Modeling and Optimization with Gaussian Processes in Reduced Eigenbases

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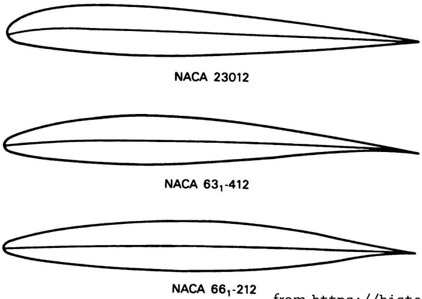
Context: costly shape optimization I

This study is presented with details in [Gaudrie et al., 2020].

Minimize the drag of an airfoil by changing its shape

$$\min_{\phi \in \mathcal{S}} f(\phi) \quad , \quad \mathcal{S} \text{ ``infinite'' dimensional space of shapes}$$



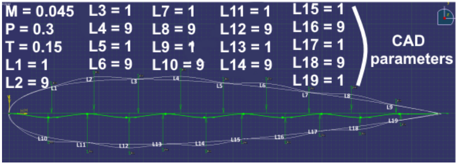
from https://history.nasa.gov/SP-468/ch5-2.htm

Context: costly shape optimization II

Computational practice

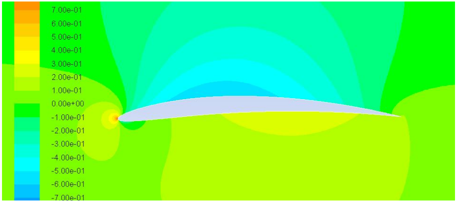
design: decide shape parameters $x \in \mathbb{R}^d$

CAD: translate them into a shape $\phi(x) \in \mathbb{R}^D$, $D \gg d$



not costly

simulate: calculate $f(\phi(x))$, e.g., by Navier-Stokes resolution



costly

Context: costly shape optimization III

A straightforward resolution of $\min_{x \in \mathcal{S} \subset \mathbb{R}^d} f(\phi(x))$ is difficult: the problem dimension d (10-100) is too large considering the computing time of f (minutes to hours).

In this work, tackle this problem through,

A) dimension reduction from $\phi(x)$ by eigenshape decomposition
B) metamodeling with Gaussian process (GP) including supervised dimension reduction (from f),
C) optimization in the reduced-dimension space of A) and B).

Intrinsic dimension reduction by eigendecomposition

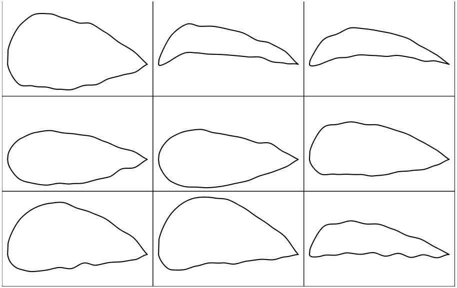
Creating shapes without evaluating their performance is fast $\Rightarrow$ calculate a hierarchical basis of eigenvectors in shape space by PCA (a.k.a. POD)

- sample CAD parameters $x^i \sim \mathcal{U}(\mathcal{S})$, $i = 1, \ldots, N$, $N \gg d$
- calculate the shapes $\phi(x^i)$, $i = 1, \ldots, N$ and create $\Phi = [\phi(x^1) \ldots \phi(x^N)]$
- PCA: (λ_i, V^i) (eigenvalues, eigenvectors) of $\frac{1}{N}\Phi\Phi^\top$ with $\lambda_1 \geq \ldots \geq \lambda_D \geq 0$
- Keep dimensions $(V^1, \ldots, V^\delta)$ where δ smallest integer such that $\frac{\sum_{i=1}^{\delta} \lambda_i}{\sum_{i=1}^{N} \lambda_i} > 0.99$

V^i: $D \times 1$ "eigenshape" (but it may not be a feasible shape)

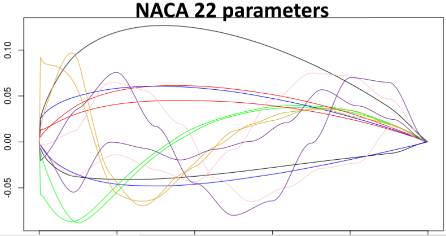
Airfoils eigenshapes

From a database of possible airfoils $[\phi(x^1), \ldots, \phi(x^{5000})]$,



...

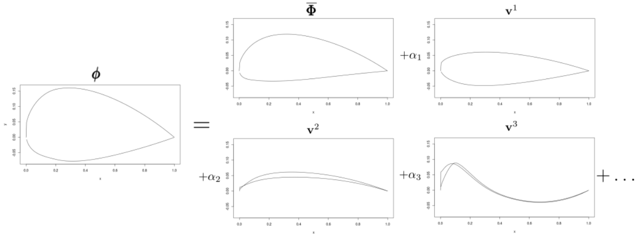
extract $\delta = 20$ eigenshapes $\{V^1, \ldots, V^\delta\}$



Working with the eigencomponents α

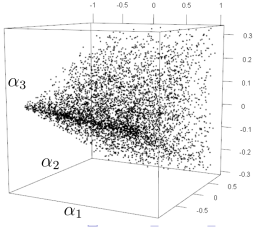
Shapes are now described with their eigencomponents α's:

$$\phi \approx \overline{\phi} + \sum_{i=1}^{\delta} \alpha_i V^i \quad \text{and} \quad \alpha_i = (\phi - \overline{\phi})^\top V^i$$



$(\alpha_1, \dots, \alpha_\delta)$ make a specific manifold

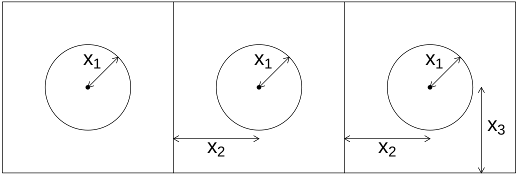
Cf. also [Raghavan et al., 2013, Li et al., 2018, Cinquegrana and Iuliano, 2018]



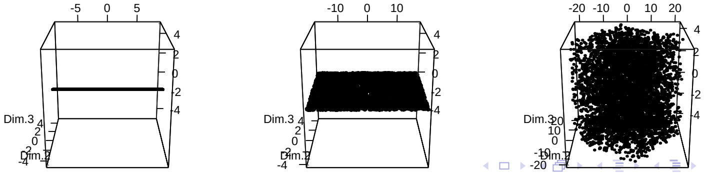
δ and the intrinsic dimension

[Gaudrie et al., 2020]: with $\phi(x)$ a vector of discretized contour points (as opposed to characteristic functions and signed distances),

δ = dimension of the α manifold $\underset{\text{empirical}}{\approx}$ intrinsic dimension of the shapes



α's



A) dimension reduction from $\phi(x)$ by eigenshape decomposition

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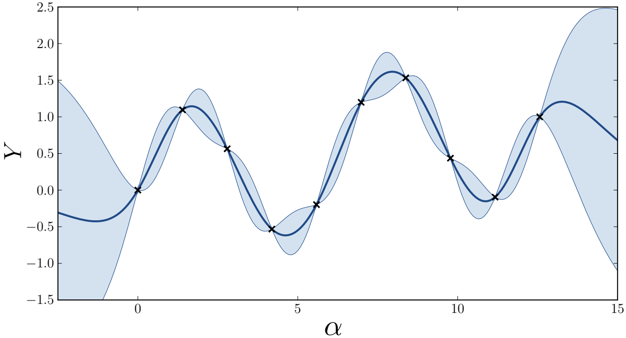
GP approximation with dimension reduction I

Approximate $f(\phi)$ (the drag) with a GP $Y(\alpha)$ where $\alpha = V^\top(\phi - \overline{\phi})$



$$Y(\alpha) \text{ learns the database } \underbrace{\left[\alpha^i = V^\top(\phi(x^i) - \overline{\phi}) \;,\; f(\phi(x^i))\right]}_{[\mathbb{\alpha}\;,\;\mathbb{F}]}, i = 1, N$$

GP approximation with dimension reduction II

- The GP is mainly controlled through its kernel, $k(\alpha, \alpha') = \text{Cov}(Y(\alpha), Y(\alpha'))$
- Kernels are parameterized by θ's and σ^2
- Anisotropic kernels have 1 θ_i per dimension

  Expl: $k_{\text{ani}}(\alpha, \alpha') = \sigma^2 \exp\left(-\sum_{i=1}^{\delta} \frac{(\alpha_i - \alpha'_i)^2}{{\theta_i}^2}\right)$
- isotropic kernels have 1 θ for all dimensions

  Expl: $k_{\text{iso}}(\alpha, \alpha') = \sigma^2 \exp\left(-\frac{(\alpha_i - \alpha'_i)^2}{\theta^2}\right)$

- Kernel parameters are learned by maximizing the likelihood of $[\mathbb{\alpha}\ ,\ \mathbb{F}]$

GP approximation with dimension reduction III

- A likelihood that favors sparsity [Yi et al., 2011]:

$$\theta^\star = \arg\max_\theta \text{ Log-Likelihood}(\theta; \mathbb{\alpha}, \mathbb{F}) - \lambda \|\theta^{-1}\|_1$$

$\Rightarrow$ active and non-active dimensions, α_a and $\alpha_{\bar{a}}$.

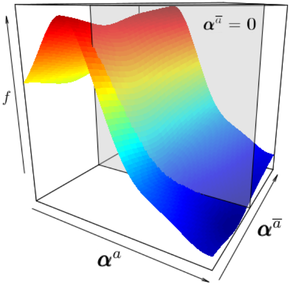
$$\begin{aligned} a &= \{i \in [1, \ldots, \delta] \mid \theta_i^\star < M \gg 1\} \\ \bar{a} &= \{1, \ldots, \delta\} \setminus a \end{aligned}$$

GP approximation with dimension reduction IV

- GP as the sum of an anisotropic and isotropic GPs [Allard et al., 2016], accurate on the active dimensions, plain but sparse otherwise:
  $k(\alpha, \alpha') = k_{\text{ani}}(\alpha_a, \alpha'_a) + k_{\text{iso}}(\alpha_{\bar{a}}, \alpha'_{\bar{a}})$

  Expl NACA22 :
  $\alpha_a = \{\alpha_1, \alpha_2, \alpha_3\}$, $\delta_a = 3$, $\delta = 20$
  $\Rightarrow$ 20 to 6 kernel parameters

  20: θ_1 to $\theta_{\delta=20}$, σ^2 by likelihood concentration formula.
  6: 3 θ_a's, 1 $\theta_{\bar{a}}$, σ^2_{iso}, σ^2_{ani}



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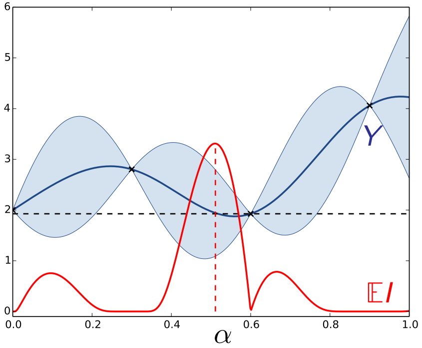
Optimizing with GPs

Measure of progress: the improvement,

$$I(x) = \max\left[0, \min(\mathbb{F}) - Y(\alpha)\right]$$

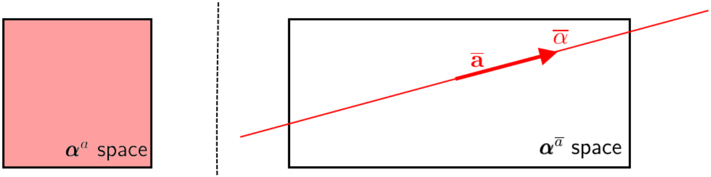
Optimization scheme : maximize the expectation of the improvement at each iteration and update the GP



$\mathbb{E}I = 0$ at data points, pushes the search away from them

Reduced dimension search

Search the full active space and search along a 1D random linear embedding in the inactive space



$$\boxed{\alpha^{(t+1)*} = \arg\max_{[\alpha_a, \overline{\alpha}]} \mathbb{E}I}$$

$\overline{\alpha}$ coordinate along a random line in non-active space,
$\delta_a + 1$ dimensions.

GP update: pre-image problem

To calculate the new objective function, $\alpha^{(t+1)*}$ needs to be transformed into a CADable shape = pre-image problem = projection of $V\alpha^{(t+1)*} + \overline{\phi}$ onto the closest CAD shape

$$x^{(t+1)} = \arg\min_{x \in \mathcal{S}} \|\mathrm{V}\alpha^{(t+1)*} + \overline{\phi} - \phi(x)\|^2$$

and evaluate $f(\phi(x^{(t+1)}))$

The next feasible eigencomponents are

$$\alpha^{(t+1)} = \mathrm{V}^\top(\phi(x^{(t+1)}) - \overline{\phi})$$

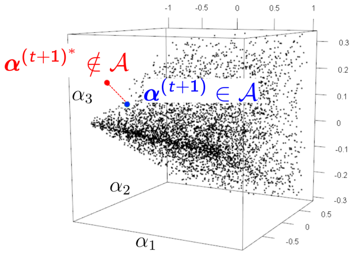
GP update: replication

Incentive for the optimization to search into the α-manifold: put the datapoint outside the manifold as $\mathbb{E}I$ will be null there afterwards

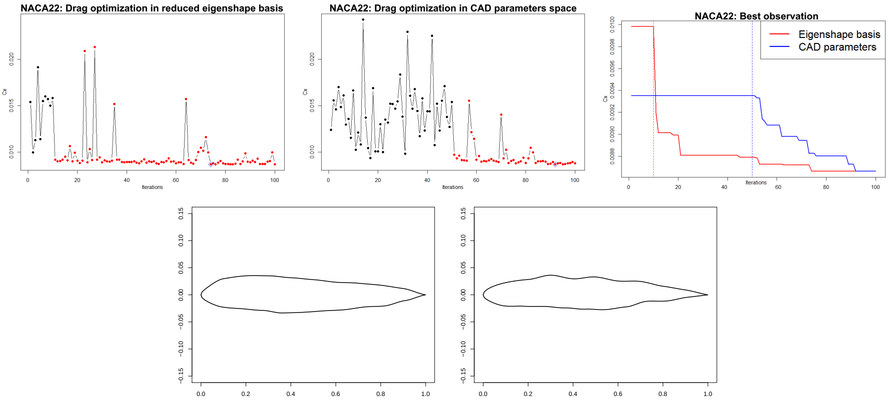
Replication

Update the GP with both $\alpha^{(t+1)*}$ and $\alpha^{(t+1)}$:

$[\mathbb{a}, \mathbb{F}] \longleftarrow [\mathbb{a}, \mathbb{F}] \cup \left[\alpha^{(t+1)}, f(\phi(x^{(t+1)}))\right] \cup \left[\alpha^{(t+1)*}, f(\phi(x^{(t+1)}))\right]$



Example: NACA 22 airfoil drag minimization



- Faster decrease of the objective function in the reduced eigenshape basis (left) compared with the standard approach (right, CAD parameter space).
- Smoother airfoils are obtained because a shape basis is considered instead of a combination of local parameters.

Summary

- We have mixed two dimension-reduction techniques: PCA and subsequent searching into an α-manifold (replication); the identification of an inactive subspace where sparse learning and searching is done (additive kernel and linear embedding).

Perspectives

- Why is the PCA dimension reduction working so well in our cases of CAD-like shape parameters?
- The approach is not specific to shapes and would apply any objective function composed as $f(\phi(x))$

$\Rightarrow$ try other cases, e.g. functional inputs.

- Investigate the 2 ideas (PCA . . . , inactive space identification . . .) separately.

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