Model Reduction using Proper Orthogonal Decomposition

PhD Summer School on Reduced Basis Methods, Ulm

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POD-Galerkin ansatz

MOTIVATION:

Find finite elements $\{u_1, ..., u_l\}$ which reflect the dynamics of the evolution equation

$$\begin{cases} \dot{y}(t) - Ay(t) & = & f(t) \\ y(0) & = & y_0 \end{cases},$$

i.e. $y^l(t) := \sum_{i=1}^{l} \mathrm{y}_i(t) u_i$ determined by solving the reduced Galerkin system

$$\begin{cases} \mathrm{M}(u)\dot{\mathrm{y}}(t) - \mathrm{A}(u)\mathrm{y}(t) & = & \mathrm{F}(u)(t) \\ \mathrm{M}(u)\mathrm{y}(0) & = & \mathrm{y}_0(u) \end{cases},$$

is a good approximation for y where l is quite small.

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Singular value decomposition

Let $y_1, \dots, y_n \in \mathbb{R}^m$ the columns of a matrix $Y \in \mathbb{R}^{m\times n}$ of rank d.

Then there are $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_d > 0$ and orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that

$$U^t Y V = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma \in \mathbb{R}^{m\times n}, \qquad D = \operatorname{diag}(\sigma) \in \mathbb{R}^{d\times d}.$$

- The columns $u_1, \dots, u_m$ of U are the eigenvectors of YY^t corresponding to the eigenvalues $\sigma_1^2, \dots, \sigma_d^2, 0, \dots, 0$.
- Analogously, the columns $v_1, \dots, v_n$ of V are the eigenvectors of Y^tY corresponding to the eigenvalues $\sigma_1^2, \dots, \sigma_d^2, 0, \dots, 0$.
- The columns of Y can be represented by

$$y_j = \sum_{i=1}^{d} \langle y_j, u_i \rangle u_i.$$

Singular value decomposition

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- The representation
$$Y = U\Sigma V^t$$
is called the Proper Orthogonal Decomposition (POD) of Y.
- The orthogonal subbasis $U^l := \{u_1, \ldots, u_l\}$ of the image $\operatorname{Im}(Y)$ is called the POD-basis of rank l ($l \leq d$).
- The optimal representation of y as a linear combination with l vectors is
$$y \approx \sum_{i=1}^{l} \langle y, u_i \rangle u_i :$$

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POD as best-approximation

THEOREM. The minimization problem

$$\begin{cases} \displaystyle\min_{(\tilde u_1,\ldots,\tilde u_l)} \sum_{j=1}^{n} \Big\| y_j - \sum_{i=1}^{l} \langle y_j, \tilde u_i\rangle \tilde u_i \Big\|^2 \\ \text{subject to } \langle \tilde u_i, \tilde u_j\rangle = \delta_{ij} \end{cases}$$

is solved by the POD-basis $(u_1, \ldots, u_l)$.

The Pythagoras theorem states that this optimization problem is equivalent to

$$\begin{cases} \displaystyle\max_{(\tilde u_1,\ldots,\tilde u_l)} \sum_{j=1}^{n} \sum_{i=1}^{l} |\langle y_j, \tilde u_i\rangle|^2 \\ \text{subject to } \langle \tilde u_i, \tilde u_j\rangle = \delta_{ij} \end{cases}$$

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POD as best-approximation

To solve the constraint maximization problem, we introduce the Lagrange function

$$\mathscr{L} : \mathbb{R}^{m\times l} \times \mathbb{R}^{l\times l}$$

by

$$\mathscr{L}(\tilde{U}, \Lambda) := \sum_{j=1}^{n} \sum_{i=1}^{l} |\langle y_j, \tilde{u}_i \rangle|^2 + \sum_{j=1}^{l} \sum_{i=1}^{l} \lambda_{ij}(\delta_{ij} - \langle \tilde{u}_i, \tilde{u}_j \rangle).$$

The first-order optimality conditions

$$\frac{\partial}{\partial \tilde{u}_i} \mathscr{L}(\tilde{U}, \Lambda) = 0$$

can be transformed into

$$\underbrace{\sum_{j=1}^{n} \langle y_j, \tilde{u}_i \rangle y_j}_{=YY^t \tilde{u}_i} = \frac{1}{2} \sum_{j=1}^{l} (\lambda_{ji} + \lambda_{ij}) \tilde{u}_i.$$

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POD as best-approximation

Together with the remaining first-order optimality conditions

$$\frac{\partial}{\partial \lambda_{ij}} \mathscr{L}(\tilde{U}, \Lambda) = \delta_{ij} - \langle \tilde{u}_i, \tilde{u}_j \rangle = 0,$$

we get $\lambda_{ij} = \lambda_{ii}\delta_{ij}$ which implies

$$YY^t \tilde{u}_i = \lambda_{ii} \tilde{u}_i.$$

Hence, $\tilde{U}^* = U$ and $\Lambda^* = \mathrm{diag}(\sigma_1^2, ..., \sigma_l^2)$ solves the optimization problem and

$$\max_{(\tilde{u}_1,\ldots,\tilde{u}_l)} \sum_{j=1}^{n} \sum_{i=1}^{l} |\langle y_j, \tilde{u}_i \rangle|^2 = \sum_{i=1}^{l} \sigma_i^2.$$

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Approximation of $\mathcal{L}^2(\Omega)$

Let $\Omega := (a, b) \subseteq \mathbb{R}^1$, $m \in \mathbb{N}$, $h := \frac{b-a}{m-1}$, $x := (x_1, \dots, x_m) \in \mathbb{R}^m$, $x_i := (i-1)h \in \overline{\Omega}$.

We approximate the infinte-dimensional Lebesgue space

$$\mathcal{L}^2(\Omega) := \{\varphi : \Omega \to \mathbb{R} \mid \langle \varphi, \varphi \rangle_{\mathcal{L}^2} < \infty\}, \qquad \langle \varphi, \psi \rangle_{\mathcal{L}^2} := \int_\Omega \varphi(x)\psi(x)\, \mathrm{d}x$$

by $\varphi \mapsto \varphi_h := \varphi(x) \in \mathbb{R}^m$,

$$\mathcal{L}^2_h(\Omega) := \mathbb{R}^m, \qquad \langle \varphi_h, \psi_h \rangle_{\mathcal{L}^2_h} := \frac{h}{2}\varphi_h^1\psi_h^1 + \sum_{i=2}^{m-1} h\varphi_h^i\psi_h^i + \frac{h}{2}\varphi_h^m\psi_h^m,$$

the trapezoidal rule for numerical integration.

Let $W := \operatorname{diag}(\frac{h}{2}, h, \dots, h, \frac{h}{2}) \in \mathbb{R}^{m\times m}$ (symmetric & positive definite). Then $\langle \cdot, \cdot \rangle_{\mathcal{L}^2_h}$ can be considered as the weighted $\mathbb{R}^m$-scalar product

$$\langle \varphi_h, \psi_h \rangle_{\mathcal{L}^2_h} = \langle \varphi_h, W\psi_h \rangle \approx \langle \varphi, \psi \rangle_{\mathcal{L}^2}.$$

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The weighted POD method in $\mathbb{R}^m$

THEOREM. Let $Y \in \mathbb{R}^{m\times n}$, $\operatorname{rank}(Y) = d$, and $W \in \mathbb{R}^{m\times m}$ symmetric & positive definite, $\langle\cdot,\cdot\rangle_W := \langle\cdot, W\cdot\rangle$.

Let $\bar{Y} := \sqrt{W}Y$ and $\bar{Y} = \bar{U}\Sigma\bar{V}^t$ the SVD of $\bar{Y}$.

Then the solution to the minimization problem

$$\begin{cases} \displaystyle\min_{(\tilde{u}_1,\ldots,\tilde{u}_l)} \sum_{j=1}^{n} \left\| y_j - \sum_{i=1}^{l} \langle y_j, \tilde{u}_i\rangle_W \tilde{u}_i \right\|_W^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j\rangle_W = \delta_{ij} \end{cases}$$

is given by $u_i = \sqrt{W}^{-1}\bar{u}_i$.

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Method of snapshots

If $n \ll m$, it is more efficient to solve the lower-dimensional eigenvalue problem

$$Y^t Y v_i = \lambda_i v_i$$

and to calculate the POD basis elements by the transformation

$$u_i = \frac{1}{\sqrt{\lambda_i}} Y v_i = \frac{1}{\sigma_i} Y v_i.$$

In the case of weighted POD, we solve

$$\bar{Y}^t \bar{Y} \bar{v}_i = Y^t W Y \bar{v}_i = \lambda_i \bar{v}_i$$

and define

$$u_i = \frac{1}{\sqrt{\lambda_i}} \sqrt{W}^{-1} (\bar{Y} \bar{v}_i) = \frac{1}{\sqrt{\lambda_i}} Y \bar{v}_i;$$

in this case, we do not have to calculate $\sqrt{W}$ or $\sqrt{W}^{-1}$.

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Finite differenced for the one-dimensional heat equation

Let $T > 0$ and $\Theta := (0, T)$. We transform the one-dimensional heat equation

$$\left\{\begin{array}{rcll} \dot{y}(t,x) - \Delta y(t,x) & = & f(t,x) & \text{on } \Theta \times \Omega \\ y_x(t,x) & = & 0 & \text{on } \Theta \times \partial\Omega \\ y(0) & = & y_0 & \text{on } \Omega \end{array}\right. \tag{pde}$$

via

$$y(t,\cdot) \approx y_h(t) \in \mathbb{R}^m, \qquad \Delta y(t,x_i) \approx \frac{y_h^{i-1}(t) - 2y_h^i(t) + y_h^{i+1}(t)}{h^2}$$

into a system of ordinary differential equations

$$\left\{\begin{array}{rcll} \dot{y}_h(t) - A_h y_h(t) & = & f_h(t) & \text{on } \Theta \\ y_h(0) & = & y_{0,h} & \end{array}\right. \tag{pde$_h$}$$

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Finite differenced for the one-dimensional heat equation

with

$$A_h = \frac{1}{h^2} \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{pmatrix}$$

and

$$f_h(t) = \begin{pmatrix} f(t, x_1) \\ f(t, x_2) \\ \vdots \\ f(t, x_{m-1}) \\ f(t, x_m) \end{pmatrix}, \qquad y_{0,h} = \begin{pmatrix} y_0(x_1) \\ y_0(x_2) \\ \vdots \\ y_0(x_{m-1}) \\ y_0(x_m) \end{pmatrix}.$$

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The continuous POD method

THEOREM: Let $y_h \in \mathcal{C}^1(\Theta, \mathbb{R}^m) \cap \mathcal{C}^0(\overline{\Theta}, \mathbb{R}^m)$ the solution to (pde$_h$).

Consider the operator $\mathcal{Y}_h \in \mathcal{L}_b(\mathcal{L}^2(\Theta, \mathbb{R}), \mathbb{R}^m)$ and the corresponding adjoint operator $\mathcal{Y}_h^* \in \mathcal{L}_b(\mathbb{R}^m, \mathcal{L}^2(\Theta, \mathbb{R}))$, given by

$$\mathcal{Y}_h \varphi := \int_\Theta \varphi(t) y_h(t) \, \mathrm{d}t \in \mathbb{R}^m, \qquad \mathcal{Y}_h^* u := \langle u, y_h(\cdot) \rangle_W \in \mathcal{L}^2(\Theta, \mathbb{R}).$$

Let $U^l = (u_1, \ldots, u_l)$ a POD-basis of rank l to the operator $\mathcal{Y}_h \mathcal{Y}_h^* : \mathbb{R}^m \to \mathbb{R}^m$.

Then U^l solves the minimization problem

$$\begin{cases} \min\limits_{\tilde{u}_1, \ldots, \tilde{u}_l} \displaystyle\int_\Theta \left\| y_h(t) - \sum_{i=1}^N \langle y_h(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \mathrm{d}t \\ \text{subject to} \qquad \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{cases}$$

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The Reduced Order Model

To solve (pde_h) approximatively with little numerical effort, we make the POD-Galerkin ansatz

$$y^l(t) := \sum_{i=1}^{l} \mathrm{y}_i^l(t) u_i \approx y_h(t).$$

The desired vector of the time-dependent coefficients, $\mathrm{y}^l(t) \in \mathbb{R}^m$, is given as the solution to the Reduced-Order Model (ROM)

$$\begin{cases} \mathrm{M}(u)\dot{\mathrm{y}}^l(t) - \mathrm{A}(u)\mathrm{y}^l(t) = \mathrm{F}(u)(t) & \text{on } \Theta \\ \mathrm{M}(u)\mathrm{y}^l(0) = \mathrm{y}_0(u) \end{cases} \qquad (\text{pde}_h^l)$$

where $\mathrm{M}(u) := (\langle u_i, u_j \rangle_W) = \mathrm{Id}(l)$, $\mathrm{A}(u) := (\langle A_h u_i, u_j \rangle_W)$, $\mathrm{F}(u) := (\langle f_h(t), u_i \rangle_W)$ and $\mathrm{y}_0(u) = (\langle y_{0,h}, u_i \rangle_W)$.

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Error analysis for continuous ROM

There exists some $C > 0$ such that

$$\int_\Theta ||y_h(t) - y^l(t)||_W^2 \, \mathrm{d}t \leq C \sum_{i=l+1}^{d} \lambda_i + C \sum_{i=l+1}^{m} \int_\Theta |\langle \dot{y}_h(t), u_i \rangle_W|^2 \, \mathrm{d}t.$$

To avoid the last term, a POD basis which also respects the time derivative of y can be determined as the solution to

$$\begin{cases} \min_{\tilde{u}_1,\ldots,\tilde{u}_l} \int_\Theta \left\| y(t) - \sum_{i=1}^{l} \langle y(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \mathrm{d}t + \int_\Theta \left\| \dot{y}(t) - \sum_{i=1}^{l} \langle \dot{y}(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \mathrm{d}t \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{cases}$$

which is given as the set of eigenvectors to the l largest eigenvalues of $\mathcal{Y}_h \mathcal{Y}_h^* + \dot{\mathcal{Y}}_h \dot{\mathcal{Y}}_h^*$,

$$\dot{\mathcal{Y}}_h \varphi := \int_\Theta \varphi(t) \dot{y}_h(t) \, \mathrm{d}t \in \mathbb{R}^m, \qquad \dot{\mathcal{Y}}_h^* u := \langle u, \dot{y}_h(\cdot) \rangle_W \in \mathcal{L}^2(\Theta, \mathbb{R}).$$

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Time discretization for the heat equation

Let $n \in \mathbb{N}$, $k := \frac{T}{n-1}$, $t_j := (j-1)k \in \Theta$ and $Y_j \approx y_h(t_j)$.

We transform (pde_h) via

$$y_h(\cdot) \approx Y \in \mathbb{R}^{m\times n}, \qquad \dot{y}_h(t_j) \approx \frac{Y_j - Y_{j-1}}{k}$$

into a linear system of equations,

$$\begin{cases} \dfrac{Y_j - Y_{j-1}}{k} - A_h Y_j & = & F \\ Y_1 & = & Y_0 \end{cases} \tag{$\text{pde}_{h,k}$}$$

where $F = (f_h(t_j))$ and $Y_0 = y_{0,h}$.

Hence, we have $y(t_j, x_i) \approx y_{h,i}(t_j) \approx Y_{ij}$.

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The discrete POD method

THEOREM: Let $\alpha = (\frac{k}{2}, k, ..., k, \frac{k}{2}) \in \mathbb{R}^n$ the corresponding trapezoidal weights.

Let $U^l = (u_1, ..., u_l)$ a POD basis to the operator

$$\bar{Y}\text{diag}(\alpha)\bar{Y}^t : u \mapsto \sum_{j=1}^{n} \alpha_j \langle Y_j, u \rangle_W Y_j \approx \int_\Theta \langle y_h(t), u \rangle_W y_h(t) \,\mathrm{d}t = \mathcal{Y}_h \mathcal{Y}_h^* u.$$

Then U^l solves the minimization problem

$$\begin{cases} \min\limits_{(\tilde{u}_1,\dots,\tilde{u}_l)} \sum_{j=1}^{n} \alpha_j \left\| Y_j - \sum_{i=1}^{l} \langle Y_j, \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{cases}$$

In general we have $||\bar{Y}\text{diag}(\alpha)\bar{Y}^t - \mathcal{Y}_h\mathcal{Y}_h^*||_{\mathcal{L}_b(\mathbb{R}^m,\mathbb{R}^m)} \stackrel{n\to\infty}{\longrightarrow} 0.$

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The homogenous one-dimensional heat equation

Let $\Omega = (0,2)$, $\Theta = (0,3)$, $m = 2500$ the number of time discretization points and $n = 7500$ the number of spatial gridpoints.

$y \in \mathbb{R}^{m\times n}$, $y_{ij} \approx y(t_i, x_j)$ denotes the approximative solution to

$$\begin{cases} \dot{y}(t,x) - \Delta y(t,x) = 0 & \text{on } \Theta \times \Omega \\ y(t,x) = 0 & \text{on } \Theta \times \partial\Omega \\ y(0,x) = y_0(x) := -x^2 + 2x & \text{on } \Omega \end{cases}$$

calculated by central differences for Δ and the implicit Euler method for $\frac{\mathrm{d}}{\mathrm{d}t}$ in **4.45 sec**.

The calculation of the first 10 pod elements takes **19.88 sec**.

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The homogenous one-dimensional heat equation

l	eigval.	time absol. / relat.	L^2 error	inform.
1	2.16e-01	0.51sec / 11.66%	2.17e-05	96.52%
2	2.16e-05	0.50sec / 11.25%	1.25e-07	99.39%
3	1.20e-07	0.55sec / 12.49%	2.80e-09	99.83%
4	2.51e-09	0.58sec / 13.06%	1.29e-10	99.94%
5	1.05e-10	0.59sec / 13.47%	9.23e-12	99.98%
6	6.63e-12	0.58sec / 13.06%	7.38e-13	99.99%
7	4.74e-13	0.58sec / 13.04%	5.17e-14	99.99%
8	3.10e-14	0.59sec / 13.31%	3.15e-15	99.99%
9	1.77e-15	0.58sec / 13.10%	1.98e-15	99.99%
10	8.81e-17	0.60sec / 13.61%	1.65e-15	99.99%

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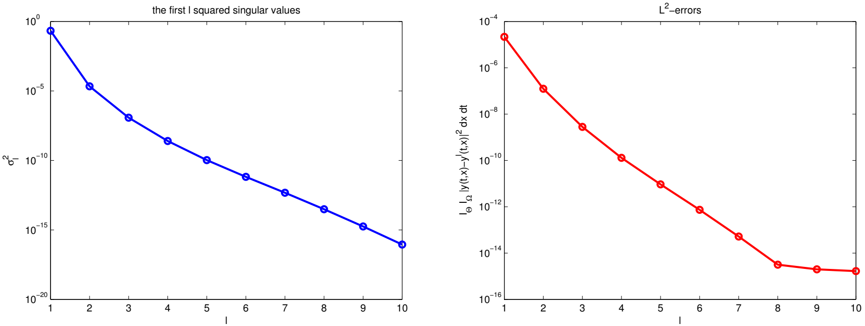
The homogenous one-dimensional heat equation



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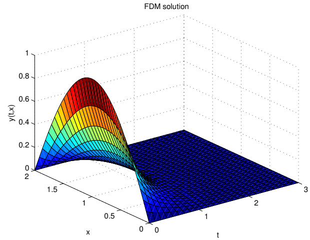
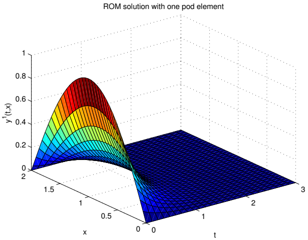
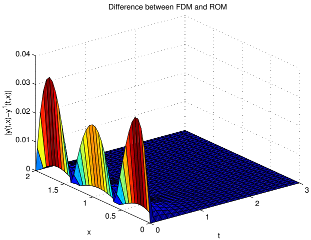
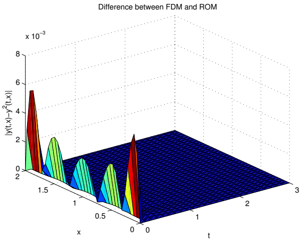
The homogenous one-dimensional heat equation









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