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Gaussian Processes Indexed by Clouds of Points: a study

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Context And Problematic

- Metamodel a function over clouds of points using Gaussian process.
- A cloud is a set of points invariant under permutation \( \{x_1, \ldots, x_n\} \) with \( x_i \in \mathbb{R}^{dim} \)

Test Function

The following test function mimics a wind-farm production:

\[
F(\{x_1, \ldots, x_n\}) = \sum_{i=1}^{n} \sum_{j \leq i} f_p(x_j, x_i) f_0(x_i)
\]

where \( f_p(x_j, x_i) \) expresses the energy loss over \( x_i \) that is caused by \( x_j \) and \( f_0 \) is a constant.

Kernels

Substitution kernel with MMD

- We want to construct a kernel between two clouds of the form \( K(X, Y) = \sigma^2 \exp(- \frac{d^2(X, Y)}{2\theta}) \) where \( d \) is an Hilbertian distance.
- For two clouds \( X = \{x_1, \ldots, x_n\} \) and \( Y = \{y_1, \ldots, y_n\} \), \( P_X = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \) and \( P_Y = \frac{1}{n} \sum_{i=1}^{n} \delta_{y_i} \) are the respective associated empirical uniform distributions.
- There exists a Reproducing Kernel Hilbert Space, \( H \) with a characteristic kernel such as \( k_H(x, \cdot) = \exp(- \frac{d^2(x, \cdot)}{2\theta}) \).
- The characteristic nature guarantees the injectivity of the embedding map [1]: \( P_X \mapsto \mu_X = \int P_X(x) k_H(x, \cdot) \, dx \).
- \( \text{MMD}^2(P_X, P_Y) = \| \mu_X - \mu_Y \|_H^2 \)
- For any kernel \( k_H \) of the RKHS, the uniform empirical laws gives \( \text{MMD}^2(P_X, P_Y) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(x_i, x_j) + \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(y_i, y_j) - 2 \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(x_i, y_j) \)
- The correlation kernel \( K_{\text{sub}_\text{mmd}}(X, Y) = \sigma \exp(- \frac{\| \mu_X - \mu_Y \|_H^2}{2\theta}) \) is symmetric and definite positive.

Geometrical Properties of the kernels

- Below is represented the correlation between a cloud and its image by a geometric transformation. Considered transformations are rotations and translations.
- We compare two scenarios: centered clouds and non-centered ones.
- The different kernels of the Hilbertian Space are the Exponential, the Gaussian(Squared Exponential), the Matern32 and the Matern52.

Prediction Results on the analytical Function F

- We metamodel the wind-farm proxy function \( F \) with a Gaussian process of kernel \( K_{\text{sub}_\text{mmd}} \).
- We consider a set of 1000 clouds of 10 points each.
- Each point of a cloud is drawn uniformly in a square.
- The kernel parameters are learned using 200 clouds by maximizing log-likelihood with BFGS.
- On each plot, we represent predicted values vs. true ones on the remaining clouds, obtained with the different kernels.
- The corresponding Q2, MAE and MSE are also displayed.

References