Dimension Reduction for the Bayesian Optimization of Shapes

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Abstract:

Parametric shape optimization aims at minimizing one (or $m \geq 2$ in a multi-objective setting) objective function $f(\mathbf{x})$ where $\mathbf{x} \in X \subset \mathbb{R}^d$ is a d-dimensional vector of CAD parameters. It is common that d is large, $d \gtrsim 50$. Optimization in such a high-dimensional design space is difficult, especially when $f(\cdot)$ is an expensive black-box function and the use of surrogate-based approaches [1] is mandatory. The ratio between the allowed budget of function evaluations ($b \approx$ 100-200) and d is also too small to perform sensitivity analysis prior to selecting $d' << d$ variables.
In this work, we exploit the fact that the computation time of a shape $\Omega_{\mathbf{x}}$ is negligible in comparison with the evaluation time of $f(\mathbf{x})$. Most often, the set of all CAD generated shapes, $\mathbf{\Omega} := \{\Omega_{\mathbf{x}}, \mathbf{x} \in X\}$ can be approximated in a $\delta << d$ -dimensional manifold where it is preferable to build the surrogate model and perform the optimization. To uncover this manifold, we apply PCA to a dataset of designs and test alternative shape representations. We then build Gaussian processes and optimize in the reduced space of eigenshapes. Such approaches have already been considered in part in [3, 4], but we provide a new integrated view of shape reduction and optimization with kernel methods. In the following, the essential elements of our approach are further introduced.

From CAD description to shape eigenbasis. Let $\phi : X \to \Phi$ be a mapping to a high-dimensional space $\Phi \subset \mathbb{R}^D$, $D >> d$. We have compared alternative $\phi : X \to \Phi$ based on their ability to uncover intrinsic dimensions through Principal Component Analysis (PCA). The ϕ studied here are the characteristic function, the signed distance to contours and the contour discretization. We proceed by uniformly sampling N designs in X. Performing a PCA of that sample in the X space would be useless. However, with a proper choice of ϕ, we have found that a few (δ) eigenshapes allow to accurately describe the sample of CAD shapes through their principal components, $\boldsymbol{\alpha}$ in the eigenbasis $(\mathbf{v}^1, \ldots, \mathbf{v}^D)$.

GP model for shrinked spaces. Instead of building a surrogate for $f(\cdot)$ using $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)} \in X \subset \mathbb{R}^d$, a GP is fitted to the principal components $\boldsymbol{\alpha}^{(1)}, \ldots, \boldsymbol{\alpha}^{(n)} \in \mathbb{R}^D$. To simultaneously emphasize the δ most important axes without entirely neglecting the $D - \delta$ remaining ones, an additive model between the (δ) active components and the residual coordinates is considered:

$$Y(\boldsymbol{\alpha}) = \mu + Y^a(\boldsymbol{\alpha}_{1:\delta}) + Y^{\overline{a}}(\boldsymbol{\alpha}_{\delta+1:D}) + \varepsilon \ .$$

$Y^a(\cdot) \sim \mathcal{GP}_\delta(0, k^a(\cdot,\cdot))$ is the main-effect GP in a δ-dimensional input space and $Y^{\overline{a}}(\cdot) \sim \mathcal{GP}_{D-\delta}(0, k^{\overline{a}}(\cdot,\cdot))$ is a sparse, isotropic GP. $Y^{\overline{a}}(\cdot)$ lives in a high dimensional space but only requires the estimation of 2 hyperparameters, θ_D and σ_D^2. It aims at taking the less relevant, though existing, effects of the remaining eigenshapes into account.

Optimization in a reduced space. The well known Expected Improvement [2] is then maximized with the full $Y(\cdot)$ to optimize the shape. It is possible to carry out this maximization in the X space thanks to the ϕ mapping, $\mathbf{x}^{(n+1)} = \underset{\mathbf{x}\in X}{\arg\max}\ \mathrm{EI}(\boldsymbol{\alpha}(\mathbf{x}))$. But such an approach does not take advantage of the space reduction beyond the construction of $Y(\cdot)$. We thus propose a redefinition of improvement to carry out the maximization in the smaller space of important eigenshapes, completed by a cheap maximization with regard to the dimensions $\delta + 1$ to D, $\boldsymbol{\alpha}^{(n+1)} = \underset{[\boldsymbol{\alpha}_{1:\delta}, \boldsymbol{\alpha}_{\delta+1:D}]\in\mathbb{R}^D}{\arg\max}\ \mathrm{EI}([\boldsymbol{\alpha}_{1:\delta}, \boldsymbol{\alpha}_{\delta+1:D}])$. The calculation of the 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 finally performed to find the next parametric design to be evaluated by the computer code.

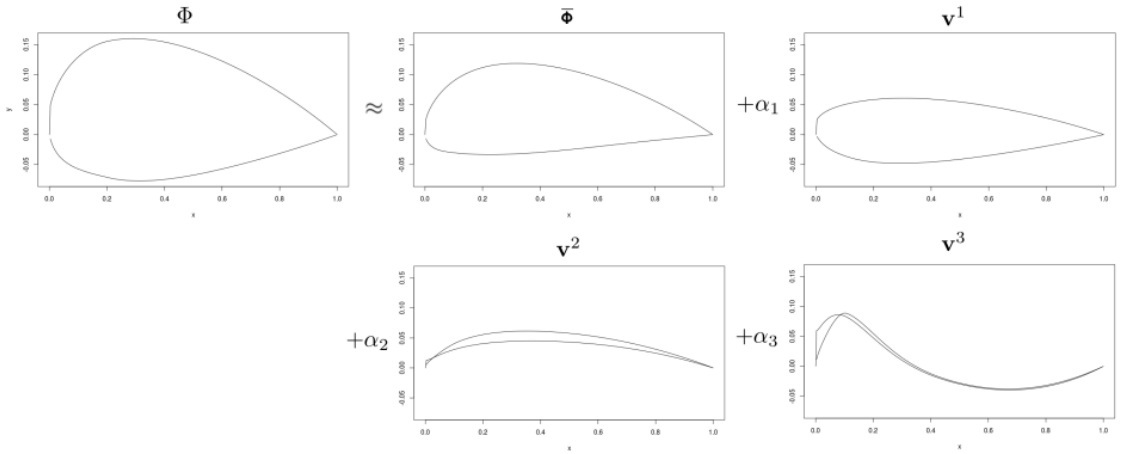

Figure 1: Shape decomposition in its eigenbasis

References

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Short biography – David Gaudrie obtained his engineering degree from INSA Toulouse in Applied Mathematics in 2016. He started a PhD thesis about high dimensional multi-objective optimization in the context of expensive computer codes in November 2016. This thesis in funded by the automotive group PSA (CIFRE convention) in collaboration with the École des Mines de Saint-Étienne.