Proper Orthogonal Decomposition: Theory and Reduced-Order Modeling

Stefan Volkwein

University of Konstanz, Department of Mathematics and Statistics, Numerics & Optimization Group

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Motivation for our Research Areas (Grimm, Gubisch, Iapichino, Mancini, Rogg, Trenz, V., Wesche)

- **Problem**: time-variant, nonlinear, parametrized PDE systems
- **Efficient and reliable numerical simulation in multi-query cases**
  → finite element or finite volume discretizations too complex
- **Multi-query examples**
  - fast simulation for different parameters on small computers
  - parameter estimation, optimal design and feedback control

  → usage of a reduced-order SURROGATE MODEL
- **Time-variant, nonlinear coupled PDEs**
  → methods from linear system theory not directly applicable
- **Nonlinear model-order reduction**
  → proper orthogonal decomposition and reduced-basis method
- **Error control for reduced-order model**
  → new a-priori and a-posteriori error analysis

PDE — Partial Differential Equation

Singular Value Decomposition (SVD)

- **Given vectors**: $y_1, \dots, y_n \in \mathbb{R}^m$
- **Data matrix**: $Y = [y_1, \dots, y_n] \in \mathbb{R}^{m \times n}$
- **Singular value decomposition**: $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ orthogonal

$$U^\top Y V = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} = \Sigma \in \mathbb{R}^{m \times n}$$

  with $D = \operatorname{diag}(\sigma_1, \dots, \sigma_d) \in \mathbb{R}^{d \times d}$
- **Singular values**: $\sigma_1 \geq \dots \geq \sigma_d > 0$, rank $Y = d$
- **Frobenius norm**:

$$\|Y\|_F = \left(\sum_{i=1}^m \sum_{j=1}^n Y_{ij}^2 \right)^{1/2} \quad \text{for } Y \in \mathbb{R}^{m \times n}$$

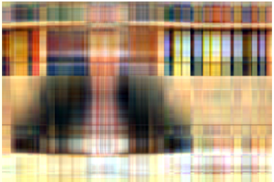
- **Approximation quality**:

$$\|Y - Y^\ell\|_F^2 = \sum_{i=\ell+1}^d \sigma_i^2$$

  with $Y^\ell = U \begin{pmatrix} D^\ell & 0 \\ 0 & 0 \end{pmatrix} V^\top$ and $D^\ell = \operatorname{diag}(\sigma_1, \dots, \sigma_\ell)$

Approximation $\|Y - Y^\ell\|_F^2 = \sum_{i=\ell+1}^{d} \sigma_i^2$ for a given Photo

0,5% der Matrixbasis –> 45% Information



1% der Matrixbasis –> 56% Information

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Outline of Lecture 1

- **The method of Proper Orthogonal Decomposition (POD)**
- **Reduced-order modeling utilizing the POD method**

The Method of Proper Orthogonal Decomposition (POD)

Topics:

- Definition of a (discrete variant of the) POD basis
- Efficient computation of a POD basis
- POD for dynamical systems
- A continuous variant of the POD basis and asymptotic analysis

POD as a Minimization Problem

- **Given multiple snapshots**: $\{y_j^k\}_{j=1}^n \subset X$, $1 \le k \le \wp$, with a (real) Hilbert space X
- **Snapshot subspace**:

$$\mathcal{V} = \operatorname{span}\Big\{ y_j^k \,\big|\, 1 \le j \le n \text{ and } 1 \le k \le \wp \Big\} \subset X$$

  with dimension $d \in \{1, \ldots, \min(n\wp, \dim X)\}$

- **Proper Orthogonal Decomposition (POD)**: for any $\ell \in \{1, \ldots, d\}$ solve

$$\min \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \, \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}^\ell)$$

  with positive weights α_j

- **Optimal solution to (P$^\ell$)**: POD basis $\{\bar\psi_i\}_{i=1}^{\ell}$ of rank ℓ
- **Orthogonal projection**: define $\mathscr{P}^\ell : X \to \mathcal{V}^\ell = \operatorname{span}\{\bar\psi_1, \ldots, \bar\psi_\ell\} \subset \mathcal{V}$ by

$$\mathscr{P}^\ell \psi = \sum_{i=1}^{\ell} \langle \psi, \bar\psi_i \rangle_X \, \bar\psi_i \quad \text{for } \psi \in X$$

$$\Rightarrow \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \, \psi_i \Big\|_X^2 = \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \| y_j^k - \mathscr{P}^\ell y_j^k \|_X^2$$

Equivalent POD Formulation

- **POD as a minimization problem**: for any $\ell \in \{1, \ldots, d\}$ solve

$$\min \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \, \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \ 1 \le i,j \le \ell \qquad (\mathbf{P}^\ell)$$

- **Orthonormal basis elements**: for $1 \le j \le n$ and $1 \le k \le \wp$ we have

$$\Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \, \psi_i \Big\|_X^2 = \| y_j^k \|_X^2 - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2$$

- **POD as a maximization problem**: for $\ell \in \{1, \ldots, d\}$ solve

$$\max \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \ 1 \le i,j \le \ell \qquad (\hat{\mathbf{P}}^\ell)$$

$\Rightarrow$ maximize the first ℓ Fourier coefficient $\Big(\sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 \Big)$ on average $\Big(\sum_{j=1}^{n} \alpha_j \Big)$ for all k

- **Lagrange functional for $(\hat{\mathbf{P}}^\ell)$**: for $\Psi = (\psi_1, \ldots, \psi_\ell) \in X^\ell$ and $\Lambda = ((\lambda_{ij})) \in \mathbb{R}^{\ell \times \ell}$ define

$$\mathscr{L}(\Psi, \Lambda) = \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 + \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \lambda_{ij} \big(\delta_{ij} - \langle \psi_i, \psi_j \rangle_X \big)$$

Lagrangian Framework in (Infinite Dimensional) Optimization

- **POD as a maximization problem**: for any $\ell \in \{1,\dots,d\}$ solve

$$\max \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \qquad (\hat{\mathbf{P}}^\ell)$$

- **Lagrange functional for $(\hat{\mathbf{P}}^\ell)$**: for $\Psi = (\psi_1,\dots,\psi_\ell) \in X^\ell$ and $\Lambda = ((\lambda_{ij})) \in \mathbb{R}^{\ell \times \ell}$ define

$$\mathscr{L}(\Psi,\Lambda) = \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 + \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \lambda_{ij} \big(\delta_{ij} - \langle \psi_i, \psi_j \rangle_X \big)$$

- **Necessary optimality conditions**: let $\bar{\Psi} = (\bar{\psi}_1,\dots,\bar{\psi}_\ell)$ denote a solution to $(\hat{\mathbf{P}}^\ell)$
- **Constraint qualification condition**: there is a Lagrange multiplier $\bar{\Lambda} = ((\bar{\lambda}_{ij}))$ with

$$\frac{\partial \mathscr{L}}{\partial \psi_i}(\bar{\Psi},\bar{\Lambda}) = 0 \text{ in } X \text{ for } 1 \le i \le \ell \quad \text{and} \quad \frac{\partial \mathscr{L}}{\partial \lambda_{ij}}(\bar{\Psi},\bar{\Lambda}) = 0 \text{ in } \mathbb{R} \text{ for } 1 \le i,j \le \ell$$

$\Rightarrow$ first-order necessary optimality conditions for $(\hat{\mathbf{P}}^\ell)$

First-Order Necessary Optimality Conditions

- **POD as a maximization problem**: for any $\ell \in \{1,\ldots,d\}$ solve

$$\max \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \qquad (\hat{\mathbf{P}}^\ell)$$

- **First-order necessary optimality conditions**: $\bar\Psi = (\bar\psi_1,\ldots,\bar\psi_\ell)$ and $\bar\Lambda = ((\bar\lambda_{ij}))$ satisfy

$$\frac{\partial \mathscr{L}}{\partial \psi_i}(\bar\Psi,\bar\Lambda) = 0 \text{ in } X \text{ for } 1 \le i \le \ell \quad \text{and} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij} \text{ for } 1 \le i,j \le \ell$$

- **Summation operator**: define $\mathscr{R}: X \to X$ as $\mathscr{R}\psi = \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \langle \psi, y_j^k \rangle_X\, y_j^k$ for $\psi \in X$

- **Theorem**: *X separable Hilbert space*
  a) *$\mathscr{R}$ is linear, compact, selfadjoint and nonnegative*
  b) *there are eigenfunctions $\{\bar\psi_i\}_{i\in\mathfrak{I}}$ and eigenvalues $\{\bar\lambda_i\}_{i\in\mathfrak{I}}$ with*

$$\mathscr{R}\bar\psi_i = \bar\lambda_i \bar\psi_i, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \ldots \ge \bar\lambda_d > \bar\lambda_{d+1} = \ldots = 0$$

  c) *$\{\bar\psi_i\}_{i=1}^{\ell}$ solves $(\hat{\mathbf{P}}^\ell)$ and $(\mathbf{P}^\ell)$*
  d) $\displaystyle\sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \sum_{i=1}^{\ell} \langle y_j^k, \bar\psi_i \rangle_X^2 = \sum_{i=1}^{\ell} \bar\lambda_i, \quad \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \bar\psi_i \rangle_X \bar\psi_i \Big\|_X^2 = \sum_{i>\ell} \bar\lambda_i$

POD Basis Computation

- **POD**: for any $\ell \in \{1,\dots,d\}$ solve

$$\min \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i\rangle_X \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j\rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}^{\ell})$$

- **Eigenvalue problem**:

$$\mathscr{R}\bar\psi_i = \sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j \langle \bar\psi_i, y_j^k\rangle_X y_j^k = \bar\lambda_i \bar\psi_i \text{ for } 1 \le i \le \ell, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \ldots \ge \bar\lambda_\ell > 0$$

- **Approximation quality**: POD basis $\{\bar\psi_i\}_{i=1}^{\ell}$ of rank ℓ

$$\sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \bar\psi_i\rangle_X \bar\psi_i \Big\|_X^2 = \sum_{i>\ell} \bar\lambda_i$$

$\Rightarrow$ for fastly decreasing $\bar\lambda_i$'s good approximation quality even for small $\ell \ll d = \dim V$

- **In practical computations**: heuristical choice for ℓ by posing

$$\mathscr{E}(\ell) = \frac{\sum_{i=1}^{\ell} \bar\lambda_i}{\sum_{i\in\mathfrak{I}} \bar\lambda_i} = \frac{\sum_{i=1}^{\ell} \bar\lambda_i}{\sum_{k=1}^{\wp}\sum_{j=1}^{n} \alpha_j \|y_j^k\|_X^2} \approx 99\,\%$$

$\Rightarrow$ $\{\bar\lambda_i\}_{i>\ell}$ not required for the computation of $\mathscr{E}(\ell)$

Example 1: POD in the Euclidean Space $X = \mathbb{R}^m$

- **Setting**: $X = \mathbb{R}^m$, $\{y_j\}_{j=1}^n \subset \mathbb{R}^m$ ($\wp = 1$), $Y := [y_1|\dots|y_n] \in \mathbb{R}^{m\times n}$, $\alpha_j = 1$ for $1 \le j \le n$
- **POD**: for any $\ell \in \{1,\dots,d\}$ solve

$$\min \sum_{j=1}^n \Big\| y_j - \sum_{i=1}^{\ell} (y_j^\top \psi_i)\,\psi_i \Big\|_{\mathbb{R}^m}^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset \mathbb{R}^m \text{ and } \psi_i^\top \psi_j = \delta_{ij},\ 1 \le i,j \le \ell$$

- **Summation operator**: $\mathscr{R}\psi = \sum_{j=1}^n (\psi^\top y_j)\, y_j = YY^\top \psi$ for $\psi \in \mathbb{R}^m$
- **Symmetric eigenvalue problem**:

$$YY^\top \bar\psi_i = \bar\lambda_i \bar\psi_i \text{ for } 1 \le i \le \ell, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \dots \ge \bar\lambda_\ell > 0$$

- **Singular value decomposition (SVD)**: $\bar\sigma_1 \ge \dots \ge \bar\sigma_d > 0$

$$\Psi^\top Y \Phi = \begin{pmatrix} \Sigma_d & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma \in \mathbb{R}^{m\times n}$$

with $\Psi = [\bar\psi_1|\dots|\bar\psi_m] \in \mathbb{R}^{m\times m}$, $\Phi = [\bar\phi_1|\dots|\bar\phi_n] \in \mathbb{R}^{n\times n}$ orthogonal, $\Sigma_d = \operatorname{diag}(\bar\sigma_1,\dots,\bar\sigma_d)$

- **Relation between POD and SVD**: for $1 \le i \le \ell$ we have

$$\underbrace{Y\bar\phi_i = \bar\sigma_i\bar\psi_i, \quad Y^\top\bar\psi_i = \bar\sigma_i\bar\phi_i,}_{\text{SVD (stability)}} \qquad \bar\sigma_i^2 = \bar\lambda_i, \qquad \underbrace{YY^\top\bar\psi_i = \bar\lambda_i\bar\psi_i,}_{\text{if } m<n} \qquad \underbrace{Y^\top Y\bar\phi_i = \bar\lambda_i\bar\phi_i}_{\text{if } n<m}$$

Example 2: POD in the Euclidean Space $X = \mathbb{R}^m$ with Weighted Inner Product

- **Setting**: $X = \mathbb{R}^m$, $\{y_j\}_{j=1}^n \subset \mathbb{R}^m$ ($\wp = 1$), $Y := [y_1|\ldots|y_n] \in \mathbb{R}^{m\times n}$
- **Inner product**: $\langle \psi, \tilde\psi\rangle_X = \langle \psi, \tilde\psi\rangle_W = \psi^\top W\tilde\psi$ for $\psi, \tilde\psi \in \mathbb{R}^m$ and $W = W^\top \succ 0$
- **POD**: for any $\ell \in \{1,\ldots,d\}$ solve

$$\min \sum_{j=1}^n \alpha_j \Big\| y_j - \sum_{i=1}^\ell \langle y_j, \psi_i\rangle_W \, \psi_i \Big\|_W^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^\ell \subset \mathbb{R}^m \text{ and } \langle \psi_i, \psi_j\rangle_W = \delta_{ij},\ 1 \le i,j \le \ell$$

- **Summation operator**: $\mathscr{R} = YDY^\top W$ and $D = \mathrm{diag}\,(\alpha_1,\ldots,\alpha_n) \in \mathbb{R}^{n\times n}$
- **Symmetric eigenvalue problem**: $\hat Y = W^{1/2}YD^{1/2}$ and $\hat Y\hat Y^\top = W^{1/2}YDY^\top W^{1/2}$

$$\hat Y\hat Y^\top \psi_i = \bar\lambda_i \psi_i \text{ for } 1 \le i \le \ell, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \ldots \ge \bar\lambda_\ell > 0$$

  and set $\bar\psi_i = W^{-1/2}\psi_i$ for $1 \le i \le \ell$
- **Singular value decomposition**: $\hat Y^\top \hat Y = D^{1/2}Y^\top WYD^{1/2}$ and $\bar\sigma_i^2 = \bar\lambda_i$

$$\hat Y^\top \hat Y \phi_i = \bar\lambda_i \phi_i \text{ for } 1 \le i \le \ell, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \ldots \ge \bar\lambda_\ell > 0$$

  and set $\bar\psi_i = YD^{1/2}\phi_i/\bar\sigma_i$ for $1 \le i \le \ell \Rightarrow$ no computation of $W^{1/2}$
- **Multiple snapshots**: set $Y_k = [y_1^k|\ldots|y_n^k] \in \mathbb{R}^{m\times n}$ and

$$\mathscr{R} = \big(Y_1DY_1^\top + \ldots + Y_\wp DY_\wp^\top\big)W \in \mathbb{R}^{m\times m}$$

Application to Nonlinear Dynamical Systems

- **Dynamical system in Hilbert space X**:
$$\dot{y}(t) = f(t, y(t); \mu) \text{ for } t \in (t_\circ, t_f], \quad y(t_\circ) = y_\circ \in X$$
with given parameter $\mu \in \mathcal{D}_{ad}$, initial value $y_\circ$ and (smooth) nonlinearity f
- **State trajectory**: there is a unique solution $y(t; \mu) \in X$ for fixed parameter $\mu \in \mathcal{D}_{ad}$
- **Multiple snapshots**: for grids $t_\circ = t_1 < \ldots < t_n \leq t_f$ and $\{\mu^k\}_{k=1}^{\wp} \subset \mathcal{D}$ let $y_j^k \approx y(t_j; \mu^k)$
- **Discrete variant of POD**: for any $\ell \in \{1, \ldots, d\}$ solve
$$\min \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \; 1 \leq i, j \leq \ell \quad (\mathbf{P}^\ell)$$
with positive weights α_j (compare Greedy-POD strategy)
- **Questions**: a) How to choose "good" time instances t_j for the snapshots?
  b) What are appropriate positive weights $\{\alpha_j\}_{j=1}^n$?
- **Continuous variant of POD**: for $y^k(t) = y(t; \mu^k)$, $1 \leq k \leq \wp$, and any $\ell \in \{1, \ldots, d\}$ solve
$$\min \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X \psi_i \Big\|_X^2 \mathrm{d}t \text{ s.t. } \{\psi_i\}_{i=1}^{\ell} \subset X, \; \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \; 1 \leq i, j \leq \ell \quad (\mathbf{P}_\infty^\ell)$$

Continuous and Discrete Variant of the POD Method

- **Dynamical system in Hilbert space X**:

$$\dot{y}(t) = f(t, y(t); \mu) \text{ for } t \in (t_\circ, t_f], \quad y(t_\circ) = y_\circ \in X$$

- **Given multiple snapshots**: solutions $y^k(t) = y(t; \mu^k) \in X$ for parameters $\{\mu^k\}_{k=1}^{\wp} \subset \mathcal{D}$
- **Snapshot subspace**:

$$\mathcal{V} = \operatorname{span}\Big\{ y^k(t) \,|\, t \in [t_0, t_f] \text{ and } 1 \le k \le \wp \Big\} \subset X \quad \text{with dimension } d^\infty \le \infty$$

- **Continuous variant of POD**: for any $\ell \in \{1, \dots, d\}$ solve

$$\min \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \mathrm{d}t \text{ s.t. } \{\psi_i\}_{i=1}^{\ell} \subset X,\ \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}_\infty^\ell)$$

- **Integral operator**: define $\mathscr{R}^\infty : X \to X$ as $\mathscr{R}^\infty \psi = \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \langle \psi, y^k(t) \rangle_X \, y^k(t) \, \mathrm{d}t$ for $\psi \in X$

- **Discrete variant of POD**: for $y_j^k \approx y^k(t_j)$ and any $\ell \in \{1, \dots, d\}$ solve

$$\min \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \Big\| y_j^k - \sum_{i=1}^{\ell} \langle y_j^k, \psi_i \rangle_X \, \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X \text{ and } \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}^\ell)$$

- **Summation operator**: $\mathscr{R}^n : X \to X$ with $\mathscr{R}^n \psi = \sum_{k=1}^{\wp} \sum_{j=1}^{n} \alpha_j \langle \psi, y_j^k \rangle_X \, y_j^k$ for $\psi \in X$

Asymptotic Analysis (Kunisch/V.'02)

- **Continuous variant of POD**: for any $\ell \in \{1,\dots,d\}$ solve

$$\min \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i\rangle_X \, \psi_i \Big\|_X^2 \mathrm{d}t \text{ s.t. } \{\psi_i\}_{i=1}^{\ell} \subset X,\ \langle \psi_i, \psi_j\rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}_\infty^\ell)$$

- **Operators**: $\mathscr{R}^\infty \psi = \sum\limits_{k=1}^{\wp} \int\limits_{t_\circ}^{t_f} \langle \psi, y^k(t)\rangle_X \, y^k(t)\,\mathrm{d}t$ and $\mathscr{R}^n \psi = \sum\limits_{k=1}^{\wp} \sum\limits_{j=1}^{n} \alpha_j \langle \psi, y_j^k\rangle_X \, y_j^k$

Theorem (Hilbert-Schmidt, Riesz-Schauder theorems; Perturbation theory (Kato'66))

X separable, $y^k \in H^1(t_\circ, t_f; X)$, choose α_j as trapezoidal weights

a) *$\mathscr{R}^\infty$ is linear, compact, selfadjoint and nonnegative*

b) *there are eigenfunctions $\{\bar\psi_i^\infty\}_{i\in\mathcal{I}}$ and eigenvalues $\{\bar\lambda_i^\infty\}_{i\in\mathcal{I}}$ with*

$$\mathscr{R}^\infty \bar\psi_i^\infty = \bar\lambda_i^\infty \bar\psi_i^\infty, \quad \bar\lambda_1^\infty \ge \bar\lambda_2^\infty \ge \ldots \ge 0, \quad \lim_{i\to\infty} \bar\lambda_i^\infty = 0$$

c) *$\{\bar\psi_i^\infty\}_{i=1}^{\ell}$ solves ($\mathbf{P}_\infty^\ell$)*

d) $$\sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \sum_{i=1}^{\ell} \langle y^k(t), \bar\psi_i^\infty\rangle_X^2 \mathrm{d}t = \sum_{i=1}^{\ell} \bar\lambda_i^\infty, \quad \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \bar\psi_i^\infty\rangle_X \, \bar\psi_i^\infty \Big\|_X^2 \mathrm{d}t = \sum_{i>\ell} \bar\lambda_i^\infty$$

e) $\lim\limits_{n\to\infty} \|\mathscr{R}^n - \mathscr{R}^\infty\|_{\mathcal{L}(X)} = 0$ *and* $\lim\limits_{n\to\infty} \bar\lambda_i^n = \bar\lambda_i^\infty$, $\lim\limits_{n\to\infty} \bar\psi_i^n = \bar\psi_i^\infty$ *for $1 \le i \le \ell$ (if $\bar\lambda_i^\infty$ seperated)*

Numerical Example: λ-ω PDE System

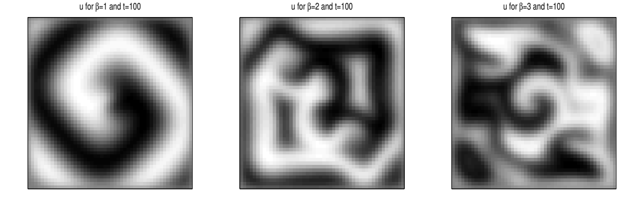
- **λ-ω PDE system**: $s = u^2 + v^2$, $\lambda(s) = 1 - s$, $\omega(s) = -\beta s$

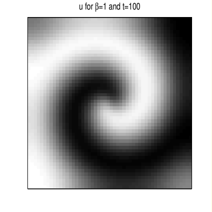
$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \lambda(s) & -\omega(s) \\ \omega(s) & \lambda(s) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} \sigma \Delta u \\ \sigma \Delta v \end{pmatrix}$$

- **Homogeneous boundary conditions**:

$$u = v = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$$

- **Initial conditions**: $u_\circ(x_1, x_2) = x_2 - 0.5$, $v_\circ(x_1, x_2) = (x_1 - 0.5)/2$





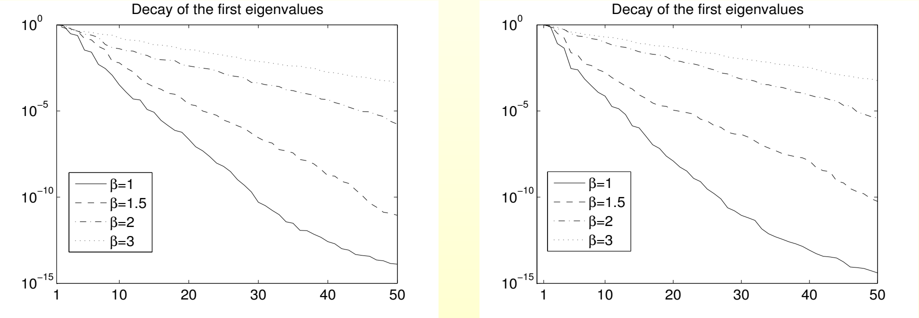
Numerical Example: Decay of the POD Eigenvalues for the λ-ω Systems

- **λ-ω PDE system**: $s = u^2 + v^2$, $\lambda(s) = 1 - s$, $\omega(s) = -\beta s$

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \lambda(s) & -\omega(s) \\ \omega(s) & \lambda(s) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} \sigma\Delta u \\ \sigma\Delta v \end{pmatrix}$$

- **Homogeneous boundary conditions**:

$$u = v = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$$



Dirichlet boundary conditions Neumann boundary conditions

Related Literature

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Reduced-Order Modeling (ROM) Utilizing the POD Method

Topics:

- POD reduced-order modeling
- A-priori error analysis for POD
- Convergence and rate of convergence results
- Extensions

Abstract Linear Evolution Problem

- **Function spaces**: H, V separable Hilbert spaces, $V \hookrightarrow H$ dense and compact
- **Gelfand triple**: $V \hookrightarrow H \equiv H' \hookrightarrow V'$
- **Time-dependent bilinear form**: $a(t;\cdot,\cdot) : V \times V \to \mathbb{R}$ satisfying

$$|a(t;\varphi,\tilde{\varphi})| \leq \gamma \|\varphi\|_V \|\tilde{\varphi}\|_V \qquad \forall \varphi, \tilde{\varphi} \in V \text{ a.e. in } [t_\circ, t_f]$$

$$a(t;\varphi,\varphi) \geq \gamma_1 \|\varphi\|_V^2 - \gamma_2 \|\varphi\|_H^2 \qquad \forall \varphi \in V \text{ a.e. in } [t_\circ, t_f]$$

  with time-independent constants γ, $\gamma_1 > 0$ and $\gamma_2 \geq 0$
- **Solution Hilbert space**: $W(t_\circ, t_f) = \{\varphi \in L^2(t_\circ, t_f; V) \,|\, \varphi_t \in L^2(t_\circ, t_f; V')\}$
  $\Rightarrow W(t_\circ, t_f) \hookrightarrow C([t_\circ, t_f]; H)$, i.e., $y(t) \in H$ is meaningful for all $t \in [t_\circ, t_f]$
- **Input/control space**: $\mathcal{U} = L^2(t_\circ, t_f; U) \simeq \mathcal{U}'$ with $U = \mathbb{R}^{N_u}$, $U = L^2(\Omega)$ or $U = L^2(\Gamma)$
- **Linear evolution problem**: find $y \in W(t_\circ, t_f)$ satisfying $y(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi \rangle_H + a(t; y(t), \varphi) = \langle (f + \mathscr{B}u)(t), \varphi \rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

  for given $y_\circ \in H$, $f \in L^2(t_\circ, t_f; V')$ and bounded, linear $\mathscr{B} : \mathcal{U} \to L^2(t_\circ, t_f; V')$
- **Solvability**: there is a unique solution $y \in W(t_\circ, t_f)$ with

$$\|y\|_{W(t_\circ,t_f)} \leq C\left(\|y_\circ\|_H + \|f\|_{L^2(t_\circ,t_f;V')} + \|u\|_{\mathcal{U}}\right)$$

  with a constant $C > 0$ independent of $y_\circ$, f, and u

Affine Linear Representation of the Solution

- **Linear evolution problem**: find $y \in W(t_\circ, t_f)$ satisfying $y(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t), \varphi\rangle_H + a(t; y(t), \varphi) = \langle (f + \mathscr{B}u)(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f) \qquad \textbf{(EVP)}$$

  for given $y_\circ \in H$, $f \in L^2(t_\circ, t_f; V')$ and bounded, linear $\mathscr{B} : \mathfrak{U} \to L^2(t_\circ, t_f; V')$

- **Particular solution**: $\hat{y} \in W(t_\circ, t_f)$ solves $\hat{y}(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{y}(t), \varphi\rangle_H + a(t; \hat{y}(t), \varphi) = \langle f(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

- **Control-to-state mapping**: $\mathscr{S} : \mathfrak{U} \to W(t_\circ, t_f)$, $w = \mathscr{S}u$ solves $w(t_\circ) = 0$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle w(t), \varphi\rangle_H + a(t; w(t), \varphi) = \langle (\mathscr{B}u)(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

  $\Rightarrow \mathscr{S}$ linear and bounded

- **Affine linear representation of the solution to (EVP)**: $y = \hat{y} + \mathscr{S}u$
- **Regularity**: $y \in C([t_\circ, t_f]; V)$ if $a(t; \cdot, \cdot) = a(\cdot, \cdot)$, $y_\circ \in V$ and $f, \mathscr{B}u \in L^2(t_\circ, t_f; H)$

Continuous Variant of POD for the Evolution Problem

- **POD setting**: $X = H$ and $X = V$, $y^1 = \mathscr{S}u$ ($\wp = 1$), $\mathcal{V} = \mathrm{span}\,\{y^1(t)\,|\,t \in [t_\circ, t_f]\}$, $d = \dim \mathcal{V}$
- **Continuous variant of POD**: for any $\ell \in \{1, \ldots, d\}$ solve

$$\min \int_{t_\circ}^{t_f} \Big\| y^1(t) - \sum_{i=1}^{\ell} \langle y^1(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \, \mathrm{d}t \quad \text{s.t.} \quad \{\psi_i\}_{i=1}^{\ell} \subset X,\ \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \qquad (\mathbf{P}_\infty^\ell)$$

- **Integral operator**: $\mathscr{R} : X \to X$ with $\mathscr{R}\psi = \int\limits_{t_\circ}^{t_f} \langle \psi, y^1(t) \rangle_X \, y^1(t)\,\mathrm{d}t$
- **POD basis of rank ℓ**: $\{\psi_i\}_{i=1}^{\ell} \subset X$, $V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\}$

$$\|y^1 - \mathscr{P}^\ell y^1\|_{L^2(t_\circ, t_f; X)}^2 = \int_{t_\circ}^{t_f} \Big\| y^1(t) - \sum_{i=1}^{\ell} \langle y^1(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \, \mathrm{d}t = \sum_{i=\ell+1}^{d} \lambda_i$$

  with $\mathscr{P}^\ell \psi = \sum\limits_{i=1}^{\ell} \langle \psi, \psi_i \rangle_X \, \psi_i$ for $\psi \in X$

- **Reduced-order model**: use V^ℓ as the solution and test space instead of V
  $\Rightarrow$ low-dimensional model since $\ell \ll \dim V = \infty$ (in practice: $\ell \ll \dim V^{\mathcal{N}} = \mathcal{N}$)
- **Regularity**: if $(\mathscr{S}u)(t) \in V$ a.e. in $[t_\circ, t_f]$, then $\{\psi_i\}_{i=1}^{\ell} \subset V$ holds even for $X = H$

POD Galerkin Scheme (Gubisch/V.'13)

- **Linear evolution problem**: find $y \in W(t_\circ, t_f)$ satisfying $y(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t), \varphi\rangle_H + a(t; y(t), \varphi) = \langle (f + \mathscr{B}u)(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

- **Particular solution**: $\hat{y} \in W(t_\circ, t_f)$ solves $\hat{y}(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{y}(t), \varphi\rangle_H + a(t; \hat{y}(t), \varphi) = \langle f(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

- **POD control-to-state mapping**: $\mathscr{S}^\ell : \mathfrak{U} \to W(t_\circ, t_f)$, $w^\ell = \mathscr{S}^\ell u$ solves $w^\ell(t_\circ) = 0$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle w^\ell(t), \psi\rangle_H + a(t; w^\ell(t), \psi) = \langle (\mathscr{B}u)(t), \psi\rangle_{V',V} \quad \forall \psi \in V^\ell \text{ a.e. in } (t_\circ, t_f]$$

  $\Rightarrow \mathscr{S}^\ell$ linear and bounded

- **POD solution form**: $y^\ell = \hat{y} + \mathscr{S}^\ell u$

  $\Rightarrow y^\ell(0) = y_\circ$ in H, i.e., no POD error in the initial condition

- **POD a-priori error**: convergence result for $\|y - y^\ell\|$ and $\|\mathscr{S} - \mathscr{S}^\ell\|_{\mathcal{L}(\mathscr{U}, W(t_\circ, t_f))}$?

POD A-Priori Estimation

- **POD setting**: $X = V$, $y^1 = \mathscr{S}u$, $V^\ell = \mathrm{span}\{\psi_1, \ldots, \psi_\ell\}$, $\mathscr{P}^\ell \psi = \sum_{i=1}^{\ell} \langle \psi, \psi_i \rangle_V \psi_i$

$$\|\mathscr{S}u - \mathscr{P}^\ell(\mathscr{S}u)\|^2_{L^2(t_\circ,t_f;V)} = \int_{t_\circ}^{t_f} \Big\| y^1(t) - \sum_{i=1}^{\ell} \langle y^1(t), \psi_i \rangle_V \psi_i \Big\|_V^2 \mathrm{d}t = \sum_{i>\ell} \lambda_i$$

- **Decomposition**:

$$\begin{aligned} y^\ell(t) - y(t) &= \hat{y}(t) + (\mathscr{S}^\ell u)(t) - \hat{y}(t) - (\mathscr{S}u)(t) \\ &= \underbrace{(\mathscr{S}^\ell u)(t) - \mathscr{P}^\ell((\mathscr{S}u)(t))}_{=:\vartheta^\ell(t) \in V^\ell} + \underbrace{\mathscr{P}^\ell((\mathscr{S}u)(t)) - (\mathscr{S}u)(t)}_{=:\rho^\ell(t) \in (V^\ell)^\perp} = \vartheta^\ell(t) + \rho^\ell(t) \end{aligned}$$

- **Estimate for ρ^ℓ**: $\int_{t_\circ}^{t_f} \|\rho^\ell(t)\|_V^2 \,\mathrm{d}t = \int_{t_\circ}^{t_f} \|\mathscr{P}^\ell((\mathscr{S}u)(t)) - (\mathscr{S}u)(t)\|_V^2 \,\mathrm{d}t = \sum_{i>\ell} \lambda_i$

- **Estimate for ϑ^ℓ**: use the evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \vartheta^\ell(t), \psi \rangle_H + a(t; \vartheta^\ell(t)(t), \psi) = \langle (\mathscr{S}u)_t(t) - \mathscr{P}^\ell((\mathscr{S}u)_t(t)), \psi \rangle_{V',V} \quad \forall \psi \in V^\ell \text{ a.e. in } (t_\circ, t_f]$$

and choose $\psi = \vartheta^\ell(t) \in V^\ell$

POD A-Priori Error for Abstract Linear Evolution Problems

Theorem (Kunisch/V.'01, Hinze/V.'08, Tröltzsch/V.'09, Gubisch/V.'13)

$X = V$, $\mathcal{V} = \mathrm{span}\,\{y^k(t)\,|\,t \in [t_\circ, t_f],\ 1 \le k \le \wp\}$, $\mathscr{P}^\ell \psi = \sum_{i=1}^{\ell} \langle \psi, \psi_i \rangle_V \, \psi_i$

a) *Snapshot* $y^1 = \mathscr{S}u$, $y = \hat{y} + \mathscr{S}u$, $y^\ell = \hat{y} + \mathscr{S}^\ell u$:

$$\|y - y^\ell\|^2_{W(t_\circ,t_f)} \le \sum_{i>\ell} \lambda_i + C_1 \, \|(\mathscr{S}u)_t - \mathscr{P}^\ell(\mathscr{S}u)_t\|^2_{L^2(t_\circ,t_f;V')}$$

b) *Snapshots* $y^1 = \mathscr{S}u$ *and* $y^2 = (\mathscr{S}u)_t \in L^2(t_\circ, t_f; V)$:

$$\|y - y^\ell\|^2_{W(t_\circ,t_f)} \le C_2 \sum_{i>\ell} \lambda_i$$

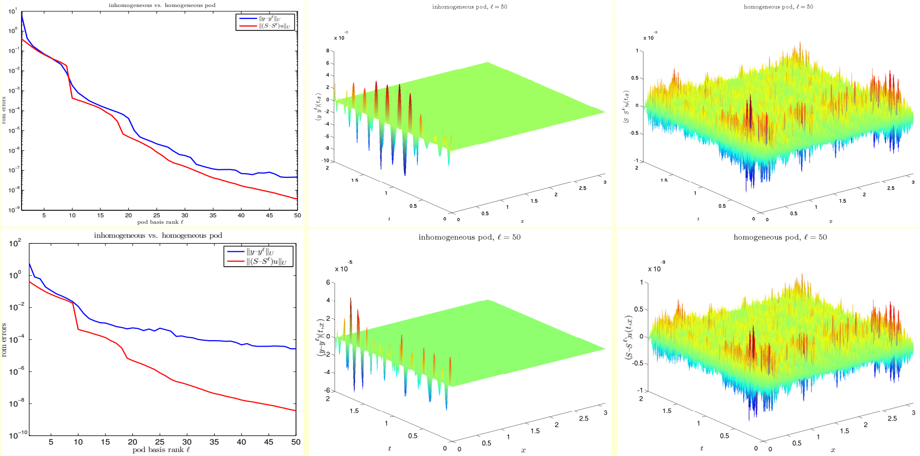
c) *If* $\mathscr{S}u \in H^1(t_\circ, t_f; V)$ *for all* $\tilde{u} \in \mathfrak{U}$, *then* $\lim\limits_{\ell \to \infty} \|\mathscr{S} - \mathscr{S}^\ell\|_{\mathscr{L}(\mathfrak{U}, W(t_\circ,t_f))} = 0$

In particular, $\lim\limits_{\ell \to \infty} \|y(\tilde{u}) - y^\ell(\tilde{u})\|_{W(t_\circ,t_f)} = 0$ *for any* $\tilde{u} \in \mathfrak{U}$

- **FE approximation quality**: $\|\varphi - \mathscr{P}^h \varphi\|_H + h\|\varphi - \mathscr{P}^h \varphi\|_V = \mathscr{O}(h^2)$ for all $\varphi \in Z \subset V$
- **POD approximation quality**: $\|\varphi - \mathscr{P}^\ell \varphi\|^2_{L^2(t_\circ,t_f;V)} = \mathscr{O}\Big(\sum_{i>\ell} \lambda_i\Big)$ for all $\varphi \in \mathcal{V} \subset V$
- **Extension for the case $X = H$** (Singler'13): $\|y - y^\ell\|^2_{W(t_\circ,t_f)} = \mathscr{O}\Big(\sum_{i>\ell} \lambda_i \, \|\psi_i - \mathscr{P}^\ell \psi_i\|^2_V\Big)$

Numerical Example for the Modified POD Galerkin Scheme (Gubisch)

- **Problem**: linear heat equation on $(t_\circ, t_f) = (0,3)$ and $\Omega = (0,2)$
- **Discretization**: piecewise linear FE and Crank-Nicolson with a total error of 10^{-5}
- **Continuous and discontinuous initial condition**: $y_\circ(x) = \sin(\pi x/2)$ without/with noise



Further Topics

- **Fully discretized problems**: temporal error, asymptotic analysis, case $X = H$
- **A-priori error analysis for nonlinear systems**: e.g., Navier-Stokes and battery models
- **A-priori error analysis with respect to the “truth” approximation**
- **Optimal snapshot locations**: goal-oriented choice of snapshots
- **Efficient POD-Galerkin for nonlinear problems**: POD-(D)EIM
- **Parameterized PDEs**: POD-Greedy algorithm
- **POD and Balancing**: utilize observability (i.e., dual) information
- ...

Literature on POD-ROM

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