VNIVERSITAT DE VALÈNCIA
Facultat de Ciències Matemàtiques
Departament d'Estadística i Investigació Operativa

Geoestadística en regiones heterogéneas con distancia basada en el coste

TESIS DOCTORAL

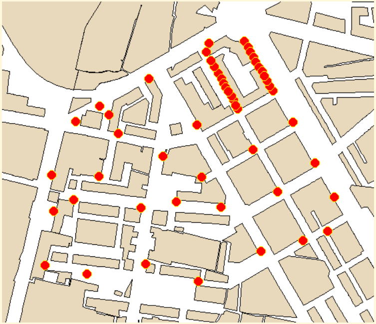
Facundo Martín Muñoz Viera

Director: Antonio López-Quílez

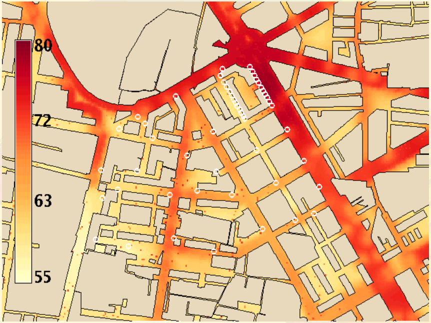
Febrero 2013

Outline

Motivation: acoustic maps and heterogeneous regions



observations



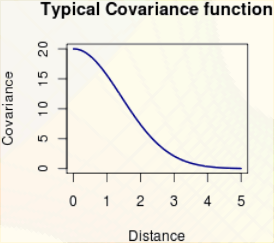
prediction

- Assessment of the uncertainty!

Covariance functions

$C(h) \overset{h=d(\boldsymbol{s}_1,\boldsymbol{s}_2)}{\overset{\downarrow}{=}} \mathbb{C}\left[Z(\boldsymbol{s}_1), Z(\boldsymbol{s}_2)\right]$ represents the relationship between the *proximity* and the statistical correlation.

We restrict to isotropic functions.



Valid covariance functions

Not all functions are permissible as covariance functions

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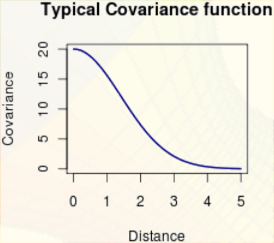

Valid covariance functions

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Positive-definite functions

Positivity condition

The covariance function must be positive-definite

$$\forall \{\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n\}, \quad \forall a_1, \ldots, a_n, \quad \sum_i \sum_j a_i a_j C(h_{ij}) = \boldsymbol{a}'\boldsymbol{\Sigma}\boldsymbol{a} \geq 0$$

In the Euclidean space $E_d = (\mathbb{R}^d, \cdot)$, the family of positive-definite functions is fully characterized by Schoenberg's (1938) theorem:

$$C(h) = \int_0^\infty \Omega_{\frac{d-2}{2}}(h\lambda)\, dG(\lambda),$$

where $\Omega_m(x) = \Gamma(m+1)(\frac{2}{x})^m J_m(x)$, J_m is the Bessel function of the first kind of order m, and G is a nondecreasing bounded measure on $[0, \infty)$.

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Bochner's Theorem (1933)

Characterizes the positive-definite (non-isotropic) functions as characteristic functions (a kind of Fourier Transform) of distribution functions in E_d.

$$\tilde{C}(\boldsymbol{h}) = \mathbb{E}\left[e^{i\boldsymbol{h}'\boldsymbol{X}}\right] = \int_{E_d} e^{i\boldsymbol{h}'\boldsymbol{x}} dF_X(\boldsymbol{x}), \quad \boldsymbol{h}, \boldsymbol{X} \in E_d \tag{1}$$

Sufficiency:

$$\begin{aligned}\sum_{i,j} a_i a_j \tilde{C}(\boldsymbol{s}_i - \boldsymbol{s}_j) &= \mathbb{E}\left[\sum_{i,j} a_i a_j e^{i(\boldsymbol{s}_i - \boldsymbol{s}_j)'\boldsymbol{x}}\right] \\ &= \mathbb{E}\left[\Big(\sum_i a_i e^{i\boldsymbol{s}_i'\boldsymbol{x}}\Big)\overline{\Big(\sum_j a_j e^{i\boldsymbol{s}_j'\boldsymbol{x}}\Big)}\right] \\ &= \mathbb{E}\left[\Big|\Big(a_i \sum_i e^{i\boldsymbol{s}_i'\boldsymbol{x}}\Big)\Big|^2\right] \geq 0.\end{aligned} \tag{2}$$

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Heterogeneous regions

In the presence of barriers, the correlation is not directly associated with the Euclidean distance.

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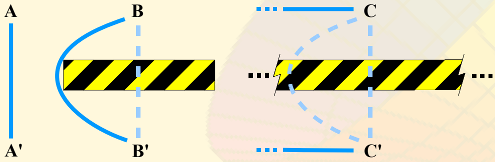

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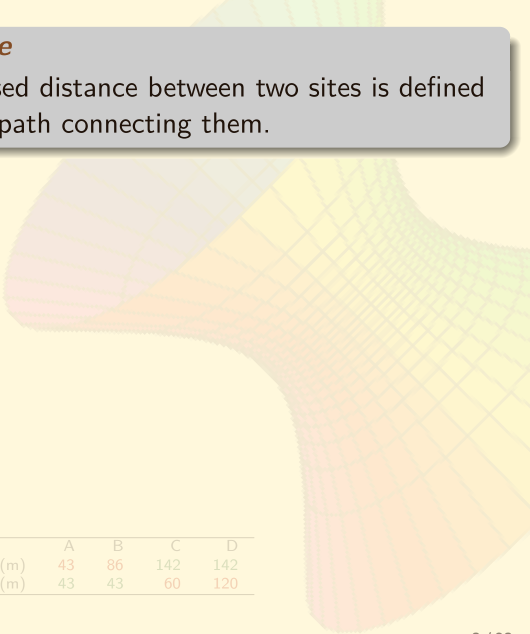
A practical approach

Definition: ***Cost-based distance***

Given a cost-surface, the cost-based distance between two sites is defined as the cost of the minimum-cost path connecting them.



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Cost-based distance (m)	43	86	142	142
Euclidean distance (m)	43	43	60	120

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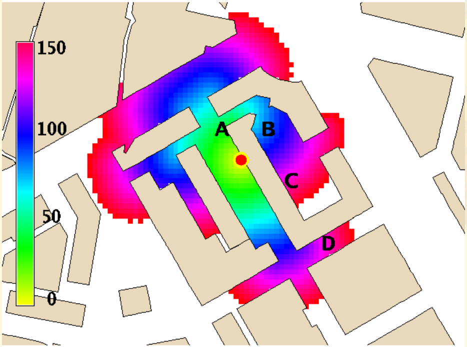

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Cost-based geostatistics

- The cost-based distance generalizes the Euclidean distance, which is a particular case where the cost surface is flat
- It accounts not only for barriers but for general heterogeneous regions
- This definition and its implementation is an original contribution of the first part of the thesis project

Implementation

- Geographic computation of cost-based distances (GRASS GIS)
- Send covariates, observations and prediction locations with cost-based distance matrices to R
- Use (modified) geoR functions to perform cost-based geostatistical prediction
- Return results to GRASS GIS and produce prediction maps

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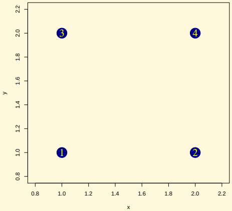
Validity: a toy example



$$\mathbf{D} = \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 2 & 1 \\ 1 & 2 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix}$$

$$\mathbf{Z} = (Z_1, Z_2, Z_3, Z_4) \sim MVN(\mathbf{0}, \mathbf{\Sigma})$$

$$\mathbf{\Sigma} = \begin{pmatrix} 20.00 & 15.58 & 15.58 & 7.36 \\ 15.58 & 20.00 & 7.36 & 15.58 \\ 15.58 & 7.36 & 20.00 & 15.58 \\ 7.36 & 15.58 & 15.58 & 20.00 \end{pmatrix}$$

$$C(h) = 20e^{-\left(\frac{h}{2}\right)^2}$$

Eigenvalues: $\{58.52, 12.64, 12.64, -3.80\}$

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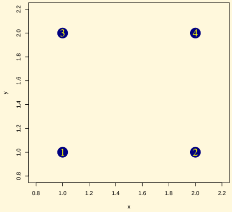

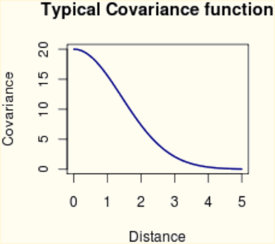

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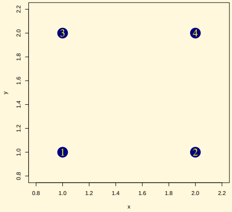

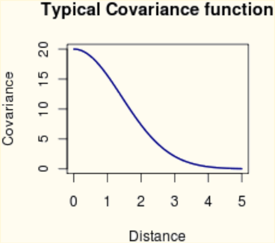

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Positive-definiteness with cost-based distances

- The positive-definite functions of the Euclidean space may not be valid with non-Euclidean distances are used
- If $\mathbf{\Sigma}$ is positive-semidefinite,
  - the kriging prediction is valid under the interpretation of a BLUP
  - it does not guarantee that C is positive-definite, thus, the underlying Gaussian field of the spatial statistical model might be invalid.
- The approach can be used safely, provided that the positive-definiteness of $\mathbf{\Sigma}$ is verified every time.

Second part of the thesis

Study the mathematical condition of positive-definiteness under cost-based distances

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Riemannian model

- Define in $D \subseteq \mathbb{R}^d$ the following Riemannian metric

$$g_p(\boldsymbol{x}, \boldsymbol{y}) := \mathfrak{f}(p)^2 \langle \boldsymbol{x}, \boldsymbol{y} \rangle, \qquad p \in D,\ \boldsymbol{x}, \boldsymbol{y} \in T_p D$$

where $\mathfrak{f}$ is the cost-surface and $\langle \cdot, \cdot \rangle$ the Euclidean inner product.

Now, given a curve α in D, its length is given by

$$L(\alpha) = \int_0^1 \sqrt{g_{\alpha(t)}(\alpha'(t), \alpha'(t))}\, dt = \int_0^1 \mathfrak{f}(\alpha(t)) \|\alpha'(t)\|\, dt.$$

This is, its *Euclidean* length weighted locally by the corresponding cost. The *metric* τ_g induced by this Riemannian metric is precisely the cost-based distance.

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Positive definiteness in Riemannian manifolds

- We are interested in the family of positive-definite functions

$$\mathcal{P}(D, \mathfrak{d})$$

- In this framework the Vector Space (and group) structure is lost
- Generalizing Bochner's and Schoenberg's theorems in such an abstract context is extremely difficult
- Strategy: embedding into more structured spaces
- Embedding into an Euclidean (or Hilbert) space is not possible in general

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Kuratowski embedding

The metric space D embeds isometrically in the Banach space $L^\infty(D)$ of bounded functions on D with the supremum norm. Fixing $x_0 \in D$, define

$$\begin{aligned} D &\hookrightarrow L^\infty(D) \\ x &\mapsto \phi_x : \, D \to \mathbb{R} \\ &\qquad\qquad y \mapsto \mathfrak{d}(x, y) - \mathfrak{d}(y, x_0). \end{aligned}$$

- ϕ_x are bounded (triangle ineq.)
- The norm $\|\cdot\|_\infty$ induces a distance in $L^\infty(D)$ compatible with the cost-based distance: $\|\phi_{x_1} - \phi_{x_2}\|_\infty = \mathfrak{d}(x_1, x_2)$
- Rudin (1991, Teo. 11.32) gives a generalization of Bochner's theorem in the context of Banach algebras
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Euclidean representation

An Euclidean representation of a distance matrix **D** $n \times n$ is a matrix **X** whose rows give the coordinates of a set of points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$ that reproduce the distances.

- Not all distance matrices admit an exact Euclidean representation.
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Pseudo-Euclidean representation

A pseudo-Euclidean inner product in $\mathbb{R}^d$ of index k is of the form

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = (x_1 y_1 + \cdots + x_k y_k) - (x_{k+1} y_{k+1} + \cdots + x_d y_d).$$

Figure: Some points and their relative quadratic distances in the pseudo-Euclidean space $E_{(1,1)}$

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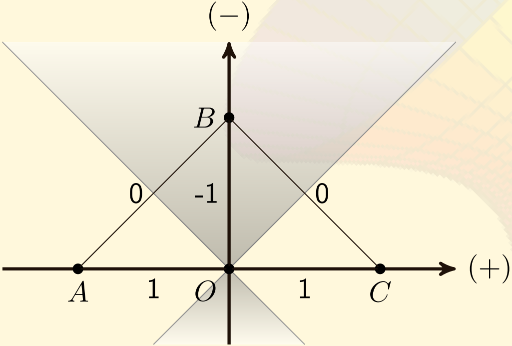

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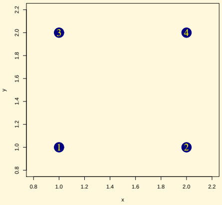
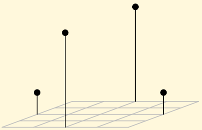
Pseudo-Euclidean representation

Theorem: All distance matrices D can be represented in a pseudo-Euclidean space

$$\mathbf{X} = \mathbf{\Gamma}(\mathbf{\Lambda}\mathbf{S}_k)^{1/2}, \quad \mathbf{HDH} = \mathbf{\Lambda}\mathbf{S}_k\mathbf{\Lambda},$$

where $\mathbf{S}_k$ is the signature of the space.





$$X = \begin{bmatrix} 0 & 1 & \frac{1}{2} \\ 1 & 0 & -\frac{1}{2} \\ -1 & 0 & -\frac{1}{2} \\ 0 & -1 & \frac{1}{2} \end{bmatrix}$$

$$d_{12}^2 = (0-1)^2 + (1-0)^2 - (\tfrac{1}{2} + \tfrac{1}{2})^2 = 1^2$$

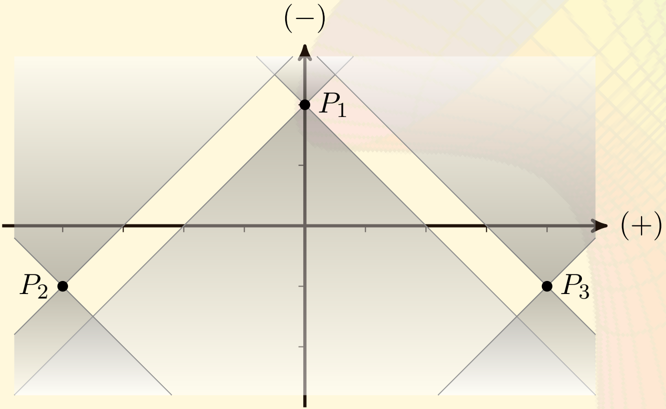
$$d_{13}^2 = (0+1)^2 + (1-0)^2 - (\tfrac{1}{2} + \tfrac{1}{2})^2 = 1^2$$

$$d_{14}^2 = (0-0)^2 + (1+1)^2 - (\tfrac{1}{2} - \tfrac{1}{2})^2 = 2^2$$

$$\ldots$$

Pseudo-Euclidean representation

- The pseudo-Euclidean embedding is not strict: there are configurations that are not representations of any cost-based problem (e.g., negative quadratic distances; violations of triangle ineq.)



Positive definiteness in pseudo-Euclidean spaces

- At least the trivial constant function is positive-definite in the pseudo-Euclidean space
- All cost-based problems can be represented in the pseudo-Euclidean space
- The Euclidean space is a particular case of cost-based manifold

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Generalizations of Bochner's and Schoenberg's theorems

- Bochner's theorem remain valid in pseudo-Euclidean spaces!

$$\tilde{C}(\boldsymbol{h}) = \int_{E_d} e^{i\boldsymbol{h}'\boldsymbol{x}} dF_X(\boldsymbol{x}), \quad \boldsymbol{h}, \boldsymbol{X} \in E_d \tag{3}$$

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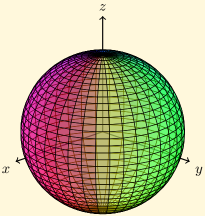

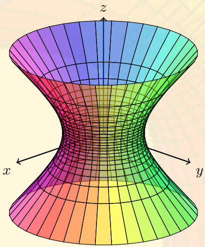

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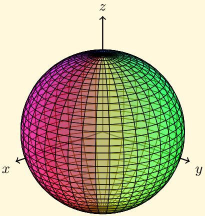

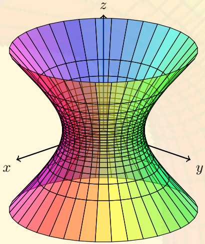

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Integrating on the hyperboloid

- The pseudo-Euclidean sphere has infinite surface, therefore the integration of a constant is divergent
- We can consider the *mean* value of the function $\tilde{C}(\boldsymbol{h})$ over the surface (which is $C(\rho)$, where $\rho = \|\boldsymbol{h}\|$).
- The mean of the right-hand side can be formally expressed as the quotient of two divergent integrals, and then change the integration order to express it as the integral of a function $M(\rho)$ with respect to the distribution F.

$$C(\rho) = \int_{S_\rho^+} \left(\int_{\mathbb{R}^d} e^{i\boldsymbol{\omega}'\boldsymbol{x}} \, F(d\boldsymbol{\omega}) \right) s(d\boldsymbol{x}) \Bigg/ \int_{S_\rho^+} s(d\boldsymbol{x}) =$$

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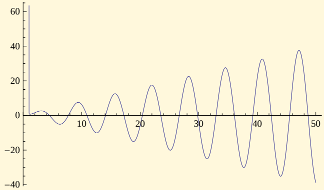
Divergence of the function M

- Defined formally as the mean value of the (bounded) complex exponential function over the (infinte) surface of the hyperboloid
- Integrate in pseudo-hyperspheric coordinates and reduce the problem to the quotient of one-dimensional integrals

$$\int_1^\infty x^{\frac{k}{2}} J_{\frac{k}{2}-1}(A_2 x)\,\frac{dx}{\sqrt{x^2-1}} \Bigg/ \int_1^\infty x^{k-1}\,\frac{dx}{\sqrt{x^2-1}},$$

  where J_ν denotes de Bessel function of the first kind, and A_2 is a constant.
- This is the quotient of two divergent functions. The numerator looks something like $(k=5)$



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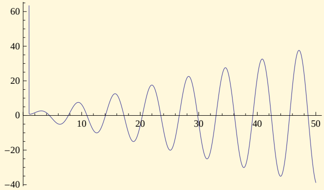

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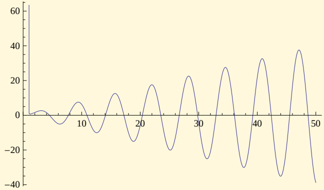

Spectral density functions of particular cases

- Isotropic correlation function in $E_{(2,1)}$

$$f(\boldsymbol{\omega}) = \begin{cases} \dfrac{1}{2\pi^2\|\boldsymbol{\omega}\|} \displaystyle\int_0^\infty R(\rho^2)\rho\Big(\cos(\|\boldsymbol{\omega}\|\rho) + e^{-\|\boldsymbol{\omega}\|\rho}\Big)\, d\rho, & (\boldsymbol{\omega},\boldsymbol{\omega}) > 0 \\ \dfrac{-1}{2\pi^2\|\boldsymbol{\omega}\|} \displaystyle\int_0^\infty R(\rho^2)\rho \sin(\|\boldsymbol{\omega}\|\rho)\, d\rho, & (\boldsymbol{\omega},\boldsymbol{\omega}) < 0 \end{cases}$$

- Exponential correlation function in $E_{(2,1)}$

$$f(\boldsymbol{\omega}) = \begin{cases} \dfrac{1}{2\pi^2\|\boldsymbol{\omega}\|}\left(\dfrac{\varphi^2 - \|\boldsymbol{\omega}\|^2}{(\varphi^2 + \|\boldsymbol{\omega}\|^2)^2} + \dfrac{1}{(\varphi + \|\boldsymbol{\omega}\|)^2}\right), & (\boldsymbol{\omega},\boldsymbol{\omega}) > 0 \\ \dfrac{-\varphi}{\pi^2(\varphi^2 + \|\boldsymbol{\omega}\|^2)^2}, & (\boldsymbol{\omega},\boldsymbol{\omega}) < 0 \end{cases}$$

where $\|\boldsymbol{\omega}\| = \sqrt{|(\boldsymbol{\omega},\boldsymbol{\omega})|}$. This goes negative for $\|\boldsymbol{\omega}\|$ large enough in $(\boldsymbol{\omega},\boldsymbol{\omega}) > 0$. The exponential function is not positive-definite in $E_{(2,1)}$.

Reparameterization of covariance matrices

- Model the elements of a reparameterization of the covariance matrix (e.g. Cholesky) as a function of the distances
- We still want covariances to be functions of the distances
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TESIS DOCTORAL

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Director: Antonio López-Quílez

Febrero 2013