PCA & Kriging for Surrogate Models

Application to 1-D Laminar Flames

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Introduction

Objective: Construction of a Reduced Order Model (**ROM**) which preserves the physics of the system.

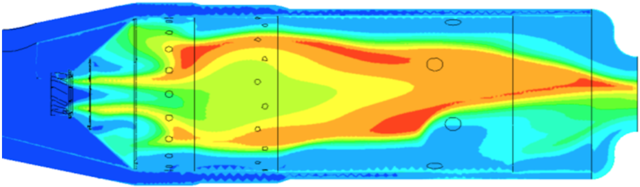
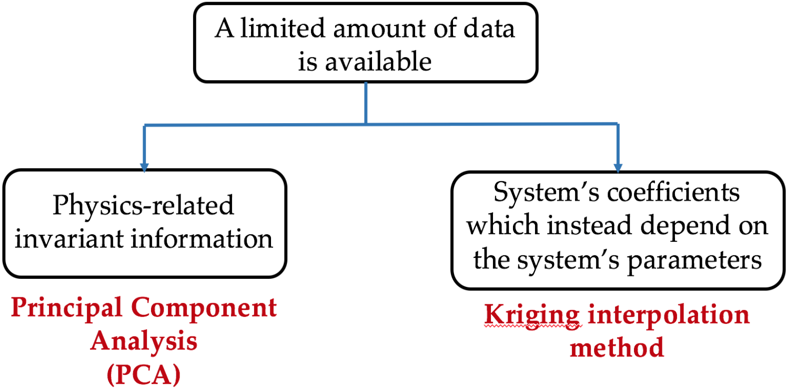


Figure: Ansaldo Turbine

Motivations:
Full-Order Models (**FOMs**) for combustion systems are available but they might be computationally expensive.

Introduction



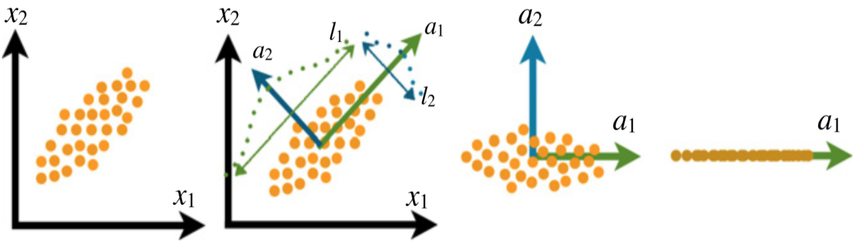
Principal Component Analysis

PCA decomposition

$$\hat{\mathbf{y}}(\mathbf{x}) = \sum_{i=1}^{q \ll N} \phi_i \alpha_i(\mathbf{x})$$

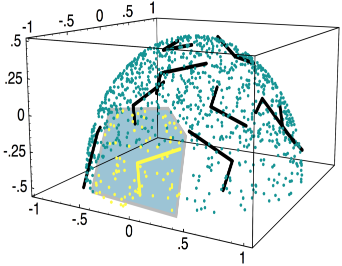
The basis functions $\Longleftarrow$ solution of an eigenproblem.

$$\mathbf{C}\phi_i = \lambda_i \phi_i$$



Local Principal Component Analysis (LPCA)

PCA is a linear combination of basis functions: when trying to represent a highly non-linear system, it may fail.



Data is divided into clusters and **PCA** is applied locally to each cluster.

Projection Partition:
$\mathrm{d}(\mathbf{x}, \mathbf{r}_i) = \|\mathbf{x} - \tilde{\mathbf{x}}^{(i)}\|^2$

If the local regions are small enough, the data manifold will not curve much over the extent of the region.

Constrained PCA

Important physical constraints: conservation of mass,

$Y_s \geq 0, \quad \sum Y_{s_i} = 1$

$\Longrightarrow$ may be violated using simple PCA.

Constrained-PCA approach:

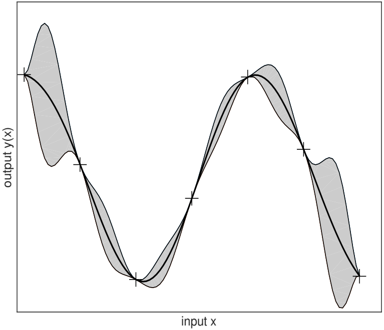
$$\begin{aligned} \text{minimize} \quad & \mathcal{J}(\boldsymbol{\alpha}) = \frac{1}{2} \parallel \mathbf{y} - \hat{\mathbf{y}} \parallel^2 \\ \text{subject to} \quad & \mathcal{L}(\boldsymbol{\alpha}) = \mathbf{0} \end{aligned}$$

Kriging

Kriging: interpolation method where the interpolated targets are modeled by a Gaussian process.

For scalar targets, the **Stochastic field model** is:

$$y(\mathbf{x}) = \sum_{i=1}^{p} \beta_i f_i(\mathbf{x}) + z(\mathbf{x})$$
$$= \mathbf{f}(\mathbf{x})^T \boldsymbol{\beta} + z(\mathbf{x})$$



- **Kriging estimator**: $y^* = \mathbf{c}^T \mathbf{y} = \mathbf{c}^T \left(\mathbf{F}\boldsymbol{\beta} + \mathbf{z} \right)$

How to evaluate the weights **c**?

The **mean square error** (MSE) is

$$\mathbb{E}\left[\left(\hat{y}(\mathbf{x}) - y(\mathbf{x})\right)^2\right] = \mathbb{E}\left[\left(\mathbf{c}^T\mathbf{z} - z(\mathbf{x})\right)^2\right]$$

Minimizing the MSE under the constraint $\mathbf{F}^T\mathbf{c} = \mathbf{f}$ will yield the wanted $\mathbf{c}$.

Application

Brief summary

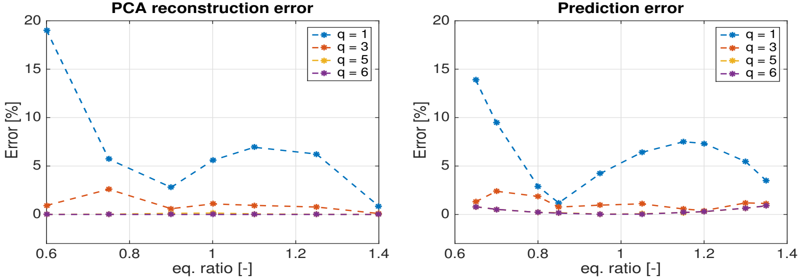
- **PCA** on the DoE points:
  $$\{\mathbf{y}^1, \dots, \mathbf{y}^M\} \underset{PCA}{\Longrightarrow} \{\boldsymbol{\alpha}^1, \dots, \boldsymbol{\alpha}^M\}$$
- **Kriging** for a prediction point:
  $$(\mathbf{x}^* \mid \boldsymbol{\alpha}^m) \underset{Kriging}{\Longrightarrow} \boldsymbol{\alpha}^* \underset{PCA^{-1}}{\Longrightarrow} \mathbf{y}^*$$
- The **PCA modes** $\{\boldsymbol{\phi}\}_{i=1}^{q}$ are not affected by the interpolation.

1-D LAMINAR FLAME:

- GRI Mech: 53 chemical species.
- Solver: OpenSMOKE (POLIMI).
- Varying parameter: **Equivalence Ratio**.
- Training points:
  {0.6, 0.75, 0.9, 1.0, 1.1, 1.25, 1.4}
- Prediction points:
  {0.65, 0.7, 0.8, 0.85, 0.95, 1.05, 1.15, 1.2, 1.3, 1.35}

Results

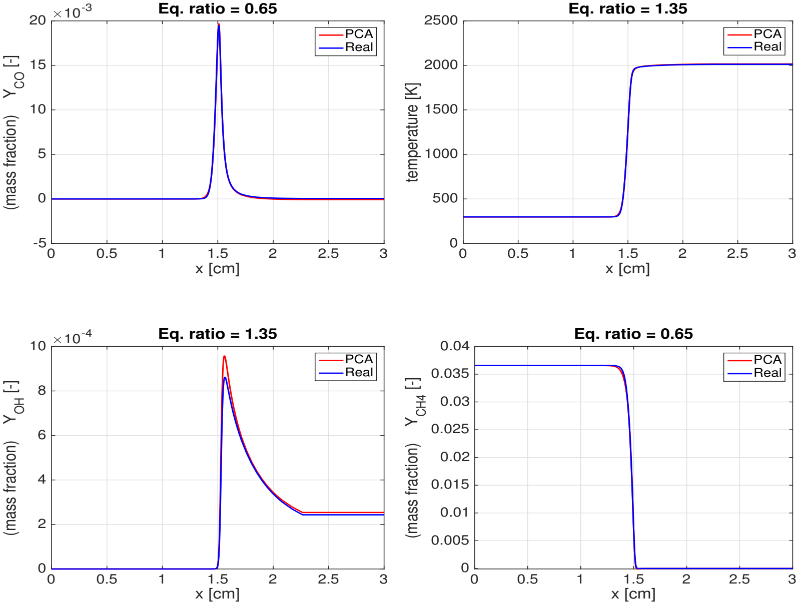
Results: PCA & Kriging



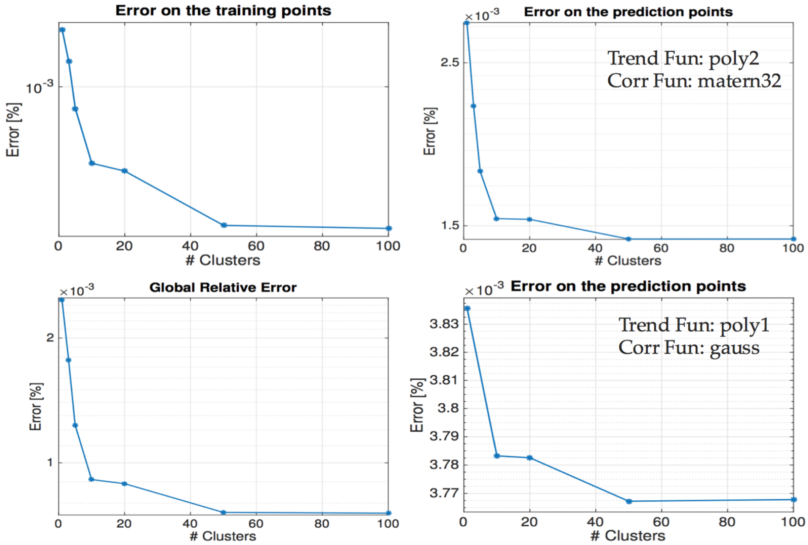
The reconstruction error of the solution on the training points is strongly reduced when more **PCA modes** are added.

The **Kriging interpolation** predicts the **PCA scores** for prediction points of the Eq. Ratio.

Results: PCA & Kriging



Results: Local-PCA$_{q=5}$ & Kriging



Conclusions

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- The **Kriging-PCA** approach turned out to be a promising method for model reduction.
- The method displays important attributes such as **low computational effort** and overall good **accuracy**.
- Further improvements are expected after the strategy for the **Local-PCA** clustering procedure is further optimized.

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Thank you.

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