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

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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 \(x_i \in \mathbb{R}^{d \times m}\).

Test Function

The following test function mimicks a wind-farm production:

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

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 \(K(F, Y) = \sigma^2 \exp(-\frac{d^2(F, Y)}{2})\) 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, \(H\) with a characteristic kernel such as \(k_H(x, .) = \exp(-\frac{d^2(x, .)}{2})\).
- The characteristic nature guarantees the injectivity of the embedding map [1]: \(P_X \mapsto \mu_X = \int P_X(x) k_H(x, .) dx\).
- \(MMD^2(P_X, P_Y) = \|\mu_X - \mu_Y\|^2_H\)
- For any kernel \(k_H\) of the RKHS, the uniform empirical laws gives \(MMD^2(P_X, P_Y) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k_H(x_i, x_j) + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} k_H(y_i, y_j) - \frac{2}{nm} \sum_{i=1}^{n} \sum_{j=1}^{m} k_H(x_i, y_j)\).
- The correlation kernel \(K_{sub\_mmd}(F, Y) = \sigma \exp(-\frac{d^2(F, Y)}{2})\) 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 \(K_{sub\_mmd}\).
- 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.

The best results are obtained when \(k_H\) is the Squared Exponential and clouds are centered. This can be explained by the fact that the quadratic modified distance with two length scales of this \(k_H\) complies better with the geometric properties of \(F\).

References