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Evolution of Covariance Functions for Gaussian Process Regression using Genetic Programming

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In this contribution we describe an approach to evolve composite covariance functions for Gaussian processes using genetic programming. A critical aspect of Gaussian processes and similar kernel-based models such as SVM is, that the covariance function should be adapted to the modeled data. Frequently, the squared exponential covariance function is used as a default. However, this can lead to a misspecified model, which does not fit the data well. In the proposed approach we use a grammar for the composition of covariance functions and genetic programming to search over the space of sentences that can be derived from the grammar. We tested the proposed approach on synthetic data from two-dimensional test functions, and on the Mauna Loa CO2 time series. The results show, that our approach is feasible, finding covariance functions that perform much better than a default covariance function. For the CO2 data set a composite covariance function is found, that matches the performance of a hand-tuned covariance function.

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