Kullback-Leibler Divergence Estimation Based on Iterative Gaussianization

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Kullback-Leibler divergence

Non-symmetric measure of the difference between two probability distributions,

$$D_{KL}(p,q) = \int_{\mathbb{R}^d} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} d\mathbf{x}$$

Problem: high dimensional KLD estimation is difficult

The proposed method is useful:

- Curse of dimensionality alleviated
- Low computational cost
- Non-parametric

Consider two distributions $p_1(\mathbf{x})$ and $q_1(\mathbf{x})$ in space X ($\mathbf{x} \in X$). Let $\mathcal{G} : X \to Y$ (linear or nonlinear) denote a differentiable and invertible mapping function that converts $\mathbf{x}$ into $\mathbf{y}$,

$$p_1(\mathbf{x}) = p_2(\mathcal{G}(\mathbf{x}))|\nabla_{\mathbf{x}}\mathcal{G}|$$

$$q_1(\mathbf{x}) = q_2(\mathcal{G}(\mathbf{x}))|\nabla_{\mathbf{x}}\mathcal{G}|$$

The KL divergence between two distributions is invariant under transformation $\mathcal{G}$,

$$D_{KL}(p_1, q_1) = D_{KL}(p_2, q_2).$$

Proposed method

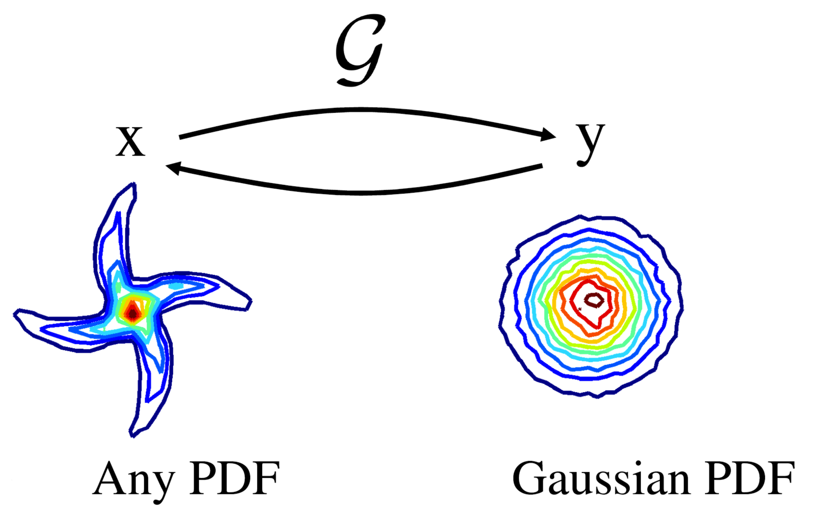
Initial objective: $D_{KL}(p_1, q_1)$

1. Find transform $\mathcal{G}_1$ that gaussianizes q_1 ($q_2 = \mathcal{N}(\mathbf{0}, \mathbf{I})$)
2. Apply $\mathcal{G}_1$ to p_1

New objective: $D_{KL}(p_2, \mathcal{N}(\mathbf{0}, \mathbf{I}))$

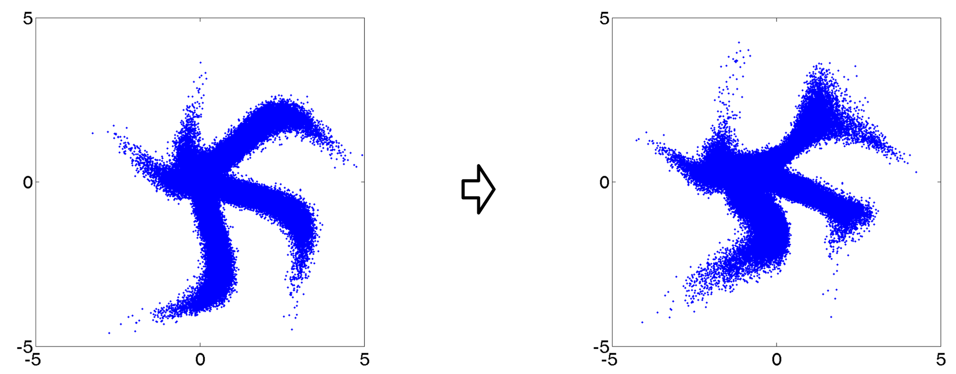
3. Find transform $\mathcal{G}_2$ that gaussianizes p_2
4. Compute objective

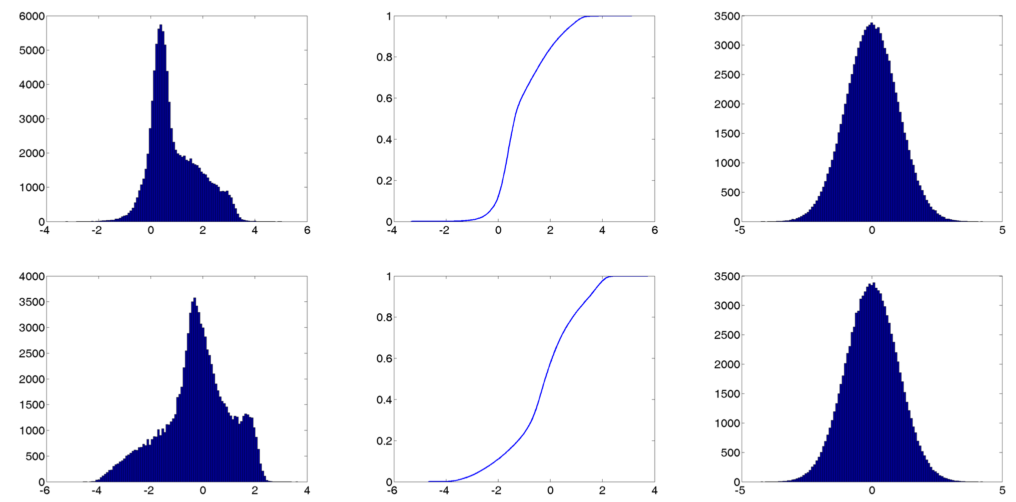
Iterative gaussianization



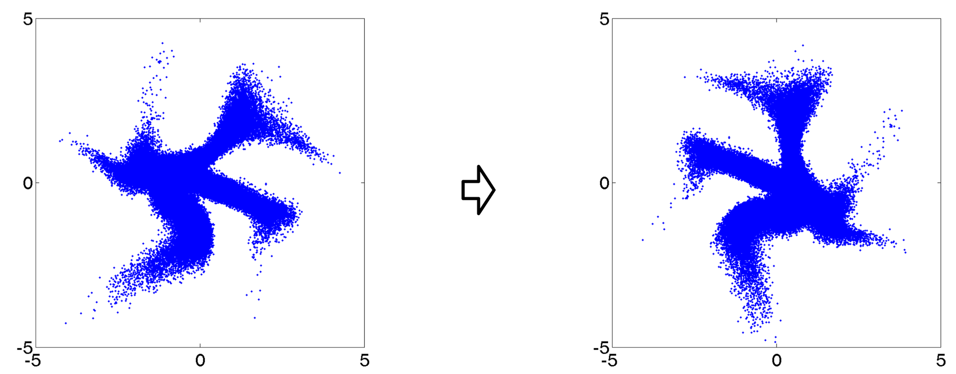
Iterative algorithm with 2 steps per iteration: $\mathbf{x}^{(k+1)} = \mathbf{R}_{(k)}\mathbf{\Psi}_{(k)}(\mathbf{x}^{(k)})$

1. Marginal Gaussianization ($\mathbf{\Psi}$)





2. Rotation ($\mathbf{R}$)



Divergence estimation

$D_{KL}(p(\mathbf{x}), \mathcal{N}(\mathbf{0}, \mathbf{I})) = I(\mathbf{x}) + D_{KLm}(\mathbf{x})$

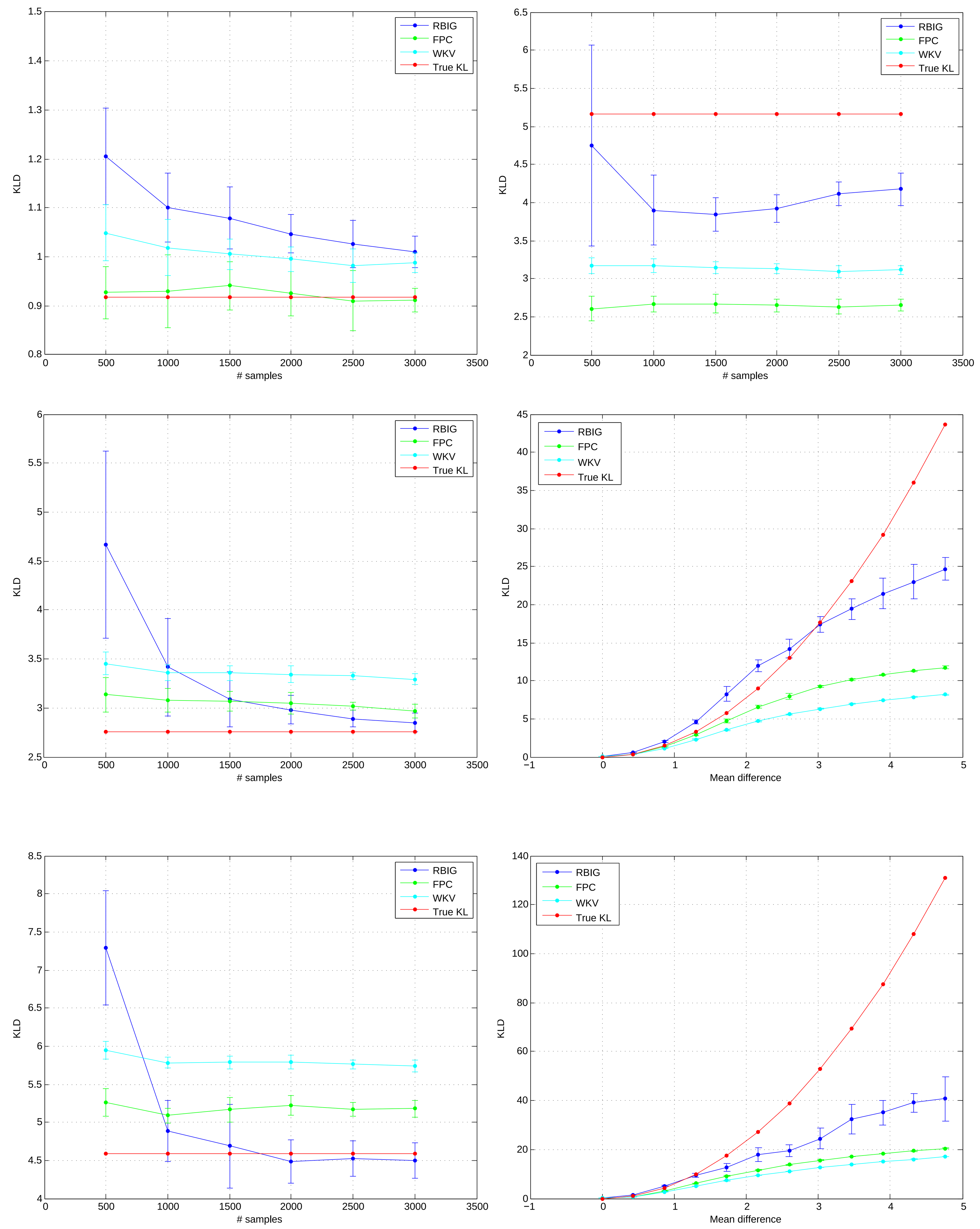
$I(\mathbf{x}) \to$ multi-information

$D_{KLm}(\mathbf{x}) \to$ marginal KL divergence

Estimation: compute $\Delta D_{KL(k)} = D_{KLm}(\mathbf{x}^{(k)}) = \Delta I_{(k-1)}$ at each iteration

Results

Estimation of KL divergence between two Gaussian densities in various shapes and with various dimensionalities. Left figures depict the experimental results for isotropic-isotropic Gaussians of 2, 6 and 10 dimensions. Top right presents isotropic-correlated Gaussians with increasing numbers of samples. Bottom right figures show how the estimation results increase with the increase of the mean difference for a fixed number of data samples.



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