Gradient-enhanced Gaussian Process Models:

What, Why and How

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Abstract

Simulations with gradient information are increasingly used in engineering and science. From a data pooling perspective, it is appealing to use the gradient-enhanced Gaussian process model for emulating such simulations. However, it is computationally challenging to fit such an emulator for large data sets because its covariance matrix has severe singular issues. I will present a theory to show why this problem happens. I will also propose a random Fourier feature method to mitigate the problem. The key idea of the proposed method is to employ random Fourier features to obtain an easily computable, low-dimensional feature representation for shift-invariant kernels involving gradients. The effectiveness of the proposed method is illustrated by several examples.