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Calibrating Prediction Intervals for Gaussian Processes using Cross-Validation method

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Gaussian Processes are considered as one of the most important Bayesian Machine Learning methods (Rasmussen and Williams [1], 2006). They typically use the Maximum Likelihood Estimation or Cross-Validation to fit parameters. Unfortunately, these methods may give advantage to the solutions that fit observations in average (F. Bachoc [2], 2013), but they do not pay attention to the coverage and the width of Prediction Intervals. This may be inadmissible, especially for systems that require risk management. Indeed, an interval is crucial and offers valuable information that helps for better management than just predicting a single value.

In this work, we address the question of adjusting and calibrating Prediction Intervals for Gaussian Processes Regression. First we determine the model's parameters by a standard Cross-Validation or Maximum Likelihood Estimation method then we adjust the parameters to assess the optimal type II Coverage Probability to a nominal level. We apply a relaxation method to choose parameters that minimize the Wasserstein distance between the Gaussian distribution of the initial parameters (Cross-Validation or Maximum Likelihood Estimation) and the proposed Gaussian distribution among the set of parameters that achieved the desired Coverage Probability.

References :

1. Rasmussen, C.E., Williams, C.K.I.: Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning). The MIT Press (2005).
2. Bachoc, F.: Cross validation and maximum likelihood estimations of hyper-parameters of gaussian processes with model misspecification. Computational Statistics & Data Analysis 66, 55–69 (2013).

Keywords

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Special/invited session

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