Exploiting Hessian matrix and trust-region algorithm in hyperparameters estimation of Gaussian process

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Abstract

Gaussian process (GP) regression is a Bayesian non-parametric regression model, showing good performance in various applications. However, it is quite rare to see research results on log-likelihood maximization algorithms. Instead of the commonly used conjugate gradient method, the Hessian matrix is first derived/simplified in this paper and the trust-region optimization method is then presented to estimate GP hyperparameters. Numerical experiments verify the theoretical analysis, showing the advantages of using Hessian matrix and trust-region algorithms. In the GP context, the trust-region optimization method is a robust alternative to conjugate gradient method, also in view of future researches on approximate and/or parallel GP-implementation.

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