

VNIVERSITAT DE VALÈNCIA



Cloud screening algorithm for MERIS and CHRIS multispectral sensors

Tesis Doctoral **PhD Thesis**
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Cloud screening algorithm for MERIS and CHRIS
multispectral sensors

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Luis Gómez Chova, 2008.

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Book cover art by Luis Gómez Chova. The picture shows the cloud mask generated by the algorithm presented in this Thesis for an ENVISAT/MERIS multispectral image acquired over The Netherlands in 2003 (ESA).

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“It is better to remain silent and be thought a fool,
than to open your mouth and remove all doubt.”
attr to George Eliot (Mary Ann Evans)

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Abstract

Earth Observation systems monitor our Planet by measuring, at different wavelengths, the electromagnetic radiation that is reflected by the surface, crosses the atmosphere, and reaches the sensor at the satellite platform. In this process, clouds are one of the most important components of the Earth's atmosphere affecting the quality of the measured electromagnetic signal and, consequently, the properties retrieved from these signals. This Thesis faces the challenging problem of cloud screening in multispectral and hyperspectral images acquired by space-borne sensors working in the visible and near-infrared range of the electromagnetic spectrum. The main objective is to provide new operational cloud screening tools for the derivation of cloud location maps from these sensors' data. Moreover, the method must provide cloud abundance maps –instead of a binary classification– to better describe clouds (abundance, type, height, subpixel coverage), thus allowing the retrieval of surface biophysical parameters from satellite data acquired over land and ocean. In this context, this Thesis is intended to support the growing interest of the scientific community in two multispectral sensors on board two satellites of the European Space Agency (ESA). The first one is the MEdium Resolution Imaging Spectrometer (MERIS), placed on board the biggest environmental satellite ever launched, ENVISAT. The second one is the Compact High Resolution Imaging Spectrometer (CHRIS) hyperspectral instrument, mounted on board the technology demonstration mission PROBA (Project for On-Board Autonomy). The proposed cloud screening algorithm takes advantage of the high spectral and radiometric resolution of MERIS, and of the high number of spectral bands of CHRIS, as well as the specific location of some bands (e.g., oxygen and water vapor absorption bands) to increase the cloud detection accuracy. To attain this objective, advanced pattern recognition and machine learning techniques to detect clouds are specifically developed in the frame of this Thesis. First, a feature extraction based on meaningful physical facts is carried out in order to provide informative inputs to the algorithms. Then, the cloud screening algorithm is conceived trying to make use of the wealth of unlabeled samples in Earth Observation images, and thus unsupervised and semi-supervised learning methods are explored. Results show that applying unsupervised clustering methods over the whole image allows us to take advantage of the wealth of information and the high degree of spatial and spectral correlation of the image pixels, while semi-supervised learning methods offer the opportunity of exploiting also the available labeled samples.

Overview

Earth Observation (EO) covers those procedures and scientific methodologies focused on monitoring our Planet by means of electromagnetic radiation sensors located on space-borne or air-borne platforms. The information these sensors provide represents spatial and temporal scales completely different to those obtained from ground measurements. Particularly, optical passive remote sensing lies on the study of the surface by means of the solar radiation reflected by the observed target and transmitted through the atmosphere to the sensor.

Materials in a scene reflect, absorb, and emit electromagnetic radiation in different ways depending on their molecular composition and shape. Remote sensing exploits this physical fact and deals with the acquisition of information about a scene at a short, medium, or long distance. The radiation acquired by a sensor is measured at different wavelengths, and the resulting spectral signature (or *spectrum*) is used to identify a given material or to retrieve surface biophysical parameters from it. The field of spectroscopy is concerned with the measurement, analysis, and interpretation of such spectra.

However, EO from remote sensing data implies accounting for the coupling between atmosphere and surface radiative effects. If there were no atmosphere around the Earth, the solar radiation would only be perturbed when it reached the surface. Therefore, incoming radiation would provide a direct representation of the surface nature and the associated dynamics when registered by a space-borne sensor. Nevertheless, the atmospheric influence on the visible (VIS) and infrared (IR) radiation is strong enough to modify the reflected electromagnetic signal, causing the loss or corruption of part of the carried information. The interaction of the solar radiation with the atmospheric components consists of absorption and scattering processes. The absorption decreases the intensity of the radiation arriving at the sensor, which causes a loss of the brightness of the target, while the scattering mainly acts modifying the propagation direction.

In this scenario, clouds are one of the most important components of Earth's atmosphere, and constitute the core focus of this work. The presence of clouds affects dramatically the quality and reliability of the measured electromagnetic signal and thus the retrieved surface properties. The corresponding cloud influence depends on the cloud type, cloud cover, cloud height, and cloud distribution in the sky. For instance, thick *opaque* clouds impede the incoming radiation reaching the surface, while thin *transparent* clouds contaminate the data with photons scattered

in the observation direction or attenuates the signal by the removal of photons in their travel to the sensor. As a result, any set of remote sensing images needs for cloud screening in the initial processing steps before exploiting the data to ensure a maximal accuracy in the results. This is the fundamental basis of cloud screening in optical remote sensing: the detection of the clouds in the observer's line of sight in order to identify the usefulness of the signal reflected by the target.

Accurate identification of clouds in remote sensing images is a key issue for a wide range of remote sensing applications, especially in the case of sensors working in the visible and near-infrared (VNIR) range of the electromagnetic spectrum. The amount of images acquired over the globe every day by the instruments on board EO satellites makes inevitable that many of these images present cloud covers, whose extent depends on the season and the geographic position of the study region. It is estimated that more than 60% of the globe is covered by clouds. Therefore, from an operational point of view, undetected clouds are the most significant source of error for ground reflectance retrieval, affecting a wide range of remote sensing applications.

On the one hand, clouds can be viewed as a source of contamination that makes the image partly useless for assessing landscape properties. Without an accurate cloud masking, undetected clouds in the scene are the most significant source of error for true ground reflectance estimation, and thus for biophysical parameter retrieval over both water and land covers. By masking only those image areas affected by cloud covers, the whole image must not be necessarily discarded, increasing usability of remote sensing data or making multitemporal studies possible. On the other hand, global scale monitoring of clouds is a key requirement for an adequate modeling of the Earth's climate. Having a global scale monitoring of clouds is becoming more and more important in climatological aspects: clouds contribute significantly to the global radiation budget with its role in the direct radiative forcing, and thin clouds are responsible for the atmospheric greenhouse effect. Therefore, clouds can be viewed as a source of contamination that makes the image partly useless for assessing landscape properties, or as a source of information for measuring important climatological parameters. In both cases, an automatic and accurate method for cloud screening in optical remote sensing is required. As a result, cloud screening represents an important preprocessing task for any EO image in order to ensure a maximal accuracy and reliability in the results inferred by the latter exploitation of the data.

Under the light of the aforementioned needs and demands, the present Thesis addresses the crucial problem in the remote sensing of environment of developing an operational, accurate and automated set of tools for the discrimination of clouds. We can clearly state different objectives in this work:

1. To analyze the problem of cloud detection under different perspectives. The intrinsic multi-disciplinary nature of this work (in the intersect of Physics, Thermodynamics, Telecommunications, Computer Science and Machine Learning) will allow us to extract different features for better understanding and modeling the problem.
2. To better understand signals provided by ENVISAT/MERIS (Rast et al., 1999) and PROBA

/CHRIS (Barnsley et al., 2004) imaging spectrometers. In particular, PROBA is a technology demonstration satellite whose sensor CHRIS provides minimally preprocessed data. Appropriate correction and calibration of CHRIS and MERIS data is a key issue for accurate cloud screening and also for other remote sensing applications.

3. To develop an automatic, robust and operational algorithm for cloud screening. The algorithm should primarily provide a cloud mask interpretable as cloud abundance.
4. To validate the proposed algorithm extensively. This is achieved through two different ways: comparing the resulting cloud masks with the official MERIS and CHRIS products and with the multi-temporal classification of cloud-covered image series.
5. To provide the remote sensing community with a set of guidelines and recommendations for developing further missions and satellite sensors.

This Thesis is organized in four different parts: (1) a thorough literature review, (2) the development of a set of robust tools for automated cloud screening, (3) the evaluation of the proposed algorithms in real situations, and (4) the elaboration of a set of guidelines and recommendations aimed to be useful for further missions:

Part I reviews the fundamental basis of passive remote sensing, cloud physical and optical properties, along with a compilation of state-of-the-art cloud screening methods. This first step identifies strengths and weaknesses of the most representative algorithms to date.

Part II addresses the proposed methodology for cloud product generation. In particular, to obtain cloud probability masks and knowledge from the extracted cloud features.

Part III deals with the validation of the proposed methodology and cloud products. A wide database of images has been included in the study in order to take into account their different characteristics: type of cloud (cumulus, cirrus, stratocumulus); geographic location (latitude/longitude); date (season); and surface types. The validation of cloud detection algorithms is not an easy task because there is no independent measurement with the same spatial resolution. For this reason, significant effort has to be done in order to validate results by using different techniques.

Part IV summarizes the accomplished objectives, discusses the main conclusions, and provides guidelines and recommendations to improve cloud screening for multispectral imaging spectrometers in future EO missions.

Part I

Introduction

Chapter 1

Remote Sensing from Earth Observation Satellites

Passive optical remote sensing relies on solar radiation as the source of illumination. This solar radiation travels across the Earth atmosphere before being reflected by the surface and again before arriving at the sensor. Thus, the signal measured at the satellite is the emergent radiation from the Earth surface-atmosphere system in the sensor observation direction.

The reflectance of the observed target should be the parameter of interest since it characterizes the surface independently of atmospheric effects and seasonal and diurnal differences in solar position. However, the estimation of the surface reflectance from the radiance measured at the satellite –also known as atmospheric correction– requires an accurate estimation of the parameters used to model the atmospheric effects and then to compensate them using a proper radiative transfer model. The main problem is that, radiative transfer modeling for surface reflectance retrieval assumes cloud-free data in order to estimate atmospheric parameters from the data themselves. Thus, results over clouds have no physical interpretation and a previous accurate cloud screening is required. Hence, *cloud screening* is the first processing step after noise reduction and radiometric calibration.

We must state here that atmospheric correction procedure is out of the scope of this Thesis. Nevertheless, since cloud screening is carried out before the atmospheric correction is done, interaction between the atmosphere and the radiation will be taken into account in order to quantify the atmospheric effects on the measured signal. Moreover, an accurate formulation of the atmospheric effects on the retrieved signal allows us to estimate useful features to discriminate clouds from surface.

In this chapter, a brief introduction to the solar electromagnetic radiation and its interaction with the Earth atmosphere is given. The absorption and scattering processes affecting the solar electromagnetic radiation in its path across the atmosphere until reaching the sensor are described. The acquisition and operation mode of common multispectral imaging spectrometers is detailed.

Finally, a brief description of ENVISAT/MERIS and PROBA/CHRIS satellite sensors is included together with discussion about current opportunities and identified problems that justify the selection of these sensors and cloud screening to be studied in the present Thesis.

1.1 Electromagnetic Radiation and Radiative Transfer

1.1.1 Electromagnetic Radiation

Electromagnetic radiation (EMR) travels through space in the form of periodic disturbances of electric and magnetic fields that simultaneously oscillate in planes mutually perpendicular to each other and to the direction of propagation through space at the speed of light ($c = 2.99792458 \times 10^8$ m/s). The electromagnetic spectrum is a continuum of all electromagnetic waves arranged according to frequency or wavelength, which are defined as the number of wave peaks passing a given point per second and the distance from peak to peak, respectively. Thus, both frequency, ν (Hz), and wavelength, λ (m), of an EMR wave are related by its propagation speed, $c = \lambda\nu$. The energy carried by EMR is contained in the photons that travel as a wave, being the energy in a photon proportional to the frequency, $E = h\nu = \hbar\omega$, where h is the Planck's constant ($h = 6.626 \times 10^{-34}$ J s) and $\hbar = h/2\pi$ is called the reduced Planck's constant.

The spectrum is divided into regions based on wavelength ranging from short gamma rays, which have wavelengths of 10^{-6} μm or less, to long radio waves which have wavelengths of many kilometers. Since the range of electromagnetic wavelengths is so vast, the wavelengths are often shown graphically on a logarithmic scale (see Fig. 1.1 for a detailed classification of the electromagnetic spectrum). Visible light is composed of wavelengths ranging from 400 to 700 nm, i.e. from blue to red. This narrow portion of the spectrum is the entire range of the electromagnetic energy to which the human visual system is sensitive to. When viewed through a prism, this range of the spectrum produces a rainbow, that is, a spectral decomposition in fundamental harmonics or frequency components (colors). Just beyond the red-end of the visible (VIS) region there is the region of infrared (IR) energy waves: near-infrared (NIR), shortwave-infrared (SWIR), middle-infrared (MIR), and the thermal-infrared (TIR).

The VIS and IR regions are commonly used in remote sensing. In particular, passive optical remote sensing is mainly focused in the VIS and NIR spectral region (VNIR), and in the SWIR since it depends on the Sun as the unique source of illumination. The predominant type of energy detection in the wavelength regions from 400 to 3000 nm (VNIR and SWIR) is based on the reflected sunlight.

1.1.2 Solar Irradiance

Energy generated by nuclear fusion in the Sun's core is the responsible for the electromagnetic radiation emitted by the Sun in its outer layer, which is known as the photosphere. It is the

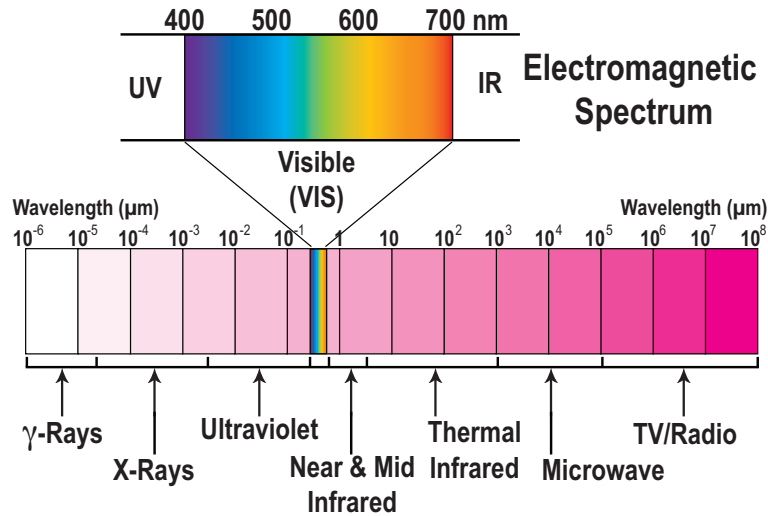


Figure 1.1: Electromagnetic spectrum classification based on wavelength range.

continuous absorption and emission of EMR by the elements in the photosphere that produces the light observed emanating from the Sun. The absorption characteristics of these elements produces variations in the continuous spectrum of solar radiation, resulting in the typical solar irradiance spectral curve. It must be stressed that 99% of the solar radiative output occurs within the wavelength interval 300-10000 nm.

The rate of energy transfer by EMR, the so-called *radiant flux*, incident per unit area is termed the *radiant flux density* or *irradiance* (W/m^2). A quantity often used in remote sensing is the irradiance per unit wavelength, and is termed the *spectral irradiance* (with units $\text{W}/\text{m}^2/\text{nm}$). The total radiant flux from the Sun is approximately 3.84×10^{26} W and, since the mean Earth-Sun distance is 1.496×10^{11} m, the total solar irradiance, over all wavelengths, incident at the top of the atmosphere (TOA), at normal incidence to the Earth's surface, is

$$F_0 = \frac{3.84 \times 10^{26}}{4\pi(1.496 \times 10^{11})^2} = 1370 \text{ W}/\text{m}^2, \quad (1.1.1)$$

which is known as the *solar constant*, although it presents a considerable variation with time. The observed variations at the Sun are due to localized events on the photosphere known as *sunspots* and *faculae*¹. An increased number of these events occurs approximately every 11 years, a period known as the solar cycle. However, the largest source of variation in the incident solar irradiance at the TOA is the orbit of the Earth around the Sun, due to the variable Earth-Sun distance that varies with the day of year.

Space-borne instruments allow us measuring the spectral variation in solar irradiance at the TOA without the effects of the Earth's atmosphere which, depending on the wavelength of the

¹*Sunspots* are dark areas on the photosphere which are cooler than surrounding regions. They have lifetimes ranging from a few days to weeks and are accompanied by strong magnetic fields. *Faculae* are regions of the photosphere which are hotter than their surroundings. They often occur in conjunction with sunspots and also possess strong magnetic fields and similar lifetimes.

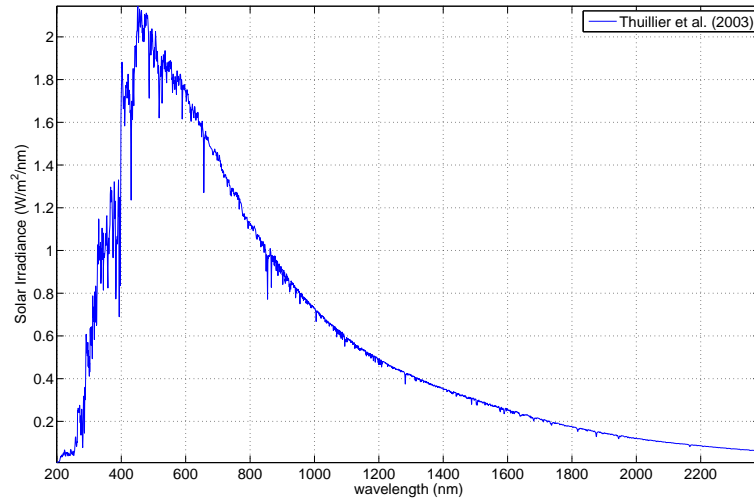


Figure 1.2: Solar spectral irradiance at the top of the Earth's atmosphere.

radiation, can reduce the intensity of the measured radiation. In this Thesis, the used solar spectral irradiance curve, $F_0(\lambda)$, comes from Thuillier et al. (2003), where the ultraviolet (UV), visible, and infrared spectra from the ATmospheric Laboratory for Applications and Science (ATLAS) and the EUropean Retrieval CARrier (EURECA) missions were merged into a single absolute solar irradiance spectrum covering the 200 to 2400 nm range. In particular, the SOLar SPECTrum (SOLSPEC) and the Solar SPECTrum (SOSP) spectrometers, on board ATLAS and EURECA missions respectively, were used to carry out the solar spectral irradiance measurements. Figure 1.2 shows the solar spectral irradiance at the top of the Earth's atmosphere (Thuillier et al., 2003).

It can be shown that the solar intensity curve resembles that of a Planck's distribution, $B(\lambda, T)$, for a blackbody at a temperature $T = 5777$ K (Fig. 1.3):

$$B(\lambda, T) = \frac{2\hbar c^2}{\lambda^5 (\exp(\frac{\hbar c}{k_B T \lambda}) - 1)}, \quad (1.1.2)$$

where, k_B is the Boltzmann's constant ($k_B = 1.38 \times 10^{-23}$ J/K). The maximum emission intensity of the curve occurs around 500 nm. This fact is consistent with Wien's displacement law, which states that the wavelength (λ_{\max}) corresponding to the peak in Planck's curve for a blackbody radiating at a temperature T are related as follows:

$$\lambda_{\max} T = 2.898 \times 10^6 \text{ (nm K)}. \quad (1.1.3)$$

Finally, the Stefan-Boltzmann law states that the total power emitted by a blackbody, per unit surface area of the blackbody, varies as the fourth power of the temperature:

$$F = \pi \int_0^\infty B(\lambda, T) d\lambda = 5.671 \times 10^{-8} T^4 \text{ (W/m}^2\text{)} \quad (1.1.4)$$

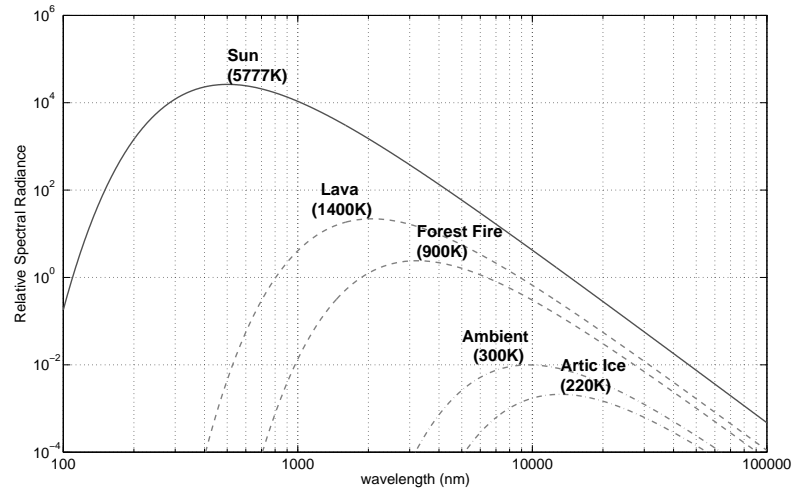


Figure 1.3: Blackbody emission of objects at typical temperatures.

Because the Sun and Earth's spectra have a very small overlap (Fig. 1.3), the radiative transfer processes for solar and infrared regions are often considered as two independent problems.

1.1.3 Earth Atmosphere

The Earth's surface is covered by a layer of atmosphere consisting of a mixture of gases and other solid and liquid particles. The principal gaseous constituents, present in nearly constant concentration, are nitrogen (78%), oxygen (21%), argon (1%), and minor constituents (<0.04%). Water vapor and an ozone layer are also present. The atmosphere also contains solid and liquid particles such as aerosols, water droplets (clouds or raindrops), and ice crystals (snowflakes). These particles may aggregate to form clouds and haze.

The vertical profile of the atmosphere is divided into four main layers: *troposphere*, *stratosphere*, *mesosphere*, and *thermosphere*. The tops of these layers are known as the *tropopause* (10 km), *stratopause* (50 km), *mesopause* (85 km), and *thermopause*, respectively. The gaseous materials extend to several hundred kilometers in altitude, though there is no well-defined limit of the atmosphere.

All the weather activities (water vapour, clouds, precipitation) are confined to the troposphere. A layer of aerosol particles normally exists near to the Earth's surface, and the aerosol concentration decreases nearly exponentially with height, with a characteristic height of about 2 km. In fact, the troposphere and the stratosphere together (first 30 km of the atmosphere) account for more than 99% of the total mass of the Earth's atmosphere. Finally, ozone exists mainly at the stratopause.

The characteristic difference between molecules and aerosols in the atmosphere is their respective size or radius (D'Almeida et al., 1991). Molecules have a radius on the order of 0.1 nm, while

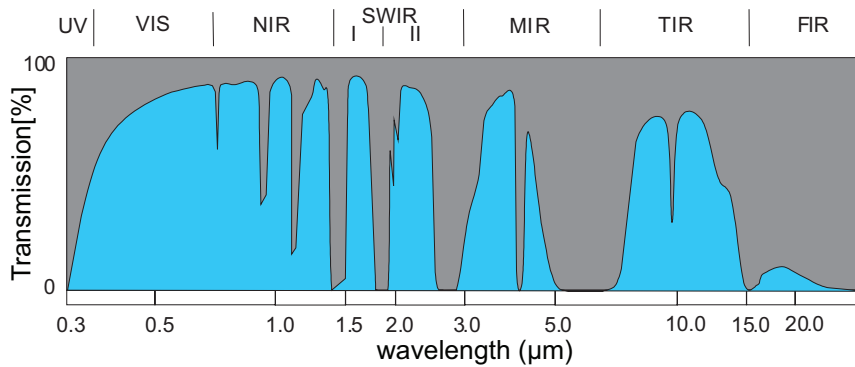


Figure 1.4: Relative atmospheric radiation transmission. Gray denotes absorption bands and blue areas denote atmospheric windows (transmission peaks).

aerosols can have a range of radii from 100 to 1000 nm. Both molecules and aerosols are optically active, causing the *absorption* and *scattering* of the electromagnetic radiation, respectively. Therefore, when the EMR from the Sun reaches Earth’s atmosphere, it may be (Hapke, 1993):

- *Absorbed:* incident radiation is taken in by the medium. A portion of the radiation is converted into internal heat energy that is emitted or radiated back at longer thermal infrared wavelengths.
- *Scattered:* incident radiation is dispersed or spread out by the particles suspended in the medium unpredictably in all directions. Radiation is absorbed and subsequently reemitted at about the same wavelength without energy transformation, changing only the spatial distribution of the radiation.
- *Transmitted:* incident radiation passes through matter with measurable attenuation (absorbed or scattered).
- *Reflected:* incident radiation bounces off the surface of a substance in a predictable (specular reflection) or unpredictable (diffuse reflection) direction. Reflection consists in the scattering of the EMR by an object.

The overall effect is the removal of energy from the incident radiation. The amount of radiant energy that the atmosphere either removes or adds to that emitted or reflected from the Earth’s surface depends on:

- the constituents of the atmosphere,
- the path length of radiation (function of the geometry of the illumination, the surface, and the observation),
- the reflectance of the surface target area and the surrounding scene.

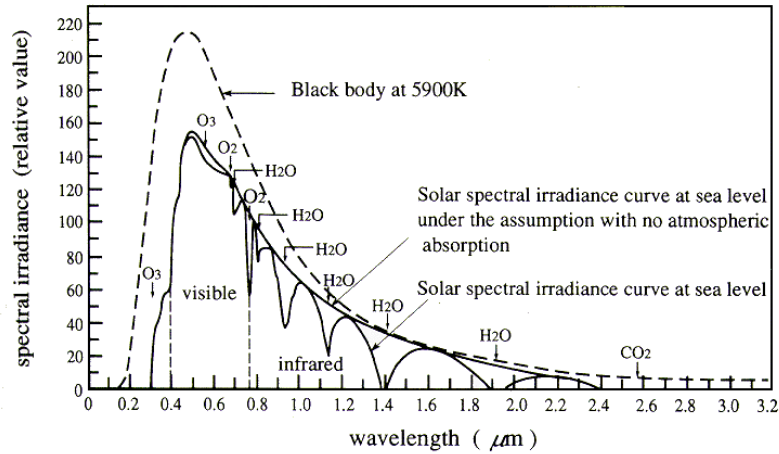


Figure 1.5: Solar irradiance at the top of the atmosphere and at the sea level, and blackbody emission spectrum at 5900 K.

Each type of molecule (constituent) has its own set of absorption bands in various parts of the electromagnetic spectrum (D’Almeida et al., 1991). Absorption by atmospheric gases is dominated by that of water vapor (H_2O), carbon dioxide (CO_2), and ozone (O_3) with smaller contributions of the methane (CH_4), carbon monoxide (CO) and other trace gases. CO_2 and CH_4 are essentially uniformly distributed in the atmosphere, hence the effect of their absorption bands can be predicted reasonably well, while the water vapor distribution is rather variable in both location and altitude. Figure 1.4 shows the relative atmospheric radiation transmission of different wavelengths. A first consequence of the atmospheric effects is that wavelength bands used in remote sensing systems are usually designed to fall within these *atmospheric transmission windows*, outside the main absorption bands of the atmospheric gases, to minimize the atmospheric effects.

Figure 1.5 shows the spectral features of the solar radiation outside the atmosphere (external line) and at the sea level (internal line). The maximum is located at $0.47 \mu\text{m}$, being about 20% of the solar energy in wavelengths lower than that, and a 44% in the visible band, between $0.40 \mu\text{m}$ and $0.76 \mu\text{m}$. It is evident that water vapor is the most important absorber in the solar NIR spectrum, which contains about 50% of the solar energy.

1.1.4 At-Sensor Radiance

Signal measured at the satellite is the emergent radiation from the Earth surface-atmosphere system in the sensor observation direction. The incoming solar radiation, $F_0(\lambda)$, that we use for the observation of the surface, travels throughout the complex Earth atmosphere medium before is reflected by the surface, and the reflected signal travels again throughout the atmosphere before it arrives at the sensor. The measured at sensor radiance is called TOA radiance, and is the information we have to deal with when working with remote sensing data before atmospheric

correction. The absorption and scattering processes affecting the solar electromagnetic radiation in its path across the atmosphere can be summarized as follows:

- Atmospheric absorption, which affects mainly the visible and infrared bands, reduces the solar radiance within the absorption bands of the atmospheric gases. The reflected radiance is also attenuated after passing through the atmosphere. This attenuation is wavelength dependent. Hence, atmospheric absorption will alter the apparent spectral signature of the target being observed.
- Atmospheric scattering is important only in the visible and near infrared regions. Scattering of radiation by the constituent gases and aerosols in the atmosphere causes degradation of the remotely sensed images. Most noticeably, the solar radiation scattered by the atmosphere towards the sensor without first reaching the ground produces a hazy appearance of the image. This effect is particularly severe in the blue end of the visible spectrum due to the stronger Rayleigh scattering for shorter wavelength radiation.
- Furthermore, the light from a target outside the field of view of the sensor may be scattered into the field of view of the sensor. This effect is known as the *adjacency effect*. Near the boundary between two regions of different brightness, the adjacency effect results in an increase in the apparent brightness of the darker region, while the apparent brightness of the brighter region is reduced.

In this section, the interaction of the solar irradiance with the molecules and aerosols in the atmosphere is described by a simplified version of the radiative transfer equation in order to quantify the different contributions to the measured signal.

Radiance and Irradiance

We describe radiation in terms of energy, power, and the geometric characterization of power (Fig. 1.6). The radiant power, Φ , is the flux or flow of energy in the stream of time, hence power is represented in watts (W). Flux density is the amount of radiant power emitted or received in a surface region. In fact, radiant *intensity*, *irradiance*, and *radiance* are different flux densities obtained by integrating the radiant power over the area, A , and/or the solid angle, ω , of the surface²:

- Irradiance, F , is defined as the received radiant power per unit area: $F = d\Phi/dA$ (W/m²).
- Intensity, I , is an angular flux density defined as the power per unit solid angle: $I = d\Phi/d\omega$ (W/sr).

²The *area* measures the surface region of a two- or three-dimensional object in square meters (m²), while the *solid angle* is the projection of an area onto a sphere, or the surface area of the projection divided by the square of the radius of the sphere, which is measured in steradians (sr).

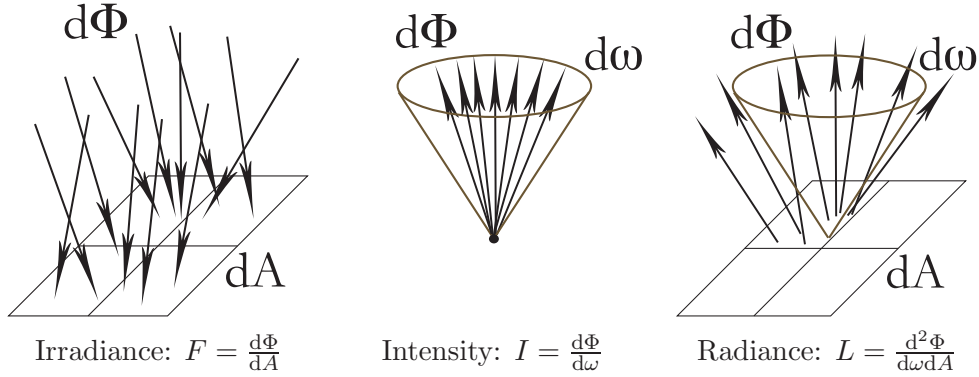


Figure 1.6: Illustration of the geometric characterization of the incident irradiance, radiant intensity, and radiance.

- Radiance, L , is an angular-area flux density defined as the power and unit area per unit solid angle ($\text{W}/\text{m}^2/\text{sr}$).

The fundamental radiometric quantity is the *radiance* that is the contribution of the electromagnetic power incident on a unit area dA by a cone of radiation subtended by a solid angle $d\omega$ at an angle θ to the surface normal. It has units $\text{W}/\text{m}^2/\text{sr}$, although *spectral radiance* (radiance per unit wavelength, $\text{W}/\text{m}^2/\text{nm}/\text{sr}$) is also commonly used, and is expressed mathematically as,

$$L(\lambda, \theta, \psi) = \frac{d^2\Phi(\lambda)}{\cos(\theta)d\omega dA}, \quad (1.1.5)$$

where θ and ψ are the *zenith* and *azimuth* angle³, respectively. Irradiance and intensity can be computed from the radiance, with appropriate integration: Irradiance is the integral of the radiance over all solid angles, and Intensity is the integral of the radiance over all areas.

If the radiance from the Sun incident at the TOA is denoted L_0 , then the at-sensor solar irradiance described in section 1.1.2 is obtained by integrating over all possible zenith angles and azimuth directions, that is,

$$F_0(\lambda) = \int_0^{2\pi} \int_0^{\pi/2} L_0(\lambda, \theta, \psi) \cos(\theta) \sin(\theta) d\theta d\psi, \quad (1.1.6)$$

where $d\omega$ is expressed in spherical polar coordinates as $\sin(\theta)d\theta d\psi$.

Defining $\mu = \cos(\theta)$, which is the inverse of the so called optical mass, (1.1.6) can be rewritten as

$$F_0(\lambda) = \int_0^{2\pi} \int_0^1 L_0(\lambda, \theta, \psi) \mu d\mu d\psi. \quad (1.1.7)$$

If a radiation field is termed *isotropic*, then at any point in the field the intensity of measured radiation is independent of the direction of observation (i.e., independent of θ and ψ). In this

³A zenith angle is a vector's angular deviation from an outward normal to the Earth's surface and azimuth is the horizontal angular variation of a vector from the direction of motion or true North.

case,

$$F_0(\lambda) = \pi L_0(\lambda), \quad (1.1.8)$$

which can be rearranged to give the expression for radiance,

$$L_0(\lambda) = F_0(\lambda)/\pi, \quad (1.1.9)$$

If the illuminating radiation is composed of parallel beams emanating from the direction (μ_0, ψ_0) , then

$$L_0(\lambda, \theta, \psi) = \frac{F_0(\lambda)}{\pi} \delta(\mu - \mu_0) \delta(\psi - \psi_0), \quad (1.1.10)$$

which is equivalent to the isotropic case when $\mu = \mu_0$ and $\psi = \psi_0$.

Radiation extinction

The energy transfer in a complex medium, such as the atmosphere, is generally affected by absorption, scattering and emission (Hapke, 1993). In the case of the Earth atmosphere and optical remote sensing, the emission process can be neglected due to the low atmosphere temperature (150-300 K), which corresponds to a blackbody emission centered in the thermal infrared wavelengths. Therefore, the two dominant mechanisms affecting the propagation of EMR of wavelengths between 400-2500 nm in the terrestrial atmosphere are absorption and scattering (Lenoble, 1993). The absorption (mainly corresponding to the gases, since aerosol absorption is comparatively marginal) acts decreasing the radiation in a given direction, while the scattering (the molecules and aerosols) may increase or decrease the intensity in the same direction, by means of the deviation of the radiation propagating towards other directions or, on the contrary, modifying the direction of the radiation into the considered direction.

The absorption and the scattering associated to the loss of energy in the considered direction can be treated as two separate events, and their combined effect is known as *extinction*. The extinction action on the radiation can be formulated by means of the Bouguer-Lambert-Beer law, which is defined by a simple differential equation considering that the radiance loss is proportional to the total energy amount and to the crossed distance. If we consider a layer of thickness dz in an absorbing and scatterer medium perpendicular to a radiation beam of radiance L , the radiance has been changed to $L + dL$, so the variation is given by

$$dL = -\beta_e L dz, \quad (1.1.11)$$

where β_e is the volume extinction coefficient, which is the sum of the volume absorption and scattering coefficients. If we integrate between two positions, z_1 and z_2

$$L(z_2) = L(z_1) \exp\left(-\int_{z_1}^{z_2} \beta_e(z) dz\right) = L(z_1) e^{-\tau} \quad (1.1.12)$$

where τ is called optical thickness. Eq. 1.1.12 is known as *Beer's exponential extinction law* and provides the expression of the *transmittance* $T(z_1, z_2)$ of the layer between z_1 and z_2 along the

direction of propagation by

$$T(z_1, z_2) = \frac{L(z_2)}{L(z_1)} = e^{-\tau}. \quad (1.1.13)$$

The *optical thickness* (often referred to as *optical depth*) serves as a measure of the opacity or turbidity of the atmosphere for a given wavelength of EMR. From an altitude z above the Earth's surface to the TOA, the total optical depth is calculated as

$$\tau_{\text{tot}}(\lambda) = \int_z^\infty \beta_e(\lambda, z) dz = \int_z^\infty \kappa_{\text{tot}}(\lambda) \delta_{\text{atm}}(z) dz, \quad (1.1.14)$$

where $\kappa_{\text{tot}}(\lambda)$ is the total extinction coefficient (which can be specified for each of the molecular species in the atmosphere) and $\delta_{\text{atm}}(z)$ is the density of the intervening atmosphere between z and the TOA. For the absorbing and scattering atmospheres we have respectively the absorbing and scattering optical thicknesses $\tau_{\text{abs}}(\lambda)$ and $\tau_{\text{dif}}(\lambda)$. The solar intensity measured at the Earth's surface assumes the form of the extinction Bouguer-Lambert-Beer law, $L_s(\lambda) = L_0(\lambda) \exp(-\tau_{\text{tot}}(\lambda))$.

TOA Signal Formulation

A simple but accurate formulation of the TOA signal measured by the space-borne sensor in terms of surface reflectance and atmospheric optical parameters is necessary for the evaluation of TOA radiance (Liou, 2002). In this formulation, the TOA radiance is expressed as a sum of radiative terms from different processes, such as the radiation scattered by the atmosphere into the sensor line of sight, or the direct radiation multiply scattered between the atmosphere and the surface.

Specifically, the contribution of the target to the upward TOA radiance can be decomposed as the sum of five terms, which are shown in Fig. 1.7: (1) the photons reflected by the atmosphere before reaching the surface, (2a) the photons directly transmitted from the Sun to the target and directly reflected back to the sensor, (2b) the photons scattered by the atmosphere then reflected by the target and directly transmitted to the sensor, (3a) the photons directly transmitted to the target but scattered by the atmosphere on their way to the sensor, and, finally, (3b) the photons having at least two interactions with the atmosphere and one with the target.

In this formulation, the direction of propagation of EMR incident at the TOA or Earth's surface from the Sun will be denoted by the illumination zenith and azimuth angle, θ_s and ψ_s . Similarly, the direction of EMR emerging from the Earth's surface-atmosphere system is denoted by the viewing zenith and azimuth angle, θ_v and ψ_v .

The TOA radiance signal registered by a sensor looking at an homogeneous *Lambertian*⁴ surface would be given by the following simplified radiative transfer equation (Tanré et al., 1979;

⁴In Lambertian surfaces the reflected radiance is isotropous or perfectly diffuse. Thus, the reflected field is the same for all of the points in the surface, and independent of the view angle.

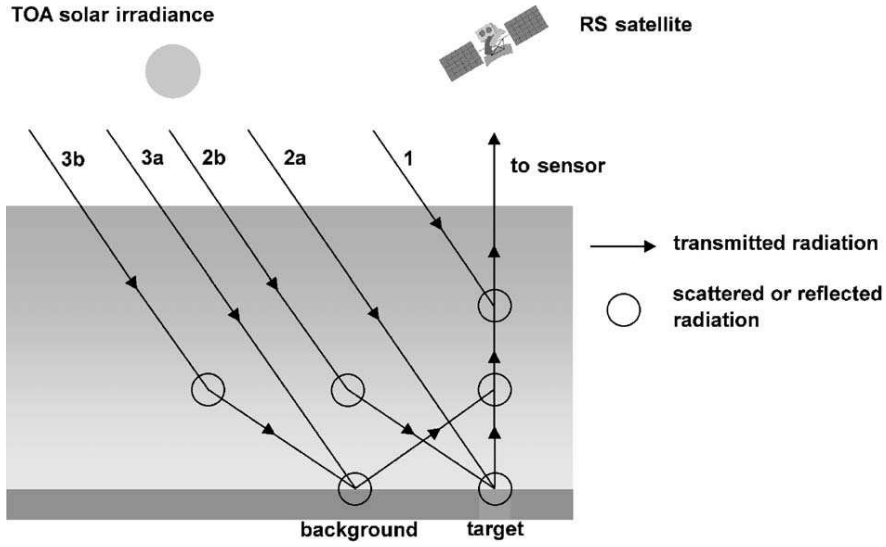


Figure 1.7: Contributions to TOA signal from surface and atmosphere (from Verhoef and Bach, 2003).

Vermote et al., 1997; Renzullo, 2004; Guanter, 2006):

$$L_{\text{TOA}} = L_p + \frac{1}{\pi} \frac{\rho_s (F_{\text{dir}} \mu_s + F_{\text{dif}}) T_{\uparrow}}{1 - s \rho_s} \quad (1.1.15)$$

where L_{TOA} is the TOA radiance; L_p is the atmospheric path radiance, component of the radiance emerging from the TOA that is independent of surface reflectance; μ_s is the cosine of the illumination zenith angle, measured between the solar ray and the surface normal; $F_{\text{dir}} \mu_s$ and F_{dif} are the direct and diffuse fluxes arriving at the surface, respectively; s is the atmospheric spherical albedo, reflectance of the atmosphere for isotropic light entering it from the surface; T_{\uparrow} is the total atmospheric transmittance (for diffuse plus direct radiation) in the observation direction; and ρ_s is the surface reflectance.

In (1.1.15), one can appreciate the complexity of the retrieval of the surface reflectance ρ_s , which is usually the parameter of interest since it characterizes the surface independently of atmospheric effects and seasonal and diurnal differences in solar position. The estimation of the surface reflectance from the TOA radiance measured at the satellite (also known as atmospheric correction), requires an accurate estimation of the parameters quantifying the atmospheric effects and then to compensate them using a proper radiative transfer model. However, in order to estimate atmospheric parameters from the data themselves, which is out of the scope of this Thesis, a previous accurate cloud screening is required. This is a *vicious circle*. Hence, an acceptable compromise is to use the TOA apparent reflectance instead of surface reflectance to perform cloud screening. TOA reflectance is estimated according to Vermote et al. (1997):

$$\rho_{\text{TOA}} = \frac{\pi L_{\text{TOA}}}{\mu_s F_0}, \quad (1.1.16)$$

which allows us to remove the dependence on particular illumination conditions (day of the year

and angular configuration) and illumination effects due to rough terrain (cosine correction). It is worth noting that illumination effects are usually higher than the atmospheric effects depending on the geometric configuration. Think for example in the huge contrast that can be appreciated on a spherical object illuminated at an angle with a lamp (Gómez-Sanchis et al., 2008d). One can see that ρ_{TOA} becomes the surface reflectance ρ_s under the following conditions: atmospheric path radiance $L_p = 0$; diffuse illumination $F_{\text{dif}} = 0$; direct illumination equal to the TOA solar irradiance $F_{\text{dir}} = F_0$; atmospheric spherical albedo $s = 0$; and total atmospheric transmittance $T_{\uparrow} = 1$. That is, when the Earth's atmosphere completely disappears.

1.2 Multispectral and Hyperspectral Imaging Spectrometers

As shown in previous sections, materials reflect, absorb, and emit electromagnetic radiation in different ways depending on their molecular composition and shape. Remote sensing exploits this physical fact and deals with the acquisition of information about a scene at a short, medium, or long distance. The radiation acquired by a sensor is measured at different wavelengths, and the resulting spectral signature (or *spectrum*) is used to identify a given material or to retrieve surface biophysical parameters by means of regression and inversion models (Gómez-Chova et al., 2001; Gómez-Chova, 2002; Camps-Valls et al., 2005, 2006c, 2008b). The field of spectroscopy deals with the measurement, analysis, and interpretation of such spectra (Richards and Jia, 1999); and it is worth noting that it can be applied to a broad range of problems not related to Earth observation, such as industrial applications (Calpe et al., 2003; Calpe-Maravilla et al., 2004b, 2005, 2006; Vila et al., 2005; Vila-Francés et al., 2005, 2006b) or food engineering (Gómez-Sanchis et al., 2008c,a,b). Figure 1.8 shows the application of imaging spectroscopy to perform satellite remote sensing. In imaging spectroscopy or hyperspectral remote sensing (Goetz et al., 1985; Schaepman et al., 2006), the resulting multispectral image consists of a simultaneous acquisition of spatially coregistered images, in several, spectrally contiguous bands, measured in calibrated radiance units, from a remotely operated platform.

Clear examples of *multispectral* sensors on-board satellite platforms are Landsat/TM, SPOT/HRV, TERRA/ASTER or IKONOS, which present a few spectral bands and with broad bandwidths (Capolsini et al., 2003). Recent satellite sensors are capable of acquiring images at many more wavelength bands. For example, the NASA's TERRA/MODIS (Salomonson et al., 1989) or ESA's ENVISAT/MERIS (Bezy et al., 1999; Rast et al., 1999) sensors acquire tens of spectral bands with narrow bandwidths, enabling the finer spectral characteristics of the targets to be captured by the sensor. This kind of sensors are commonly called *superspectral* sensors. Finally, a *hyperspectral* image consists of about a hundred or more narrow and contiguous spectral bands. The precise spectral information contained in a hyperspectral image enables better characterization and identification of targets (Gómez-Chova et al., 2001, 2004a; Calpe-Maravilla et al., 2004a; Camps-Valls et al., 2003, 2004a, 2007b). Figure 1.8 shows a typical example of an hyperspectral image consisting of over a hundred contiguous spectral bands, forming a three-dimensional (two

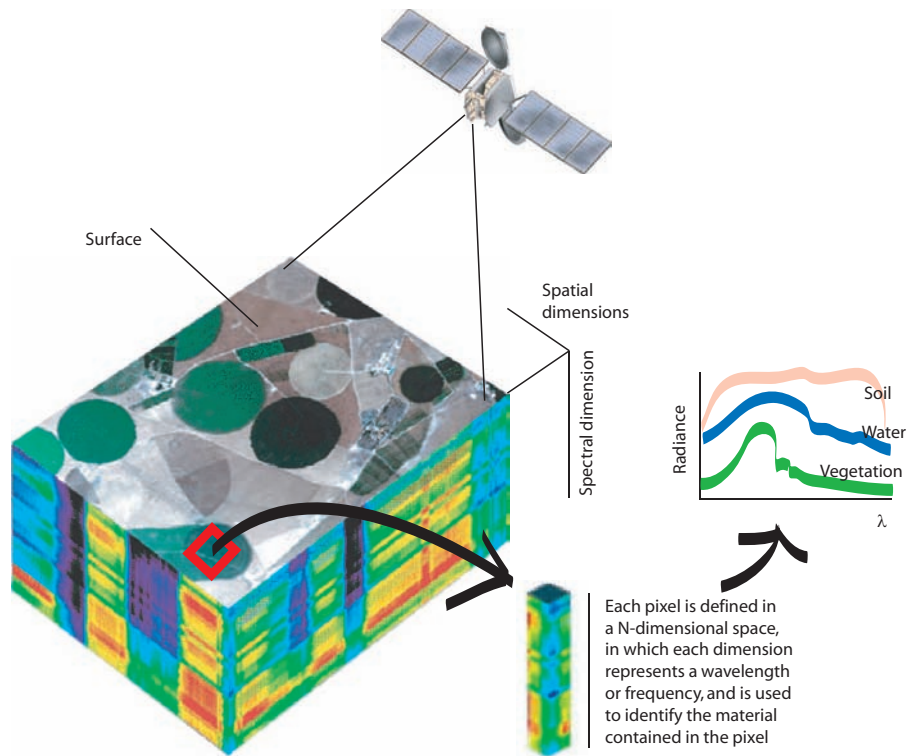


Figure 1.8: Principle of imaging spectroscopy.

spatial dimensions and one spectral dimension) image cube. Each pixel is associated with a complete spectrum of the imaged area.

Currently, space-borne hyperspectral imagery is not commercially available. There are only experimental satellite-sensors that acquire hyperspectral imagery for scientific investigation such as NASA’s EO1/Hyperion (Ungar et al., 2003) and ESA’s PROBA/CHRIS (Barnsley et al., 2004; Cutter, 2004b). However, future planned Earth Observation missions (submitted for evaluation and approval) point to a new generation of hyperspectral sensors (Schaeppman et al., 2006): EnMAP (Environmental Mapping and Analysis Program, GFZ/DLR, Germany) (Stuffer et al., 2007; Kaufmann et al., 2008), FLEX (ESA Earth Explorer proposal) (Stoll et al., 2003; Moreno, 2006), HypIRI (NASA GSFC proposal) (Green et al., 2008a,b), SpectraSat (Full Spectral Landsat proposal), ZASat (South African proposal, University of Stellenbosch), HIS (Chinese Space Agency), etc. Figure 1.9 shows a comparison of current multi- and hyperspectral systems in terms of information content, spatial resolution, and number of spectral bands.

In particular, coming hyperspectral instruments on-board EnMAP (Kaufmann et al., 2008) and FLEX (Moreno, 2006) missions, in addition to acquire a set of spectrally contiguous bands in the spectral region of interest for the mission applications, include dedicated bands specifically designed to perform an accurate cloud screening. This fact remarks the increasing importance of cloud screening in operational EO missions.

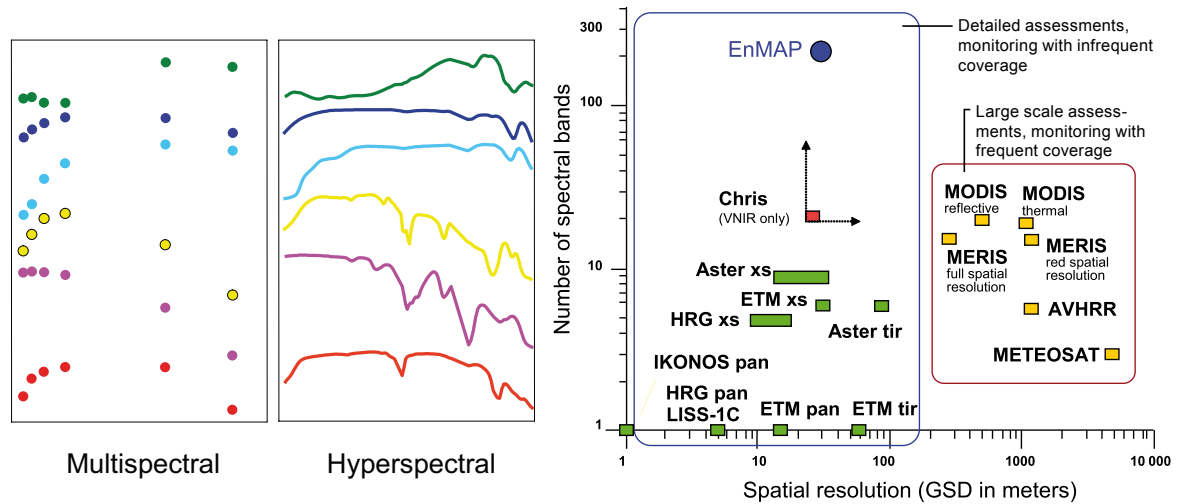


Figure 1.9: Comparison of multispectral and hyperspectral data and instruments (credits: <http://www.enmap.de/>). *Left:* Comparison of multispectral and hyperspectral measuring data. *Right:* Performance comparison of main air- and space-borne multi- and hyperspectral systems in terms of spectral and spatial resolution.

1.3 Push-broom Imaging Spectrometers

Many of the multispectral and hyperspectral sensors are push-broom imaging spectrometers. Push-broom line imagers consist of an optical system that focalizes the light coming from a portion of the Earth's surface onto the focal plane where the sensor is placed. The system includes a long and narrow slit that limits the area being imaged to a stripe aligned with one of the sensor's axis, while a diffractive medium (prism, grid, etc.) forms a spectrum of the line along the orthogonal axis. Usually, the detector is a charge coupled device (CCD) two-dimensional array whose rows separate wavelengths and columns separate resolved points in the Earth image (Mouroulis et al., 2000). Figure 1.10 shows the push-broom operation mode for the acquisition of spectral images. The optical system collects the light arriving from a long and narrow strip of the surface below by means of a thin slit. The slit is oriented perpendicularly to the direction of motion of the sensor, and the sequential acquisition of lines generates the image as the platform moves forward. The image of the land strip is spectrally spread out (diffracted for gratings and dispersed for prisms), separating the different wavelengths, and projected onto a properly aligned CCD array, so the line is parallel to the horizontal axis (spatial) while the spectral spread out is produced along the perpendicular axis (spectral).

Therefore, a hyperspectral image consists of two spatial dimensions (along-track and across-track) and one spectral dimension (wavelength). This hyperspectral image is registered by the instrument in a data-cube where: the along-track dimension at the Earth surface, y , corresponds to the image-lines dimension l (distributed in the vertical direction of the image); the surface across-track dimension, x , corresponds to the line-pixels dimension p (distributed in the horizon-

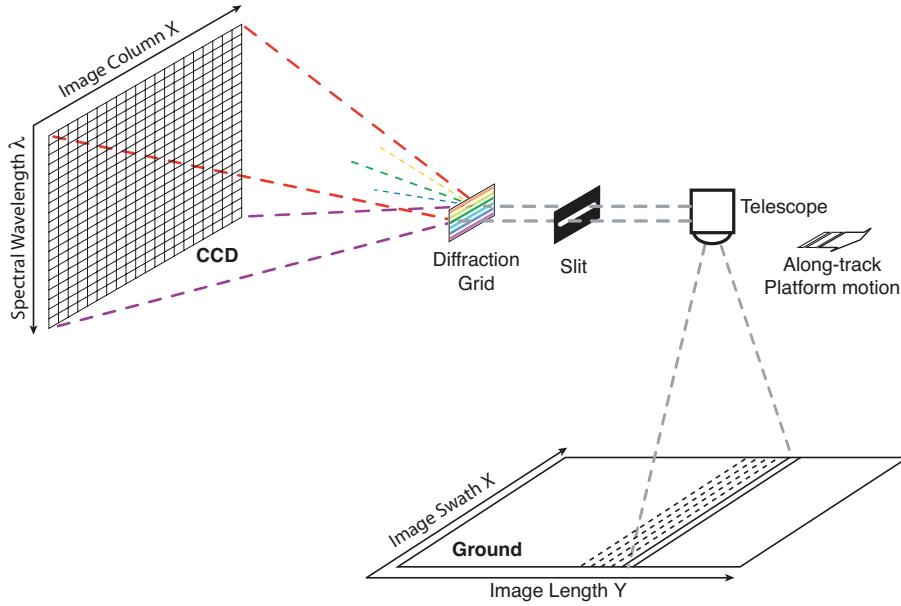


Figure 1.10: Design of a push-broom imaging spectrometer that shows its operation mode.

tal direction of the image and CCD); and the spectral dimension, λ , corresponds to the image band b (distributed in the vertical direction of the CCD). These correspondences among Earth surface, instrument CCD, and hyperspectral data-cube are depicted in Fig. 4.3. The size of the hyperspectral data-cube can be written in the form $N_l \times N_p \times N_b$, where N_l is the number of image lines, N_p is the number of pixels per line, and N_b is the number of spectral bands. The incoming radiance is integrated over the spatial and spectral response of the system for a given detector element (p, b) of the CCD array. The relation between the incoming *at sensor* radiance from the Earth surface, $L(x, y, \lambda)$ ($\text{W}/\text{m}^2/\text{sr}$), and the registered value by the CCD, $I(l, p, b)$ (Digital Number, DN), can be defined as:

$$I(l, p, b) = S(p, b) \int_{y \in l} \int_{x \in p} \int_{\lambda \in b} L(y, x, \lambda) H(x, \lambda) dy dx d\lambda + S_0(l, p, b), \quad (1.3.1)$$

where $H(x, \lambda)$ represents the optical system response, $S(p, b)$ is the CCD sensitivity, and $S_0(l, p, b)$ contains all the analog offset errors and random noise. In this equation, it is worth noting that the vertical dimension of the image is related to the time when the image line, l , was acquired. In addition, the image values, I , and CCD sensitivity, S , are expressed as a function of the image pixels and bands, (p, b) . Hence, assuming a one-to-one correspondence between the image pixels and bands and the CCD columns and rows, respectively. However, usually a certain number of CCD columns or rows are binned to form the final image (e.g. reducing the spatial or spectral resolution to increase the radiometric accuracy). In this case, some lines and columns of $I(l, p, b)$ would be summed, but all the presented formulation is still valid.

The physical interpretation of satellite data needs an accurate sensor calibration that converts the recorded digital number (DN) of $I(l, p, b)$ into radiance values as close as possible to the true

radiance $L(l, p, b)$. Most of existing CCD sensors allow an accurate correction of dark current offsets, thus making $S_0(l, p, b)$ negligible (remaining only a zero mean, low amplitude random noise). Therefore, the calibration procedure consists in finding a set of calibration coefficients to retrieve the true radiance:

$$L(l, p, b) = a(p, b)I(l, p, b), \quad (1.3.2)$$

where $a(p, b)$ is the calibration coefficient at band b on the pixel p , which depends on the optical system response, H , and the CCD sensitivity, S .

If the instrument works correctly (Mouroulis et al., 2000), the spatial and the spectral dimensions (orthogonal dimensions of the CCD), are independent and they can be processed separately. Therefore, the optical system response can be expressed as $H(x, \lambda) = H(x)H(\lambda)$, where $H(x)$ represents the slit response and $H(\lambda)$ represents the instrument chromatic response, which in turn defines the wavelength and bandwidth of each band. Thus, the slit response is constant for all the lines and bands of a given image, and independent from pixel-to-pixel. This is known as uniformity.

Assuming a smooth optical response, the integral of the incoming radiance over the optical response of the system in (1.3.1), which represents the radiance at the focal plane array of the CCD, can be approximated as:

$$\int_{y \in l} \int_{x \in p} \int_{\lambda \in b} L(y, x, \lambda) H(x) H(\lambda) dy dx d\lambda = L(l, p, b) H_x(p) H_\lambda(b) \quad (1.3.3)$$

where $H_x(p)$ and $H_\lambda(b)$ represent the contribution of the spatial and spectral response to the calibration coefficient of the detector element (p, b) . Then, the relation between the incoming radiance and the registered value by the CCD of (1.3.1) can be written as:

$$I(l, p, b) = L(l, p, b) H_x(p) H_\lambda(b) S(p, b) + S_0(l, p, b), \quad (1.3.4)$$

and the different contributions to the ideal calibration coefficients ($S_0(l, p, b) \simeq 0$) would be:

$$a(p, b) = \frac{L(l, p, b)}{I(l, p, b)} = \frac{1}{H_x(p) H_\lambda(b) S(p, b)}. \quad (1.3.5)$$

Summarizing, the complete optical design is optimized so that monochromatic images of the slit fall on straight CCD rows, and line spectra of resolved ground areas fall on CCD columns. In this case, each pixel in a line of the image at a given wavelength has been acquired by a different element of the CCD; while every column of the image for that wavelength has been measured by the same element of the CCD. Would be the CCD and the slit ideally built then all the CCD elements would have the same sensitivity and response, producing even and noise-free images. However, in real devices, deviations from these design conditions produce the following problems:

- Optical aberrations and misalignments in the CCD integration with optics cause the spectrometer entrance slit image to be projected as a curve on the detector array. This causes a bending of spectral lines across the spatial axis and of the spatial lines across the spectral axis (Goetz et al., 2003).

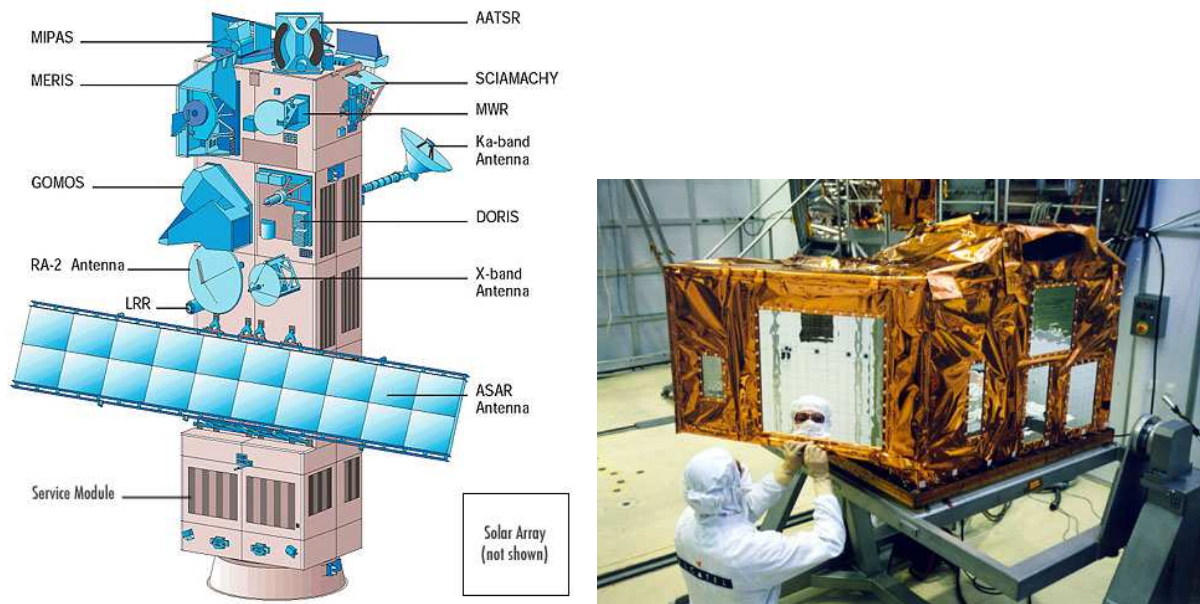


Figure 1.11: ENVISAT/MERIS system. *Left:* Location of MERIS on ENVISAT. *Right:* MERIS instrument. (Credits: ESA)

- Deviations of the monochromatic images of the slit from the CCD rows are known as *smile* (curved up) or *frown* (curved down). It causes a non-linear variation in the wavelength in the across-track direction, which results in a spectral shift from nominal spectral band positions along the CCD columns.
- Deviations of the line spectra of resolved ground areas from the CCD columns are known as *chromatic keystone*. It causes images of the slit at different wavelengths to differ in length depending on where the ray propagates with respect to the center of the lens.
- Sensitivity variations between neighboring elements of the CCD and variations on the width of the slit along its length results in the intensity of an homogeneous area to be slightly different in each column of the CCD array (Barducci and Pippi, 2001).
 - The effect of these imperfections in the resulting image is a vertical pattern known as *vertical striping*.

A more detailed description of the sensor calibration and the proposed correction of presented errors is given in chapter 4 for the imaging spectrometers used in this Thesis.

1.3.1 The MEdium Resolution Imaging Spectrometer (MERIS)

The MEdium Resolution Imaging Spectrometer (MERIS) instrument (Rast et al., 1999) is mounted on board the ENVironmental SATellite (ENVISAT) Earth Observation Satellite launched

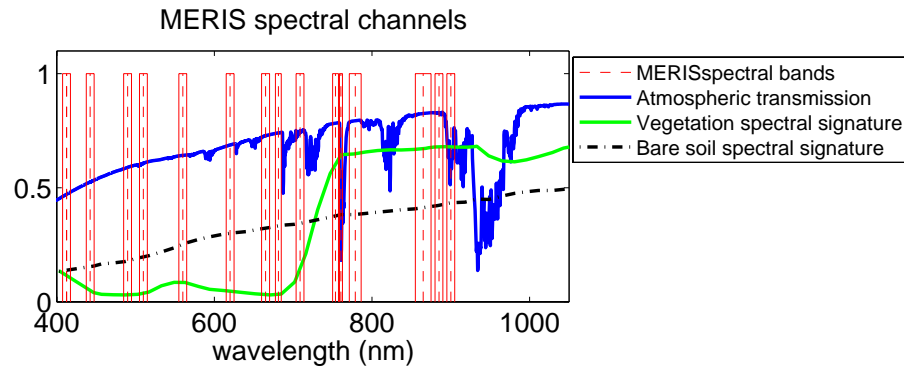


Figure 1.12: MERIS band locations (red) superimposed to a reflectance spectra of healthy vegetation (green), bare soil (black), and the atmospheric transmittance (blue).

by the European Space Agency in March 2002. MERIS on ENVISAT is a programmable medium resolution imaging spectrometer operating in the VNIR spectral range (400-900 nm). The ENVISAT/MERIS system is depicted in Fig 1.11.

The instrument scans the Earth's surface in a push-broom mode. The satellite's motion provides scanning in the along-track direction, and the scene is imaged simultaneously across the entire spectral range through a dispersing system onto a CCD array, resulting the spatial sampling in the across-track direction. MERIS is designed so that it can acquire data over the Earth whenever illumination conditions are suitable (illumination angles below 80°) with high radiometric (1% to 5%) and spectrometric (1 nm) performance. Fifteen spectral bands can be selected by ground command, each of them has a programmable width and location in the 390 nm to 1040 nm spectral range (Merheim-Kealy et al., 1999). However, a fixed set of bands was recommended by the Science Advisory Group and frozen before launch. It is presented in Table 1.1 and depicted in Fig 1.12. The Level 2 ESA products are being developed and will be validated for this set of bands, although it is possible to use alternative band sets for experimental campaigns of a few weeks duration.

The MERIS' 68.5° field of view (FOV) around nadir covers a swath width of 1150 km at a nominal altitude of 800 km. It allows global coverage of the Earth in 3 days. The instantaneous FOV is divided into five segments, each of them is imaged by one of the corresponding five cameras. A slight overlap exists between the FOVs of adjacent optical cameras. An area CCD detector is used, with an instantaneous detector element FOV of 1.149 arcmin.

MERIS provides either full spatial resolution data (FR) or reduced spatial resolution data (RR). These two spatial resolutions, for the nominal orbit are:

- *Full spatial resolution:* 260 m across track, 290 m along track. Full FR scenes have 2241×2241 pixels and cover 582 km (swath) by 650 km (azimuth). Quarter scenes have 1153×1153 pixels and cover 300 km (swath) by 334 km (azimuth).
- *Reduced spatial resolution:* 1040 m across track, 1160 m along track. A reduced spatial

Table 1.1: MERIS fixed set of bands.

#	Band centre (nm)	Bandwidth (nm)	Application
1	412.5	10	Yellow substance and detrital pigments
2	442.5	10	Chlorophyll absorption maximum
3	490	10	Chlorophyll and other pigments
4	510	10	Suspended sediment, red tides
5	560	10	Chlorophyll absorption minimum
6	620	10	Suspended sediment
7	665	10	Chlorophyll absorption and fluorescence reference
8	681.25	7.5	Chlorophyll fluorescence peak
9	708.75	10	Fluorescence reference, atmosphere corrections
10	753.75	7.5	Vegetation, cloud
11	760.625	3.75	O ₂ R-branch absorption band
12	778.75	15	Atmosphere corrections
13	865	20	Vegetation, water vapor reference
14	885	10	Atmosphere corrections
15	900	10	Water vapor, land

resolution pixel is obtained by averaging the signal of 16 full spatial resolution pixels. More precisely, 4 adjacent pixels across-track for 4 successive pixel lines along-track are used. Resolution scenes have 1121×1121 pixels and cover 1165 km (swath) by 1300 km (azimuth).

1.3.2 The Compact High Resolution Imaging Spectrometer (CHRIS)

The Compact High Resolution Imaging Spectrometer (CHRIS) instrument (Barnsley et al., 2004) is mounted on board the European Space Agency small satellite platform called PROBA (*Project for On Board Autonomy*) launched on 22 October 2001 (Fig. 1.13). PROBA is a technology-proving experiment to demonstrate the on-board autonomy of a generic platform suitable for small scientific or application missions.

The platform provides pointing in both across-track and along-track directions, as well as a fixed scanning speed on the ground during imaging in order to increase the CHRIS integration time, thus increasing the radiometric resolution. In this way, the system CHRIS/PROBA has multiangular capabilities, acquiring five consecutive images at time when the satellite projection on the surface is closest to the target. This position corresponds to a minimum zenith observation angle (MZA), that is negative in the case of target locations East of the ground track. The images are acquired from a set of Fly-by-Zenith Angles (FZA): 0° , $\pm 36^\circ$, and $\pm 55^\circ$, which are related to the actual view zenith angles by the MZA. The sign refers to along track position. The acquisition geometry is depicted in Fig. 1.14. The CHRIS imaging spectrometer system has been designed mainly to provide remote sensing data for land applications, and it is intended to demonstrate that low cost compact imaging spectrometers can be viable instruments when combined with



Figure 1.13: *Left:* Artistic image of the PROBA platform. *Right:* CHRIS picture. (Credits: SIRA)

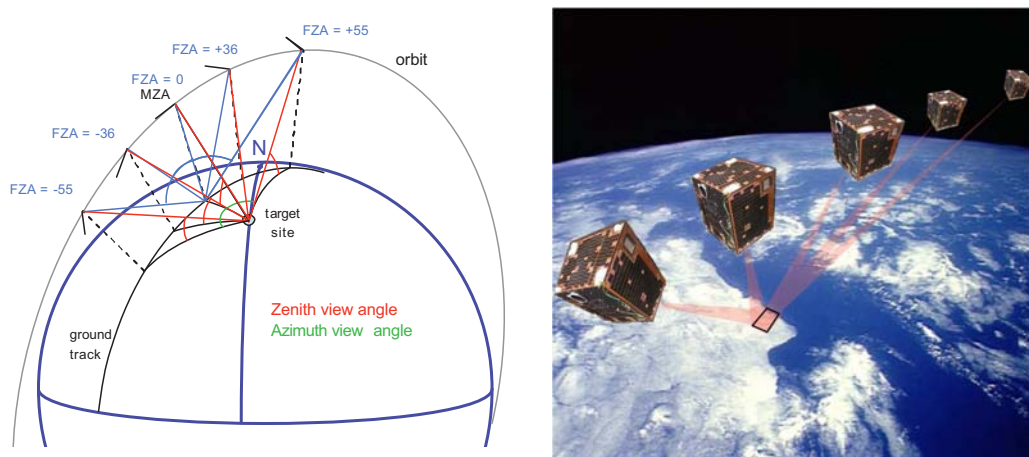


Figure 1.14: Pointing capabilities of the PROBA platform in both across-track and along-track directions.

agile small satellite platforms (dimensions: $200 \times 260 \times 790$ mm; weighting under 14 kg; power consumption less than 8 W).

The CHRIS instrument is a conventional push-broom imaging spectrometer with a telescope forming an image of the Earth's surface onto the entrance slit of a spectrometer, and an area-array detector at the spectrometer focal plane. The detector is a thinned, back-illuminated, frame-transfer charge coupled device, with the CCD rows being assigned to different wavelengths and the CCD columns to separate resolved areas on the Earth's surface. From a 600 km orbit, CHRIS can image the Earth in a 13.5 km swath with a spatial resolution of 17 m (at perigeo, this is somewhat variable as the altitude varies around the orbit from 688 km to 553 km). Using PROBA's agile steering capabilities in along- and across-track directions enables observation of selectable targets (Fig. 1.15). CHRIS operates over the VNIR spectral range from 400 nm to 1050 nm and can operate in 62 spectral bands at a spatial resolution of 34 m, or with 18 bands at 17 m, with a spectral sampling interval ranging between 1.25 (@400 nm) and 11 nm (@1000 nm).

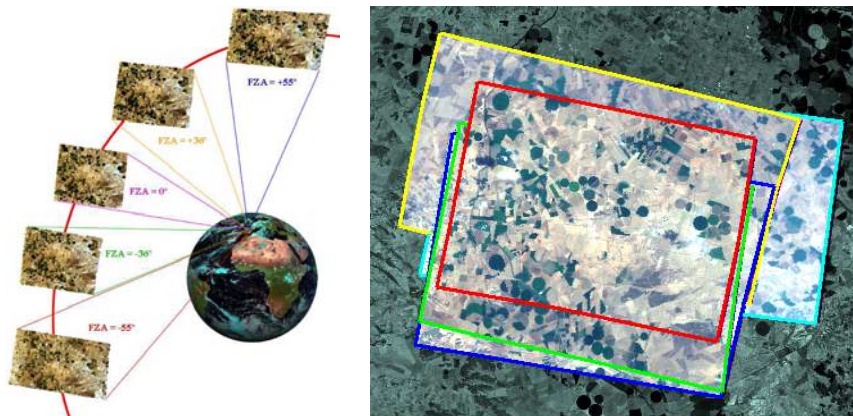


Figure 1.15: CHRIS/PROBA multiangular image acquisition of five consecutive images per surface target.

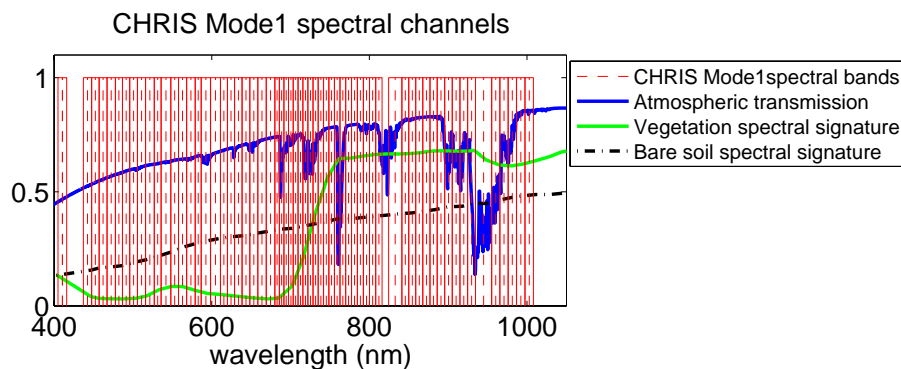


Figure 1.16: CHRIS Mode1 band locations (red) superimposed to a reflectance spectra of healthy vegetation (green), bare soil (black), and the atmospheric transmittance (blue).

The instrument is very flexible and different sets of bands can be used for different applications. There is a trade-off between the number of bands that can be output and the spatial resolution because there is a finite data transfer rate between the platform and the ground station.

The spatial and spectral resolutions can be altered by binning elements on the CCD detector array. Data rates can be reduced by limiting the number of across-track pixels output or by operating at a coarse along track resolution or by reducing the number of spectral channels. The along track resolution is determined by the detector integration time. By controlling the pitch of the platform the integration time can be varied so that signal to noise ratio can be increased for low albedo targets. Each CHRIS image represents about 131 Mbits of data so that the 1 Gbit of mass memory that is assigned to CHRIS can store several images taken at different view angles. There are several operation modes, with different band configurations (number, center location and width) and spatial resolution. The data we have worked with correspond to Mode 1, consisting of 34 m pixel and 62 bands between 400 and 1000 nm, which are displayed in Fig. 1.16 (see <http://earth.esa.int/proba/> for a detailed description of the available operation modes).

1.4 Motivation

This Thesis is intended to support the scientific and technological interest in MERIS and CHRIS (or other VIS/IR multispectral sensors) data for Earth observation studies. For an accurate exploitation of remote sensing data provided by these sensors, the ideal situation would be the availability of additional products containing relevant information about cloud characteristics simultaneous to the image acquisition and with the same spatial resolution. This can be accomplished if cloud detection is achieved directly from the data by means of the measured radiances in some properly selected wavelengths. Therefore, the main objective is to provide new operational cloud screening tools for the derivation of cloud location and abundance maps, thus allowing the retrieval of atmospheric and surface biophysical parameters from satellite data taken over land and ocean.

Several aspects of these sensors justify the approach. Two of the key features of MERIS are its temporal resolution (revisit time of 3 days) and its spatial coverage (swath width of 1150 km). In addition, MERIS also provides data at an unprecedented combination of spectral and spatial resolutions: 15 narrow bands and 300 m pixel size in full resolution (FR) mode. Therefore, MERIS has a great potential for multitemporal studies both at regional and global scales. The operational use of MERIS images is, however, hampered by the presence of clouds because this instrument works in the VNIR part of the electromagnetic spectrum. On this matter, an automatic and accurate cloud screening method is essential in order to use partially cloudy images facilitating the elaboration of MERIS products and also improving the usability of MERIS temporal series.

Two major points motivate the selection of MERIS data and cloud screening to be put together in this Thesis. On the one hand, MERIS offers a unique spectral configuration for the retrieval of both atmosphere and surface parameters: two fine bands at the oxygen (O₂-A) and water vapor atmospheric absorptions are combined with other thirteen channels providing high-accuracy measurements from the blue to the near-infrared spectral regions (see Rast et al. (1999) for further technical information). The accurate characterization of the O₂-A absorption at MERIS band 11 enables the estimation of cloud top height from MERIS data (Preusker et al., 2006). On the other hand, the lack of operative methods for the cloud screening of MERIS data, as well as identified problems in the corresponding ESA Official Level 2 cloud mask products, are known (Santer et al., 1999).

The other sensor included in this study is the CHRIS hyperspectral instrument mounted on board PROBA. Thanks to the PROBA platform pointing capabilities and small CHRIS spatial coverage (typical image areas about 13 km²), the acquisition plan of CHRIS tries to avoid acquisitions with cloud coverage, but usually images are partially affected by clouds. In these cases, users that requested the acquisition have a special interest in an accurate cloud screening in order to identify the cloud-free areas of the scene. In addition, the high spectral and spatial resolution of CHRIS makes it a good choice in order to propose and validate cloud detection methodologies for next generation of satellite hyperspectral instruments.

Chapter 2

Cloud Screening from Earth Observation Images

Clouds can be defined as a mass of condensed water vapor or ice particles suspended above the Earth's surface. Accurate identification of clouds in remote sensing images is a key issue for a wide range of remote sensing applications, especially in the case of sensors working in the VNIR range of the electromagnetic spectrum due to the severe absorption and scattering of cloud constituents at these wavelengths. The amount of images acquired over the globe every day by the instruments on board Earth Observation satellites makes inevitable that many of these images present cloud covers, whose extent depends on the season and the geographic position of the study region. According to the observational estimates from the International Satellite Cloud Climatology Project (ISCCP) data set (Zhang et al., 2004), the global annual-mean cloud cover is around 66%. Other studies report higher rates of cloud covers over the globe analyzing data from a worldwide meteorological network with a large number of stations at different latitudes and seasons (Bréon and Colzy, 1999). Figure 2.1 shows the total cloud amount (%) from the ISCCP-D2 monthly mean dataset for the period July 1983 through June 2005 (products from the ISCCP-D2 dataset are available and can be generated on-line at <http://isccp.giss.nasa.gov>).

The presence of clouds drastically affects the measured electromagnetic signal and thus the retrieved information about the observed target. The corresponding cloud influence depends on the cloud type, cloud cover, cloud height and cloud distribution in the sky, e.g. thick *opaque* clouds impede the incoming radiation reaching the surface, while thin *transparent* clouds contaminate the data by photons scattered in the observation direction, or attenuate the signal by the removal of photons in their travel to the sensor. An important issue here is to stress that, depending on the remote sensing application, clouds can be either viewed as a source of contamination that makes the image partly useless for assessing landscape properties, or a source of information for measuring important climatological parameters (Peixoto and Oort, 1992).

- Without an accurate cloud masking, undetected clouds in the scene are the most significant

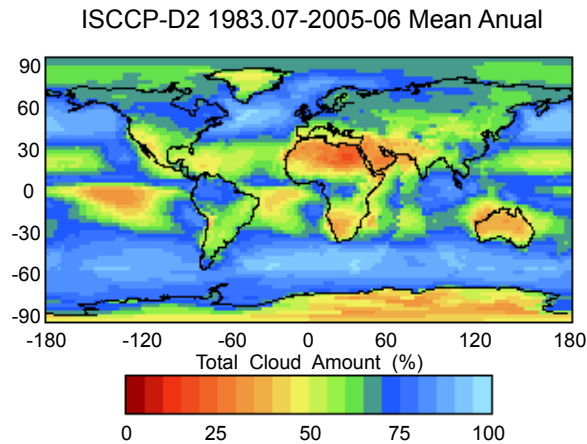


Figure 2.1: Total cloud amount (%) from the ISCCP-D2 monthly mean dataset for the period July 1983 through June 2005. (Credits: <http://isccp.giss.nasa.gov>)

source of error for true ground reflectance estimation, and thus for biophysical parameter retrieval over both sea and land covers. By masking only the image areas affected by cloud covers, the whole image is not necessarily discarded, making multitemporal studies possible.

- Having a global scale monitoring of clouds is becoming more and more important in climatology studies: clouds contribute significantly to the global radiation budget with its role in the direct radiative forcing, and thin clouds are responsible for the atmospheric greenhouse effect.

The starting point for the subject of this Thesis is that any set of optical remote sensing images needs to carry out a cloud screening process in the initial processing steps to ensure accuracy in results extracted from them.

In this chapter, a brief introduction of the cloud types and the traditional characteristics used to classify them is given. The main effects of cloud types on the EMR that travels through the Earth's atmosphere and, thus, its effects on the Earth's radiation budget and climate are introduced. Then, most relevant cloud optical properties measurable from remote sensing systems are described. Finally, a review of cloud screening approaches presented in the literature is carried out, paying special attention to the reference cloud screening algorithms developed for the sensors studied in this Thesis.

2.1 Cloud Types and Characteristics

Clouds may be classified by their visual appearance, height, or form. A classification of clouds was first introduced by Howard (1804) who used Latin words to describe their characteristics (*Cirrus*, *Cumulus*, *Stratus*, and *Nimbus*). There are now ten main types of cloud (Fig. 2.2), which can be separated into three broad categories according to the height of their base above the ground:

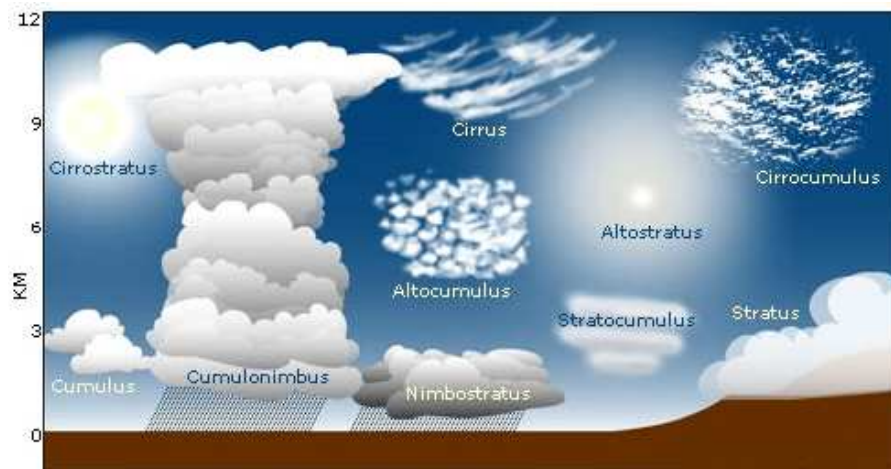


Figure 2.2: Types of cloud according to the height of their base above the ground and their vertical distribution (Credits: BBC Weather).

high clouds, medium clouds and low clouds (Stephens, 2003). Most of the main cloud types are often subdivided further on the basis of their shape, structure and degree of transparency:

- *High clouds.* These are usually composed solely of ice crystals and have a base between 7000 and 18000 m.
 - *Cirrus* - white filaments.
 - *Cirrocumulus* - small rippled elements.
 - *Cirrostratus* - transparent sheet, often with a halo.
- *Medium clouds.* These are usually composed of water droplets and ice crystals, and have a base between 2000 and 7000 m.
 - *Altostratus.* - thin layer, grey, allows sun to appear as if through ground glass.
 - *Nimbostratus.* - thick layer, low base, dark, rain or snow may fall from it.
- *Low clouds.* These are usually composed of water droplets, though cumulonimbus clouds include ice crystals, and have a base usually below 2000 m.
 - *Stratocumulus* - layered, series of rounded rolls, generally white with some shading.
 - *Stratus* - layered, uniform base, grey.
 - *Cumulus* - individual cells, vertical rolls or towers, flat base.
 - *Cumulonimbus* - large cauliflower-shaped towers, often 'anvil tops' sometimes giving thunderstorms, or showers of rain or snow.

Figure 2.3 shows pictures of the ten main types of cloud sorted according to the four main levels of taxonomical classes. The reader can appreciate the particular characteristics described for each type of cloud and the huge variability of cloud’s appearance when viewed from ground.

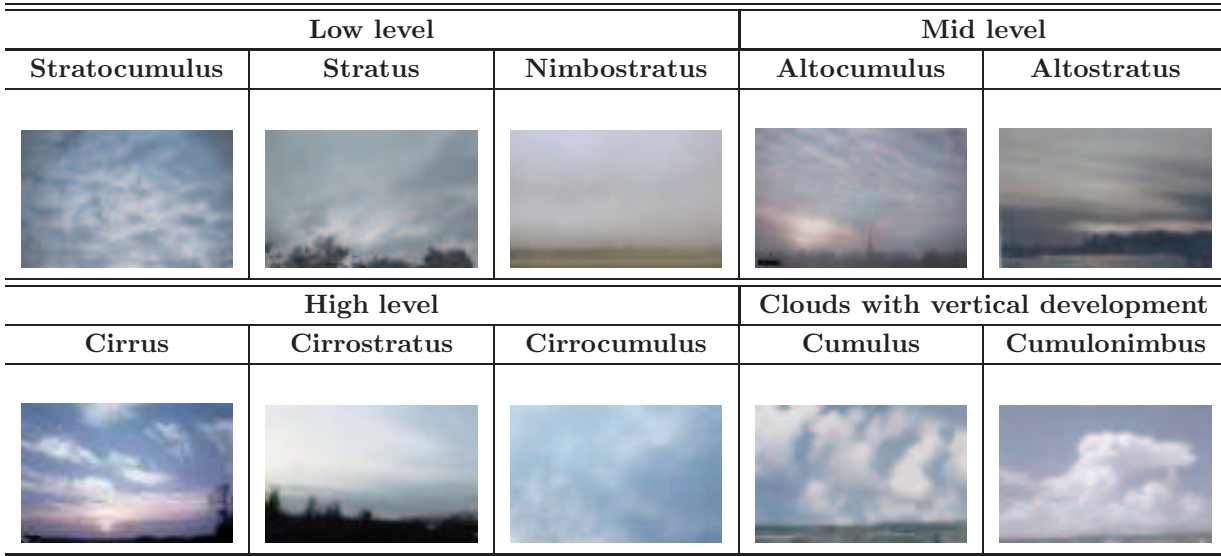


Figure 2.3: Pictures of ten main types of cloud.

In addition to the huge variability of cloud types and characteristics, one of the reasons that makes cloud screening of paramount relevance in remote sensing is the broad coverage of the

Table 2.1: Frequency of occurrence and percentage of coverage over land and over ocean for the ten main types of cloud.

Cloud Type	Height of base (km)	Freq.[%] over land / ocean	Coverage[%] over land / ocean
Low level			
Stratocumulus (Sc)	0-2	27 / 45	18 / 34
Stratus (St)			
Nimbostratus (Ns)	0-4	6 / 6	5 / 6
Mid level			
Altostratus (As)	2-7	35 / 46	21 / 22
Altostratus (As)			
High level			
Cirrus (Ci)	7-18	47 / 37	23 / 13
Cirrostratus (Cs)			
Cirrocumulus (Cc)			
Clouds with vertical development			
Cumulus (Cu)	0-3	14 / 33	5 / 12
Cumulonimbus (Cb)	0-3	7 / 10	4 / 6

Earth's surface by clouds when viewed from the space. Clouds cover more than 60% of the Earth's surface (Zhang et al., 2004). In particular, average global coverage over the oceans is about 65% and over the land is about 52%. Table 2.1 provides a frequency of occurrence and percentage of coverage over land and over ocean depending on the type of cloud.

For the subject of this Thesis, the interest on cloud types comes from the effect of different clouds on the solar radiation that is used by remote sensing sensors to observe the Earth. Low and high clouds have different effects on the radiation field with contrary effects on the Earth's radiation budget. Whether a given cloud will heat or cool the surface depends on several factors, including the cloud's altitude, its size, and the make-up of the particles that form the cloud. Moreover, cloud detection will not be concerned in identifying cloud type but only presence (and probability) of clouds.

2.2 Clouds and the Energy Cycle

The Sun's radiant energy is the fuel that drives Earth's climate engine. Energy received from the Sun is mostly in the visible (or shortwave) part of the electromagnetic spectrum. About 30% of the solar energy that comes to Earth is reflected back to space. The ratio of reflected-to-incoming energy is called *albedo*¹ from the Latin word meaning whiteness. The solar radiation absorbed by the Earth causes the planet to heat up until it radiates (or emits) as much energy back into space as it absorbs from the Sun. The Earth's thermal emitted radiation is mostly in the infrared (or longwave) part of the spectrum. The top of the clouds is usually colder than the Earth's surface. If a cloud is formed in a previously clear sky, the cold cloud top reduces the longwave emission to space, and energy is trapped beneath the cloud top. The trapped energy increases the temperature of the Earth's surface and atmosphere until the longwave emission to space once again balances the incoming absorbed shortwave radiation. This process is called the *greenhouse effect* and, taken by itself, causes a heating of the Earth's climate.

The balance between incoming and outgoing energy is called the Earth's radiation budget. As shown in figure 2.4, the Earth's atmosphere system constantly tries to maintain a balance between the energy that reaches the Earth from the Sun and the energy that flows from Earth back out to space.

The most important components of the Earth's system to the radiation budget are the planet's surface, atmosphere, and clouds. The effect of clouds on the Earth's radiation balance is measured as the difference between the clear-sky and total-scene radiation results. This difference is defined as cloud-radiative forcing (Kiehl, 1992). Mainly, two cloud effects in the radiation budget can be distinguished (Fig. 2.5):

- Shortwave rays from the sun are scattered in a cloud. Many of the rays return to space.

¹*Albedo* indicates the fraction of the total solar radiation incident to a body that is reflected by it.

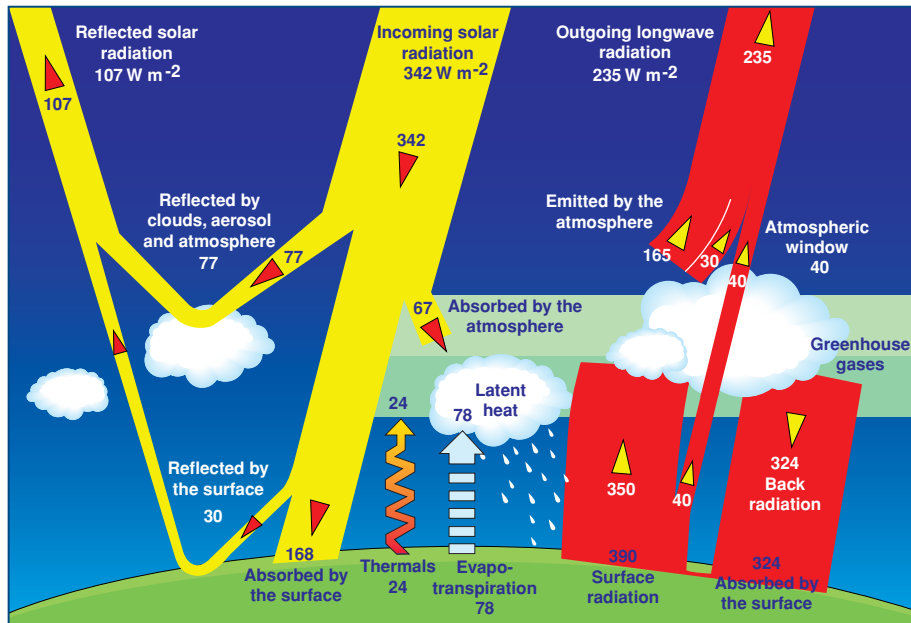


Figure 2.4: Radiation Balance of the Earth. (Credits: Kiehl (1992))

The resulting “cloud albedo forcing” tends to cause a cooling of the Earth.

- Longwave rays emitted by the Earth are absorbed and reemitted by a cloud, with some rays going to space and some going to the surface. The resulting “cloud greenhouse forcing” tends to cause Earth’s warming.

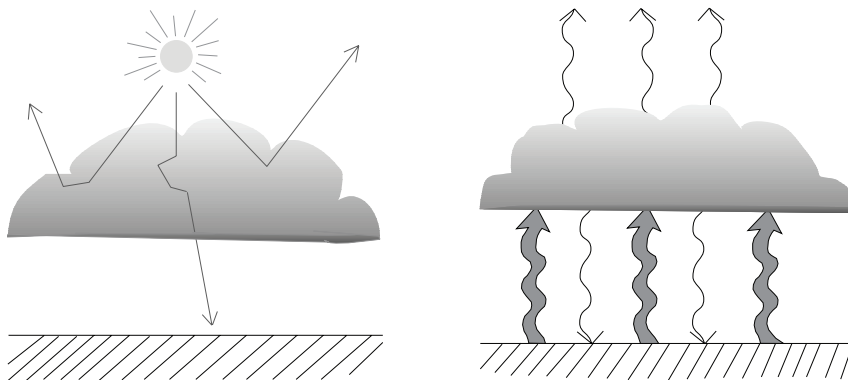


Figure 2.5: Cloud albedo forcing due to the reflection of shortwave radiation (straight arrows) by clouds (left) and cloud greenhouse forcing due to the absorption and reemission of longwave radiation (wavy arrows) by clouds (right). (Credits: NASA Facts (1999))

The balance of the opposing cloud albedo forcing and cloud greenhouse forcing determines whether a certain cloud type will produce a warming or a cooling effect. As explained below, the high thin clouds tend to enhance the heating effect, and low thick clouds have the opposite effect, while deep convective clouds are neutral (Fig. 2.6):

- Low thick clouds reflect more shortwave radiation back to space than the darker surface would in the absence of the cloud, and thus, less solar energy is available to heat the surface and atmosphere that tends to cool the Earth's climate.
- High thin cirrus clouds have a warming effect because they transmit most of the incoming solar radiation while, simultaneously, they absorb some of the Earth's infrared radiation and radiate it back to the surface.
- Deep convective clouds, such as those associated with thunderstorms, have neither a warming nor a cooling effect because their cloud greenhouse effect, although large, is nearly balanced by the effect due to the convective clouds' high albedo.

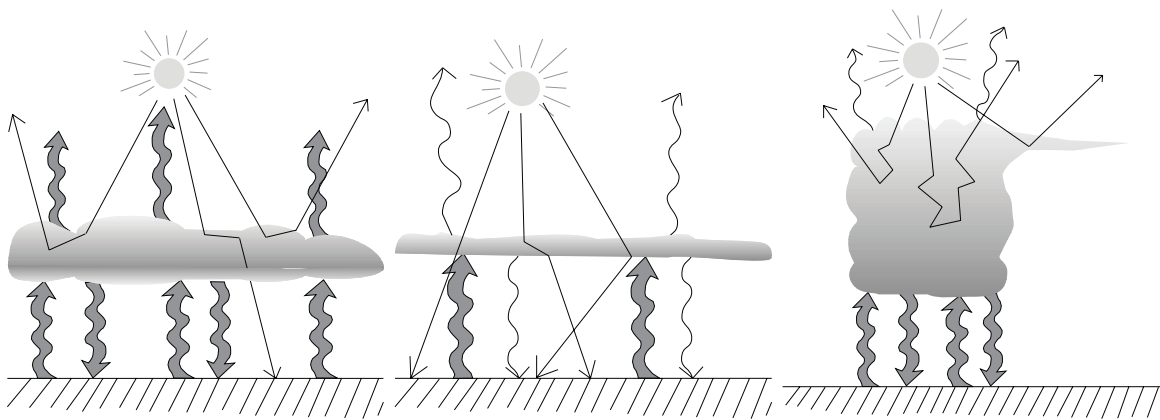


Figure 2.6: Cloud albedo forcing (straight arrows, which indicate shortwave rays) and cloud greenhouse forcing (wavy arrows, which indicate longwave rays) of low thick clouds (*left*), high thin cirrus clouds (*middle*), and deep convective clouds (*right*). (Credit: NASA Facts (1999))

2.3 Cloud Properties

As shown in the previous section, clouds have an important role in energy budget studies due to its effect on the EMR crossing the Earth's atmosphere. The cloud cover fraction, cloud type and the cloud top height have to be known accurately to better quantify the global mean effect of clouds cooling the climate system and also the effect of clouds on the EMR detected by the remote sensing sensors. The properties of clouds can vary widely with location, with time of day, with changing weather, and with season. For these reasons, satellite data play an important role in the study of clouds as the most effective method to observe clouds on a large scale and to estimate their impact on the Earth's climate. The most important cloud optical properties that can be estimated from remote sensing data are the cloud optical thickness, cloud albedo, and cloud top pressure:

- *Cloud optical thickness:* The cloud optical thickness is a measure of the opacity of the cloud. The cloud optical thickness is an important parameter for the surface and atmospheric

energy budget since the variation of cloud optical thickness alters the amount of reflected radiation and hence the energy that reaches the surface. In addition, the intensity of the thermal emission from a cloud varies with its temperature and the optical depth or thickness of the cloud. The optical thickness of a cloud is a measure of not only the physical thickness of the cloud but also of the amount and phase of water in the cloud. A cloud can be physically thin, but contain water at a density high enough to produce a high optical thickness. Clouds that allow most of the sunlight hitting them to pass through them are considered optically thin. Clouds that reflect most of the sunlight hitting them are considered to be optically thick. The cloud optical thickness can be determined directly from reflectance data, but its retrieval depends on the particle size and shape.

- *Cloud albedo*: The most important cloud parameter for energy budget studies is the cloud albedo. The cloud albedo is a measurement of the amount of radiation reflected by clouds. The cloud albedo varies from less than 10 to more than 90 percent of the insolation and depends on the cloud optical thickness, the size distribution of the cloud droplets, the liquid water content, the water vapor content, and the Sun's zenith angle. The smaller the drops and the greater the liquid water content, the greater the cloud albedo, if all other factors are the same.
- *Cloud top pressure*: The cloud top pressure is a measurement of pressure that represents the location of the radiating top of the clouds (if there is a very tenuous upper portion, this value may be below where the first cloud particles are found). It can be considered as equivalent to cloud top height above mean sea level.

By using a simple relationship between the presented cloud optical properties, the ISCCP has suggested an alternative method of classifying clouds into the traditional cloud types. This method classifies clouds based upon how optically thick they are and how high they are in the sky. Figure 2.7 shows how this method classifies clouds based on their optical thickness and cloud top pressure (cloud top height). The cloud type names represent only an approximate climatological relationship between the satellite-measured optical parameters and the classical morphological cloud types. However, a detailed comparison of the satellite and surface-based cloud observations supports this assignment of names.

The estimation of cloud optical properties involves the use of radiative transfer models and also an accurate localization of clouds in the image is required. However, it would be advantageous that the cloud screening algorithm, in addition to detecting clouds accurately, also provided a cloud abundance index *per* pixel instead of a binary classification. This added-value information may be used as follows:

1. To better describe clouds in order to include their properties (abundance, type, height, subpixel coverage) in radiation models (Tian et al., 1999).

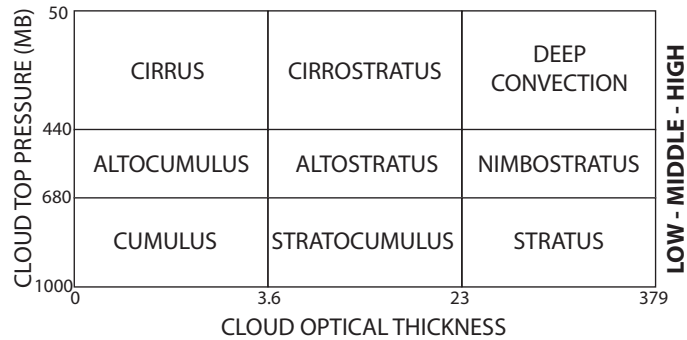


Figure 2.7: International Satellite Cloud Climatology Project (ISCCP) definition of cloud types used in remote sensing of clouds.

2. It can be converted into a binary cloud mask by setting thresholds that can be changed depending on the application restrictions.

In general, cloud screening algorithms can be separated into *clear sky conservative* and *cloud conservative* algorithms. Clear sky conservative algorithms minimize the clear sky detection error, i.e. if a pixel is detected as clear the probability of cloudiness should be very low. This often has the side effect that many cloud free pixels are detected as cloudy. The opposite is true for cloud conservative algorithms, which try to minimize the cloud detection error, with the side-effect that many cloudy pixels are missed. The selection of the type of cloud detection algorithm usually depends on the posterior remote sensing application. The proposed cloud abundance product would allow users to adjust the trade-off between clear sky and cloud detection errors.

2.4 Review of Cloud Screening Algorithms

Cloud screening approaches, also referred to as *cloud masking* or *cloud detection*, are generally based on the assumption that clouds present some useful features for its identification (Rossow, 1993): clouds are usually brighter and colder than the underlying surface, clouds increase the spatial variability of detected radiance, and the spectral response is different from that of the surface covers. But, individually, as shown in chapter 1, each of these features in a given image is strongly conditioned by the sun elevation, variable path length, atmospheric water vapor, aerosol concentrations, variable reflectance, and subpixel clouds produced on the same pixel by cloud structures over land or sea (Yhann and Simpson, 1995). Some of these problems can be mitigated in the cloud screening algorithm by including specific corrections (e.g. sun elevation or path length), avoiding bands with severe atmospheric effects, and providing the user with information about subpixel coverage. The atmospheric features, though viewed as a problem by most of the cloud screening approaches, can provide useful information about cloud height that can be included in the screening approach.

After stating the cloud screening problem, it is clear that the selection of an approach heavily

depends on the characteristics of the instrument. The spectral range, along with the spectral and spatial resolutions are also critical factors in the selection of the best approach. For example, the presence of channels in the thermal infrared range enables detection based on thermal contrasts (Simpson and Gobat, 1996; Papin et al., 2002). Sensors with narrow spectral channels beyond $1 \mu\text{m}$ have demonstrated good capabilities to detect high clouds because of the strength of the water vapor absorption (McIntire and Simpson, 2002; Gao et al., 1998). In the spectral range of $1.38\text{-}1.50 \mu\text{m}$, both the thin cirrus clouds and the lower-level cumulus clouds can be seen; however, the surface features are eliminated due to additional absorption of solar radiation by atmospheric water vapor between clouds and the surface cover (even in presence of ice or snow). In fact, new generation EO satellites, such as the Global Monitoring for Environment and Security (GMES) Sentinel 2 and 3 (European Space Agency, 2007), include dedicated bands specifically designed to perform an accurate cloud screening. These features can not be exploited by recently developed multispectral sensors that work in the spectral range between $400\text{-}1000 \text{ nm}$, such as CHRIS and MERIS. However, even in these cases, one can take advantage of their high spectral and radiometric resolution and the specific band locations to increase the cloud detection accuracy, and to properly describe detected clouds.

In the literature, the simplest approach to mask clouds in a particular scene is the use of a set of static thresholds (e.g. over features such as albedo or temperature) applied to every pixel in the image and ultimately providing a binary flag (Wang and Shi, 2006). These methods can fail for several reasons, such as subpixel clouds, high reflectance surfaces, illumination and observation geometry, sensor calibration, variation of the spectral response of clouds with cloud type and height, etc. (Simpson et al., 1998). Spatial coherence methods have an advantage over static threshold methods because they use the local spatial structure to determine cloud free and cloud covered pixels. Usually, these algorithms are based on extracted textural features (Tian et al., 1999; Christodoulou et al., 2003), contextual approaches (Papin et al., 2002), or simple thresholds applied to the spatial variability of spectral bands (Martins et al., 2002), which is mainly applicable over the ocean where the surface background is sufficiently homogeneous. However, spatial coherence methods can fail when the cloud system is multi-layered (which is often the case), the clouds over the scene are smaller than the instrument spatial resolution, or the scene presents cirrus clouds (which are not opaque). As a consequence, researchers have turned to developing adaptive threshold cloud-masking algorithms (Simpson et al., 1998; Di Vittorio and Emery, 2002; Yang et al., 2007). Some other algorithms take advantage of the multi-angular (Yang et al., 2007; Mazzoni et al., 2007) or the multi-temporal (Saitwal et al., 2003) information depending on the instrument characteristics and the application constraints. In this context, few works using more sophisticated machine learning tools have been presented so far, such as Bayesian methods (Murtagh et al., 2003; Li et al., 2003; Merchant et al., 2005), fuzzy logic (Ghosh et al., 2006), artificial neural networks (Yhann and Simpson, 1995; Tian et al., 1999; McIntire and Simpson, 2002; Torres Arriaza et al., 2003), or recently kernel methods (Srivastava and Stroeve, 2003; Lee et al., 2004; Mazzoni et al., 2007).

Given the extreme complexity of cloud screening, most of the operational cloud masking applications of current satellite multispectral systems, such as Moderate Resolution Imaging Spectroradiometer (MODIS) (Ackerman et al., 1998; Platnick et al., 2003), Advanced Very High Resolution Radiometer (AVHRR) (Saunders and Kriebel, 1988), Along Track Scanning Radiometer (ATSR) (Simpson et al., 1998), POLarization and Directionality of the Earth's Reflectances (POLDER) (Buriez et al., 1997), or MERIS (Santer et al., 1997), consist in a series of cloud detection threshold tests, which can vary depending on surface type, solar illumination, geographic location, or climatological criteria.

2.4.1 Reference Cloud Screening Algorithms

The choice of the cloud screening approach is conditioned by the instrument characteristics. CHRIS and MERIS are optical sensors working in the VNIR range of the spectrum. Two major points motivate the selection of these instruments and cloud screening to be put together in this work.

In the case of MERIS, it offers a unique spectral configuration for the retrieval of both atmosphere (Guanter et al., 2008a) and surface (Guanter et al., 2007) parameters: two fine bands at the oxygen (O₂-A) and water vapor atmospheric absorptions are combined with thirteen other spectral bands providing high-accuracy measurements from the blue to the near-infrared spectral regions (see Rast et al. (1999) for further technical information). Also, the accurate characterization of the O₂-A absorption at MERIS channel 11 enables the estimation of cloud-top pressure (which is related to cloud height) from MERIS data (Santer et al., 1999; Naud et al., 2003). However, there is a well-known lack of accurate methods for the cloud screening of MERIS data, as well as clearly identified problems in the corresponding ESA official Level 2 cloud mask products (Ramon et al., 2003; MERIS Quality Working Group, 2006).

In the case of CHRIS, it covers a spectral range from 400 nm to 1050 nm with a high number of spectral bands (up to 62 spectral channels) and with a high spatial resolution (17 or 34 m at nadir) depending on the acquisition mode. Owing to the PROBA platform pointing capabilities, the acquisition plan tries to avoid acquisitions with cloud coverage, but occasionally images are partially affected by clouds. However, since PROBA is an experimental mission, official Level 2 algorithms and products have not been developed and a cloud mask is not provided with CHRIS products.

Summarizing, as far as author's knowledge, no cloud screening algorithm have been proposed in the literature for CHRIS instrument. In the case of MERIS, in addition to the ESA official Level 2 cloud mask products, several approaches have been proposed in the literature in order to mitigate identified problems in the standard ESA product (Ranera et al., 2005; Preusker et al., 2006; Guanter et al., 2008a). In the following, the MERIS Level 2 Cloud Masking (the official ESA product) and the Cloud Probability Processor (made available to the user community in the BEAM software) are described in detail.

MERIS Level 2 Cloud Masking

MERIS Level 2 products (European Space Agency, 2006) are obtained by further processing MERIS TOA radiance. In order to take into account the effect of clouds, image pixels clear enough to pursue atmospheric corrections are first identified as ‘*clear sky*’ or ‘*cloud free*’. The classification process uses the a priori knowledge of a land/ocean map indexed by longitude and latitude, and the information in the TOA radiance bands to classify each valid pixel into four pixel classes: ‘*clear sky*’ or ‘*bright pixel*’ over both ‘*ocean*’ or ‘*land*’. In this classification, *bright pixels* include clouds, bright sand or soil, ice, snow, sunglint, etc. Then there is also a need, for bright pixels, to separate clouds from bright land and ocean surfaces. The proposed pixel identification algorithm is based on a succession of tests on reflectance in the MERIS bands:

- For pixels identified as *land*, identification of homogeneous clouds is based on (i) tests on the ratio of Rayleigh-corrected reflectance at several wavelengths; and (ii) the apparent pressure estimated in the O₂ absorption by two independent methods (a polynomial regression and an artificial neural network).
- Over *ocean*, apparent pressure is used to discriminate between cloud and ice or sun glint. In this case, thresholds are defined as a function of geometrical conditions due to the strong effects of clouds on the scattering of radiation.

In addition to this classification, some flags are also defined for the possible occurrence of cirrus clouds or finite clouds. Since the final L2 cloud classification is a hard classification (i.e. no information about cloud transparency/contamination is given), these flags are proposed as a warning for the quality of the atmospheric corrections. Over *ocean*, a first flag is set from correlations between apparent pressure in O₂ channels and reflectances at 865 nm with a threshold in pressure corresponding to a too high contribution of the cirrus reflectance. A similar flag is implemented for *land* observations.

All these flags (bright pixel, low pressures, pressure confidences, and reflectance ratios) are finally used to index a decision table which provides the *Cloud-Free* flag. Pixels flagged as cloudy are further processed in order to retrieve the cloud albedo, the cloud optical thickness, and the cloud top pressure. Finally, a simple classification table indexed by the cloud optical thickness and cloud top pressure is used to provide a cloud type index.

BEAM Cloud Probability Processor

As aforementioned, ESA official Level 2 cloud mask products have shown clearly identified problems when considering critical cloud screening issues such as cloud borders and bright surfaces (Ramon et al., 2003; MERIS Quality Working Group, 2006). In consequence, recent alternative algorithms have been proposed (Ranera et al., 2005; Preusker et al., 2006).

The *Basic ERS & ENVISAT (A)ATSR and MERIS (BEAM) Toolbox* is a collection of executable tools (Fomferra and Brockmann, 2005) that was originally developed by ESA to facilitate the utilization, viewing, and processing of ESA MERIS, (A)ATSR and others (<http://envisat.esa.int/resources/softwaretools/> or <http://www.brockmann-consult.de/beam/>).

This software includes the BEAM Cloud Probability Processor, which uses a clear sky conservative cloud detection algorithm which is based on artificial neural networks (Preusker et al., 2006).

The cloud probability algorithm uses nine spectral bands of MERIS, the ratio of band 11 and 10, which is an indication of the absorption due to oxygen, the ECMWF² surface pressure and the exact wavelength of band 11 as input. As an output, it yields a probability value $\in [0, 1]$ indicating if a pixel can be regarded as a cloud or not. Such a probability permits a more flexible way to work with identified clouds compared to a binary cloud mask.

The algorithm uses two different artificial neural nets for prediction purposes. The first one is used over the open ocean and the second one over land. The distinction between ocean and land is done using the altitude information. If the altitude is lower than -50 m the ocean net is used.

During development of the algorithm, the *Matrix Operator Model* (MOMO), a radiative transfer model (Fischer and Grassl, 1991) based on the Matrix Operator Method, was used to simulate cloud and non-cloud TOA radiance and an artificial neural net was trained. The output of the neural net is finally scaled into a probability value. The final cloud classification indicates pixels that are cloudy (*probability* > 80%), cloud free (*probability* < 20%) or where it is uncertain ($20\% < \textit{probability} < 80\%$).

This algorithm provides a more accurate cloud mask than the MERIS Level 2 Cloud Masking algorithm, but it still misclassifies bright surfaces such as ice and snow covers. Moreover, the cloud probability provided by the artificial neural net, which may be useful for the users to decide *what is a cloud* depending on the application requirements or image conditions, is usually unevenly distributed around zero and one, and thus, the information provided is equivalent to a binary cloud mask.

²European Centre for Medium-Range Weather Forecasts: <http://www.ecmwf.int/>.

Part II

Methodology for Cloud Identification

Chapter 3

Proposed Methodology for Cloud Screening

The main objective of this PhD Thesis is to develop an accurate cloud screening algorithm using the full spectral information provided by MERIS and by CHRIS imaging spectrometers. The proposed cloud screening algorithm takes advantage of the high spectral and radiometric resolutions of MERIS, or the high number of spectral bands of CHRIS, and the specific location of some bands to increase the cloud detection accuracy, such as the oxygen and water vapor absorption bands. This chapter summarizes the proposed cloud screening procedure and briefly introduces the different modules that constitute it. Chapters 4, 5, and 6 will be devoted to analyze in greater detail these parts.

The method should be capable of: *(i)* detecting clouds accurately; and *(ii)* providing probability or cloud abundance rather than merely cloud flags. The cloud abundance product provided is not directly related to the retrieval of cloud optical properties (Kokhanovsky et al., 2007b), such as the cloud optical thickness, which usually relies on radiative transfer models. This added value product allows the user to apply an adjustable cloud mask depending on the further processing stages and final use of the image. For example, undetected cloudy pixels heavily affect biophysical parameter retrieval methods based on the evaluation of the measurements in the shortest wavelengths, such as aerosol retrieval, or estimation of water pigments or suspended matter, as well as to methods relying on temporal composites (Saitwal et al., 2003; Ranera et al., 2005; Plummer, 2005). Slight over-masking of potential cloudy pixels –conservative cloud masking– would be preferred to guarantee a minimum admissible quality of the final product (Guanter et al., 2008a; Kaufman et al., 2005; Martins et al., 2002), while other applications such as land use classification are less sensitive to thin clouds, and thus the associated areas should not be necessarily discarded (Gómez-Chova et al., 2006f, 2007c; Camps-Valls et al., 2008a). As a result, the method should be scalable and allow different levels of masking. Hence, a probabilistic mask indicating the cloud contamination is proposed.

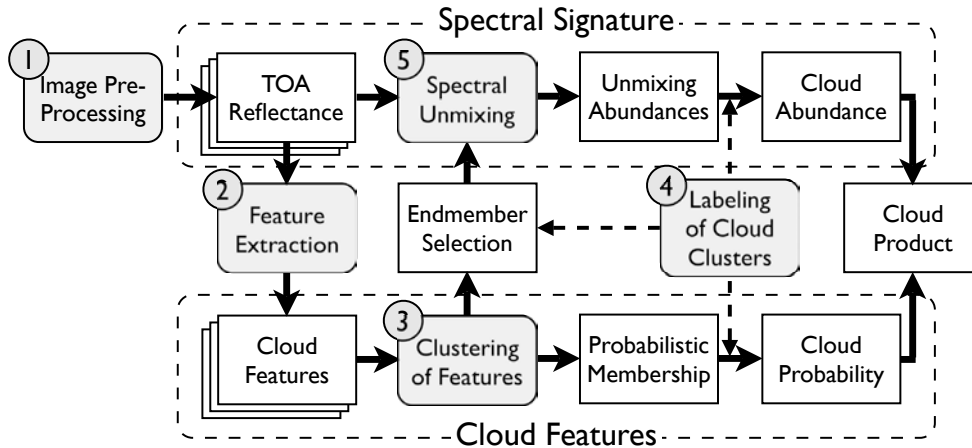


Figure 3.1: Scheme of the cloud screening algorithm constituted by the preprocessing (TOA reflectance derivation) and four main processing steps (grey boxes).

To achieve the objectives of accuracy and cloud probability, we propose a scheme based on some building blocks and processing steps (see Fig 3.1). Firstly, a feature extraction based on meaningful physical facts is carried out (e.g. clouds are bright and white). Then, a semi-supervised or unsupervised classification is applied to these features and the resulting clusters are subsequently labeled as *cloud* or *cloud-free*. Finally, a spectral unmixing is applied to the classified image. Summarizing, the cloud screening procedure is constituted by the following steps:

1. *Image pre-processing*: TOA reflectance is derived.
2. *Feature extraction*: physically-inspired features are extracted to increase separability of clouds and surface.
3. *Image clustering*: an unsupervised clustering is performed on the extracted features in order to separate clouds from the ground-cover.
4. *Cluster labeling*: resulting clusters are subsequently labeled (by the user or by an automatic classifier) into geo-physical classes according to their extracted features and spectral signatures.
5. *Spectral unmixing*: a spectral unmixing is applied to the segmented image in order to obtain an abundance map of the cloud content in the cloudy pixels.

Image pre-processing

Both MERIS and CHRIS products are provided in TOA radiance, that is, radiometrically calibrated data. However, uncorrected errors, deviations from nominal calibration values, and high levels of noise affect the performance of cloud screening significantly. Hence, a particular attention is paid in this Thesis to the pre-processing of images, especially for CHRIS data, which

present high levels of noise. In addition, the method must work under many situations. Therefore, TOA reflectance is estimated to remove the dependence on particular illumination conditions (day of the year and angular configuration).

Feature Extraction

The measured spectral signature depends on the illumination, the atmosphere, and the surface. Spectral bands free from atmospheric absorptions contain information about the surface reflectance, while others are mainly affected by the atmosphere. Physically-inspired features that increase separability of clouds and surface covers can be extracted independently from the bands that are free from atmospheric effects and from the bands affected by the atmosphere.

With regard the reflectance of the surface, one of the main characteristics of clouds is that they present *bright* and *white* spectra:

- A *bright* spectrum means that the intensity of the spectral curve (related to the albedo) should present high values. Therefore, cloud brightness is calculated as the integral of the spectrum.
- A *white* spectrum means that the spectral curve is flat, and thus, the first derivative of the spectral curve should present low values.

Concerning the atmospheric absorptions present in the spectrum of a pixel, another meaningful feature is the fact that clouds are at a higher altitude than the surface. It is worth noting that atmospheric absorption depends on the atmospheric components and the optical path. Since light reflected on high clouds crosses a shorter section of the atmosphere, the consequence would be an abnormally short optical path, thus weaker atmospheric absorption features. Atmospheric oxygen or water vapor absorptions (at 760 nm and 940 nm respectively) can be used to estimate this optical path.

This approach tries to overcome one of the critical issues in cloud detection: the presence of bright pixels, such as ice/snow in the surface. Bright land covers and clouds have a similar reflectance behavior, but the atmospheric absorption suffered by cloud pixels is lower than for the surface pixels due to their height.

Image Clustering and Labeling

At this step, two different approaches have been proposed and analyzed: a fully unsupervised method and a semi-supervised approach:

1. *Unsupervised classification algorithm.* In this approach, we use the Expectation-Maximization (EM) algorithm (Dempster et al., 1977) to estimate the parameters of a Gaussian mixture

model (GMM) since it considers the full relationship among variables and provides probability maps for each cluster. At this point of the process, the obtained clusters can be labeled into geo-physical classes taking into account three complementary sources of information: the thematic map with the distribution of the clusters in the scene, the spectral signatures of the cluster, and their distribution in the image. Once all clusters have been related to a class with a geo-physical meaning, it is straightforward to merge all the clusters belonging to a cloud type. Since the EM algorithm provides posterior probabilities, a probabilistic cloud index, based on the clustering of the extracted features, can be computed as the sum of the posteriors of the cloud-clusters. However, if the clusters are well separated in the feature space, the posteriors decrease drastically from one to zero in the boundaries between clusters. Therefore, this cloud probability index indicates the probability that one pixel belongs to a cloud-cluster more likely than to one of the other clusters found in the image, but it does not give information about the cloud content at a subpixel level, which in turn becomes very important when dealing with thin clouds or partially covered pixels.

2. *Semi-supervised classification algorithm.* In this second approach, we develop a semi-supervised kernel-based method that incorporates labeled and unlabeled data in a general-purpose learner. The problem of learning from labeled and unlabeled data (semi-supervised learning) has attracted considerable attention in recent years (Joachims, 2003; Chapelle et al., 2006). In particular, we focus on two semi-supervised extensions of support vector machines (SVM) (Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004; Camps-Valls et al., 2007c): the so called Laplacian SVM (LapSVM), which introduces an additional regularization term on the geometry of both labeled and unlabeled samples by using the graph Laplacian (Belkin et al., 2006; Gómez-Chova et al., 2007b, 2008c); and a novel generative semi-supervised method based on composite kernels and mean kernel theory (Camps-Valls et al., 2006d, 2008a; Gómez-Chova et al., 2008a, 2009).

Spectral Unmixing

In order to obtain a cloud abundance map for every pixel in the image, rather than flags or a binary classification, a spectral unmixing algorithm is applied to the image using the full spectral information (Chang, 2003). The computed abundances are related to a cluster with a geo-physical meaning, and the abundance of cloud is computed as the sum of the abundances of the cloud-clusters. An improved cloud abundance map can be obtained when combining the cloud abundance and the cloud probability by means of a pixel-by-pixel multiplication. That is, combining two complementary sources of information processed by independent methods: the degree of cloud abundance or mixing (obtained from the spectra) and the cloud probability that is close to one in the cloud-like pixels and close to zero in remaining areas (obtained from the extracted features). As a result, the proposed algorithm should provide a probabilistic map of cloud abundance rather than a binary cloud presence flag at a pixel level.

Chapter 4

Image Pre-processing and Feature Extraction

When working with remote sensing images at different times and locations, a desirable characteristic is to have data independent of the sensor system and image acquisition conditions. This is also true for cloud screening. On the one hand, correcting image data for uncertainties in sensor calibration has the advantage that then these data are independent of differences in sensor system conditions. On the other hand, converting TOA radiance data into TOA reflectance has the advantage that then these data are corrected for seasonal and diurnal differences in solar position.

Once the image data are expressed in TOA reflectance, we can further process the reflectance spectra in order to extract features that increase the separability of clouds and surface covers. These features are physically-inspired and their meaning is independent of differences in the number, location, and bandwidth of the sensor channels, which is a desirable characteristic for a cloud screening algorithm intended to work in images acquired by multi and hyperspectral sensors, such as MERIS and CHRIS.

4.1 Pre-processing (I): TOA Radiance Corrections

Earth observation images acquired by remote sensing instruments are generally affected by two kinds of noise. The first one can be defined as standard random noise (Aiazzi et al., 2002), which varies with time and determines the minimum image signal-to-noise ratio (SNR). In addition, hyperspectral images can present non-periodic partially deterministic disturbance patterns, which come from the image formation process and are characterized by a high degree of spatial and spectral coherence (Barducci et al., 2005).

Usually, the whole system is fully characterized after assembly, obtaining the actual gain correction factors that would produce an even image in operational situations. However, in some occasions, especially after launch, the system is affected in such a way that the characterization

does not remove completely the noise. In addition, this type of sensors degrade with time, and thus require a recalibration, which is not always possible. In those cases, a noise reduction algorithm must be applied after image reception in the pre-processing phase.

In this first section of the chapter, we focus on presenting, modeling, and correcting the coherent spatial and spectral noise patterns produced by these systematic, yet hardly predictable, disturbances in both the operational MERIS and the experimental CHRIS instruments.

4.1.1 Corrections for MERIS

ENVISAT is the most important EO satellite ever launched by ESA. The calibration and validation activities of all ENVISAT instruments represent a long-term effort, which has been carried out by ESA in parallel to the algorithms improvement (Baudin et al., 1996; Merheim-Kealy et al., 1999; Delwart et al., 2004).

Calibration involves both pre-launch and post-launch measurements to fully characterize the payload instruments, and subsequent activities to configure the ground processors to provide calibrated (Level-1b) data products. MERIS Level 1b (L1b) products are provided in *top of the atmosphere* radiance and two different calibration approaches are used to radiometrically calibrate the data. The primary calibration is the *in-flight calibration* and characterization of the instrument that uses the onboard sunlit calibration diffuser plates (Dubuisson et al., 2003; Ramon et al., 2003; Delwart et al., 2007). Validation of TOA radiances measured by MERIS are also achieved by comparison with TOA radiance values determined through a number of *vicarious calibration* independent methods: simultaneous in-situ measurements of natural targets (Hagolle and Cabot, 2004); analysis of Rayleigh scattering over clear water (Martiny et al., 2005); simulation of radiance data with radiative transfer models (Antoine and Chami, 2004); data acquisition over stable deserts sites (Govaerts and Clerici, 2004); or simultaneous acquisition by other sensors (Acarreta and Stammes, 2005; Kokhanovsky et al., 2007c).

The scene is acquired simultaneously across the entire spectral range, through a dispersing system, onto the CCD array (cf. section 1.3). Signals read out from the CCD pass through several processing steps in order to achieve the required image quality. These CCD processing tasks include dumping of spectral information from unwanted bands, and spectral integration to obtain the required bandwidth. Onboard analog electronics perform pre-amplification of the signal and correlated double sampling and gain adjustment before digitization. The onboard digital electronics system has three major functions: it completes the spectral integration, it performs offset and gain corrections in full processed mode, and it creates the reduced-resolution data when required.

The calibration of MERIS is performed at the orbital south pole, where the calibration diffuser is illuminated by the Sun by rotating a calibration mechanism. In particular, onboard spectral calibration is based on the use of absorption bands (Delwart et al., 2007): pink panel that is an

Erbium doped panel with well-defined absorption peaks; the Fraunhofer lines; and the oxygen bands. In the calibration mode, correction parameters such as offset and gain are generated, which are then used to correct the recorded spectra. This correction can be carried out either on-board or on the ground segment.

A spectral characterization was performed before MERIS launch, which showed a spectral shift mainly due to the CCD integration with optics during the spatial registration. The so-called smile effect has a maximum spectral dispersion of 1.5 nm and can be observed at any wavelength. In fact, MERIS smile is the sole acquisition error that is not corrected in the provided images and has an important effect in the proposed cloud screening algorithm. However, MERIS smile has been well characterized in previous works with both in-flight (Dubuisson et al., 2003) and vicarious (Martiny et al., 2005) calibration methods. This accurate characterization of the spectral shift produced by the smile can be introduced in the formulation of the cloud screening algorithm in order to compensate its effects as it will be explained later.

4.1.2 Corrections for CHRIS

PROBA was designed as a technology demonstrator satellite and, originally, CHRIS data was a secondary objective of the mission. ESA has renewed its support to the PROBA/CHRIS acquisition plan year by year thanks to the interest of the scientific community, but originally CHRIS data were not available in the ESA catalogues, and even nowadays CHRIS has no standard processing algorithms defined. In fact, the only pre-processing step performed to the CHRIS data before delivering image products is the radiometric calibration¹. Thus, CHRIS images present a certain number of problems and errors that are commonly removed from most of the remote sensing data.

As a push-broom sensor, the radiometric response of the CHRIS instrument is determined by two overlapping components: the optical system response (a telescope forming an image onto the entrance slit together with the spectrometer) and the CCD response (a thinned, back-illuminated, frame-transfer CCD) (Bernaerts et al., 2000). With regard to the CCD response, the different pixel-to-pixel response comes from non-uniformities on dark current generation, non-uniformities on pixel sensitivity, threshold variations, and gain and off-set differences (Theuwissen, 1995). But, in practice, these CCD imperfections are relatively stable with temperature and time (Cutter, 2004a) resulting in a spatially fixed-pattern noise in the image that should be removed, e.g. the dark signal offsets are removed by subtracting a generic dark image. However, with regard to the optical system response, changes in temperature, due to the seasonal variation of the in-orbit CHRIS instrument temperature (Cutter, 2004a), produce a dilation of the slit and change its width and moves the image of the slit across the detector. Therefore, the effect of the slit adds up

¹CHRIS products are provided in *top of the atmosphere* radiance in a HDF v4 file format, which includes additional acquisition information (image date, azimuth and zenith angles, etc) contained in the metadata attributes of the CHRIS HDF file (Cutter and Johns, 2005b).

to the vertical pattern in a complex way, as it is dependent on the sensors temperature heavily (see Fig. 4.1), and thus it must be modeled and corrected.

Several vertical stripping (VS) reduction approaches have been proposed in the literature. Our approach falls in the field of the *scene-based non-uniformity corrections* (SNUCs), since it provides relative calibration factors directly computed from the acquired image. Methods based on large uniform areas in the scene or methods assuming constant-static noise patterns (Torres et al., 2003; Pezoa et al., 2006) are not appropriate for CHRIS due its spatial resolution (17 to 34 m) and its noise dependence on the sensor’s temperature, respectively. Other methods assume that all sensor elements observe similar subscenes in a given image and adjust the distributions of values acquired by each sensor to some reference distribution by means of histogram or moment matching (Gadallah et al., 2000), but also the high CHRIS spatial resolution and the moderate number of lines per image dissuade us from its use. Finally, most related methods assume that noise contribution changes from one pixel to another (high spatial frequency) in the across-track direction while surface contribution presents smoother profiles (lower spatial frequencies) in the across-track dimension (Barducci and Pippi, 2001; Garcia and Moreno, 2004; Settle and Cutter, 2005; Mlsna and Becker, 2006). This approach is described in more detail in section 4.1.2 but the reader is referred to Leathers et al. (2005) for a full description of SNUC methods for push-broom sensors. A novelty of the proposed vertical striping correction method is that it explicitly introduces a technique for excluding the contribution of the surface’s spatial high frequencies from the destriping process. The proposed approach is ‘CHRIS-oriented’ since it takes advantage of the hyperspectral and multiangular capabilities of CHRIS, and also can include the platform temperature information in order to improve the results. However, the general nature of the procedure allows it to be applied to any push-broom imaging spectrometer data.

In addition to the VS noise produced at the image formation process, the transmission of CHRIS channel 2 (odd and even pixels from each CCD row are read in parallel) randomly fails producing anomalous odd pixels in some image rows called ‘*drop-outs*’. These errors must be identified (masked and unmasked drop-outs) and corrected by making use of both spatial and spectral information of the anomalous pixel and its neighbors. Drop-outs hamper the operational use of CHRIS images since later processing stages are drastically affected by these anomalous pixels. For this reason, version 4.1 of the CHRIS data HDF file (Cutter and Johns, 2005a) includes a quality mask that indicates pixel saturation and occurrence of errors: useful pixels, drop-out pixel (Ch2 reset), and saturated pixel. The problem is that this mask sometimes fails to mark drop-out pixels and, in addition, older versions of CHRIS products do not include the mask at all.

The cloud screening module requires the CHRIS image already noise-corrected: *drop-outs* cannot be processed since they present anomalous values in some bands, and the *vertical striping* introduces differences between bands that affect features extracted from the spectra. Figure 4.2 shows an example of the effects of both types of noises and the images after the correction. In the following sections, the correction algorithm proposed in this Thesis is described in detail. It

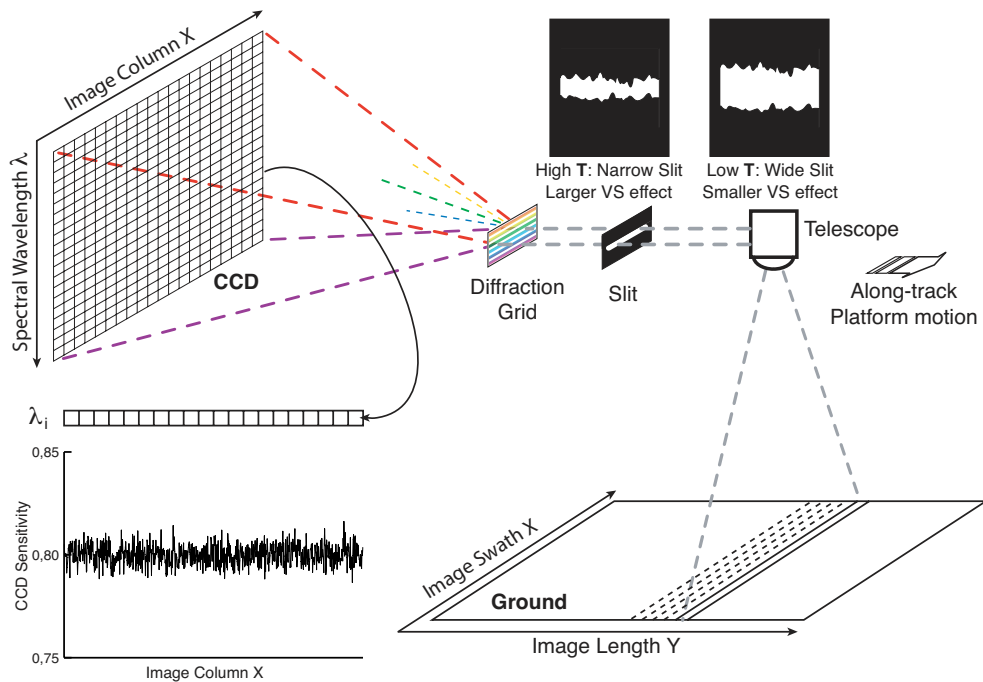


Figure 4.1: Design of a push-broom imaging spectrometer that shows its operation mode and the sources of the coherent spatial noise patterns.(Credit: figure based on an original of Barducci and Pippi (2001))

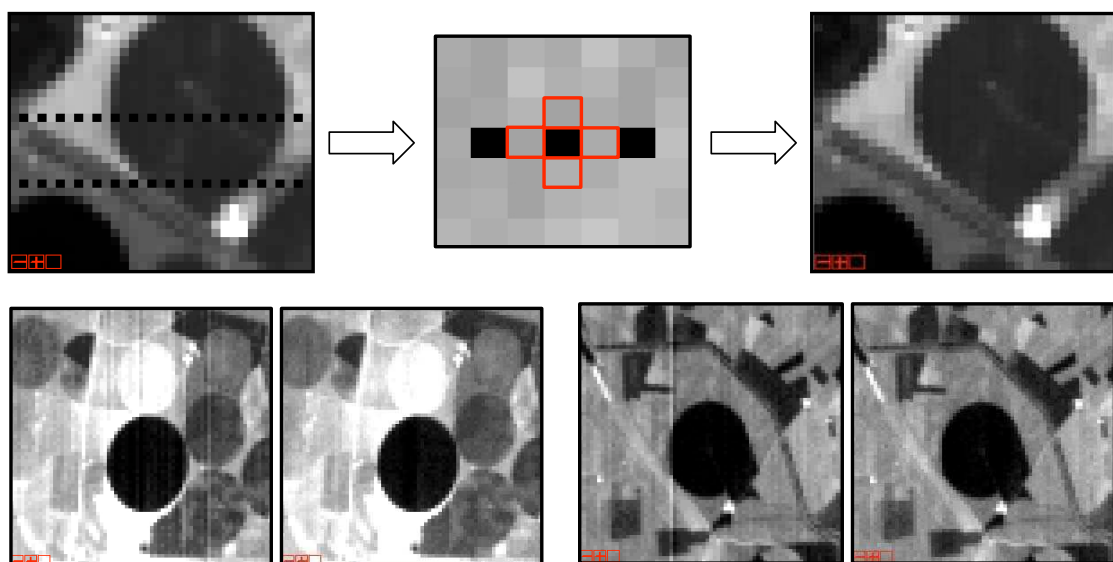


Figure 4.2: Illustration of the correction of the drop-out errors based on the four-connected neighbors (*top*) and the vertical striping (*bottom*). Credits: Garcia and Moreno (2004).

is being implemented in the BEAM Toolbox (Fomferra and Brockmann, 2005) in the framework of an ESA project² for the official CHRIS products.

No-data Mask Generation

From version release 4.1, CHRIS data includes an image quality mask, which has the same dimensions in terms of number of pixels than the CHRIS image of the HDF file, that is, a data-cube $M(l, p, b)$ of size $N_l \times N_p \times N_b$. In this mask, each pixel has one of three possible values indicating the usability of the pixel with the following meaning³: ‘0’ indicates that the pixel is a useful image pixel; ‘1’ indicates that the pixel is a channel 2 reset pixel and holds no valuable data (Drop-Out); or ‘2’ indicates that the pixel has saturated and holds no valuable data (Saturation).

If the mask is not available (versions previous to v4.1) we have to create an empty mask of the same size than the image and find rows with drop-out pixels. Moreover, although we have the mask with the drop-outs (channel 2 reset), in some images there may also be invalid pixels that are not masked. The problem with these unmasked pixels is that they do not present negative values (their values are in the order of magnitude of the signal) but they always occur in odd columns. Therefore, whether the mask with the drop-outs is available or not, we need to improve/create the mask adding undetected drop-outs.

The anomalous pixels (drop-outs) are found for all the image lines N_l of all the spectral bands N_b as follows:

1. We assume that the difference between contiguous pixels in a row is small. The difference between a correct pixel with its neighbor should be equal or smaller than with the pixel of two columns away, except in the case that the neighbor is a drop-out. This assumption should be true for all the odd pixels of the row.

- Square difference of odd pixels, which may be drop-outs, with neighboring even pixels that are certainly correct:

$$D_{\text{all}}(l, b) = (I(l, p, b) - I(l, p + 1, b))^2 \quad p = 1, 2, \dots, N_p - 1, \quad (4.1.1)$$

where high differences are expected in presence of drop-outs.

- Square difference of even pixels, which are certainly correct, with the following even pixel:

$$D_{\text{even}}(l, b) = (I(l, p, b) - I(l, p + 2, b))^2 \quad p = 2, 4, \dots, N_p - 2, \quad (4.1.2)$$

where low differences are expected in all cases (depending on the surface changes in the across-track direction).

²Development of CHRIS/PROBA Modules for the BEAM Toolbox (ESRIN Contract No. 20442/07/I-LG).

³The meaning of the quality mask values is also provided in the “Key to Mask” annotation in the HDF file metadata of the CHRIS products as a simple line of text: “0 = useful pixels; 1 = Ch2 reset pixels; 2 = Saturated data pixel”.

2. Surface and vertical striping affect differences between contiguous columns, thus the ‘median’ is used to obtain a robust estimator of the average difference between pixels for the whole line.
3. Finally, all odd pixels of the line are labeled as drop-out noise if the difference between neighbours is 50% higher than between even pixels:

$$\text{IF } \frac{\text{median}(D_{\text{all}}(l, b))}{\text{median}(D_{\text{even}}(l, b))} > 1.5 \text{ THEN } M(l, p, b) = 1 \quad p = 1, 3, \dots, N_p \quad (4.1.3)$$

Drop-out Correction

Once the drop-out errors have been detected, they must be corrected by using both spatial and spectral information of the anomalous pixel and its neighbors. Each invalid pixel value is replaced by a weighted average of the values of the neighboring pixels. In order to avoid the poor performance of spatial filters (local average) in border or inhomogeneous areas (Larsen et al., 1998; Garcia and Moreno, 2004), the contribution of each pixel (i, j) of a given neighborhood (C) of size 3×3 , is weighted by its similarity to the corrected pixel, $I(l, p, b)$. In particular, this similarity weight is the inverse of the Euclidean distance between the spectral signature of the pixels, which is calculated locally using the n_b upper and bottom spectral bands closer to the corrected band b :

$$W(i, j) = \left(\sum_k (I(l, p, b) - I(l + i, p + j, b + k))^2 \right)^{-1/2} \quad k = -n_b, \dots, -1, 1, \dots, n_b. \quad (4.1.4)$$

The final weight matrix, W_C is modified to have zero values for the pixels not belonging to the given neighborhood C and it is normalized in order to sum to one, i.e. , $W_C(i, j) = C(i, j)W(i, j) / \sum_{i, j} C(i, j)W(i, j)$. Finally, the new value of the drop-out is calculated as:

$$I(l, p, b) = \sum_{i, j} I(l + i, p + j, b)W_C(i, j) \quad i, j = -1, 0, 1. \quad (4.1.5)$$

The result of this process is similar to a spatial interpolation but taking into account the similarity with neighbors. It is worth noting that the values of bands with errors (indicated by the CHRIS quality mask) are not considered during this process. The inputs required by the drop-out correction algorithm are the CHRIS image, I , the improved quality mask, M , the definition of the neighborhood, C , and the number of spectral bands n_b used to compute the local spectral distance.

The correction of the drop-out errors can be carried out independently of the vertical striping correction. However, the vertical striping noise introduces different multiplicative factors in image columns that can affect the new pixel value if the local average is performed by using contiguous columns. Therefore, if drop-out correction is performed before the vertical striping correction, only the values of the vertical neighbors (C_2) must be used in order to avoid the effect of vertical

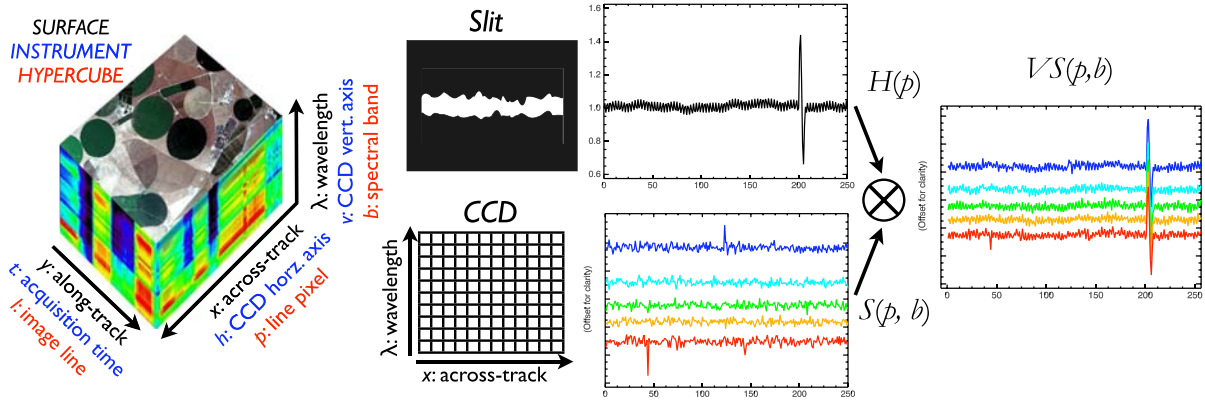


Figure 4.3: Vertical striping formation process from the combination of the non-uniform CCD pixel response $S(p, b)$ and the slit optical response $H_x(p)$, which are constant in columns.

striping. After the vertical striping removal, it is possible to perform a second correction based on the four-connected (C_4) or eight-connected (C_8) neighbors.

$$C_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad C_4 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad C_8 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} \quad (4.1.6)$$

Vertical Striping Correction

As it has been previously shown (cf. section 1.3), a spectral band b will be acquired by the same row of CCD elements. Therefore, each image column p will be affected by a different CCD pixel response $S(p, b)$, and a different optical slit response $H_x(p)$, which is equal for all spectral bands. The combination of these non-uniform spatial responses, which are constant in columns, superimposes a systematic pattern of noise organized by vertical lines (the formation of the stripe noise is depicted in Fig. 4.3). Therefore, the relation between the desired at-sensor radiance, $L_{\text{TOA}}(l, p, b)$, and the provided (radiometrically calibrated) product, $I(l, p, b)$, can be expressed from (1.3.4) as:

$$I(l, p, b) = L_{\text{TOA}}(l, p, b)H_x(p)H_\lambda(b)S(p, b) + S_0(l, p, b) = L_{\text{TOA}}(l, p, b)\nu(p, b) + S_0(l, p, b), \quad (4.1.7)$$

where $\nu(p, b)$ is a multiplicative noise coming from the slit and CCD, and $S_0(l, p, b)$ represents an additive noise. In the particular case of CHRIS, the provided level 1a images are radiometrically corrected (so the units of I are radiance units instead of DN), and images processed at version 4.1 of the CHRIS HDF files present an improved radiometric calibration (Cutter, 2004a; Cutter and Johns, 2005b) which was poor in previous versions (underestimation up to a factor two of the sensor measurements in the NIR). Therefore, one can assume that images present an accurate spectral radiometric calibration with $H_\lambda(b) \simeq 1$, and are corrected of dark current offsets, thus making $S_0(l, p, b)$ negligible, i.e. remaining only random noise of zero mean and low

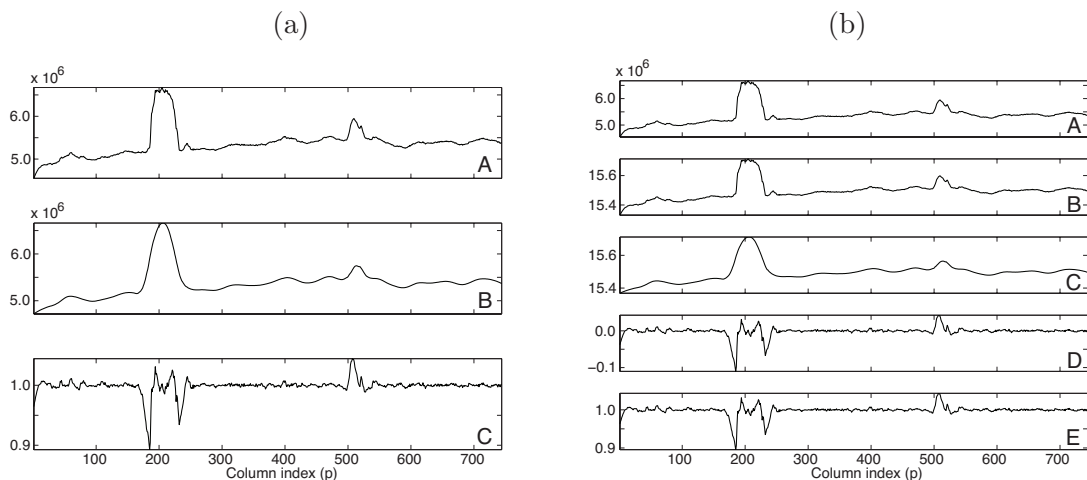


Figure 4.4: Example of the processing steps of two different vertical striping correction methods proposed by Barducci and Pippi (2001) (a) and Settle and Cutter (2005) (b): profiles of the last band of CHRIS_EL060130_63A1.41 image taken over Heron Island.

amplitude. Hence, (4.1.7) is reduced to:

$$I(l, p, b) = L_{\text{TOA}}(l, p, b)H(p)S(p, b) = L_{\text{TOA}}(l, p, b)\nu(p, b). \quad (4.1.8)$$

The objective of vertical striping (VS) correction methods is to estimate the correction factor, $\nu(p, b) = H(p)S(p, b)$, of each spectral band to correct all the lines of this band. The main assumption consists in considering that both slit (H) and CCD (S) contributions change from one pixel to another (high spatial frequency) in the across-track (p) but are constant in the along-track (l); while surface contribution (L_{TOA}) presents smoother profiles (lower spatial frequencies) in the across-track dimension.

Vertical striping correction methods. In the literature, all the vertical striping reduction approaches take advantage of the constant noise factors in the image columns (Barducci and Pippi, 2001; Garcia and Moreno, 2004; Settle and Cutter, 2005; Mlsna and Becker, 2006). Basically, the image is averaged in lines (along-track) and then the noise profile is estimated in the across-track direction for each band. By averaging image lines (*integrated line profile*) the surface contribution is smoothed, the additive random noise is cancelled, and the VS profile remains constant. Consequently, the surface contribution presents lower spatial frequencies in the integrated line profile and can be easily separated from the VS (high frequencies) applying a filter with a suited cut-off frequency.

Figure 4.4a shows the three steps of the method proposed by Barducci and Pippi (2001):

- A. Each band is averaged in lines (along-track direction) obtaining one integrated line profile per band: $\alpha(p, b) = \int_1^{N_l} I(l, p, b)dl = \nu(p, b) \int_1^{N_l} L(l, p, b)dl = \nu(p, b)\beta(p, b)$.

- B. A low pass filter (LPF) is applied using a moving-window algorithm that flattens the profile $\alpha(p, b)$ by convolving it with a Gaussian weighting function w : $\hat{\beta}(p, b) = \text{LPF}\{\alpha(p, b)\} = \int w(p - k)\alpha(p, b)dk$. In this kind of filter, the cut-off frequency f_c defines the standard deviation of the Gaussian window, $\sigma \sim 1/f_c$.
- C. Since $\hat{\beta}(p, b)$ mainly contains the surface contribution, the shape of the VS factors can be obtained by the ratio $\hat{\nu}(p, b) = \alpha(p, b)/\hat{\beta}(p, b)$. Thus, the corrected image is calculated as $\hat{L}(l, p, b) = I(l, p, b)/\hat{\nu}(p, b)$.

Figure 4.4b shows the method that is used by SIRA Technology Ltd. to correct CHRIS images (Settle and Cutter, 2005). The main difference with the previous method is the use of logarithms to transform the multiplicative noise into additive noise in order to improve the filtering as follows:

- A. Each band is averaged in lines obtaining one integrated line profile per band, $\alpha(p, b)$.
- B. Log-transform the averaged profile: $\log_\alpha(p, b) \equiv \log(\alpha(p, b)) = \log(\nu(p, b)) + \log(\beta(p, b))$
- C. Applying a low pass filter in order to eliminate high frequency variations (coming from the noise ν) and estimate surface contribution: $\hat{\log}_\beta(p, b) = \text{LPF}\{\log_\alpha(p, b)\}$.
- D. Obtaining high frequency variations (considered as the noise): $\hat{\log}_\nu(p, b) = \log_\alpha(p, b) - \hat{\log}_\beta(p, b)$
- E. The vertical striping factors are obtained calculating the inverse of the logarithm $\hat{\nu}(p, b) = \exp(\hat{\log}_\nu(p, b))$.

Theoretically, the first approach should give poor results when filtering the line profile because it is affected by a multiplicative noise and this is equivalent to a convolution in the frequency domain. This is the main reason to propose the second approach but, in practice, both approaches give equivalent results. This can be explained because features of the multiplicative noise, which present a mean close to one ($f = 0$ and $A = 1$) and high frequency components of low amplitude (high f and $A \simeq 0.1$). Therefore, when performing the convolution of the signal and noise in the frequency domain, the power spectral density of the signal at low frequencies is not affected. Since both methods provide equivalent results, we consider them as a single method and hereafter we refer to them as the *standard method*.

The standard method can fail for several reasons, such as high amplitude changes in the VS, which affect the performance of the low pass filter (wrong estimation of the surface contribution) producing an overestimation or underestimation in the correction factors of the neighboring columns. Garcia and Moreno (2004) presented an iterative method that corrects the effect of these high striping values. However, as proposed in the next section, these effects can be also avoided using more advanced filtering techniques that use a weight function.

Robust vertical striping correction method. One of the main drawbacks of the methods proposed in the literature is the fact that they do not take into account the possible high frequency components of the surface explicitly. In images presenting structures or patterns in the vertical direction, the averaged profile $\alpha(p, b)$ may present high frequency contributions due to the surface. This will be interpreted as vertical striping when estimating $\nu(p, b)$ (see the selected example in Fig. 4.4), and some columns will be corrected with wrong values, worsening the final image.

The proposed correction method is also based on the hypothesis that the vertical disturbance presents higher spatial frequencies than the surface radiance. However, it models the noise pattern by suppressing the surface contribution in the across-track in two different ways: first, avoiding the high frequency changes due to surface edges, and then subtracting the low frequency profile.

The surface can present high spatial frequencies due to: the surface texture, which has low amplitude changes; or changes in the land-cover type, which can produce great changes in amplitude being a problem in the destriping process. In principle, in one spectral band, both the surface and noise contributions are mixed and is not possible to distinguish which of them causes the changes in the radiance amplitude between contiguous columns. However, the spectral signature of pixels from current hyperspectral sensors can provide helpful information about the land cover changes. Considering the spectra of two contiguous pixels, p_1 and p_2 , just in the boundary between two land-cover types, there are three factors affecting the spectral change: (i) differences between the true spectra of both surfaces (in shape and magnitude); (ii) the different CCD sensitivity $S(p, b)$, which modulates the spectral signature as a multiplicative noise of low variance; and (iii) the different multiplicative factor due to the slit $H(p)$, which scales the magnitude of the whole spectral signature. Among these three factors, the first one will produce the greater change, the second one will be a second-order factor when comparing the spectral similarity, and the third one will not affect the final result if the selected spectral distance is invariant to scaling by a positive factor. Therefore, we can apply a filter in the across-track direction of the hyperspectral image in order to find the surface borders that introduce high frequencies in the across-track profile. The next sections explain how pixels corresponding to borders are not employed when computing the integrated line profiles.

Spatio-Spectral Edge Detection. We propose a spatio-spectral filter based on spatial convolution filters, which are commonly used in grayscale image processing, like the *Derivation filter* or the *Gradient-Roberts filter* (Pratt, 2001). These spatial convolution filters which calculate a weighted average of the cells in the current filter window. The spatial filter response, R , contains the array of weighting coefficients used in the calculation. To find edges in the horizontal direction (across-track) the edge detection matrix R of these methods can be $\begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}$ for the derivation filter, $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ or $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ for the Roberts filter, or a combination of them. To apply these techniques to hyperspectral images, taking into account the spectral dimension, it is not possible to directly calculate the convolution of the edge detection matrix and the three-dimensional hypercube. In our proposal, a spectral distance is first computed between the spectrum of the

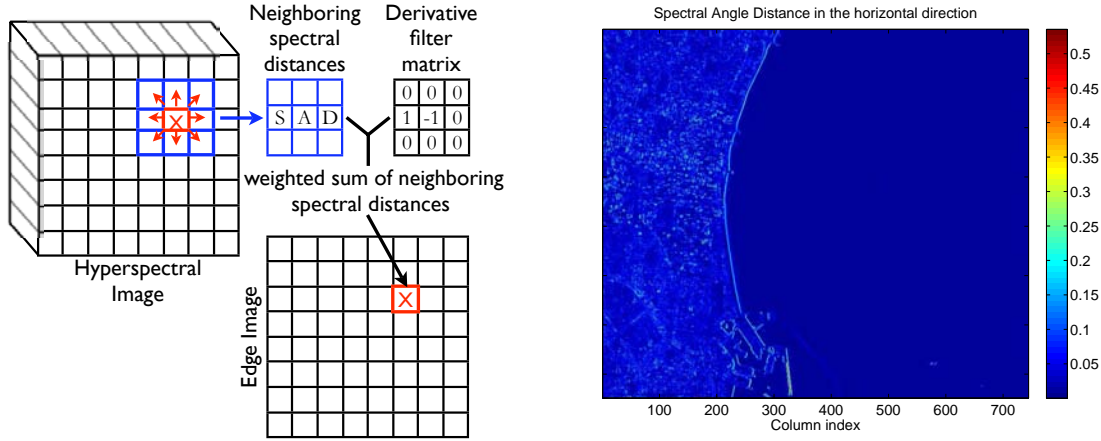


Figure 4.5: Approach followed to find edges in the hyperspectral image using a spatio-spectral derivative filter in the horizontal direction (Image CHRIS_PC_050518_540B_41 acquired over the port of Valencia).

pixel linked to the position with value $R(i, j) = -1$ in the edge detection matrix (reference pixel), and the rest of neighboring pixels (forming a matrix D of distances with value $D(i, j) = 0$ for the reference pixel). Then, the sum of the product of the elements of the edge detection matrix and the distance matrix is computed, $\sum_{i,j} R(i, j)D(i, j)$, and the resulting value is assigned to the reference pixel (i, j) . The main difference of this method compared to the case of grayscale image processing is that only one position of R can present the value -1 , which indicates at each moment the pixel that is being used as a reference to compute the spectral distances. Once this process is applied to all the pixels, a sensitivity threshold is defined. All pixels with values higher than the threshold (i.e. pixels whose spectral signatures differ from that of their neighbors) are identified as edges.

Figure 4.5 shows the approach followed to find the edge values in the processed hyperspectral images, which uses the derivative filter in the horizontal direction $R = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}$. Concerning the spectral distance D , the spectral angle distance (SAD) is used since it is invariant to multiplicative scaling (Keshava, 2004) and will be not affected by the vertical striping of the slit:

$$D(\mathbf{x}_1(\lambda), \mathbf{x}_2(\lambda)) = \arccos (\langle \mathbf{x}_1, \mathbf{x}_2 \rangle / (\|\mathbf{x}_1\| \|\mathbf{x}_2\|)), \quad (4.1.9)$$

where \mathbf{x}_1 and \mathbf{x}_2 are the vectors containing the spectral signature of the pixels whose spectral distance is being calculated, $\langle \cdot, \cdot \rangle$ is the dot product operator, and $\|\cdot\|$ is the quadratic norm. Finally, in order to find an optimum threshold for each image, but also accounting for a significant number of lines to compute the smoothed integrated line profiles, an iterative empirical procedure is followed. The procedure starts with a threshold equal to zero iteratively increased until a 60% of non-edge pixels in the column that presents more edge pixels is ensured, i.e.:

$$\text{IF } \sum_{i,j} R(i, j)D(\mathbf{x}(l, p), \mathbf{x}(l + i, p + j)) > \text{threshold} \text{ THEN } \text{Edge}(l, p) = 1 \quad (4.1.10)$$

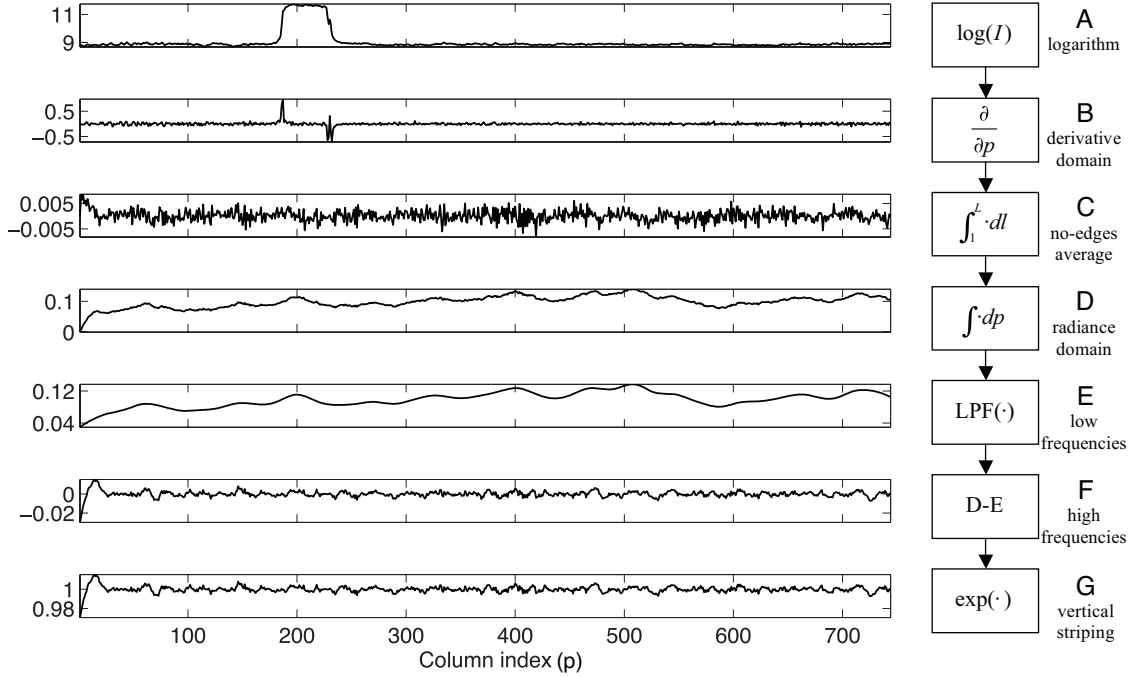


Figure 4.6: Example of the processing steps of proposed vertical striping correction method (profiles of the last band of CHRIS_EL060130_63A1_41 image taken over Heron Island).

Vertical Striping Removal. A critical point of the proposed approach is how to remove edge pixels when computing the integrated line profiles. If all image lines that present at least one edge pixel are removed, it is probable that only few or even none of the lines can be used in the averaging. On the other hand, if the edge pixels are removed and only the remaining pixels of the line are used for averaging, then the problem is not solved since the high frequencies are still there (think in a step profile where only one point is removed). The only way to remove the edges is to work in the across-track spatial derivative domain, where the homogeneous areas before and after the edge present values close to zero and the spikes of edge pixels can be substituted interpolating prior to the integration in the along-track direction. In this simple way, all high frequency contribution by the surface is removed from the integrated line profile before the low pass filtering, and then the estimated VS is independent to the surface patterns.

Figure 4.6 shows the steps of the proposed method, which are detailed below:

- A. To apply logarithms in order to transform the multiplicative noise in additive: $\log(I(l, p, b))$.
- B. To transform the data-cube into the across-track spatial derivative domain, which is equivalent to high-pass filtering: $\theta(l, p, b) = \frac{\partial}{\partial p} \log(I(l, p, b)) = \log(I(l, p, b)) - \log(I(l, p - 1, b))$, for $p > 1$ (note that the first column derivative is fixed to zero, $\theta(l, 1, b) = 0$).
- C. The lines of each band are averaged in the along-track direction but avoiding the edge pixels found with the spatio-spectral edge detection: $\xi(p, b) = \int_1^{N_l} \theta(l, p, b) dl$. To work in

the derivative domain has allowed our method to avoid edge pixels, and it also leads to increase the noise level temporarily because the surface power spectrum is concentrated in the low frequency region, whereas the vertical striping is spread all over the spatial frequency spectrum (Othman and Qian, 2006). Nevertheless, if the LPF is applied in the derivative domain, the committed errors by the LPF will accumulate throughout the integration in the across-track direction. Therefore, after applying the along-track LPF, data is integrated across-track to retrieve the signal in the radiance domain.

- D. Integration in the across-track direction (cumulative sum in p): $\phi(p, b) = \sum_{i=1}^p \xi(i, b)$, i.e. the integration bias is corrected at the end of the process.
- E. To apply a LPF in the across-track direction in order to eliminate the high frequency variations coming from the noise ν and estimate the surface contribution: $\varphi(p, b) = \text{LPF}\{\phi(p, b)\}$.
- F. To obtain the high frequency variations (considered to be the noise) by subtracting the low frequencies: $\psi(p, b) = \phi(p, b) - \varphi(p, b)$. The error committed during the integration process consists in a constant value for each band. Nevertheless, as the vertical striping is corrected independently for each band, the vertical striping in the logarithmic domain should present zero mean (gain close to 1 in the radiance image). Therefore, the offset errors are corrected subtracting the mean value: $\psi(p, b) = \psi(p, b) - \frac{1}{N_p} \sum_p \psi(p, b)$.
- G. Finally, the VS factors are obtained calculating the inverse of the logarithm $\hat{\nu}(p, b) = \exp(\psi(p, b))$.

Multiangular Vertical Striping Removal. Thanks to the sequential acquisition of CHRIS of the same scene from five different angles, we can also improve the robustness of the proposed algorithm using together all the multiangular images of one acquisition. As mentioned before, the VS due to the instrument slit is temperature-dependent. Although temperature recorded for different acquisitions has shown differences higher than 8°C , the changes are less than 0.5°C within a single acquisition (5 multi-angular images). Therefore, images of one acquisition present the same vertical striping pattern while they are recording different spatial patterns from the same Earth area (due to perspective, platform motion and Earth rotation). One can take advantage of this fact in order to improve the estimation of the vertical striping by considering the five images as a single longer hyperspectral image, which is formed by stacking the multiangular images in the along-track direction, i.e. an hyper-cube with the same number of columns N_p and bands N_b , but with $5 \times N_l$ lines with different spatial distribution of similar surface types (similar spectra). When processing together a higher number of lines, the surface contribution is smoother and the estimation of the VS is more accurate.

Vertical Striping Characterization and Correction of the Slit Effect. An extensive analysis of the performance of the proposed vertical striping method was carried out with more than

300 CHRIS images of several acquisition modes in (Gómez-Chova et al., 2006a; Gómez-Chova et al., 2008). Details about the vertical striping results will be omitted in this Thesis, but a result of great value is the characterization of the vertical striping and its dependence on temperature. With this purpose, we corrected a significant number of CHRIS images of the database obtaining an estimation of the vertical striping pattern, $\hat{\nu}(p, b) = H(p)S(p, b)$, per image. The sensitivity of the CCD array, $S(p, b)$, is assumed to be characterized by a Gaussian distribution with unit mean. However, by applying the logarithmic transformation to the estimated VS, the multiplicative nature of both terms is changed to additive one, $\log(\hat{\nu}(p, b)) = \log(H(p)) + \log(S(p, b))$, where the term $\log(S(p, b))$ can be safely considered additive noise with zero mean distribution. As a consequence, the VS profile due to the slit, which is constant in columns, can be obtained by averaging in the spectral direction of the CCD and then reverting the logarithm: $H(p) = \exp(\int_1^{N_b} \log(\hat{\nu}(p, b))db)$. Moreover, the slit-VS profiles of the five angular images can be averaged to obtain only one $H(p)$ per acquisition, which will be associated to the platform temperature for this given acquisition: $H(p, T)$. Changes in temperature produce an expansion of the slit, changing its width and moving the image of the slit across the detector. These two effects produce a scaling of the slit-VS factors and a shift of its shape in the across-track direction, respectively, causing a temperature dependent vertical striping. Figure 4.7, on the left side, shows a peak of the obtained $H(p)$ profiles for all the analyzed Mode 2 acquisitions (Mode 2 is shown because it is not binned and presents higher across-track resolution than Mode 1). The ‘*’ symbols represent the actual $H(p)$ values for each pixel column p , and the curves (continuous lines) are the corresponding spline interpolations in the across-track direction x , which provide a continuous subpixel resolution model of the striping $H(x)$ for each measured temperature T : $H(x, T)$. The curves clearly show the shift and scaling of the VS amplitude with temperature. Taking the VS at $T_0 = 5.5^\circ\text{C}$ as a reference, we compute the shift in the across-track looking for the lag, $\Delta_x(T)$, of the maximum of the cross-correlation sequence between the analyzed vertical striping, $H(x, T)$, and the reference one, $H(x, T_0)$. Once the shift is corrected, the scaling factor $G_H(T)$ is computed as the slope of the linear regression that better fits $H(x, T)$ with $H(x, T_0)$ in a least-squares sense. In the central and right plots of Fig. 4.7 we represent the shift $\Delta_x(T)$ and scale $G_H(T)$ of the slit-VS as a function of temperature, respectively.

The estimated $\Delta_x(T)$ and $G_H(T)$ values are used to compensate the shift and scale of the slit-VS $H(x, T)$ and obtain the corresponding slit-VS for each acquisition of the database, but expressed at the reference temperature T_0 . The average of all these curves provides us a model of the “real” slit-VS at the reference temperature, denoted by $\tilde{H}(x)$, minimizing the estimation errors. The modeled slit-VS for a given temperature T can be recovered from $\tilde{H}(x)$ as:

$$H(x, T) = G_H(T)\tilde{H}(x - \Delta_x(T)) \quad (4.1.11)$$

where $\Delta_x(T_0) = 0$ and $G_H(T_0) = 1$. The value for a given pixel column p is obtained integrating the width of the pixel photo-sensible area:

$$H(p, T) = \int_{p-1/2}^{p+1/2} H(x, T)dx \quad (4.1.12)$$

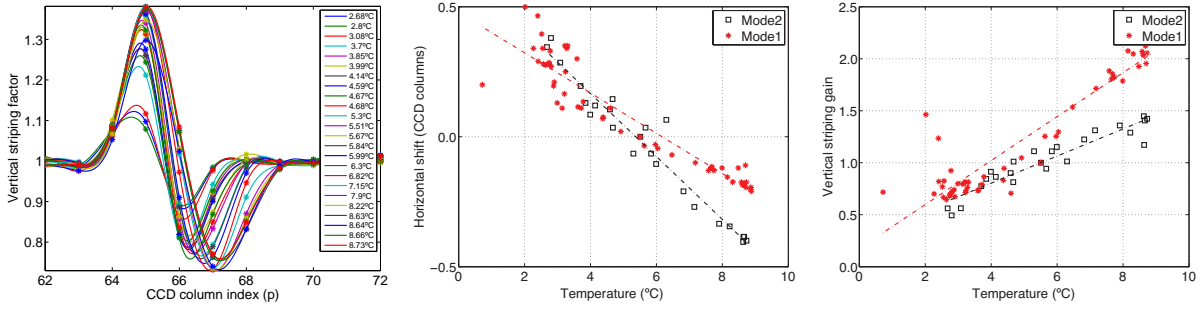


Figure 4.7: Dependence of CHRIS slit vertical striping on temperature. From left to right: (a) detail of the slit-VS profiles for all the Mode 2 acquisitions of the database; (b) across-track shift of the slit-VS shape as a function of temperature; (c) scaling of the slit-VS factors as a function of temperature.

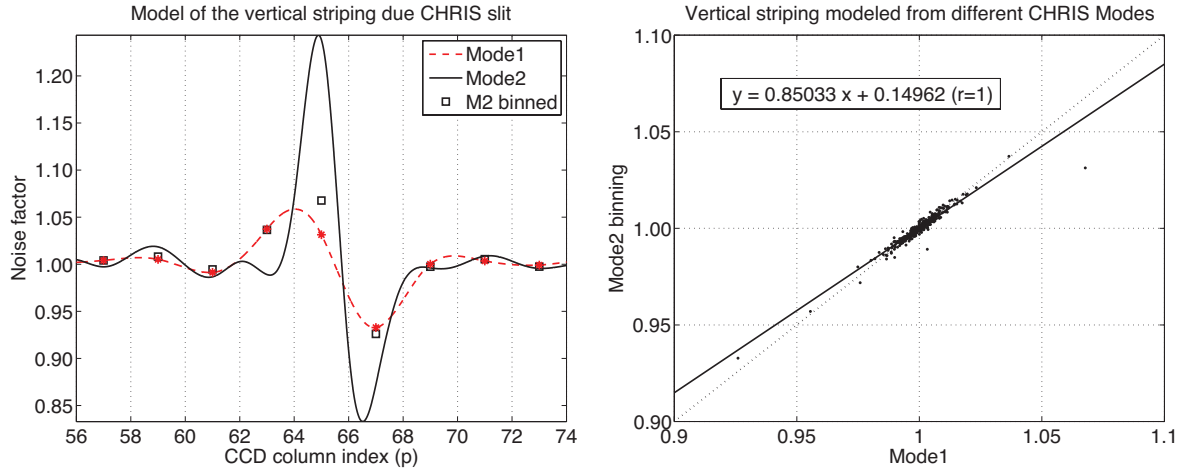


Figure 4.8: Detail of the “real” slit-VS modeled from Mode 1 and Mode 2 CHRIS images, and the binning of Mode 2 ‘x’ closely matching Mode 1 curve (left). Scatterplot of the modeled Mode 1 and Mode 2 “real” slit-VS.

It is worth noting that Mode 1 performs a binning of columns in pairs. Therefore, for Mode 1 images, we have to simulate the binning in order to obtain the slit-VS factors for each image column:

$$H_1(p_{\text{binned}}) = 1/2(H_2(p - 1) + H_2(p)) \tag{4.1.13}$$

where $p = \{2, 4, 6, \dots, 744\}$, and p_{binned} is the pixel number in Mode 1 images (372 columns).

Figure 4.8 shows a segment of the slit-VS curves modeled independently from Mode 1 and Mode 2 acquisitions $\tilde{H}_1(x)$ and $\tilde{H}_2(x)$ (Fig. 4.8[left]) and the scatterplot of Mode 1 vs. Mode 2 (Fig. 4.8[right]). Agreement between both results is excellent, except in the highest and lowest anomalous values (VS peaks) where probably the interpolation used to obtain $H(x)$ produces underestimated VS peaks, being this effect more noticeable in the binned Mode 1.

Algorithm Implementation in the BEAM Toolbox. Currently, the proposed correction algorithm is being implemented in the free BEAM Toolbox⁴ software (Fomferra and Brockmann, 2005) under the framework of the ESA contract “Development of CHRIS/PROBA modules for the BEAM toolbox” (ESA ITT SoW ENVI-DTEX-EOPS-SW-06-0008).

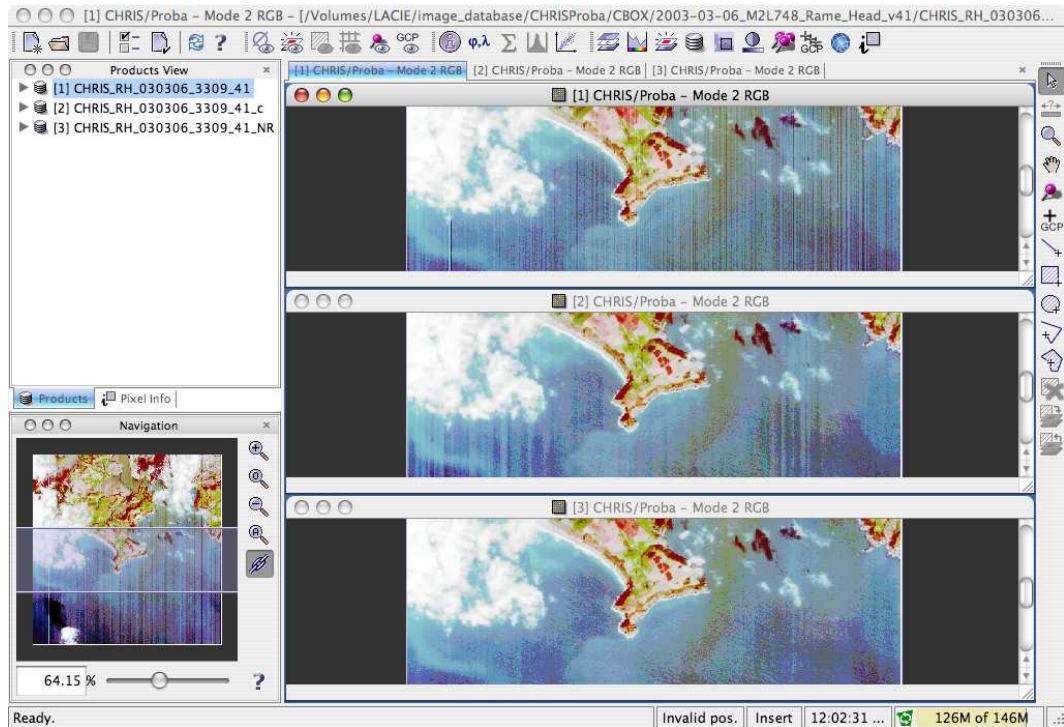


Figure 4.9: Screenshot with an example of the CHRIS/PROBA noise reduction module implemented in the ESA BEAM Toolbox software.

The approach followed in this project takes advantage of the results presented in previous sections. First, all drop-outs are corrected. Then, a rough correction of the vertical striping due to the entrance slit is performed. For a given CHRIS image, the estimation of the slit vertical striping $H(p, T)$ is obtained from the characterization of the vertical striping pattern $\tilde{H}(x)$ stored in a look-up-table (LUT) by using Eq. (4.1.11) to include the dependence on the platform temperature T at the given CHRIS acquisition, and Eq. (4.1.12) if the acquisition mode is binned. In Eq. (4.1.11), we assume a linear dependence of the shift in columns and the gain factor with the temperature: $\Delta_x(T) = -0.12T + 0.65$ and $G_H(T) = 0.13T + 0.28$, respectively, where the coefficients of the linear regression are obtained directly from Mode 2 data presented in Fig. 4.7. After this preliminary correction of the vertical striping due to the entrance slit, the robust vertical striping correction method proposed in section 4.1.2 is used to estimate directly

⁴The *Basic ERS & ENVISAT (A)ATSR and MERIS* (BEAM) Toolbox is a collection of executable tools developed by ESA to facilitate the utilization, viewing, and processing of ESA Earth observation data (<http://envisat.esa.int/resources/softwaretools/> or <http://www.brockmann-consult.de/beam/>).

from the image (or multiangular acquisition) the remaining vertical striping for each band $\hat{v}(p, b)$. Finally, obtained factors are used to correct the image column values .

Figure 4.9 shows an screenshot of the ESA BEAM Toolbox software. In this example we display the same area for the original CHRIS product (*top*), the image corrected with the algorithm implemented by Settle and Cutter (2005) (*middle*), and the image processed with the CHRIS/PROBA noise reduction module proposed in this work and implemented in the BEAM Toolbox (*bottom*). One can easily appreciate how the vertical patterns are reduced from top to bottom pictures.

4.2 Pre-processing (II): TOA Reflectance

Once the data have been corrected of errors and uncertainties, these data are independent of differences in sensor system conditions. Hence, it is no longer necessary to express this information in terms of the image-sensor lines and columns. Now, the multispectral image can be expressed in terms of pixels with spatial coordinates (x, y) , and the spectral information of each sensor channel in terms of the central wavelength λ_b and bandwidth Λ_b of the band. Only for some precise spectral calculations, which require the exact central wavelength for each pixel, information about the original detector elements will be used, mainly when dealing with narrow absorption bands where a small spectral shift affects the measure.

As already mentioned, both MERIS and CHRIS Level 1b products are provided in *top of the atmosphere* (TOA) radiance. The corrected TOA radiance is further processed in order to estimate TOA reflectance. This allows us to remove in practice the dependence on particular illumination conditions (day of the year and angular configuration) and illumination effects due to rough terrain (cosine correction), since the method is intended to work under many situations. TOA apparent reflectance is estimated as follows:

$$\rho_{\text{TOA}}(x, y, \lambda) = \frac{\pi L_{\text{TOA}}(x, y, \lambda)}{\mu_s(x, y) F_0(\lambda)}, \quad (4.2.1)$$

where $L_{\text{TOA}}(x, y, \lambda)$ is the provided at-sensor upward radiance at the image location (x, y) , $F_0(\lambda)$ is the extraterrestrial instantaneous solar irradiance, and $\mu_s(x, y)$ is the cosine of the angle between the illumination direction (solar zenith angle) and the vector perpendicular to the surface. Finally, the Sun irradiance, $F_0(\lambda)$, is taken from Thuillier et al. (2003), corrected for the acquisition day, and convolved with the spectral response of the sensor channels (see Fig. 4.10).

4.2.1 Day-of-Year Correction

The largest source of variation in F_0 at the TOA is the orbit of the Earth around the Sun (cf. section 1.1.2). The Sun is located at one of the foci of the Earth's orbit (an ellipse with eccentricity $\epsilon = 0.01673$), and the value of F_0 is expected to vary as the reciprocal of the Earth-Sun distance squared. The mean Earth-Sun distance is referred to as 1 Astronomical Unit (AU)

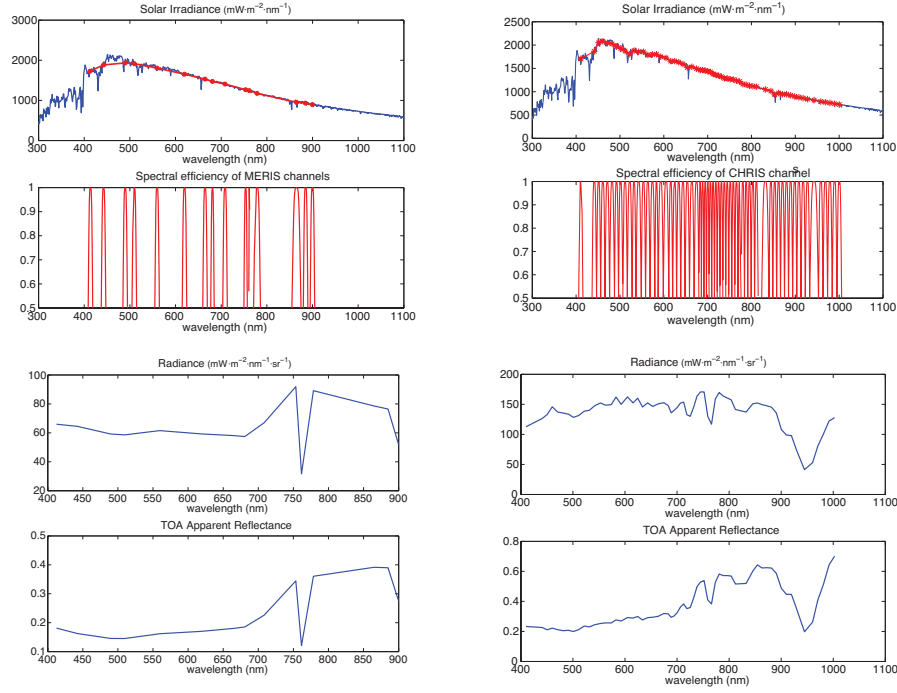


Figure 4.10: Sun irradiance corrected for the day of the year (*1st row*) and the spectral channels (*2nd row*) used to estimate from the at sensor radiance (*3rd row*) the TOA apparent reflectance (*4th row*) for MERIS (*left*) and CHRIS (*right*) instruments.

and corresponds to a distance of 1.496×10^{11} m. The factor to adjust F_0 for intra-annual variations in Earth-Sun distance is inversely proportional to the square of the Earth-Sun distance. Thus the corrected solar irradiance is given by the following approximate formula (Vermote et al., 1997):

$$F_0(\lambda) = \frac{1}{(1 - \epsilon \cos(0.9856(J - 4)\pi/180))^2} F_0(\lambda), \quad (4.2.2)$$

where J is the Julian day of year (DOY). The solar intensity at *perhelion* (January 3, minimum Earth-Sun distance) and *aphelion* (July 4, maximum Earth-Sun distance) can differ by as much as 4% relative to the mean Earth-Sun distance.

Since the reference extraterrestrial solar irradiance presents a different spectral sampling, it is resampled to fit the spectral channels of the sensor. In both MERIS and CHRIS sensors, a specific band, b , consists of the addition of one or more CCD detector pixel elements depending on the desired bandwidth. Therefore, the spectral response for a given band, $H_b(\lambda)$, is the sum of the spectral response $H_i(\lambda)$ of the corresponding detectors, i , of the CCD array. Then, the mean solar irradiance for a given band, $F_0(b)$, is obtained by integrating the extraterrestrial solar irradiance times its spectral response:

$$F_0(\lambda_b) = \frac{\int_0^\infty H_b(\lambda) F_0(\lambda) d\lambda}{\int_0^\infty H_b(\lambda) d\lambda}. \quad (4.2.3)$$

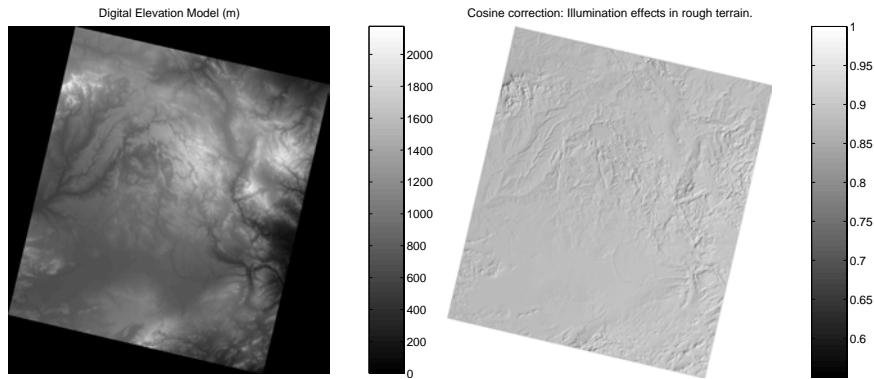


Figure 4.11: *Left:* DEM altitude of the BR-2003-07-14 image. *Right:* Cosine of the angle between the illumination vector and a vector perpendicular to the surface (cosine correction).

In CHRIS sensor, the theoretical full-width half-maximum (FWHM) of the instrument line-spread functions correspond to spectral resolutions of 1.25 nm at 415 nm, increasing to 11.25 nm at 1050 nm. In MERIS, the CCD covers the spectral range with a nominal 1.25 nm spectral sampling interval and with a FWHM equal to 1.25 nm. For both instruments, one could assume that $H_i(\lambda)$ is a Gaussian response function whose width is equal to the FWHM of each element i , and sum up all the elements of the band. In this Thesis, the spectral response of a band, $H_b(\lambda)$ is approximated as a *bell-shaped* function (that combines properties of both Gaussian and trapezoidal functions) depending on the mid-wavelength, λ_b , and the bandwidth, Λ_b , of the band, directly:

$$H_b(\lambda) = \frac{1}{1 + |2(\lambda - \lambda_b)/\Lambda_b|^4} \quad \lambda_b - \Lambda_b < \lambda < \lambda_b + \Lambda_b, \quad (4.2.4)$$

where both the exact mid-wavelength and the bandwidth values for each channel are included in the image metadata.

4.2.2 Rough Surface Correction

In this Thesis, the angle between the illumination direction and the vector perpendicular to the surface, which defines $\mu_s(x, y)$, is computed in a different way depending on the sensor:

- In MERIS, it is computed for each pixel using the *Sun Azimuth* and *Sun Zenith* angles, which are available in the *Tie Point Location and Auxiliary Data* of the MERIS product, and the vector perpendicular to the surface, which can be computed from a Digital Elevation Model (DEM). The free GETASSE30 DEM included in the BEAM ESA software (Fomferra and Brockmann, 2005) may be used for this purpose (Fig. 4.11). In this step, however, we assume a flat surface because, by using a DEM, illumination effects in the surface are corrected but the characteristics of clouds over rough terrain may change.
- In CHRIS, this correction is approximated by the *Solar Zenith Angle* provided in the CHRIS HDF file attributes since, due to the small field of view of CHRIS, one can assume a flat

landscape and a constant illumination angle for the area observed. Information from a DEM could be easily incorporated, but automatic geocoding and co-registration of CHRIS images using telemetry, which is needed in the case of cloudy images since other methods can not be applied, is a not solved problem (Alonso and Moreno, 2005; Alonso et al., 2005).

4.3 Feature Extraction

Converting image data into TOA reflectances has the advantage that these data, yet not being free of atmospheric effects (Guanter et al., 2008a), are corrected for seasonal and diurnal differences in solar position, and are independent of differences in sensor systems This is a desirable characteristic for a cloud screening algorithm intended to work in any new image acquired by the studied sensors.

In the following, all radiance signals and reflectance are referred to the top of atmosphere so, in order to simplify the notation, $L(\lambda)$ and $\rho(\lambda)$ are used instead of $L_{\text{TOA}}(\lambda)$ or $\rho_{\text{TOA}}(\lambda)$. Therefore, the image is defined by $\{\rho_i(\lambda)\}_{i=1}^n \in \mathbb{R}^{N_b}$, where n is the total number of pixels, and the spectral signature is sampled at N_b narrow bands of the VNIR spectral region. It is important to remark that, in the case of MERIS (cf. section 1.3.1), the set of bands is fixed, $\{\lambda_b\}_{b=1}^{15} = \{412.5, 442.5, 490, 510, 560, 620, 665, 681.25, 708.75, 753.75, 760.625, 778.75, 865, 885, 900\}$ nm, and in the case of CHRIS (cf. section 1.3.2), the number of bands, the location, and the bandwidth are variable depending on the acquisition mode. For this reason, in this section, numeric values of used bands are provided only for MERIS. A detailed description of the different CHRIS band sets is provided at the end of the chapter (section 4.3.3).

The measured spectral signature depends on the illumination, the atmosphere, and the surface. Figure 4.12 shows sensor channel locations compared to the spectral curve of healthy vegetation, bare soil, and the atmospheric transmittance. The spectral bands free from atmospheric absorptions contain information about the surface reflectance, while others are mainly affected by the atmosphere.

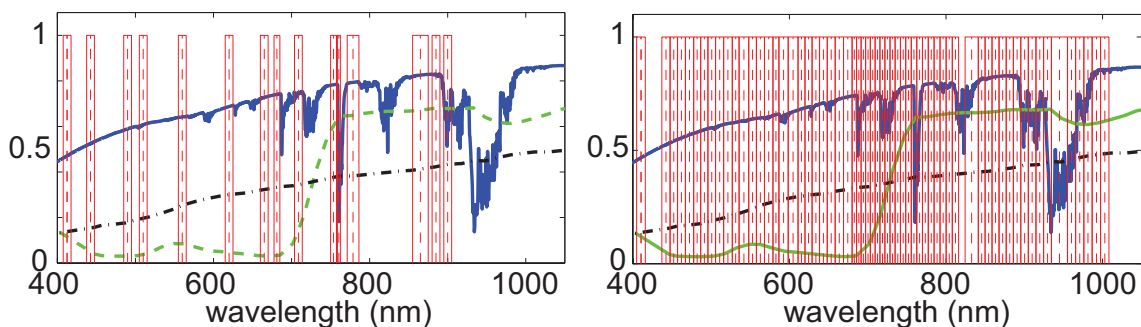


Figure 4.12: MERIS (*left*) and CHRIS Mode 1 (*right*) channel locations (boxes) superimposed to a reflectance spectra of healthy vegetation (dashed), bare soil (dash-dotted), and the atmospheric transmittance (solid).

At this step, rather than working with the spectral reflectance only, physically-inspired features are used in order to increase the separability of clouds and surface covers, which is a common strategy in remote sensing classification (Gómez-Chova et al., 2003c,a). These features are extracted independently from the channels that are free from strong gaseous absorptions ($\lambda_b \subset B_S$) and from the channels substantially affected by the atmosphere ($\lambda_b \subset B_A$). In the case of MERIS, which presents a fixed band configuration, the *atmospheric* channels, B_A , are $b = \{11, 15\}$ and the *surface* channels, B_S , are $b = \{1, \dots, 10, 12, \dots, 14\}$. A detailed analysis of the extracted features is given in the following subsections. For illustration purposes, only the extracted features from one CHRIS image (CHRIS-BR-050717-576C-41, section 7.1.1) and one MERIS image (BR-2003-07-14, section 7.2.1) are provided.

4.3.1 Surface Spectral Features

Regarding reflectance of the surface, one of the main characteristics of clouds is that they present *bright* and *white* spectra (Fig. 4.13). We can exploit bands in B_S in order to extract information about the target reflectance, i.e. cloud brightness and cloud whiteness for cloudy pixels:

- A *bright* spectrum means that the intensity of the spectral curve (related to the albedo) should present relatively high values. Therefore, cloud brightness is calculated for each pixel as the integral of spectrum, $f_{Br} = \int \rho(\lambda)d\lambda$, which can be approximated with a trapezoidal numerical integration:

$$\hat{f}_{Br} = \frac{1}{\lambda_{\max} - \lambda_{\min}} \sum_{\lambda_b \subset B_S} \frac{\rho(\lambda_{b+1}) + \rho(\lambda_b)}{2} (\lambda_{b+1} - \lambda_b), \quad (4.3.1)$$

which differs from the average of the spectral channels since it takes into account the distribution of the energy along the spectrum.

- A *white* spectrum means that the spectral signature must be flat along the spectrum. The first derivative of the spectral curve should present low values, but noise and calibration errors may reduce the accuracy in the estimation of the spectrum flatness when computing the spectral derivative in channels with similar wavelengths. Therefore, we compute for each pixel the deviation from the flatness as the (trapezoidal approximate) integral of $e(\lambda) = |\rho(\lambda) - \hat{f}_{Br}|$:

$$f_{Wh} = \frac{1}{\lambda_{\max} - \lambda_{\min}} \sum_{\lambda_b \subset B_S} \frac{e(\lambda_{b+1}) + e(\lambda_b)}{2} (\lambda_{b+1} - \lambda_b) \quad (4.3.2)$$

Further surface features can be obtained by considering independently the VIS ($\lambda_{VIS} \in [400 - 700]$ nm) and NIR ($\lambda_{NIR} \in [700 - 1000]$ nm) spectral ranges, where surface covers present different reflectance properties. Therefore, instead of working with f_{Br} and f_{Wh} , we can obtain 2+2 features from (4.3.1) and (4.3.2) respectively: $f_{Br,VIS}$ and $f_{Wh,VIS}$, computed using $\lambda_b \subset (B_S \cap VIS)$; and

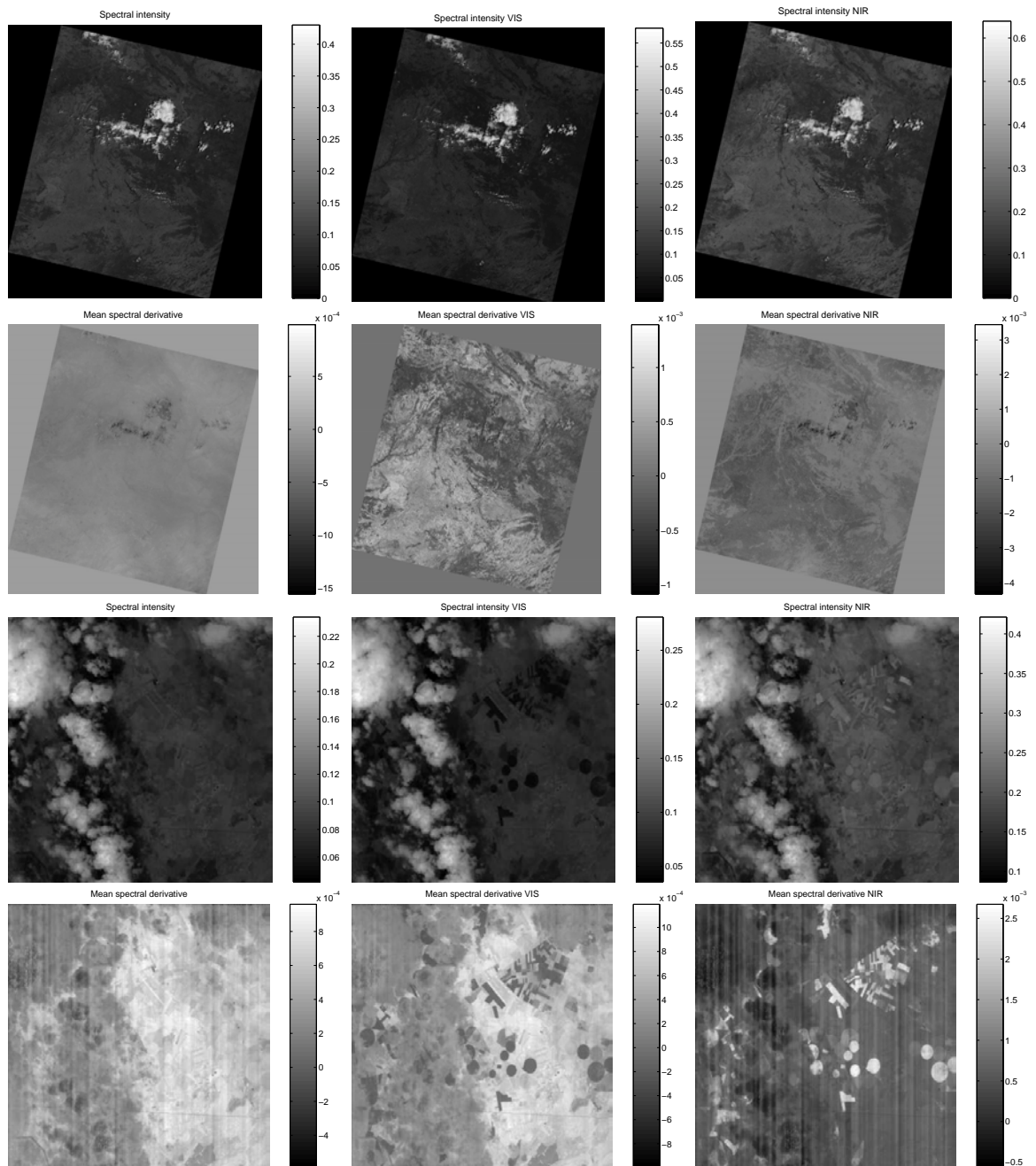


Figure 4.13: Cloud brightness (*up*) and whiteness (*down*) features extracted from the TOA reflectance, for VNIR (*left*), VIS (*center*) and NIR (*right*), of the MERIS BR-2003-07-14 (*top*) and the CHIRS CHRIS-BR-050717-576C-41 (*bottom*) images.

$f_{Br,NIR}$ and $f_{Wh,NIR}$, computed using $\lambda_b \subset (B_S \cap NIR)$. For example, clouds over land should be better recognized in $f_{Br,VIS}$ than in $f_{Br,NIR}$ since land covers have less reflectance in the VIS range, while the opposite is true for clouds over sea.

4.3.2 Atmospheric Features

Regarding atmospheric absorptions, another meaningful feature is the fact that clouds are at a higher altitude than the surface. It is worth noting that atmospheric absorption depends on the atmospheric constituents and the optical path. Since light reflected on high clouds crosses a shorter section of the atmosphere, the consequence would be an abnormally short optical path, thus weaker atmospheric absorption features. Atmospheric oxygen absorption and even water vapor absorption (at 760 nm and 940 nm respectively) are candidate bands to be used in the optical path estimation.

The use of atmospheric absorption in the oxygen-A band to infer cloud pressure, which is related to cloud-top height, has been suggested by several authors (Yamamoto and Wark, 1961; Chapman, 1962). In fact, cloud top height retrieval from the oxygen-A band using instruments conceived to yield global distributions of atmospheric constituents, such as GOME and SCIAMACHY, is an active field of research (Kokhanovsky et al., 2007b,a). In the case of medium resolution imaging spectrometers, several studies have shown that the oxygen-A band is potentially efficient for determining the cloud-top pressure (Fischer and Grassl, 1991; Buriez et al., 1997; Ramon et al., 2003). All these studies assume that the two spectral channels located at the oxygen-A band (one outside and another inside the absorption band) allow the derivation of an apparent pressure which roughly represents the cloud pressure. In particular, apparent pressure is calculated using an empirical polynomial function of the oxygen transmission derived from the reflectance ratio $\rho(\lambda_{in})/\rho(\lambda_{out})$. However, to obtain reliable estimations of the cloud-top height is still a challenging problem affected by the instrument radiometric and spectral resolution, the influence of ground reflectance, and the need of a reliable surface pressure reference, e.g. from the ECMWF. These difficulties explain the little attention paid to this helpful feature in cloud screening.

In the case of MERIS, the accurate characterization of the O₂-A absorption at MERIS channel 11 (bandwidth of 3.75 nm) makes the inclusion of this atmospheric feature in the cloud screening scheme mandatory, as pointed out by Ramon et al. (2003) and Preusker et al. (2006). In the case of CHRIS modes 1 and 5, at least one spectral band is affected by the O₂-A absorption, which makes the inclusion of this atmospheric feature in the cloud screening scheme possible. However, its wavelength is not necessarily centered in the maximum absorption and its bandwidth is too high, making difficult an accurate estimation of the optical path. Therefore, when using the oxygen absorption band in CHIRS images, only high clouds are well distinguished from the surface and low clouds present almost the same values as the surface. In the following paragraphs, we present the formulation proposed to extract an atmospheric feature directly related to the optical path.

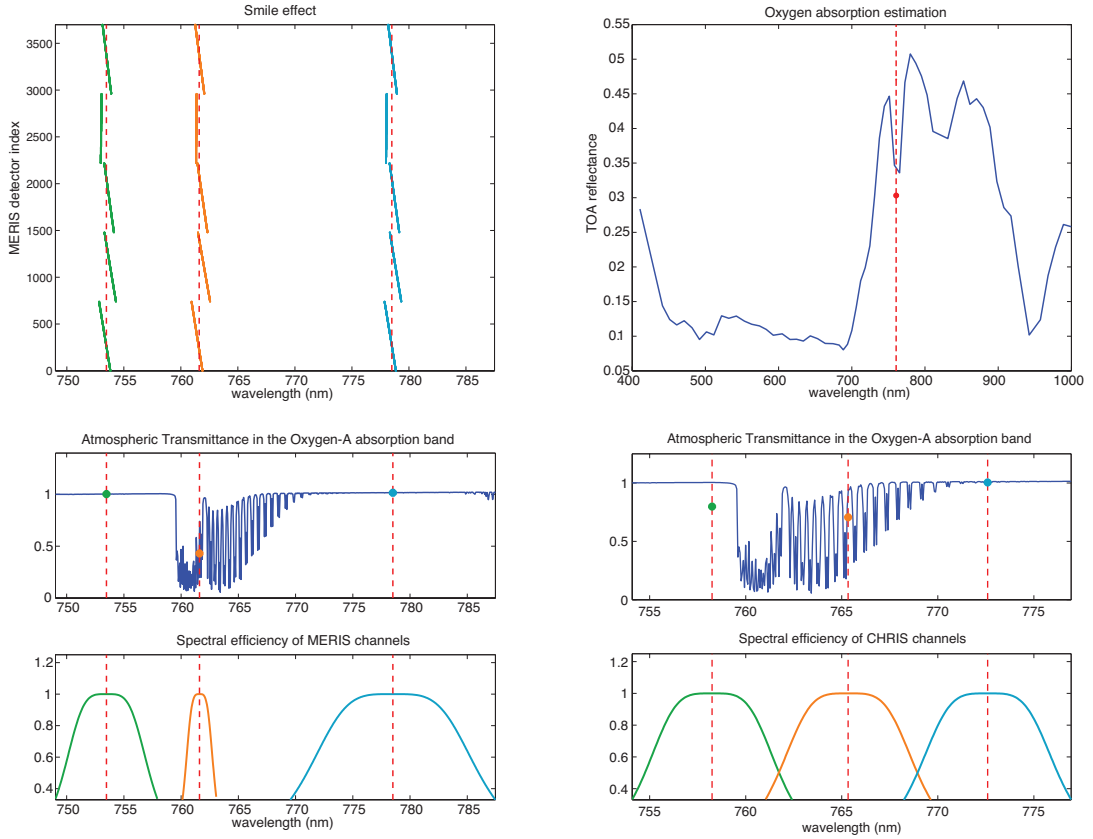


Figure 4.14: Estimation of the optical path, δ_{atm} , from the O_2 absorption band. *Left:* Correction of the spectral shift on the MERIS response due to the smile effect. *Top-Left* Nominal wavelength λ_b of the channels $b = 10, 11, 12$ (dashed lines), and the corrected one for each MERIS detector index (constant in a given image column), $\lambda_b + \Delta\lambda_b(x)$. *Middle-Left:* Effective atmospheric vertical transmittance, $\exp(-\tau_0(\lambda))$, estimated from a high resolution curve taking into account the spectral response (efficiency) of MERIS channels *Bottom-Left*. *Top-Right:* CHRIS example of the TOA reflectance inside the oxygen band, and the estimated reflectance at the maximum absorption ($\lambda=760.625$ nm). *Middle-Right:* Effective atmospheric vertical transmittance, $\exp(-\tau_0(\lambda))$, estimated from a high resolution curve taking into account the spectral response (efficiency) of CHRIS channels *Bottom-Right*.

The light transmitted through a non-dispersive medium can be expressed using the Bouguer-Lambert-Beer law:

$$L(\lambda) = L_0(\lambda) \exp\left(-\frac{\tau(\lambda)}{\mu}\right), \quad (4.3.3)$$

where $L_0(\lambda)$ is the light entering into the medium, the term $\exp(-\tau(\lambda)/\mu)$ is the transmittance factor, $1/\mu$ is the optical mass obtained from the illumination and observation zenith angles, and $\tau(\lambda)$ is the atmospheric optical depth. Since most of the radiation measured by the sensor has been reflected by the surface, (4.3.3) can not be used to model the at-sensor radiance. However, it provides a physical basis for the definition of a non-dimensional parameter that accounts for atmospheric absorptions in typical remote sensing scenarios. In our case, the reference radiance $L_0(\lambda)$ will be the radiance outside the absorption feature, calculated by interpolating the nearby channels that are unaffected by absorptions, and $L(\lambda)$ will be the radiance affected by gaseous absorptions after crossing the TOA-surface-sensor path. The inversion of (4.3.3) provides $\tau(\lambda)$, which is a measure of the strength of the gaseous absorptions in a certain spectral range. The assumption is that variations in $\tau(\lambda)$ are driven by sharp changes in elevation as those due to transitions between cloud-free and cloud-covered areas. Horizontal variations in the atmospheric state are considered as a second-order effect compared to cloud-to-surface elevation changes. An equivalent atmospheric transmittance parameter could be calculated as the ratio $L(\lambda)/L_0(\lambda)$, but the contribution of illumination and observation geometries would not be normalized.

The atmospheric path radiance is an additional contribution to take into account, which is the radiation reflected by the atmosphere into the sensor's line-of-sight. Further refinement of (4.3.3) is achieved by removing the atmospheric path radiance, $L_p(\lambda)$, from $L(\lambda)$ and $L_0(\lambda)$, as L_p is mainly associated to scattering processes rather than to absorption ones. In particular, L_p is calculated at each pixel using the exact pixel geometry (solar zenith angle, viewing geometry, and surface height) from a look-up table generated with the MODTRAN4 radiative transfer code (Berk et al., 1998). A default visibility value of 23 km is assumed for the aerosol loading, but changes in illumination and observation angles are properly considered (Guanter, 2006).

The foundations for the procedure are solid but the performance of the instruments severely affects the robustness of the method. Sensor spectral calibration is a major source of uncertainty when dealing with gaseous absorptions. In the case of MERIS, even though it has two specific spectral bands in the oxygen-A absorption region (channels 10 and 11), the oxygen absorption is extremely narrow and small variations of the spectral wavelength of each pixel along the CCD lines (*smile* effect) have a large impact on any variable derived from the oxygen-A. Fortunately, this spectral shift on the MERIS response has been well characterized (Dubuisson et al., 2003), and the spectral shift values for each pixel column in the across-track direction ($p \equiv x$) of the five MERIS detectors, $\Delta\lambda_b(x)$, have been provided to the user community (D'Alba et al., 2005; Delwart et al., 2007). This allows us an easy introduction of the spectral shift in our formulation. In the case of CHRIS, the broader bandwidth makes the estimation of the oxygen absorption less accurate but less sensitive to spectral shifts (moreover CHRIS optical system is designed to minimize the smile). However, residual vertical striping noise is critical when ratios between

bands with low values are computed.

The atmospheric optical depth is decoupled into two contributions,

$$\tau(\lambda) = \tau_0(\lambda)\delta_{\text{atm}}, \quad (4.3.4)$$

where τ_0 is an optical thickness reference spectrum at sea level for nadir illumination and observation, and δ_{atm} is a factor accounting for elevated surfaces such as clouds. The reference $\tau_0(\lambda)$ values are estimated from a high spectral resolution curve following the same procedure that in (4.2.3). The approach followed here for the so-called Oxygen-A band can be devised from Fig. 4.14, and the extracted feature is derived from (4.3.3) and (4.3.4) as:

$$f_{\text{O}_2}(x, y) = -\frac{\mu(x, y)}{\tau_{\text{atm}}(\lambda_{\text{in}})} \log \left(\frac{L(x, y, \lambda_{\text{in}})}{L_0(x, y, \lambda_{\text{in}})} \right), \quad (4.3.5)$$

where the interpolated radiance at the absorption band is estimated from nearby channels, $L_0(\lambda_{\text{in}}) = L(\lambda_{\text{out_inf}}) + (\lambda_{\text{in}} - \lambda_{\text{out_inf}})(L(\lambda_{\text{out_sup}}) - L(\lambda_{\text{out_inf}}))/(\lambda_{\text{out_sup}} - \lambda_{\text{out_inf}})$. In the case of MERIS, the fix set of band locations *out_inf*, *in*, and *out_sup* for the oxygen absorption corresponds to channels 10, 11, and 12, respectively; and $\tau_0(\lambda)$ has been corrected for the smile effect, $\lambda_b(x) = \lambda_b + \Delta\lambda_b(x)$. Note that the smile correction can be easily implemented by calculating the atmospheric features for each detector column x separately.

An additional estimation of the optical path can be obtained from the water vapor absorption in the NIR, close to the end of the valid range of the sensors. In the case of the water vapour absorption, the maximum absorption (940 nm) is acquired by CHRIS Modes 1 and 5 only, but is located outside the MERIS range. In addition, the water vapor distribution is extremely variable, and thus it is not straightforward to relate this feature to the real altitude. However, it is still valid for relative measurements inside the same image since almost all the atmospheric water vapor is distributed in the first 2-3 km of the atmosphere below most of the cloud types; and, in the case of CHRIS, one can fairly assume small differences because of the small CHRIS spatial coverage (15 km swath). Therefore, the optical path estimated from water vapor absorption provides better cloud discrimination in CHRIS images since this band is broader than the oxygen band and more CHRIS bands are completely affected. Finally, snow presents higher absorption than clouds at 900 nm and this behavior can be appreciated in the extracted feature.

The same approach than in the O₂ case has been followed to obtain this feature (Fig. 4.15):

$$f_{\text{WV}}(x, y) = -\frac{\mu(x, y)}{\tau_0(\lambda_{\text{in}})} \log \left(\frac{L(x, y, \lambda_{\text{in}})}{L(x, y, \lambda_{\text{out_inf}})} \right), \quad (4.3.6)$$

where we assume that $L_0(\lambda_{\text{in}}) = L(\lambda_{\text{out_inf}})$ since the interpolation at the end of the spectral range of the sensor is sometimes not possible in CHRIS, and completely impossible in MERIS where only the last two channels, $\lambda_{\text{out_inf}} = \lambda_{14}$ and $\lambda_{\text{in}} = \lambda_{15}$, can be used.

It is worth noting that the extracted atmospherical features are not intended to estimate altitude of clouds. They are just an estimation of the optical path by taking into account important

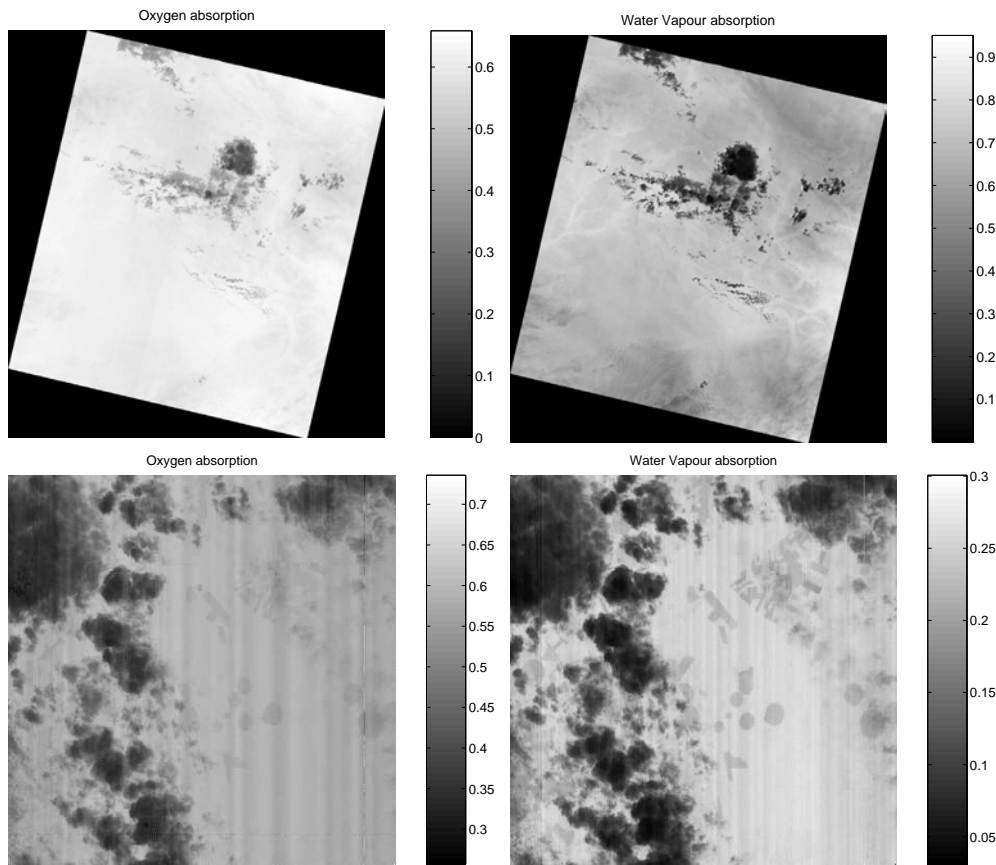


Figure 4.15: Estimation of the optical path from the oxygen absorption (*left*) and water vapor (*right*) bands for the MERIS BR-2003-07-14 (*top*) and the CHIRS CHRIS-BR-050717-576C-41 (*bottom*) images.

issues such as the viewing geometry, atmospheric transmission, and sensor calibration. However, this estimation is affected by the background reflectance of the surface and the atmospheric conditions (Guanter et al., 2008a), which change from one image to another. For example, at the oxygen absorption band, solar-induced chlorophyll fluorescence emitted by terrestrial vegetation (Gómez-Chova et al., 2006b; Vila-Francés et al., 2006a, 2007; Amorós-López et al., 2006b, 2007, 2008a) fills the absorption in those wavelengths and thus green vegetation fields can present lower optical path values (Alonso et al., 2006, 2007, 2008), comparable to low altitude clouds (Guanter et al., 2006b,c; Guanter et al., 2007). All these problems preclude the use of these features in simple approaches based on static thresholds.

As it happened with the surface features, we found differences for the retrieved atmospheric absorption features over land and ocean, which are mainly due to the coupling between scattering and absorption. Over dark surfaces with low reflectance, such as oceanic water, an important part of the light coming into the instrument is scattered in the atmosphere. Therefore, the extracted features do not measure the direct oxygen or water vapor transmittance anymore, thus resulting in a biased optical path (Ramon et al., 2003, 2004; Ranera et al., 2005). Despite of these differences over land and over ocean, the extracted features are still capable of discriminating cloud pixels

in both cases for a given image. These differences on feature values over land and ocean suggest that these two different cases should be better managed separately, that is, clustering pixels of each surface type separately.

4.3.3 Remarks on CHRIS Acquisition Modes

One of the main advantages of the CHRIS instrument is its high operation mode configurability. In fact, the number of bands and their nominal wavelength allocations changes to a great extent from one mode to another. However, this advantage is a problem for the detection of clouds since the method has to take into account the number and configuration of the spectral bands for each CHRIS acquisition mode. For example, the oxygen and water vapour atmospheric absorptions are only present in the spectral region registered by Modes 1 and 5. The spectral coverage of bands acquired by the main CHRIS modes is depicted in Fig. 4.16.

Table 4.1: Available features depending on CHRIS mode and number of bands used to compute them.

Characteristic	Range	Feature	Mode 1	Mode 2	Mode 3	Mode 4	Mode 5
Spectral Brightness	VIS	$f_{Br,VIS}$	22	10	7	5	8
Spectral Brightness	NIR	$f_{Br,NIR}$	11	4	6	8	10
Spectral Brightness	VNIR	f_{Br}	33	14	13	13	18
Spectral Whiteness	VIS	$f_{Wh,VIS}$	22	10	7	5	8
Spectral Whiteness	NIR	$f_{Wh,NIR}$	11	4	6	8	10
Spectral Whiteness	VNIR	f_{Wh}	33	10	13	13	18
Oxygen absorption	760 nm	f_{O_2}	3	–	–	–	3
Water vapor absorption	940 nm	f_{WV}	2	–	–	–	2

The proposed cloud masking algorithm has been designed for CHRIS Modes with full spectral information (Modes 1 and 5). Table 4.1 shows the available features depending on the CHRIS acquisition mode. In the case of the brightness and whiteness, the number of spectral bands used to compute them is lower for modes 2, 3, and 4. Therefore the robustness and the discrimination power of these features will be poorer for these modes. Moreover, the absorption features can not be computed at all for these modes. In consequence, the proposed algorithm could present a poor performance for Modes 2-3-4 images in critical cloud screening situations, such as over bright surfaces (ice, snow, sand, etc) and around cloud borders or thin semi-transparent clouds.

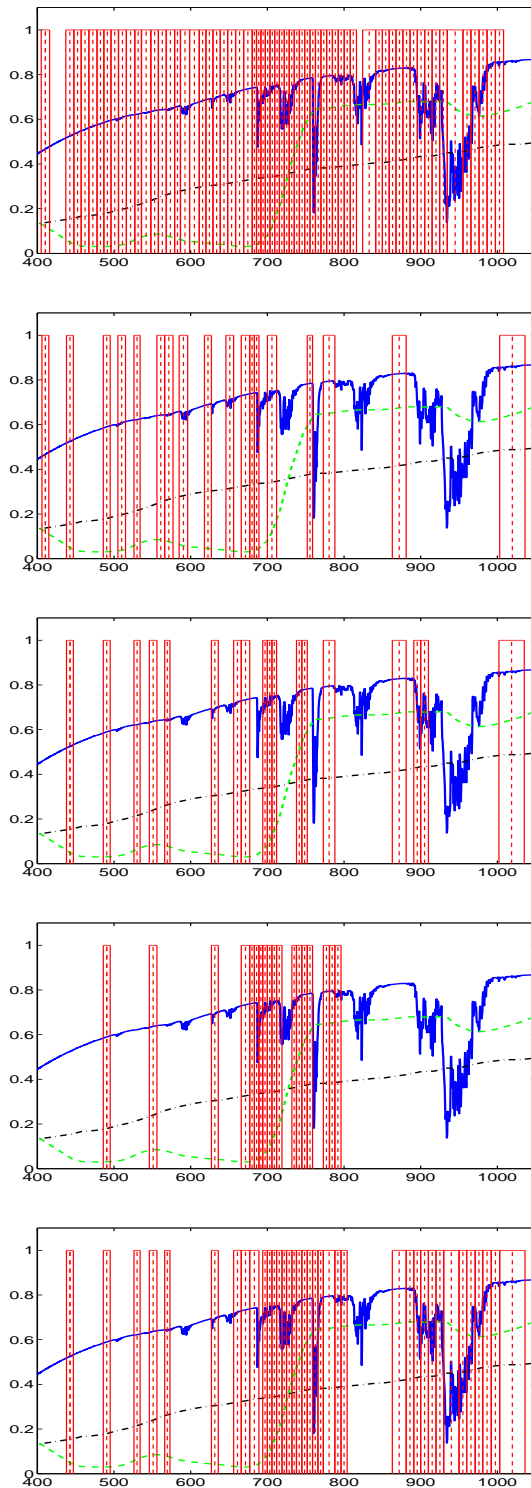


Figure 4.16: *Top-to-bottom:* Modes 1–5 CHRIS band locations (boxes) superimposed to a reflectance spectra of healthy vegetation (dashed), bare soil (dash-dotted), and atmospheric transmittance (solid).

Chapter 5

Unsupervised Cloud Classification

As previously discussed, cloud screening based on static thresholds applied to every pixel in the image can fail due to subpixel cloud coverage, sensor calibration, variation of the spectral response of clouds with cloud type and height, etc. In this context, the following step in our methodology considers the use of classification methods to find groups of similar pixels in the image. Clustering methods assume that the input data is organized into a number of groups or clusters according to a given distance measure in some representation space (Duda and Hart, 1973). An excellent review of clustering algorithms can be found in Xu and Wunsch (2005). In this work, we use the Expectation–Maximization (EM) algorithm (Dempster et al., 1977) to estimate the parameters of a Gaussian mixture model.

5.1 Pixel Identification and ROI Selection

Before applying a clustering algorithm, we should stress the fact that if clouds were not statistically representative in a given image, clustering methods could not find small clouds or cloud pixels could be mixed with other similar covers. Therefore, in addition to using representative features along with the spectral bands, clustering performance improves when applied over the regions of the image where clouds are statistically representative, which are defined as the *regions of interest* (ROIs).

5.1.1 Water/Land Identification

Differences of reflectance over land and ocean produce significant differences on the extracted features. As a consequence, splitting image pixels into two different clustering problems reduces the types of clusters and speeds up the clustering process itself. In order to do that, Geographical Information Systems (GIS), both tools and products, are very useful since they provide additional information of the geographical areas observed by the sensor, which can be combined with

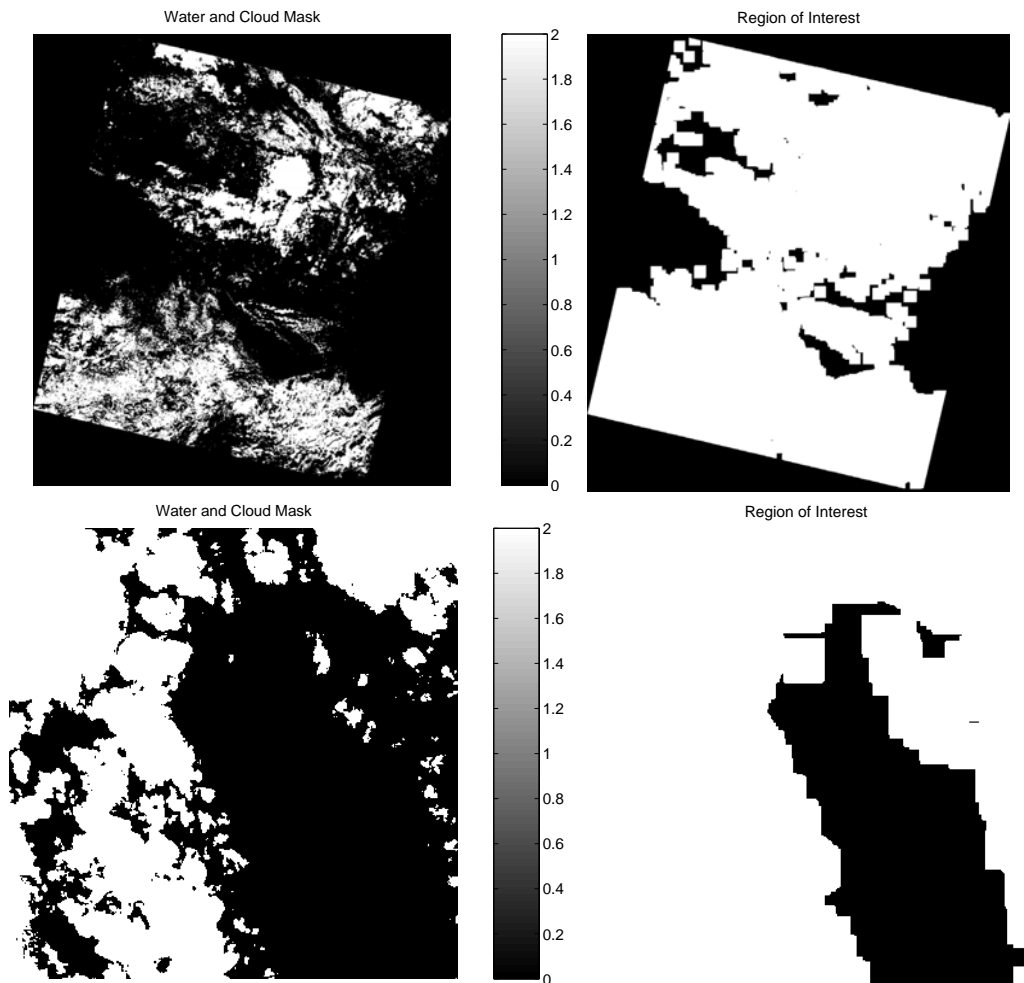


Figure 5.1: Result of the threshold-based cloud/land/water classification (*left*) and the growing algorithm (*right*) for the MERIS BR-2003-07-14 (*top*) and the CHIRS CHRIS-BR-050717-576C-41 (*bottom*) images (significant pixels in white).

the image data (Izquierdo-Verdiguier et al., 2008; Amorós-López et al., 2008b). The so called ‘land/ocean’ and ‘coastline’ flags attached to the MERIS L1b product could be used to separate land and water pixels present in the image. However, this geographical product can not be directly used for this purpose due to inaccuracies in the image geo-referentiation (Brockmann et al., 2002). Therefore, a refinement process of the ‘land/ocean’ flag is carried out on a per pixel basis using the TOA reflectance in order to accurately classify the inland waters and coast intertidal areas. Once image pixels are separated according to the surface type (‘land’ or ‘water’), the clustering is carried out. This process is further described in the following subsections.

5.1.2 Region of Interest with Cloud Covers

In order to find regions that could potentially contain clouds, we apply hard non-restrictive thresholds to provide a first map of cloud-like pixels¹. These absolute thresholds were obtained empirically and were applied to well-defined features: the brightness in the VIS and the NIR region, the estimated water vapor absorption, and the NDVI (in order to exclude areas with vegetation). Then, a region growth algorithm is carried out, along with a morphological process that dilates cloudy areas. This way, we ensure that all possible clouds and their contiguous areas will be considered in the clustering. The result of this process is far from providing a classification map, but just an overlay that identifies areas with presence of clouds (Fig.5.1).

5.2 Unsupervised Classification with the EM Algorithm

The clustering algorithm is applied to all the pixels in the ROI $\mathcal{X} = \{\mathbf{x}_i\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^d$ is the vector of extracted features for each pixel: $\mathbf{x}_i = [f_{\text{Br,VIS}}, f_{\text{Br,NIR}}, f_{\text{Wh}}, f_{\text{O}_2}, f_{\text{WV}}]^\top$, which correspond to the target spectral brightness in the VIS and NIR, the target spectral whiteness, and the oxygen and water vapor atmospheric absorptions, respectively. Basically, the aim of the clustering is to associate each input \mathbf{x}_i to one of the clusters ω_k , $k = 1, \dots, c$, in order to separate different classes (or at least clouds and ground-cover) present in the scene. We impose the following requirements to the clustering method: (i) it should take advantage of all available features (including atmospheric absorptions); (ii) it should consider the full relationship among variables (without applying independent tests to each feature); and (iii) it should provide for each input a *soft* association with the clusters (membership or probability value) between zero and one, h_{ik} , with the requirement that the memberships sum to one.

5.2.1 EM Algorithm

In multispectral and hyperspectral image processing, the assumption that the distribution of image data can be approximated as a mixture of normally distributed samples is commonly accepted (Shahshahani and Landgrebe, 1994; Jackson and Landgrebe, 2001; Landgrebe, 2002). In this chapter, we make such assumption for the extracted features. Therefore, we consider the input as a mixture of normal distributions and use the EM algorithm to obtain the maximum likelihood estimation of the probability density function (pdf) of the Gaussian mixture (Duda and Hart, 1973).

The EM algorithm estimates the mixture coefficient π_k , the mean $\boldsymbol{\mu}_k$, and the covariance matrix $\boldsymbol{\Sigma}_k$ for each component of the mixture. The final pdf describes both the class of interest and the ground-cover class, and is worth noting that both heterogeneous classes can be made up

¹Note that, in the case of MERIS, the ‘bright’ flag could be directly used to determine these regions and, therefore, to speed up the process.

of more than one mode, each representing a different subclass.

In a mixture model, the probability density function is given by (Duda and Hart, 1973):

$$p(\mathbf{x}|\Theta) = \sum_{k=1}^c p(\mathbf{x}|\omega_k, \Theta)P(\omega_k) \quad (5.2.1)$$

where ω_k are the components, $P(\omega_k)$ are their prior probabilities, or mixing parameters, and $p(\mathbf{x}|\omega_k, \Theta)$ are the conditional pdf associated to the k th component, being Θ the vector of parameters. Sometimes Θ also includes $P(\omega_k)$. The log likelihood of the independently and identically distributed (i.i.d.) sample \mathcal{X} is:

$$\mathcal{L}(\Theta|\mathcal{X}) = \sum_i \log p(\mathbf{x}_i|\Theta) = \sum_i \log \sum_k p(\mathbf{x}_i|\omega_k, \Theta)P(\omega_k) \quad (5.2.2)$$

This has not a straightforward solution, but the mixture parameters can be estimated using the EM algorithm, which involves two consecutive iterative steps.

In the E-step, we compute the posteriors as follows:

$$P(\omega_k|\mathbf{x}_i, \Theta) = \frac{p(\mathbf{x}_i|\omega_k, \Theta)P(\omega_k)}{\sum_l p(\mathbf{x}_i|\omega_l, \Theta)P(\omega_l)} \quad (5.2.3)$$

which will be also referred to as h_{ik} hereafter for the shake of simplicity in the notation. If the component densities are taken to be d -variate Gaussian, $p(\mathbf{x}|\omega_k, \Theta) \sim \mathcal{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$:

$$p(\mathbf{x}|\omega_k, \Theta) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}_k|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x} - \boldsymbol{\mu}_k)\right) \quad (5.2.4)$$

then we have

$$h_{ik} = \frac{\pi_k |\boldsymbol{\Sigma}_k|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k)\right)}{\sum_l \pi_l |\boldsymbol{\Sigma}_l|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_l)^\top \boldsymbol{\Sigma}_l^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_l)\right)} \quad (5.2.5)$$

where we re-define $\pi_k \equiv P(\omega_k)$.

In the M-step, we update the component parameters Θ :

$$\begin{aligned} \boldsymbol{\mu}_k &= \frac{\sum_i h_{ik} \mathbf{x}_i}{\sum_i h_{ik}} \\ \boldsymbol{\Sigma}_k &= \frac{\sum_i h_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^\top}{\sum_i h_{ik}} \\ \pi_k &= \frac{1}{n} \sum_i h_{ik} \end{aligned} \quad (5.2.6)$$

EM initialization

The EM algorithm has to be started with a set of initial values for the parameters of the pdf. In this work, the k -means algorithm is used to obtain a first approach to the structure of the data in clusters. This algorithm only needs the number of clusters c to be fixed, and minimizes the

Euclidean distance of the samples in one cluster to its mean. In k -means, input is associated only with the cluster having the nearest center (*crisp* labels). The cluster center is the mean of all inputs associated with that cluster. Once the cluster centers are updated, samples may change to a different cluster so an iterative procedure is followed until centers do not change significantly.

MAP classification

Once we have estimated the Gaussian components of the pdf of the data, we perform a Gaussian maximum likelihood classification on the whole image. The algorithm assigns the pixel to the cluster with the maximum *a posteriori* probability (MAP) generating a map with the clusters in the image. The final estimates of the cluster membership for each pixel in the image h_{ik} represent the estimates of the posterior probabilities, which are used to compute the optimal cluster label as:

$$h_i \equiv \underset{k}{\operatorname{argmax}} \{h_{ik}\} \quad (5.2.7)$$

Remarks on the number of clusters

The proposed image clustering process relies on the key step of selecting the number of clusters, c . Several statistical criteria can be used to assess partitions produced by the EM clustering algorithm. In (Bezdek et al., 1997) a good review of cluster validity indices, both crisp and probabilistic, for choosing the correct number of components in a mixture of normal distributions can be found. A well known statistically motivated index is the crisp *Davies-Bouldin* (DB) index (Davies and Bouldin, 1979), which consists in maximizing the between-cluster separation while minimizing the within-cluster scatter using an Euclidean metric. There are several information-based criteria aimed at determining the model (number of Gaussian components) that best describes the data (in terms of the maximum likelihood estimate) while reduces model's complexity (i.e. number of independently adjusted parameters within the model) to account for the over-fitting of high order models. The most common criterion of this type is the *Akaike's Information Criterion* (AIC) (Akaike, 1974), which adds to the *log-likelihood* of the model parameters Θ with respect to the set of samples, $\mathcal{L}(\Theta|\mathcal{X})$, a penalty term depending of the number of free parameters of the model, $n_p = c(1 + d + (d + 1)d/2) - 1$, and looks for the model with lowest value: $-2\mathcal{L}(\Theta|\mathcal{X}) + 2n_p$. The Rissanen's *Minimum Description Length* (MDL) criterion (Rissanen, 1986) includes in the penalty term the total number of samples, n , in order to obtain a consistent estimator that converges when the number of observations tends to infinity: $-2\mathcal{L}(\Theta|\mathcal{X}) + n_p \log(n)$. Some variants of the MDL penalize free parameters more strongly than the previous one: $-2\mathcal{L}(\Theta|\mathcal{X}) + n_p \log(nd)$.

Another possibility for the user (and not explored in this work) is to initialize the mean of the clusters with the spectral signature of the class of interest using a spectral library. Obviously, the problem of selecting c vanishes if a training labeled set is available.

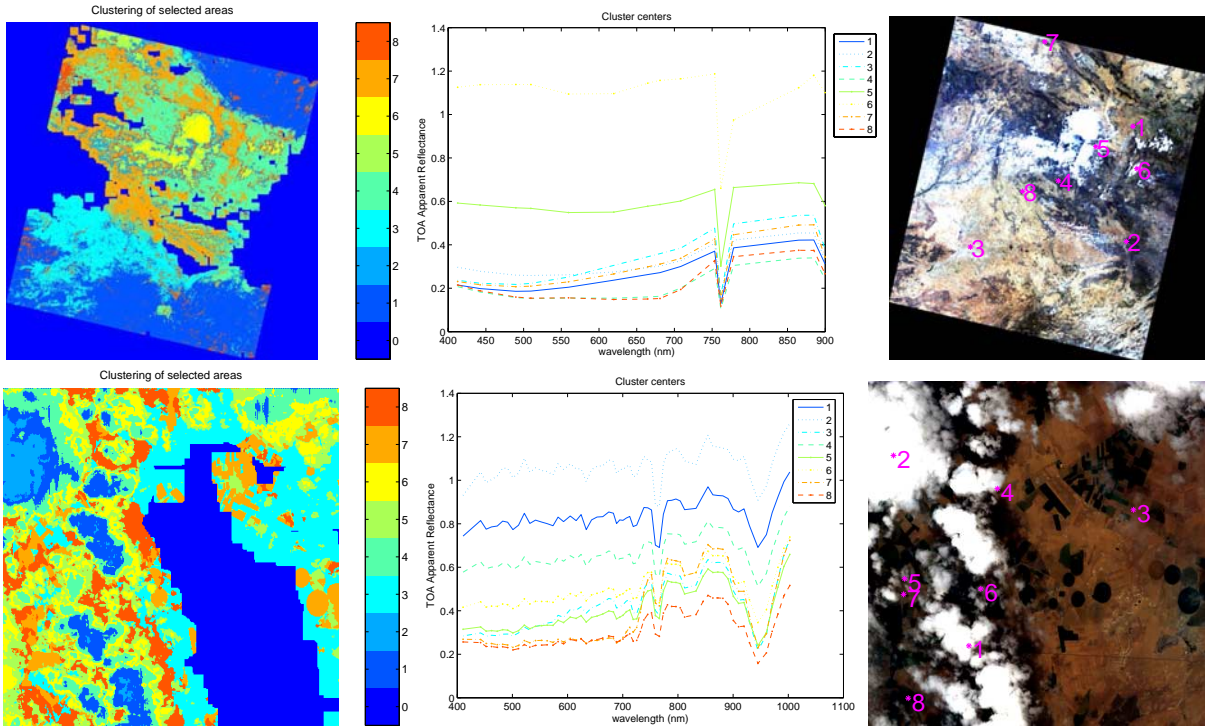


Figure 5.2: Thematic map with the distribution of the clusters in the scene (*left*), the spectral signatures of the clusters (*center*), and the location in the image of the pixels with the most similar spectra (*right*) for the MERIS BR-2003-07-14 (*top*) and the CHIRS CHRIS-BR-050717-576C-41 (*bottom*) images.

5.2.2 Cloud Identification

Once clusters are determined in the previous step, the spectral signature for each cluster, $\mathbf{s}_k(\lambda)$, is estimated as the average of the spectra of the cluster pixels. This step excludes those pixels with abnormally low membership values or posterior probability h_{ik} . It is important to emphasize that these spectral signatures of each cluster could differ a lot from the spectra obtained when applying the EM algorithm over the image using the spectral bands rather than the extracted features. The extracted features used to find the clusters are optimized to increase separability between clouds, C , and any-other surface type, \overline{C} , while in the spectral domain these clusters could present a high degree of overlapping. Therefore, the obtained clusters can be labeled (or identified) as ‘cloud’ or ‘cloud-free’ (or into more detailed geo-physical classes) to take into account four complementary sources of information (Fig. 5.2): (i) the cluster centers $\boldsymbol{\mu}_k$ of the extracted features; (ii) the spectral signatures of cluster, \mathbf{s}_k ; (iii) the thematic map with the distribution of the clusters in the scene; and (iv) the location in the image of the pixels with the spectral signature closer to \mathbf{s}_k . At this point of the process, two different labeling strategies can be followed depending on whether the method is applied to a large number of scenes in an operational mode or it is used by an operator to improve cloud screening on regional and case studies. In the first case, found clusters are labeled by using a set of threshold tests over $\boldsymbol{\mu}_k$ and \mathbf{s}_k values (these tests can be similar to the ones used by the MERIS standard algorithm (Santer et al., 1997)). This

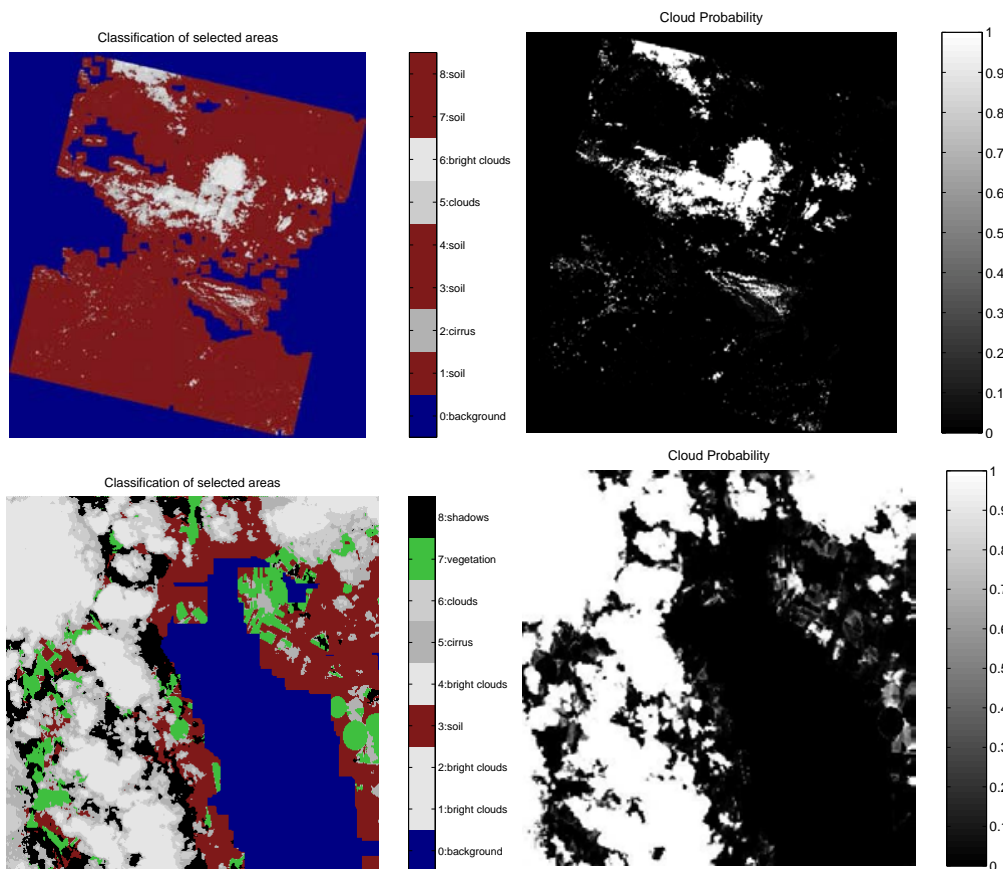


Figure 5.3: Thematic map with the distribution in the scene of the classes of the clusters (*left*) and *Cloud Probability* index computed from the posteriors of the cloud-clusters (*right*) for the MERIS BR-2003-07-14 (*top*) and the CHIRS CHRIS-BR-050717-576C-41 (*bottom*) images.

cluster-based approach provides a more accurate cloud screening than the standard approach (applied on a per pixel basis) since classifying the centers of the clusters should be easier than classifying single pixels, e.g. pixels close to the decision boundaries. It is worth noting that, in this case, different classification criteria can be used for clusters found over ‘land’ and over ‘water’. For regional and case studies, the cluster information can be analyzed directly by the user for the given image. This can help significantly to identify clusters corresponding to extremely thin clouds or ice/snow covers misclassified by the automatic labeling. In the following processing steps of the method, both ‘land’ and ‘water’ clusters are used together to obtain the final probability and abundance fraction of clouds for all image pixels, and thus obtaining a cloud product map without discontinuities between land and water.

Once all clusters have been related to a class with a geo-physical meaning (Fig. 5.3[*left*]), it is straightforward to merge all the clusters belonging to a cloud type. Since the EM algorithm provides posterior probabilities ($h_{ik} \in [0, 1]$ and $\sum_{k=1}^c h_{ik} = 1$), a probabilistic cloud index, based on the clustering of the extracted features, can be computed as the sum of the posteriors of the

cloud-clusters C :

$$h_{iC} = \sum_{\omega_k \subset C} h_{ik} \quad (5.2.8)$$

However, if the clusters are well separated in the input space, the posteriors decrease drastically from one to zero in the boundaries between clusters (Fig. 5.3[*right*]). Therefore, this *Cloud Probability* index indicates the probability that one pixel more likely belongs to a cloud-cluster, C , than to one of the other clusters, \overline{C} , found in the image, but it does not give information about the cloud content at subpixel level, which is very important when dealing with thin clouds or partially covered pixels.

5.3 Cloud Abundance

In order to obtain a cloud abundance map for every pixel in the image, instead of flags or a binary classification, a spectral unmixing algorithm is applied to the MERIS image. The linear spectral unmixing algorithm (LSU) (Chang, 2003) allows decomposing each pixel of the image, $\rho_i(\lambda)$, into a collection of constituent spectra or *endmembers*, and a set of corresponding abundances that indicate the proportion of each endmember in the pixel.

5.3.1 Linear Spectral Unmixing

The algorithm used to perform the spectral unmixing is the Fully Constrained Linear Spectral Unmixing (FCLSU) (Heinz and Chang, 2001; Chang, 2003), which guarantees a physical (yet linear) interpretation of the results and can be formalized as follows:

$$\rho_i(\lambda_b) = \sum_{q=1}^Q m_q(\lambda_b) a_{iq} + \varepsilon_b \quad (5.3.1)$$

subject to

$$0 \leq a_{iq} \leq 1 \text{ and } \sum_q a_{iq} = 1 \quad (5.3.2)$$

where $\rho_i(\lambda_b)$ is the value of the pixel i for band b ; Q represents the number of endmembers that are being unmixed; and coefficients a_{iq} are the unmixing coefficients, which can be interpreted as the abundance fractions of materials in a pixel. Finally, the term ε_b represents the residual error per band. Equation (5.3.1) can be expressed in a matrix form as $\rho_i = \mathbf{M} \cdot \mathbf{a}_i + \varepsilon$, where the spectral signatures of materials, \mathbf{m}_q , are expressed as the columns of matrix \mathbf{M} . The FCLSU algorithm solves a constrained linear least-squares problem:

$$\min_{\mathbf{a}_i} \|\mathbf{M} \cdot \mathbf{a}_i - \rho_i\| \quad (5.3.3)$$

subject to (5.3.2), i.e. the vector \mathbf{a}_i of independent variables is restricted to being nonnegative and sum to one. This is because \mathbf{a}_i represents the contribution of reflectance signatures \mathbf{m}_q and it is

supposed that \mathbf{M} represents all the constituents in the image with at least one pure independent spectrum.

Remarks on endmember extraction for cloud screening

In the literature, there are different approaches to determine the spectra of the different pure constituents in the image (Keshava and Mustard, 2002; Plaza and Chang, 2006). However, in a cloud screening framework, two specific considerations have to be taken into account. First, only one endmember must be selected to represent clouds. This constraint contrasts with the selection of the number of clusters, in which more clusters should model better such an heterogeneous class as clouds. In the classification, most of the cloud-clusters consists of mixed pixels of thin clouds and ground or borders and subpixel clouds. In the LSU method, we assume that clouds represent pure constituents and consequently only one endmember must represent them. Some examples of the negative effects of including mixed thin cloud spectra as endmembers were reported by Gómez-Chova et al. (2005a). In this work, the *cloud endmember*, \mathbf{m}_1 , is selected among all the cloud pixels, $\rho_i \in C$, looking for the brightest and whitest one. The second issue is related to the total number of endmembers. If the value of Q is selected to be too low, then not all constituents will be extracted. On the other hand, if the value of Q is selected to be too high, some extracted endmembers may be unwanted non-pure signatures. However, this does not constitute a critical problem since we are not interested in obtaining accurate abundances for *all* the constituents present in the image, but basically in the cloud abundance. For this reason, obtaining some unpure *ground endmembers*, i.e. those mixture of two or more ground constituents, is not a problem as this will only affect the abundances related to ground endmembers.

Endmember initialization algorithm

Taking into account the previous considerations, we use the Automated Target Generation Process (ATGP) (Ren and Chang, 2003) to select the rest of endmembers, $\{\mathbf{m}_q\}_{q=2}^Q$, from the ground pixels, $\rho_i \in \overline{C}$. The ATGP finds the endmembers in accordance with an orthogonal subspace projection criteria and it normally outperforms the other common endmember initialization algorithms (Amorós-López et al., 2006a; Plaza and Chang, 2006). In particular, the ATGP is well-suited to our problem since it starts with the initial endmember signature, \mathbf{m}_1 , then finds the next endmember signature, \mathbf{m}_2 , looking for the ground pixel with the maximum absolute projection in the space orthogonal to $\mathbf{M} = [\mathbf{m}_1]$, adds the new endmember to $\mathbf{M} = [\mathbf{m}_1, \mathbf{m}_2]$, and repeats the procedure until a set of Q endmembers $\{\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_Q\}$ is extracted.

5.3.2 Cloud Abundance fraction

After the endmember selection, we apply the FCLSU to the image using all the available spectral bands except those MERIS bands particularly affected by atmospheric absorptions ($\lambda_b \in$

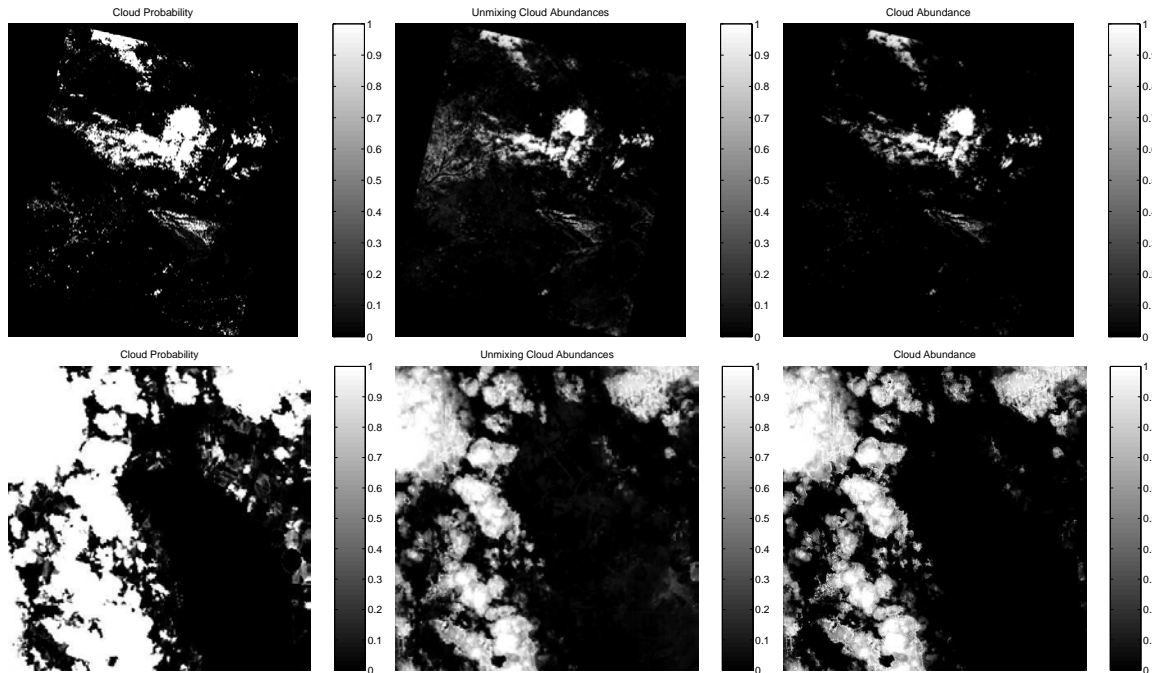


Figure 5.4: *Cloud Probability* index computed from the posteriors of the cloud-clusters (*left*); *Cloud Abundance* computed from the unmixing coefficients of the cloud clusters (*center*); and cloud abundance product (*left*) for the MERIS BR-2003-07-14 (*top*) and the CHRIS-BR-050717-576C-41 (*bottom*) images.

B_A , $b = \{11, 15\}$), since the *linear* mixing assumption is not appropriate at those bands. The FCLSU provides the vector \mathbf{a}_i of abundances for each sample pixel i . As it happens with the probabilities of the clusters, the abundance $a_{iq} \in [0, 1]$ and $\sum_{q=1}^Q a_{iq} = 1$. Therefore, the *Cloud Abundance* is the sum of the abundances of the cloud-clusters which, in our case, represents the abundance of the cloud-endmember (Fig. 5.4[*center*]):

$$a_{iC} = \sum_{q \in C} a_{iq} = a_{i1} \quad (5.3.4)$$

As in the case of the probabilities, a threshold of a_{iC} would give a good cloud mask, but some false detections could appear since unmixing has been performed on the basis of spectral signatures that could be non-pure pixels or, at least, not completely independent, thus providing relatively high cloud abundances in ground covers with similar spectral signatures.

5.3.3 Cloud Final Product

An improved cloud product map can be obtained when combining the *Cloud Abundance*, a_{iC} , and the *Cloud Probability*, h_{iC} , by means of a pixel-by-pixel multiplication (Fig. 5.4[*right*]).

$$\vartheta_i = a_{iC} h_{iC} \quad (5.3.5)$$

That is, combining two complementary sources of information processed by independent methods: the degree of cloud abundance or mixing (obtained from the spectra) and the cloud probability

that is close to one in the cloud-like pixels and close to zero in remaining areas (obtained from the extracted features). Note that, by performing a pixel-by-pixel multiplication, errors in the sub-pixel cloud abundance would lead to similar errors in the cloud abundance product. For example, if an endmember is selected from a ground cover with similar reflectance signature to the cloud endmember, it could introduce significant errors in the estimated cloud abundance. However, the endmember selection performed by the ATGP algorithm reduces to some extent the risk of selecting such spectra. In addition, besides abundance fractions, the unmixing algorithm provides the unmixing residual error, ε , which informs us about the accuracy of the unmixing on a per-pixel basis.

Chapter 6

Semi-supervised Cloud Classification

Applying unsupervised clustering methods over the whole image allows us to take advantage of the wealth of information and the high degree of spatial and spectral correlation of the image pixels. However, the cluster labeling strategy presented in the previous chapter (cf. section 5.2.2) is conceived for scenarios where there is an operator to improve cloud screening on regional and case studies, but it is not practical when applied to a large number of scenes in an operational mode. This solution is mostly image oriented and concerned with obtaining more accurate cloud masks than the standard approach (applied on a per pixel basis), which underperforms in some critical problems, such as cloud borders and bright surfaces.

When the aim is to process a large number of scenes in an automatic way, we should turn to robust supervised methods, which learn from a reliable set of labeled training samples in order to define a decision function that correctly classifies cloudy pixels. However, few labeled samples are typically available or likely to be obtained in an operational basis. Our aim is to take advantage of the benefits shown by both supervised and unsupervised methods. For this reason, in this chapter, we explore the opportunities offered by semi-supervised learning (SSL) that exploits the few labeled samples and the wealth of unlabeled samples in the images.

In remote sensing image classification, we are usually given a reduced set of labeled samples to develop the classifier. Learning in these conditions is more challenging when dealing with *ill-posed* problems, i.e. working with less labeled samples than the input dimension of the pixels. Supervised support vector machines (SVMs) (Schölkopf and Smola, 2001; Camps-Valls et al., 2007c) excel in using the labeled information, since they are (regularized) maximum margin classifiers also equipped with an appropriate loss function (Vapnik, 1998; Shawe-Taylor and Cristianini, 2004; Camps-Valls and Bruzzone, 2005). These methods, nevertheless, need to be reformulated in order to exploit the information contained in the wealth of unlabeled samples, a.k.a. *semi-supervised classification*. In semi-supervised learning, the algorithm is provided with some available supervised information in addition to the unlabeled data.

Cloud screening constitutes a clear example of these situations, since few labeled cloud pixels

are typically available, and cloud features change to a great extent depending on the cloud type, thickness, transparency, height, or background, as shown in previous chapters. In addition, cloud screening must be carried out before atmospheric correction, being the input data affected by the variable atmospheric conditions.

Semi-supervised Learning Framework When working with semi-supervised methods, the number of reliable labeled samples is usually small and semi-supervised learning methods try to use the large amount of available unlabeled data by making some assumptions. Only if the imposed model assumption meets the problem structure, it is possible to learn from unlabeled samples and to improve classifier performance. The main assumptions made in SSL are the following:

- The *cluster* assumption can be roughly stated as “If samples are in the same cluster, they are likely to belong to the same class”. Nearby points are likely to have the same label (local consistency), while points on the same data structure are likely to have the same label (global consistency).
- The *manifold*¹ (smoothness) assumption can be stated as “If two samples in a high-density region are close, then so should be the corresponding outputs”. If two points are linked by a path of high density then their outputs are likely to be close (global consistency), but the contrary is not necessarily true.

The framework of semi-supervised learning is very active and has recently attracted a considerable amount of research (Zhu, 2005; Chapelle et al., 2006). Essentially, two different classes of SSL algorithms are encountered in the literature.

1. *Generative models* involve estimating the conditional distribution by means of modeling the class-conditional distributions explicitly, such as expectation-maximization (EM) algorithms with finite mixture models (Dempster et al., 1977), which have been extensively applied in the context of remotely sensed image classification (Shahshahani and Landgrebe, 1994; Jackson and Landgrebe, 2001; Gómez-Chova et al., 2002, 2003b).
2. *Discriminative models* estimate the conditional distribution directly and there is no need to explicitly specify the class-conditional distributions. Two subgroups of SSL algorithms can be distinguish within these models:
 - *Low density separation algorithms* maximize the margin for labeled and unlabeled samples simultaneously, such as Transductive SVM (TSVM) (Vapnik, 1998), which has been recently applied to hyperspectral image classification (Bruzzone et al., 2006);

¹A manifold is a topological space that is locally Euclidean, but in which the global structure may be more complex. Formally, in a “ d -dimensional topological manifold” \mathcal{M} , for each point \mathbf{x} in the manifold \mathcal{M} there is an open subset S with $\mathbf{x} \in S$, for which there exists a homeomorphic mapping g that maps S into a d -dimensional open subset S' in a d -dimensional Euclidean space \mathbb{R}^d (Bachmann et al., 2005, 2006).

- *Graph-based methods*, in which each sample spreads its label information to its neighbors until a stable state is achieved on the whole dataset (Chung, 1997) also adapted to remote sensing image classification by Camps-Valls et al. (2007a).

In the recent years, TSVM and graph-based methods have captured great attention. However, some specific problems are identified in both of them. In particular, the TSVM is sensitive to local minima and requires convergence heuristics by using an (unknown) number of unlabeled samples. Graph-based methods are computationally demanding and generally do not yield a final decision function but only prediction labels.

In the following sections, we first provide an introduction to kernel-based methods, which have been selected as the core of the semi-supervised classification algorithms proposed in this Thesis. Then, we describe a semi-supervised discriminative algorithm based on the *graph Laplacian* and SVMs that we propose for its use in cloud screening. Finally, a novel semi-supervised algorithm based on composite kernels and kernel mean mappings is presented and analyzed in detail.

6.1 Introduction to Kernel Methods

In this section, we first state the general problem of learning from samples, the need of introducing regularization in the classifiers, and the important concept of kernel feature space. After this, the formulation and characteristics of each kernel-based method are briefly reviewed. For a full theoretical description of these (and other) kernel-based methods, the reader is referred to Schölkopf (1997); Müller et al. (2001) and for the analysis of hyperspectral image classification with kernels to Camps-Valls et al. (2003, 2004b); Camps-Valls and Bruzzone (2004); Camps-Valls et al. (2004a); Camps-Valls and Bruzzone (2005); Camps-Valls et al. (2006a); Bruzzone et al. (2007).

6.1.1 Learning from Samples, Regularization, and Kernel feature space

Let us consider a two-class problem, where a labeled training data set $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, being $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, +1\}$, is generated according to an (unknown) probability distribution $p(\mathbf{x}, y)$. The problem is to find a function f that minimizes the expected error (or risk)

$$R(f) = \int V(f(\mathbf{x}), y) dp(\mathbf{x}, y) \quad (6.1.1)$$

where V represents a pre-defined cost (or loss) function of the errors committed by f . Since the risk cannot be minimized directly, one follows an inductive principle. A common one consists in approximating the minimum of the risk by the *empirical risk* $R_{\text{emp}}(f)$, i.e. the error in the training data set:

$$R_{\text{emp}}(f) = \frac{1}{n} \sum_{i=1}^n V(f(\mathbf{x}_i), y_i) \quad (6.1.2)$$

However, convergence of the empirical risk to the actual risk is only ensured as n goes to infinity and, since this is not possible in real applications, the well-known problem of overfitting may arise. This is specially significant in hyperspectral image classification given the low ratio between the number of training samples and the size of the input feature space, and the high spatial variability of the spectral signature.

In order to control the capacity (or excess of flexibility) of the models and to avoid overfitting, the solution is usually regularized (Tikhonov and Arsenin, 1977), which is carried out in practice by minimizing an l -norm of the decision function given by the model parameters, $\|\mathbf{w}\|_l$, in the corresponding feature space where the function is defined. This is intuitively equivalent to find the estimator which uses the minimum possible energy of the data to estimate the output, i.e. by minimizing this term one forces smooth solutions by using small weights, which reduces the tendency of the model to overfit the training data. The resulting functional should take into account both this complexity term and an empirical error measurement term defined according to an *a priori* determined cost function V of the committed errors. Hence, the regularized minimizing functional can be written as

$$R_{\text{reg}}(f) = R_{\text{emp}}(f) + \gamma \|\mathbf{w}\|_l^2, \quad (6.1.3)$$

where the parameter γ tunes the trade-off between model complexity and minimization of training errors. It is worth noting that different loss functions V and norms can be adopted for solving the problem, involving completely different families of models and solutions.

The problem of minimizing the regularized functional in (6.1.3) can be solved following different minimization procedures. Neural networks are trained to minimize the empirical risk, and therefore, they follow the empirical risk minimization (ERM) principle (Soria-Olivas et al., 2003). However, on the one hand, in order to attain significant results on the test set, early-stopping criteria or pruning techniques must be used (Haykin, 1999; Camps-Valls et al., 2006e). On the other hand, the structural risk minimization (SRM) principle (Vapnik, 1998) states that a better solution in terms of generalization capabilities can be found by minimizing an upper bound of the generalization error.

Statistical learning theory points out that learning can be simpler using low complexity classifiers in high dimension (possibly infinite) spaces \mathcal{H} instead of working in the original input space \mathbb{R}^d , i.e. not the dimensionality but the complexity of the function class, which maps input data into \mathcal{H} , matters (Vapnik, 2000). Thus, all the potential and richness that a classifier needs can be introduced by a mapping ϕ to a Hilbert space \mathcal{H} . For instance, in a Radial Basis Function Neural Network (RBFNN), the Hilbert space \mathcal{H} is spanned by the RBF centers, whereas in the case of SVMs it is expanded by the training samples (Camps-Valls et al., 2004c; Camps-Valls and Bruzzone, 2005). It is worth noting, nevertheless, that in the machine learning community, one only refers to *kernel methods* as those that take advantage of the “kernel trick”, which allows us to work in the mapped *kernel space* without explicitly knowing the mapping ϕ ,

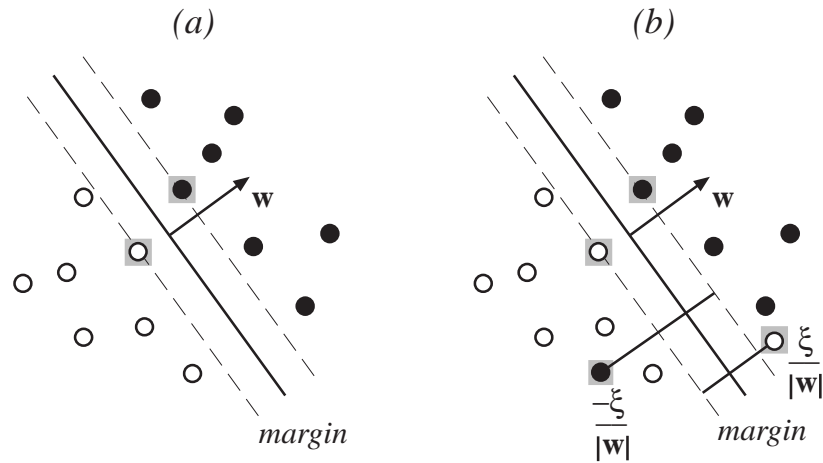


Figure 6.1: (a) The Optimal Decision Hyperplane (ODH) in a linearly separable problem. Optimal margin hyperplane is equivalent to minimizing $\|\mathbf{w}\|$. Only support vectors (gray-squared samples) are necessary to define the ODH. (b) Linear decision hyperplanes in nonlinearly separable data can be handled by including slack variables ξ_i to allow classification errors.

but only the kernel function formed by the dot product of mapping functions. In the following, we will always refer to the reproducing kernel Hilbert space (RKHS), where the data is mapped, as the “kernel space”. Further detailed information on this issue can be found in the next subsections where kernel-based methods are briefly reviewed. Among all the available kernel machines, we focus on SVMs, which have recently demonstrated superior performance in the context of hyperspectral image classification (Camps-Valls and Bruzzone, 2004, 2005). For all methods, we only review the standard binary formulation since cloud screening can be considered a binary classification problem.

6.1.2 Support Vector Machines

The classification methodology of SVMs attempts to separate samples belonging to different classes by tracing maximum margin hyperplanes in the kernel space where samples are mapped to (see Fig. 6.1(a)). Maximizing the distance of samples to the optimal decision hyperplane is equivalent to minimizing the norm of \mathbf{w} , and thus this becomes the first term in the minimizing functional. For better manipulation of this functional, the quadratic norm of the weights is preferred. Therefore, following previous notation, the SVM method solves the following primal problem:

$$\min_{\mathbf{w}, \xi_i, b} \left\{ \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i \right\} \quad (6.1.4)$$

constrained to:

$$y_i (\langle \phi(\mathbf{x}_i), \mathbf{w} \rangle + b) \geq 1 - \xi_i \quad \forall i = 1, \dots, n \quad (6.1.5)$$

$$\xi_i \geq 0 \quad \forall i = 1, \dots, n \quad (6.1.6)$$

where \mathbf{w} is the normal to the optimal decision hyperplane defined as $\langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b = 0$, and b represents the bias or closest distance to the origin of the coordinate system. These parameters define a linear classifier in the kernel space \mathcal{H} :

$$\hat{y}_* = f(\mathbf{x}_*) = \text{sgn}(\langle \mathbf{w}, \phi(\mathbf{x}_*) \rangle + b) \quad (6.1.7)$$

The non-linear function ϕ maps samples to a higher dimensional space, which in accordance with Cover's theorem (Cover, 1965), guarantees that the transformed samples are more likely to be linearly separable. The regularization parameter C controls the generalization capabilities of the classifier, and ξ_i are positive slack variables allowing to deal with permitted errors (see Fig. 6.1(b)).

The above problem is solved by introducing Lagrange multipliers ($\xi_i \geq 0, \mu_i \geq 0$) for each constraint:

$$\min_{\mathbf{w}, \xi, b} \left\{ \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i [y_i (\langle \mathbf{w}, \phi(\mathbf{x}_i) \rangle + b) + \xi_i - 1] - \sum_{i=1}^n \mu_i \xi_i \right\} \quad (6.1.8)$$

Now, by making zero the gradient of this primal-dual functional \mathcal{L}_{pd} with respect to the primal variables (\mathbf{w}, b, ξ_i), we obtain the following conditions:

$$\frac{\partial \mathcal{L}_{pd}}{\partial \mathbf{w}} = 0 \quad \rightarrow \quad \mathbf{w} = \sum_i y_i \alpha_i \phi(\mathbf{x}_i) \quad (6.1.9)$$

$$\frac{\partial \mathcal{L}_{pd}}{\partial b} = 0 \quad \rightarrow \quad \sum_i y_i \alpha_i = 0 \quad (6.1.10)$$

$$\frac{\partial \mathcal{L}_{pd}}{\partial \xi_i} = 0 \quad \rightarrow \quad C = \alpha_i + \mu_i, \quad i = 1, \dots, n \quad (6.1.11)$$

If constraints (6.1.9)-(6.1.11) are included in the Lagrange functional \mathcal{L}_{pd} (Eq. (6.1.8)) in order to remove the primal variables, the dual problem \mathcal{L}_d to be solved is obtained:

$$\max_{\alpha} \left\{ \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle \right\}, \quad (6.1.12)$$

constrained to $0 \leq \alpha_i \leq C$ and $\sum_i \alpha_i y_i = 0, \forall i = 1, \dots, n$. In this way, one gets rid of the explicit usage of very high dimensional vectors, \mathbf{w} . This constitutes a quadratic programming (QP) problem with linear constraints, and can be solved with many available software packages.

It is worth noting that all ϕ mappings used in the SVM learning occur in the form of inner products. This allows us to define a kernel function K :

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle, \quad (6.1.13)$$

and then, without considering the mapping ϕ explicitly, a non-linear SVM can be defined. Note

that the pair $\{\mathcal{H}, \phi\}$ will only exist if the kernel function K fullfils Mercer's conditions² as will be detailed in the following section.

After solving the QP problem with a given kernel function, one obtains the optimal Lagrange multipliers, α_i , which reflect the relative relevance of each sample for classification. The key issue is that we have worked implicitly in the higher dimensional feature space, and retrieve a weight vector in the original input space. Note that, by solving the optimization problem, the feature-space model parameters \mathbf{w} are expressed as a linear expansion of the mapped samples $\phi(\mathbf{x}_i)$ through the dual parameters α_i , i.e. $\mathbf{w} = \sum_{i=1}^n y_i \alpha_i \phi(\mathbf{x}_i)$ (Eq. (6.1.9)).

By plugging (6.1.9) into (6.1.7), the decision function for any test vector \mathbf{x}_* is given by:

$$\hat{y}_* = f(\mathbf{x}_*) = \text{sgn} \left(\sum_{i=1}^n y_i \alpha_i K(\mathbf{x}_i, \mathbf{x}_*) + b \right), \quad (6.1.14)$$

where b is calculated using the primal-dual relationship, and where only samples with non-zero Lagrange multipliers α_i account for the solution. This leads to the very important concept of *sparsity*, i.e. the solution is expressed as a function only of the most critical training samples in the distribution, namely *support vectors* (SV). For deeper analysis and application of SVMs in RS image classification refer to Gualtieri and Crompt (1998); Gualtieri et al. (1999); Camps-Valls et al. (2004a); Camps-Valls and Bruzzone (2005).

6.1.3 Composite Kernels Framework

The bottleneck for any kernel method is the definition of a suitable kernel mapping function that accurately reflects the similarity (distance, resemblance) between samples. However, not all metric distances are permitted. In fact, valid kernels are only those fulfilling the Mercer's Theorem (Mercer, 1905; Aizerman et al., 1964).

Some popular kernels fulfilling these conditions are:

- *Linear kernel:*

$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle \quad (6.1.15)$$

- *Non-homogeneous Polynomial:*

$$K(\mathbf{x}_i, \mathbf{x}_j) = (\langle \mathbf{x}_i, \mathbf{x}_j \rangle + 1)^p, \quad p \in \mathbb{Z}^+ \quad (6.1.16)$$

²According to Hilbert-Schmidt theory, $K(\mathbf{x}_i, \mathbf{x}_j)$ can be any symmetric function satisfying Mercer's conditions. This was firstly stated by Courant and Hilbert (1953). The same idea was used by Aizerman et al. (1964) for the analysis of the convergence properties of the method of potential functions, and happened at the same time as the method of the optimal hyperplane was developed by Vapnik and Chervonenkis (1964). Full details on the Mercer's conditions can be obtained from Vapnik (2000).

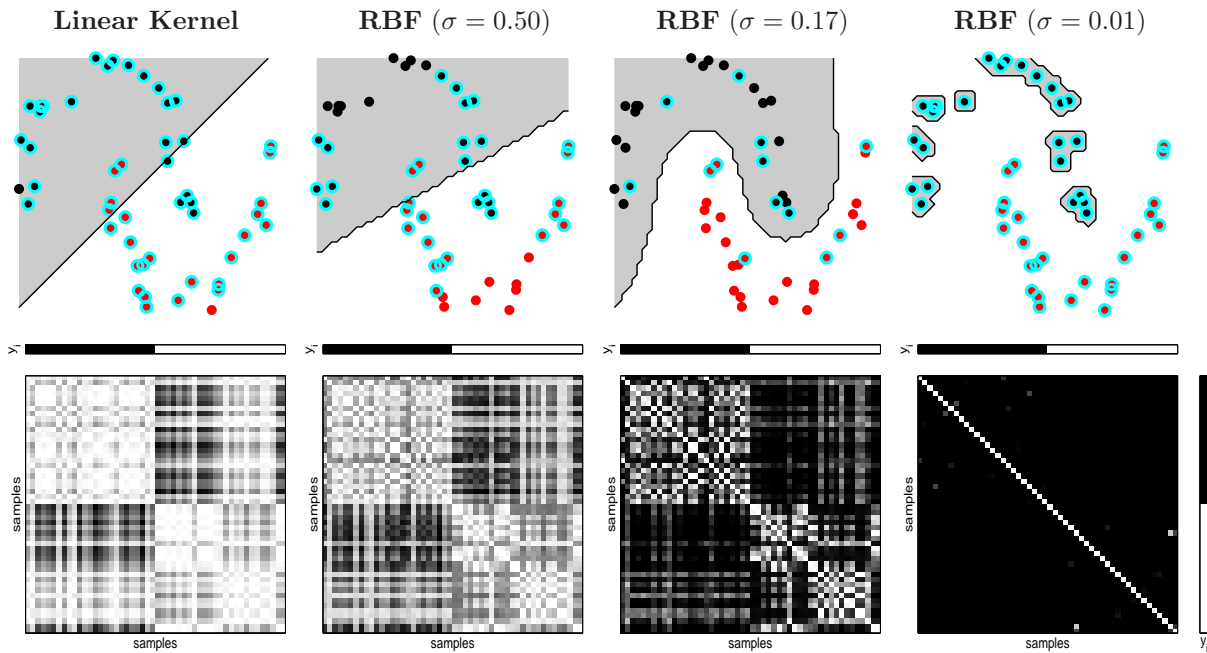


Figure 6.2: Illustrative example of the use of different kernel functions in a two-dimensional two-class problem where training data are generated from the so called ‘two moons’ nonlinear problem. Upper part of the figure shows the classification results for the standard SVM with the linear kernel and the RBF kernel with different widths. In these plots, *red* and *black points* represent the training samples; *blue circles* indicate the samples used as support vectors in each SVM; and *black line* shows the classification boundary of the trained classifiers. Bottom part of the figure shows the kernel matrix of the training samples for each trained model (samples are sorted by class for a proper interpretation).

- *Radial Basis Function (RBF) kernel:*

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma^2), \quad \sigma \in \mathbb{R}^+ \quad (6.1.17)$$

In order to illustrate the relevance of the adequate definition of the kernel function, Fig. 6.2 shows the classification results obtained for the so called ‘two moons’ nonlinear problem when using a linear kernel or an RBF kernel with different widths. The linear kernel function is directly the dot product of the input vectors $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ and thus ϕ corresponds to the identity function and input data are not mapped to a different space. As a consequence, the linear kernel provides a regularized maximum margin linear classifier in the input space as we can observe in Fig. 6.2. The RBF kernel implies a nonlinear mapping to a higher dimensional Hilbert space. In fact, it can map data to so many spaces as values can take the kernel width σ , which is the standard deviation of a Gaussian function. It is worth noting that the similarity between samples in the RBF kernel comes from dividing their squared distances by the kernel width (σ^2) in the exponent. Therefore, σ is a scale parameter that is directly related to the local variability of the data. Figure 6.2 shows results obtained with a standard SVM when fixing the value of σ to a *large*, *optimum*, or *small* value (data ranges between -1 and 1 in both dimensions). In practice, a σ greater than half the

maximum Euclidean distance between all samples will provide results similar to the linear kernel since a high value ($\sigma = 0.5$) would imply low variability or local structure. On the other hand, a σ smaller than half the smallest Euclidean distance between training samples would make samples go too far from each other (with respect to the Gaussian) to extract the structure of data. This is shown for $\sigma = 0.01$, where the imposed data locality leads to *overfit*³ training samples. For this case, classification boundary clearly overfits the training data, all training samples are selected as support vectors (*blue circles*), and the kernel matrix is almost diagonal (no class structure is observed). Finally, the value $\sigma = 0.17$ is selected through cross-validation in the training set. In this case, a nonlinear classifier is obtained while optimizing its generalization capabilities, and the kernel matrix structure reflects the class information. Summarizing, when using RBF kernels, the more local data structure is, the smaller σ should be.

In this section, we review the main properties of kernels and the framework of composite kernels, which will be explained to later present a novel semi-supervised kernel algorithm for cloud classification.

Properties of Mercer's kernels

In the context of SVMs in particular and kernel methods in general, one can use any kernel function $K(\cdot, \cdot)$ that fulfills Mercer's condition, which can be stated formally in the following theorem:

Theorem 1. Mercer's kernel. *Let \mathcal{X} be any input space and $K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a symmetric function, K is a Mercer's kernel if and only if the kernel matrix formed by restricting K to any finite subset of \mathcal{X} is positive semi-definite, i.e. having no negative eigenvalues.*

The Mercer condition constitutes the key requirement to obtain a unique global solution when developing kernel-based classifiers (e.g. SVMs) since they reduce to solving a convex optimization problem (Cristianini and Shawe-Taylor, 2000). In addition, important properties for Mercer's kernels can be derived from the fact that they are positive-definite (affinity) matrices, as follows:

Property 1. *Be K_1 and K_2 valid Mercer's kernels over $\mathcal{X} \times \mathcal{X}$, with $\mathbf{x}_i \in \mathcal{X} \subseteq \mathbb{R}^d$, with \mathbf{A} being a symmetric positive semi-definite $n \times n$ matrix, and $\alpha > 0$. Then, the following kernels:*

$$K(\mathbf{x}_i, \mathbf{x}_j) = K_1(\mathbf{x}_i, \mathbf{x}_j) + K_2(\mathbf{x}_i, \mathbf{x}_j) \quad (6.1.18)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \alpha K_1(\mathbf{x}_i, \mathbf{x}_j) \quad (6.1.19)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{A} \mathbf{x}_j \quad (6.1.20)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = K_1(\mathbf{x}_i, \mathbf{x}_j) K_2(\mathbf{x}_i, \mathbf{x}_j) \quad (6.1.21)$$

³Overfitting consists in perfectly fitting available data with a false model by increasing its complexity, i.e. its number of parameters, but reducing the ability of the model to generalize beyond the fitting data. Therefore, it will not be able to predict the correct output for other examples, thus it will not generalize to situations not presented during the training process.

are valid Mercer's kernels. \square

Therefore, one can design kernels by summing, weighting, or multiplying dedicated kernels. This intuitive idea is formally expressed in the following. It is worth noting that the size of the training kernel matrix is $n \times n$ and each position (i, j) of the kernel matrix \mathbf{K} contains the similarity between all possible pairs of training samples measured with a suitable kernel function K fulfilling Mercer's conditions. As shown before, some popular kernels are: linear, polynomial, or radial basis function. This (distance or similarity) matrix is precomputed at the very beginning of the minimization procedure, and thus, one usually works with the transformed input data, \mathbf{K} , rather than the original input space samples, \mathbf{x}_i . This fact allows us to easily combine positive definite kernel matrices taking advantage of the properties in Proposition 1, as will be shown in the next section.

Composite kernels for hyperspectral image classification

In (Camps-Valls et al., 2006d), we explicitly formulated a full family of kernel-based classifiers that combine different kernels in order to simultaneously take into account spectral, spatial, and local cross-information in a hyperspectral image. This framework was further extended in (Camps-Valls et al., 2008a) to multitemporal and multisource classification and change detection problems. Basically, we take advantage of two specially interesting properties of kernel methods: (i) their good performance when working with high input dimensional spaces (Camps-Valls et al., 2004a; Camps-Valls and Bruzzone, 2005), and (ii) the properties derived from Mercer's conditions by which a scaled summation of (positive definite) kernel matrices is a valid kernel, which have provided good results in other domains (Mak et al., 2004; Sun et al., 2004).

A full family of composite kernels for the combination of different information types is presented in this section. The following composite kernels are defined for two types of information only \mathcal{A} and \mathcal{B} . In any case, the formulations proposed in this section can be easily extended to any number of information types. For this purpose, three steps are followed:

1. *Pixel definition.* A pixel entity \mathbf{x}_i is defined simultaneously in both informative domains \mathcal{A} , $\mathbf{x}_i^{\mathcal{A}} \in \mathbb{R}^{d_{\mathcal{A}}}$, and \mathcal{B} , $\mathbf{x}_i^{\mathcal{B}} \in \mathbb{R}^{d_{\mathcal{B}}}$.
2. *Kernel computation.* Once that both input vectors $\mathbf{x}_i^{\mathcal{A}}$ and $\mathbf{x}_i^{\mathcal{B}}$ are constructed, different kernel matrices can be easily computed using any suitable kernel function that fulfills Mercer's conditions.
3. *Kernel combination.* At this point, we take advantage of the *direct sum* of Hilbert spaces by which two (or more) Hilbert spaces \mathcal{H}_k can be combined into a larger Hilbert space, $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \oplus \mathcal{H}_N$.

In the following, we present three different kernel approaches for hyperspectral image classification.

The stacked-features approach A good example of the applicability of composite kernels to remote sensing is the combination of spectral and contextual information of the pixels. The most commonly adopted approach in hyperspectral image classification is to exploit the spectral content of a pixel, defined as \mathbf{x}_i^A . However, performance can be improved by including also the textural information in the classifier, defined as \mathbf{x}_i^B . This is usually done by means of the ‘stacked’ approach, in which feature vectors are built from the concatenation of both types of features. Note that if the chosen mapping ϕ is a transformation of the concatenation $\mathbf{x}_i \equiv \{\mathbf{x}_i^A, \mathbf{x}_i^B\}$, then the corresponding ‘stacked’ kernel matrix is:

$$K_{\{\mathcal{A}, \mathcal{B}\}} \equiv K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle, \quad (6.1.22)$$

which does not include explicit cross relations between different information features \mathbf{x}_i^A and \mathbf{x}_j^B .

The direct summation kernel A simple composite kernel combining two types of information naturally comes from the concatenation of nonlinear transformations of \mathbf{x}_i^A and \mathbf{x}_i^B . Let us assume two nonlinear transformations $\varphi_1(\cdot)$ and $\varphi_2(\cdot)$ into Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , respectively. Then, the following transformation can be constructed:

$$\phi(\mathbf{x}_i) = \{\varphi_1(\mathbf{x}_i^A), \varphi_2(\mathbf{x}_i^B)\} \quad (6.1.23)$$

and the corresponding dot product can be easily computed as follows:

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j) &= \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle \\ &= \langle \{\varphi_1(\mathbf{x}_i^A), \varphi_2(\mathbf{x}_i^B)\}, \{\varphi_1(\mathbf{x}_j^A), \varphi_2(\mathbf{x}_j^B)\} \rangle \\ &= K_{\mathcal{A}}(\mathbf{x}_i^A, \mathbf{x}_j^A) + K_{\mathcal{B}}(\mathbf{x}_i^B, \mathbf{x}_j^B) \end{aligned} \quad (6.1.24)$$

Note that the solution is expressed as the sum of positive definite matrices, with $\dim(\mathbf{x}_i^A) = d_{\mathcal{A}}$, $\dim(\mathbf{x}_i^B) = d_{\mathcal{B}}$, and $\dim(\mathbf{K}) = \dim(\mathbf{K}_{\mathcal{A}}) = \dim(\mathbf{K}_{\mathcal{B}}) = n \times n$.

The weighted summation kernel By exploiting Property (2) in Proposition 1, a composite kernel that balances both information types in (6.1.24) can also be created, as follows:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \nu K_{\mathcal{A}}(\mathbf{x}_i^A, \mathbf{x}_j^A) + (1 - \nu) K_{\mathcal{B}}(\mathbf{x}_i^B, \mathbf{x}_j^B) \quad (6.1.25)$$

where ν is a positive real-valued free parameter ($0 < \nu < 1$), which is tuned in the training process and constitutes a trade-off between the spatial and spectral information to classify a given pixel. This composite kernel allows introducing *a priori* knowledge in the classifier or allows extracting some information from the best tuned ν parameter.

6.2 Semi-supervised Classification with the Laplacian SVM

In this section, we present a recently introduced semi-supervised framework that incorporates labeled and unlabeled data in any general-purpose learner (Belkin and Niyogi, 2004; Belkin et al.,

2006). We focus on a semi-supervised extension of the SVM, which introduces an additional regularization term on the geometry of both labeled and unlabeled samples by using the *graph Laplacian* (Chung, 1997), thus leading to the so-called Laplacian SVM (LapSVM) (Belkin et al., 2006). This methodology follows a *non-iterative optimization procedure*, in contrast to most transductive learning methods, and provides a closed-form classification function for testing on novel samples not used in the training phase (*out-of-sample predictions*), in contrast to graph-based approaches. In addition, the Laplacian SVM constitutes a general framework for SSL, in which supervised SVM and other methods can be regarded just as particular cases. Hard-margin SVM, directed graph methods, label propagation methods, and spectral clustering solutions (Shawe-Taylor and Cristianini, 2004; Chapelle et al., 2006) are obtained for particular free parameters of the LapSVM.

The use of the Laplacian SVM algorithm in the field of remote sensing was introduced for the first time in (Gómez-Chova et al., 2007b) for cloud screening of MERIS data, and was extended in (Gómez-Chova et al., 2008c) for a urban monitoring application combining multispectral and SAR data from LANDSAT/TM and ERS (Gómez-Chova et al., 2004b,c, 2006e) or from MERIS and ASAR (Gómez-Chova et al., 2005d). The reason for using LapSVM is that it permits using the labeled samples, and efficiently exploiting the information contained in the high number of available unlabeled pixels to characterize the *marginal distribution* of data. This is particularly interesting in practical remote-sensing applications since obtaining additional unlabeled samples is cheap and easy, while labeling is expensive, difficult, or even impossible.

6.2.1 Manifold Regularization Learning Framework

Regularization is necessary to produce smooth decision functions and thus avoiding overfitting to the training data. Since the work of Tikhonov (1963), many regularized algorithms have been proposed to control the capacity of the classifier (Evgeniou et al., 2000; Schölkopf and Smola, 2001). The regularization framework has been recently extended to the use of unlabeled samples (Belkin et al., 2006) as follows.

Notationally, we are given a set of ℓ labeled samples, $\{\mathbf{x}_i, y_i\}_{i=1}^{\ell}$, and a set of u unlabeled samples $\{\mathbf{x}_i\}_{i=\ell+1}^{\ell+u}$, where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, +1\}$. Let us now assume a general-purpose decision function f . The regularized functional to be minimized is defined as:

$$R_{\text{reg}}(f) = \frac{1}{\ell} \sum_{i=1}^{\ell} V(f(\mathbf{x}_i), y_i) + \gamma_L \|f\|_{\mathcal{H}}^2 + \gamma_M \|f\|_{\mathcal{M}}^2, \quad (6.2.1)$$

where V represents a generic cost function of the committed errors on the labeled samples, γ_L controls the complexity of f in the associated Hilbert space \mathcal{H} , and γ_M controls its complexity in the intrinsic geometry of the marginal data distribution $p(\mathbf{x})$. For example, if the probability distribution is supported on a low-dimensional manifold, $\|f\|_{\mathcal{M}}^2$ penalizes f along that manifold \mathcal{M} . Note that this functional constitutes a general regularization framework that takes into account all the available knowledge.

6.2.2 Laplacian Support Vector Machines

The previous semi-supervised learning framework allows us to develop many different algorithms just by playing around with the loss function, V , and the regularizers for the function f . In this work, we focus on the Laplacian SVM formulation, which basically uses SVM as the core learner and the graph Laplacian for manifold regularization. In the following, we review all the ingredients of the formulation.

Cost function of the errors

The Laplacian SVM uses the same hinge loss function as the traditional SVM:

$$V(f(\mathbf{x}_i), y_i) = \max\{0, 1 - y_i f(\mathbf{x}_i)\}, \quad (6.2.2)$$

where f represents the decision function implemented by the selected classifier and predicted labels are $y_* = \text{sgn}(f(\mathbf{x}_*))$.

Decision function

We use as the decision function $f(\mathbf{x}_*) = \langle \mathbf{w}, \phi(\mathbf{x}_*) \rangle + b$, where $\phi(\cdot)$ is a nonlinear mapping to a higher (possibly infinite) dimensional Hilbert space \mathcal{H} , and \mathbf{w} and b define a linear regression in that space. By means of the Representer Theorem (Schölkopf and Smola, 2001), weights \mathbf{w} can be expressed in the dual problem as the expansion over labeled and unlabeled samples $\mathbf{w} = \sum_{i=1}^{\ell+u} \alpha_i \phi(\mathbf{x}_i) = \Phi \alpha$, where $\Phi = [\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_{\ell+u})]^\top$ and $\alpha = [\alpha_1, \dots, \alpha_{\ell+u}]$. Then, the decision function is given by:

$$f(\mathbf{x}_*) = \sum_{i=1}^{\ell+u} \alpha_i K(\mathbf{x}_i, \mathbf{x}_*) + b, \quad (6.2.3)$$

and \mathbf{K} is the kernel matrix formed by kernel functions $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$. The key point here is that, without considering the mapping ϕ explicitly, a non-linear classifier can be constructed by selecting the proper kernel. Also, the regularization term can be fully expressed in terms of the kernel matrix and the expansion coefficients:

$$\|f\|_{\mathcal{H}}^2 = \|\mathbf{w}\|^2 = (\Phi \alpha)^\top (\Phi \alpha) = \alpha^\top \mathbf{K} \alpha. \quad (6.2.4)$$

Manifold regularization

The geometry of the data is typically modeled with a graph whose nodes represent both labeled and unlabeled samples connected by weights W_{ij} (Jordan, 1999; Chapelle et al., 2006). Regularizing the graph follows from the smoothness (or manifold) assumption and intuitively is

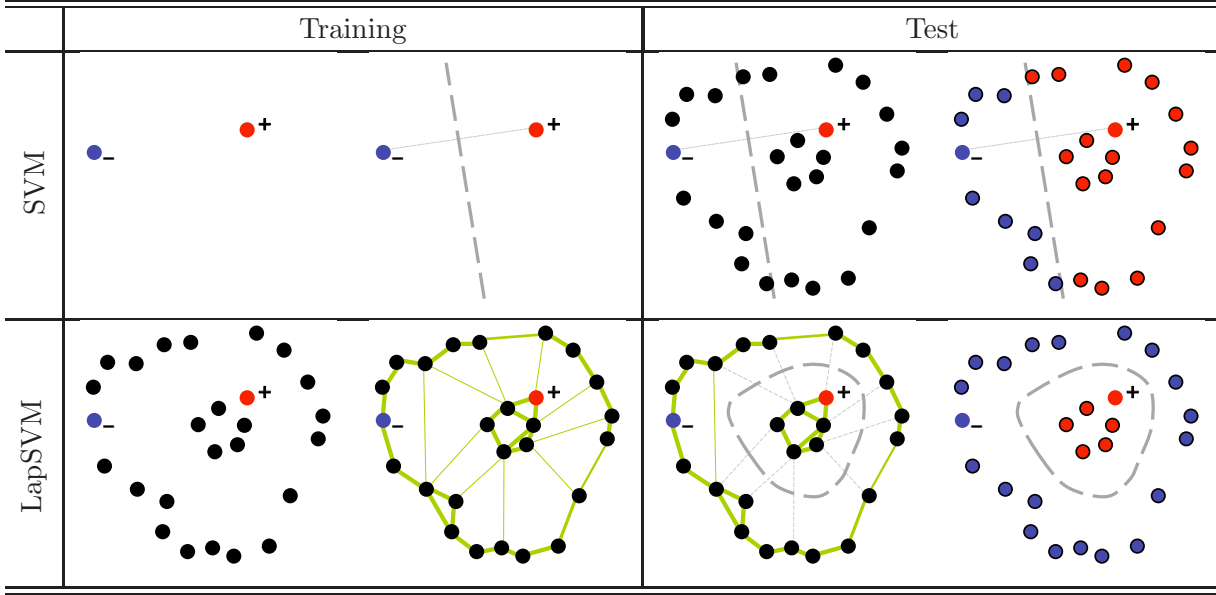


Figure 6.3: Illustrative example of the use of the graph Laplacian for manifold regularization. Upper part of the figure shows the learning and classification process using only the two labeled samples (signed balls). Bottom part of the figure shows how LapSVM efficiently exploits the information contained in the available unlabeled samples (unsigned balls) to characterize the *marginal distribution* of data by means of a graph.

equivalent to penalize the “rapid changes” of the classification function evaluated between close samples in the graph (Fig. 6.3):

$$\|f\|_{\mathcal{M}}^2 = \frac{1}{(\ell + u)^2} \sum_{i,j=1}^{\ell+u} W_{ij} (f(\mathbf{x}_i) - f(\mathbf{x}_j))^2 = \frac{1}{(\ell + u)^2} \mathbf{f}^\top \mathbf{L} \mathbf{f}, \quad (6.2.5)$$

where $\mathbf{L} = \mathbf{D} - \mathbf{W}$ is the graph Laplacian; \mathbf{D} is the diagonal degree matrix of \mathbf{W} given by $D_{ii} = \sum_{j=1}^{\ell+u} W_{ij}$ and $D_{ij} = 0$ for $i \neq j$; the normalizing coefficient $\frac{1}{(\ell+u)^2}$ is the natural scale factor for the empirical estimate of the Laplace operator (Belkin et al., 2006); and $\mathbf{f} = [f(\mathbf{x}_1), \dots, f(\mathbf{x}_{\ell+u})]^\top = \mathbf{K}\boldsymbol{\alpha}$, where we have deliberately dropped the bias term b .

Formulation

By plugging (6.2.2), (6.2.4), and (6.2.5) into (6.2.1), we obtain the regularized function to be minimized:

$$\min_{\substack{\boldsymbol{\xi} \in \mathbb{R}^\ell \\ \boldsymbol{\alpha} \in \mathbb{R}^{\ell+u}}} \left\{ \frac{1}{\ell} \sum_{i=1}^{\ell} \xi_i + \gamma_L \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha} + \frac{\gamma_M}{(\ell + u)^2} \boldsymbol{\alpha}^\top \mathbf{K}^\top \mathbf{L} \mathbf{K} \boldsymbol{\alpha} \right\} \quad (6.2.6)$$

subject to:

$$y_i \left(\sum_{j=1}^{\ell+u} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + b \right) \geq 1 - \xi_i, \quad i = 1, \dots, \ell \quad (6.2.7)$$

$$\xi_i \geq 0 \quad i = 1, \dots, \ell \quad (6.2.8)$$

where ξ_i are slack variables to deal with committed errors in the labeled samples. Introducing restrictions (6.2.7)-(6.2.8) into the primal functional (6.2.6) through Lagrange multipliers, β_i and η_i , and taking derivatives w.r.t. b and ξ_i , we obtain:

$$\min_{\alpha, \beta} \left\{ \frac{1}{2} \alpha^\top \left(2\gamma_L \mathbf{K} + \frac{2\gamma_M}{(\ell+u)^2} \mathbf{K}^\top \mathbf{L} \mathbf{K} \right) \alpha - \alpha^\top \mathbf{K} \mathbf{J}^\top \mathbf{Y} \beta + \sum_{i=1}^{\ell} \beta_i \right\}, \quad (6.2.9)$$

where $\mathbf{J} = [\mathbf{I} \ \mathbf{0}]$ is an $\ell \times (\ell + u)$ matrix with \mathbf{I} as the $\ell \times \ell$ identity matrix (the first ℓ points are labeled) and $\mathbf{Y} = \text{diag}(y_1, \dots, y_\ell)$. Taking derivatives again w.r.t. α , we obtain the solution (Belkin et al., 2006):

$$\alpha = \left(2\gamma_L \mathbf{I} + 2 \frac{\gamma_M}{(\ell+u)^2} \mathbf{L} \mathbf{K} \right)^{-1} \mathbf{J}^\top \mathbf{Y} \beta^* \quad (6.2.10)$$

Now, substituting again (6.2.10) into the dual functional (6.2.9), we obtain the following quadratic programming problem to be solved:

$$\beta^* = \max_{\beta} \left\{ \sum_{i=1}^{\ell} \beta_i - \frac{1}{2} \beta^\top \mathbf{Q} \beta \right\} \quad (6.2.11)$$

subject to $\sum_{i=1}^{\ell} \beta_i y_i = 0$ and $0 \leq \beta_i \leq \frac{1}{\ell}$, $i = 1, \dots, \ell$, where

$$\mathbf{Q} = \mathbf{Y} \mathbf{J} \mathbf{K} \left(2\gamma_L \mathbf{I} + 2 \frac{\gamma_M}{(\ell+u)^2} \mathbf{L} \mathbf{K} \right)^{-1} \mathbf{J}^\top \mathbf{Y} \quad (6.2.12)$$

Therefore, the basic steps for obtaining the weights α_i for the solution in (6.2.3) are: (i) build the weight matrix \mathbf{W} and compute the graph Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{W}$, (ii) compute the kernel matrix \mathbf{K} , (iii) fix regularization parameters γ_L and γ_M , and (iv) compute α using (6.2.10) after solving the problem (6.2.11).

Relation with other classifiers

The Laplacian SVM is intimately related to other unsupervised and semi-supervised classifiers. This is because the method incorporates both the concepts of kernels and graphs in the same classifier, thus having connections with transduction, clustering, graph-based and label propagation methods. The minimizing functional used in the standard TSVM considers a different regularization parameter for labeled and unlabeled samples, which is the case in the proposed framework. Also, LapSVM is directly connected with the soft-margin SVM ($\gamma_M = 0$), the hard

margin SVM ($\gamma_L \rightarrow 0, \gamma_M = 0$), the graph-based regularization method ($\gamma_L \rightarrow 0, \gamma_M > 0$), the label-propagation regularization method ($\gamma_L \rightarrow 0, \gamma_M \rightarrow 0, \gamma_M \gg \gamma_L$), and spectral clustering ($\gamma_M = 1$). In conclusion, by optimizing parameters γ_L and γ_M over a wide enough range, the LapSVM theoretically outperforms the aforementioned classifiers. See (Belkin et al., 2006) for deeper details and theoretical comparison.

6.2.3 Remarks on Laplacian SVM

This method brings together the ideas of spectral graph theory, manifold learning, and kernel-based algorithms in a coherent and natural way to incorporate geometric structure with a kernel-based regularization framework. The solution of the LapSVM constitutes a convex optimization problem and results in a natural out-of-sample extension from the labeled and unlabeled training samples to novel examples, thus solving the problems of previously proposed methods.

The potential of this classification method in remote sensing image classification increases when reduced labeled training sets are available. In particular, in cloud screening, it becomes very difficult to obtain a representative training set for all possible situations, motivating the introduction of a semi-supervised method exploiting the unlabeled data.

The main problem is related to the computational cost, since a huge matrix consisting of labeled and unlabeled samples must be inverted (see Eqs. 6.2.10 and 6.2.12). Note, however, that in this method it is not necessary to incorporate all unlabeled samples in the image so the computational load is easily scalable. However, smart sampling strategies developed to select the most informative unlabeled samples could yield improve performance. In this respect, a modified manifold regularization method for large-scale problems has been recently presented by Tsang and Kwok (2007).

Another problem when using the Laplacian SVM in cloud screening is that it assumes that considered problems hold a non-linear manifold. However, distribution of remote sensing data, and of clouds in particular, can differ to a great extent from a manifold, making the cluster assumption more suitable in these cases.

6.3 Semi-supervised Classification with Composite Mean Kernels

In previous sections, we introduced kernel-based classification methods and pointed out the advantages offered by SSL in EO applications. However, SSL approaches make some model assumptions to improve classification performance by using unlabeled data that do not necessarily hold in our problem. Consequently, when selecting or developing an SSL method, one has to verify that the imposed model assumptions meet the problem data structure.

In this section, we propose a semi-supervised kernel-based classification method that takes

into account the particularities and problems found in practical cloud screening of EO images. The main issues to be considered before presenting the method can be summarized as follows:

Data Structure. The main assumptions made about data structure in SSL are that data are organized into a number of groups or clusters according to a given distance measure in some representation space (*cluster assumption*) or that data hold a manifold forming a non-linear complex global structure (*manifold assumption*) (Bachmann et al., 2005, 2006). In the case of clouds, and most natural land covers, distribution of remote sensing data is smooth and spectra of pixels of the same land cover are similar, making the cluster assumption more suitable to model each class. This is why the proposed method assumes that data are organized into a number of groups or clusters according to a given distance measure in some representation space. If the correspondence between sample and cluster is known for some training samples, one can reinforce samples in the same cluster to belong to the same class by taking into account the similarity between clusters.

SSL Model. In general, SSL methods aim to retrieve information from unlabeled data by estimating its conditional distribution, and one can distinguish between *generative models* and *discriminative models* to accomplish that. In multispectral image processing, the assumption that the data distribution can be approximated as a mixture of normally distributed samples is commonly accepted (Shahshahani and Landgrebe, 1994; Jackson and Landgrebe, 2001). Hence, generative models, which estimate the conditional distribution by modeling the class-conditional distributions explicitly, may provide a good performance in cloud screening and perfectly fit the cluster assumption.

Basic Operations in the Kernel Space. One of the basic ideas when working with kernel methods is that the mapping $\phi(\mathbf{x})$ into the kernel-defined feature space \mathcal{H} needs not to be explicitly known. Although we do not have access to the representation of samples in this space, it is possible to perform some elementary calculations in the kernel space, such as computing means and distances.

Training Set Representativeness. In many remote sensing image classification problems, it is difficult to collect a sufficient number of statistically significant ground-truth samples to define a complete training set for developing robust supervised classifiers. In this setting, two main different conditions are usually considered: (1) few training samples are available for characterizing the image to be classified; and (2) no training samples are available for the test image to be classified. In the later case, one-class classifiers can be used (Muñoz-Marí et al., 2007, 2008). We instead adopt another strategy by which training data extracted from other images modeling similar problems can be exploited. In both situations, unlabeled samples of test image can be jointly used with the available training samples for increasing the reliability and accuracy of the classifier.

All these issues are addressed in this section. First, some recommendations about how to use

clustering methods to extract information from unlabeled samples of the test image are given. Then, the concept of mean kernel is introduced to compute cluster similarities and then it is extended under the framework of composite kernels (Camps-Valls et al., 2006d). Finally, the proposed solution is presented. It is based on the idea that clouds in the test image present features that form compact clusters, and unlabeled data coming from similar images can help to model these clusters and to improve classification performance at pixel level by reinforcing samples in the same cluster to belong to the same class. Consequently, the aim of the algorithm is to compute and combine both similarity between samples and similarity between clusters in the kernel space, while performing the classification at a sample or pixel level. The section closes with a comprehensive comparison of the benchmarked kernel-based methods with special emphasis on the *pros* and *cons* of the proposed method.

6.3.1 Image Clustering

It is worth noting that the distribution of remote sensing data over natural land covers is usually smooth and spectra of pixels of the same land cover are locally similar, making the cluster assumption more suitable in the general case. In this work, clusters of the analyzed image are found by applying a clustering algorithm, which provides for each sample \mathbf{x}_i a *crisp* or *soft* association, h_{ik} , with each cluster ω_k . In particular, we consider the input image as a mixture of normal distributions so the EM algorithm can be used to obtain the maximum likelihood estimation of the probability density function (pdf) of the Gaussian mixture. The EM algorithm estimates the mixture coefficient π_k , the mean $\boldsymbol{\mu}_k$, and the covariance matrix $\boldsymbol{\Sigma}_k$ for each component of the mixture. Then, the algorithm assigns each pixel to the cluster with the maximum *a posteriori* probability (MAP); and the cluster membership h_{ik} represents the estimates of the posterior probabilities; that is, membership or probability value between zero and one, with the requirement that the memberships of one sample to all the clusters sum to one $\sum_k h_{ik} = 1$. Hence, the optimal cluster label for each sample is found as $h_i = \underset{k}{\operatorname{argmax}} \{h_{ik}\}$, i.e. $h_i = k$ if the sample \mathbf{x}_i is assigned to the cluster ω_k .

The suitability of the Expectation-Maximization algorithm with finite Gaussian mixture models (GMM) for remotely sensed image classification has been extensively demonstrated in the literature (Shahshahani and Landgrebe, 1994; Jackson and Landgrebe, 2001) and its use in cloud screening problems was justified in Chapter 5. Applying unsupervised clustering methods over the whole image allows us to take advantage of the wealth of information and the high degree of spatial and spectral correlation in the image pixels.

6.3.2 Cluster Similarity and the Mean Map

Given a finite subset of training samples $S = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ laying in an input space \mathcal{X} and a kernel $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \boldsymbol{\phi}(\mathbf{x}_i), \boldsymbol{\phi}(\mathbf{x}_j) \rangle$, let $\boldsymbol{\Phi}(S) = \{\boldsymbol{\phi}(\mathbf{x}_1), \dots, \boldsymbol{\phi}(\mathbf{x}_n)\}$ be the image of S under

the map ϕ . Hence $\Phi(S)$ is a subset of the inner product space \mathcal{H} . Significant information about the embedded data set $\Phi(S)$ can be obtained by using only the inner product information contained in the kernel matrix \mathbf{K} of kernel evaluations between all pairs of elements of S : $\mathbf{K}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$, $i, j = 1, \dots, n$. In particular, the centre of mass of the set S in the kernel space is the vector:

$$\phi_\mu(S) = \frac{1}{n} \sum_{i=1}^n \phi(\mathbf{x}_i) \quad (6.3.1)$$

where $\phi_\mu(\cdot)$ denotes the *mean map*. The concept of the mean map has been recently extended and led to a full family of kernel methods known under the framework of *mean kernels*, which has mainly been used for the comparison of distributions in the kernel space (Gretton et al., 2007b,a).

We should stress that there is not an explicit vector representation of the centre of mass, since, in this case, there may also not exist a point in the input space \mathcal{X} whose image under ϕ is $\phi_\mu(S)$. In other words, we are now considering points that potentially lie outside $\phi(\mathcal{X})$, that is, the image of the input space \mathcal{X} under the mapping ϕ .

Let us now consider two finite subsets of samples $S_1 = \{\mathbf{a}_1, \dots, \mathbf{a}_m\}$ and $S_2 = \{\mathbf{b}_1, \dots, \mathbf{b}_n\}$ belonging to two different clusters ω_1 and ω_2 , respectively. We are interested in defining a *cluster similarity* function that estimates the proximity between them in a sufficiently rich feature space. A straightforward kernel function reflecting the similarity between clusters is obtained by evaluating the kernel function between the means of the clusters in the input space \mathcal{X} :

$$K_\mu^{\mathcal{X}}(S_1, S_2) \equiv \langle \phi(\boldsymbol{\mu}_1), \phi(\boldsymbol{\mu}_2) \rangle = K(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2), \quad (6.3.2)$$

but then we lose the advantage of working in the kernel space \mathcal{H} implicitly.

The centre of mass of the sets S_1 and S_2 in the kernel space are the vectors $\phi_\mu(S_1) = \frac{1}{m} \sum_{i=1}^m \phi(\mathbf{a}_i)$ and $\phi_\mu(S_2) = \frac{1}{n} \sum_{i=1}^n \phi(\mathbf{b}_i)$. Despite the apparent inaccessibility of the points $\phi_\mu(S_1)$ and $\phi_\mu(S_2)$ in the kernel space \mathcal{H} , we can compute the *cluster similarity* in \mathcal{H} using only evaluations of the *sample similarity* contained in the kernel matrix:

$$\begin{aligned} K_\mu^{\mathcal{H}}(S_1, S_2) &\equiv \langle \phi_\mu(S_1), \phi_\mu(S_2) \rangle \\ &= \left\langle \frac{1}{m} \sum_{i=1}^m \phi(\mathbf{a}_i), \frac{1}{n} \sum_{j=1}^n \phi(\mathbf{b}_j) \right\rangle \\ &= \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n K(\mathbf{a}_i, \mathbf{b}_j) \end{aligned} \quad (6.3.3)$$

Note how significant information about the cluster similarities can be obtained by using only the inner product information contained in the kernel matrix, $K_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$, of kernel evaluations

between all pairs of elements in S_1 and S_2 :

$$\mathbf{K} = \left[\begin{array}{ccc|ccc} K(\mathbf{a}_1, \mathbf{a}_1) & \cdots & K(\mathbf{a}_1, \mathbf{a}_m) & K(\mathbf{a}_1, \mathbf{b}_1) & \cdots & K(\mathbf{a}_1, \mathbf{b}_n) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{a}_m, \mathbf{a}_1) & \cdots & K(\mathbf{a}_m, \mathbf{a}_m) & K(\mathbf{a}_m, \mathbf{b}_1) & \cdots & K(\mathbf{a}_m, \mathbf{b}_n) \\ \hline K(\mathbf{b}_1, \mathbf{a}_1) & \cdots & K(\mathbf{b}_1, \mathbf{a}_m) & K(\mathbf{b}_1, \mathbf{b}_1) & \cdots & K(\mathbf{b}_1, \mathbf{b}_n) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{b}_n, \mathbf{a}_1) & \cdots & K(\mathbf{b}_n, \mathbf{a}_m) & K(\mathbf{b}_n, \mathbf{b}_1) & \cdots & K(\mathbf{b}_n, \mathbf{b}_n) \end{array} \right] \quad (6.3.4)$$

which is reduced to \mathbf{K}_μ by applying (6.3.3):

$$\mathbf{K}_\mu^{\mathcal{H}} = \left[\begin{array}{c|c} K_\mu^{\mathcal{H}}(S_1, S_1) & K_\mu^{\mathcal{H}}(S_1, S_2) \\ \hline K_\mu^{\mathcal{H}}(S_2, S_1) & K_\mu^{\mathcal{H}}(S_2, S_2) \end{array} \right] \quad (6.3.5)$$

6.3.3 Composite Pixel-Cluster Kernels

The concept of computing similarities between sets of vectors in the kernel space has been previously explored in several application fields. For example, in (Gärtner et al., 2002), a kernel on sets is proposed to solve multi-instance problems, where individuals are represented by structured sets; in (Kondor and Jebara, 2003), the Bhattacharyya's measure is computed in the Hilbert space between the Gaussians obtained after mapping the set of vectors into \mathcal{H} ; in (Jebara et al., 2004), kernel machines are combined with generative modeling using a kernel between distributions called Probability Product Kernel (PPK); in (Zhou and Chellappa, 2006), expressions for the most common probabilistic distance measures in the reproducing kernel Hilbert space are presented; and, in (Li et al., 2007), the PPK is used to develop a Support Cluster Machine for large-scale classification problems, where the labeled samples are clustered and the obtained labeled clusters are used to train the model instead of the training samples. However, all these works consider the sets of samples or distributions as a single entity with a given label and no information is provided for each individual sample. In our approach, classifying clusters is not the goal since we seek a detailed classification at a pixel level. This approach thus it falls into the field of *cluster kernels*, which are focused on changing the representation given to a classifier by taking into account the structure described by the unlabeled data (Szummer and Jaakkola, 2002; Zhu and Ghahramani, 2002; Chapelle et al., 2003; Weston et al., 2005). Let us remind that the bottleneck for any kernel method is the definition of a suitable kernel function that accurately reflects the similarity between samples. Hence, the proposed algorithm should compute and combine both similarity between samples and similarity between clusters in the kernel space.

Notationally, we are given a set of ℓ labeled samples, $\{\mathbf{x}_i, y_i\}_{i=1}^\ell$, and a set of u unlabeled samples $\{\mathbf{x}_i\}_{i=\ell+1}^{\ell+u}$, where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, +1\}$. In the proposed semi-supervised method, the u unlabeled training samples coming from the test image are used to describe the clusters and to compute the similarity between clusters, which is used to weight the similarity between the ℓ labeled training samples that define the classes. The similarity between clusters is included

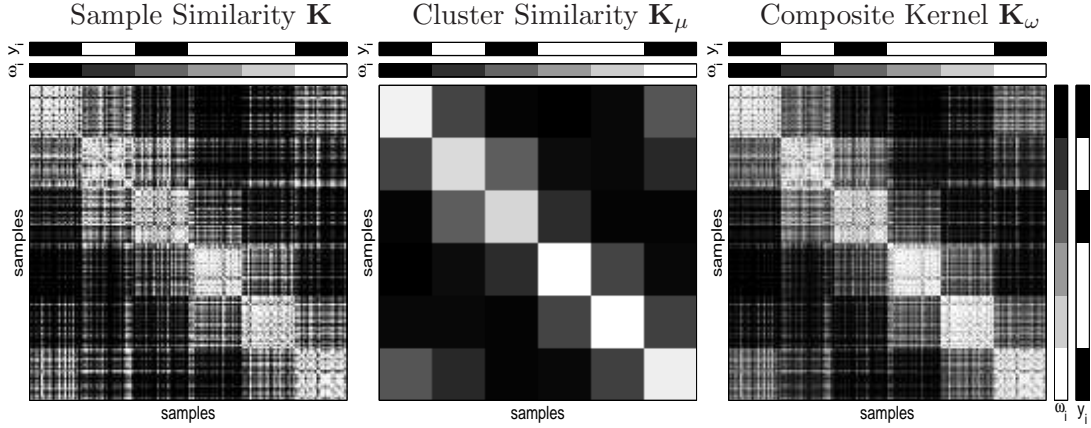


Figure 6.4: Illustrative example of the three involved kernel matrices: *sample similarity* accounted by the kernel of the training samples \mathbf{K} ; *cluster similarity* accounted by the mean map kernel of the clusters \mathbf{K}_μ ; and the *composite kernel* \mathbf{K}_ω obtained by combining the sample and the cluster similarities for each sample. Note that samples are sorted by class y_i and by cluster ω_i for a proper interpretation.

through the use of a composite kernel that balances both similarity distances

$$K_\omega(\mathbf{x}_i, \mathbf{x}_j) = \nu K(\mathbf{x}_i, \mathbf{x}_j) + (1 - \nu) K_\mu(S_{h_i}, S_{h_j}) \quad \forall i, j = 1, \dots, \ell \quad (6.3.6)$$

where ν is a positive real-valued free parameter ($0 \leq \nu \leq 1$), which is tuned in the training process and constitutes a trade-off between the sample and corresponding cluster information. It is worth noting that the size of the kernel matrix of all the training samples \mathbf{K} is $(\ell + u) \times (\ell + u)$, and not $\ell \times \ell$, because unlabeled samples allow us to compute the cluster similarities by summing elements of the kernel matrix. On the other hand, the size of the kernel matrix with the cluster similarities \mathbf{K}_μ is only $c \times c$. However, the size of the final kernel matrix \mathbf{K}_ω used to train the standard SVM (6.2.3) is $\ell \times \ell$ (the first ℓ samples are labeled). Summarizing, each position (i, j) of matrix \mathbf{K}_ω contains the similarity between all possible pairs of the ℓ labeled training samples (\mathbf{x}_i and \mathbf{x}_j) and their corresponding clusters (defined by h_i and h_j), which are measured with suitable kernel functions K and K_μ fulfilling Mercer's conditions.

Figure 6.4 shows an illustrative example of the three kernel matrices involved in the proposed method: *sample similarity* accounted by the kernel of the training samples \mathbf{K} ; *cluster similarity* accounted by the mean map kernel of the clusters \mathbf{K}_μ ; and the *composite kernel* \mathbf{K}_ω obtained by combining the sample and the cluster similarities for each sample. It is worth noting that the proposed composite kernel K_ω maintains the sample similarity at pixel level while making pixels in the same cluster more similar, thus reinforcing them to belong to the same class. It may be interpreted as a smoothing of K attending to the cluster structure in K_μ .

Even that cluster information could be also included in the classification process by stacking the input features of each pixel \mathbf{x}_i with the mean of its corresponding cluster $\boldsymbol{\mu}_{k=h_i}$. However, it has been shown in previous works that the use of composite kernels provides better results if

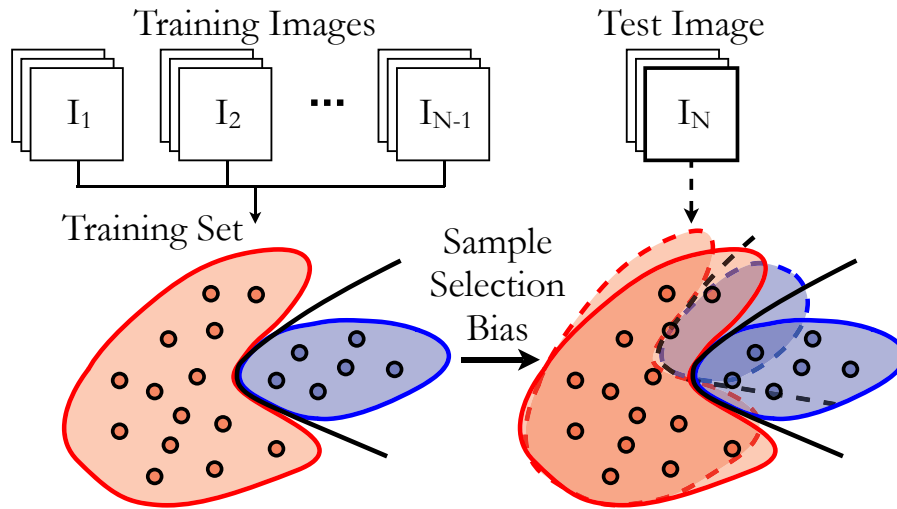


Figure 6.5: Illustrative example of the *sample selection bias* produced when the distributions on training and test sets might not match, which is a common situation in remote sensing image classification if no labeled training set is available for the test image.

different information entities are treated separately and combined in feature spaces (Mak et al., 2004; Camps-Valls et al., 2006d, 2008a).

6.3.4 Sample Selection Bias and the Soft Mean Map

SSL methods learn from both labeled and unlabeled samples constituting the training set to build a model that is used to classify the test set. So far we have assumed that training and test data are independently and identically distributed (i.i.d.) from the same pdf, but in reality the distributions on training and test sets might not match, which is known in the literature as the *sample selection bias* (Heckman, 1979; Huang et al., 2007; Bickel et al., 2007) or *covariate shift* (Shimodaira, 2000; Sugiyama and Müller, 2005; Sugiyama et al., 2007, 2008). Obviously, if the training and the test data have nothing in common there is no chance to learn anything. Thus, we assume that both follow a similar conditional distribution $p(y|x)$ and the input distributions $p(x)$ differ, yet not completely (see Fig. 6.5). In remote sensing, this is a likely situation since usually no training samples are available for the image to be classified and labeled data is extracted from other images modeling similar problems. In these situations, not all training samples are equally reliable. In the literature, the training samples are weighted in different ways in order to avoid the sample selection problem: by deriving the conditional density to maximize the log-likelihood function (Shimodaira, 2000); by changing the criterion to be maximized for learning, such as the nonparametric kernel mean matching method presented in (Huang et al., 2007) that tries to match the first momentum of training and test sets in the kernel space; or by modifying the model selection criteria (*importance weighted cross validation* estimate of risk) to obtain unbiased results (Sugiyama et al., 2007).

In the proposed method, the most reliable samples in terms of maximum likelihood in the input space are used to compute a kernel function that accurately reflects the similarity between clusters in the kernel space. Therefore, the relative reliability of training samples is trimmed by weighting the contribution of each sample \mathbf{x}_i to the definition of the centre of mass of each cluster in the kernel space \mathcal{H} with the EM estimated posterior probabilities h_{ik} , that is:

$$\phi_{\mu_s}(S_k) = \frac{\sum_i h_{ik} \phi(\mathbf{x}_i)}{\sum_i h_{ik}}, \quad (6.3.7)$$

which we call the *soft mean map*. The corresponding kernel can be easily computed as:

$$\begin{aligned} K_{\mu_s}^{\mathcal{H}}(S_k, S_l) &= \langle \phi_{\mu_s}(S_k), \phi_{\mu_s}(S_l) \rangle \\ &= \left\langle \frac{\sum_i h_{ik} \phi(\mathbf{x}_i)}{\sum_i h_{ik}}, \frac{\sum_j h_{jl} \phi(\mathbf{x}_j)}{\sum_j h_{jl}} \right\rangle \\ &= \frac{\sum_i \sum_j h_{ik} h_{jl} K(\mathbf{x}_i, \mathbf{x}_j)}{\sum_i h_{ik} \sum_j h_{jl}}, \end{aligned} \quad (6.3.8)$$

and now, when computing cluster similarities, all training samples contribute to all clusters but with different relative weights with a posteriori probability sense. The main advantage of the proposed method is that weights for the training samples are directly computed by taking advantage of the full statistical information of the test data distribution without modifying the classification problem to be solved, i.e. the same QP problem of the SVM is solved with the available standard optimization tools. We should stress that, with this approach, the EM algorithm is applied to the entire image in order to properly characterize the test data distribution and compute the sample weights, but the number of unlabeled samples used to describe the clusters in the soft mean map can be selected by the user to reduce the size of the kernel matrix and thus controlling the computational effort.

Note that the mean map kernel in (6.3.3) is a particular case of the proposed soft mean map kernel in (6.3.8) when the training samples are associated only with one cluster (*crisp* association), i.e. when $h_{ik} = 1$ if \mathbf{x}_i belongs to cluster ω_k and $h_{ik} = 0$ otherwise. In addition, the expression of the soft mean map kernel in (6.3.8) can be rewritten in matrix notation as follows:

$$\mathbf{K}_{\mu}^{\mathcal{H}} = \mathbf{D}\mathbf{H}^{\top}\mathbf{K}\mathbf{H}\mathbf{D} \quad (6.3.9)$$

where \mathbf{K} is the $(\ell + u) \times (\ell + u)$ kernel matrix of both labeled and unlabeled training samples; \mathbf{H} is a $(\ell + u) \times c$ matrix containing the membership value h_{ik} of each training sample to each cluster of the analyzed image; and \mathbf{D} is a $c \times c$ diagonal matrix with normalization factors for each cluster $D_{kk} = \sum_i h_{ik}$. Note that the computational effort is directly controlled by the number of unlabeled samples u included in \mathbf{K} to describe the clusters.

The size of the matrix containing the similarity between clusters \mathbf{K}_{μ} is $c \times c$. Thus, it has to be expanded to match the number of labeled samples, in order to obtain the final $\ell \times \ell$ kernel matrix \mathbf{K}_{ω} in (6.3.6) used to train the classifier:

$$\mathbf{K}_{\omega} = \nu \mathbf{J}\mathbf{K}\mathbf{J}^{\top} + (1 - \nu) \mathbf{W}\mathbf{K}_{\mu}\mathbf{W}^{\top} \quad (6.3.10)$$

Table 6.1: Particular cases of the proposed method depending on: 1) the sample-cluster similarity balance (free parameter ν), 2) in which space the cluster similarities are computed (input or kernel space), and 3) how the unlabeled training samples contribute to each cluster (crisp or soft association).

Method	Kernel	Mapping	Similarity	Eq.
SVM	K	$\phi(\mathbf{x})$	$\nu = 1$	(6.1.13)
μ -SVM in \mathcal{X}	$K_{\omega}^{\mathcal{X}} = \nu K + (1 - \nu)K_{\mu}^{\mathcal{X}}$	$\{\sqrt{\nu}\phi^{\top}(\mathbf{x}), \sqrt{1 - \nu}\phi^{\top}(\boldsymbol{\mu})\}^{\top}$	$0 < \nu < 1$	(6.3.6)
	$K_{\mu}^{\mathcal{X}}$	$\phi(\boldsymbol{\mu})$	$\nu = 0$	(6.3.2)
μ -SVM in \mathcal{H}	$K_{\omega}^{\mathcal{H}} = \nu K + (1 - \nu)K_{\mu}^{\mathcal{H}}$	$\{\sqrt{\nu}\phi^{\top}(\mathbf{x}), \sqrt{1 - \nu}\phi_{\mu}^{\top}(S)\}^{\top}$	$0 < \nu < 1$	(6.3.6)
	$K_{\mu}^{\mathcal{H}}$	$\phi_{\mu}(S)$	$\nu = 0$	(6.3.3)
μ_s -SVM in \mathcal{H}	$K_{\omega_s}^{\mathcal{H}} = \nu K + (1 - \nu)K_{\mu_s}^{\mathcal{H}}$	$\{\sqrt{\nu}\phi^{\top}(\mathbf{x}), \sqrt{1 - \nu}\phi_{\mu_s}^{\top}(S)\}^{\top}$	$0 < \nu < 1$	(6.3.6)
	$K_{\mu_s}^{\mathcal{H}}$	$\phi_{\mu_s}(S)$	$\nu = 0$	(6.3.8)

where $\mathbf{J} = [\mathbf{I} \ \mathbf{0}]$ is an $\ell \times (\ell + u)$ matrix with \mathbf{I} as the $\ell \times \ell$ identity matrix (the first ℓ samples are labeled); and \mathbf{W} is a $\ell \times c$ sparse matrix that stores the cluster of each labeled sample h_i , i.e. $W_{ik} = 1$ if sample \mathbf{x}_i belongs to cluster ω_k and $W_{ik} = 0$ otherwise.

6.3.5 Summary of Composite Mean Kernel Methods

The proposed method brings together the ideas of unsupervised clustering, mean map kernel, composite kernel, and SVM in a simple and natural way, improving classification performance by exploiting the information contained in the unlabeled samples. Essentially, the method tries to: 1) to reinforce both the local and global consistencies, and 2) to mitigate the sample selection bias problem. The method combines the expectation-maximization (EM) algorithm for fitting Gaussian mixture models (GMM) and the *mean map kernel*, which uses the most reliable samples in terms of maximum likelihood to compute a kernel function that accurately reflects the similarity between clusters in the kernel space. The final classification model is obtained by solving a standard SVM (a convex optimization problem) but the kernel of the labeled training samples (local consistency) is previously deformed to take into account the similarities between clusters (global consistency), which are easily computed from the unlabeled samples of the analyzed image.

Table 6.1 shows several particular cases of the proposed method depending on: 1) the balance between the sample similarity and the cluster similarity (free parameter ν), 2) in which space the cluster similarities are computed (input or kernel space), and 3) how the unlabeled training samples contribute to each cluster (crisp or soft association). In this table we indicate the kernel function used in the SVM, the mapping function whose dot product generates the corresponding composite kernel (cf. section 6.1.3), and the value of ν that constitutes a trade-off between the sample ($\nu = 1$) and the cluster information ($\nu = 0$).

6.3.6 Performance on Synthetic Data

Figure 6.6 shows an illustrative example of how the proposed method efficiently exploits the information contained in the available unlabeled samples to characterize the *marginal distribution* of data by means of the cluster structure. In order to demonstrate the robustness of the method in the sample selection bias problem, we used a two-dimensional non-linear classification problem where training and test data are generated by two slightly different mixture models composed of six Gaussian components (Fig. 6.6[*top*]). Three different models are obtained in order to illustrate the trade-off between the sample ($\nu = 1$) and the cluster information ($\nu = 0$) provided by the proposed method (Fig. 6.6[*bottom*]). In particular, we have depicted results of the pixel-based approach ($\nu = 1$) equivalent to a standard SVM trained with K (*left*); the cluster-based approach ($\nu = 0$) of the μ_s -SVM trained with $K_{\mu_s}^{\mathcal{H}}$ (*center*); and the composite pixel-cluster approach ($0 < \nu < 1$) of the μ_s -SVM trained with $K_{\omega_s}^{\mathcal{H}}$ (*right*).

Selected models are compared with the classification boundary of the maximum likelihood classifier (MLC) built with the true mixture models (upper-bound of the classification performance) of both the training distribution and the test distribution, respectively. In the three plots at the bottom part of the figure, we can observe from the sample-similarity based approach to the cluster-similarity based approach, how the classification boundary changes. On the one hand, Fig. 6.6(d) corresponds to the standard SVM looking for a maximum margin classifier of the training samples. In this case, the classification boundary matches the MLC boundary of the training set (*gold line*). On the other hand, Fig. 6.6(e) corresponds to the cluster-based approach that trains a SVM using as kernel matrix the cluster similarity $K_{\mu_s}^{\mathcal{H}}$ of the associated clusters. In this case, classification boundary is dominated by the cluster distribution of the unlabeled samples from the test set, and thus it matches the MLC boundary of the test set (*blue line*). It is worth noting that in the case where both sample and cluster similarities are combined (Fig. 6.6(f)) we obtain an intermediate solution, that is: 1) in regions densely populated by labeled training samples, the μ_s -SVM follows the optimal MLC boundary of the training data (middle-left part of the plot); and 2) in regions without labeled training samples forcing the output class, μ_s -SVM follows the optimal MLC boundary of the test data (bottom-right corner of the plot). The value of ν can be tuned by the user in the training process or selected through cross-validation in the training set, as is commonly done with the other free parameters of SVMs, such as C and σ . We should note, however, that the model selection in semi-supervised methods applied to problems affected by sample selection bias is not well-solved since, if the training and test distributions are significantly different, selected model will be biased towards the training samples when performing cross-validation in the training set.

To provide an exhaustive analysis of the proposed method's performance, the experiment described in Fig. 6.6 was repeated for a series of realizations varying the following parameters:

- *Data Generation*: the width σ of the Gaussian components used in the mixture model to generate the training and test data. Different σ correspond to different levels of data overlap

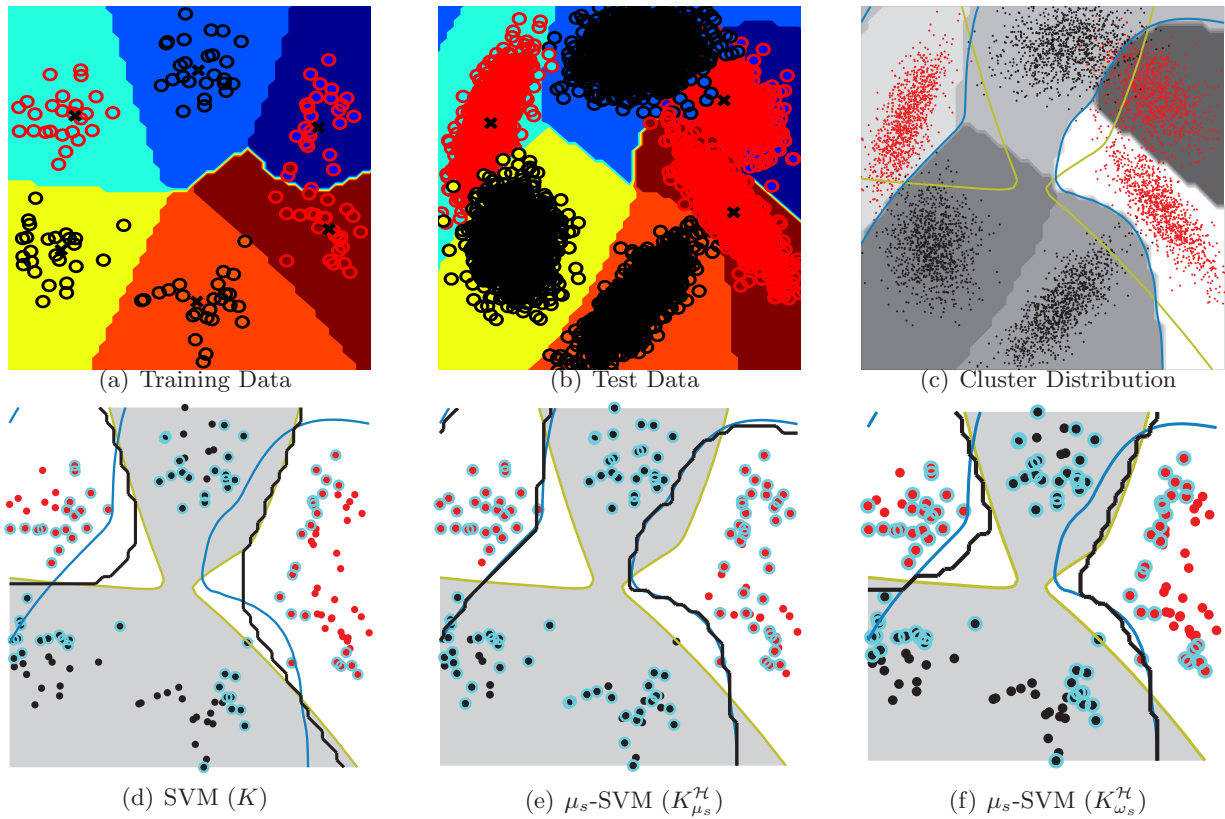


Figure 6.6: Illustrative example of the use of composite mean kernel in a two-dimensional two-classes problem where training and test data are generated by two slightly different mixture models composed of six Gaussian components. Upper part of the figure (*left* and *center*) shows the samples (circles) and the distribution (colored areas) of each Gaussian component of the the training (6×25 samples) and test (6×1000 samples) sets, respectively. Upper-right plot shows test samples with the true class labels (*red* and *black points*) and the distribution (*shaded areas*) of the found clusters by the EM algorithm. Bottom part of the figure shows the classification results of the proposed composite kernel using the soft mean map for three different situations: pixel-based approach ($\nu = 1$) equivalent to a standard SVM trained with K (*left*); cluster-based approach ($\nu = 0$) of the μ_s -SVM trained with $K_{\mu_s}^{\mathcal{H}}$ (*center*); and composite pixel-cluster approach ($0 < \nu < 1$) of the μ_s -SVM trained with $K_{\omega_s}^{\mathcal{H}}$ (*right*). In these plots, *red* and *black points* represent the training samples; *blue circles* indicate the samples used as support vectors in each model; *golden line* and *shaded areas* indicate the classification boundary of the maximum likelihood classifier (MLC) built with the true mixture model of the training data (upper-bound of the classification performance); *blue line* indicates the classification boundary of the MLC built with the true mixture model of the test data; and *black line* shows the classification boundary of the trained models.

that determine the classification complexity. In particular, using the true pdf that generated the test data with $\sigma = \{0.2, 0.275, 0.35, 0.425, 0.5\}$, the maximum likelihood classifier results in a kappa statistic $\kappa = \{0.97, 0.90, 0.81, 0.71, 0.63\}$, respectively. Fig. 6.7(a) shows the κ obtained when classifying test data with the MLC using the true pdf of the test data (*dashed line*), which provides an upper-bound of the classification performance, and using the true pdf of the training data (*dotted line*), which informs us about the difference between the mixture models used to generate training and test data (sample selection bias problem).

- *Supervised Information*: the number of labeled samples ℓ used to train the models. By decreasing the number of labeled training samples ℓ , one can analyze how the SSL method efficiently exploits the information contained in the available unlabeled samples. In the experiments, the number of unlabeled samples is fixed to $u = 300$ and we explore from ill-posed situations with only 3 labeled samples per class ($\ell = 6$) up to almost supervised cases with 300 labeled samples per class ($\ell = 600$).
- *Unsupervised Clustering*: the number of clusters c , i.e. the number of Gaussian components fixed in the EM algorithm. The proposed method requires as input the clusters presents in the test data, which are obtained from the unlabeled data using the EM algorithm. Therefore, the proposed method relies on the clustering performance and assumes that clusters present in the test data are correctly identified. In order to analyze the robustness of the method to inaccurate clustering results, the number of Gaussian components in the EM algorithm is set to $c = \{2, 4, 6, 8, 10\}$ instead of the actual six components of the mixture model that generated the data.

As mentioned above, for the experiments, we generated training sets consisting of $\ell = 600$ labeled samples (300 samples *per class*), and added $u = 300$ unlabeled (randomly selected) samples from the analyzed test data to the training set for the SSL methods. We focus on the ill-posed scenario and vary the rate of labeled samples, i.e. $\{1, 2, 4, 8, 14, 27, 52, 100\}\%$ of the labeled samples of the training set were used to train the models in each experiment. In order to avoid skewed conclusions, for each combination of parameters σ , ℓ , and c , the experiments were run for ten realizations where the used training samples were randomly selected. All classifiers are compared using the estimated kappa statistic κ as a measure of robustness in the classification of 6000 independent validation samples. Free parameter ν was varied in steps of 0.1 in the range $[0.01, 0.99]$, and the Gaussian width for the RBF kernel was tuned in the range $\sigma_{\text{RBF}} = \{10^{-3}, \dots, 10\}$. The selection of the best subset of free parameters was done by cross-validation.

Fig. 6.7 shows the validation results for the analyzed SVM-based classifiers when the number of clusters in the EM is fixed to the $c = 6$ actual clusters and only class overlap σ and labeled training samples ℓ are varied. Fig. 6.7(b) and 6.7(c) show the κ surface as a function of σ and ℓ for the proposed μ_s -SVM method when using as kernel $K_{\mu_s}^{\mathcal{H}}$ ($\nu = 0$) and $K_{\omega_s}^{\mathcal{H}}$ ($0 < \nu < 1$), respectively. These plots illustrate how the most separated are the classes (low σ) and supervised information is available (high ℓ), the most accurate is the classification for all methods. Fig. 6.7[*bottom*] shows

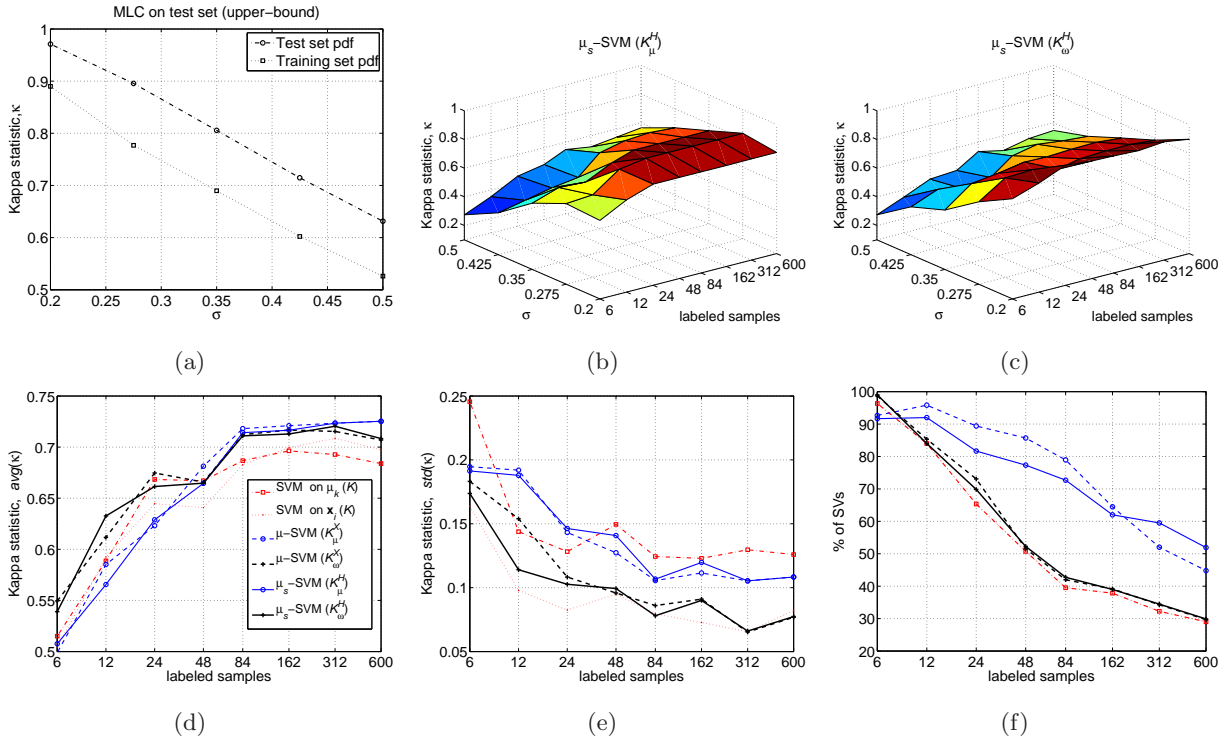


Figure 6.7: Validation results for the analyzed SVM-based classifiers when the number of clusters in the EM is fixed to the actual clusters ($c = 6$) and only class overlap σ and labeled training samples ℓ are varied. *Top, from left to right:* MLC kappa statistic (κ) for different levels of data overlap σ using the test and the training pdfs, and κ surface as a function of σ and number of labeled samples ℓ for the proposed μ_s -SVM method when using as kernel $K_\mu^{\mathcal{H}}$ ($\nu = 0$) and $K_w^{\mathcal{H}}$ ($0 < \nu < 1$). *Bottom, from left to right:* results averaged over σ for all the analyzed methods: $avg(\kappa)$, $std(\kappa)$, and the percentage of training samples used as support vectors SVs[%].

the results for all the analyzed methods averaged over σ : $avg(\kappa)$, $std(\kappa)$, and the percentage of training samples used as support vectors (SVs) in the selected models. Note that, in addition to the standard SVM and the variations of the proposed method, we have include classification results obtained when using the trained standard SVM (K) to classify the centers of the clusters (μ_k) and then assigning the same class label to all the samples belonging to the same cluster ω_k . Several conclusions can be obtained from these plots. First (Fig. 6.7(d)), composite mean kernels classifiers (black '+' lines), which combine both sample and cluster similarities, produce better classification results than SVM (red dotted line) in all cases for both the $K_w^{\mathcal{X}}$ and $K_w^{\mathcal{H}}$ kernels (note that SVM is a particular case of the μ -SVM for $\nu = 1$). The cluster-based approaches $K_\mu^{\mathcal{X}}$ and $K_\mu^{\mathcal{H}}$ (blue 'o' lines) provide accurate classifications when there are enough labeled samples to describe the class conditional distribution of the clusters (otherwise a whole cluster can be misclassified). In addition, cluster-based approaches are not equivalent to a simple classification of the centers of the clusters (red dash-dotted line). Regarding the standard deviation of kappa $std(\kappa)$ (Fig. 6.7(e)), the SVM provide the most stable results, but composite mean kernels provide

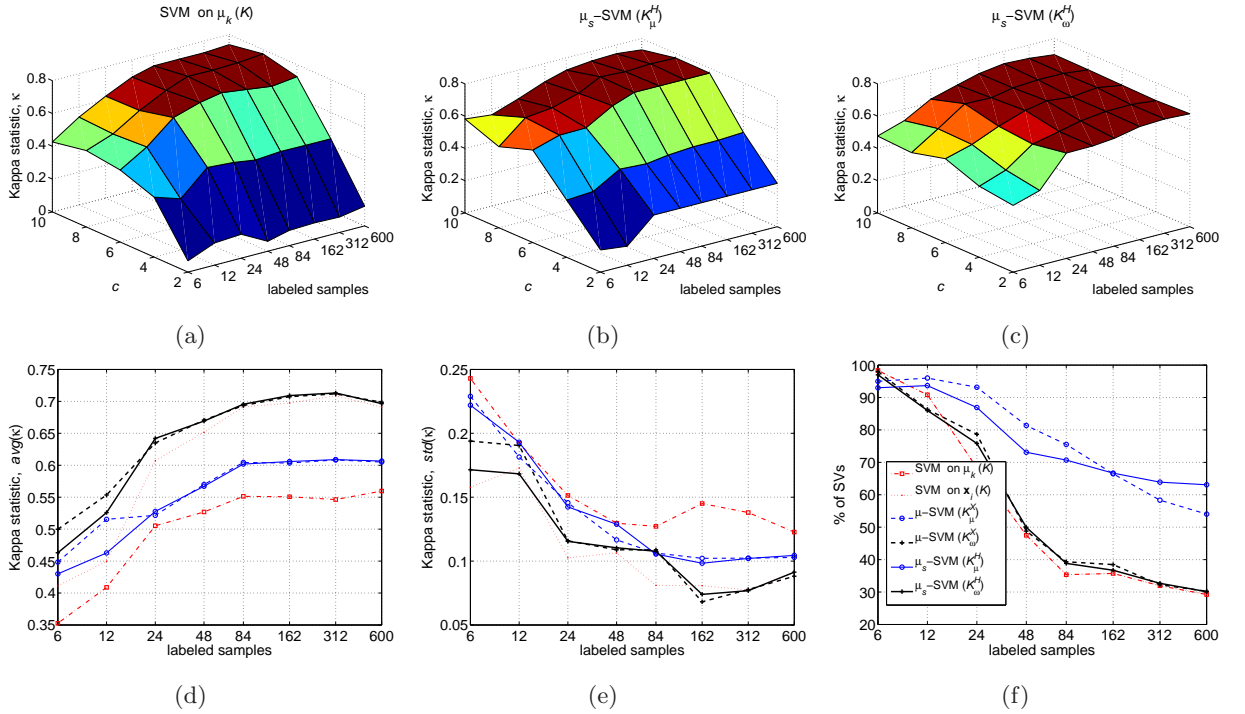


Figure 6.8: Validation results when the class overlap is fixed to $\sigma = 0.35$ (MLC accuracy of $\kappa = 0.81$) and the number of clusters in the EM c and labeled training samples ℓ are varied. *Top, from left to right:* the kappa (κ) surface as a function of the number of clusters c and number of labeled samples ℓ for the result of classifying cluster centers μ_k with the standard SVM, the cluster-based μ_s -SVM using as kernel $K_{\mu_s}^{\mathcal{H}}$ ($\nu = 0$), and the composite kernel μ_s -SVM using as kernel $K_{\omega_s}^{\mathcal{H}}$ ($0 < \nu < 1$). *Bottom, from left to right:* results averaged over c for all the analyzed methods: $avg(\kappa)$, $std(\kappa)$, and the percentage of training samples used as support vectors SVs[%].

similar results that the SVM and significantly better than the cluster-based methods. Finally, a similar behavior can be observed with the number of SVs (Fig. 6.7(f)), SVM and composite mean kernels produce sparse models with low number of support vectors (note that both red lines are overlapped since the resulting SVM model is the same), while the cluster-based methods require more SVs to correctly weight the cluster similarities.

In the previous results, we have used in the EM algorithm the actual number of Gaussian components that generated the data. Hence, with enough unlabeled samples and a proper initialization, we can assume that the clustering algorithm is modeling the class conditional distribution almost perfectly. However, this is not usually the case and we can obtain misleading clustering results. To analyze the robustness of the methods to the clustering accuracy, Fig. 6.8 shows the validation results when the class overlap is fixed to $\sigma = 0.35$ (MLC accuracy of $\kappa = 0.81$) and the number of clusters in the EM c and labeled training samples ℓ are varied. Fig. 6.8[*top*] shows the κ surface as a function of c and ℓ for the result of classifying cluster centers with the standard SVM, the cluster-based μ_s -SVM using as kernel $K_{\mu_s}^{\mathcal{H}}$ ($\nu = 0$), and the composite kernel μ_s -SVM

using as kernel $K_{\omega_s}^{\mathcal{H}}$ ($0 < \nu < 1$), from left to right, respectively. In these plots, contrarily to Fig. 6.7, one can observe clear differences between the exclusively cluster-based approaches and the proposed composite mean kernel. When the number of found clusters goes under the actual number of clusters in the data, it is possible to merge clusters corresponding to different classes in one cluster, and thus, in cluster-based approaches, one entire cluster is misclassified. However, composite mean kernel provides an excellent trade-off between the sample and the cluster information and, even when samples of different classes are merged in the same estimated cluster, the labeled samples of the training set allow the proposed method to define the classification boundary correctly. Fig. 6.8[*bottom*] shows the results for all the analyzed methods averaged over c . The obtained $avg(\kappa)$ validate the fact that composite kernels provide the best results together with the standard SVM, and that they are robust to inaccuracies in the data clustering, which produces the worsening the classification performance of cluster-based methods. Regarding the $std(\kappa)$ and the number of SVs, the same conclusions than in Fig. 6.7 can be extracted. Summarizing, results confirm that the proposed SSL method efficiently exploits the information contained in the available unlabeled samples to improve classification accuracy of supervised methods by means of reinforcing samples in the same cluster to belong to the same class. The algorithm requires to estimate the clusters present in the test data, but it has demonstrated to be robust to errors in the data clustering. In addition, it retains the good SVM properties of stability and sparsity.

6.4 Remarks on Semi-supervised Cloud Classification

Two different strategies have been proposed in Chapter 5 and Chapter 6 in order to classify image pixels as cloud-free and cloud-contaminated pixels:

- In previous chapter, an unsupervised approach has been proposed. The method relies on using representative features along with the spectral bands to perform a clustering of the analyzed image, and then to label the found clusters instead of directly finding the class of each single pixel. For regional and case studies, the cluster information can be analyzed directly by the user for the given image. This approach is intended for being used by an operator to improve cloud screening on particular cases. For example, this user-driven approach can help significantly to identify clusters corresponding to extremely thin clouds or ice/snow covers misclassified by the automatic labeling.
- In this chapter, a semi-supervised approach has been proposed. In this case, some supervised information is available and it is used together with the unlabeled samples of the analyzed image to develop a classifier that provides the class of each pixel but taking also into account the image data distribution. Therefore, this method can be applied automatically to a large number of scenes in an operational mode.

Both cloud classification approaches perfectly fit in the cloud screening scheme proposed in Fig. 3.1. After the cloud labeling, the following processing step of the method consisted of ob-

taining the final abundance fraction of clouds for all image pixels. In the unsupervised approach, the improved cloud product map was obtained combining the *Cloud Abundance*, a_{iC} , and the *Cloud Probability*, h_{iC} , by means of a pixel-by-pixel multiplication, $\vartheta_i = a_{iC}h_{iC}$. The procedure followed in section 5.3 to obtain the cloud final product is still valid for the semi-supervised approach. The main difference now is that, instead of obtaining h_{iC} from the posterior probabilities of the cloud-clusters for each sample provided by the EM algorithm, we define h_{iC} as the hard classification label \hat{y}_i provided for each sample by the semi-supervised cloud classifier. That is, $h_{iC} = 1$ if the sample \mathbf{x}_i is classified as cloud-contaminated (C) and $h_{iC} = 0$ if is cloud-free. It is worth noting that now h_{iC} is a binary label instead of a continuous probability value, but it indicates more accurately the presence of cloud. In addition, the posterior probabilities also decreased drastically from one to zero in the boundaries between clusters. Therefore, both the cloud probability and the cloud classification label indicate if one pixel is cloudy, C , or cloud-free, \bar{C} , but none of them give information about the cloud content at subpixel level. In the cloud final product, $\vartheta_i = a_{iC}h_{iC}$, h_{iC} indicates the cloudy pixels and a_{iC} indicates their cloud abundance.

Part III

Experimental Results

Chapter 7

Unsupervised Cloud Screening Validation

The third part of the work deals with the validation of the proposed methodology and cloud products. A wide database of images has been included in the study in order to take into account the different peculiarities of the problem: geographic location, date and season, type of cloud, and type of surface. The selected images allow us to validate method's performance since they include different landscapes, vegetation, bare soils, and two critical cases given the especial characteristics of the induced problems: ice and snow covers.

The validation of cloud screening algorithms is not an easy task because, in the unsupervised case (i.e. with no labeled data), there are no simultaneous independent measurements with the same spatial resolution. In most cases, the performance of cloud detection algorithms has been evaluated against visual analysis of the original satellite images. The human eye is able to recognize cloud structures in a satellite image much better than any automatic algorithm does, which justifies this validation approach. However, human cloud recognition may miss the difficult cases (thin clouds, broken cloudiness) and is far from being operational. In addition, visual comparison requires a large amount of tedious work, which is unsuited for a quantitative validation on a large dataset. For these reasons, a significant effort has been done in order to validate results by using different techniques:

- The simplest approach consists in comparing the final cloud mask and abundance with a false color composite of the images. Therefore, the resulting products are validated by visual inspection on CHRIS and MERIS data in section 7.1 and section 7.2, respectively. Following this validation approach, we are simultaneously testing the generalization ability of the proposed cloud screening algorithm, because a general methodology for cloud detection should be valid for different sensors working in the VNIR range. In particular, in Gómez-Chova et al. (2005b,a), performance of the proposed approach is tested on images from the CHRIS instrument, which presents completely different characteristics than

MERIS, tested in Gómez-Chova et al. (2005c, 2006d, 2007a).

- In the case of MERIS, we can also compare results with the official MERIS Level 2 Cloud Flag. In section 7.3, a representative set of MERIS images is processed and compared to the Level 2 products (used for validation purposes only) by comparing its cloud flag product to the cloud mask produced by the presented method. Preliminary test of this approach were carried out in previous works (Gómez-Chova et al., 2005c, 2006d, 2007a) by testing critical situations in cloud detection (e.g. ice/snow covers). Results were encouraging since the proposed algorithm classifies difficult cloud pixels more accurately; especially thin cirrus clouds and clouds over ice/snow.
- The lack of a real *ground truth*, and the low accuracy shown by the official MERIS Level 2 Cloud Flag in some situations prevent the validation of the cloud screening in fair conditions. Therefore, new validation approaches are required in order to test the proposed cloud screening algorithm. In section 7.4, the performance of the cloud screening is tested with a multitemporal validation approach proposed in Gómez-Chova et al. (2006f). In particular, pairs of cloud-free and cloud-covered images over the same area are used to detect cloud-pixels by identifying pixels with spectral changes between both dates. The spectral change is detected by using the spectral angle distance (SAD) as it is invariant to multiplicative scaling (being less affected by atmospheric and illumination changes). Image pairs are selected to be close in time, so spectral changes due to temporal evolution of the surface are avoided. However, images taken from orbits within three or six days present a significant variation in the viewing geometry. Therefore, pixels with significant changes in composition ($> 10\%$) due to the different observation angle are not considered in the multi-temporal cloud screening validation.

In the following sections, we present results of the unsupervised cloud screening scheme proposed in Chapter 5. The results were obtained for all images and scenarios as follows. The number of clusters found by the EM clustering was automatically determined as the maximum of suggested numbers by the DB and MDL indices (cf. section 5.2.1). However, we did not observe a critical dependence of the results on the number of clusters; note that even if a low number of clusters is selected, some of them should correspond to different cloud types, since the (overgrown) ROI is typically well-identified. Clusters were labeled into geo-physical classes by an operator considering the extracted features (cf. section 5.2.2). The number of endmembers was equal to the number of cloud-free clusters (cf. section 5.3.1). Finally, cloud screening results are presented in terms of the *cloud probability* h_{iC} in (5.2.8), the *cloud abundance* a_{iC} in (5.3.4), and the hard classification between clouds and ground was obtained applying a threshold of 0.05 to the *cloud final product* ϑ in (5.3.5) (cf. section 5.3.3).

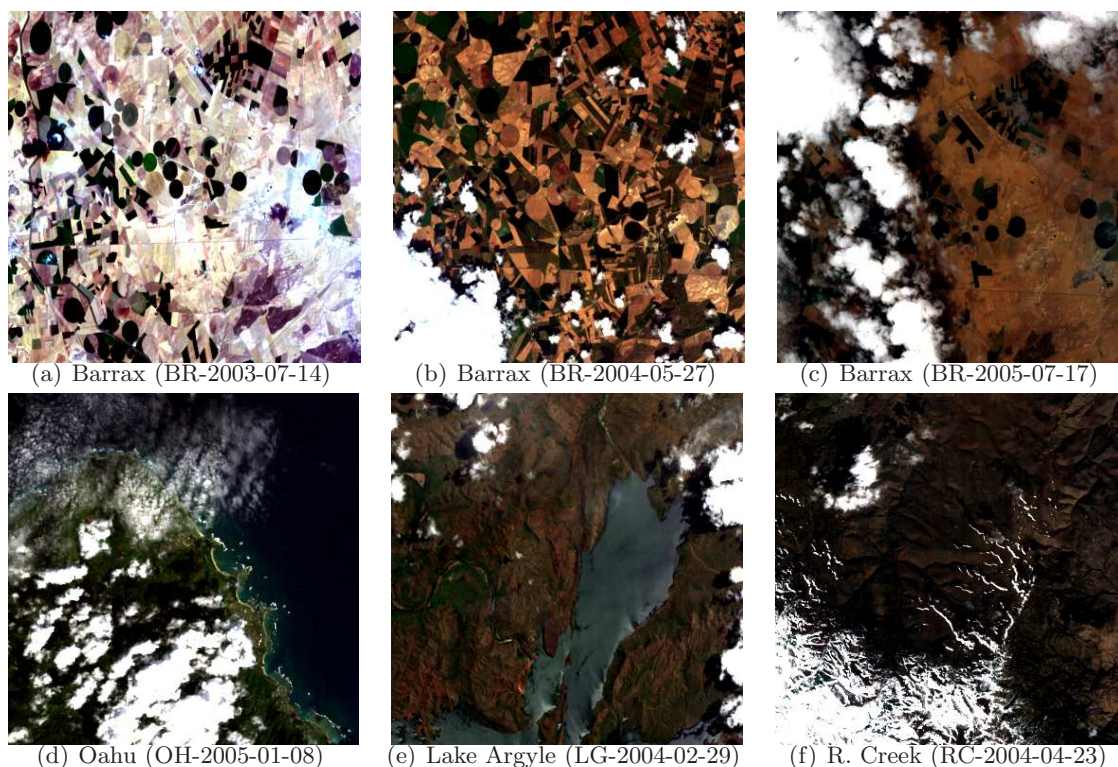


Figure 7.1: RGB composite of the CHRIS images (Mode 1, FZA 0°) over different test sites.

7.1 Visual Inspection of PROBA/CHRIS Images

7.1.1 CHRIS Sample Products

A dataset consisting of six CHRIS Mode 1 acquisitions (five multi-angular images per acquisition) over four of the core sites of the PROBA mission is considered. In particular, images taken over Barrax (BR, Spain), Oahu (OH, Hawaii, USA), Lake Argyle (LG, Australia), and Reynold's Creek (RC, USA) have been included in the study (Fig.7.1) in order to take into account their different characteristics: geographic location (latitude/longitude); date and season; type of cloud (cumulus, cirrus, stratocumulus); and surface types (soil, vegetation, sand, ice, snow, lakes, sea, etc). Fig. 7.1 shows an RGB composite of the images over the test sites (BR-2003-07-14, BR-2004-05-27, BR-2005-07-17, OH-2005-01-08, LG-2004-02-29, and RC-2004-04-23) with an histogram stretching such that 10% of data is saturated at both low and high reflectance (10%-90%) in order to increase the contrast of the cloudy images. These images are useful to validate the performance of the algorithm since they include different landscapes, land covers, and also ice and snow.

7.1.2 CHRIS Cloud Screening Results

We have tested the proposed scheme for the aforementioned images. All the method has been implemented in Matlab programming language and it is capable to handle directly the CHRIS HDF original files and process them automatically producing the results in an ENVI standard format. Intermediate images of the method have been shown in Chapter 5. This section analyzes the performance of the method on the six images by means of the thematic map of the clusters and the cloud abundance product (Fig.7.2).

The following conclusions about the method results are depicted in Fig.7.2. The three images over the Barrax (BR, Spain) site are a good example of an easy cloud detection problem, when clearly defined clouds are well contrasted with soil and vegetation. The ROI selection can be easily appreciated in the classified images, being more important in the BR-2003-07-14 image where small clouds could be mixed in a cluster with other classes if the whole image is considered. At the OH-2005-01-08 image (Oahu, Hawaii), waves and beach sand pixels belong to a cluster labeled as cloud due to their high reflectance and whiteness, but they present low probabilities and abundances. In addition, this image presents cirrus clouds over land and over sea that are well detected since specific clusters describe them and have been correctly classified. One of the weak points of the algorithm is the use of thresholds to select the ROI, because some thin or small clouds can be excluded from the ROI. A solution is to relax thresholds at the risk of considering as ROI the whole image like in the image of LG-2004-02-29 (Lake Argyle, Australia). But, even in this case, results are good if clouds cover a sufficient percentage of the image or the number of clusters is high enough. The image of RC-2004-04-23 (Reynold's Creek, United States) is an example of one of the critical issues in cloud detection, the presence of ice/snow in the surface. These covers and clouds have a similar reflectance behavior. However, the atmospheric absorption suffered by cloud pixels is lower than for the case of surface pixels due to their height, thus different clusters are found for these two classes in the image. Thanks to the extracted atmospheric features, ice/snow pixels present low *cloud probability* values although the *cloud abundance* provided by the spectral unmixing could be relatively high due to the spectral similarities. In consequence, both information types are combined improving the final classification accuracy.

The use of CHRIS data allows us to assess algorithm performance in favorable spatial resolution (34 m) and number of bands (62 channels). The extrapolation to the ENVISAT MERIS sensor will be very valuable in order to simulate the subpixel effects due to the MERIS coarse spatial resolution (300m at Full Resolution). In addition, MERIS allows an accurate oxygen absorption estimation (11th/10th band ratio) and presents narrower bands to enhance detection and knowledge discovery.

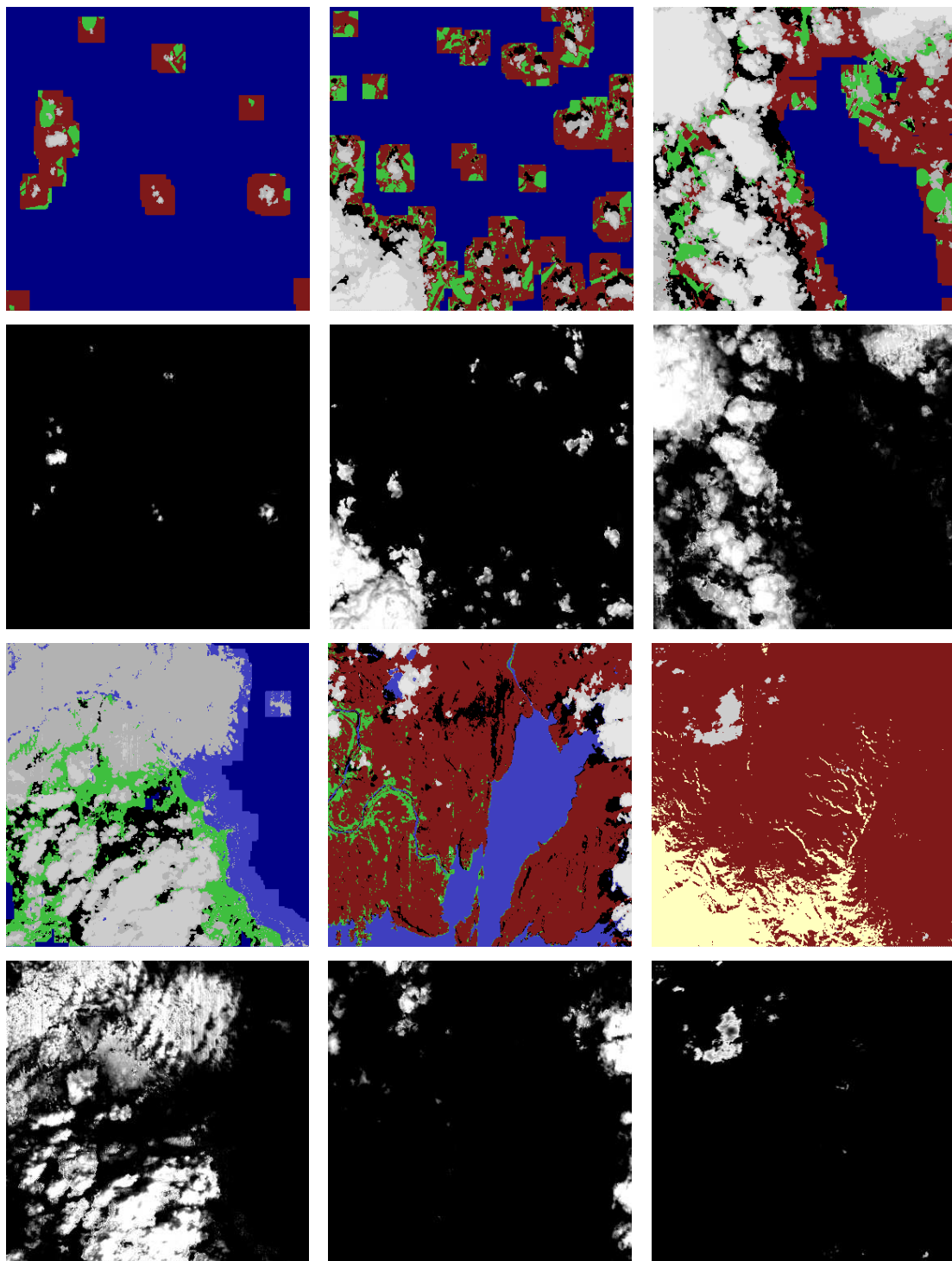


Figure 7.2: Cloud screening results on CHRIS images: BR-2003-07-14, BR-2004-05-27, BR-2005-07-17, OH-2005-01-08, LG-2004-02-29, and RC-2004-04-23 (from left to right). *First and third rows:* Thematic maps obtained after the cluster labeling (colors have been manually assigned to match land cover colors: clouds in grey, ground in brown, ice/snow in yellow, and background in blue). *Second and fourth rows:* Cloud abundance product.

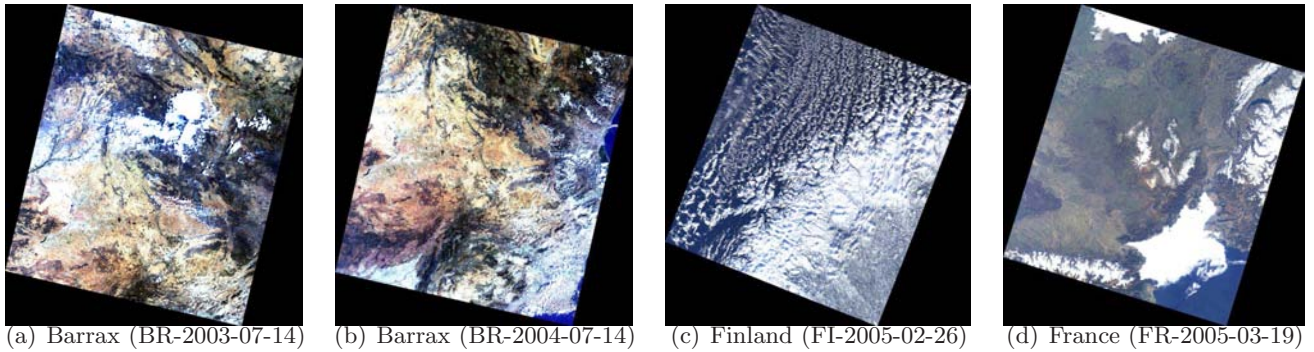


Figure 7.3: RGB composite of the MERIS images over the test sites of Barrax, Finland, and France.

7.2 Visual Inspection of ENVISAT/MERIS Images

7.2.1 MERIS Sample Products

A dataset consisting of four acquisitions over three sites has been selected to perform the visual validation on MERIS data. Both Level 1b (L1b) and Level 2 (L2) products were available for all MERIS Full Resolution (FR) images (300 m). In particular, the site of Barrax (BR, Spain) was selected as the main test site since it has been the core site of previous Earth observation campaigns and the analyzed cloudy images are part of the data acquired in the framework of the SPARC 2003 and 2004 ESA campaigns (ESA-SPARC Project, contract ESTEC-18307/04/NL/FF) (Moreno et al., 2005). These two images were acquired on July 14th of two consecutive years (BR-2003-07-14 and BR-2004-07-14). Additionally, MERIS acquisitions over France (FR-2005-03-19) and Finland (FI-2005-02-26) have been included in the study in order to take into account their different characteristics: geographic location, date and season, type of cloud, and type of surface. Again, the selected images represent different scenarios extremely useful to validate the performance of the method, including different landscapes; soils covered by vegetation or bare; and two critical cases given the special characteristics of the induced problems: ice and snow. Fig. 7.3 shows an RGB composite of the images over the test sites (BR-2003-07-14, BR-2004-07-14, FI-2005-02-26, and FR-2005-03-19) with an histogram stretching such that 10% of data is saturated at both low and high reflectance (10%-90%) in order to increase the contrast of the cloudy images.

The proposed method is only applied to the MERIS L1b products (TOA radiance) because the top of aerosols reflectance provided on MERIS L2 products does not include information at the oxygen and water vapor absorptions (MERIS channels 11 and 15 are not corrected from atmosphere due to the strong gaseous absorptions). Besides, L2 products are processed from L1b using a cloud pixel classification that could be inaccurate. Therefore, L2 products are only used for validation purposes by comparing the official L2 cloud flag with the cloud mask produced by our method.

7.2.2 MERIS Cloud Screening Results

Easy cloud screening situations

The two images over Barrax (Spain) are a good example of an easy cloud detection problem, where opaque clouds are well contrasted with bare soil and vegetation (Fig. 7.4[*first and second columns*]). At the BR-2003-07-14 image, dry soil pixels belong to a cluster labeled as cloud due to their high reflectance and whiteness, but they present low probabilities and abundances. The BR-2004-07-14 image presents thin and small clouds over land and over sea, which are well detected since a specific cluster describes them. The ROI selection can be easily seen in the classification images (Fig. 7.4[*second row*]), being more significant in the BR-2004-07-14 image where small clouds could be mixed in a cluster with other ground covers if the whole image is considered. The use of thresholds to select the ROI could be interpreted as one of the weak points of the algorithm, since some thin or small clouds could be potentially excluded from the ROI. However, the ROI selection can be seen as an eventual improvement. The obvious solution is to relax the thresholds or even consider the whole image. In this case, results are accurate if clouds cover a sufficient percentage of the image or the found number of clusters is high enough (as in the image over Finland, FI-2005-02-26).

Challenging cloud screening situations

The images over Finland and France have been included in the study to test one of the critical issues in cloud screening for which the proposed algorithm was intended for. In particular, the presented approach is designed to overcome the presence of bright pixels, such as ice and snow in the surface. Bright land covers and clouds have a similar reflectance behavior, thus thresholds on reflectance values or unmixed fractions do not solve the problem. However, the atmospheric absorption suffered by cloud pixels is lower than for the surface pixels due to their height. For this reason, when using together all the features in the clustering algorithm, different clusters are found for these two classes in the image. Thanks to the extracted atmospheric features, ice/snow pixels present low *cloud probability* values although the *cloud abundance* provided by the spectral unmixing could be relatively high due to the spectral similarities.

Consequently, both information types are combined improving the final cloud abundance product provided to the users (Fig. 7.4[*third row*]). Figure 7.4[*fourth column*] shows a case example result for an image over France (FR-2005-03-19) that presents opaque clouds at south and north France, and snowy mountains at various altitudes (Pyrenees, Massif Central, and the Alps), which are well-distinguished from clouds. The cloud product for these regions presents low values because the low cloud probability, $h_{iC} \sim 0$, obtained for these pixels.

In the case of Finland (FI-2005-02-26, Fig. 7.4[*third column*]), we have a different scenario where a cirrus cloud, often found in advance of a warm front, is moving from sea to the icy coast of Finland. In this image, we have a difficult cloud identification problem, even for an expert

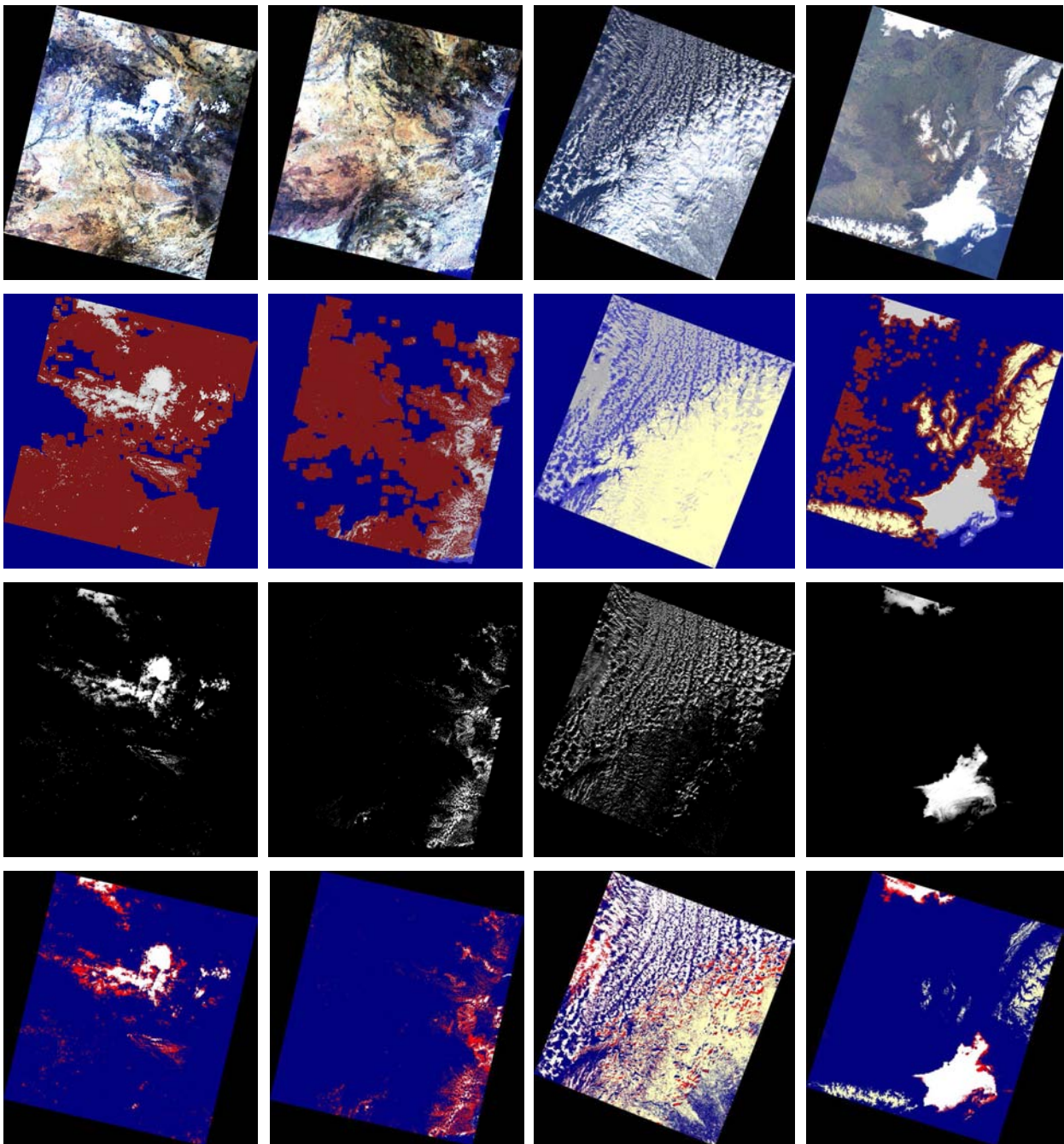


Figure 7.4: MERIS images over the test sites of BR-2003-07-14, BR-2004-07-14, FI-2005-02-26, and FR-2005-03-19 displayed in columns from left to right. *First row:* RGB composite with an histogram stretching such that 10% of data is saturated at both low and high reflectance (10%-90%) in order to increase the contrast of the cloudy images. *Second row:* Classification of the relevant regions (clouds in grey, ground in brown, ice/snow in yellow, and background in blue). *Third row:* Cloud abundance product. *Fourth row:* Comparison of MERIS L2 Cloud Flag with the obtained cloud mask (discrepancies are shown in red where our algorithm detects cloud and in yellow where pixels are classified as cloud free).

analyst. Incoming radiance from transparent cirrus clouds is mostly affected by the surface contribution, and it ranges from very low to extremely high values depending on whether cirrus cloud is over water or ice, respectively. However, the highest altitude clouds in the atmosphere are cirrus clouds located at altitudes between 5 and 14 km (cf. section 2.1). Despite the variability of the spectral behavior, the atmospheric features allow us to cluster transparent cirrus clouds correctly. Summarizing, the use of the oxygen-A absorption allows thick and high/middle-level clouds to be detected unambiguously. Very low level clouds, very thin cirrus clouds and broken clouds could be undetected when using only the oxygen feature, but its combined use with surface reflectance features solves these problems to a great extent. Finally, although the water vapor absorption feature is less accurate than the oxygen feature for cloud height estimations, it provides an alternative independent estimation. Besides, it is extremely useful to discriminate clouds from ice/snow covers due to the incipient absorption of these types of covers in the NIR region above 900 nm (Gao et al., 1998).

7.3 Comparison with MERIS Standard Products

One of the motivations to propose the presented cloud screening algorithm is to solve some critical problems where the operational MERIS L2 algorithm shows clear deficiencies, as reported by the user community elsewhere (Ramon et al., 2003; Brockmann, 2006), and by the MERIS Quality Working Group (MERIS Quality Working Group, 2006). For this reason, we illustrate the proposed methodology in different scenarios presenting critical cloud screening problems, and compare it to the MERIS L2 flag solution (cf. section 2.4.1).

Images in the last row of Fig. 7.4 show a comparison of MERIS L2 Cloud Flag with the results obtained by our algorithm. Pixels where both algorithms agree are depicted in *white* for the cloudy pixels and in *blue* for the cloud free pixels. The agreement between both methods is shown in Table 7.1 on the basis of the confusion matrices, which are expressed in terms of percentage of pixels in each image, and the overall accuracy (OA) and estimated kappa statistic¹ (κ) derived from them. Although overall agreement between both classifications is good enough for most of these images, the low values of kappa indicate that significant differences between methods exist. These differences can be better analyzed looking at the confusion matrices and comparison maps in Fig. 7.4. From these results, two main discrepancies are found. On the one hand, pixels classified as cloudy pixels (C) by our method but not by the MERIS flag (\overline{C}) are plotted in *red*, showing a good agreement with cloud borders. Therefore, one can assume that the proposed method provides better recognition in cloud borders and in small and thin clouds, which is the situation in the images acquired over Spain. On the other hand, discrepancy pixels

¹The use of estimated kappa statistics, κ , is more appropriate than the overall accuracy for testing whether agreement for both binary cloud classifiers exceeds chance levels (Congalton and Green, 1999). A value of $\kappa = 1$ means complete agreement and $\kappa \leq 0$ reflects no agreement. Following this criterion, a classification can be considered ‘good’ for $\kappa > 0.8$ and ‘poor’ for $\kappa < 0.7$.

Table 7.1: Confusion matrices between the proposed method in the whole scene using the MERIS L2 Cloud Flag as reference (given in % of pixels). In the bottom, the overall agreement (OA[%]) and estimated kappa statistics (κ) are given for all images.

MERIS L2 Cloud Flag	Proposed Method								
	Spain'03		Spain'04		Finland		France		
	C	\overline{C}	C	\overline{C}	C	\overline{C}	C	\overline{C}	
Conf. Matrix	C	3.8	0.0	1.3	0.0	27.6	30.2	7.4	4.4
	\overline{C}	5.4	90.8	6.2	92.5	9.8	32.4	1.8	86.4
OA[%]	94.58		93.84		59.98		93.78		
κ	0.56		0.29		0.23		0.66		

classified by our algorithm as cloud-free (\overline{C}) are shown in *yellow*. These areas correspond to ice covers (Finland image) and snow over high mountains (Pyrenees, Massif Central, and Alps in the France image). These results explain all discrepancies found in the confusion matrices and indicate the goodness of our approach.

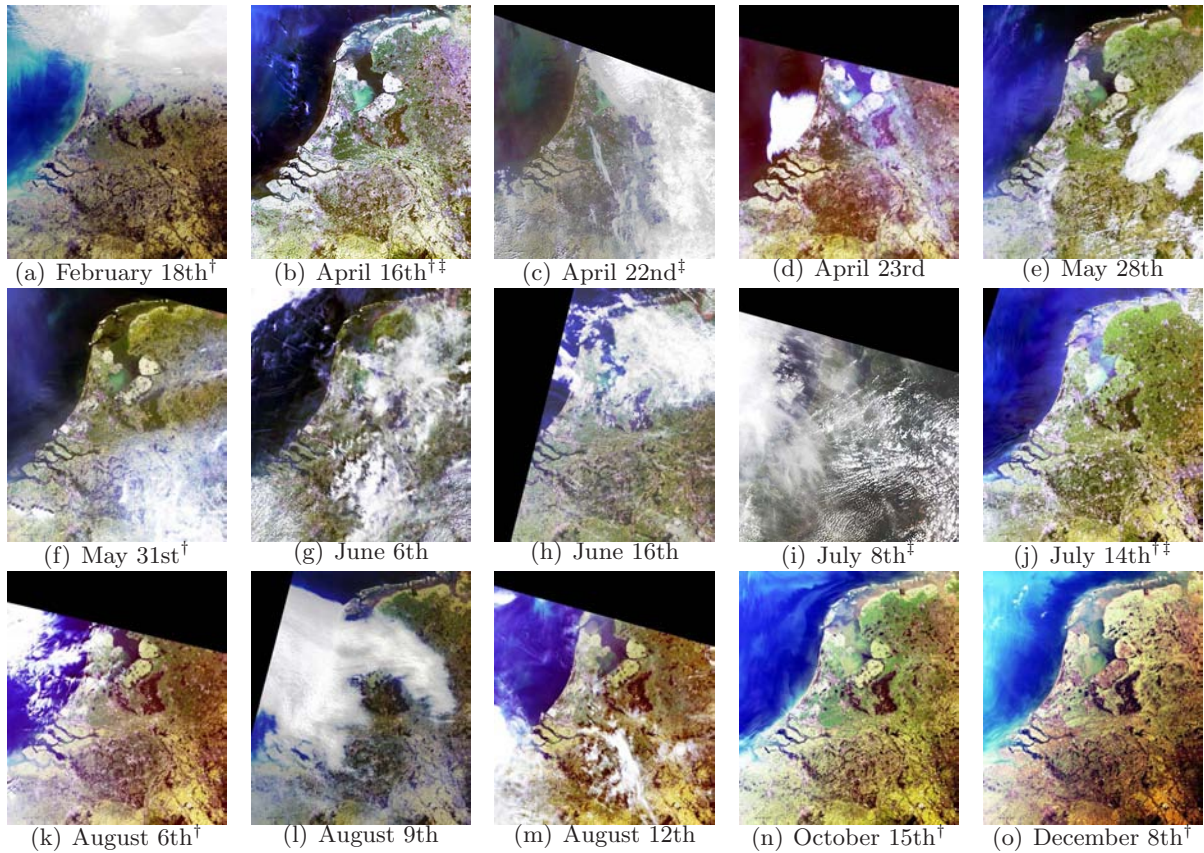
For the sake of a fair comparison between both algorithms, we want to remark that the proposed algorithm is less efficient than the MERIS standard cloud masking scheme in terms of computational burden (mainly due to the clustering and unmixing processes). However, when considering critical cloud screening problems, our algorithm provides better results. The algorithm has not been specifically designed to process a large number of images like the operational MERIS L2 algorithm or recent pragmatic solutions proposed for MERIS (Ranera et al., 2005; Preusker et al., 2006). Our proposal is more concerned with obtaining abundance and accurate cloud masks when the thresholds used in the MERIS L2 algorithm are not representative.

7.4 Multitemporal Validation on MERIS Series

In order to test the performance of the proposed cloud screening algorithm, we set up a real multitemporal land cover mapping application over cloudy areas. In particular, a temporal series of MERIS images is used to derive sub-pixel land cover composition by means of linear spectral unmixing techniques. The final objective of this validation approach is two-fold: to propose a cloud screening validation based on temporal series, and to evaluate the impact of a cloud screening algorithm in a multitemporal unmixing application.

7.4.1 MERIS Time Series over The Netherlands

A temporal series of MERIS FR Level 1b images acquired over the Netherlands in 2003 is selected to illustrate our approach (Fig. 7.5). The Netherlands is selected as study area because of the heterogeneity of its landscapes, frequent cloud coverage, and the availability of an up-to-



† Dates selected for the multitemporal unmixing in the multitemporal land cover mapping application, which are chosen throughout the year according to its low cloud coverage.

‡ Pairs of cloudy and cloud-free dates used to validate the cloud screening algorithm.

Figure 7.5: Coregistered MERIS FR L1b temporal series acquired over The Netherlands in 2003.

date high spatial resolution land use database. The availability of this high resolution land use map over The Netherlands is really convenient because it can be used to validate the subpixel classification results provided by the unmixing, but also as an input of the validation methodology in order to improve the accuracy of the cloud screening validation.

Most of the acquisition dates of the temporal series presented extensive clouded areas. Therefore, the selected dates for the multitemporal unmixing are chosen according to two criteria: (i) to maximize the number of cloud free pixels in each scene and (ii) to get, at least, one image per month so that the vegetation phenological cycle is fully captured. Unfortunately, no suitable MERIS FR scene was found for the months of January, March, June, September, and November. Therefore, an uneven temporal series of seven images is considered for the unmixing: February 18th, April 16th, May 31st, July 14th, August 6th, October 15th, and December 8th. In addition, images of the 22nd of April and the 8th of July are only used to validate the cloud screening algorithm. These dates were the closest clouded dates to the 16th of April and 14th of July, respectively, and thus are needed in order to set up pairs of cloudy and cloud-free images (marked

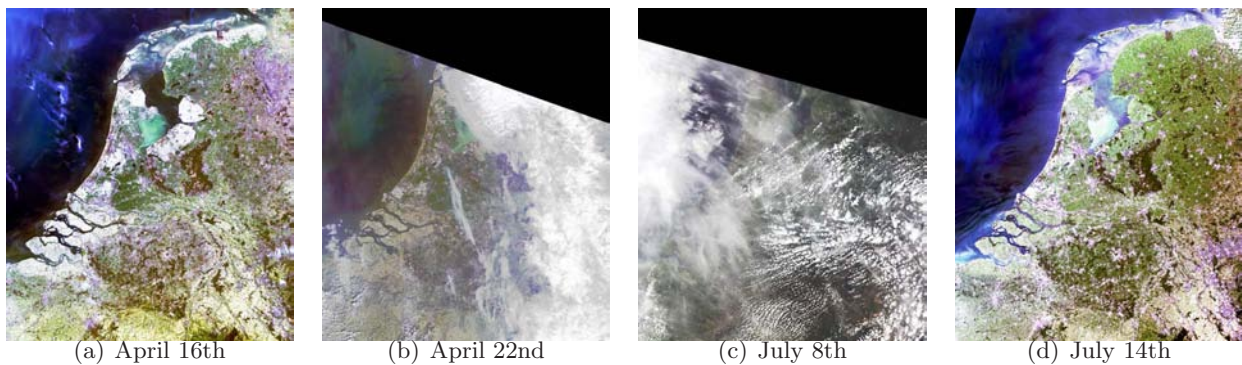


Figure 7.6: Co-registered MERIS FR L1b images acquired the 16th and 22nd of April (a and b), and the 8th and 14th of July (c and d).

by ‡ in Fig. 7.5 and shown in Fig. 7.6).

Reference dataset

The LGN5 Dutch land use database is used as a reference in this study. This geographical database is based on a multi-temporal classification of high resolution satellite data acquired in 2002 and 2003; several types of ancillary data were also used to produce the LGN5 land use database (Hazeu, 2005, 2006). The LGN5 has a pixel size of 25m and maps 39 classes. The unmixing of all these classes would be unrealistic, since some of the classes are rather small and/or sparsely distributed and/or heavily based on available ancillary data, which mainly describes land uses rather than land cover types. Consequently, the LGN5 was thematically aggregated into the main 9 land cover types of The Netherlands. The aggregation to 9 classes is meant to offer a detailed distribution of the following classes: grassland, arable land, deciduous forest, coniferous forest, water, built-up, greenhouses, bare soil (including sand dunes), and natural vegetation.

Image co-registration

First, the LGN5 is spatially aggregated in order to match the nominal MERIS FR pixel size (Fig. 7.7). To do so, a majority filter with a window of 12 by 12 LGN5 pixels is used, obtaining a land cover classification map of 300 m (*LCC*). During this spatial aggregation process, abundances of the different land cover types present in the final pixel of 300 m are recorded (*LCA*).

The second step in the pre-processing of the images is the co-registration. Multitemporal studies require an accurate co-registration so that the correspondence between pixels at different dates is ensured. Nevertheless, a perfect correspondence is very difficult to obtain because of differences in observation angles (in our case each MERIS acquisition date belongs to a different ENVISAT orbit) and because of the so-called resampling effects (e.g., Moirée patterns). In order to minimize these effects, we compute the ‘real’ land cover abundances as seen by MERIS for

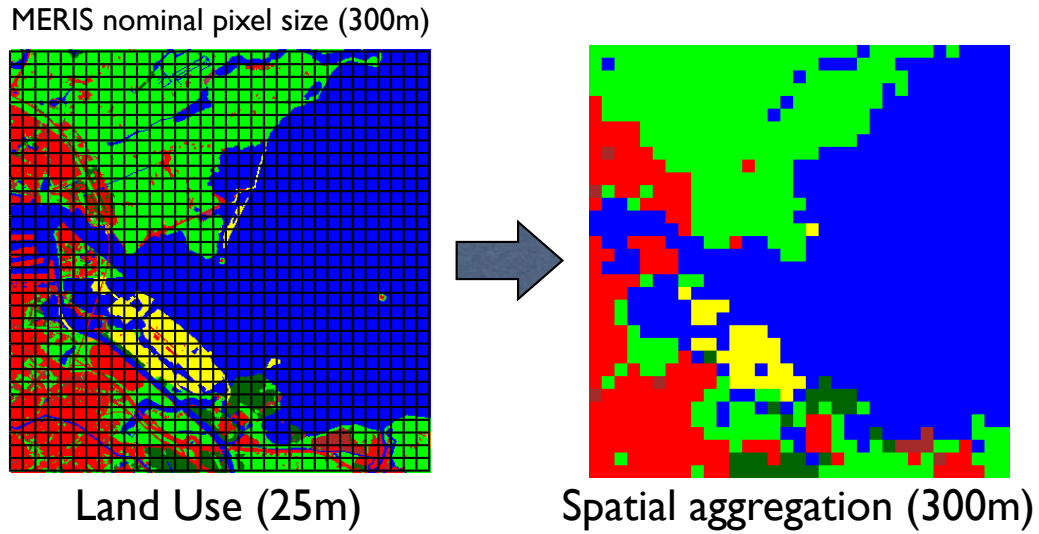


Figure 7.7: Illustration of the spatial aggregation of the LGN5 land use database to the nominal MERIS FR pixel size.

each date. This provides us with slightly different abundances for each date that can be used to do a fair validation of the unmixing results. Figure 7.8 illustrates how the ‘real’ abundances are computed. First, each MERIS image is projected into the original 25m grid of the reference dataset (LGN5). Then, the abundances of the different land cover types present in the area observed by each MERIS detector element are computed. The class having the highest abundance is also used to produce a land cover classification for each date, t , so that both a sub-pixel and a per-pixel validation of the results could be done. After this, each MERIS image (t) and its corresponding sub-pixel abundances (LCA^t) and land cover map (LCC^t) are projected into the same coordinate system of the reference LGN5 dataset but this time with a grid of 300 by 300 m (i.e., MERIS nominal pixel size). A nearest neighbor interpolation method is used so that the original values recorded by MERIS are not modified.

7.4.2 Temporal Cloud Screening based on Change Detection

Once all MERIS images are co-registered, the performance of the cloud screening is tested with a multitemporal validation approach. In particular, pairs of cloud-free and cloud-covered images (Fig. 7.6) are used to detect cloud-pixels by identifying pixels with spectral changes between both dates (t_1 and t_2) higher than a given threshold. Concerning the spectral change, the spectral angle distance (SAD) is used since it is invariant to multiplicative scaling (Keshava, 2004), and thus is less affected by atmospheric and illumination changes:

$$D(\rho_i^{t_1}, \rho_i^{t_2}) = \arccos \left(\frac{\langle \rho_i^{t_1}, \rho_i^{t_2} \rangle}{\|\rho_i^{t_1}\| \|\rho_i^{t_2}\|} \right) \quad (7.4.1)$$

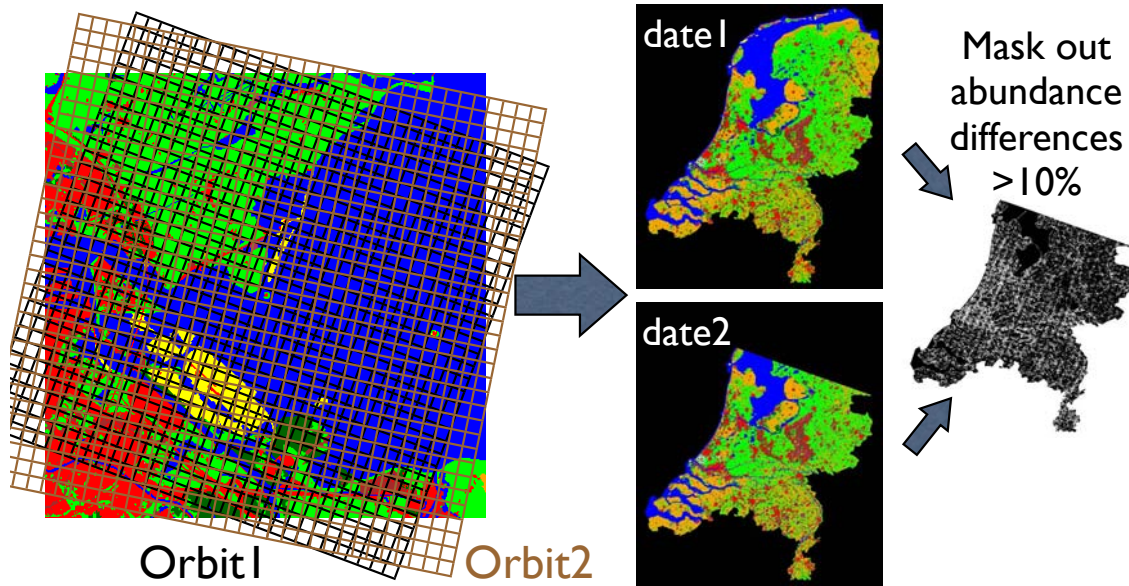


Figure 7.8: Illustration of the projection and spatial aggregation of the LGN5 land use database to the actual area observed by the MERIS pixels depending on the observation angles from the given orbit.

where $\rho_i^{t_1}$ and $\rho_i^{t_2}$ represent the spectra of a given pixel location i for dates t_1 and t_2 , respectively; $\langle \cdot, \cdot \rangle$ is the dot product operator; and $\| \cdot \|$ is the squared norm. Image pairs are selected to be close in time in order to avoid spectral changes due to temporal evolution of the surface. However, images with only three or six days of difference are taken from different orbits and thus present a significant variation in the viewing angles. Although images are co-registered and a one-to-one correspondence between the pixels of the two dates can be found, the area observed at each date is not exactly the same. If the land cover types present in the observed areas change from one date to the other, then the spatial shift can produce significant spectral changes between $\rho_i^{t_1}$ and $\rho_i^{t_2}$. In consequence, pixels with significant changes in composition, i.e. differences between LCA^{t_1} and LCA^{t_2} derived from de LGN5 higher than 10%, are masked out in the multitemporal cloud screening validation (Fig. 7.8).

Cloud screening results

A hard cloud mask is obtained for each date t by applying the same threshold of 0.05 to the cloud abundance product maps ϑ^t of the proposed algorithm, which are shown in Fig. 7.9. Since no ground truth indicating cloudy pixels can be generated for all dates, we first analyze the performance of the proposed method by visual inspection. The analysis of the results showed an excellent cloud screening performance even in thin clouds and cloud borders. The only exception is a small amount of pixels belonging to the classes greenhouses (sun glint on glass roofs) and bare soil (sand dunes). These pixels were identified as clouds because these classes have similar

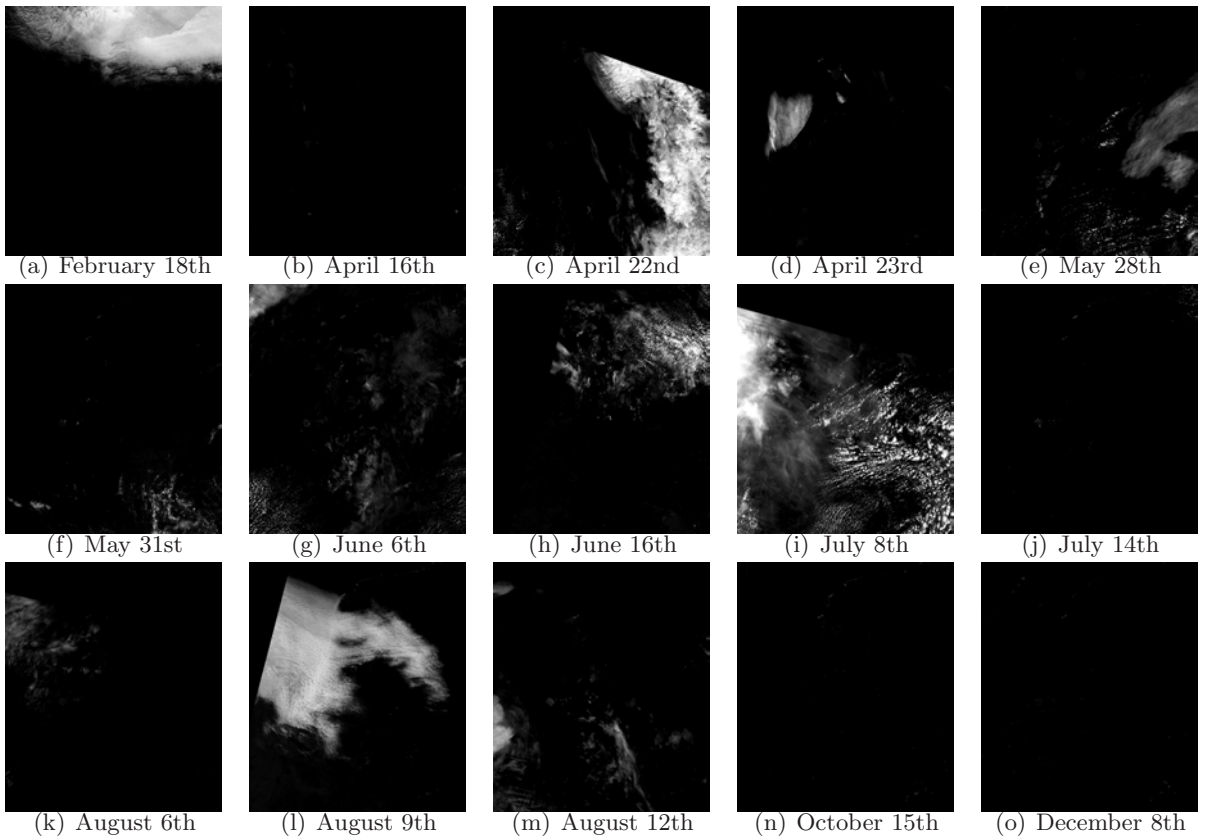


Figure 7.9: Cloud product provided by the proposed cloud screening algorithm for the temporal series of MERIS images shown in Figure 7.5 (same order and dates).

reflectance behavior to clouds. However, the classes that were misclassified represent less than 0.5% of The Netherlands and, therefore, were not statistically representative in the clustering process used by the cloud screening algorithm.

In addition to the visual analysis, image pairs covering the same area acquired within few days can be used to perform the temporal validation of the cloud screening. The performance of the cloud screening algorithm is validated over the cloudy images acquired the 16th of April and the 14th of July using as reference the cloud-free images of the 22nd of April and 8th of July, respectively (Fig. 7.6). Figure 7.10 shows on the left the temporal spectral change computed with (7.4.1) and on the right the final cloud product as provided by the proposed cloud screening algorithm. From this figure, one can easily appreciate the high correlation between both magnitudes. However, it is worth noting that in the temporal spectral change images: (i) the surface contribution is still visible, and (ii) differences between surface and cloud values are lower than in the proposed cloud screening product, which suggests the consistency of our approach.

In order to obtain a quantitative validation of the proposed approach, the cloud screening accuracy is assessed by comparing the hard cloud mask ($\vartheta^t > 0.05$) with a ‘true mask’, which is obtained by applying an empirical threshold to the temporal spectral change (SAD). Considering

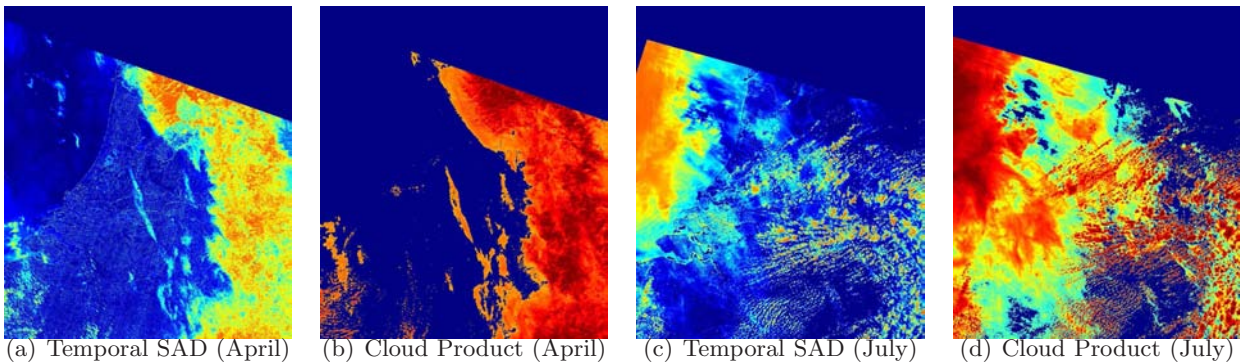


Figure 7.10: Temporal spectral change (SAD) computed from image pairs of April 16th-22nd (a) and July 8th-14th (c). Cloud product provided by the proposed cloud screening algorithm for April 22nd (b) and July 8th (d).

the cloud mask as a binary classification, the overall accuracy (OA[%]) and the kappa statistic (κ) show an excellent detection accuracy for April 22nd (OA=91%, $\kappa=0.82$), and slightly worst results for July 8th (OA=87%, $\kappa=0.67$), since this presents a complex cloud screening problem with thin transparent clouds at different layers. However, ‘true mask’ obtained with the multitemporal approach is not 100% accurate, and thus one has to interpret this assessment as a simple comparison between the multitemporal approach and the proposed method. Figure 7.11[*top*] shows the comparison of both cloud masks. On the one hand, when our algorithm detects more cloudy pixels (*blue*), good agreement with cloud borders can be seen. Therefore, one can assume that the proposed method provides better recognition in cloud borders and thin clouds. On the other hand, differences when our algorithm classifies as cloud-free are shown in *red*. One can see that these areas correspond to the boundaries between land cover types, where spectral changes are probably due to the different viewing geometry of the two dates. Therefore, one can conclude that, despite the fact that the proposed method only uses the information of the ‘cloudy image’, our method offers a better discrimination than the multitemporal change detection approach.

For the studied MERIS temporal series over The Netherlands, only MERIS FR Level 1b products is available. Therefore, it is not possible to compare the official L2 cloud flag with the cloud mask produced by our method. However, further validation can be performed by comparing results with the *Cloud Flag* provided by the *Cloud Probability Processor* of the *Basic ENVISAT AATSR and MERIS* (BEAM) Toolbox (cf. section 2.4.1). The BEAM Cloud Probability Processor uses a clear sky conservative cloud detection algorithm, which is based on artificial neural nets (NN). Figure 7.11[*bottom*] shows the comparison of our method against a flag that indicates cloudy when NN *probability* > 20%, which is the lowest threshold recommended by the authors of the algorithm (Preusker et al., 2006). Also, in this comparison a good agreement with cloud borders can be seen in the *blue* areas where only our algorithm detects cloudy pixels.

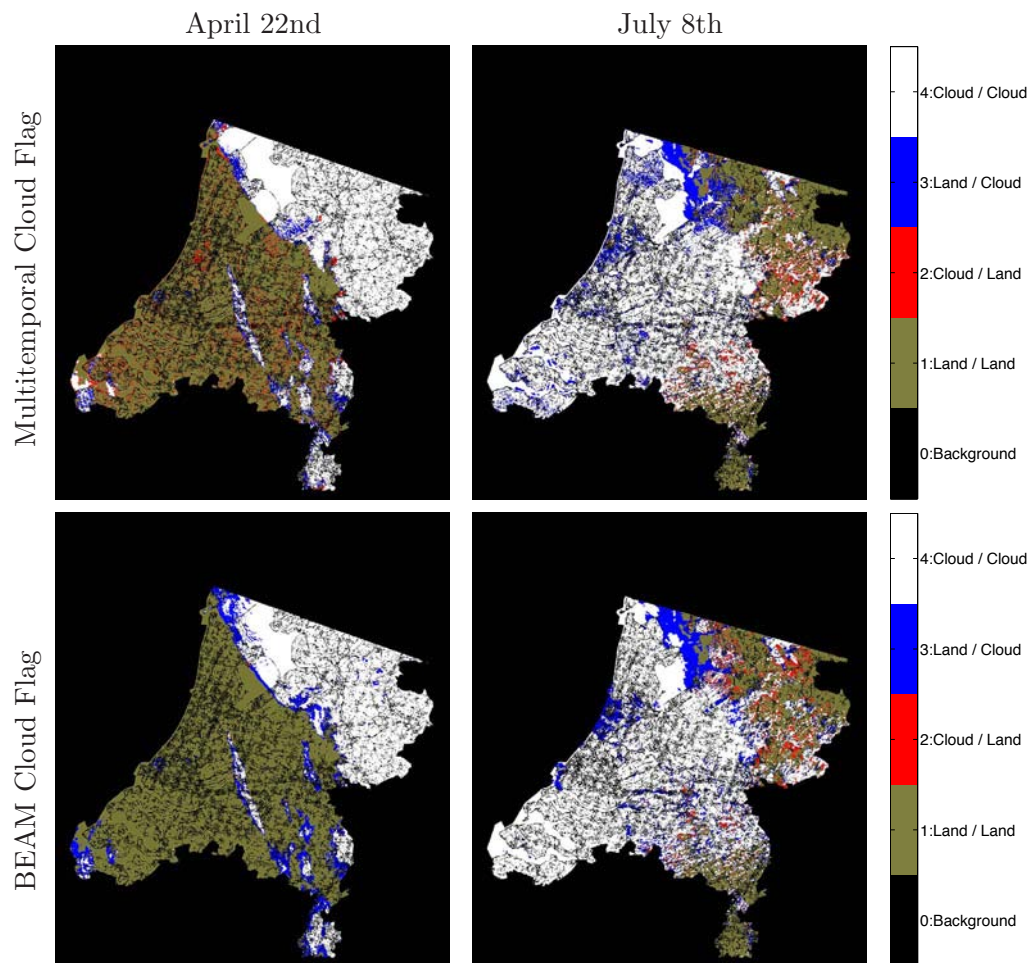


Figure 7.11: Comparison of the obtained cloud mask against the multitemporal cloud flag (*top*) and against the BEAM Cloud Probability Processor Flag (*bottom*) for the images of April 22nd (*left*) and July 8th (*right*). Discrepancies between methods are shown in blue when our algorithm detects cloud and in red when pixels are classified as cloud-free.

7.4.3 Spectral Unmixing of Multitemporal Series

An indirect procedure to test cloud screening performance consists in analyzing its effect in a real application. Undetected clouds are one of the most significant sources of error in both sea and land cover biophysical parameter retrieval. For example, in a land use classification application based on spectral unmixing of multitemporal series, undetected clouds can hamper the selection of endmembers and seriously affect the quality of the unmixing of cloud contaminated pixels. Therefore, cloud screening is needed to remove all the cloudy pixels from the final analysis. As a consequence, an accurate cloud screening should significantly increase the classification accuracy.

The algorithm used to perform the spectral unmixing is the fully constrained linear spectral unmixing (Heinz and Chang, 2001) presented in section 5.3.1, which can be applied to each MERIS

image (mono-temporal case) as well as to a multitemporal composite (stacked approach) of all the MERIS images. The FCLSU guarantees a physical interpretation of the results, and can be formalized as follows:

$$\rho_i^t(\lambda_b) = \sum_{q=1}^Q m_q^t(\lambda_i) a_{iq}^t + \varepsilon \quad (7.4.2)$$

subject to $0 \leq a_{iq}^t \leq 1$ and $\sum_q a_{iq}^t = 1$; where $\rho_i^t(\lambda_b)$ is pixel i value for band b at date t , Q represents the number of class endmembers, \mathbf{m}_q^t , that are being unmixed, being the coefficients of this combination, a_{iq}^t , the unmixing coefficients, which can be interpreted as the abundance fractions of materials or classes in a pixel. Finally, the term ε represents the residual error per band, assumed constant for all bands.

In the multitemporal case, the spectral signature of each class, \mathbf{m}_q , is the stacked vector formed by the class endmember of all dates, $\mathbf{m}_q = [\mathbf{m}_q^{t_1}, \mathbf{m}_q^{t_2}, \dots]$, and the pixel to be unmixed, ρ_i , is the stacked vector $\rho_i = [\rho_i^{t_1}, \rho_i^{t_2}, \dots]$. Now, (7.4.2) can be expressed in a matrix form as $\rho_i = \mathbf{M} \cdot \mathbf{a}_i + \varepsilon$, where the spectral signatures of materials, \mathbf{m}_q , are expressed in the columns of matrix \mathbf{M} .

Multitemporal unmixing results

After applying the cloud screening algorithm to all the selected images, identified cloud contaminated pixels are masked out and the spectral unmixing is carried out. Figure 7.12(a) shows the spectral signature of the endmembers for the seven dates selected in this study. Grassland presents the highest NIR reflectance all year around. During the months of May, July, and August the endmember of deciduous forest also shows high reflectance (high greening of vegetation). The rest of the vegetated classes appear to have a very similar spectral signature. High confusion is, therefore, expected among these classes. On the one hand, in the spectral unmixing of one image, the land cover abundances cannot be obtained over clouded areas or outside the field of view of the sensor. On the other hand, in the multitemporal unmixing, each pixel is formed as the stacked vector of the spectra for all the available dates. This allows us to obtain the abundance fractions in all the pixels of the studied area, but the number of dates used in multitemporal unmixing is pixel dependent since each pixel is unmixed with the maximum number of valid cloud free dates. This means that the quality of the unmixing is also pixel-dependent and that, whenever critical (phenological) dates are missing for a number of pixels (e.g. clouded areas), the accuracy of the results on those pixels (areas) might be lower. Figure 7.12(b) shows the number of usable dates for each pixel after masking out the clouds and cloud borders. It should be noted that the northern and south-eastern parts of The Netherlands have less usable pixels than the rest of the country. This is not only because of the cloud coverage but also because some of the MERIS FR images did not cover the whole of The Netherlands.

A detailed description of the multitemporal spectral unmixing and the obtained results is given in Gómez-Chova et al. (2006f). Here, we have only focused on the impact of cloud screening in

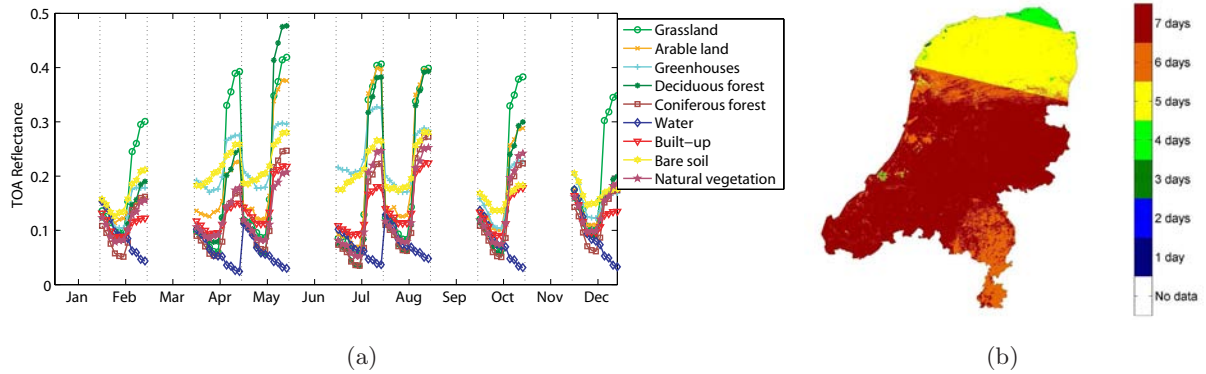


Figure 7.12: (a) Pure temporal endmembers selected from the multitemporal dataset for each land cover class. (b) Per-pixel number of usable dates.

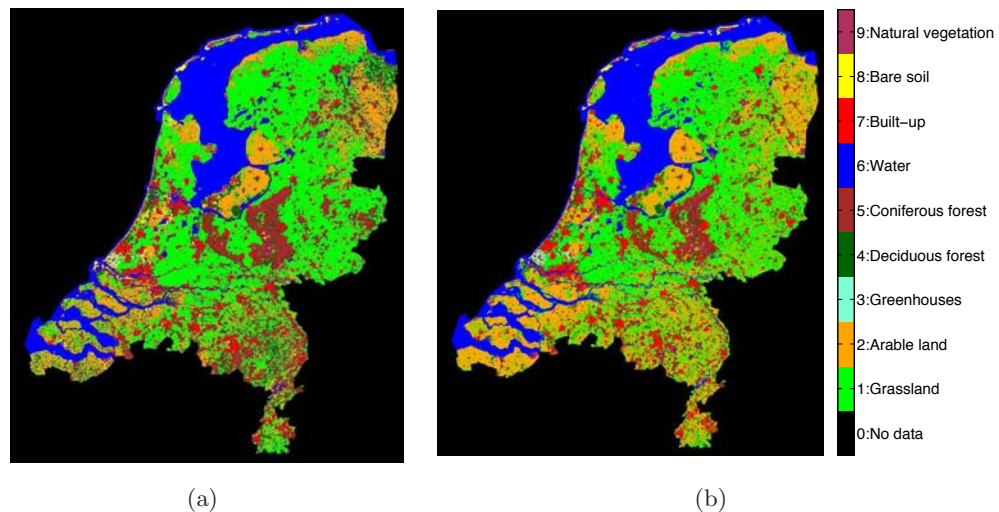


Figure 7.13: (a) Classification obtained from the multitemporal unmixing abundances. (b) LGN5 resampled to 9 classes and 300 m used as ground truth.

the multitemporal unmixing. However, in the following, we summarize the main unmixing results in order to show the importance of an accurate cloud screening. The unmixed abundances for each date, \mathbf{a}_i^t , and the multitemporal approach, \mathbf{a}_i , are compared to the abundances computed during the spatial aggregation of the LGN5 database, LCA . Then, the classification obtained from the abundances (Fig. 7.13) is used to compute the overall classification accuracy and the kappa statistic using the LCC as ground truth (Table 7.2). As expected, the multitemporal approach yielded the highest classification results, since adding the temporal evolution (phenology) simplifies the discrimination of spectrally similar land cover types. However, the difference between the classification results of the best (monotemporal) image [April] and the multitemporal approach is not very large. These errors in the multitemporal case should be produced by the within class heterogeneity (land covers with different phenology mixed in one class, e.g. arable

Table 7.2: Performance of the land cover classification using the FCLU at per pixel scale (overall accuracy, OA[%], and kappa statistics, κ) for each single date and the multitemporal series.

Data	Feb	Apr	May	Jul	Aug	Oct	Dec	Multitemporal
Kappa	0.36	0.49	0.39	0.45	0.36	0.37	0.35	0.52
OA[%]	46.44	58.58	50.33	56.10	46.81	49.88	47.55	62.29

land class) or by the procedure used to elaborate the LGN5 used as ground truth. In conclusion, the accurate cloud screening performed by the proposed algorithm enables a more efficient use of MERIS images.

7.5 The Cloud Abundance Product

Finally, one of the requirements imposed to the proposed cloud screening methodology was to provide information about the contribution of clouds to the spectra of image pixels (for both transparent clouds or subpixel coverage situations). This type of information may be very useful for the users in order to decide *what is a cloud* depending on the application requirements or image conditions. In this work, we classify as cloud all pixels presenting values higher than 0.05 in the obtained *cloud abundance product*. It should be noted that this threshold is the same for all images analyzed in order to demonstrate the general applicability of the method. This value is so low because the classification probability makes almost zero the cloud abundance product for all the cloud-free pixels. However, if the user is not interested in excluding pixels slightly affected by clouds in a given application, the threshold value can be increased.

In order to show the potential of the cloud abundance product, Fig. 7.14 shows the histograms of the obtained values of posterior probability h_{iC} (*dark*) and cloud product ϑ_i (*white*) for all images. The smooth distribution of ϑ_i values differs to a great extent from the output of the probabilistic classifier, which has no physical meaning and is usually unevenly distributed around zero and one.

Finally, we can also validate our abundance product against the cloud probability provided by the *Cloud Probability Processor* implemented in the BEAM Toolbox, which is the most similar cloud product available for MERIS data. Figure 7.15 shows the histograms of the proposed cloud product (*white*) and the BEAM cloud probability (*dark*) values. Again, our algorithm provides a smoother distribution of ϑ values, which differs to a great extent from the output of the probabilistic NN classifier that is concentrated around one.

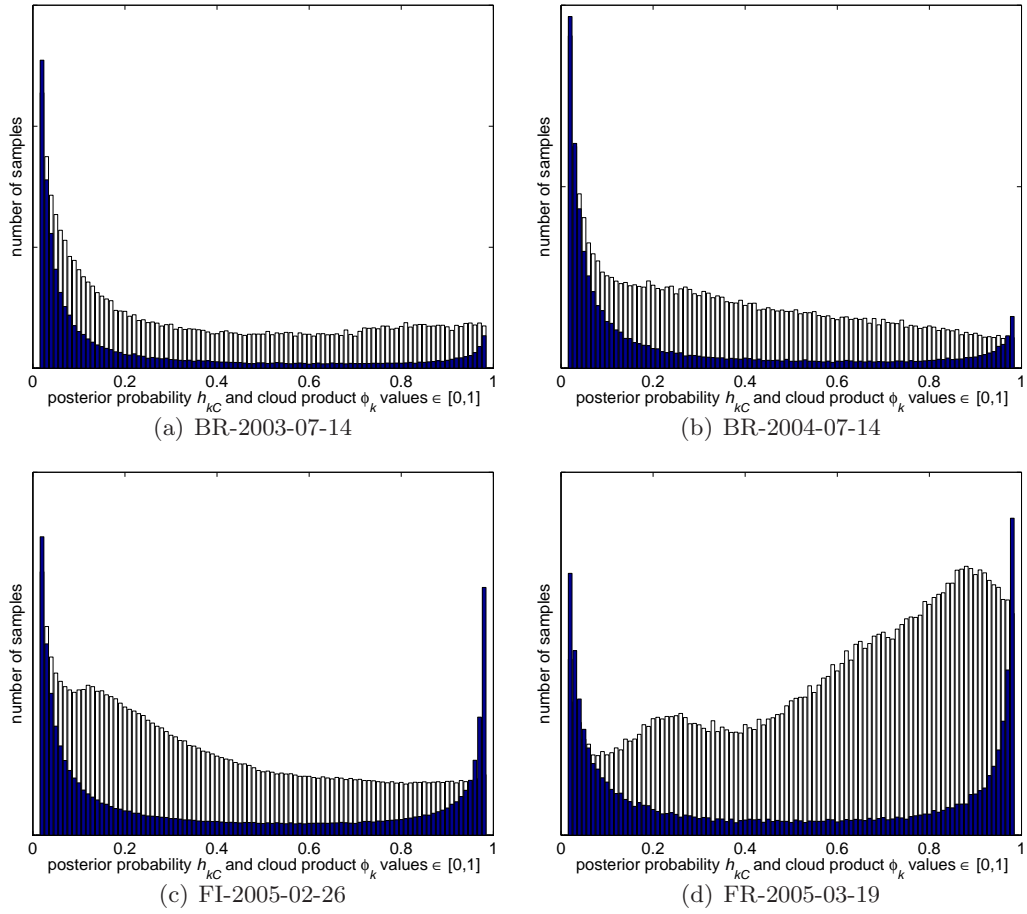


Figure 7.14: Histogram of the posterior probability h_{iC} (*dark*) and cloud product ϑ_i (*white*) values for the images of BR-2003-07-14 (a), BR-2004-07-14 (b), FI-2005-02-26 (c), and FR-2005-03-19 (d). Extreme low and high values have been excluded for a proper visualization.

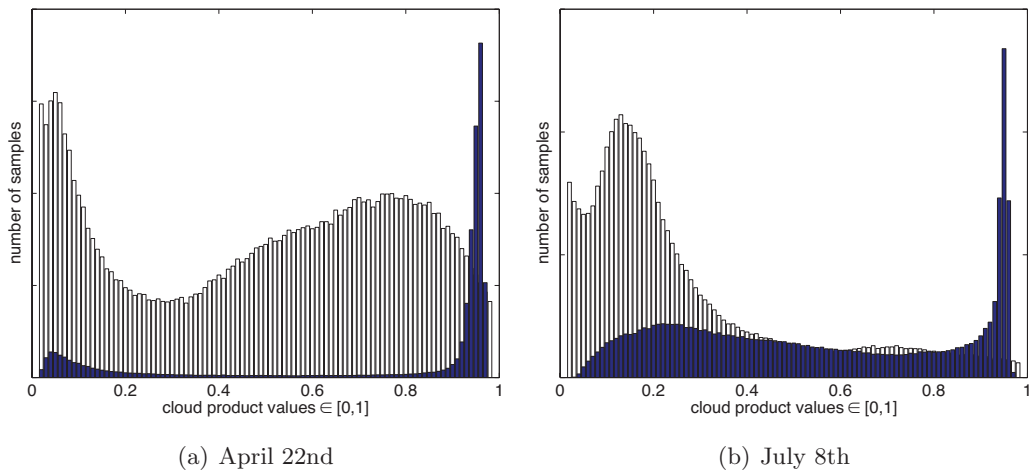


Figure 7.15: Histogram of the proposed cloud product (*white*) and the BEAM cloud probability (*dark*) values for the images of April 22nd (a) and July 8th (b). Extreme low and high values have been excluded for a proper visualization.

Chapter 8

Semi-supervised Cloud Screening Validation

The user-driven approach proposed in Chapter 5 has shown an excellent cloud screening performance in the results as presented in Chapter 7. However, this approach is best suited to case studies due to its computational cost and the optional interaction of the user during the labeling process. In operational cloud screening applications, methods that automatically and accurately classify clouds are mandatory. Therefore, supervised or semi-supervised methods should be more appropriate due to their typically enhanced performance. This chapter describes the cloud screening results obtained with the novel kernel methods presented in Chapter 6. All these methods are supervised or semi-supervised classifiers, and thus they require a representative set of labeled samples to train and validate the models.

As we mentioned in previous chapters, in a real cloud screening classification problem, no simultaneous independent assessment measurement of cloud presence at the same image spatial resolution is usually available. Therefore, it is not easy to obtain the true label (cloud or cloud-free) for the image pixels. In the case of MERIS images, only two cloud mask products (obtained in an operational basis) can be used as a reference in order to compare the results of the proposed cloud screening approaches. These two cloud masks, which are derived directly from the MERIS image, are the official MERIS L2 Cloud Flag and the BEAM Cloud Probability Processor Flag that provides a more accurate cloud mask than the official product. However, results presented in Chapter 7 revealed that both methods have deficiencies. In fact, the analysis carried out in Chapter 7 showed that the method based on unsupervised clustering proposed in Chapter 5 is the most accurate cloud screening method, especially when the labeling of the found clusters is done by the user (user-driven approach). Therefore, the true labels and true maps used to train and validate the classifiers presented in this chapter are based on the proposed cloud abundance product (see section 5.3.3).

8.1 Experimental Setup

In a real cloud screening classification problem, it is difficult to collect a statistically significant number of ground-truth samples to define a complete training set for developing robust supervised classifiers. This usually leads to a poor representation of the problem by the training set that can induce the so-called *sample selection bias problem*, i.e. the available training set is not representative enough of the test set. For this reason, the proposed kernel methods are benchmarked in two different conditions: (1) few labeled training samples are available for characterizing the image to be classified; and (2) no labeled training samples are available for the test image to be classified. In the latter case, training data extracted from other images modeling similar problems are exploited to develop the classifiers. In both situations, unlabeled samples of the test image can be jointly used with the available training samples to increase the reliability and accuracy of the classifier. In this context, two scenarios are further considered: labeled and unlabeled training samples might belong to the image to be classified, or to different images coming from different locations and acquired in eventually very different conditions. The most realistic situation in operational remote sensing applications is, nevertheless, to obtain the labeled samples from previous images and the unlabeled samples from the image to be classified. Summarizing, two challenging scenarios are considered:

Single-Image Approach. In these experiments, labeled and unlabeled training samples belong to the image to be classified. This is a common scenario in remote sensing, when a single image is available or is going to be analyzed, and the training set is built by labeling some representative samples, usually by an expert or by using additional ground measurements. In this case, both the training and test data come from the same marginal distribution, and thus the classifiers are not affected by the sample selection bias problem. We call this procedure the *single-image approach*.

Image-Fold Approach. A completely different (and more realistic) situation is to obtain the labeled training samples from previous images or from physical model simulations, and then apply the developed models to a test set, which usually consists of several images. In this case, the available training set can be not representative enough for the test (sample selection bias problem) and the unlabeled samples from the image to be classified should help to improve the classification accuracy. In order to analyze this scenario, in this chapter, we carry out some experiments where classifiers are trained using both labeled samples from the $N - 1$ out of N available images, and unlabeled samples from the image to be classified. We call this procedure the *image-fold approach* (see Fig. 8.1).

Table 8.1 describes the data sets used to develop the kernel classifiers and the experimental setup followed to obtain the cloud screening results. The input features used by all the methods are extracted from the MERIS L1b images, as described in Chapter 4. The labels of the image pixels are obtained from the cloud abundance product (cf. section 5.3.3), which has been analyzed

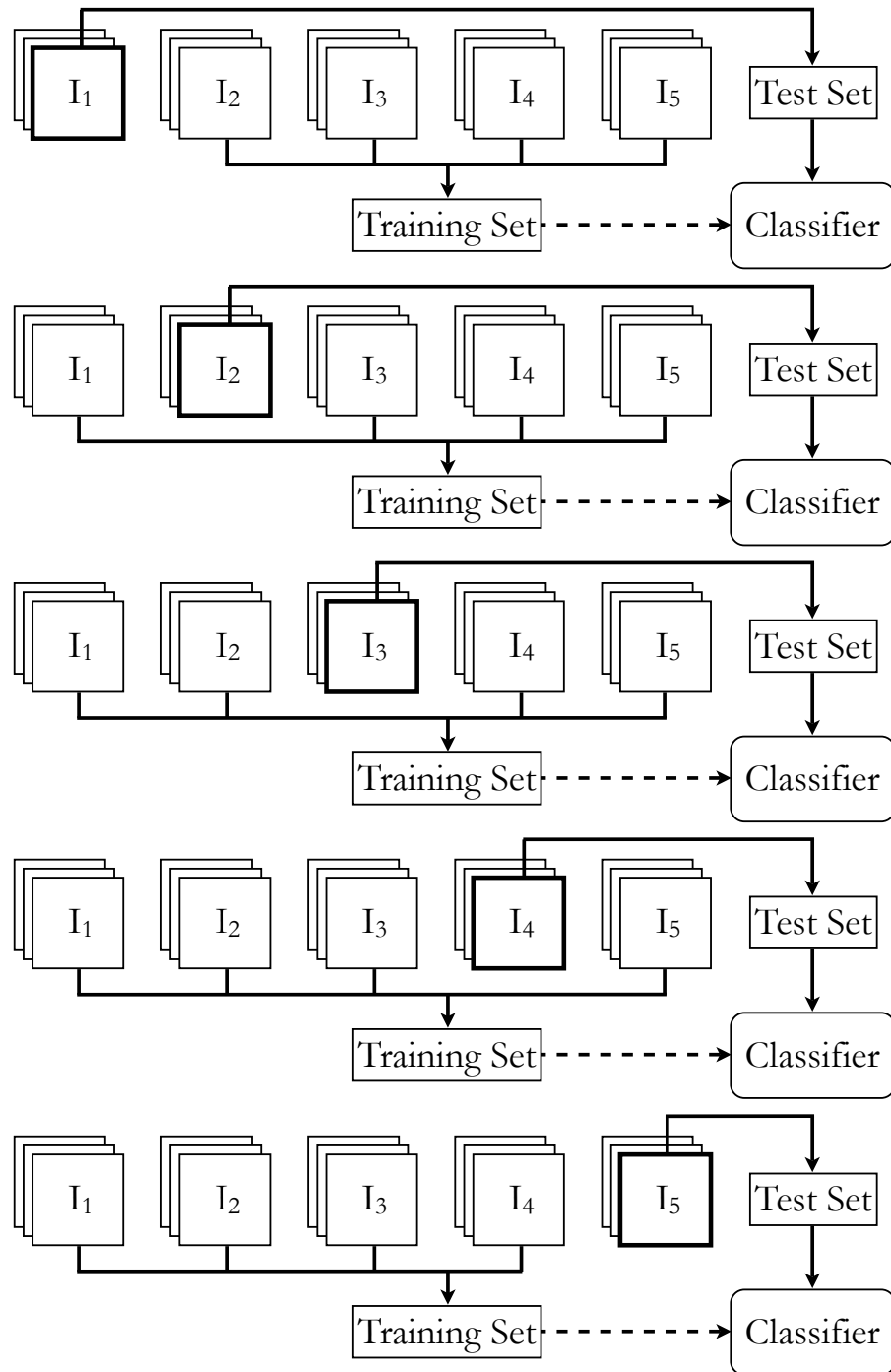


Figure 8.1: *Image-fold approach* followed in the experiments in order to induce the *sample selection bias* in the training process. Classifiers are trained using both labeled samples from the $N - 1$ out of N available images, and unlabeled samples from the image to be classified. The scheme depicts a 5-image-fold approach, where a different classifier is trained for each image. Finally, classification results on test are averaged for the 5 images to evaluate the robustness of the classifiers to the sample selection bias.

Table 8.1: Experimental setup and data used to develop the kernel classifiers and to obtain the cloud screening results.

Data Sets	
Input Features	All methods are applied to the vector of extracted features for each pixel: $\mathbf{x}_i = [f_{\text{Br,VIS}}, f_{\text{Br,NIR}}, f_{\text{Wh}}, f_{\text{O}_2}, f_{\text{WV}}]^\top$, which correspond to the target spectral brightness in the VIS and NIR, the target spectral whiteness, and the oxygen and water vapor atmospheric absorptions, respectively.
Labels (y_i)	Supervised information defining the labels (cloud/cloud-free) of the image pixels is obtained by applying a threshold of 0.05 to the <i>cloud abundance product</i> (cf. section 5.3.3), presented in Chapter 7: $y_i = \text{sgn}(\vartheta_i - 0.05)$.
Samples (\mathbf{x}_i)	10000 labeled samples covering the full range of ϑ values are selected from each image. These samples are used to generate the different training and validation sets used to develop and compare the models.
Clusters (ω_k)	The EM algorithm is applied to each image in order to obtain the clusters present in the image, together with the cluster membership h_{ik} , and assigned cluster h_i for each sample \mathbf{x}_i .
Training Set	A given number of samples is used to develop the models during the training process. For all models, a set of ℓ labeled samples $\{\mathbf{x}_i, y_i\}_{i=1}^\ell$ is used. For semi-supervised models, a set of u unlabeled samples $\{\mathbf{x}_i\}_{i=\ell+1}^{\ell+u}$ is also included in the training set. In the later case, we assume that the unlabeled samples come from the image to be classified, and their labels y_i are unknown, but their cluster membership h_i has been obtained. In the experiments, the number of unlabeled samples is fixed to $u = 800$ and we explore from ill-posed situations with only 4 labeled samples per class ($\ell = 8$) up to well-posed supervised cases with 200 labeled samples per class ($\ell = 400$). The best model for each experiment is selected by 10-fold cross-validation over the labeled training samples evaluating the averaged κ statistics.
Validation Set	An independent dataset of 5000 labeled samples from the test image is used to compare the performance of the classifiers. These samples are used to compute the κ classification accuracy of the different models but not to tune the free parameters of the models, i.e. validation samples are not used during the training phase since the best model is selected with the 10-fold cross-validation approach. In addition, in order to avoid skewed conclusions, we run all experiments for a number of realizations where the used training samples were randomly selected. Therefore, the validation results are averaged for 10 realizations in order to measure the robustness of the methods in the classification.
Test Set	The developed classifiers are finally applied to all the pixels of the test image in order to obtain the classification maps.

in Chapter 7. The training and validation sets are built in a different manner for each experiment depending on whether a *single-image approach* or an *image-fold approach* is followed. In addition, the number of labeled samples ℓ used to train the models is also different for each experiment. By decreasing the number of labeled training samples ℓ , one can analyze how the SSL methods efficiently exploit the information contained in the available unlabeled samples compared to the labeled samples. Regarding the validation results, in order to avoid skewed conclusions, we run all the experiments several times using randomly selected train samples, and the validation results, obtained over unseen data, are averaged for ten realizations in order to measure the robustness of the classification methods. Finally, the developed models are applied to all the pixels of the test image in order to obtain the classification maps.

8.2 Kernel Methods and Model Development

The kernel methods analyzed in this chapter are the supervised and semi-supervised classifiers presented in Chapter 6. The novel kernel methods based on the composite and mean kernels are benchmarked against the standard SVM, which is used as a reference for supervised methods (cf. 6.1), and the Laplacian SVM, which is used as a reference for semi-supervised methods as it is a general regularization framework that contains as particular cases several unsupervised and semi-supervised methods (cf. 6.2). The main characteristics of these methods (corresponding kernel and mapping functions) are summarized in Table 6.1. Here, a brief description of these methods, and the abbreviations and legend used in the results of this chapter are provided in Table 8.2. In addition to the standard SVM (denoted by “SVM on \mathbf{x}_i ”), the proposed methods are also compared with the classification results obtained when using the trained standard SVM (with kernel K) to classify the centers of the clusters ($\boldsymbol{\mu}_k$) and then assigning the same class label to all the samples belonging to the same cluster ω_k (denoted by “SVM on $\boldsymbol{\mu}_k$ ”). Note that this is the standard approach in unsupervised classification problems, where first a clustering algorithm is applied to the data and later clusters are classified. For all the experiments, we used the Radial Basis Function (RBF) kernel, $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma^2)$, where $\sigma \in \mathbb{R}^+$ is the kernel width for SVM, LapSVM, and μ -SVM, and can be different for K and K_μ . In addition, in the LapSVM, the graph Laplacian \mathbf{L} consisted of $\ell + u$ nodes connected using 6 nearest neighbors, and the edge weights W_{ij} are computed using the Euclidean distance among samples.

The parameters of the maximum-margin hyperplane defining a linear classifier in the kernel space are derived by solving the corresponding quadratic programming (QP) optimization problem in its dual form. For all the analyzed kernel methods, the dual optimization problem is solved by using the LibSVM software package (Chang and Lin, 2001), which follows a sequential minimal optimization (SMO) procedure. In order to adjust the free parameters of the SVM (C, σ), μ -SVM (C, σ, ν), and LapSVM ($\gamma_L, \gamma_M, \sigma$), a cross-validation strategy with ten folds in the training set is applied. A summary of the parameters to be tuned during the training process is provided in Table 8.2, indicating also their variation range. Once classifiers are trained and adjusted, they are

Table 8.2: Summary of the analyzed kernel methods and the parameters to be tuned during the training.

Kernel Methods (see Table 6.1)		
SVM on \mathbf{x}_i	$\cdots\cdots K_{\ell \times \ell}$	SVM trained with the ℓ labeled samples and applied to each sample \mathbf{x}_j to obtain its class label: $K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$.
SVM on $\boldsymbol{\mu}_k$	$\cdots\cdots K_{\ell \times \ell}$	SVM trained with the ℓ labeled samples but applied to each cluster center $\boldsymbol{\mu}_k$ in order to obtain its class label that is propagated to all the samples belonging to this cluster: $K(\mathbf{x}_i, \boldsymbol{\mu}_k)$.
LapSVM	$\cdots\cdots K_{n \times n}$	Laplacian SVM trained with the $n = \ell + u$ labeled and unlabeled samples of the training set (see 6.2 for details).
μ -SVM in \mathcal{X}	$\cdots\cdots K_{\mu}^{\mathcal{X}}$	Mean-Map SVM based on the cluster similarity in \mathcal{X} , i.e. computed between the cluster centers $\boldsymbol{\mu}_k$ in the input space: $K_{\mu}^{\mathcal{X}} = \langle \phi(\boldsymbol{\mu}_1), \phi(\boldsymbol{\mu}_2) \rangle$
	$\cdots\cdots K_{\omega}^{\mathcal{X}}$	Mean-Map SVM combining both the sample similarity and the cluster similarity in \mathcal{X} through composite kernels: $K_{\omega}^{\mathcal{X}} = \nu K + (1 - \nu)K_{\mu}^{\mathcal{X}}$.
μ -SVM in \mathcal{H}	$\cdots\cdots K_{\mu}^{\mathcal{H}}$	Mean-Map SVM based on the cluster similarity in \mathcal{H} , i.e. computed between the clusters S_k in the kernel space by using the mean map: $K_{\mu}^{\mathcal{H}}(S_1, S_2) = \langle \phi_{\mu}(S_1), \phi_{\mu}(S_2) \rangle$.
	$\cdots\cdots K_{\omega}^{\mathcal{H}}$	Mean-Map SVM combining both the sample similarity and the cluster similarity in \mathcal{H} through composite kernels: $K_{\omega}^{\mathcal{H}} = \nu K + (1 - \nu)K_{\mu}^{\mathcal{H}}$.
μ_s -SVM in \mathcal{H}	$\cdots\cdots K_{\mu_s}^{\mathcal{H}}$	Mean-Map SVM based on the cluster similarity in \mathcal{H} , i.e. computed between the clusters S_k in the kernel space by using the soft mean map: $K_{\mu_s}^{\mathcal{H}}(S_1, S_2) = \langle \phi_{\mu_s}(S_1), \phi_{\mu_s}(S_2) \rangle$.
	$\cdots\cdots K_{\omega_s}^{\mathcal{H}}$	Mean-Map SVM combining both the sample similarity and the soft cluster similarity in \mathcal{H} through composite kernels: $K_{\omega_s}^{\mathcal{H}} = \nu K + (1 - \nu)K_{\mu_s}^{\mathcal{H}}$.
Free Parameters		
SVM	Kernel width $\sigma \in \mathbb{R}^+$ of the RBF kernel, $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\ \mathbf{x}_i - \mathbf{x}_j\ ^2/2\sigma^2)$, was tuned in the range $\{10^{-3}, \dots, 10\}$. Regularization parameter C was varied in the range $\{10^{-1}, \dots, 10^2\}$.	
LapSVM	Kernel width σ was varied as in the SVM. γ_L and γ_M were varied in steps of one decade in the range $\{10^{-4}, \dots, 10^4\}$. The graph Laplacian L was computed using 6 neighbors.	
μ -SVM	Kernel width σ and C were varied as in the SVM. Weight ν was tuned in the range $\{0.01, \dots, 0.99\}$ for composite kernels.	

compared using the overall accuracy OA[%] and the kappa statistic κ as a measure of robustness in the classification over the validation set and the test image.

8.3 Semi-supervised Cloud Screening Validation Results

In this section, we show the validation results for the set of MERIS images presented in section 7.2.1 (four MERIS Level 1b images taken over Spain, Finland, and France) plus an image over Tunisia (TU-2004-07-15). For our experiments, we used as the input the 6 physically-inspired features extracted from MERIS bands normalized between zero and one: cloud brightness and whiteness in the visible (VIS) and near-infrared (NIR) spectral ranges, along with atmospheric oxygen and water vapor absorption features.

As mentioned above, we generated training sets consisting of $\ell = 400$ labeled samples (200 samples *per* class), and added $u = 800$ unlabeled (randomly selected) samples from the analyzed test data to the training set for the SSL methods. We focus on the ill-posed scenario and vary the rate of labeled samples, i.e. $\{2, 4, 7, 14, 27, 52, 100\}\%$ of the labeled samples of the training set were used to train the models in each experiment. In order to avoid skewed conclusions, for each value of ℓ , the experiments are run for ten realizations using randomly selected training samples. Then, classifiers are compared using the overall accuracy OA[%] and the estimated kappa statistic κ in the classification of 5000 independent validation samples.

8.3.1 Single-Image Approach Results

First, we are going to analyze the classification results when following the *single-image approach*, i.e. each test image is classified with a model built with labeled and unlabeled samples coming from the same test image. This procedure is aimed at comparing the different algorithms in an ideal situation where both training and test data come from the same distribution. Hence, one can assess which method learns best from the labeled samples, and how the semi-supervised methods take advantage of the available unlabeled samples. In the following paragraphs, we discuss results obtained for the single-image approach. Average results over ten realizations are shown in Fig. 8.2. Several conclusions are obtained from these plots.

Figure 8.2(a) shows the κ statistic for the five images obtained with the standard SVM. This plot provides us with a reference on how difficult is the classification problem or the cloud screening problem in each MERIS image. From the results one can conclude that the classification complexity of the images increases in the following order: Barrax (BR-2003-07-14) that presents a bright and thick cloud in the center of the image; Barrax (BR-2004-07-14) that presents small clouds over land and sea in the right part of the image; Tunisia (TU-2004-07-15) that presents clouds and bright desertic areas; France (FR-2005-03-19) that presents opaque clouds at south and north France, but also snowy mountains at various altitudes; and, finally, Finland (FI-2005-02-26), which presents cirrus clouds over the sea and the icy coast of Finland. Therefore, we

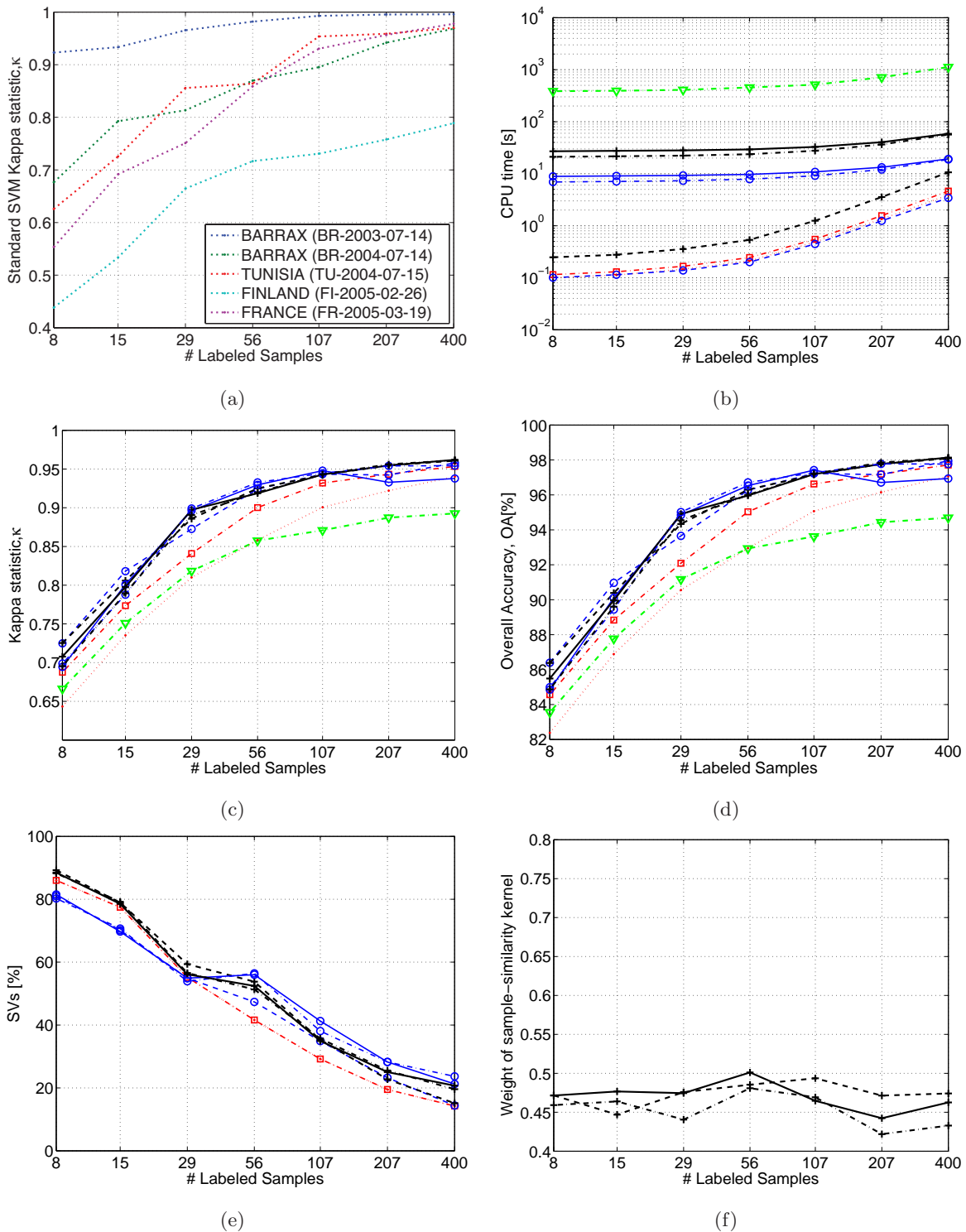


Figure 8.2: Average cloud classification results for the 5 MERIS sample images training the models with labeled and unlabeled (800) samples from the image to be classified (*single-image approach*): κ of the standard SVM for each image, CPU time [s], $\text{avg}(\kappa)$, $\text{avg}(\text{OA})$, SVs[%], and weight ν of the sample-similarity kernel of labeled samples K . Symbols correspond to the legend in Table 8.2.

are including in the experiments both easy cloud screening problems, where few labeled samples are enough to obtain accurate classifications, and extremely complex cloud screening scenarios, where a reasonable number of labeled samples is required to correctly detect clouds when using a standard supervised classifier. In the remaining plots of Fig. 8.2, the results obtained for these five scenes are averaged in order to discover which method performs best in most of the scenarios.

Figure 8.2(b) shows the average CPU time consumed by each method during the training phase. All experiments were carried out in a 64-bit dual-core Intel[®] Xeon[™] CPU 2.80GHz processor under Linux, and all methods are based on MATLAB implementations with a QP/SMO algorithm programmed in C++ (Chang and Lin, 2001). In this plot, three groups of methods are easily distinguished. Firstly, the best performance in terms of CPU time is obtained by the standard SVM and the μ -SVM in \mathcal{X} , which only require to compute the kernel matrix for the labeled samples $K_{\ell \times \ell}$. In fact, $K_{\mu}^{\mathcal{X}}$ method is slightly faster than the SVM since it only computes the kernel matrix over the cluster centers μ_k in the input space ($K_{\mu}^{\mathcal{X}} = \langle \phi(\mu_1), \phi(\mu_2) \rangle$) and the number of clusters c in the image is usually much lower than the number of labeled samples ℓ . On the other hand, $K_{\omega}^{\mathcal{X}} = \nu K + (1 - \nu)K_{\mu}^{\mathcal{X}}$ is slightly slower than these methods since the weighting parameter ν is also tuned during the training phase. Secondly, the proposed μ_s -SVM classifiers in \mathcal{H} provide an acceptable performance but are slower than previous methods since, in order to compute the similarity between clusters in the kernel space $K_{\mu}^{\mathcal{X}}$, they have to compute the kernel matrix for the labeled and unlabeled samples $K_{(\ell+u) \times (\ell+u)}$. However, this difference is reduced when the number of labeled samples ℓ approaches the number of unlabeled samples $u = 5000$. Again, the weighted versions of the μ -SVM ('+' markers) are slower than the versions based on clusters exclusively ('o' markers) because of the tuning of ν . Finally, LapSVM is around a thousand times more demanding than SVM in terms of CPU time, and a thousand times more demanding than μ -SVM. It can be explained because the training of LapSVM models requires tuning more free parameters than in the SVM case, but the main problem is that a $(\ell+u) \times (\ell+u)$ matrix consisting of labeled and unlabeled samples must be inverted.

Figures 8.2(c) and 8.2(d) show the average κ and OA for all the methods. The first conclusion extracted from the curves is that the proposed μ -SVM method clearly improves the results of the other methods. The mean kernels classifiers produce better classification results than the reference provided by the supervised SVM in all cases (note that SVM is a particular case of the μ -SVM for $\nu = 1$). These results are a consequence of taking into account the distribution of image data to define the clusters. In consequence, μ -SVM classifiers can be considered as a good trade-off between computational cost and classification accuracy. In addition, μ -SVM classifiers working in the kernel space provide slightly better results, supporting the idea that we can find a richer space \mathcal{H} for separating classes. In ill-posed situations, with a low number of labeled samples, the performance of μ -SVM in \mathcal{H} is reversed and μ -SVM in \mathcal{X} provide better results. This fact can be explained since, when working with a low number of labeled samples, v -fold cross-correlation techniques are less efficient at tuning the kernel width σ , which actually defines the mapping to \mathcal{H} . Therefore, the cluster similarity $K_{\mu}^{\mathcal{H}}$, computed only from the unlabeled samples in \mathcal{H} , is less

meaningful than $K_\mu^\mathcal{X}$, computed by using the cluster centers μ_k obtained when applying the EM algorithm to the whole image. We can also observe that the proposed method is not equivalent to a simple segmentation of the image by classifying the centers of the clusters (*red dash-dotted line*), that is, classifying μ_k is not a good option but still better than purely supervised SVM (*red dotted line*). This indicates that the EM clustering of the image provides a good image segmentation, which is mainly due to the physically-inspired extracted features described in Chapter 4. Finally, LapSVM classifiers produce worse classification results than SVM in some cases. In principle that is not possible since SVM is a particular case of the LapSVM for $\gamma_M = 0$. However, we explicitly avoid this combination by varying γ_L and γ_M in the range $\{10^{-4}, \dots, 10^4\}$. These results suggest that LapSVM assumes that considered problems hold a complex manifold, but distribution of remote sensing data and clouds, can differ to a great extent from a manifold, making the cluster assumption more suitable in these cases. Nevertheless, LapSVM performs better than the standard SVM when a low number of labeled samples is available and unlabeled samples help estimating the geometry of data.

Figure 8.2(e) shows the average percentage of support vectors (SVs) for each method, i.e. the number of labeled training samples used as SVs in the selected models. In these experiments, all SVM methods produce sparse models with low number of support vectors. Note that the LapSVM is not included in the analysis since it does not produce sparse models and all the training samples (both labeled and unlabeled) contribute to the final model. This fact makes LapSVM computationally expensive in both the training and test phases. The trend of all methods is coherent, since as the number of labeled samples in the training set increases, the rate of samples (SVs) required to correctly classify decreases. The only significant difference between methods is that, in ill-posed situations with a low number of labeled samples, the classifiers based on cluster similarity require less SVs since the class distribution is approximated by the cluster distribution. However, when increasing the number of labeled samples, simple spaces (such as that of SVM) increase sparsity, but also worsens models in terms of kappa.

Finally, Fig. 8.2(f) shows the relative weight ν of the sample-similarity kernel of labeled samples K with respect to the cluster-similarity kernel of the unlabeled samples in the selected $K_\omega^\mathcal{X}$, $K_\omega^\mathcal{H}$, and $K_{\omega_s}^\mathcal{H}$ models. The value of ν can be tuned by the user in the training process, but we have selected it through cross-validation in the training set. In these experiments, the sum of Hilbert spaces (i.e. different mapping and kernel functions) leads approximately to an average weighting as optimal solution ($\nu \sim 0.5$). Intuitively, this means that both the labeled information and the cluster information show similar importance in the classification. Hence, taking into account the excellent classification accuracy obtained in the experiments, we can conclude that both the labeled samples included in the training set and the clusters from unlabeled samples properly describe the class distribution in the test image. This situation is coherent in the context of the *single-image approach* followed to obtain the results presented in Fig. 8.2.

8.3.2 Image-Fold Approach Results

Now, we analyze the classification results when following the *image-fold approach*, i.e. each test image is classified according to a model built with labeled samples from the other 4 images and unlabeled samples coming from the same test image. This procedure is aimed at testing the robustness of the algorithm to differences between the training and test distributions.

Figure 8.3(a) shows the κ statistic for the five images obtained with the standard SVM. This plot provides us a reference of how difficult is the classification problem in each MERIS image, but now it also depends on how well are the labeled samples from the other images in the training set representing the classes in the test image. Now, the order of the images depending on its classification complexity is very similar: Barrax (BR-2003-07-14), Barrax (BR-2004-07-14), Tunisia (TU-2004-07-15), France (FR-2005-03-19), and Finland (FI-2005-02-26). Also poorer classification accuracy is obtained in all images as expected. However, it remains almost independent of the number of labeled samples, which indicates that, from the very beginning, labeled samples from other images roughly describe the type of clouds in the test image, and these situations do not improve by adding more labeled samples with the same information. Therefore, we can conclude that, following the proposed image-fold approach, the experiments for the five images are affected by sample selection bias problem. In the remaining plots of Fig. 8.3, the results obtained for these five scenes are averaged in order to discover which method performs better in most of the scenarios.

Figure 8.3(b) shows the average CPU time consumed by each method during the training phase. The results in this plot are almost identical to the results in Fig. 8.2, since the computational burden mainly depend on the amount and type of data, and the experiments were carried out in the same computer.

Figures 8.3(c) and 8.3(d) show the average κ and OA for all the methods. The situation now is completely different to the previous experiments following the single-image approach. Almost all the methods provide moderate classification results, and all of them provide poor results in ill-posed situations. However, a great difference can be observed between the μ -SVM classifiers based on clusters exclusively ('o' markers) and the rest. Several conclusions can be obtained from these curves. The standard SVM is affected by the sample selection bias and this can not be solved since it relies on the training labeled samples exclusively. When using the standard SVM to directly classify the centers of the clusters from the EM algorithm, classification results improve since, if the training and the test data are different, it is difficult to learn from training samples and then unsupervised approaches can be useful. Again, the main impediment is the SVM classifier used to label the cluster centers. The LapSVM provides moderate classification results, but generates better classification accuracy than the SVM in all cases since it incorporates in the solution the geometry of the unlabeled samples that come from the test image. The μ -SVM classifiers based exclusively on cluster-based approaches $K_{\mu}^{\mathcal{X}}$, $K_{\mu}^{\mathcal{H}}$, and $K_{\mu_s}^{\mathcal{H}}$ provide excellent results when there are enough labeled samples to describe the class conditional distribution of the clusters (with

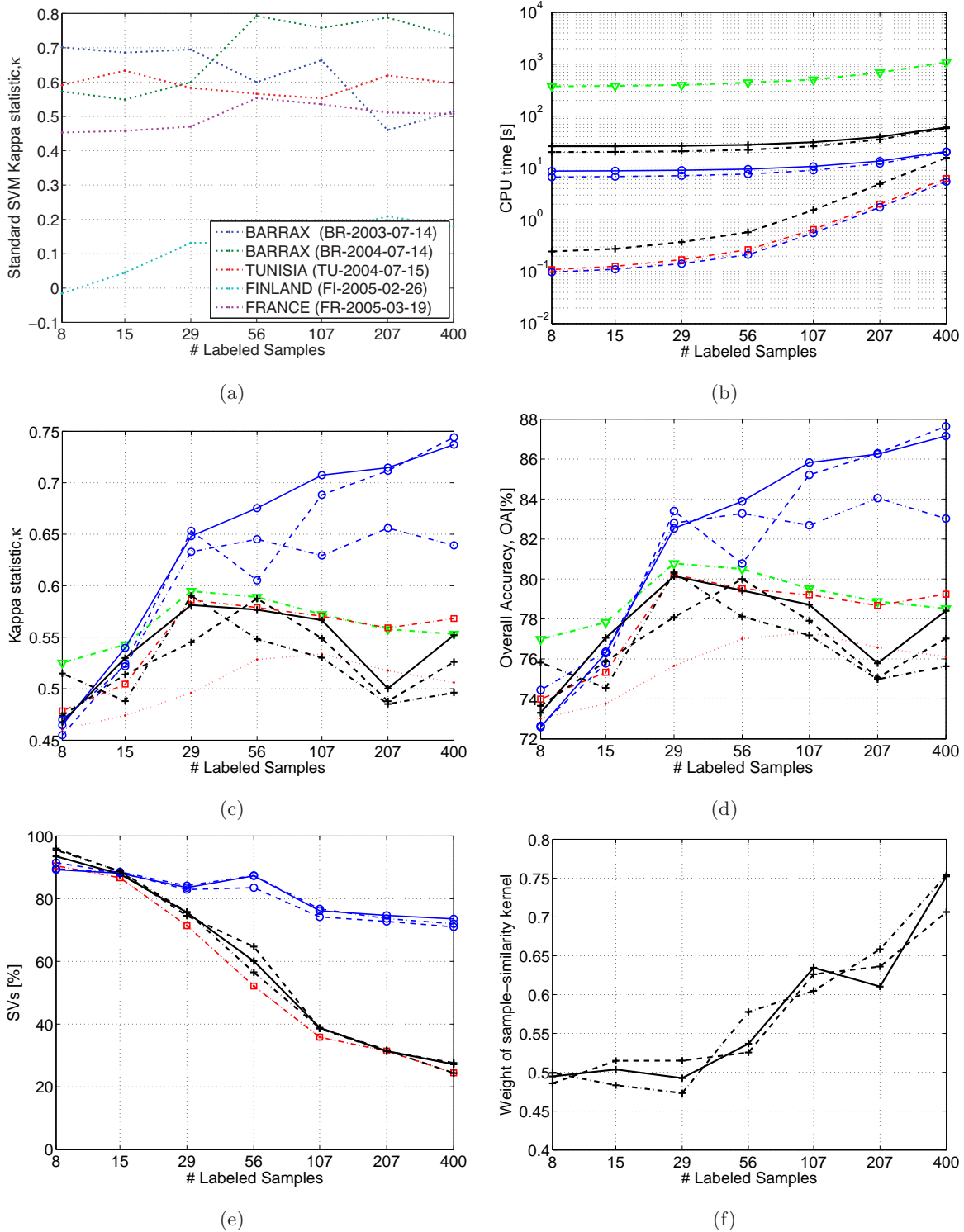


Figure 8.3: Average cloud classification results for the 5 MERIS sample images training the models with labeled samples from the other 4 images and 800 unlabeled samples from the image to be classified (*image-fold approach*): κ of the standard SVM for each image, CPU time [s], $\text{avg}(\kappa)$, $\text{avg}(\text{OA})$, SVs[%], and weight ν of the sample-similarity kernel of labeled samples K . Symbols correspond to the legend in Table 8.2.

few labeled samples a whole cluster can be misclassified). Among these three classifiers, $K_\mu^{\mathcal{H}}$ produce worse results. This can be explained since the selection of the mapping function to \mathcal{H} , i.e. the selection of kernel free parameters, depends on the classification accuracy in the training set. Therefore, an inappropriate training set produces an inappropriate mapping (in terms of class separability in test). As a consequence, $K_\mu^{\mathcal{H}}$ is more affected by the sample selection bias since all the unlabeled samples in the training set are used to compute the cluster similarity in an inappropriate kernel space. On the other hand, $K_\mu^{\mathcal{X}}$ is more robust to the sample selection bias because it approximates the cluster similarity to the similarities of the cluster centers μ_k already defined in the input space, and thus it is less dependent on how the unlabeled samples that represent the clusters are mapped into \mathcal{H} . In this context, $K_{\mu_s}^{\mathcal{H}}$ provides the best results and is also more robust to the sample selection bias because it uses the soft mean map to compute the cluster similarity in the kernel space. The soft mean map weights the contribution of each sample to the definition of the centre of mass of each cluster in the kernel space \mathcal{H} with the EM estimated posterior probabilities. This is equivalent to eliminate the samples that do not properly represent the cluster in the input space, and thus the estimation of the cluster center in \mathcal{H} is less influenced by the selection of an inappropriate mapping. Finally, the μ -SVM classifiers based on composite mean kernels $K_\omega^{\mathcal{X}}$, $K_\omega^{\mathcal{H}}$, and $K_{\omega_s}^{\mathcal{H}}$ (*black '+' lines*) produce significant worse results than the cluster-based approaches K_μ . These approaches combine both sample and cluster similarities and, intuitively, should produce better classification results than standard SVM (K) and K_μ , which are a particular case of K_ω for $\nu = 1$ and $\nu = 0$, respectively. Therefore, the divergence in the results should be explained because the tuning of ν , and we have to analyze also the selected ν value for the different experiments.

Fig. 8.3(f) shows the relative weight ν of the sample-similarity kernel of labeled samples K with respect to the cluster-similarity kernel K_μ . In this plot, we can observe that for a low number of labeled samples ($\ell \leq 30$) the sample-similarity and cluster-similarity has the same weight ($\nu = 0.5$), and then the weight of the sample-similarity kernel of labeled samples K increases exponentially with the number of labeled samples. As the number of labeled samples increases, K becomes more important than the cluster information (the exponential value of labeled samples in supervised classifiers is analyzed in detail by Castelli and Cover (1995)). However, the opposite behavior is observed in the classification accuracy (Fig. 8.3(c) and 8.3(d)) that starts to decrease when ν increases. As mentioned above, the labeled samples in the training set used to compute K come from different images and are affected by the sample selection bias. For this reason, high values of ν (more weight of K) produce worse values. The key point is why high values of ν are selected during the training. The reason is that ν has been selected through v -fold cross-validation in the labeled training samples, thus the selected model (ν , σ , and C) will be biased towards the training samples, which produces worse results in test if the training and test distributions are significantly different. It should be noted that the model selection in semi-supervised methods applied to problems affected by sample selection bias is not well-solved yet. A solution would be to select the best model by cross-validation in a labeled validation set coming from the image to

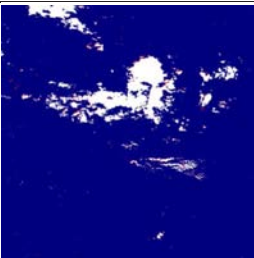
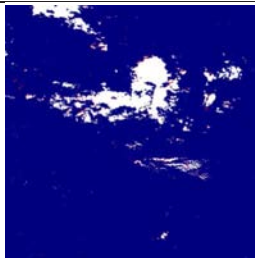
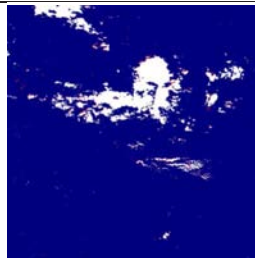
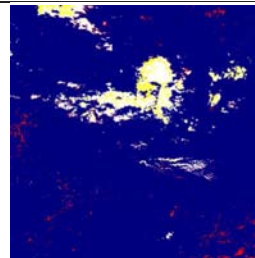
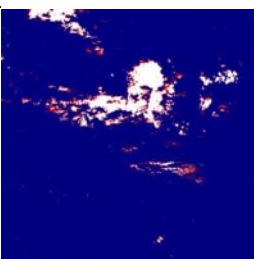
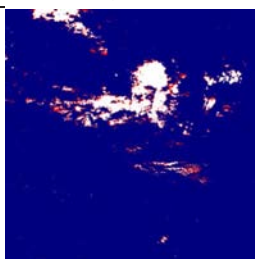
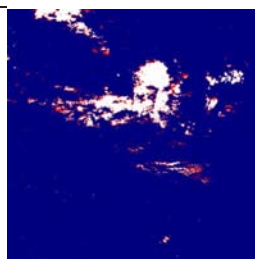
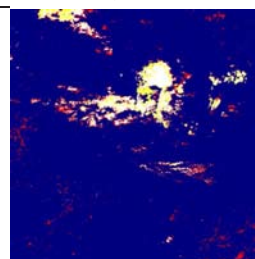
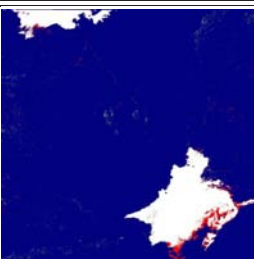
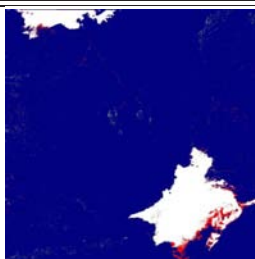
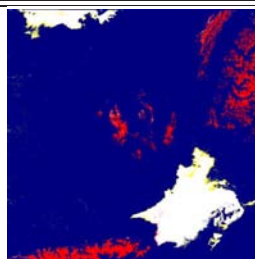
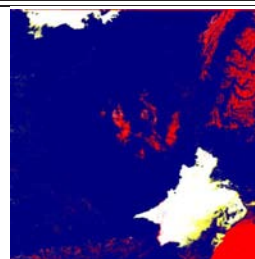
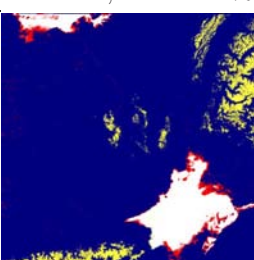
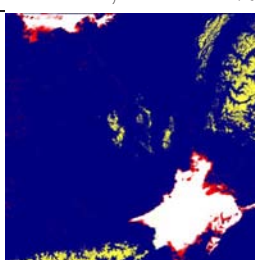
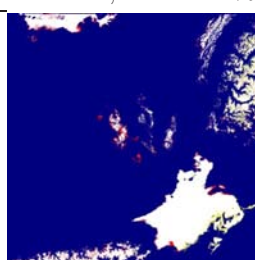
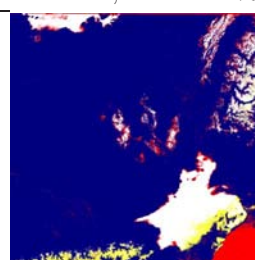
be classified, but this is an unrealistic situation since, in this case, these data can be used in the training. The results suggest that a trade-off is to equally weight the sample and cluster similarity ($\nu = 0.5$), which provides good results in standard semi-supervised scenarios (Fig. 8.2) and it is not biased towards the training set when dealing with sample selection biased problems (Fig. 8.3).

Finally, Fig. 8.3(e) shows the average percentage of support vectors (SVs) for each method. Again, most of the methods produce sparse models with low number of support vectors. The only exception are the three cluster-based methods that require more SVs to correctly weight the cluster similarities. Here we can clearly observe the trade-off between sparsity and accuracy, with the over-sparse solutions that provide low classification accuracy and the moderately sparse (80% over 400 samples) models that provide better classification accuracy. The high number of SVs in cluster-based methods can be explained since in this image-fold experiment the information (similarities) in K and K_μ are contradictory because the class distribution in training and the cluster distribution in test do not match. Hence, a higher number of samples is needed to find a maximum-margin hyperplane in the kernel space.

8.4 Comparison with MERIS Standard Products

Results shown in the previous section have been obtained by using the validation set (5000 labeled samples from the test image used to compare the performance of the classifiers). In this section, a quantitative and a visual analysis of the corresponding classification maps of the test images are carried out.

The obvious cloud reference to compare the results obtained by our algorithm is the official MERIS L2 Cloud Flag. However, it shows clear deficiencies, as reported by the user community elsewhere (Ramon et al., 2003; Brockmann, 2006), and by the MERIS Quality Working Group (MERIS Quality Working Group, 2006). In section 7.3, we assessed this poor performance of the MERIS L2 Cloud Flag when compared to the proposed user-driven cloud screening based on clustering and spectral unmixing (cf. Chapter 5). For this reason, we illustrate the proposed semi-supervised kernel methods in the same five scenarios presenting critical cloud screening problems, but now we compare it to the unsupervised cloud screening results shown in section 7.3. In addition, a further validation can be performed by comparing results with the *Cloud Flag* provided by the *Cloud Probability Processor* of the *Basic ENVISAT AATSR and MERIS* (BEAM) Toolbox (cf. section 2.4.1). With this approach we can compare our results against both an accurate cloud screening (in which the labeling of the clusters has been carried out by an operator) and an independent cloud screening (the BEAM Cloud Probability Processor is based on NN and uses the reflectance values as input). It should be noted that benchmarking the proposed kernel algorithms against a completely independent cloud screening method is relatively important in our case since the semi-supervised kernel methods use the same extracted features and cluster information than the unsupervised approach. In addition, the labels of the training set of the kernel methods are obtained from the *cloud abundance product* of the unsupervised approach.

		Single-Image Approach		Image-Fold Approach	
		$K_{\mu_s}^{\mathcal{H}}$	$K_{\omega_s}^{\mathcal{H}}$	$K_{\mu_s}^{\mathcal{H}}$	$K_{\omega_s}^{\mathcal{H}}$
BARRAX (easy)	User-driven Method	 $\kappa=0.96$; OA=99.5%	 $\kappa=0.93$; OA=98.7%	 $\kappa=0.96$; OA=99.5%	 $\kappa=0.75$; OA=96.9%
	BEAM Cloud Processor	 $\kappa=0.81$; OA=97.8%	 $\kappa=0.65$; OA=92.4%	 $\kappa=0.81$; OA=97.8%	 $\kappa=0.60$; OA=95.6%
FRANCE (difficult)	User-driven Method	 $\kappa=0.93$; OA=98.7%	 $\kappa=0.93$; OA=98.7%	 $\kappa=0.69$; OA=93.5%	 $\kappa=0.54$; OA=89.1%
	BEAM Cloud Processor	 $\kappa=0.65$; OA=92.5%	 $\kappa=0.65$; OA=92.5%	 $\kappa=0.90$; OA=97.8%	 $\kappa=0.66$; OA=91.1%

Proposed / Reference: Cloud / Cloud Land / Cloud Cloud / Land Land / Land

Color Legend Bar:



Figure 8.4: Comparison of the cloud mask of kernel methods proposed in Chapter 6 against two reference cloud flags obtained from the user-driven unsupervised method proposed in Chapter 5 (*top*) and the BEAM Cloud Probability Processor Flag (*bottom*) for the MERIS images over Barrax (BR-2003-07-14) and France (FR-2005-03-19). Discrepancies between methods are shown in red when proposed kernel methods detect cloud and in yellow when pixels are classified as cloud-free.

Figure 8.4 shows the comparison of the μ_s -SVM methods (both composite $K_{\omega_s}^{\mathcal{H}}$ and cluster-based $K_{\mu_s}^{\mathcal{H}}$ classifiers) against the cloud masks from the two cloud screening references. The cloud flag of the user-driven method is computed by applying a threshold of 0.05 to the *cloud abundance product* (cf. section 5.3.3), which in fact are the true labels for the trained models; and the flag of the BEAM Cloud Processor indicates cloudy when the NN output is higher than 20%, which is the lowest threshold recommended by the authors of the algorithm (Preusker et al., 2006). The images selected to illustrate the results are one image over Barrax (BR-2003-07-14) and the France image (FR-2005-03-19), which present different cloud screening problems and are differently affected by the sample selection bias problem. In the case of the unprojected MERIS FR images, the quarter scenes have 1153×1153 pixels (e.g. BR-2003-07-14) and the full scenes have 2241×2241 pixels (e.g. FR-2005-03-19). The selected images are classified using the best models (realization with best validation results) trained with 400 labeled samples for both the single-image approach and the image-fold approach (last point in the figures 8.2 and 8.3, respectively). Pixels where compared algorithms agree are depicted in *white* for the cloudy pixels and in *blue* for the cloud free pixels; discrepancies are shown in *yellow* and *red*. The agreement between both methods is expressed in terms of the overall accuracy (OA) and kappa statistic (κ) for the whole image.

Classification accuracies higher than 90% are obtained for most cases, but the lower values of κ for some cases reflect that classification results are unbalanced due to the misclassification of a significant number pixels of one class. Note that the overall accuracy is directly interpretable as the ratio of pixels being classified correctly, while the kappa coefficient allows for a statistical test of the significance of the divergence between two algorithms (Congalton and Green, 1999). The best kappa result (>0.9) for each experiment is bold faced. First, we are going to analyze the classification on the Barrax image, which represents an easy cloud screening problem. Looking at the comparisons with both the ‘User-driven Method’ and the ‘BEAM Cloud Processor’ references, one can observe that the kernel methods and the user-driven unsupervised method show a good agreement, while the BEAM product misclassifies the cloud borders (*red* pixels) where only our algorithms detect cloudy pixels. When comparing the two kernel methods with the user-driven reference, the cluster-based classifier $K_{\mu_s}^{\mathcal{H}}$ provides good results even in the image-fold approach, which means that training samples from the other images are useful to correctly classify the clusters found in the test image. However, the composite kernel classifier $K_{\omega_s}^{\mathcal{H}}$ works properly in the single-image approach, while results are worse for the image-fold approach, which means that the model is biased towards the labeled samples of the other images instead of to the cluster structure (see explanation of Fig. 8.3(f)).

The second image is the ‘France image’, which presents opaque clouds at south and north and also snow in the Alps, the Pyrenees, and the Massif Central. Attending to the image-fold experiments, μ_s -SVM methods agree with the user-driven cloud mask, and the discrepancies with the BEAM Processor show evidence of the errors committed by the BEAM Processor that misclassifies all the snowy areas as clouds. In the image-fold approach, neither the cluster-based classifier $K_{\mu_s}^{\mathcal{H}}$ nor the composite kernel classifier $K_{\omega_s}^{\mathcal{H}}$ produce an accurate cloud screening. This can

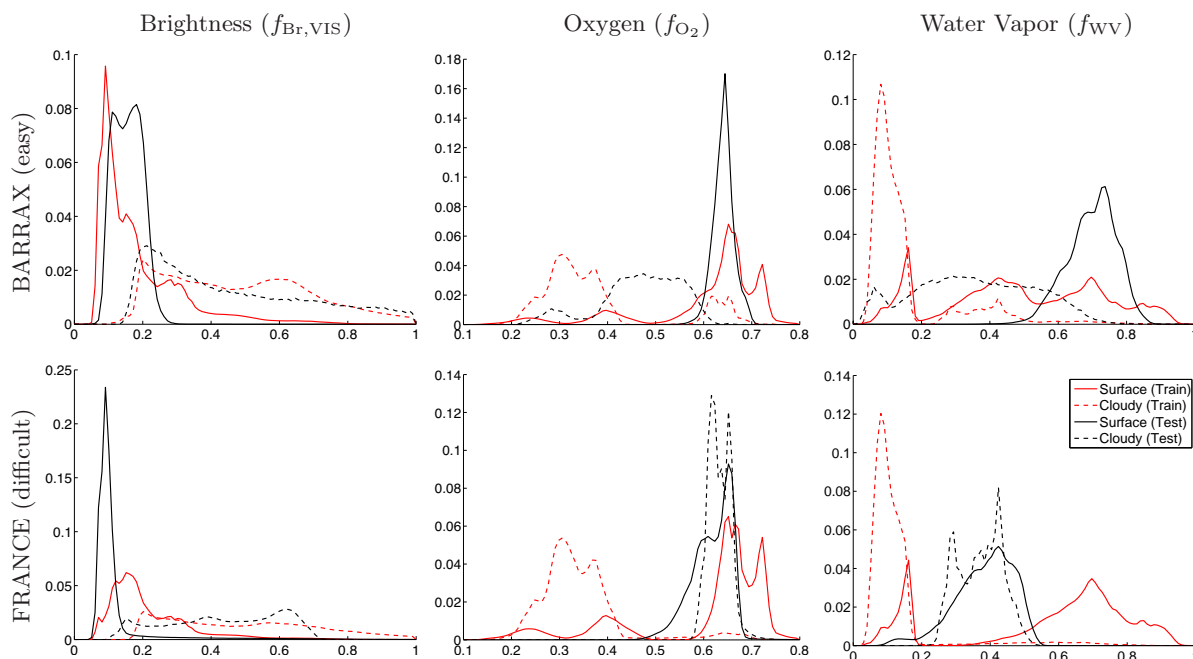


Figure 8.5: Comparison of the class conditional distributions of the brightness ($f_{Br,VIS}$, *right*), oxygen (f_{O_2} , *center*), and water vapor (f_{WV} , *left*) features for the MERIS images over Barrax (BR-2003-07-14, *top*) and France (FR-2005-03-19, *bottom*). The class conditional distributions are obtained from the normalized histograms of each class; and, in the case of the training distributions (*red* curves), the histograms of each experiment were obtained with all the pixels from the other four images (*image-fold approach*).

be explained since, in the image-fold approach, no training samples from the other images model the difference between clouds and snowy mountains, thus the classifier can not learn this difference (as probably happens with the NN trained for BEAM). Therefore, although the proposed semi-supervised methods benefit from the inclusion of unlabeled samples by estimating the marginal data distribution, these methods are limited by the quality of the available labeled information and can not alleviate situations with a dramatic sample selection bias problem.

Figure 8.5 illustrates the origin of the sample selection bias caused when the training set is formed by samples coming from images different to the image to be classified (*image-fold approach*). In this figure, the class conditional distributions (pdf) of some extracted features for the training images and test image are displayed. Two main conclusions can be extracted from these plots. On the one hand, the distributions of the two classes (*solid-line* for ‘Surface’ and *dashed line* for ‘Cloudy’) in the test image (*black* color) are more overlapped for all the extracted features from the France image, which confirms the higher difficulty to classify the France image than the Barrax image. On the other hand, the ‘Surface’ and ‘Cloudy’ distributions on training (*image-fold approach*, *red*) are much more different than the ‘Surface’ and ‘Cloudy’ distributions on test (*black*), respectively, for the case of France image classification. Summarizing, the France image is intrinsically more difficult to classify due to the class overlap, and it is more affected

by the sample selection bias due to the lack of representativeness of the test class conditional distribution in the training images.

8.5 Results on MERIS Temporal Series

Let us start by formally reviewing the main differences between the *single-image* approach and the *image-fold* approach in a multitemporal classification context. In multitemporal classification, one tries to classify the pixels of an image at the observation time t_N by using the available (instantaneous or previous) information $t \leq t_N$. In these experiments, we follow a cascade strategy for classification, i.e. only the previous acquired information is used to classify a given image. This strategy differs from a strategy in which the posterior images are also used. Therefore, under the semi-supervised learning framework, two main situations may arise, depending on the availability of information at the classification time $t = t_N$.

1. Labeled information is available only for $t < t_N$. This is the most common scenario and discourages the use of fully supervised classifiers, such as the SVM, that learn to discriminate classes at $t < t_N$ and then are used to extrapolate their predictions at $t = t_N$. This scenario is simulated in the experiments by a *multitemporal image-fold approach* where models are trained using both labeled samples from t_1 to t_{N-1} images, and unlabeled samples from the image to be classified t_N .
2. Labeled information is available for $t = t_N$. This *single-image* situation makes the use of supervised classifiers, such as SVM, more appropriate, but unlabeled data still can help in the classification when a reduced number of labeled data is available.

For the experiments, the temporal series of MERIS FR Level 1b images acquired over The Netherlands in 2003 are used to illustrate our approach. Most of the images are the same as in Fig. 7.5, but different dates/images are chosen since the criterion now is to select images with both cloudy and cloud-free areas. In addition, now we are not restricting ourselves to use one image per month in order to capture the phenological cycle of land covers. In fact, close dates are better suited for an image-fold approach since land covers should not change. Therefore, an uneven temporal series of 12 images is considered in the *multitemporal image-fold approach*: February 18th, April 22nd, April 23rd, May 28th, May 31st, June 6th, June 16th, August 6th, August 8th, August 9th, and August 12th. In addition, no co-registration or even projection of the images is required, since now we are not interested in land properties and the proposed multitemporal approach requires samples from different dates but not all the dates for a given location. In this context, the models are trained using both labeled samples from the t_{N-2} and t_{N-1} available images, and unlabeled samples from the image to be classified t_N , i.e. 2-image-fold approach where only the two closest previous images are used. Note that, following this approach, only ten images will be classified since the images of 18th February and 22nd April are only used

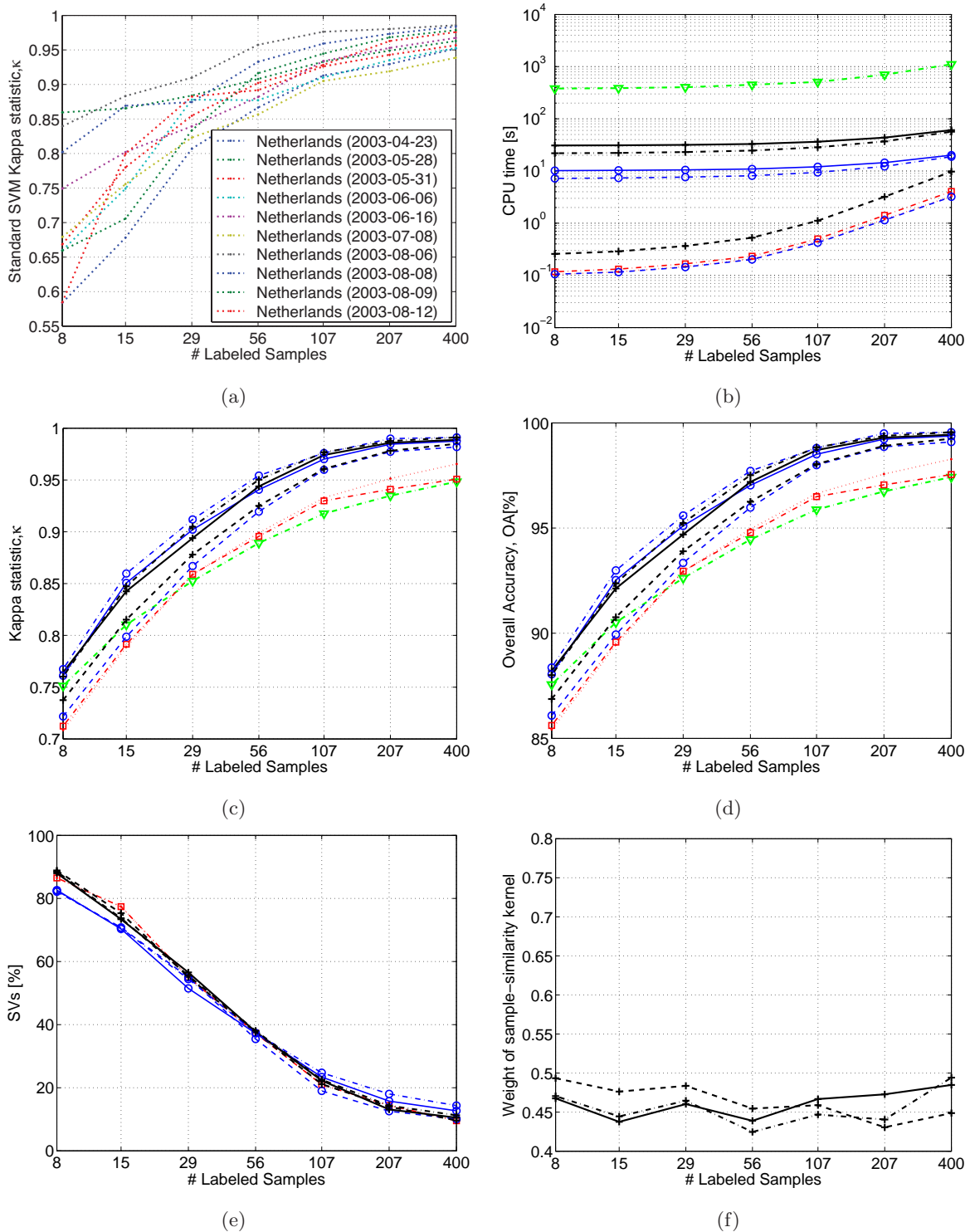


Figure 8.6: Average cloud classification results for 10 MERIS images over The Netherlands training the models with labeled and unlabeled (800) samples from the image to be classified (*single-image approach*): κ of the standard SVM for each image, CPU time [s], avg(κ), avg(OA), SVs[%], and weight ν of the sample-similarity kernel of labeled samples K . Symbols correspond to the legend in Table 8.2.

to generate the training set of 23rd April and half of the training set of 28th May. For additional details about the experimental setup see section 8.1 and for the used kernel methods and the model development see section 8.2.

The same procedure that in section 8.3 is followed in order to analyze the performance of the classifiers on the temporal series of MERIS images acquired over The Netherlands. Average results over ten realizations for different rates of labeled samples are shown in Fig. 8.6 and Fig. 8.7 for the *single-image* and the *image-fold* approach, respectively. Several conclusions can be obtained from these plots.

Figure 8.6(a) shows the κ statistic for the ten images obtained with the standard SVM, which indicates that the classification complexity of the images is almost the same except for ill-posed situations where semi-supervised methods should provide better results. In the remaining plots of Fig. 8.6, the results obtained for the ten dates are averaged in order to discover which method performs better in most situations. The discussion about the CPU time consumed by each method in Fig. 8.6(b) has already been done for Fig. 8.2. The average κ and OA for all the methods are shown in Fig. 8.6(c) and 8.6(d), respectively. The main conclusion extracted from the curves is that the proposed μ -SVM method clearly improves the results of the other methods, especially when the cluster similarity is computed in the kernel space \mathcal{H} by using the mean map. In fact, the μ -SVM classifiers follow a similar trend that the purely supervised SVM (*red dotted line*), which means that the labeled information is crucial to obtain accurate results, but the cluster structure of the test image properly adapts the classification mapping if the EM produces a good image segmentation. In the case of the LapSVM, different behaviors can be observed depending on the labeled samples. Only when a low number of labeled samples is available LapSVM performs better than the standard SVM thanks to the unlabeled samples that help estimating the geometry of data distribution. Finally, the percentage of SVs for all the methods (Fig. 8.6(e)) is almost the same since, in the single image approach, the class distribution is well-defined by the labeled samples in the training set and the same key samples are used in all the methods to define the class boundary. The gain in accuracy of the semi-supervised μ -SVM classifiers is not obtained by adding more labeled samples to the final model but taking also into account the similarities between the clusters of the selected SVs. This can be observed in Fig. 8.6(f) that shows how the sample-similarity K and cluster-similarity K_μ equally contribute in the best models ($\nu \sim 0.5$).

Figure 8.7 shows the classification results for the same images when following the *multitemporal image-fold approach*. The κ statistic for the ten images obtained with the standard SVM (Fig. 8.7(a)) evidences the decrease in the classification accuracy, which is also much more variable, due to the sample selection bias (i.e., in some cases, the labeled samples from the two previous images do not represent the classes in the test image). However, the worsening of the results now is lower than for the images of section 8.3 since the problems in contiguous images of the temporal series are similar (land covers, location, etc.). The CPU times in Fig. 8.7(b) are almost identical to the results in Fig. 8.2, since the computational burden mainly depends on the amount and type of data, and the labeled samples are the same and experiments were carried out in the same

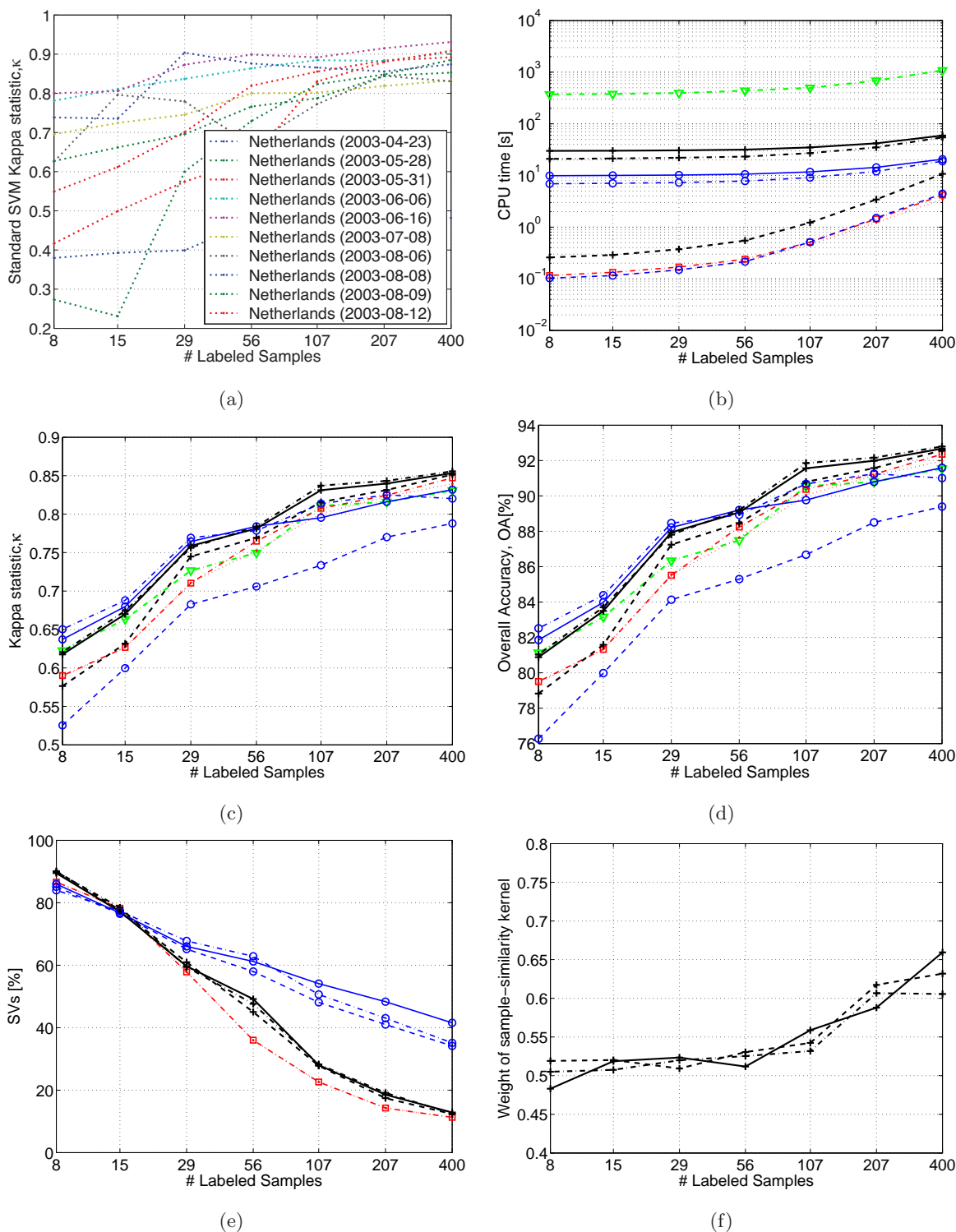


Figure 8.7: Average cloud classification results for 10 MERIS images over The Netherlands training the models with labeled samples from the two previous images over The Netherlands and 800 unlabeled samples from the image to be classified (temporal *image-fold approach*): κ of the standard SVM for each image, CPU time [s], $\text{avg}(\kappa)$, $\text{avg}(\text{OA})$, SVs[%], and weight ν of the sample-similarity kernel of labeled samples K . Symbols correspond to the legend in Table 8.2.

computer. Figures 8.7(c) and 8.7(d) show the average κ and OA for all the methods. Again, the situation is less dramatic than in the previous experiments of section 8.3 since the images of the temporal series are less affected by the sample selection bias problem. For this reason, although the mean classification accuracy is lower, the differences among methods are similar to those of the single-image approach in Fig. 8.6. Only for the μ -SVM cluster-based classifier K_μ^χ a significant lower classification accuracy is observed, which suggests that, for the image-fold approach, the centers of the clusters of previous images μ_k^{t-i} can not properly model the clusters of the test image and better results are obtained when computing the cluster similarity in the kernel space.

Regarding the average percentage of SVs in Fig. 8.7(e), the three cluster-based methods require more SVs to correctly weight the cluster similarities. This result agrees with the curves found for the previous image-fold experiments (Fig. 8.3), where the information (similitudes) in K and K_μ are contradictory because the class distribution in training and the cluster distribution in test do not match. Hence, a higher number of samples is needed to find the optimum classifier.

Finally, the relative weight ν of the sample-similarity kernel of labeled samples K with respect to the cluster-similarity kernel K_μ (Fig. 8.7(f)) shows the expected behavior for the image-fold experiments. Again, the weight of the sample-similarity kernel of labeled samples K increases exponentially with the number of labeled samples (with more labeled samples K becomes more important than the cluster information). Nevertheless, since in the temporal series of images the sample selection bias problem is not so hard, ν increases slowly with the number of labeled samples and the classification accuracy is less affected. Therefore, although the selected model (ν) is biased towards the training samples, results in test are not so bad because the training and test distributions are not so different.

Once the classification results over the validation set (5000 labeled samples from the test image used to compare the performance of the classifiers) have been discussed, the classification maps are generated for the ten test images. For the studied MERIS temporal series over The Netherlands, only MERIS FR Level 1b products are available. Therefore, it is not possible to compare the official L2 cloud flag with the cloud mask produced by the kernel methods. The cloud mask provided by the BEAM Cloud Probability Processor is available but, as we have shown in sections 7.4.2 and 8.4, this algorithm fails in some critical cloud screening problems. In consequence, we restrict ourselves to compare the classification maps of the composite mean kernel classifier ($K_{\omega_s}^{\mathcal{H}}$) with the user-driven cloud screening method that provides the most accurate ground truth (computed by applying a threshold of 0.05 to the *cloud abundance product*). The images are classified using the best model (realization with best validation results) trained with 400 labeled samples for the single-image approach (last point in Fig.8.6).

Figure. 8.8 shows the RGB color images for the temporal series of MERIS images with cloud covers over The Netherlands in 2003 together with the cloud mask provided by the proposed kernel method based on composite and mean kernels, $K_{\omega_s}^{\mathcal{H}}$. Note that the images are not projected in any geo-reference system and thus the image size of all the MERIS FR scenes is 2241×2241 and the

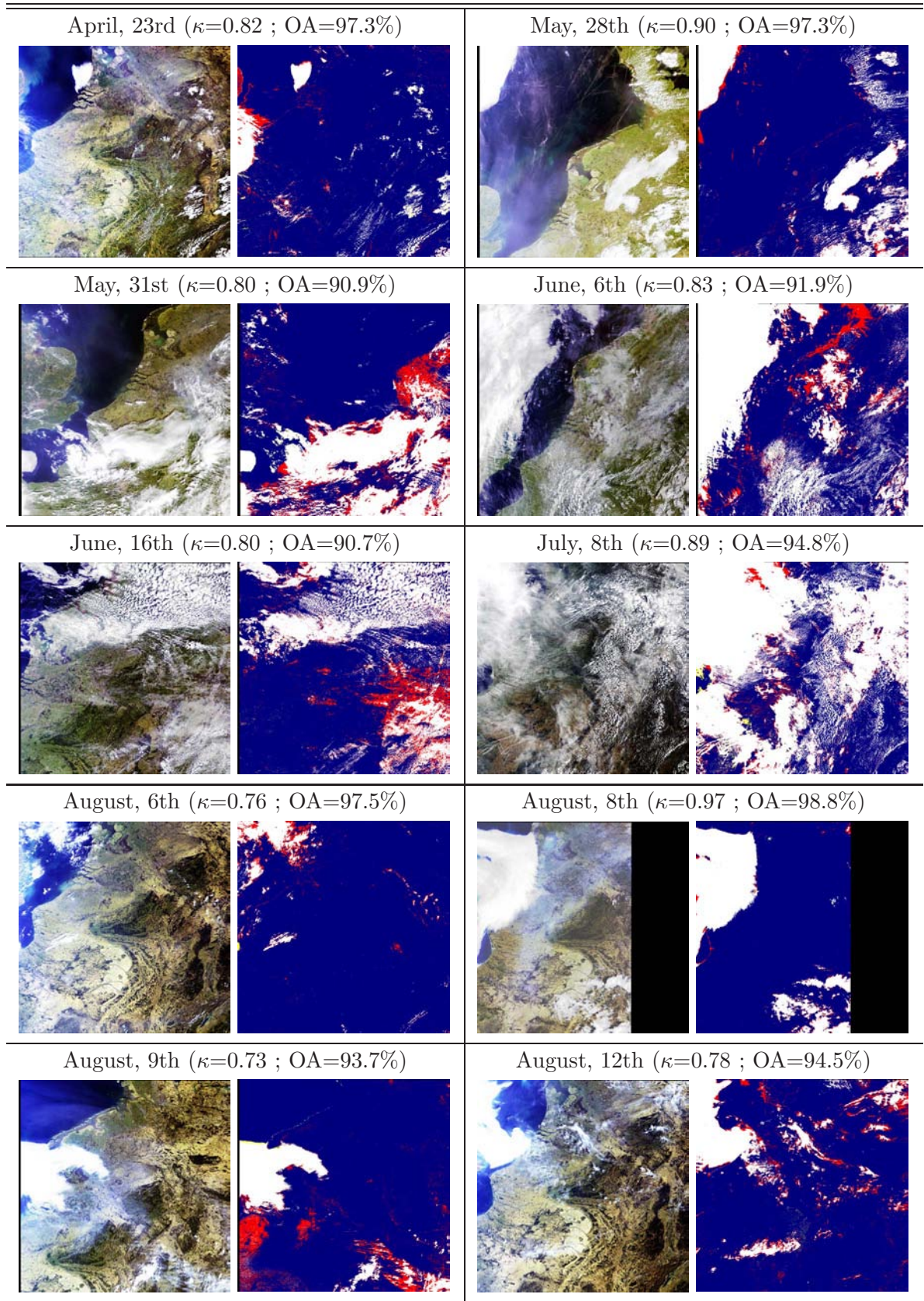


Figure 8.8: Cloud mask provided by the proposed kernel method based on composite and mean kernels, $K_{\omega_s}^{\mathcal{H}}$, for the temporal series of MERIS images with cloud covers over The Netherlands in 2003.

area displayed is not exactly the same. Pixels where compared algorithms agree are depicted in *white* for the cloudy pixels and in *blue* for the cloud free pixels; discrepancies are shown in *yellow* and *red*. The agreement between both methods is expressed in terms of the overall accuracy (OA) and estimated kappa statistic (κ) for the whole image. In the figure, we can appreciate the excellent classification accuracies higher than 90% obtained for all cases. Also κ shows balanced classification results higher than 0.7 even in the worst cases. In addition, one can observe that the kernel methods and the user-driven unsupervised method show an excellent agreement, and most of the discrepancies correspond to the cloud borders (*red* pixels) where it is really difficult to distinguish the level of cloud contamination in the measured pixel.

8.6 On the Relative Importance of Labeled and Unlabeled Samples

In the previous sections, performance of the supervised and semi-supervised kernel methods in different situations has been analyzed. In the experiments, we have explored the robustness of the classifiers to the number of labeled samples available during the training process; from ill-posed situations with only 4 labeled samples per class ($\ell = 8$) up to well-posed supervised cases with 200 labeled samples per class ($\ell = 400$). In addition, for the semi-supervised methods, the number of unlabeled samples (randomly selected from the analyzed test image) used in the training of the models is fixed to $u = 800$. However, in the case of semi-supervised learning, it is also interesting to analyze the capability of the different SSL methods to exploit the information contained in the wealth of unlabeled samples. Therefore, additional experiments have been carried-out, in which the number of both labeled and unlabeled samples is varied independently, in order to see how efficiently the classifiers learn from the unlabeled samples, and how much the classifier performance improves.

Fig. 8.9 shows the κ surface of the different methods as a function of the number of labeled (ℓ) and unlabeled (u) samples used in the training phase. Note that the variation of u is two times the variation of ℓ since unlabeled samples can be easily obtained from the test image. Moreover, all experiments consider a minimum number of one hundred unlabeled samples since the cluster-based methods require a proper representation of the clusters found in the test image in order to provide reasonable classification results (though this is not a critical requirement). The κ surface is shown for the standard SVM, the LapSVM, and the proposed μ_s -SVM classifiers $K_{\omega_s}^{\gamma_\ell}$ ($0 < \nu < 1$) and $K_{\mu_s}^{\gamma_\ell}$ ($\nu = 0$). It is worth noting that the SVM is a fully supervised method and it is only based on labeled samples. Therefore, the κ surface in Fig. 8.9(a) represents actually a single curve since it is independent on the number of unlabeled samples. Results in Fig. 8.9 illustrate only the *image-fold approach* since the value of unlabeled samples can be better evaluated when labeled samples do not perfectly define the class distribution in the test image (sample selection bias problem).

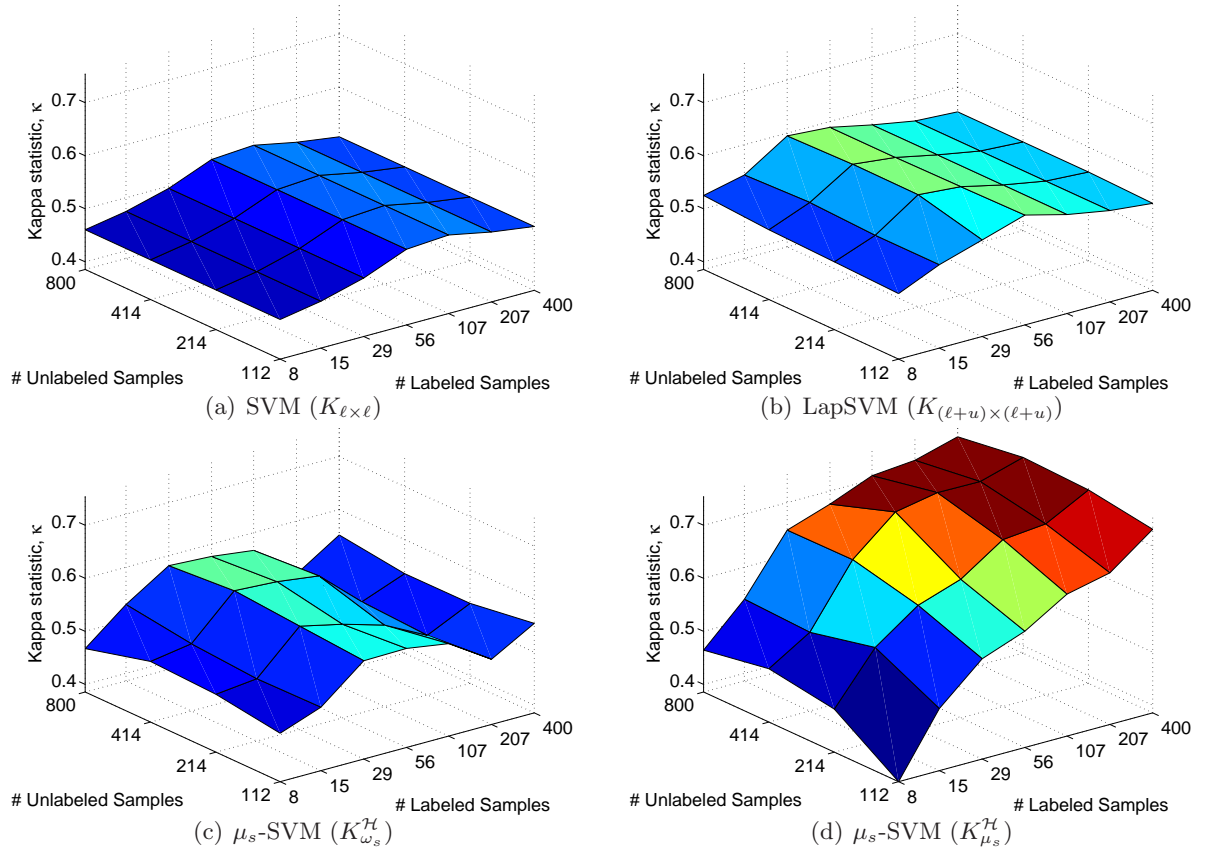


Figure 8.9: Average cloud classification results for the 5 MERIS sample images (BR-2003-07-14, BR-2004-07-14, TU-2004-07-15, FR-2005-03-19, and FI-2005-02-26) training the model for each image with labeled samples from the other 4 images and unlabeled samples from the image to be classified (*image-fold approach*): Kappa statistic surface over the validation set for the SVM, LapSVM, and μ_s -SVM as a function of the number of labeled (ℓ) and unlabeled (u) samples.

The κ surface for the standard SVM (Fig. 8.9(a)) provides us with a baseline of κ and shows its dependence on the number of labeled samples. This plot illustrates how the more supervised information is available (high ℓ), the more accurate should be the classification for all methods. However, due to the sample selection bias problem, when ℓ is high enough, the model is biased towards the labeled training samples, which produces worse results in test since the training and test distributions are significantly different. On Fig. 8.9(b), the κ surface for the LapSVM confirms, in general terms, the importance of the labeled information in this problem. The LapSVM benefits from the information of unlabeled samples, since it provides better results than the standard SVM in all cases. However, classification accuracy slightly improves with the number of unlabeled samples, which suggests a preference for the regularization of the classifier (supervised information) than for the regularization of the geometry of the marginal data distribution (unsupervised information). Finally, the κ surfaces obtained for both μ -SVM methods are significantly different. The $K_{\omega_s}^H$ classifier (Fig. 8.9(c)) is affected by the sample selection bias problem for high values of ℓ as the standard SVM. As explained in section 8.3.2, in the image-fold experiments, the $K_{\mu_s}^H$ model is

also biased towards the labeled training samples since ν is selected through v -fold cross-validation in the labeled training samples. On the other hand, $K_{\mu_s}^{\mathcal{H}}$ (Fig. 8.9(d)) confirms the importance of both labeled and unlabeled information in this problem. It uses both the labeled samples to fix a support for the class distribution, and the unlabeled samples to characterize (parametrize) the *marginal distribution* of data. The key point is that the proposed μ -SVM methods integrate the test data distribution through the cluster distribution of the test image, which has been estimated with the EM algorithm for GMM using the information contained in the high number of available unlabeled pixels (or even all the image pixels) and not only with the unlabeled samples included in the training set that the μ -SVM uses to determine cluster similarities.

The observed facts confirm the fact that semi-supervised learning methods require a much more unlabeled samples than labeled for a noticeable gain in the classification accuracy, as suggested by Castelli and Cover (1995, 1996) and Sinha and Belkin (2008). However, this implies an extremely high computational cost in kernel methods. We have mitigated these problems by using the EM algorithm as a preprocessing stage of the μ -SVM (note that the simplest and best understood situation is when the data is described by an identifiable mixture model and each class comes from a pure component). This approach falls in the field of *cluster kernels*, which are focused on changing the representation given to a classifier by taking into account the structure described by the unlabeled data (Szummer and Jaakkola, 2002; Zhu and Ghahramani, 2002; Chapelle et al., 2003; Weston et al., 2005). We should note that even though the approach alleviates the problem, there is still more room for improvement in the form of ‘learned’ kernels for specific datasets, or by increasing the computational capabilities of kernel methods. We should stress here that novel, fast, and linearly scalable SSL kernel methods are still required for remote sensing applications. Recently, a great interest has been put on large scale kernel machines (Bottou et al., 2007).

Part IV

Conclusions

Chapter 9

Discussion and Conclusions

9.1 Summary and Conclusions

This Thesis presented a novel methodology in order to solve the challenging problem of cloud screening in optical Earth Observation images acquired by multispectral and hyperspectral spaceborne sensors working in the visible and near-infrared range of the electromagnetic spectrum. Sensors on board two European Space Agency environmental satellites are used in this work: the MEdium Resolution Imaging Spectrometer (MERIS), placed on board the biggest environmental satellite ever launched (ENVISAT); and the Compact High Resolution Imaging Spectrometer (CHRIS) hyperspectral instrument, mounted on board the technology demonstration mission PROBA.

The proposed methodology identifies clouds in the image and produces a cloud abundance map in order to quantify how cloud presence affects the measured spectra. The cloud screening algorithm is based on well-founded physical features, which are intended to increase separability between clouds and ground covers, and are extracted from the converted TOA reflectance in order to reduce dependence on illumination and geometric acquisition conditions. A significant effort has been done to correct and calibrate images from the selected sensors in order to ensure the quality of data. In this respect, a novel algorithm has been proposed for the pre-processing of push-broom hyperspectral sensors, which is especially relevant in the case of the CHRIS sensor.

The final objective has been to develop an accurate and automated set of tools for the discrimination of clouds. For this purpose, two different approaches have been proposed depending on whether the algorithm has to be applied on an operational basis to automatically classify a significant number of images, or the classification process can be driven by an operator to accurately identify even the most critical cloud screening problems. Both approaches use, as the starting point, an unsupervised clustering method based on the extracted features in order to adapt the cloud screening procedure to the situation of each image, mainly the atmospheric conditions, the background, and the existing cloud types. This step allows to easily discriminate

between cloud-free and cloudy regions, providing a cloud abundance product based on a spectral unmixing algorithm.

In the following paragraphs, several remarks and conclusions are drawn from the different modules and algorithms developed in this Thesis.

Image Pre-processing. The first step of the process is to correct remote sensing data in order to obtain an accurate TOA radiance signal. Note that correcting and compensating image data from uncertainties in sensor calibration makes data to be independent from the sensor system. This requires a deep understanding of the signals provided by ENVISAT/MERIS and PROBA/CHRIS imaging spectrometers in order to adapt the cloud screening algorithm, or even developing completely new correction algorithms.

- The smile effect produces small variations of the spectral wavelength of each pixel in the across-track direction that have a large impact on the oxygen absorption feature, which is extremely narrow. Therefore we have proposed a novel feature extraction algorithm that allows the introduction of the spectral shift on the MERIS response in our formulation.
- PROBA is a technology demonstration satellite and several noise reduction algorithms have been developed ad-hoc since CHRIS provides minimally preprocessed data.
- A new technique has been presented in order to detect pixels presenting drop-outs and correct them by making use of both spatial and spectral information of the drop-out pixel and its neighbors. Although it is a ‘cosmetic’ correction, it is needed since later processing stages are drastically affected by these anomalous pixel values.
- A new technique has been presented to reduce the coherent noise known as vertical striping, which is usually found in hyperspectral images acquired by push-broom sensors such as CHRIS. The main novelty of our proposal consists in reducing the vertical striping pattern using a new algorithm robust to surface changes.
- The proposed destriping approach has proven to be robust, stable, and permitted to successfully model the relationship of the sensor temperature with the magnitude and distribution of the vertical striping.

Feature Extraction. When working with remote sensing images at different times and locations, a desirable characteristic is having data independent of the image acquisition conditions. Converting TOA radiance data into TOA reflectance has the advantage that these data are corrected for seasonal and diurnal differences in solar position. Moreover, extracting appropriate physically-based features increases separability between clouds and ground covers, which improves the classification performance and allows a better understanding of the problem.

We should note that, in addition to the brightness and whiteness radiometric properties of clouds, one critical feature introduced in this work is the use of the atmospheric oxygen and water vapor absorption bands to improve cloud screening results.

- The use of atmospheric absorption in the oxygen-A band to infer cloud pressure, which is related to cloud-top height, is well-known in atmospheric studies. Here, we proposed a formulation to extract an atmospheric feature directly related with the optical path by using the exact pixel geometry.
- The oxygen absorption band is extremely narrow and, despite the high spectral and radiometric resolution of MERIS, small variations of the spectral wavelength of each pixel have a large impact on any variable derived from the oxygen-A. As mentioned, this spectral shift has been accounted for in order to correct the *smile effect*.
- In the case of CHRIS, the oxygen band is not so necessary because of CHRIS broader bandwidths. However, some CHRIS acquisition modes present an excellent characterization of the water vapor absorption.
- The maximum water vapor absorption (940 nm) is located outside the MERIS range but absorption at 900 nm is still valid for relative measurements inside the same image. Moreover, snow presents higher absorption than clouds at 900 nm and this behavior can be observed in the extracted feature.
- Results obtained by using these absorption features suggest that it would be advantageous to see those bands included in future sensors.
- Specifically, the study has led to a qualitative list of key issues and physical features which can potentially enhance cloud detection in remote sensing sensors working in the visible and near-infrared spectrum: the target spectral brightness and whiteness in the VIS and the NIR region, and the oxygen and water vapor atmospheric absorptions.

Cloud Screening. A central objective of the Thesis has been to provide new operational cloud screening tools for the derivation of cloud location maps from the selected sensors' data. In order to achieve this objective, advanced pattern recognition and machine learning techniques have been specifically developed.

- Two different cloud screening approaches have been proposed based on the assumption that the available unlabeled samples in the remote sensing images have to be exploited.
- An unsupervised cloud screening approach based on classical pattern recognition methods is proposed.

- Applying unsupervised clustering methods to the whole image allows us to take advantage of the wealth of information and the high degree of spatial and spectral correlation of the image pixels.
- The EM algorithm applied to the extracted features has shown an excellent ability to segment the image pixels allowing to easily discriminate between cloudy and cloud-free regions.
- A specific procedure has been defined to label the found clusters in order to assist an operator to identify even the most critical cloud screening problems in regional and case studies.
- Advanced semi-supervised learning methods are explored since they offer the opportunity of exploiting available labeled samples and the wealth of unlabeled samples. In this case, some supervised information is available and is used together with the unlabeled samples of the analyzed image to develop a classifier that provides the class of each pixel but taking also into account the image data distribution. Since class distribution is partially fixed by a training set, this method can be automatically applied to a large number of scenes in an operational mode.
- A novel family of kernel methods based on the composite and mean kernels is proposed and benchmarked to the standard SVM, which is used as a reference for supervised methods, and the Laplacian SVM, which is used as a reference for semi-supervised methods.
- The proposed mean-map SVM (μ -SVM) combines both the *sample similarity*, computed from the labeled samples in the training set, and the *cluster similarity*, computed from the unlabeled samples of the test image in the kernel space through composite kernels.
- With this approach, the *class distribution* of typically low number of labeled samples is adapted to the *data distribution* in the analyzed image estimated from the unlabeled samples. As a consequence, the proposed approach is more robust to the sample selection bias, which is a common statistical problem in real Earth Observation applications.

Cloud Abundance. One of the key requirements imposed to the proposed cloud screening methodology was to provide information about the contribution of clouds to the spectra of image pixels (for both transparent clouds or subpixel coverage situations). Therefore, an important aspect of the proposed cloud screening methodology is that it provides a cloud abundance product.

- The cloud abundance product provides maps with the level of cloud contamination on a per pixel basis instead of a binary classification.
- The cloud product map is obtained combining the cloud abundance, computed with a spectral unmixing algorithm, and the cloud probability, obtained from the clustering algorithm, by means of a pixel-by-pixel multiplication.

- The proposed approach combines two complementary sources of information processed by independent methods: the degree of cloud abundance or mixing (obtained from the spectra) and the cloud probability that is close to one in the cloud-like pixels and close to zero in remaining areas (obtained from the extracted features).
- The cloud abundance product can be used to better describe detected clouds (subpixel coverage, transparency, cloud type) and to generate cloud masks with different restrictive levels depending on the application.

Validation Approaches. The validation of cloud detection algorithms is not an easy task because there is no independent measurement with the same spatial resolution. For this reason, a significant effort has been required to validate results by using different techniques.

- The simplest approach consisted in validating the resulting products by visual inspection, comparing the final cloud mask and abundance with a false color composite of the images.
- In the case of MERIS, we also compared results with the official MERIS Level 2 Cloud Flag, comparing the cloud flag against the cloud mask produced by the presented method in terms of classification accuracy.
- A multitemporal validation approach has been proposed to test the performance of the cloud screening. Pairs of cloud-free and cloud-covered images over the same area have been used to detect cloud-pixels by identifying pixels with spectral changes between both dates.
- The advantages provided by an accurate cloud screening have also been shown for a sub-pixel land cover mapping application. In particular, the unmixing of MERIS FR time series have been shown to outperform the unmixing of single dates.
- We have also validated the abundance product against the cloud probability provided by the Cloud Probability Processor implemented in the BEAM Toolbox, which is the most similar cloud product available for MERIS data.
- In the case of the semi-supervised approach, more classical classification results (κ and OA[%] for all the methods) have been provided by using true labels and true maps to train and validate the classifiers.
- The proposed kernel methods have been benchmarked in two different conditions: first when few labeled training samples are available for characterizing the image to be classified; and second when no labeled training samples are available for the test image to be classified. In the later case, an image-fold experimental setup has been proposed in order to induce and analyze the so-called sample selection bias problem.

Results and Recommendations. Following these validation approaches, a series of experiments has been carried out to obtain a comprehensive collection of results. A wide database of images has been included in the study in order to take into account the different peculiarities of the problem (geographic location, date and season, type of cloud, and type of surface) for both sensors.

- Results have demonstrated that the proposed user-driven algorithm accurately classifies difficult cloud-pixels, especially thin cirrus clouds and clouds over ice/snow.
- Clear deficiencies have been observed in the MERIS L2 Cloud Flag over bright covers, such as bare soils, ice, and snow, which are classified as clouds; and more accurate results have been obtained by the presented method in thin transparent clouds and cloud borders, which are misclassified by the official ESA product.
- The algorithm has also been validated against a cloud mask obtained with a temporal change detection approach and, despite the fact that the proposed method only uses the information of the ‘cloudy image’, results show that our method offers a better discrimination of thin clouds and cloud borders. This accurate cloud screening algorithm enables a more efficient use of MERIS images and temporal series.
- The histograms of the proposed cloud abundance product show a smooth distribution, which differs to a great extent from the output of the cloud probabilistic NN implemented in BEAM toolbox that is concentrated around one, and thus provides a more useful information.
- The mean kernel classifiers produce better classification results than the reference provided by the supervised SVM and the semi-supervised LapSVM in all cases. Note that SVM is a particular case of the μ -SVM, which also takes into account the distribution of image data in order to define the clusters.
- Due to its relatively low CPU time consumed, the μ -SVM classifiers have a good trade-off between computational cost and classification accuracy.
- In addition, μ -SVM classifiers working in the kernel space provide slightly better results, supporting the idea that we can find a richer space \mathcal{H} for separating classes.
- In ill-posed situations, with a low number of labeled samples, the wealth of unlabeled samples helps to improve the performance of μ -SVM and to provide better results.
- The proposed μ -SVM method based exclusively on the cluster similarity is not equivalent to a simple segmentation of the image by classifying the centers of the clusters with a purely supervised SVM. We observed that its performance depends on the quality of the image segmentation provided by the EM clustering.

- In the case of the image-fold experiments, the standard SVM is drastically affected by the sample selection bias since it relies exclusively on labeled samples that do not represent the classes in the test image.
- A common problem for all the kernel methods is that the selection of kernel free parameters depends on the training set and thus it is drastically affected by the sample selection bias problem.
- The μ -SVM classifiers based exclusively on cluster-based approaches $K_{\mu}^{\mathcal{X}}$, $K_{\mu}^{\mathcal{H}}$, and $K_{\mu_s}^{\mathcal{H}}$ provide excellent results in the image-fold experiments. However, a sufficient number of labeled samples is required to describe the class conditional distribution of the clusters (with fewer labeled samples a whole cluster might be misclassified).
- The soft mean map is more robust to the sample selection bias because it weights the contribution of each sample to the definition of the centre of mass of each cluster in the kernel space \mathcal{H} with the posterior probabilities. This is equivalent to eliminate the samples that do not properly represent the cluster in the input space, and thus the estimation of the cluster center in \mathcal{H} is less affected by the selection of an inappropriate mapping.
- Results also suggest that a compromise solution in composite μ -SVM classifiers is to equally weight the sample and cluster similarity, which provides good results in standard semi-supervised scenarios, and it is not biased towards the training set when dealing with sample selection biased problems.
- Finally, results show a trade-off between model sparsity (number of SVs) and classification accuracy. Over-sparsified solutions provide low classification accuracy while the moderately sparse models provide better classification accuracy. Especially in image-fold experiments, a higher number of samples is needed since the information of class distribution in training and the cluster distribution in test do not match or are even contradictory.
- The main limitation of the proposed semi-supervised methods is that, although they benefit from the inclusion of unlabeled samples by estimating the marginal data distribution, the available labeled information cannot alleviate situations with a dramatic sample selection bias problem, such as in the shown cases of France or Finland images where ice and snow covers are not well-represented in the training set.
- In the case of temporal series of images, the sample selection bias problem is not that hard, and results in test are acceptable because the training and test distributions do not differ significantly.

Summarizing, a full principled cloud screening methodology has been proposed. The methodology is versatile and consists of an arrangement of different purpose-designed modules, which have been formulated in terms of operational algorithms that cover the essential requirements

for the cloud screening process. These modules can be updated to more advanced algorithms or modified to adapt to the characteristics of other sensors. Consequently, this procedure can serve to develop a cloud screening algorithm for other imaging spectrometers working in the VNIR spectral range with proper spectral characterization of the atmospheric absorptions, such as NASA's EO1/Hyperion, the future GMES/Sentinel-3 and EnMAP Earth observation missions, and the FLEX ESA Earth explorer proposal. In fact, an important outcome of this Thesis consists in a series of guidelines and recommendations provided for MERIS and CHRIS instruments, which may be useful for developing further missions and satellite sensors. Specifically, the study has led to a qualitative list of key issues and physical features which can potentially enhance cloud detection in remote sensing sensors working in the visible and near-infrared spectrum.

9.2 Further Work

The list of objectives proposed at the beginning of this Thesis has been completely fulfilled. However, the presented methodology for cloud screening opens many future directions of research due to its natural modularity. In this respect, our next steps are tied to the inclusion of further refinements addressed to enhance its robustness. For instance, the inclusion of dynamic thresholds might be useful to find the regions to analyze, while the inclusion of contextual and textural information might enhance the clustering module. Some other directions will consider the inclusion of sun position to relate cloud and shadow positions.

An important remark is that the methodology has been implemented to use self-contained information provided with MERIS or CHRIS level 1 products. This pre-requisite is one of the advantages of the proposed methods. However, in the experiments, we have discovered some difficulties of the automatic classifiers to distinguish bright surface covers at different altitudes from clouds, such as snowy mountains and ice at high latitudes. These problems cannot be completely solved with the information contained in the spectral range covered by MERIS and CHRIS, but sensors with narrower spectral channels beyond $1 \mu\text{m}$ have demonstrated good capabilities to detect clouds because of the magnitude of the water vapor absorption. For this reason, our new lines of research are tied to the synergistic use of complementary data coming from different sensors. For example, the presence of channels in the thermal infrared range enables detection based on thermal contrasts. Currently, we are defining and will implement a cloud screening scheme combining information from both AATSR and MERIS instruments on board ENVISAT. The simultaneous acquisition and similar spatial resolution allows the synergy of MERIS and AATSR. The inclusion of the AATSR SWIR band at $1.6 \mu\text{m}$ in the cloud screening scheme is of paramount importance (McIntire and Simpson, 2002). Also the presence of channels in the thermal infrared range (TIR) provided by AATSR in nadir and forward views enables cloud detection based on thermal contrast (Simpson and Gobat, 1996; Papin et al., 2002), and based on the spatial variability over oceans (Martins et al., 2002).

Furthermore, in the spectral range of $1.38\text{-}1.50 \mu\text{m}$, both thin cirrus clouds and lower-level

cumulus clouds can be seen, but the surface features are eliminated due to additional absorption of solar radiation by atmospheric water vapor between clouds and the surface cover (even in presence of ice or snow). New generation EO satellites, such as the Global Monitoring for Environment and Security (GMES) Sentinel 2 and 3 (European Space Agency, 2007), include dedicated bands specifically defined to perform an accurate cloud screening. Currently, we are also analyzing the benefits of including the so-called cirrus band ($1.38 \mu\text{m}$) in the cloud screening scheme in the frame of the preparatory studies for the FLEX Earth explorer proposal (Moreno, 2006).

Finally, it is worth noting that, although the proposed techniques have been developed with remote sensing applications in mind, some algorithms and breakthroughs can be applied to other fields related to data clustering and classification.

9.3 Achievements and Relevance

Applicability of the developed methodology is crucial for a successful outcome. In this sense, we should stress here the following achievements.

Cloud screening constitutes itself both a research and technical opportunity, which has led to important publications in the field, and attracted the interest of the international scientific community. Several publications cover the most relevant issues of this Thesis:

- The preprocessing of EO data from multispectral and hyperspectral sensors has led to different algorithms for noise reduction in (Gómez-Chova et al., 2006a; Gómez-Chova et al., 2008) and atmospheric correction in (Guanter et al., 2006a, 2007, 2008a).
- The presented method was tested in (Gómez-Chova et al., 2005b, 2006c, 2005a) on CHRIS Mode 1 hyperspectral images in order to propose and validate cloud detection methodologies in favorable spatial resolution (34 m) and number of bands (62 channels).
- Preliminary test of MERIS cloud screening was carried out in (Gómez-Chova et al., 2005c, 2006d, 2007a) by testing critical situations in cloud detection (e.g. ice/snow covers).
- Temporal series have been employed for cloud screening in (Gómez-Chova et al., 2006f, 2007c), subpixel classification through unmixing techniques in (Zurita-Milla et al., 2007), and classification of remote sensing data in (Camps-Valls et al., 2006b, 2008a).
- Theoretical background of the advanced kernel methods used in this Thesis is based on the carried out work in (Camps-Valls et al., 2004a, 2006d, 2008a).
- The performance of semi-supervised techniques such as the LapSVM and mean kernels has been analyzed in (Gómez-Chova et al., 2007b, 2008c) and (Gómez-Chova et al., 2008a), respectively.

The knowledge acquired about this multi-disciplinary field of research has led to the publication of three chapters in international books:

- *Hyperspectral Image Classification with Kernels* in “Kernel Methods in Bioengineering, Signal and Image Processing” Idea Group Publishing (Bruzzone et al., 2007).
- *Kernel Machines in Remote Sensing Image Classification* in “Intelligent Systems: Techniques and Applications” Shaker Publishing (Camps-Valls et al., 2008c).
- *Kernel Mean for Semi-supervised Remote Sensing Data Classification* in “Kernel methods for Remote Sensing Data Analysis” Wiley & Sons (Gómez-Chova et al., 2009).

Finally, the present Thesis is devoted to developing scientific as well as technical innovative tools. As a consequence, the Thesis is also framed in three different *European Space Agency* (ESA) contracts:

- *Development of CHRIS/PROBA modules for the BEAM toolbox* (ESRIN Contract No. 20442/07/I-LG). Currently, the method presented for the PROBA/CHRIS instrument is being implemented in ESA BEAM software as a part of a toolbox for the pre-processing of CHRIS/PROBA data. Particularly, the methods presented in section 4.1.2 and chapter 5 are being implemented as two different BEAM modules in the Work Packages “2.3 Noise Reduction Definition” and “2.4 Cloud Masking Definition” of the project, which are managed by the author of this Thesis. The decision of ESA to implement the proposed algorithms derived from this work for real application in the *Basic ENVISAT Toolbox for (A)ATSR and MERIS* (BEAM toolbox¹) is definitely a significant achievement and also demonstrates the interest and applicability of the pursued work.
- *Atmospheric Corrections for Fluorescence Signal Retrieval* (ESTEC Contract No. 20882/07/NL/LvH). The gained knowledge about cloud screening of hyperspectral images during the work carried out in this Thesis is being applied in this project (Guanter et al., 2008b) to define and implement a cloud screening scheme for the FLEX candidate mission. Cloudy pixels must be masked for fluorescence studies (Gómez-Chova et al., 2006b; Guanter et al., 2007; Guanter et al., 2007), as they may contaminate the retrieval of the fluorescence signal to be investigated. In the WP “3.1 Cloud screening method”, which is managed by the author of this Thesis, a method for the derivation of probabilistic cloud masks will be developed, and the expected improvements associated to the SWIR imager to be installed onboard FLEX platform will be estimated for descoping purposes.
- *MERIS/AATSR Synergy Algorithms for Cloud Screening, Aerosol Retrieval, and Atmospheric Correction* (ESRIN Contract No. 21090/07/I-LG). The extension of the work of this Thesis for the MERIS instrument is being investigated in the frame of this project

¹<http://www.brockmann-consult.de/beam/>

(North et al., 2008). The cloud screening method proposed in this project exploits the combined information of both AATSR and MERIS features in order to improve current cloud masking products of both sensors (Gómez-Chova et al., 2008b). The author of this Thesis is the principal investigator of this project at the University of Valencia and is responsible for the definition of a novel MERIS/AATSR synergy algorithm for cloud screening (WP 2.1) and all the related cloud issues. In addition, he participates in the *MERIS and AATSR Cloud Screening Working Group*, which was established by ESA in order to combine forces and use existing know-how to develop novel cloud screening approaches.

9.4 Acknowledgements

Besides the importance of the above mentioned outcomes, it is also necessary to acknowledge the institutions and projects related to this work that have made this Thesis possible. In particular, the author of this Thesis acknowledges the support by a PhD fellowship from the Spanish Ministry of Education and Science (Beca de postgrado FPU del Ministerio de Educación, Cultura y Deporte, AP2000-2838).

The author has also participated actively in several projects, related to the work described in this Thesis, that have supported the research carried out during these years. The following list briefly introduces these projects and the relation with this Thesis:

SMARTSPECTRA *Smart Multispectral System for Commercial Applications.*

“Multispectral systems with an affordable cost and proven robustness are needed in order to achieve a broad use of multispectral techniques in several commercial areas and applications. These sensors must have the capability to be integrated in currently established production systems. Moreover, they have to be flexible enough to be applicable a wide range of applications.”

In this project, a Smart Multispectral System was designed and implemented, developing different electronic and processing techniques to achieve a system with the above mentioned features (Vila et al., 2005). This provided us an excellent opportunity to apprehend the physics and electronics fundamentals of the different imaging spectrometer systems.

Project funded by IST, European Union (2002-2005)

IST-2001-37306

<http://www.smartspectra.com/>

ESA CATEGORY-1 *Development of an Expert Classification System for Urban Monitoring at Regional Scale Based on ASAR and MERIS data.*

“The objective of this project is twofold: on the one hand, to explore the capabilities of ENVISAT ASAR and MERIS data to map urban area at European scale; on the other

hand, and based on the results derived from the previous analysis, an expert classification system was prototyped being able to map urban areas over Europe on a regular basis.”

In this project, the operation modes, image acquisition, and data products of ASAR synthetic aperture radar and the MERIS multispectral imaging spectrometer were investigated in depth (Gómez-Chova et al., 2005d, 2006e). The author of this Thesis was the principal researcher of this project, which was carried out in the context of an ESA internship programme at the ESA-ESRIN research center.

Project funded by the European Space Agency (2003-2004)
ESA CAT-1 ID2489
<http://eopi.esa.int/>

SPARC *Technical assistance for CHRIS/PROBA measurements during Spectra Barrax Campaign (SPARC).*

“The SPARC field campaign is the frame for several activities, planned over Barrax (Spain) the summer of 2004, originated from the combination of a number of initially not connected initiatives: Field activities of the EU projects DEMETER, EAGLE and SMARTSPECTRA; MERIS/ASAR synergy studies within an ENVISAT AO project; MERIS validation activities within the framework of another ESA project; CHRIS/PROBA acquisitions and data analysis; MSG/SEVIRI validation activities under funding by EUMETSAT LSA SAF; Barrax as an additional site for VALERI activities; Background activities for vegetation fluorescence modelling and validation studies; Background activities for SPECTRA studies; and other national projects.”

This project represents the starting point for the research of this Thesis related to the CHRIS/PROBA signal acquisition, data calibration, and image correction, which lead to the development of a set of tools for processing CHRIS images (Gómez-Chova et al., 2008).

Project funded by the European Space Agency (2003-2005)
RFQ/3-10824/03/NL/FF
<http://gpds.uv.es/sparc/>

HYPERTEL *Contribution to the design of future Earth Observation ESA missions with optimal use of new hyperspectral sensors.*

“This project aims to contribute to the development of theoretical models for hyperspectral data interpretation, and to the implementation of multiangular geometric registration methods and atmospheric corrections, compression techniques, automatic classification and other elements in the Ground Segment of the SPECTRA mission. In addition, some aspects of design and enhancement of the acquisition tools will be developed. On one hand, the aim is to introduce computing elements in the sensor that carry out common image

corrections. At this stage, we will use the technology developed under the European project entitled “SmartSpectra” for the acquisition of remote sensed imagery. On the other hand, a complementary goal is the analysis and modeling of directional effects over the estimation of the Earth surface temperature at a global scale (from data supplied by on-board sensors, such as AATSR in ENVISAT, and SEVIRI in 2nd Generation Meteosat), but also at a local scale (from foreseen multiangular sensors in future ESA missions; e.g. SPECTRA).”

This project aimed at the incorporation of Spanish research teams to the start-up design stages of the future European Space Agency (ESA) missions. It allowed us to play an important role in the context of the preliminary hyperspectral and multi-angular future missions, or in the experimentation stage of current missions such as PROBA.

Project funded by the Spanish Ministry of Education and Science CICYT (2005)
ESP2004-06255-C05-02

HYPERCLASS *Advanced Methods for Hyperspectral Image Classification.*

“This project deals with the consolidation of knowledge and the state of the art in processing hyperspectral imaging, as well as proposing innovative remote sensing techniques. The study will take place through the research and development of techniques based on kernel methods and their implementation in a set of routines integrated in an hyperspectral image processing environment.”

This project allowed establishing the theoretical basis and investigate the experimental performance of the supervised kernel methodologies used in this Thesis such as the support vector machines with composite kernels (Camps-Valls et al., 2004a, 2006d, 2008a).

Project funded by the Generalitat Valenciana, Grups Emergents (2005-2006)
GVA/11/2005

SEN2FLEX *SENTinel-2 and FLuorescence EXperiment Campaign (SEN2FLEX).*

“The SENTinel-2 and FLuorescence EXperiment (SEN2FLEX) is a campaign that combines different activities in support of initiatives related both to fluorescence experiments (AIR-FLEX) for observation of solar induced fluorescence signal over multiple surface targets and to GMES Sentinel-2 initiative for prototyping of spectral bands, spectral widths, and spatial/temporal resolutions to meet mission requirements. Both initiatives require simultaneous airborne hyperspectral and ground measurements for interpretation of fluorescence signal levels (AIRFLEX), and simulation of an optical observing system capable to assess geo- and bio-physical variables and to classify target surfaces by spectral, spatial and temporal distinction (Sentinel-2).”

One of the aims of this project was the analysis of fluorescence signal retrieval (Alonso et al., 2008; Amorós-López et al., 2008a) from satellite remote sensing data in the frame of the

preparatory studies for the FLEX mission. This study has revealed that undetected clouds have a negative impact in the retrieval of vegetation fluorescence (Guanter et al., 2007), and have favored the assignment of several ESA projects in order to investigate the development of cloud screening methods to be applied to imaging spectrometers with high spectral resolution (Guanter et al., 2008b).

Project funded by the European Space Agency (2005-2006)
19187/05/I-EC, 17628/03/NL/CB, and 17336/03/NL/CB
<http://www.uv.es/leo/sen2flex/>

AC.INT. ES-IT *Classification of hyperspectral remote sensing images based on semi-supervised kernel methods.*

“Earth observation is a crucial aspect in today’s life. Nowadays, satellites offer many possibilities for the analysis of the Earth surface, such as the analysis of climate changes, urbanization, fire detection, coastal monitoring, water quality assessment, observation and detection of crop fields, detection of contaminants and pollution elements, temperature maps, etc. Despite the good capabilities of multispectral sensors (those with a reduced number of spectral channels or bands) to address these problems, in the last years the development of hyperspectral sensors has offered improved performance for the detection and classification of the Earth land-cover classes. The information contained in hyperspectral images allows the characterization, identification, and classification of the land-covers with improved accuracy and robustness. However, several critical problems should be considered in classification of hyperspectral data, among which: (i) the high number of spectral channels, (ii) the spatial variability of the spectral signature, (iii) the high cost of true sample labeling, and (iv) the quality of data. In particular, the high number of spectral channels and low number of labeled training samples pose the problem of the curse of dimensionality, (i.e. the Hughes phenomenon) and, as a consequence, result in the risk of overfitting the training data. These problems have been recently alleviated by the introduction of kernel classifiers. However, further improvement in the classification accuracy could be achieved by taking into account the information provided by the high number of unlabeled samples in the image. Recent years have seen considerable attention on semi-supervised learning, which differs from traditional supervised learning by making use of unlabeled data.”

The main objective and motivation guiding this project was to extend the use of kernel methods to the semi-supervised classification framework. Most of the new semi-supervised kernel methods proposed in this Thesis have been developed in the frame of this project, such as the Laplacian support vector machines (Gómez-Chova et al., 2008c) and the mean kernels (Gómez-Chova et al., 2008a).

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Acción integrada España-Italia: MEC/HI2005-0228

DATASAT *Development of an Integrated Processing System for Earth Observation Data, Applicable to Design of Future Hyperspectral ESA Missions.*

“One of the main current problems in Earth Observation satellite data exploitation is the development of appropriate algorithms for data interpretation and information extraction, as well as the optimization of such algorithms to allow a proper storage, indexing, processing and distribution of remote sensing data and products to the final user. At the same time, this optimization of advanced algorithms would have an impact on a better design of future sensors and Earth Observation systems to make more easy and efficient its data usage. This project intends to use the SPARC database (ESA campaigns for the simulation of future missions) to develop and validate new algorithms for the processing of remote sensing data, and to implement these algorithms in the processing chain of ENVISAT/MERIS-AATSR, CHRIS/PROBA, APEX, ARES, AHS, AIRFLEX and future missions in preparation such as FLEX (always in the context of systems with high spectral resolution).”

The aim was to contribute to the development of theoretical models for hyperspectral data interpretation, and to the implementation of geometric registration methods, cloud screening and atmospheric corrections, band selection techniques, automatic classification, estimation of biophysical parameters, among others. All such algorithms, including the ones of this Thesis, were validated thanks to the access to the SPARC data previously mentioned (Gómez-Chova et al., 2007a). The activities proposed in this project were under the scope and framework of on-going ESA projects, with guaranteed access to data and resources needed from ESA for such activities.

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ESP2005-07724-C05-03

<http://www.vision.uji.es/datasat>

Part V

Appendices

Appendix A

Acronyms

AATSR Advanced Along Track Scanning Radiometer

AERONET AErosol RObotic NETwork

AIC Akaike's Information Criterion

AOT Aerosol Optical Thickness

ATGP Automated Target Generation Process

ATLAS ATmospheric Laboratory for Applications and Science mission

AVHRR Advanced Very High Resolution Radiometer

AVIRIS Airborne Visible/Infrared Imaging Spectrometer

BEAM Basic ERS & ENVISAT (A)ATSR and MERIS

BRDF Bidirectional Reflectance Distribution Function

CCD Charge Coupled Device

CHRIS Compact High Resolution Imaging Spectrometer

COT Cloud Optical Thickness

CTP Cloud Top Pressure

DB Davies-Bouldin index

DEM Digital Elevation Model

DN Digital Number

DOY Day Of Year

ECMWF	European Center for Medium range Weather Forecasting
EM	Expectation–Maximization
EMR	ElectroMagnetic Radiation
EnMAP	Environmental Mapping and Analysis Program
ENVISAT	ENVIronmental SATellite
EO	Earth Observation
ERM	Empirical Risk Minimization
ERS	European Remote Sensing satellite
ESA	European Space Agency
EURECA	EUropean Retrieval CARrier mission
FCLSU	Fully Constrained Linear Spectral Unmixing
FLEX	FLuorescence EXperiment
FOV	Field Of View
FR	Full Resolution
FWHM	Full Width at Half Maximum
GETASSE30	Global Earth Topography And Sea Surface Elevation at 30 arc second resolution
GMES	Global Monitoring for Environment and Security
GMM	Gaussian Mixture Model
HDF	Hierarchical Data Format
IR	InfraRed
ISCCP	International Satellite Cloud Climatology Project
LapSVM	Laplacian Support Vector Machine
LCC	Land Cover Classification
LCA	Land Cover Abundances
LPF	Low Pass Filter
LSU	Linear Spectral Unmixing

LUT Look-Up Table

MAP Maximum A Posteriori Probability

MDL Minimum Description Length criterion

MERIS ME^Dium RE^Solution IM^Aging SP^Ectrometer

MERIS FR MERIS Full Resolution (300m)

MERIS RR MERIS Reduced Resolution (1200m)

MLC Maximum Likelihood Classifier

MIR Middle-InfraRed

MODIS Moderate Resolution Imaging Spectroradiometer

MODTRAN MODerate Resolution TRANsmittance

MOMO Matrix Operator Model

NASA National Aeronautics and Space Administration

NDVI Normalize Difference Vegetation Index

NIR Near InfraRed

NDOI Normalized Difference at Oxygen-A absorption Index

NN Neural Network

OA Overall Accuracy

ODH Optimal Decision Hyperplane

OLCI Ocean and Land Colour Instrument

pdf Probability Density Function

POLDER POLarization and Directionality of the Earth's Reflectances

PROBA PRoject for On-Board Autonomy

RBF Radial Basis Function

RGB Red-Green-Blue

RKHS Reproducing Kernel in Hilbert Space

ROI Region Of Interest

RR	Reduced Resolution
RT	Radiative Transfer
RTM	Radiative Transfer Model
RMSE	Root Mean Square Error
SAA	Sun Azimuth Angle
SAD	Spectral Angle Distance
SLST	Sea and Land Surface Temperature
SNR	Signal-to-Noise Ratio
SOLSPEC	SOLar SPECTrum spectrometer
SOSP	SOLar SPECTrum spectrometer
SPARC	SPECTra bARrax Campaign
SPECTRA	Surface Processes and Ecosystem Changes Through Response Analysis
SRF	Spectral Response Function
SRM	Structural Risk Minimization
SSL	Semi-Supervised Learning
SV	Support Vector
SVM	Support Vector Machine
SWIR	ShortWave InfraRed
SZA	Sun Zenith Angle
TM	Thematic Mapper
TIR	Thermal InfraRed
TOA	Top Of Atmosphere
TOC	Top Of Canopy
TSVM	Transductive Support Vector Machine
VIS	VISible
VISAT	VISualisation and Analysis Tool

VNIR Visible and Near InfraRed

VS Vertical Striping

VZA View Zenith Angle

WV Water Vapor

Appendix B

List of Notational Symbols

Symbols Introduced in Chapter 1

λ	wavelength	ν	frequency
c	speed of light	\hbar	Planck's constant
F_0	solar constant	$F_0(\lambda)$	solar spectral irradiance
$B(\lambda, T)$	Planck's distribution	k_B	Boltzmann's constant
Φ	radiant power	I	radiant intensity
A	area	ω	solid angle
F	irradiance	L	radiance
θ	zenith angle	ψ	azimuth
μ	$\cos(\theta)$	$1/\mu$	optical mass
β_e	volume extinction coefficient	τ	optical thickness or depth
\log	natural logarithm	e	base of the natural log
T	transmittance	ρ	reflectance
y	surface along-track dimension	x	surface across-track dimension
l	image-lines dimension	p	line-pixels dimension
N_l	number of image lines	N_p	number of pixels per line
b	image-bands dimension	N_b	number of spectral bands
$H(x, \lambda)$	optical system response	$S(p, b)$	CCD sensitivity
$I(l, p, b)$	image values	$a(p, b)$	calibration coefficients

Symbols Introduced in Chapter 4

$\nu(p, b)$	vertical striping factors	$\alpha(p, b)$	integrated line profile
f	profile frequency	A	profile amplitude
D	spectral distance	R	spatial filter response
λ_b	channel mid-wavelength	Λ_b	channel bandwidth

Symbols Introduced in Chapter 5

\mathbb{R}	real numbers	\mathbb{N}	natural numbers
\mathbf{x}	input feature vector	\mathcal{X}	input feature space
$\mathbf{x}^\top, \mathbf{X}^\top$	transpose of a vector/matrix	$\ \mathbf{x}\ $	squared norm
n	number of samples	d	number of input features
i	sample index	k	cluster index
ω_k	cluster k	c	number of clusters
$\boldsymbol{\mu}_k$	mean feature vector	$\boldsymbol{\Sigma}_k$	covariance matrix
$p(\mathbf{x} \boldsymbol{\Theta})$	probability density function	$\boldsymbol{\Theta}$	vector of parameters
$p(\mathbf{x} \omega_k, \boldsymbol{\Theta})$	conditional pdf	$P(\omega_k)$ or π_k	prior probability
\mathcal{L}	log likelihood	$\mathcal{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$	d -variate Gaussian
$P(\omega_k \mathbf{x}_i, \boldsymbol{\Theta})$	posterior probability	h_{ik}	posterior or membership
C	cloud	\overline{C}	cloud-free
h_{iC}	cloud probability	h_i	optimal cluster label
\mathbf{a}_i	vector of abundance fractions	\mathbf{m}_q	endmember
q	endmember index	Q	number of endmembers
a_{iC}	cloud abundance	ϑ_i	cloud product

Symbols Introduced in Chapter 6

$\mathbf{x} \in \mathcal{X}$	input and input space	$y \in \mathcal{Y}$	output and output space
$f(\mathbf{x})$	real-valued function	\mathcal{F}	class of real-valued functions
$R_{\text{emp}}(f)$	empirical risk	$V(f(\mathbf{x}), y)$	cost function
\mathcal{H}	Hilbert space	ϕ, φ	mapping functions to \mathcal{H}
\mathbf{w}	weight vector	b	bias
ξ	slack variables	C	regularization parameter
\mathcal{L}_d	Lagrangian dual problem	$\boldsymbol{\alpha}$	Lagrange multipliers
$\langle \mathbf{x}, \mathbf{z} \rangle$	inner product of \mathbf{x} and \mathbf{z}	$K(\mathbf{x}, \mathbf{z})$	kernel $\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$
ℓ	labeled training samples	u	unlabeled training samples
γ_L, γ_M	regularization parameters	$\boldsymbol{\beta}, \boldsymbol{\eta}$	Lagrange multipliers
\mathbf{K}	kernel matrix	\mathbf{L}	graph Laplacian
S	subset of training set	$\Phi(S)$	S in kernel space
$\phi_\mu(S)$	mean of S in kernel space	ϕ_μ	mean map
$K_\mu^\mathcal{X}$	mean kernel in \mathcal{X}	$K_\mu^\mathcal{H}$	mean kernel in \mathcal{H}
$K_{\mu_s}^\mathcal{H}$	smooth mean kernel in \mathcal{H}	K_ω	weighted kernel
σ	Gaussian width	κ	kappa statistic

Part VI

Summary in Spanish

Resumen

Esta Tesis aborda el problema de la detección de nubes en imágenes multispectrales adquiridas desde satélites por instrumentos que trabajan en el rango visible e infrarrojo del espectro electromagnético.

Los sistemas de observación de la Tierra observan nuestro planeta midiendo en diferentes longitudes de onda la radiación electromagnética reflejada por la superficie que cruza la atmósfera hasta el satélite. La cantidad de imágenes adquiridas todos los días por los instrumentos a bordo de los satélites de observación de la Tierra hace inevitable que muchas de estas imágenes estén cubiertas de nubes. Se estima que más de 60% del globo está cubierto por nubes. De hecho, las nubes son uno de los componentes más importantes de la atmósfera de la Tierra y que más afecta a la calidad de la señal electromagnética medida y, por tanto, también a las propiedades derivadas de ella. Desde el punto de vista operativo, las nubes son la fuente más significativa de error para la obtención de la reflectividad de la superficie y afectan a una amplia gama de aplicaciones en teledetección. Enmascarando en las imágenes las zonas afectadas por nubes, no es necesario descartar toda la imagen. Por otro lado, la observación de las nubes a escala mundial es un requisito fundamental para establecer un modelo adecuado del clima de la Tierra. Por tanto, las nubes se pueden ver como una fuente de error que hace que la imagen adquirida solo sirva parcialmente para obtener propiedades de la cubierta terrestre, pero también como una fuente de información que permite medir importantes parámetros climatológicos. En ambos casos es imprescindible disponer de un método que permita enmascarar de forma precisa las nubes presentes en las imágenes de sensores ópticos de teledetección. Como resultado, la detección de nubes representa una importante tarea en el preprocesado de cualquier imagen óptica de teledetección con el fin de garantizar una máxima precisión y fiabilidad en los resultados inferidos de la explotación de los datos.

En este contexto, esta Tesis está también dirigida a cubrir el creciente interés de la comunidad científica en dos sensores a bordo de dos de los satélites de la Agencia Espacial Europea (ESA). El primero es el *MEdium Resolution Imaging Spectrometer* (MERIS), instalado en ENVISAT que es el satélite medioambiental más grande jamás lanzado. El segundo es el *Compact High Resolution Imaging Spectrometer* (CHRIS), que es un instrumento hiperespectral único montado a bordo de la misión de demostración tecnológica PROBA.

El objetivo principal es el de proporcionar nuevas herramientas operativas de enmascaramiento de nubes que proporcionen mapas con la localización de las nubes a partir de las propias imágenes. Además, el método debe proporcionar mapas con la proporción de nube para cada píxel (en lugar de una clasificación binaria) para describir mejor las nubes (proporción, tipo, altura, superficie cubierta). Permitiendo así la estimación de parámetros biofísicos de la superficie a partir de las imágenes de satélite. El algoritmo de detección de nubes propuesto aprovecha la excepcional resolución espectral y radiométrica de MERIS o el gran número de bandas espectrales de CHRIS junto con la posición específica de la longitud de onda de alguna de sus bandas (como por ejemplo las que coinciden con las absorciones del oxígeno o el vapor de agua atmosféricos) que permiten mejorar la precisión de la detección de nubes.

Para alcanzar este objetivo, diferentes técnicas de reconocimiento de patrones y aprendizaje automático han sido específicamente desarrolladas en el marco de esta Tesis para la detección de nubes. Primero, se extraen de los datos características físicas significativas de las nubes para proporcionar a los algoritmos unas entradas con la mejor información posible. A continuación, se propone un algoritmo de detección de nubes partiendo de la suposición de que se debe explotar la riqueza de las muestras de las imágenes analizadas aunque no se disponga de información de su clase. Por lo tanto, se exploran métodos de aprendizaje no supervisado y semisupervisado. En primer lugar, la aplicación de métodos de agrupamiento (*clustering*) sobre la imagen completa nos permite aprovechar la riqueza de la información de la distribución de los datos y el alto grado de correlación espacial y espectral de los píxeles de la imagen. En segundo lugar, los métodos de aprendizaje semisupervisados ofrecen la oportunidad de explotar también las muestras etiquetadas disponibles.

La validación de los algoritmos de detección de nubes no es una tarea fácil ya que, por lo general, no hay medidas independientes y con la misma resolución que informen sobre la existencia o no de nubes en el momento de la adquisición de la imagen. Por estas razones, se ha de realizar un esfuerzo importante para validar los resultados usando diferentes técnicas: por medio de un análisis visual de las imágenes en color originales, comparando la máscara de nubes resultante con los productos oficiales de la ESA (*MERIS Level 2 Cloud Flag*) y empleando algoritmos de detección de cambios aplicados a series multitemporales.

Para concluir, un resultado importante de esta Tesis incluye la elaboración de un conjunto de directrices y recomendaciones para misiones futuras. En concreto, el estudio ha dado lugar a una lista cualitativa de las principales cuestiones y características físicas que pueden mejorar la detección de nubes en los sensores de teledetección que trabajan en el visible e infrarrojo cercano.

Visión General

Observación de la Tierra

La observación de la Tierra comprende aquellos procedimientos y metodologías científicas centradas en observar nuestro planeta por medio de la radiación electromagnética medida por sensores situados en plataformas espaciales. La información que proporcionan estos sensores representa escalas espaciales y temporales completamente diferentes de las obtenidas a partir de mediciones sobre el terreno. En particular, la teledetección óptica pasiva se basa en el estudio de la superficie por medio de la radiación solar reflejada por el área observada y transmitida a través de la atmósfera hasta llegar al sensor.

Los materiales en una escena reflejan, absorben y emiten la radiación electromagnética de diferentes maneras dependiendo de su composición molecular y su forma. La teledetección explota este hecho físico y tiene que ver con la adquisición de información a corta, media o larga distancia. La radiación adquirida por el sensor se mide en diferentes longitudes de onda, y la consiguiente firma espectral (*espectro*) se utiliza para identificar un determinado material o estimar parámetros biofísicos de la superficie. El campo de la espectroscopía se refiere a la medición, análisis e interpretación de esos espectros.

Efectos radiativos de las nubes

Sin embargo, la observación de la Tierra a partir de datos de teledetección implica tener en cuenta el acoplamiento de los efectos radiativos entre la atmósfera y la superficie. Si no hay atmósfera alrededor de la Tierra, la radiación solar sólo se perturba cuando alcanza la superficie. Por lo tanto, la radiación medida proporcionaría una representación de la superficie e indirectamente de la dinámica de la naturaleza. Sin embargo, la influencia de la atmósfera sobre la radiación en el visible (VIS) e infrarrojo (IR) es lo suficientemente fuerte como para modificar la señal electromagnética reflejada, causando la pérdida o corrupción de parte de la información transportada. La interacción de la radiación solar con los componentes atmosféricos consiste básicamente en procesos de absorción y dispersión. La absorción disminuye la intensidad de la radiación que llega al sensor, lo que provoca una pérdida en la luminosidad del objetivo observado, mientras que la dispersión actúa principalmente modificando la dirección de propagación.

En este escenario, las nubes son uno de los componentes más importantes de la atmósfera de la Tierra, y constituyen el núcleo central de este trabajo. La presencia de nubes, afecta drásticamente a la calidad y fiabilidad de las mediciones de la señal electromagnética y, por tanto, a la estimación de las propiedades de la superficie. La influencia correspondiente a las nubes depende de su tipo, cubierta, altura y distribución en el cielo. Por ejemplo, nubes gruesas *opacas* impiden la entrada de radiación en su camino a la superficie, mientras que nubes finas *transparentes* contaminan los datos con fotones dispersados en la dirección de observación o atenúan la señal eliminando

los fotones en su camino hacia el sensor. Como resultado, cualquier conjunto de imágenes de teledetección requiere una detección de nubes precisa en las primeras etapas de procesamiento, antes de la explotación de los datos, para garantizar una máxima precisión en los resultados derivados. Ésta es la base fundamental del enmascaramiento de nubes en la teledetección óptica: la detección de las nubes en la línea de visión del observador con el fin de determinar la utilidad de la señal reflejada por el objetivo.

Motivación de la Tesis

La identificación de las nubes en las imágenes de teledetección es una cuestión clave para una amplia gama de aplicaciones de la teledetección, especialmente en el caso de sensores que trabajan en el visible e infrarrojo cercano (VNIR) del espectro electromagnético. La cantidad de imágenes adquiridas todos los días por los instrumentos a bordo de los satélites de observación de la Tierra hace inevitable que muchas de estas imágenes presenten cubiertas nubosas, cuyo alcance depende de la estación y la posición geográfica de la región de estudio.

Por un lado, las nubes pueden ser vistas como una fuente de contaminación que hace que la imagen sea en parte inútil para evaluar las propiedades de la superficie. Sin una detección exacta de las nubes, las nubes no detectadas en la escena son la fuente más significativa de error para estimar la reflectividad real de la superficie y, por tanto, para la recuperación de parámetros biofísicos tanto oceánicos como terrestres. Enmascarando sólo las zonas de la imagen afectadas por nubes, no es necesario descartar toda la imagen, aumentando la usabilidad de los datos de teledetección y facilitando la realización de estudios multitemporales. Por otro lado, las nubes pueden ser vistas como una fuente de información importante para medir los parámetros climatológicos. La observación de las nubes a escala mundial es cada vez más importante en los aspectos climatológicos: las nubes contribuyen de manera significativa al balance de radiación global con un papel importante en la reflexión de la radiación directa, y las nubes delgadas son también responsables del efecto invernadero en la atmósfera. Como resultado, la teledetección por satélite de las nubes no es sólo un paso en el proceso de enmascaramiento de nubes, sino también un requisito para un adecuado modelado de el clima de la Tierra.

Objetivos de la Tesis

Atendiendo a las mencionadas necesidades y demandas, la presente Tesis aborda el problema fundamental en teledetección de desarrollar un conjunto de herramientas operativas, precisas y automatizadas para la discriminación de las nubes. Podemos distinguir distintos objetivos en este trabajo:

1. Analizar el problema de la detección de nubes bajo diferentes perspectivas. La naturaleza multidisciplinar intrínseca de este trabajo (en la intersección entre la física, la termodinámica, las telecomunicaciones, la informática y el aprendizaje máquina) nos permitirá

extraer diferentes características para un mejor entendimiento y modelización del problema.

2. Entender mejor las señales proporcionadas por los espectrómetros de imagen ENVISAT/MERIS y PROBA/CHRIS. En particular, PROBA es un satélite de demostración tecnológica cuyo sensor CHRIS proporciona datos mínimamente preprocesados. La adecuada corrección y calibración de los datos de CHRIS y MERIS es una cuestión clave para una adecuada detección de las nubes y también para cualquier otra aplicación.
3. Desarrollar un algoritmo de detección de nubes automático, robusto y operacional. El algoritmo debe principalmente proporcionar una máscara de nubes interpretable como la abundancia de nube en cada píxel.
4. Validar el algoritmo propuesto. Comparando los resultados del enmascaramiento de nubes con productos oficiales de los diferentes satélites y con la clasificación multi-temporal de las cubiertas de nubes en series de imágenes.
5. Proporcionar un conjunto de directrices y recomendaciones para el desarrollo de nuevos sensores y misiones de satélites.

Organización de la Tesis

Esta Tesis está organizada en cuatro partes: (1) una profunda revisión bibliográfica, (2) el desarrollo de un conjunto robusto de herramientas automatizadas para la detección de nubes, y (3) la evaluación de los algoritmos propuestos en situaciones reales:

- La primera parte del trabajo está dedicada a una revisión de los aspectos generales de la física y propiedades ópticas de las nubes junto con una recopilación de los métodos de detección actuales. En este primer paso se identifican los puntos fuertes y débiles de los algoritmos más representativos propuestos hasta la fecha.
- La segunda parte de este trabajo aborda la metodología propuesta para la generación de productos de nubes. En particular, para producir una máscara de probabilidad de nubes y obtener conocimiento de las características extraídas de las nubes.
- La tercera parte del trabajo se ocupa de la validación de la metodología propuesta y los productos de nubes. Una amplia base de datos de imágenes se ha incluido en el estudio con el fin de tener en cuenta sus diferentes características: ubicación geográfica (latitud / longitud); fecha y estación; tipo de nubes (cúmulos, cirros, stratocumulus), y tipos de superficie.
- La última parte del trabajo resume los objetivos conseguidos, examina las principales conclusiones, y proporciona recomendaciones para mejorar la detección de nubes en imágenes multispectrales para espectrómetros de futuras misiones de observación de la Tierra.

Teledetección Mediante Satélites de Observación de la Tierra

La teledetección óptica pasiva se basa en la radiación solar como fuente de iluminación. Esta radiación solar viaja a través de la atmósfera terrestre antes de ser reflejada por la superficie y de nuevo antes de llegar al sensor. Por lo tanto, la señal medida en el satélite es la radiación emergente del sistema *tierra-atmósfera* en la dirección de observación del sensor.

La reflectividad del objeto observado es el parámetro de interés, ya que caracteriza la superficie independientemente de los efectos atmosféricos y las diferencias estacionales y diurnas en la posición solar. Sin embargo, la estimación de la reflectividad de la superficie a partir de la radiancia medida en el satélite (proceso conocido como corrección atmosférica) requiere una estimación precisa de los parámetros utilizados para modelar los efectos atmosféricos y, a continuación, compensarlos usando un buen modelo de transferencia radiativa. El principal problema es que, para estimar los parámetros atmosféricos desde los propios datos, previamente es necesaria una detección de nubes precisa. Por lo tanto, la detección de nubes es el primer paso después de la reducción del ruido y la calibración radiométrica de los datos.

Debemos señalar aquí que el procedimiento de corrección atmosférica está fuera del marco de esta Tesis. Sin embargo, dado que la detección de nubes se lleva a cabo antes de que se realice la corrección atmosférica, la interacción entre la atmósfera y la radiación se tendrá en cuenta a fin de cuantificar los efectos atmosféricos en la señal medida. Por otra parte, una formulación precisa de los efectos atmosféricos sobre la señal a recuperar nos permite estimar características útiles para discriminar las nubes de la superficie.

En el capítulo 1, se hace una breve introducción sobre la energía solar, la radiación electromagnética y su interacción con la atmósfera terrestre. Se describen los procesos de absorción y dispersión que afectan a la radiación electromagnética solar en su camino a través de la atmósfera hasta llegar al sensor. Se detalla la adquisición y el modo de funcionamiento de los espectrómetros de imagen multispectrales. Por último, se incluye una breve descripción de los sensores de satélite ENVISAT/MERIS y PROBA/CHRIS junto con una discusión sobre las oportunidades y problemas identificados que justifican la decisión de estudiar en la presente Tesis la detección de nubes en este tipo de sensores.

Detección de Nubes en Imágenes de Teledetección

Las nubes se pueden definir como una masa de vapor de agua condensada o partículas de hielo en suspensión por encima de la superficie terrestre. Debido a las intensas absorciones de las nubes en las longitudes de onda del visible e infrarrojo cercano, la mayor parte de las aplicaciones en teledetección que usan datos de sensores sensibles a este rango del espectro electromagnético requieren la identificación de las nubes en las imágenes. La cantidad de imágenes adquiridas a lo largo del mundo todos los días por los instrumentos a bordo de los satélites de observación de la

Tierra hace inevitable que muchas de estas imágenes presenten nubes, cuyo alcance depende de la estación y la posición geográfica de la región de estudio. De acuerdo con estimaciones de las observaciones obtenidas en el International Satellite Cloud Climatology Project (ISCCP) (Zhang et al., 2004), la media global anual de nubosidad es de 66% aproximadamente. Otros estudios reportan tasas más altas de nubes en el planeta analizando los datos de una red meteorológica en todo el mundo con un gran número de estaciones en diferentes latitudes (Bréon and Colzy, 1999).

La presencia de nubes afecta drásticamente la señal electromagnética medida y, por tanto, a la información obtenida de la superficie observada. Por ejemplo, nubes espesas opacas impiden la entrada de radiación hasta la superficie, mientras que nubes finas transparentes contaminan los datos de fotones dispersados en la dirección de observación y atenúan la señal debido a la eliminación de los fotones en su viaje hacia el sensor. Una cuestión importante aquí es subrayar que, dependiendo de la aplicación de teledetección, las nubes pueden ser vistas como una fuente de contaminación que hace que la imagen sea en parte inútil para estudiar la superficie, o como una fuente de información importante para medir parámetros climatológicos (Peixoto and Oort, 1992).

- Sin una máscara de nubes precisa, las nubes no detectadas en la escena son la fuente más significativa de error para la estimación de la reflectividad de superficie y, por tanto, para la recuperación de parámetros biofísicos. Enmascarando sólo las zonas de la imagen afectadas por las nubes, no es necesario descartar toda la imagen, lo que hace posible realizar estudios multitemporales.
- La monitorización de las nubes a escala mundial es cada vez más importante en estudios de la climatología (las nubes contribuyen de manera significativa a la radiación global).

La conclusión más importante para el tema de esta Tesis es que cualquier conjunto óptico de imágenes de teledetección necesita llevar a cabo un proceso de detección de nubes en las primeras etapas de procesamiento para garantizar la exactitud en los resultados extraídos de las imágenes.

En el capítulo 2, se da una breve introducción de los tipos de nubes y las características clásicas utilizadas para clasificarlas. Se presentan los principales efectos de los tipos de nubes en la radiación electromagnética que viaja a través de la atmósfera terrestre y, por tanto, sus efectos sobre el balance radiativo de la Tierra y el clima. Entonces, se describen la mayoría de las propiedades ópticas de las nubes medibles por los sistemas de teledetección. Por último, se lleva a cabo un examen de los enfoques presentados en la literatura para detectar nubes, prestando especial atención a los algoritmos de detección de nubes desarrollados para los sensores estudiados en esta Tesis.

Metodología de Detección de Nubes Propuesta

El objetivo principal de esta Tesis es desarrollar un algoritmo de detección de nubes utilizando toda la información espectral proporcionada por las imágenes de los espectrómetros MERIS y CHRIS. El algoritmo de detección de nubes propuesto se aprovecha de la alta resolución espectral y radiométrica de MERIS o el elevado número de bandas espectrales de CHRIS, así como de la ubicación específica de algunas bandas para aumentar la precisión en la detección de nubes, como por ejemplo las bandas de absorción del oxígeno y del vapor de agua. En el capítulo 3, se resume el procedimiento de detección de nubes propuesto y se introducen brevemente los diferentes módulos que lo constituyen.

El método debe ser capaz de: (i) detectar con precisión las nubes, y (ii) proporcionar probabilidad o abundancia de nubes en lugar de limitarse a indicar los píxeles que presentan nubes con una máscara binaria. El producto de abundancia de nube proporcionado no está directamente relacionado con las propiedades ópticas de las nubes, como por ejemplo el espesor óptico (Kokhanovsky et al., 2007b), que generalmente se basan en modelos de transferencia radiativa. Este producto de valor añadido permite al usuario aplicar una máscara de nubes ajustable en función de las siguientes etapas de procesamiento y uso final que se le dé a la imagen. Por ejemplo, píxeles nubosos no detectados afectan en gran medida a la recuperación de parámetros biofísicos y a métodos basados en medidas en las longitudes de onda más corta, como la estimación de aerosoles, o la estimación de pigmentos o materia en suspensión en agua, así como a los métodos que dependen de composiciones temporales (Saitwal et al., 2003; Ranera et al., 2005; Plummer, 2005). Un ligero sobre-enmascaramiento de los posibles píxeles contaminados por nubes (detección de nubes conservadora) sería preferible para garantizar un mínimo admisible en la calidad del producto final (Guanter et al., 2008a; Kaufman et al., 2005; Martins et al., 2002), mientras que otras aplicaciones, tales como la clasificación de los tipos de cubiertas, son menos sensibles a nubes delgadas, y por lo tanto, las áreas con nubes muy finas no deben ser necesariamente descartadas (Gómez-Chova et al., 2006f, 2007c; Camps-Valls et al., 2008a). Como resultado, el método debe ser escalable y permitir diferentes niveles de enmascaramiento. Por lo tanto, se propone una máscara probabilística que indique el nivel de contaminación por nubes en cada píxel.

Para lograr los objetivos de exactitud en la clasificación y en el índice de contaminación, se propone un esquema basado en bloques. En primer lugar, se lleva a cabo una extracción de características basada en propiedades físicas (por ejemplo, las nubes son brillantes y blancas). Entonces, un algoritmo de clasificación semisupervisado o no supervisado se aplica a estas características y los agrupamientos resultantes son posteriormente etiquetados como *nube* o *libre de nube*. Por último, se aplica a la imagen clasificada un algoritmo de desmezclado espectral. Resumiendo, el procedimiento de detección de nubes está constituido por los siguientes pasos:

1. *Preprocesado de la Imagen*: se obtiene la reflectividad de la superficie en el techo de la atmósfera (TOA) libre de ruidos.

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2. *Extracción de Características*: se extraen características físicas para aumentar la separabilidad de las nubes y la superficie.
 3. *Segmentación de Imagen*: se aplica un algoritmo de agrupamiento no supervisado a las características extraídas a fin de separar las nubes de la superficie.
 4. *Etiquetado de los Agrupamientos*: los agrupamientos resultantes son posteriormente etiquetados en clases geo-físicas en función de sus características extraídas y su firma espectral.
 5. *Desmezclado Espectral*: finalmente se aplica un algoritmo de desmezclado espectral a la imagen segmentada con el fin de obtener un mapa de abundancias indicando el contenido de nube por píxel.

En los capítulos 4, 5, y 6 se analizan los diferentes bloques en mayor detalle.

Preprocesado de la Imagen y Extracción de Características

Cuando se trabaja con imágenes de teledetección adquiridas en diferentes momentos y lugares, una característica deseable es contar con datos independientes del sensor y de las condiciones de adquisición de la imagen. Esto también es válido para la detección de nubes. Por una parte, corregir los datos de la imagen de las incertidumbres en la calibración del sensor tiene la ventaja de que así los datos son independientes de las diferencias en el sensor. Por otro lado, la conversión de datos de radiancia a reflectividad en el techo de la atmósfera tiene la ventaja de que estos datos se corrigen de diferencias estacionales y diurnas en la posición solar.

Una vez que los datos de la imagen se expresan en reflectancia, podemos procesar los espectros de reflectividad con el fin de extraer características que aumenten la separabilidad de las nubes y la superficie. Estas características están inspiradas en hechos físicos y su significado es independiente de las diferencias en el número, la ubicación y el ancho de banda de los canales espectrales del sensor, que es una característica deseable para un algoritmo de detección de nubes destinado a trabajar en imágenes adquiridas por sensores multi e hiperespectrales, como MERIS y CHRIS.

Clasificación no supervisada de las nubes

Los métodos basados en aplicar umbrales estáticos a cada píxel de la imagen para detectar las nubes pueden fallar debido a una cobertura parcial del píxel, a la calibración del sensor, a la variación de la respuesta espectral de las nubes con el tipo y altura de las nubes, etc. En este contexto, el siguiente paso en nuestra metodología considera la utilización de métodos de clasificación para encontrar grupos similares de píxeles en la imagen. Los métodos no supervisados de clasificación suponen que los datos de entrada están organizados en una serie de grupos de acuerdo a una determinada distancia medida en un determinado espacio (Duda and Hart, 1973). Una revisión excelente de los algoritmos de agrupamiento se puede encontrar en (Xu and Wunsch,

2005). En este trabajo, utilizamos el algoritmo Expectation-Maximization (Dempster et al., 1977) para estimar los parámetros de una distribución mezcla de Gaussianas.

Clasificación semisupervisada de las nubes

La aplicación de métodos de agrupamiento no supervisados a toda la imagen nos permite aprovechar la riqueza de la información y el alto grado de correlación espacial y espectral de los píxeles de la imagen. Sin embargo, la estrategia de etiquetado de los grupos obtenidos por métodos no supervisados se concibe para escenarios donde un usuario etiqueta manualmente los grupos con el fin de mejorar la detección de nubes en estudios de casos particulares o regionales, pero no es práctico cuando se aplica a un gran número de escenas de modo operacional. Esta solución está principalmente orientada a obtener, para la imagen en cuestión, una mayor precisión en la máscara de nubes que con el enfoque estándar (que se aplica píxel a píxel), que produce resultados insatisfactorios en algunos problemas críticos, como en los bordes de las nubes o cuando hay superficies brillantes.

Cuando el objetivo es procesar un gran número de escenas de manera automática debemos recurrir a los métodos supervisados, en los que se aprende de un conjunto fiable de muestras etiquetadas con el fin de definir una función de decisión que clasifique correctamente los píxeles con nubes. Sin embargo, típicamente hay pocas muestras etiquetadas disponibles o que se puedan obtener de forma regular. Nuestro objetivo es aprovechar los beneficios que muestran tanto los métodos supervisados como no supervisados. Por esta razón, en el capítulo 6, se exploran las oportunidades ofrecidas por el aprendizaje semisupervisado basado en métodos kernel que explota las pocas muestras con etiqueta y también la riqueza de las muestras sin etiqueta de la imagen a clasificar.

Resultados

La tercera parte del trabajo se ocupa de la validación de la metodología propuesta y de los productos de nubes obtenidos. Una amplia base de datos de imágenes se ha incluido en el estudio con el fin de tener en cuenta las distintas peculiaridades del problema: la ubicación geográfica, fecha y estación, el tipo de nube y tipos de superficie. Las imágenes seleccionadas nos permiten validar el método, ya que incluyen diferentes cubiertas, vegetación, suelos desnudos, y casos críticos para la detección de nubes como son el hielo y la nieve.

Validación de los métodos no supervisados

La validación de algoritmos de detección de nubes no es una tarea fácil porque, en el caso no supervisado (es decir, sin datos etiquetados), no suelen existir mediciones simultáneas independientes de las nubes con la misma resolución espacial que la imagen a clasificar. En la mayoría

de los casos, el rendimiento de los algoritmos de detección de nubes ha sido evaluado mediante el análisis visual de las imágenes de satélite. El ojo humano es capaz de reconocer las estructuras de nubes en una imagen de satélite mucho mejor que cualquier algoritmo automático, lo que justifica este enfoque de validación. Sin embargo, el reconocimiento de las nubes puede ser difícil en ciertos casos (nubes delgadas, nubosidad discontinua) y está lejos de ser operativo. Además, la comparación visual requiere una gran cantidad de trabajo tedioso, lo cual es inadecuado para una validación cuantitativa en un gran conjunto de datos. Por estas razones, se ha hecho un esfuerzo significativo con el fin de validar los resultados mediante el uso de diferentes técnicas:

- La aproximación más simple consiste en comparar la máscara y abundancia de nubes con las imágenes en color. Por lo tanto, los productos resultantes son validados por inspección visual de las imágenes de CHRIS y MERIS.
- En el caso de MERIS, también podemos comparar los resultados con los productos oficiales de MERIS de nivel 2 ‘Cloud Flag’ (utilizado solo para la validación, no para el entrenamiento).
- La falta de un mapa de *verdad terreno* y la escasa precisión mostrada por los productos oficiales de MERIS de nivel 2 en algunas situaciones (Santer et al., 1999) impiden la validación de la máscara de nubes en condiciones fiables. Por lo tanto, son necesarios nuevos enfoques de validación para poner a prueba el algoritmo de detección de nubes propuesto. En particular, se propone una aproximación multitemporal en la que pares de imágenes con y sin nubes sobre la misma zona se utilizan para la detección de píxeles con nubes mediante la identificación de píxeles con cambios espectrales entre ambas fechas. Los pares son seleccionados para estar cerca en el tiempo, por lo que se evitan los cambios debidos a la evolución temporal de la superficie. Sin embargo, las imágenes tomadas de las órbitas con solo tres o seis días de diferencia presentan una importante variación en la geometría de observación. Por lo tanto, píxeles con cambios significativos en su composición debido al diferente ángulo de observación no se consideran en el método multi-temporal de validación de detección de nubes.

En el capítulo 7, se presentan los resultados del método propuesto en el capítulo 5.

Validación de los métodos semisupervisados

El método propuesto en el capítulo 5 ha demostrado un excelente comportamiento en los resultados de detección de nubes tal como se presenta en el capítulo 7. Sin embargo, esta aproximación es más adecuada para estudios de casos particulares debido a su coste computacional y a la interacción opcional del usuario durante el proceso de etiquetado de los agrupamientos. En aplicaciones de detección de nubes operativas, se requiere métodos que clasifiquen automáticamente con precisión las nubes. Por lo tanto, los métodos supervisados o semisupervisados deberían ser más

adecuados. En el capítulo 8 se describen los resultados del enmascaramiento de nubes obtenidos con los nuevos métodos presentados en el capítulo 6. Todos estos métodos son clasificadores supervisados o semisupervisados y, por tanto, requieren un conjunto representativo de muestras etiquetadas para entrenar y validar los modelos.

Discusión y Conclusiones

Resumen y Conclusiones

Esta Tesis presenta una nueva metodología con el fin de resolver el difícil problema de la detección de nubes en imágenes adquiridas por sensores de satélite multiespectrales e hiperespectrales que trabajan en el rango visible e infrarrojo cercano del espectro electromagnético. Los sensores a bordo de dos satélites de la Agencia Espacial Europea se utilizan en este trabajo: el *MEdium Resolution Imaging Spectrometer* (MERIS), a bordo del satélite ENVISAT, y el instrumento hiperespectral *Compact High Resolution Imaging Spectrometer* (CHRIS), a bordo de PROBA.

La metodología propuesta identifica la ubicación de las nubes en la imagen y produce una abundancia de nube con el fin de cuantificar la forma en que la presencia de nubes afecta a la medición de espectros. El algoritmo de detección se basa en las características físicas extraídas, que están destinadas a aumentar la separabilidad entre las nubes y la superficie, y se extraen de la reflectividad en el techo de la atmósfera que pretende reducir la dependencia de la iluminación y las condiciones geométricas de adquisición. Se ha hecho un importante esfuerzo para corregir y calibrar las imágenes de los sensores seleccionados con el fin de garantizar la calidad de los datos. En este sentido, un nuevo algoritmo se ha propuesto para el tratamiento previo de sensores hiperespectrales, que es especialmente pertinente en el caso del sensor CHRIS.

El objetivo final ha sido el de desarrollar un conjunto de herramientas preciso y automático para la discriminación de las nubes. De esta manera, dos aproximaciones diferentes se han propuesto en función de si el algoritmo tiene que ser aplicado de forma operativa para clasificar automáticamente un número importante de imágenes, o el proceso de clasificación puede ser guiado por un operador para identificar con precisión incluso los casos más críticos en problemas de detección de nubes. Ambas aproximaciones usan, como punto de partida, un algoritmo de agrupamiento no supervisado basado en las características extraídas con el fin de adaptar el enmascaramiento de nubes a la situación de cada imagen, sobre todo a las condiciones atmosféricas, el escenario de fondo, y los tipos de nubes. Este paso permite discriminar fácilmente entre regiones con y sin nubes, proporcionando un producto de abundancia de nube basado en un algoritmo de desmezclado espectral.

En los párrafos siguientes se destacan varias observaciones y conclusiones se han extraído de los diferentes módulos y algoritmos desarrollados en esta Tesis.

Preprocesado de la imagen. El primer paso del proceso es corregir los datos de teledetección a fin de obtener una señal de radiancia en el techo de la atmósfera lo más precisa posible. Hay que tener en cuenta que corregir y compensar los datos de la imagen de incertidumbres en la calibración de los datos del sensor hace que estos datos sean independientes del sistema. Esto requiere una profunda comprensión de las señales proporcionadas por los espectrómetros de imagen ENVISAT/MERIS y PROBA/CHRIS para adaptar el algoritmo de detección de nubes, o incluso para desarrollar nuevos algoritmos de corrección.

- El *efecto sonrisa* (*smile effect*) produce pequeñas variaciones de la longitud de onda espectral medida por cada píxel en la dirección horizontal del sensor que tienen un gran impacto en la característica de la absorción de oxígeno, que es sumamente estrecha. Por lo tanto, hemos propuesto un nuevo algoritmo de extracción de características que permite la introducción de este desplazamiento de la respuesta espectral de MERIS en nuestra formulación.
- PROBA es un satélite de demostración de tecnología y se han desarrollado varios algoritmos de reducción de ruido en esta Tesis ya que CHRIS proporciona datos mínimamente preprocesados.
- Se ha presentado una nueva técnica para detectar píxeles con errores y corregirlos haciendo uso de la información espacial y espectral del píxel erróneo y sus vecinos. Aunque se trata de una corrección cosmética, es necesaria ya que las etapas de procesado posteriores se ven afectadas drásticamente por estos píxeles con valores anómalos.
- Se ha presentado una nueva técnica para reducir el ruido coherente conocido como *vertical striping*, que se encuentra normalmente en las imágenes hiperespectrales adquiridos por sensores como CHRIS. La principal novedad de nuestra propuesta consiste en reducir el patrón de bandas verticales usando un nuevo algoritmo robusto a cambios en la superficie.
- La aproximación propuesta de eliminación de patrones de ruido verticales ha demostrado ser robusta, estable, y permite modelizar con éxito la dependencia del ruido con la temperatura del sensor.

Extracción de características. Cuando se trabaja con imágenes de teledetección adquiridas en diferentes momentos y lugares, una característica deseable es tener datos independientes de las condiciones de adquisición. La conversión de datos de radiancia en reflectividad en el techo de la atmósfera tiene la ventaja de que estos datos se corrigen de diferencias en la posición solar estacionales y diurnas. Por otra parte, la extracción de características físicas adecuadas, aumenta la separabilidad entre las nubes y la superficie, lo que mejora la clasificación y permite una mejor comprensión del problema.

Debemos tener en cuenta que, además de propiedades comunes de las nubes como ser radiométricamente blancas y brillantes, una característica crítica presentada en este trabajo es el

uso de las bandas de absorción del oxígeno atmosférico y del vapor de agua para mejorar los resultados de la detección de nubes.

- La utilización de la absorción atmosférica del oxígeno para inferir la presión de las nubes, la cual se relaciona con la altitud de las nubes, es bien conocida en estudios atmosféricos. En este sentido, se propone una fórmula para extraer una característica atmosférica relacionada directamente con el camino óptico mediante el uso de la geometría de observación exacta de cada píxel.
- La banda de absorción del oxígeno es muy estrecha y, a pesar de la alta resolución espectral y radiométrica de MERIS, las pequeñas variaciones de la longitud de onda espectral de cada píxel tienen un gran impacto en cualquier variable derivada de la banda del oxígeno. Como se ha mencionado, este cambio espectral se ha tenido en cuenta con el fin de corregir el *smile effect*.
- En el caso de CHRIS, la banda del oxígeno no es tan útil por el mayor ancho de banda de los canales de CHRIS. Sin embargo, algunos modos de adquisición de CHRIS presentan una excelente caracterización de la absorción de vapor de agua.
- La máxima absorción de vapor de agua (940 nm) se encuentra fuera del rango de MERIS, pero la absorción a 900 nm sigue siendo válida para medidas relativas dentro de la misma imagen. Por otra parte, la nieve presenta mayor absorción que las nubes a 900 nm y este comportamiento puede observarse en las características extraídas.
- Los resultados obtenidos mediante la absorción de estas características sugieren que sería ventajoso ver esas bandas incluidas en futuros sensores.
- Resumiendo, el estudio ha dado lugar a una lista cualitativa de las principales cuestiones y características físicas que pueden mejorar la detección de nubes en los sensores de teledetección que trabajan en el visible e infrarrojo cercano del espectro.

Detección de nubes. Un objetivo central de la Tesis ha consistido en dar un conjunto de herramientas de detección de nubes para la obtención de mapas de nubes para los datos de los sensores seleccionados. Con el fin de lograr este objetivo, técnicas avanzadas de reconocimiento de patrones y de aprendizaje automático han sido desarrolladas.

- Dos aproximaciones diferentes de detección de nubes se han propuesto basadas en la idea de aprovechar las muestras sin etiqueta disponibles en las imágenes de teledetección.
- Inicialmente se propone una aproximación no supervisada de detección de nubes basada en métodos clásicos de reconocimiento de patrones.

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- La aplicación de métodos de agrupamiento no supervisados a toda la imagen nos permite aprovechar la riqueza de la información y el alto grado de correlación espacial y espectral de los píxeles de la imagen.
 - El algoritmo EM, que se aplica a las características extraídas, ha demostrado una excelente capacidad para segmentar la imagen permitiendo discriminar fácilmente entre regiones con y sin nubes.
 - Se ha definido un procedimiento específico para etiquetar los grupos encontrados a fin de ayudar al usuario a identificar incluso los problemas de detección de nubes más críticos.
 - Se han explorado métodos de aprendizaje semisupervisados, ya que ofrecen la oportunidad de explotar las muestras etiquetadas disponibles y la riqueza de las muestras sin etiqueta. En este caso, hay información supervisada disponible y se utiliza junto con las muestras sin etiqueta de la imagen analizada para desarrollar un clasificador que proporciona la clase de cada píxel, pero teniendo también en cuenta la distribución de los datos de la imagen. Dado que la distribución de las clases está fijada por el conjunto de entrenamiento, este método puede ser aplicado automáticamente a un gran número de escenas de modo operativo.
 - Se ha propuesto una nueva familia de métodos kernel basados en *kernels promedio* (μ -SVM) tomando como referencia la SVM estándar, que se utiliza como referencia de los métodos supervisados, y la SVM Laplaciana, que se utiliza como referencia de los métodos semisupervisados.
 - Los clasificadores μ -SVM propuestos combinan la similitud entre muestras, basada en las muestras etiquetadas del conjunto de entrenamiento, y la similitud entre agrupamientos, basada en las muestras sin etiqueta de la imagen analizada, que se calculan en el espacio kernel gracias a un *kernel compuesto*.
 - Con esta aproximación, la distribución de las clases, estimada típicamente a partir de un bajo número de muestras etiquetadas, se adapta a la distribución de los datos de la imagen analizada, estimada a partir de todas las muestras sin etiqueta. Como consecuencia de ello, el enfoque propuesto es más robusto al *sesgo en la selección de las muestras*, que es un problema común en aplicaciones reales de observación de la Tierra.

Abundancia de nubes. Una de las principales exigencias impuestas a la metodología propuesta de detección de nubes era proporcionar información sobre la contribución de las nubes a los espectros medidos de los píxeles de la imagen (para cuantificar situaciones con nubes semi-transparentes o con cobertura parcial de un píxel). Por lo tanto, un aspecto importante de la metodología de detección de nubes es que proporcione un producto de abundancia de nube.

- El producto de abundancia de nubes ofrece mapas con el nivel de contaminación de nubes para cada píxel en lugar de una clasificación binaria.

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- El producto final de nubes se obtiene combinando la abundancia de nubes, calculada con un algoritmo de desmezclado espectral, y la probabilidad de nubes, obtenida a partir del algoritmo de agrupamiento, por medio de una multiplicación píxel a píxel.
 - La aproximación propuesta combina dos fuentes complementarias de información procesada por métodos independientes: la abundancia de nubes (obtenida a partir de los espectros) y la probabilidad de nube (obtenida a partir de las características extraídas), que se aproxima a uno en los píxeles con nubes y es cercana a cero en el resto de zonas.
 - El producto de abundancia de nubes puede ser usado para describir mejor las nubes detectadas (cobertura subpíxel, transparencia, tipo de nubes) y para generar máscaras de nubes con diferentes niveles de restricción en función de la aplicación.

Aproximaciones de Validación de los Resultados. La validación de algoritmos de detección de nubes no es una tarea fácil porque no hay una medición independiente con la misma resolución espacial. Por esta razón, hay que hacer un esfuerzo importante para validar los resultados mediante el uso de diferentes técnicas.

- La aproximación más simple consiste en la validación de los productos resultantes mediante inspección visual, comparando la máscara de nubes y abundancia con las imágenes en color.
- En el caso de MERIS, también puede hacerse una comparación con los resultados oficiales de MERIS de nivel 2, comparando la máscara de nubes producida por el método presentado en términos de acierto en la clasificación.
- Se ha propuesto una aproximación multitemporal de validación para analizar el resultado de detección de nubes. Se han utilizado pares de imágenes sobre la misma zona, una cubierta con nubes y otra sin nubes, para detectar los píxeles con nubes mediante la identificación de píxeles con un cambio espectral significativo entre ambas fechas.
- Las ventajas previstas de una detección precisa de nubes también se han demostrado con una aplicación de clasificación de la cubierta terrestre a nivel subpíxel. En particular, se ha demostrado que el desmezclado de series temporales de imágenes MERIS supera al desmezclado de fechas independientes.
- También hemos validado los productos de abundancia y probabilidad de nube respecto a la probabilidad de nube proporcionada por el programa *BEAM Toolbox*, que es el producto de nubes más parecido disponible para datos de MERIS.
- En el caso de los métodos de clasificación semisupervisados, se ha proporcionado resultados más clásicos de acierto en la clasificación (κ y acierto promedio [%] para todos los métodos) obtenidos utilizando etiquetas y mapas de verdad terreno para entrenar y validar los clasificadores.

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- Los métodos kernel de clasificación propuestos han sido examinados en dos diferentes situaciones: en primer lugar, cuando hay disponibles muestras etiquetadas para caracterizar la imagen que debe ser clasificada y, en segundo lugar, cuando no hay muestras etiquetadas para la imagen a ser clasificada. En éste último caso, una configuración experimental se ha propuesto con el fin de inducir y analizar el llamado sesgo en la selección de las muestras.

Resultados y Recomendaciones. A raíz de estos criterios de validación, una serie de experimentos se han llevado a cabo para obtener una colección completa de resultados. Una amplia base de datos de imágenes se ha incluido en el estudio con el fin de tener en cuenta las distintas peculiaridades del problema (localización geográfica, fecha y estación, tipos de nube y tipos de superficie) para ambos sensores.

- Los resultados han demostrado que la aproximación guiada por usuario clasifica con precisión los casos más difíciles de píxeles de nubes, especialmente cirros y nubes sobre el hielo o nieve.
- Se ha observado claras deficiencias en la máscara oficial de nubes de MERIS de nivel 2 en las superficies más brillantes, como suelos desnudos, hielo y nieve, que se clasifican como nubes, y también se han obtenido resultados más precisos con el método presentado en nubes semitransparentes o bordes de nubes, que son incorrectamente clasificadas por el producto oficial de la ESA.
- El algoritmo también ha sido validado comparándolo con una máscara de nubes basada en la detección de cambios temporales. A pesar de que el método propuesto sólo utiliza la información de la imagen analizada, los resultados demuestran que nuestro método ofrece una mejor discriminación de las nubes y sus bordes. Esto permite una utilización más eficiente de las imágenes y series temporales de MERIS.
- Los histogramas del producto de abundancia de nube propuesto muestran una distribución de valores adecuada, que difiere en gran medida de la salida probabilística de la red neuronal del programa BEAM que se concentra en torno a uno y cero, y por lo tanto proporciona una información más útil para el usuario.
- Los clasificadores basados en kernels promedio (μ -SVM) producen mejores resultados que la clasificación de la referencia proporcionada por las SVM supervisadas y las LapSVM semisupervisadas en todos los casos. Hay que tener en cuenta que la SVM es un caso particular de la μ -SVM, que además tiene en cuenta la distribución de datos de la imagen con el fin de definir los grupos.
- Debido a que el tiempo de CPU consumido es relativamente bajo, los clasificadores μ -SVM tienen una buena relación entre el coste computacional y la precisión en la clasificación.
- Además, los clasificadores μ -SVM que trabajan en el espacio kernel proporcionan mejores resultados, lo que apoya la idea de que podemos encontrar un espacio más rico en términos

de separación de clases.

- En situaciones extremas, con un bajo número de muestras etiquetadas, la información de las muestras sin etiqueta ayuda a mejorar el comportamiento de la μ -SVM y a proporcionar mejores resultados.
- El método μ -SVM basado exclusivamente en similitud entre agrupamientos no es equivalente a una simple segmentación de la imagen y posterior clasificación de los centros de los grupos con una SVM supervisada. Hemos observado que su rendimiento depende de la calidad de la segmentación de la imagen proporcionada por el algoritmo EM.
- En los experimentos en los que la imagen se clasifica a partir de datos de otras imágenes, la SVM se ve drásticamente afectada por el sesgo en la selección de las muestras de entrenamiento (*sample selection bias*), ya que se basa exclusivamente en las etiquetas de muestras que no representan a las clases en la imagen analizada.
- Un problema común para todos los métodos kernel es que la selección de los parámetros libres del kernel depende de las muestras de entrenamiento y, por tanto, se ve drásticamente afectada por el *sample selection bias*.
- Los clasificadores μ -SVM basados exclusivamente en los grupos encontrados proporcionan excelentes resultados. Sin embargo, se requiere un número suficiente de muestras etiquetadas para describir la distribución de las clases (con un menor número de muestras el grupo podría ser clasificado incorrectamente).
- El mapeado propuesto es el más robusto frente al sesgo en la selección de muestras debido a que la contribución de cada una de las muestras en la definición del centro de masa de cada grupo en el espacio kernel \mathcal{H} se pesa con las probabilidades a posteriori. Esto es equivalente a eliminar las muestras que no representan adecuadamente el agrupamiento en el espacio de entrada, y, por tanto, la estimación del centro del agrupamiento en \mathcal{H} se ve menos afectada por la selección de un mapeado inadecuado.
- Los resultados también sugieren que los clasificadores μ -SVM que promedian los kernels con las similitud entre muestras y entre grupos son una solución de compromiso, ya que proporcionan buenos resultados en escenarios semisupervisado, y no están sesgados hacia el conjunto de entrenamiento cuando se trata con problemas con selección de muestras sesgadas.
- Por último, los resultados muestran una relación inversa entre la simplicidad del modelo (número de vectores soporte) y la precisión en la clasificación. Los modelos excesivamente simples ofrecen malos resultados, mientras que modelos moderadamente simples proporcionan una mejor clasificación.

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- La principal limitación de los métodos semisupervisados es que, aunque se benefician de la inclusión de las muestras sin etiqueta para estimar la distribución de datos, las etiquetas disponibles no pueden aliviar las situaciones con un excesivo sesgo de selección de las muestras, ya que los datos de la imagen de test a clasificar no están bien representados en el conjunto de entrenamiento.
 - En el caso de series temporales de imágenes, el sesgo de selección de las muestras no es tan crítico (la superficie observada es la misma), y los resultados obtenidos en los experimentos son aceptables porque las distribuciones de entrenamiento y de test no difieren significativamente.

Resumiendo, se ha propuesto una metodología de detección de nubes. La metodología es muy versátil y se compone de diferentes módulos diseñados específicamente que se han formulado en términos de algoritmos operativos que cubren los requisitos esenciales para el proceso de detección de las nubes. Estos módulos se pueden actualizar con algoritmos más avanzados o modificarse para adaptarse a las características de otros sensores. En consecuencia, este procedimiento puede servir para desarrollar un algoritmo de detección de nubes para otros espectrómetros de imagen que trabajen en el rango espectral VNIR con una adecuada caracterización espectral de las absorciones atmosféricas, como EO1/Hyperion de la NASA, las futuras misiones de observación de la Tierra GMES/Sentinel-3 y EnMAP, o la propuesta FLEX del explorador de la Tierra de la ESA.

Trabajo Futuro

La lista de objetivos propuestos al comienzo de esta Tesis ha sido totalmente cubierta. Sin embargo, la metodología para la detección de nubes presentada abre muchas direcciones futuras de investigación debido a su modularidad. En este sentido, nuestros próximos pasos están vinculados a la inclusión de modificaciones dirigidas a mejorar su robustez. Por ejemplo, la inclusión de umbrales dinámicos podría ser útil para encontrar las regiones a analizar, mientras que la inclusión de información contextual y de textura podría mejorar el agrupamiento. Algunas otras líneas de investigación consisten en la inclusión de la posición del sol respecto a las nubes para encontrar sombras.

Una importante observación es que la metodología se ha limitado para usar únicamente la información proporcionada por los productos de MERIS o CHRIS de nivel 1. Este requisito previo es una de las ventajas de los métodos propuestos. Sin embargo, en los experimentos, hemos descubierto algunas dificultades de los clasificadores automáticos para distinguir superficie brillantes a diferentes altitudes de las nubes, como por ejemplo montañas nevadas y el hielo en latitudes altas. Estos problemas no pueden resolverse por completo con la información contenida en el rango espectral cubierto por MERIS y CHRIS, pero los sensores con canales espectrales estrechos más allá de $1 \mu\text{m}$ han demostrado una buena capacidad para detectar las nubes gracias a la absorción del vapor de agua. Por esta razón, nuestras nuevas líneas de investigación están

vinculadas a la utilización de datos complementarios procedentes de diferentes sensores. Por ejemplo, la presencia de canales en el infrarrojo térmico (TIR) permite la detección basada en contrastes térmicos. Actualmente, estamos definiendo e implementando un sistema de detección de nubes que combina la información procedente de los instrumentos AATSR y MERIS a bordo de ENVISAT. La adquisición simultánea y similar resolución espacial permite la sinergia de MERIS y AATSR. La inclusión de la banda de AATSR SWIR a $1.6 \mu\text{m}$ en el sistema de detección de nubes es de suma importancia (McIntire and Simpson, 2002). También la presencia de canales en el rango infrarrojo térmico permite la detección basada en contraste térmico (Simpson and Gobat, 1996; Papin et al., 2002) y en la variabilidad espacial sobre el mar (Martins et al., 2002).

Por otra parte, en el rango espectral de $1.38\text{-}1.50 \mu\text{m}$, cirros y cúmulos bajos de nubes pueden ser detectados, ya que las características de la superficie se eliminan debido a la absorción adicional de radiación solar por el vapor de agua de la atmósfera entre las nubes y la superficie (incluso en presencia de hielo o nieve). La nueva generación de satélites, como los GMES Sentinel 2 y 3 (European Space Agency, 2007), incluyen bandas dedicadas específicamente definidas para realizar una detección precisa de cirros. Actualmente, también estamos analizando las ventajas de incluir la llamada banda de cirros ($1,38 \mu\text{m}$) en el sistema de detección de nubes en el marco de los estudios preparatorios de la misión FLEX (Moreno, 2006).

Por último, cabe señalar que, a pesar de que se han propuesto y desarrollado técnicas con aplicaciones de teledetección en mente, algunos algoritmos propuestos se puede aplicar a otros campos relacionados de agrupamiento y clasificación de datos.

Relevancia de la Tesis

La aplicabilidad de la metodología propuesta es crucial para completar con éxito el trabajo realizado en esta Tesis. En este sentido, debemos destacar aquí los siguientes logros.

La detección de nubes constituye en sí misma una oportunidad a nivel científico y técnico, lo que ha dado lugar a importantes publicaciones en el campo. Varias publicaciones abarcan los temas más relevantes de esta Tesis:

- El preprocesado de datos de teledetección de sensores hiperespectrales y multiespectrales ha dado lugar a diferentes algoritmos para la reducción del ruido en (Gómez-Chova et al., 2006a; Gómez-Chova et al., 2008) y de corrección atmosférica en (Guanter et al., 2006a, 2007, 2008a).
- El método propuesto ha sido probado en (Gómez-Chova et al., 2005b, 2006c, 2005a) en imágenes hiperespectrales de CHRIS con el fin de proponer y validar las metodologías de detección de nubes en situaciones favorables de resolución espacial (34 m) y número de bandas (62 canales).
- En (Gómez-Chova et al., 2005c, 2006d, 2007a) se llevó a cabo un estudio preliminar de

detección de nubes con MERIS, analizando situaciones críticas como por ejemplo la presencia de hielo o nieve.

- Se han empleado series temporales para la detección de nubes en (Gómez-Chova et al., 2006f, 2007c), clasificación subpíxel a través de técnicas de unmixing (Zurita-Milla et al., 2007), y clasificación de los datos de teledetección en (Camps-Valls et al., 2006b, 2008a).
- La teoría de los métodos kernel utilizados en esta Tesis se basa en la labor llevada a cabo en (Camps-Valls et al., 2004a, 2006d, 2008a).
- La utilización de técnicas semisupervisadas como la LapSVM y los kernel promedio ha sido analizada en (Gómez-Chova et al., 2007b, 2008c) y (Gómez-Chova et al., 2008a, 2009), respectivamente.

Los conocimientos adquiridos acerca de este campo de investigación multidisciplinar ha dado lugar a la publicación de tres capítulos en libros internacionales:

- *Hyperspectral Image Classification with Kernels* en “Kernel Methods in Bioengineering, Signal and Image Processing” (Bruzzone et al., 2007).
- *Kernel Machines in Remote Sensing Image Classification* en “Intelligent Systems: Techniques and Applications” (Camps-Valls et al., 2008c).
- *Kernel Mean for Semi-supervised Remote Sensing Data Classification* en “Kernel methods for Remote Sensing Data Analysis” (Gómez-Chova et al., 2009).

Por último, la presente Tesis se ha orientado tanto a la investigación científica como al desarrollo de herramientas técnicas innovadoras. Como consecuencia de ello, la Tesis también se enmarca en tres contratos diferentes de la *Agencia Espacial Europea* (ESA):

- *Development of CHRIS/PROBA modules for the BEAM toolbox* (ESRIN Contract No. 20442/07/I-LG). Actualmente, el método presentado se está aplicando al sensor CHRIS como parte del software *Basic ENVISAT Toolbox for (A)ATSR and MERIS* (BEAM toolbox¹) para el tratamiento previo de datos de CHRIS. En particular, los métodos presentados en la sección 4.1.2 y capítulo 5 están siendo implementados como dos módulos independientes de BEAM en los subproyectos “2.3 Noise Reduction Definition” y “2.4 Cloud Masking Definition” del proyecto, que son gestionados por el autor de esta Tesis. La decisión de la ESA de implementar los algoritmos derivados de este trabajo en el BEAM es, sin duda, un logro significativo y demuestra también el interés y la aplicabilidad de la investigación realizada.

¹<http://www.brockmann-consult.de/beam/>

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- *Atmospheric Corrections for Fluorescence Signal Retrieval* (ESTEC Contract No. 20882/07/NL/LvH). El conocimiento adquirido sobre la detección de nubes en imágenes hiperespectrales durante la labor llevada a cabo en esta Tesis se aplica en este proyecto (Guanter et al., 2008b) para definir y aplicar un enmascaramiento de nubes para el sistema FLEX. Los píxeles con nubes deben ser enmascarado en los estudios de fluorescencia (Gómez-Chova et al., 2006b; Guanter et al., 2007; Guanter et al., 2007; Alonso et al., 2008; Amorós-López et al., 2008a), ya que pueden contaminar la medida de la señal de fluorescencia investigada. En el subproyecto “3.1 Cloud screening method”, que es dirigido por el autor de esta Tesis, se está desarrollando un método para la obtención de máscaras de nubes probabilísticas, y se está analizando en profundidad las mejoras esperadas asociadas a la presencia de bandas en el SWIR que medirá la plataforma FLEX.
 - *MERIS/AATSR Synergy Algorithms for Cloud Screening, Aerosol Retrieval, and Atmospheric Correction* (ESRIN Contract No. 21090/07/I-LG). La extensión del trabajo de esta Tesis para el instrumento MERIS está siendo investigada en el marco de este proyecto (North et al., 2008). En el método propuesto en este proyecto se aprovecha la información combinada de ambos sensores AATSR y MERIS con el fin de mejorar los productos actuales de nubes de los dos sensores (Gómez-Chova et al., 2008b). El autor de esta Tesis es el investigador principal de este proyecto en la Universidad de Valencia y es responsable de la definición de un algoritmo de detección de nubes que combine MERIS y AATSR. Además, participa en el *MERIS and AATSR Cloud Screening Working Group*, que fue creado por la ESA con el fin de aunar sus esfuerzos y utilizar los conocimientos técnicos existentes para desarrollar nuevos métodos de detección de nubes.

Part VII

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