Gaussian Processes Indexed by Clouds of Points: a study Babacar SOW (EMSE, LIMOS), Rodolphe LE RICHE (CNRS, LIMOS)

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To cite this version:
Babacar Sow, Rodolphe Le Riche, Julien Pelamatti, Sanaa Zannane, Merlin Keller. Gaussian Processes Indexed by Clouds of Points: a study Babacar SOW (EMSE, LIMOS), Rodolphe LE RICHE (CNRS, LIMOS). MASCOT-NUM, Jun 2022, Clermont Ferrand, France. emse-03720276

HAL Id: emse-03720276
https://hal-emse.ccsd.cnrs.fr/emse-03720276
Submitted on 11 Jul 2022

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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 \( \{x_1, ..., x_n\} \) with \( x_i \in \mathbb{R}^{dim} \).

Test Function

The following test function mimics a wind-farm production:

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

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

Prediction Results on the analytical Function F

- We metamodel the wind-farm proxy function \( F \) with a Gaussian process of kernel \( K_{\text{sub-MMD}} \).
- 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.

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.

References