Construction of Parametrically-Robust Reduced-Order Models via Nonlinear Programming

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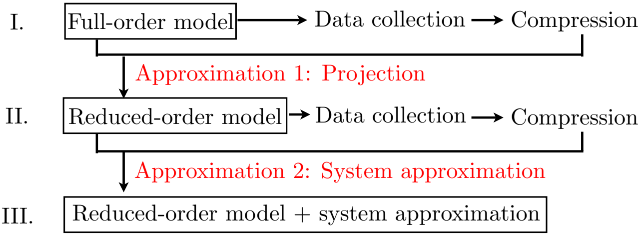
Outline

Model Order Reduction (MOR) Hierarchy



We consider the discretization of a *steady* PDE:

$$\mathbf{c}(\mathbf{w}, \mathbf{p}) = 0,$$

where $\mathbf{c} : \mathbb{R}^{N_w} \times \mathbb{R}^p \rightarrow \mathbb{R}^{N_w}$, $\mathbf{p} \in \mathcal{D} \subseteq \mathbb{R}^p$ is a vector of parameters, and N_w is typically very large. This will be referred to as the High-Dimensional Model (HDM) or Model I.

Let us denote the solution of the Reduced-Order Model (ROM) and hyperreduced ROM as:

- $\mathbf{c}_r(\mathbf{w}_r, \mathbf{p}) = 0$ Model II
- $\mathbf{c}_h(\mathbf{w}_r, \mathbf{p}) = 0$ Model III

respectively, where $\mathbf{c}_r : \mathbb{R}^{k_w} \times \mathbb{R}^p \rightarrow \mathbb{R}^{k_w}$ and $\mathbf{c}_h : \mathbb{R}^{k_w} \times \mathbb{R}^p \rightarrow \mathbb{R}^{k_w}$.

Model Order Reduction Assumption

MOR assumption: the solution of $\mathbf{c}(\mathbf{w}, \mathbf{p}) = 0$ lies in a low-dimensional affine subspace

$$\mathbf{w} = \bar{\mathbf{w}} + \mathbf{V}\mathbf{w}_r \tag{1}$$

where

$$\mathbf{V} \in \mathbb{R}^{N_w \times k_w} \text{ -- right basis}$$
$$\mathbf{w}_r \in \mathbb{R}^{k_w} \text{ -- reduced coordinates}$$
$$k_w \ll N_w.$$

Substituting this assumption into the HDM yields the overdetermined nonlinear system of equations

$$\mathbf{c}(\bar{\mathbf{w}} + \mathbf{V}\mathbf{w}_r, \mathbf{p}) = 0 \tag{2}$$

Reduced Order Model (ROM)

Now, we close the previous equation by requiring that the residual be orthogonal to the subspace spanned by the columns of some matrix $\mathbf{W} \in \mathbb{R}^{N_w \times k_w}$

$$\mathbf{c}_r(\mathbf{w}_r, \mathbf{p}) = \mathbf{W}^T \mathbf{c}(\bar{\mathbf{w}} + \mathbf{V}\mathbf{w}_r, \mathbf{p}) = 0. \quad (3)$$

Two standard choices for $\mathbf{W}$:

- $\mathbf{W} = \mathbf{V}$ Galerkin ROM
  - "Optimal" for problems with SPD Jacobians
- $\mathbf{W} = \frac{\partial \mathbf{c}}{\partial \mathbf{w}} \mathbf{V}$ Least-Squares Petrov-Galerkin ROM
  - "Optimal" for problems with non-SPD Jacobians

Outline

ROM Construction Philosophy

- ROM Construction usually considered an “offline” cost
  - Computation time allowed to be very large
    - Real-time ROM applications
- In many-query analyses with ROMs, the only important time is the total time from the beginning of ROM training to the end of the ROM optimization
  - ROM construction is time-critical
    - Optimization
    - Uncertainty Quantification

ROM Construction: Method of Snapshots

The following is a standard algorithm for constructing a Reduced Order Model.

Algorithm 1 Generic ROM Construction

Input: k_w, size of the Reduced Order Basis
Output: $\mathbf{V}$, the Reduced Order Basis
Select k training points: $\{\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_k\} \subset \mathcal{D}$
for j = 1, 2, . . . , k **do**
    Solve $\mathbf{c}(\mathbf{w}, \mathbf{p}_j) = 0 \rightarrow \hat{\mathbf{w}}_j$
end for
$\mathbf{X} = \begin{bmatrix} \hat{\mathbf{w}}_1 & \hat{\mathbf{w}}_2 & \cdots & \hat{\mathbf{w}}_k \end{bmatrix}$
Compute SVD of $\mathbf{X}$: $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$
$\mathbf{V} = \mathbf{U}(:, 1 : k_w)$ (Compression)

Non-Robustness of ROMs from Training Points

Suppose we construct a ROM from sampling k training points $\{\mathbf{p}_1, \ldots, \mathbf{p}_k\}$.

- ROM is likely to perform well for test points, $\bar{\mathbf{p}}$, "close" to one of the training points, i.e. for $\bar{\mathbf{p}} \in \{\mathbf{p} \in \mathcal{D} \mid \exists j \in \{1, \ldots, k\} \text{ such that } ||\mathbf{p} - \mathbf{p}_j|| < \epsilon_j\}$
- It is well-documented that, for test points not satisfying this criterion, ROMs tend to perform poorly.

Thus, ROMs suffer from non-robustness from training points.

ROM Optimization

- The overall goal of this project is the use of ROMs as a surrogate for the HDM in an optimization algorithm
- Optimization algorithms all reduce to a search in the parameter space for a local optimum

For ROMs to be useful for optimization, they must have parametric-robustness and their construction cannot be prohibitively expensive

Design of Experiments

Due to the large cost required to train a ROM and the general lack of parametric robustness, we state the design of experiments goal:

Construct a parametrically-robust ROM using as few sample points as possible

We use a greedy, optimization-based algorithm for the training of a ROM.

Outline

ROM Construction via Progressive Sampling

Suppose $\mathbf{V}$ is constructed from $\{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_k\}$, a *very coarse* sampling of the parameter space.

Algorithm 2 Progressive Sampling ROM Construction

Input: original ROM, $\mathbf{V}, \{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_k\}$
Output: new ROM, $\mathbf{V}$

1: **while** Not Converged **do**
2: Determine $\mathbf{p} \in \mathcal{D}$, where ROM error is largest $\rightarrow \mathbf{p}^*$
3: Solve $\mathbf{c}(\mathbf{w}, \mathbf{p}^*) = 0 \rightarrow \hat{\mathbf{w}}$ (Snapshots)
4: Use $\hat{\mathbf{w}}$ to update $\mathbf{V}$
5: **end while**

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5: **end while**

HDM-Constrained Sampling Approach

Given $\mathbf{V}$ generated from a very coarse sampling of parameters $\{\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_k\}$, solve

$$\begin{aligned} \underset{\mathbf{p}\in\mathcal{D},\, \mathbf{w}\in\mathbb{R}^{N_w},\, \mathbf{w}_r\in\mathbb{R}^{k_w}}{\text{maximize}} \quad & \frac{1}{2}\left|\left|\mathbf{w} - (\bar{\mathbf{w}} + \mathbf{V}\mathbf{w}_r)\right|\right|_2^2 \\ \text{subject to} \quad & \mathbf{c}(\mathbf{w}, \mathbf{p}) = 0 \\ & \mathbf{c}_r(\mathbf{w}_r, \mathbf{p}) = 0. \end{aligned} \tag{4}$$

Output: A parameter $\mathbf{p}^*$ where the error is largest.

Cost: Every iteration requires HDM and ROM solution.

ROM-Constrained Sampling Approach

Given $\mathbf{V}$ generated from a very coarse sampling of parameters $\{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_k\}$, solve

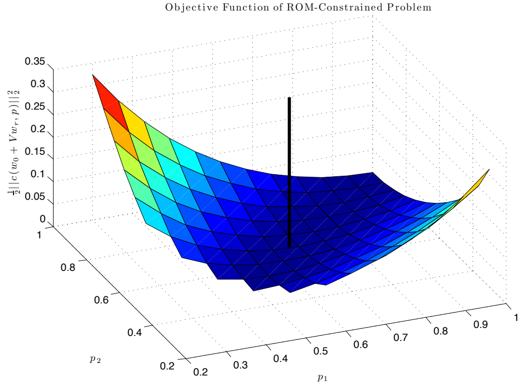
$$\begin{aligned} &\underset{\mathbf{p}\in\mathcal{D},\, \mathbf{w}_r\in\mathbb{R}^{kw}}{\text{maximize}} && \frac{1}{2}\,||\mathbf{c}(\bar{\mathbf{w}} + \mathbf{V}\mathbf{w}_r, \mathbf{p})||_2^2 \\ &\text{subject to} && \mathbf{c}_r(\mathbf{w}_r, \mathbf{p}) = 0 \end{aligned} \tag{5}$$

Output: A parameter $\mathbf{p}^*$ where the HDM residual evaluated at ROM solution is largest.

Cost: Every iteration requires ROM solution.

Difficulty of ROM-Constrained Sampling Objective

The objective function in (5) is, in general, non-concave and not even defined throughout the entire domain because the ROM may fail away from training points.



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LHS Demonstration

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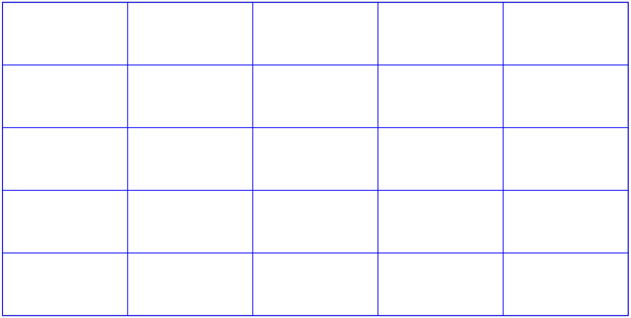

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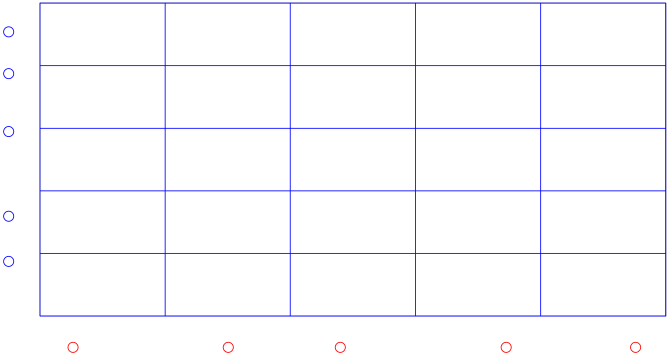

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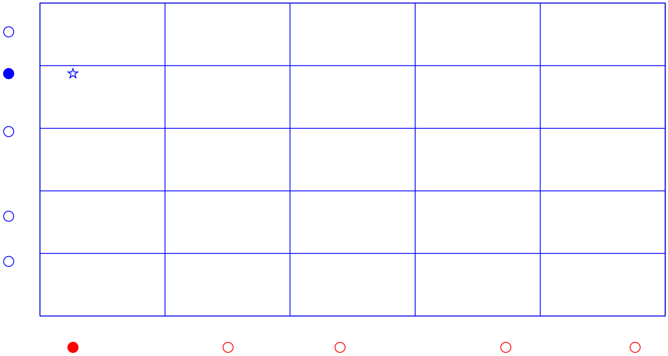

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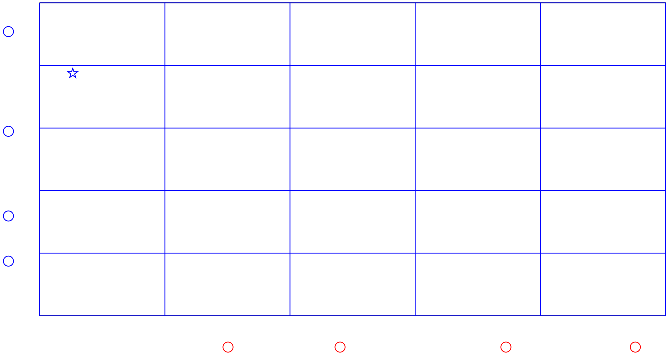

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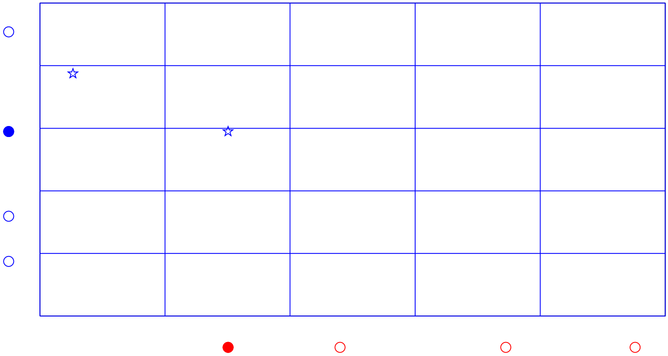

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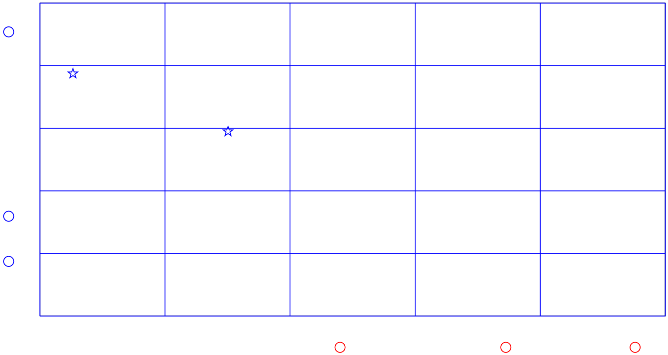

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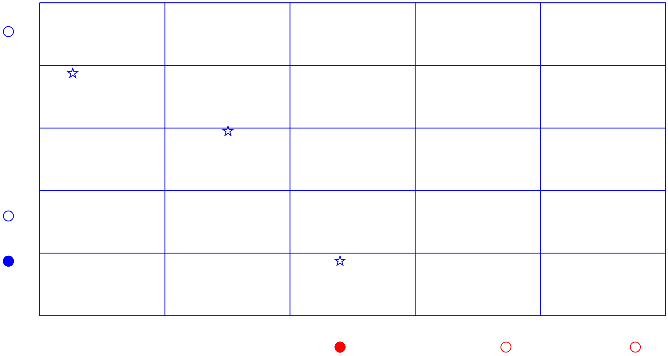

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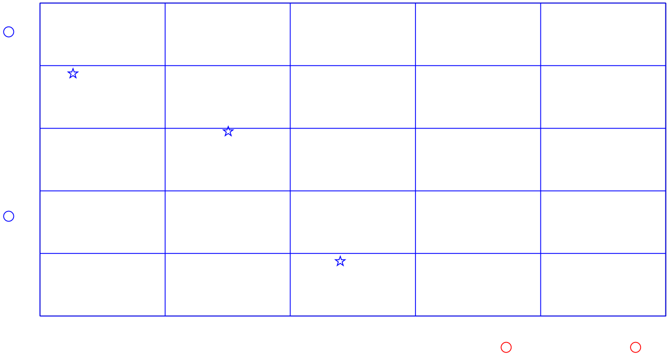

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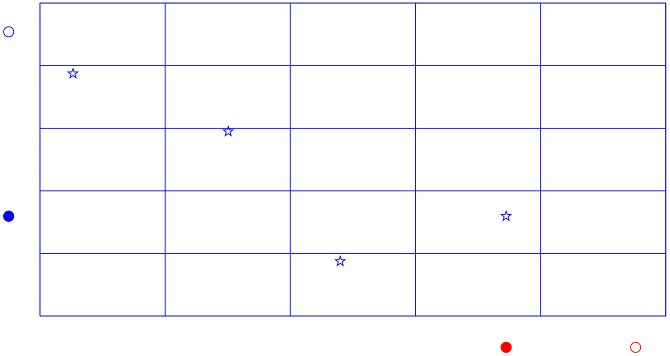

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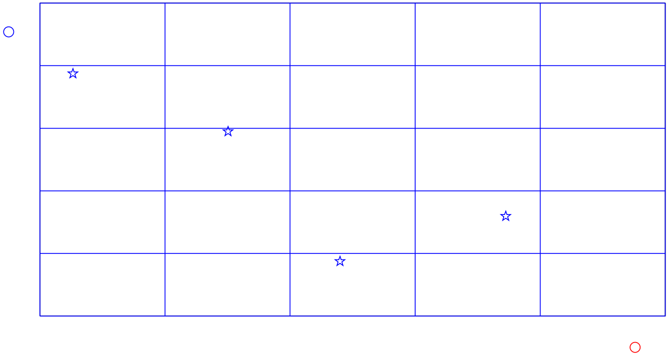

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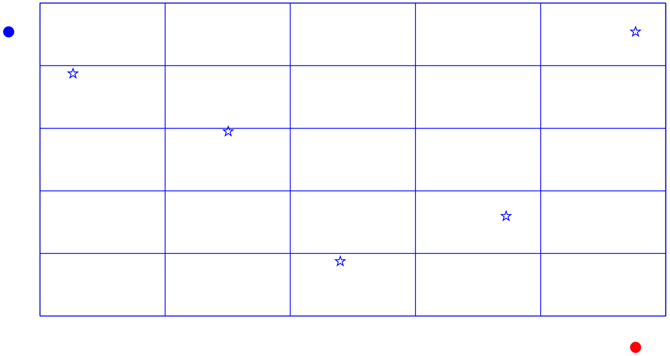

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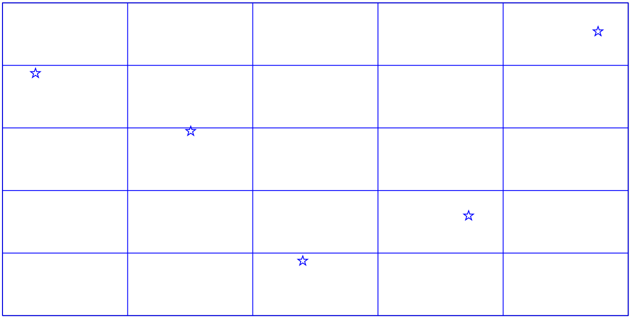
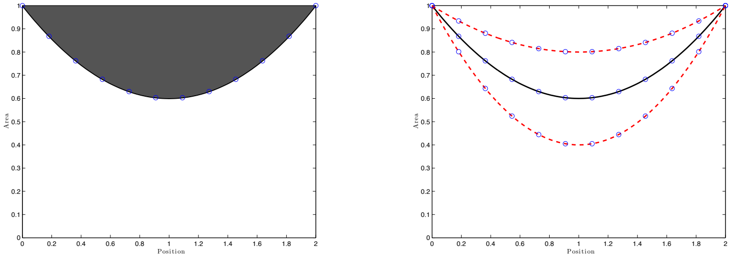


Outline

Potential Nozzle Flow - Cubic Spline Parametrization

$$\frac{d}{dx}\left(A(x)\rho(x)u(x)\right) = 0 \tag{6}$$

Nozzle Configuration and Bounds



ROMOpt Sample Numerical Experiment

- Here, we construct two of ROMs: $\mathcal{R}$ and $\tilde{\mathcal{R}}$.
- $\mathcal{R}$ is constructed with n_s sample points using the ROM-Constrained sampling and $\tilde{\mathcal{R}}$ is constructed with n_s sample points using LHS sampling.
- Generate set $\mathcal{Z} \subset \mathcal{D}$, where $|\mathcal{Z}| = 500$. This is the test set.
- $\mathcal{R}_i$ and $\tilde{\mathcal{R}}_i$ are tested on the set of parameters $\mathcal{Z}$

Sampled Nozzle Shapes

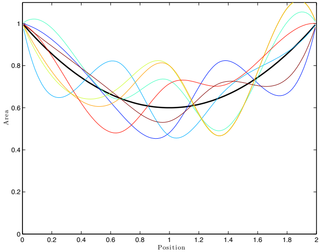


Figure: Optimization-Based Sampling

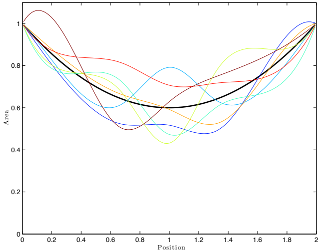
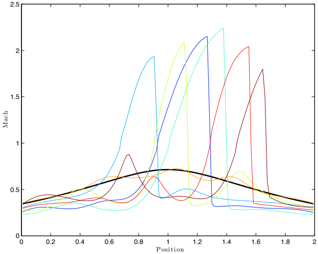


Figure: Latin Hypercube Sampling

Mach Distribution of Sampled Nozzle Shapes



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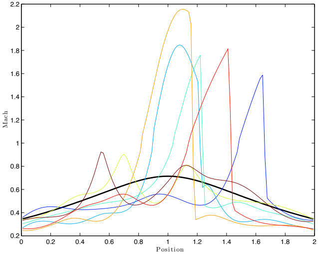

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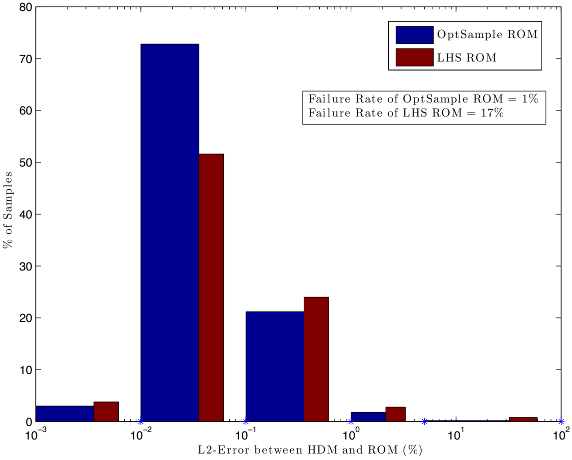
ROMOpt Sample Experiment Results



Outline

Conclusions

- Implementation of ROM optimization-based sampling builds Reduced Order Models that tend to cover the parameter space much better than a simple randomized sampling algorithm