



Contribution ID: 66

Type: **not specified**

New Estimation Algorithm for More Reliable Prediction in Gaussian Process Regression: Application to an Aquatic Ecosystem Model

Wednesday, 13 September 2023 09:10 (20 minutes)

In the framework of emulation of numerical simulators with Gaussian process (GP) regression [1], we proposed in this work a new algorithm for the estimation of GP covariance parameters, referred to as GP hyperparameters. The objective is twofold: to ensure a GP as predictive as possible w.r.t. to the output of interest, but also with reliable prediction intervals, i.e. representative of its prediction error.

To achieve this, we propose a new constrained multi-objective algorithm for the hyperparameter estimation. It jointly maximizes the likelihood of the observations as well as the empirical coverage function of GP prediction intervals, under the constraint of not degrading the GP predictivity [2]. Cross validation techniques and advantageous update GP formulas are notably used.

The benefit brought by the algorithm compared to standard algorithms is illustrated on a large benchmark of analytical functions (up to twenty input variables). An application on a EDF R&D real data test case modeling an aquatic ecosystem is also proposed: a log-kriging approach embedding our algorithm is implemented to predict the biomass of the two species. In the framework of this particular modeling, this application shows the crucial interest of well-estimated and reliable prediction variances in GP regression.

[1] Marrel et al. (2022). The ICSCREAM Methodology: Identification of Penalizing Configurations in Computer Experiments Using Screening and Metamodel. Applications in Thermal Hydraulics. Nucl. Sci. Eng., 196(3):301–321.

[2] Demay et al. (2022). Model selection for Gaussian process regression: an application with highlights on the model variance validation. Qual. Reliab. Eng. Int., 38:1482-1500.

Keywords

Computer experiments, Metamodel, Gaussian process (GP) regression, estimation of GP hyperparameters.

Classification

Both methodology and application

Primary authors: MARREL, Amandine (CEA); Dr IOOSS, Bertrand (EDF R&D)

Presenter: MARREL, Amandine (CEA)

Session Classification: CONTRIBUTED Biostatistics and Machine Learning

Track Classification: Machine learning