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Matrix-Free Hyperparameter Optimization for Gaussian Processes

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Gaussian processes (GPs) are a crucial tool in machine learning and their use across different areas of science and engineering has increased given their ability to quantify the uncertainty in the model. The covariance matrices of GPs arise from kernel functions, which are crucial in many learning tasks and the matrices are typically dense and large-scale. Depending on their dimension even computing all their entries is challenging and the cost of matrix-vector products scales quadratically with the dimension, if no customized methods are applied. We present a matrix-free approach that exploits the computational power of the non-equispaced fast Fourier transform (NFFT) and is of linear complexity for fixed accuracy. With this, we cannot only speed up matrix-vector multiplications with the covariance matrix but also take care of the derivatives needed for the gradient method avoiding Hadamard products of the Euclidean distance matrix and the kernel matrix. This arises when differentiating kernels as the squared-exponential kernel with respect to the length-scale parameter in the denominator of the exponential expression. Our method introduces a derivative kernel which is then well suited for multiplying with the Hadamard product. By applying our NFFT-based fast summation technique, fitting the kernel and the derivative kernel, will allow for fast tuning of the hyperparameters.

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