Bayesian Optimization in Reduced Eigenbases

David Gaudrie[1] Rodolphe Le Riche[2] Victor Picheny[3]

[1]Groupe PSA, France, david.gaudrie@mpsa.com
[2]CNRS LIMOS, Mines Saint-Étienne, France
[3]Prowler.io, United Kingdom

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Parametric shape optimization aims at minimizing a function $f(\mathbf{x})$ where $\mathbf{x} \in X \subset \mathbb{R}^d$ is a vector of d Computer Aided Design parameters, representing diverse characteristics of the shape $\Omega_{\mathbf{x}}$. It is common for d to be large, $d \gtrsim 50$, 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 $\phi : X \to \Phi \subset \mathbb{R}^D$, $D \gg d$. With a proper choice of ϕ, few *eigenshapes* allow to accurately describe the sample of CAD shapes through their principal components $\boldsymbol{\alpha}$ in the eigenbasis $\mathbf{V} = [\mathbf{v}^1, \dots, \mathbf{v}^D]$.

A Gaussian Process is fitted to the principal components $\boldsymbol{\alpha}^{(1)}, \dots, \boldsymbol{\alpha}^{(n)} \in \mathbb{R}^D$ instead of $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)} \in X$. The δ most important eigenshapes are selected by maximizing a likelihood with a L_1 regularization. These δ active dimensions with components $\boldsymbol{\alpha}^a$ are emphasized without entirely neglecting the $D - \delta$ remaining dimensions by constructing an additive GP [3]: $Y(\boldsymbol{\alpha}) = Y^a(\boldsymbol{\alpha}^a) + Y^{\overline{a}}(\boldsymbol{\alpha}^{\overline{a}})$. Y^a is the main-effect δ-dimensional anisotropic GP and $Y^{\overline{a}}$ 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 $\boldsymbol{\alpha}^{\overline{a}}$ through an embedding strategy [4], $\boldsymbol{\alpha}^{(n+1)} = \arg\max \mathrm{EI}([\boldsymbol{\alpha}^a, \boldsymbol{\alpha}^{\overline{a}}])$. Its pre-image, $\mathbf{x}^{(n+1)} = \underset{\mathbf{x} \in X}{\arg\min} \, \|\mathbf{V}^\top \phi(\mathbf{x}) - \boldsymbol{\alpha}^{(n+1)}\|^2$, is the next evaluated design. A new replication strategy is described that guides the optimization to the manifold of the observed $\boldsymbol{\alpha}^{(i)}$, $i = 1, \dots, n$. It is based on the repelling property of EI and the addition of both $\boldsymbol{\alpha}^{(n+1)}$ and $\mathbf{V}^\top \phi(\mathbf{x}^{(n+1)})$ to the pool of components conditioning the GP.

References

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