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

Babacar Sow, Rodolphe Le Riche, Julien Pelamatti, Sanaa Zannane, Merlin Keller

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
Submit on 11 Jul 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Gaussian Processes Indexed by Clouds of Points: a study

Julien PELAMATTI (EDF R&D), Sanaa ZANNANE (EDF R&D), Merlin KELLER (EDF R&D)

Universités: Ecole Nationale Supérieure des Mines de Saint-Etienne (EMSE), Université Clermont Auvergne (UCA)

Laboratoire: LIMOS

Email of contact: babacar.sow@emse.fr

Gaussian Processes Indexed by Clouds of Points: a study

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 \( x_i \in \mathbb{R}^{3d} \)

Test Function

The following test function mimics a wind-farm production:

\[
F((x_1, ..., x_n)) = \sum_{i=1}^{n} \sum_{j \neq i}^n f_p(x_j, x_i) f_0(x_i) \quad \text{where} \quad x_{i,j} \leq x_{i,1}
\]

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 \( K(X, Y) = \sigma^2 \exp(-\frac{d(X, Y)}{2\rho}) \) 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 empirical uniform distributions.
- There exists a Reproducing Kernel Hilbert Space, \( \mathcal{H} \) with a characteristic kernel such as \( k_H(x, \cdot) = \exp(-\frac{d(x, \cdot)}{\rho}) \).
- The characteristic norm guarantees the injectivity of the embedding map [1]: \( P_X \mapsto \mu_X = \int P_X(x) k_H(x, \cdot) dx \).
- \( \text{MMD}^2(P_X, P_Y) = \|\mu_X - \mu_Y\|_{\mathcal{H}} \)
- For any kernel \( k_H \) of the RKHS, the uniform empirical laws gives \( \text{MMD}^2(P_X, P_Y) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(x_i, x_j) + \frac{1}{m} \sum_{j=1}^{m} \sum_{k=1}^{m} k_H(y_j, y_k) - 2 \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(x_i, y_j) \)
- The correlation kernel \( K_{\text{sub}}_{\text{mmd}}(X, Y) = \sigma \exp(-\frac{\|\mu_X - \mu_Y\|^2}{2\rho}) \) 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