Bayesian Optimization in Reduced Eigenbases

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Parametric shape optimization aims at minimizing a function \(f(x)\) where \(x \in X \subset \mathbb{R}^d\) is a vector of \(d\) Computer Aided Design parameters, representing diverse characteristics of the shape \(\Omega_x\). It is common for \(d\) to be large, \(d \gg 50\), making the optimization difficult, especially when \(f\) is an expensive black-box and the use of surrogate-based approaches [1] is mandatory.

Most often, the set of considered CAD shapes resides in a manifold of lower dimension where it is preferable to perform the optimization. We uncover it through the Principal Component Analysis of a dataset of \(n\) designs, mapped to a high-dimensional shape space via \(\phi : X \rightarrow \Phi \subset \mathbb{R}^D, D \gg d\). With a proper choice of \(\phi\), few eigenshapes allow to accurately describe the sample of CAD shapes through their principal components \(\alpha\) in the eigenbasis \(V = [v^1, \ldots, v^D]\).

A Gaussian Process is fitted to the principal components \(\alpha^{(1)}, \ldots, \alpha^{(n)} \in \mathbb{R}^D\) instead of \(x^{(1)}, \ldots, x^{(n)} \in X\). The \(\delta\) most important eigenshapes are selected by maximizing a likelihood with a \(L_1\) regularization. These \(\delta\) active dimensions with components \(\alpha^a\) are emphasized without entirely neglecting the \(D - \delta\) remaining dimensions by constructing an additive GP [3]: \(Y(\alpha) = Y^a(\alpha^a) + Y^\pi(\alpha^\pi)\). \(Y^a\) is the main-effect \(\delta\)-dimensional anisotropic GP and \(Y^\pi\) is a coarse, isotropic high \((D - \delta)\) dimensional GP which only requires 2 hyperparameters.

A redefinition of the Expected Improvement [1] is proposed to take advantage of the space reduction and to carry out the maximization in the smaller space of important eigenshapes, completed by a cheap maximization with regard to \(\alpha^T\) through an embedding strategy [4], \(\alpha^{(n+1)} = \arg \max_{\alpha^T} EI(\alpha^o, \alpha^\pi)\). Its pre-image, \(x^{(n+1)} = \arg \min_{x \in X} \|V^\top \phi(x) - \alpha^{(n+1)}\|^2\), is the next evaluated design. A new replication strategy is described that guides the optimization to the manifold of the observed \(\alpha^{(i)}\), \(i = 1, \ldots, n\). It is based on the repelling property of EI and the addition of both \(\alpha^{(n+1)}\) and \(V^\top \phi(x^{(n+1)})\) to the pool of components conditioning the GP.

References


