# Model order reduction via Proper Orthogonal Decomposition

Reduced Basis Summer School 2015

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## Motivation

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# Introduction

Let $\mathcal{X}$ be a Hilbert space and $\Theta$ be a time interval.

For a given function $y \in L^2(\Theta, \mathcal{X})$ we want to find a reduced basis

$$\Psi^\ell = \{\psi_1, ..., \psi_\ell\} \subseteq \mathcal{X}$$

of $\mathcal{X}$-orthonormal elements $\psi_1, ..., \psi_\ell$ such that $y$ admits an optimal representation in $L^2(\Theta, \operatorname{span} \Psi^\ell)$, in the sense that $\psi_1, ..., \psi_\ell$ solve

$$\min_{\psi_1,\ldots,\psi_\ell \in \mathcal{X}} \int_\Theta \left\| y(t) - \sum_{l=1}^{\ell} \langle y(t), \psi_l \rangle_{\mathcal{X}} \psi_l \right\|_{\mathcal{X}}^2 \mathrm{d}t \quad \text{s.t.} \quad \langle \psi_k, \psi_l \rangle_{\mathcal{X}} = \delta_{kl} \tag{1}$$

where $\delta$ denotes the Kronecker-Delta $\delta_{kl} = 1$ for $k = l$ and 0 elsewise.

A solution to (1) is called a rank-$\ell$ POD basis.

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# Introduction

The minimization problem (1) is equivalent to maximizing the averaged projection of the snapshots $y(t),\ t \in \Theta$, onto the reduced space span $\Psi^\ell$:

$$\max_{\psi_1,\ldots,\psi_\ell} \sum_{l=1}^{\ell} \int_\Theta \langle y(t), \psi_l \rangle_{\mathcal{X}}^2 \,\mathrm{d}t \quad \text{s.t.} \quad \langle \psi_k, \psi_l \rangle_{\mathcal{X}} = \delta_{kl}; \tag{2}$$

especially, a given rank-$\ell$ POD basis $\Psi^\ell$ can be expanded to a rank-$(\ell + 1)$ basis by a solution $\psi_{\ell+1}$ to

$$\max_{\psi \in (\operatorname{span} \Psi^\ell)^\perp} \int_\Theta \langle y(t), \psi \rangle_{\mathcal{X}}^2 \,\mathrm{d}t, \tag{3}$$

choosing $\Psi^{\ell+1} = \Psi^\ell \cup \{\psi_{\ell+1}\}$; it is not required to calculate $\ell + 1$ new basis elements.

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## Basis construction

Since problem (2) is a constrained optimization problem in a Banach space, we apply the Lagrange calculus: We define the Lagrange function $\mathscr{L} : \mathcal{X}^\ell \times \mathbb{R}^{\ell\times\ell} \to \mathbb{R}$ by

$$\mathscr{L}(\psi,\lambda) = \sum_{l=1}^{\ell} \int_\Theta \langle y(t), \psi_l\rangle_{\mathcal{X}}^2 \, \mathrm{d}t + \sum_{k,l=1}^{\ell} \lambda_{kl}(\langle \psi_k, \psi_l\rangle_{\mathcal{X}} - \delta_{kl}) \tag{4}$$

and receive the necessary first-order optimality conditions

$$\int_\Theta \langle y(t), \psi_l\rangle_{\mathcal{X}} y(t) \, \mathrm{d}t = \lambda_{ll}\psi_l : \tag{5}$$

The POD basis elements solve an eigenvalue problem [4].

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## Basis construction

Furthermore, the maximal value of (2) is

$$\int_\Theta \left\| y(t) - \sum_{l=1}^{\ell} \langle y(t), \psi_l\rangle_{\mathcal{X}} \psi_l \right\|_{\mathcal{X}}^2 \mathrm{d}t = \sum_{l=1}^{\ell} \int_\Theta \langle y(t), \psi_l\rangle_{\mathcal{X}}^2 \, \mathrm{d}t = \sum_{l>\ell} \lambda_{ll}, \tag{6}$$

so we look for eigenvectors corresponding to the $\ell$ largest eigenvalues of (5).

The eigenvalue problem (5) admits a solution in $\mathcal{X}^\ell \times \mathbb{R}^\ell$ since the operator $\mathcal{R}(y) : \mathcal{X} \to \mathcal{X}$,

$$\mathcal{R}(y)\phi = \int_\Theta \langle y(t), \phi\rangle_{\mathcal{X}} y(t) \, \mathrm{d}t \qquad (\phi \in \mathcal{X}) \tag{7}$$

is nonnegative, selfadjoint and compact.

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# Projection error

Let $\mathcal{P}^\ell_{\mathcal{X}} : \mathcal{X} \to \operatorname{span} \Psi^\ell$ denote the orthogonal projection on the POD space, i.e.

$$\mathcal{P}^\ell_{\mathcal{X}}\phi = \underset{\tilde{\psi}\in\operatorname{span}\Psi^\ell}{\arg\min} \|\phi - \tilde{\phi}\|^2_{\mathcal{X}} = \sum_{l=1}^{\ell} \langle \phi, \psi_l \rangle_{\mathcal{X}} \psi_l \tag{8}$$

for each $\phi \in \mathcal{X}$. Then we have a formula for the POD projection error [10]:

$$\boxed{\int_\Theta \|y(t) - \mathcal{P}^\ell_{\mathcal{X}} y(t)\|^2_{\mathcal{X}} = \sum_{l>\ell} \lambda_l \quad \xrightarrow{\ell\to\infty} \quad 0. \qquad (9)}$$

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# Projection error

Let $V, H$ be Hilbert spaces with dense and continuous embedding $V \hookrightarrow H$ and let $y \in L^2(\Theta, V)$. Choose $\mathcal{X} = H$, then the $V$-orthogonal projection $\mathcal{P}^\ell_V : V \to \operatorname{span} \Psi^\ell$ has the following representation in the $H$-orthonormal basis $\Psi^\ell$:

$$\mathcal{P}^\ell_V\phi = \underset{\tilde{\phi}\in\operatorname{span}\Psi^\ell}{\arg\min} \|\phi - \tilde{\phi}\|^2_V = \sum_{k,l=1}^{\ell} \mathrm{M}_V^{-1}(\psi)_{lk} \langle \phi, \psi_k \rangle_H \psi_l \tag{10}$$

where $\mathrm{M}_V(\psi) \in \mathbb{R}^{\ell\times\ell}$ is the weights matrix $\mathrm{M}_V(\psi)_{lk} = \langle \psi_l, \psi_k \rangle_V$. We get [15]

$$\boxed{\int_\Theta \|y(t) - \mathcal{P}^\ell_V y(t)\|^2_V \, \mathrm{d}t = \sum_{l=\ell+1}^{\infty} \lambda_l \|\psi_l - \tilde{\mathcal{P}}^\ell_V \psi_l\|^2_V \quad \xrightarrow{\ell\to\infty} \quad 0. \qquad (11)}$$

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# Projection error

Let again be $\mathcal{X} = H$. Then we have the error formula [1]

$$\int_\Theta \|y(t) - \mathcal{P}_H^\ell y(t)\|_V^2 \,\mathrm{d}t = \sum_{l=\ell+1}^{\infty} \lambda_l \|\psi_l\|_V^2 \quad \xrightarrow{\ell\to\infty} \quad 0. \tag{12}$$

The estimates (11) and (6) allow to bound the projection errors in $V$ allthough the POD basis elements are orthogonal in $H$. This will be useful when POD is applied to partial differential equations.

If $y \in H^1(\Theta, V)$, then (6) will allow not only to approximate $y$, but also its time derivative $\dot{y}$ as we will see later.

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# Method of snapshots

We define the multiplication operator $\mathcal{Q}(y) : L^2(\Theta, \mathbb{R}) \to \mathcal{X}$ and it's adjoints $\mathcal{Q}(y)^\star : \mathcal{X} \to L^2(\Theta, \mathbb{R})$,

$$\mathcal{Q}(y)\phi = \int_\Theta \phi(t) y(t) \,\mathrm{d}t, \qquad (\mathcal{Q}(y)^\star \phi)(t) = \langle \phi, y(t) \rangle_{\mathcal{X}}. \tag{13}$$

Then the composition satisfies $\mathcal{R}(y) = \mathcal{Q}(y)\mathcal{Q}(y)^\star : V \to V$.

Let $\mathcal{K}(y) = \mathcal{Q}(y)^\star \mathcal{Q}(y) : L^2(\Theta, \mathbb{R}) \to L^2(\Theta, \mathbb{R})$. Since $\mathcal{R}(y)$ and $\mathcal{K}(y)$ have the same eigenvalues with the same multiplicities (except of possible 0), a POD basis is also given by a spectral decomposition $(\lambda_l, \phi_l)_{l=1,\ldots,\ell} \subseteq L^2(\Theta, \mathbb{R})^\ell \times \mathbb{R}^\ell$ of

$$(\mathcal{K}(y)\phi)(t) = \left\langle \int_\Theta \langle \phi(s) y(s) \,\mathrm{d}s, y(t) \right\rangle_{\mathcal{X}} = \int_\Theta \phi(s) \langle y(s), y(t) \rangle_{\mathcal{X}} \,\mathrm{d}s, \tag{14}$$

choosing $\psi_l = \frac{1}{\sqrt{\lambda_l}} \mathcal{Q}(y)\phi_l \in V$.

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# Discretization

Let $\mathcal{X}_n \subseteq \mathcal{X}$ be a finite-dimensional subspace of $\mathcal{X}$ spanned by the linearly independent elements $\varphi_1, \ldots, \varphi_n \in V$ with mass matrix $\mathrm{M}(\varphi) \in \mathbb{R}^{n\times n}$, $\mathrm{M}(\varphi)_{\mathrm{jj}} = \langle \varphi_j, \varphi_{\mathrm{j}} \rangle_{\mathcal{X}}$. Let $\{t_1, \ldots, t_m\} \subseteq \Theta$.

We replace $y \in L^2(\Theta, V)$ by $\mathrm{y} \in \mathbb{R}^{n\times m}$ such that $y(t_i) \approx \sum_{j=1}^n \mathrm{y}_{ji}\varphi_j$ and consider

$$\min_{\psi_1,\ldots,\psi_\ell \in \mathbb{R}^n} \sum_{i=1}^m \alpha_i \left\| \mathrm{y}_{\cdot i} - \sum_{l=1}^{\ell} \langle \mathrm{y}_{\cdot i}, \psi_l \rangle_{\mathbb{R}^n_\varphi} \psi_l \right\|^2_{\mathbb{R}^n_\varphi} \qquad \text{s.t.} \qquad \langle \psi_k, \psi_l \rangle_{\mathbb{R}^n_\varphi} = \delta_{kl} \tag{15}$$

with the weighted scalar product $\langle \cdot, \cdot \rangle_{\mathbb{R}^n_\varphi} = \langle \cdot, \mathrm{M}(\varphi) \cdot \rangle_{\mathbb{R}^n}$ and time weights $\alpha_i > 0$.

Then a POD basis can be calculated by a decomposition of one of the matrices

$$\mathrm{R}(\mathrm{y}) = \mathrm{y}\mathrm{M}(\alpha)\mathrm{y}^{\mathrm{T}}\mathrm{M}(\varphi) \in \mathbb{R}^{n\times n}, \qquad \mathrm{K}(\mathrm{y}) = \mathrm{y}^{\mathrm{T}}\mathrm{M}(\varphi)\mathrm{y}\mathrm{M}(\alpha) \in \mathbb{R}^{m\times m} \tag{16}$$

where $\mathrm{M}(\alpha)_{\mathrm{jj}} = \alpha_j \delta_{\mathrm{jj}}$ [4].

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# Discretization

1. Let $(\tilde{\psi}_l, \lambda_l)$ be a decomposition of the symmetrized matrix

$$\tilde{\mathrm{R}}(\mathrm{y}) = \mathrm{M}(\varphi)^{1/2}\mathrm{y}\mathrm{M}(\alpha)\mathrm{y}^{\mathrm{T}}\mathrm{M}(\varphi)^{1/2},$$

   then appropriate POD elements are $\psi_l = \mathrm{M}(\varphi)^{-1/2}\tilde{\psi}_l \in \mathbb{R}^n$. We require the decomposition of an $n \times n$ matrix, the root of the mass matrix and solution steps for the transformation $\tilde{\psi} \to \psi$.

2. Let $(\tilde{\psi}_l, \lambda_l)$ be a decomposition of the symmetrized matrix

$$\tilde{\mathrm{K}}(\mathrm{y}) = \mathrm{M}(\alpha)^{1/2}\mathrm{y}^{\mathrm{T}}\mathrm{M}(\varphi)\mathrm{y}\mathrm{M}(\alpha)^{1/2},$$

   then appropriate POD elements are $\psi_l = \lambda_l^{-1/2}\mathrm{y}\mathrm{M}(\alpha)^{1/2}\tilde{\psi}_l$: An $m \times m$ matrix has to be decomposed, but no matrix roots or solving steps are needed.

3. A singular value decomposition $(\tilde{\psi}_l, \tilde{\lambda}_l, \psi_l)$ of $\mathrm{M}(\varphi)^{1/2}\mathrm{y}\mathrm{M}(\alpha)^{1/2}$ is costly, but more robust; the eigenvalues corresponding to the POD elements $\psi_l$ are $\lambda_l = \tilde{\lambda}_l^2$.

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# Discretization

```
% --------------------------------------------------------------------------
% POD determines a weighted POD matrix by solving the eigenvalue problem
%    R(Y)*psi = Y*diag(T)*Y'*W*psi = lambda*psi.
%
% Input:
% Y .......................................... nxm snapshot matrix
% l .......................................... 1x1 pod basis rank
% W .......................................... nxn space weights
% T .......................................... mx1 time weights
%
% Output:
% Psi ........................................ nxl pod basis
% Lambda ..................................... lx1 eigenvalues
% --------------------------------------------------------------------------

function [Psi,Lambda] = pod(Y,l,W,T)

% Build up pod operator R(Y)
Alpha = spdiags(T,0,size(T,1),size(T,1));          % Alpha ........... mxm
R = Y*Alpha*Y'*W;                                  % R ................ nxn
% Solve eigenvalue problem by EIG
[Psi,Lambda] = eig(R);
  [Lambda,Ord] = sort(diag(Lambda),'descend');     % Lambda ........... nx1
  Lambda = Lambda(1:l,1);                          % Lambda ........... lx1
  Psi = Psi(:,Ord);                                % Psi .............. nxn
  Psi = Psi(:,1:l);                                % Psi .............. nxl

end
```

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# Application: Filtering and compression of frogs

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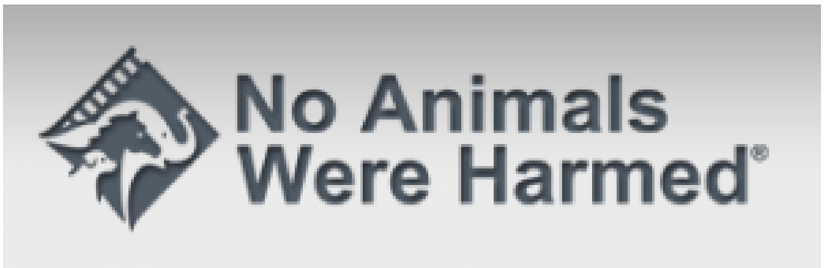
# Application: Filtering and compression of frogs

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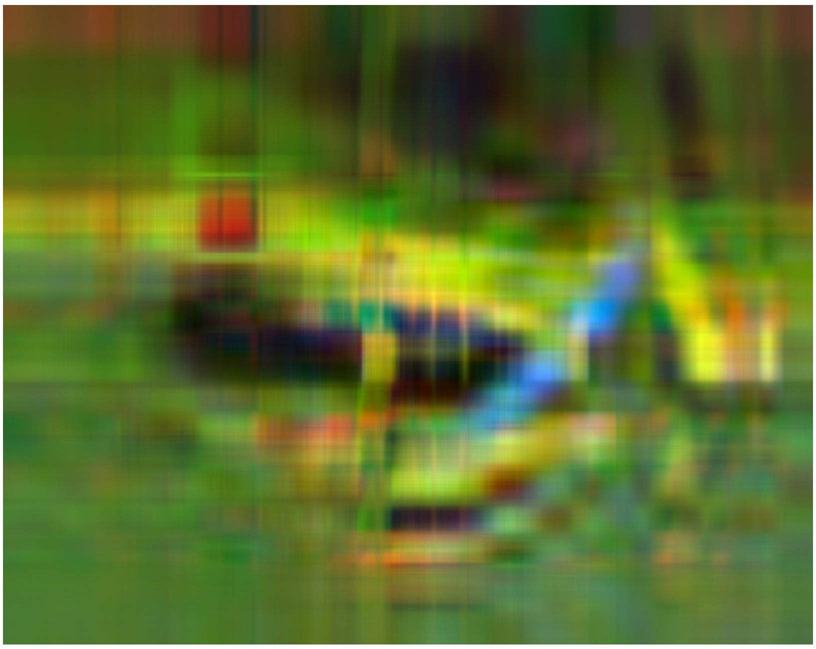
# Application: Filtering and compression of frogs



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## Application: Filtering and compression of frogs

| $l$ | Rel. Error | Rel. Size | Rel. SVs |
|---:|---:|---:|---:|
| 5 | 12.31% | 0.51% | 1.08e-01 |
| 10 | 7.81% | 1.02% | 6.68e-02 |
| 20 | 4.44% | 2.04% | 3.88e-02 |
| 50 | 1.92% | 5.09% | 1.50e-02 |
| 100 | 0.91% | 10.18% | 7.10e-03 |
| 200 | 0.39% | 20.36% | 3.09e-03 |

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# Application: Filtering and compression of random data

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# Application: Filtering and compression of random data

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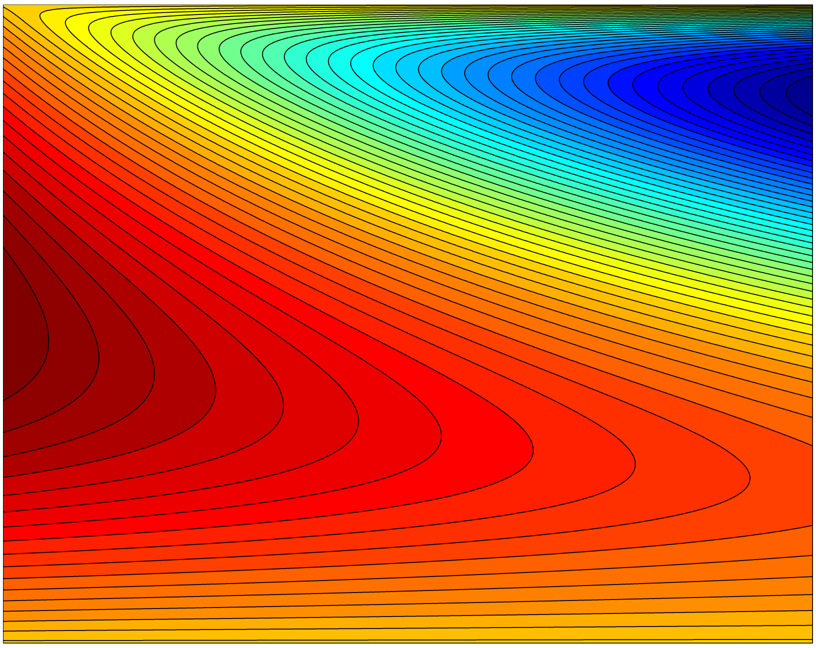
# Application: Filtering and compression of dynamical flows



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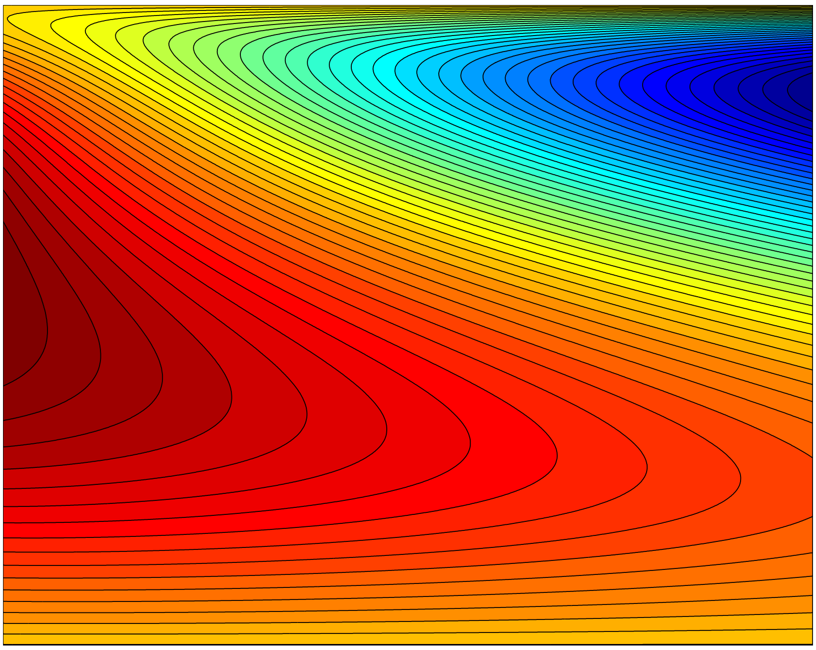
# Application: Filtering and compression of dynamical flows



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# Application: Frogs, randoms and dynamics

1. Photo compression with POD works quite well: from 10% of the original data onwards, the visible approximation errors vanish.
2. For random data, POD is completely useless (and it should be: it recognizes structurs only if they are there ...). Taking 95% of the original data still does not lead to appropriate results although the original data storage is exceeded by 150%.
3. Dynamical flows in nice settings (such as diffusion dominated processes with smooth data) are reconstructed perfectly: In the example above, we just used two POD basis functions ...

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# Reduced order modeling

Let $\Psi^\ell = \{\psi_1, ..., \psi_\ell\}$ be an orthonormal system in $\mathcal{X} \in \{V, H\}$. In the following, we interprete the parabolic partial differential equation

$$\dot{y}(t) + Ay(t) = f(t) \text{ in } V', \qquad y(0) = y_\circ \text{ in } H \tag{17}$$

as a variational problem in the reduced space span $\Psi^\ell \subseteq V$:

$$\langle \dot{y}(t), \phi \rangle_{V',V} + a(y(t), \phi) = \langle f(t), \phi \rangle_{V',V}, \qquad \langle y(0), \phi \rangle_H = \langle y_\circ, \phi \rangle_H \tag{18}$$

for all $\phi \in$ span $\Psi^\ell$.

The solution to (18) has the form

$$y^\ell \in H^1(\Theta, V), \qquad y^\ell(t) = \sum_{l=1}^{\ell} \mathrm{y}_l(t)\psi_l \tag{19}$$

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# Reduced order modeling

The coefficient function $\mathrm{y} \in H^1(\Theta, \mathbb{R}^\ell)$ is given by the system of ordinary differential equations

$$\mathrm{M}(\psi)\dot{\mathrm{y}}(t) + \mathrm{A}(\psi)\mathrm{y}(t) = \mathrm{f}(\psi; t), \qquad \mathrm{M}(\psi)\mathrm{y}(0) = \mathrm{y}_\circ(\psi); \tag{20}$$

$\mathrm{M}(\psi), \mathrm{A}(\psi) \in \mathbb{R}^{\ell\times\ell}$ are defined as

$$\mathrm{M}(\psi)_{kl} = \langle\psi_k, \psi_l\rangle_H, \qquad \mathrm{A}(\psi)_{kl} = a(\psi_k, \psi_l)$$

and the reduced data functions are $\mathrm{f}(\psi) \in L^2(\Theta, \mathbb{R}^\ell)$, and $\mathrm{y}_\circ(\psi) \in \mathbb{R}^\ell$,

$$\mathrm{f}(\psi; t)_l = \langle f(t), \psi_l\rangle_{V',V}, \qquad \mathrm{y}_\circ(\psi)_l = \langle y_\circ, \psi_l\rangle_H.$$

(20) admits the unique solution

$$\mathrm{y}(t) = e^{-t\mathrm{M}(\psi)^{-1}\mathrm{A}(\psi)}\mathrm{y}_\circ + \int_0^t e^{(\tau-t)\mathrm{M}(\psi)^{-1}\mathrm{A}(\psi)}\mathrm{M}(\psi)^{-1}\mathrm{f}(\psi;\tau)\,\mathrm{d}\tau. \tag{21}$$

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# Model reduction error

Assume $y_\circ = 0$. Let $\mathcal{X} = V$, $(\psi_1, ..., \psi_\ell)$ be a POD basis satisfying the problem

$$\int_\Theta \langle\psi_l, y(t)\rangle_V y(t)\,\mathrm{d}t = \lambda_l\psi_l$$

and let $\mathrm{y} \in H^1(\Theta, \mathbb{R}^\ell)$ be the solution to the reduced problem (20). Then there exists a constant $C > 0$ just depending on the final time and the geometric data such that the ROM error can be estimated by

$$\boxed{\left\| y - \sum_{l=1}^{\ell} \mathrm{y}_l\psi_l \right\|^2_{L^2(\Theta,V)\cap H^1(\Theta,V')} \le C\left(\sum_{l=\ell+1}^{\infty}\lambda_l + \|\dot{\tilde{y}}(t) - \mathcal{P}_V^\ell\dot{\tilde{y}}(t)\|^2_{L^2(\Theta,V')}\right). \quad (22)}$$

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# Model reduction error

Let $\mathcal{X} = V$, $(\psi_1, ..., \psi_\ell)$ be a POD basis satisfying the problem

$$\int_\Theta \langle \psi_l, y(t) \rangle_V y(t)\,\mathrm{d}t + \int_\Theta \langle \psi_l, \dot{y}(t) \rangle_V \dot{y}(t)\,\mathrm{d}t = \lambda_l \psi_l$$

and let $\mathrm{y} \in H^1(\Theta, \mathbb{R}^\ell)$ be the solution to the reduced problem (20). Then there exists a constant $C > 0$ just depending on the final time and the geometric data such that the ROM error can be estimated by

$$\boxed{\left\| y - \sum_{l=1}^{\ell} \mathrm{y}_l \psi_l \right\|^2_{L^2(\Theta,V)\cap H^1(\Theta,V')} \leq C \sum_{l=\ell+1}^{\infty} \lambda_l. \qquad (23)}$$

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# Model reduction error

Let $\mathcal{X} = H$, $(\psi_1, ..., \psi_\ell)$ be a POD basis satisfying the problem

$$\int_\Theta \langle \psi_l, y(t) \rangle_H y(t)\,\mathrm{d}t + \int_\Theta \langle \psi_l, \dot{y}(t) \rangle_H \dot{y}(t)\,\mathrm{d}t = \lambda_l \psi_l$$

and let $\mathrm{y} \in H^1(\Theta, \mathbb{R}^\ell)$ be the solution to the reduced problem (20). Then there exists a constant $C > 0$ just depending on the final time and the geometric data such that the ROM error can be estimated by

$$\boxed{\left\| y - \sum_{l=1}^{\ell} \mathrm{y}_l \psi_l \right\|^2_{L^2(\Theta,V)\cap H^1(\Theta,V')} \leq C \sum_{l=\ell+1}^{\infty} \lambda_l \|\psi_l - \tilde{\mathcal{P}}_V^\ell \psi_l\|_V^2. \qquad (24)}$$

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# Model reduction error

Let $\mathcal{X} = V$, $(\psi_1, ..., \psi_\ell)$ be a POD basis satisfying the problem

$$\int_\Theta \langle \psi_l, y(t) \rangle_V y(t)\, \mathrm{d}t = \lambda_l \psi_l$$

and let $\mathrm{y} \in H^1(\Theta, \mathbb{R}^\ell)$ be the solution to the reduced problem (20). Then there exists a constant $C > 0$ just depending on the final time and the geometric data such that the ROM error can be estimated by

$$\boxed{\left\| y - \sum_{l=1}^{\ell} \mathrm{y}_l \psi_l \right\|^2_{L^2(\Theta,V)} \leq C \sum_{l=\ell+1}^{\infty} \lambda_l \|\psi_l\|^2_V. \qquad (25)}$$

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# Motivation

1. Combination of POD with nonlinear PDE solvers such as Sequential Quadratic Programming [2], Trust Region Method [14] or Primal Dual Active Set Method [5].
2. How does the reduction error react if the state $y$ which builds up $\mathcal{R}(y)$ corresponds to a different source term $f$ then the reduced system [6]?
3. In this case, the presented a-priori estimates are not valid any more. The design of efficient a-posteriori error bounds [16], especially for nonlinear equations [7], is in work.
4. The a-priori bounds [10] and convergence rates [9] are available if an appropriate POD basis update strategy (OS-POD) [11], [3] is used.
5. Applications to optimal control [5], parameter identification [12] and inverse problems [13].
6. Combination of POD model reduction and Greedy algorithm in the reduced basis context [8].

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