Randomized Model Order Reduction

Alessandro Alla work in collaboration with J. Nathan Kutz



Data-Driven Methods for Reduced-Order Modeling and Stochastic Partial Differential Equations

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Randomized MOR

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Problem Settings

Dynamical System

$$\mathbf{M} \, \dot{\mathbf{y}}(t) = \mathbf{A} \mathbf{y}(t) + \mathbf{f}(t, \mathbf{y}(t)), \ t \in (0, T],$$

 $\mathbf{y}(0) = \mathbf{y}_{\mathbf{0}}.$

Assumptions

- $\mathbf{y_0} \in \mathbb{R}^n$ is a given initial data,
- $\mathbf{M}, \mathbf{A} \in \mathbb{R}^{n \times n}$ given matrices,
- f: [0, T] × ℝⁿ → ℝⁿ a continuous function in both arguments and locally Lipschitz-type with respect to the second variable.

WARNING: High dimensional problems are computationally expensive.

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Introduction

Low-rank approximation requires:

- Solutions of the original high-dimensional system (snapshots),
- Dimensionality-reduction produced by SVD,
- Galerkin projection of the dynamics on the low-rank subspace.

WARNING:

Offline stages are exceptionally expensive, but enable the (cheap) online stage to potentially run in real time.

GOAL: To improve the efficiency of the offline stage

Randomized techniques attempt to construct low-rank matrix decompositions, fast and accurate approximations of QR and SVD.

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Outline



Model Order Reduction

- Proper Orthogonal Decomposition
- Discrete Empirical Interpolation Method
- Dynamic Mode Decomposition
- Coupling POD and DMD methods
- 2 Randomized Linear Algebra in Model Order Reduction
 - Compressed Model Order Reduction Techniques
 - Compressed POD
 - Compressive Sampling DMD

Numerical Tests

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2) Randomized Linear Algebra in Model Order Reduction

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Numerical Tests

Proper Orthogonal Decomposition and SVD

Proper Orthogonal Decomposition (POD), [L. Sirovich '87]

- Simulate at different time instances,
- Take snapshots of the state,
- Perform POD (Proper Orthogonal Decomposition) using SVD (Singular Value Decomposition),
- Use the POD basis functions as (non local) FEM ansatz functions.

Proper Orthogonal Decomposition and SVD

Given snapshots $(y(t_0), \ldots, y(t_n)) \in \mathbb{R}^m$

We look for an orthonormal basis $\{\psi_i\}_{i=1}^{\ell}$ in \mathbb{R}^m with $\ell \ll \min\{n, m\}$ s.t.

$$J(\psi_1,\ldots,\psi_\ell) = \sum_{j=1}^n \alpha_j \left\| \mathbf{y}_j - \sum_{i=1}^\ell \langle \mathbf{y}_j,\psi_i \rangle \psi_i \right\|^2 = \sum_{i=\ell+1}^d \sigma_i^2$$

reaches a minimum where $\{\alpha_j\}_{j=1}^n \in \mathbb{R}^+$.

$$\min J(\psi_1, \dots, \psi_\ell) \quad s.t. \langle \psi_i, \psi_j \rangle = \delta_{ij}$$

Singular Value Decomposition: $Y = \Psi \Sigma V^T$.

For $\ell \in \{1, ..., d = rank(Y)\}$, $\{\psi_i\}_{i=1}^{\ell}$ are called **POD basis** of rank ℓ . **ERROR INDICATOR:** $\mathcal{E}(\ell) = \frac{\sum_{i=1}^{\ell} \sigma_i}{\sum_{i=1}^{d} \sigma_i}$ with σ_i singular values of the SVD.

Reduced Order System

POD-Galerkin ansatz

$$\mathbf{y}(t) pprox \mathbf{\Psi}^{ extsf{POD}} \mathbf{y}^{\ell}(t), \quad \mathbf{\Psi}^{ extsf{POD}} \in \mathbb{R}^{n imes \ell}.$$

POD dynamical system

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$$\begin{cases} \mathbf{M}^{\ell} \dot{\mathbf{y}}^{\ell}(t) = \mathbf{A}^{\ell} \mathbf{y}^{\ell}(t) + (\mathbf{\Psi}^{\text{POD}})^{T} f(t, \mathbf{\Psi}^{\text{POD}} \mathbf{y}^{\ell}(t)), \\ \mathbf{y}^{\ell}(0) = \mathbf{y}_{\mathbf{0}}^{\ell}. \end{cases}$$

Dimension of the entries

•
$$(\mathsf{M}^{\ell})_{ij} = \langle \mathsf{M}\psi_i, \psi_j \rangle \in \mathbb{R}^{\ell \times \ell},$$

• $(\mathsf{A}^{\ell})_{ij} = \langle \mathsf{A}\psi_i, \psi_j \rangle \in \mathbb{R}^{\ell \times \ell},$

•
$$\mathbf{y}_{\mathbf{0}}^{\ell} = (\mathbf{\Psi}^{\text{pod}})^T \mathbf{y}_{\mathbf{0}} \in \mathbb{R}^{\ell}.$$

Problem:

Reduction of the nonlinearity is **NOT** independent from *n*:

$$\mathbf{F}(t, \mathbf{y}^{\ell}(t)) := (\mathbf{\Psi}^{\mathsf{POD}})^{\mathsf{T}} \mathbf{f}(t, \mathbf{\Psi}^{\mathsf{POD}} \mathbf{y}^{\ell}(t)) = \langle \mathbf{f}(t, \mathbf{y}(t)), \mathbf{\Psi}^{\mathsf{POD}} \rangle.$$

IDEA:

Do not evaluate the nonlinearity everywhere, but select the *most important* points via the **greedy** procedure.

References

- M. Barrault, Y. Maday, N.C. Nguyen, A.T. Patera, An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations, 2004.
- S. Chatarantabut, D. Sorensen, *Nonlinear Model Reduction via Discrete Empirical Interpolation*, 2010.

- Compute **y**(*t_j*) from the dynamical system,
- Evaluate $\mathbf{f}(t_j, \mathbf{y}(t_j))$,
- $\mathbf{U} \in \mathbb{R}^{n \times k}$ the POD basis function of rank *k* of the nonlinear part.
- The DEIM approximation of **f**(*t*, **y**(*t*)) is as follows

$$\mathbf{f}^{\mathsf{DEIM}}(t, \mathbf{y}^{\mathsf{DEIM}}(t)) := \mathbf{U}(\mathbf{S}^{\mathsf{T}}\mathbf{U})^{-1}\mathbf{f}(t, \mathbf{y}^{\mathsf{DEIM}}(t))$$

where $\mathbf{S} \in \mathbb{R}^{n \times k}$ and $\mathbf{y}^{\text{DEIM}}(t) = \mathbf{S}^{\mathcal{T}} \Psi^{\text{POD}} \mathbf{y}^{\ell}(t) \in \mathbb{R}^{k}$.

Interpolation Points: Matrix S tells where evaluate the nonlinearity.

- LU decomposition with pivoting (Chatarantabut, Sorensen, 2010),
- QR decomposition with pivoting (Drmac, Gugercin, 2015).

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Let us define $\Psi^{\text{DEIM}} := \mathbf{U}(\mathbf{S}^T \mathbf{U})^{-1} \in \mathbb{R}^{n \times k}$. The reduced nonlinearity may be expressed as:

$$(\mathbf{\Psi}^{\mathsf{POD}})^{\mathsf{T}}\mathbf{f}^{\mathsf{DEIM}}(t,\mathbf{y}^{\mathsf{DEIM}}(t)) = (\mathbf{\Psi}^{\mathsf{POD}})^{\mathsf{T}}\mathbf{\Psi}^{\mathsf{DEIM}}\mathbf{f}(t,\mathbf{y}^{\mathsf{DEIM}})$$

where we only select a small (**sparse**) number of rows of $\Psi^{POD} \mathbf{y}^{\ell}(t)$.

Computational expenses

$$\mathbf{S}^{T} \mathbf{\Psi}^{\text{POD}} \in \mathbb{R}^{k \times \ell}, \, (\mathbf{S}^{T} \mathbf{U})^{-1} \in \mathbb{R}^{k \times k} \text{ and } (\mathbf{\Psi}^{\text{POD}})^{T} \mathbf{\Psi}^{\text{DEIM}} \in \mathbb{R}^{\ell \times k}$$

Remark

Precomputed quantities are **independent** of the full dimension *n*.

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POD dynamical system

$$\mathbf{M}^{\ell} \dot{\mathbf{y}}^{\ell}(t) = \mathbf{A}^{\ell} \mathbf{y}^{\ell}(t) + (\mathbf{\Psi}^{\text{POD}})^{T} f(t, \mathbf{\Psi}^{\text{POD}} \mathbf{y}^{\ell}(t)),$$
$$\mathbf{y}^{\ell}(0) = \mathbf{y}_{0}^{\ell}$$

POD-DEIM dynamical system

$$\begin{cases} \mathbf{M}^{\ell} \dot{\mathbf{y}}^{\ell}(t) = \mathbf{A}^{\ell} \mathbf{y}^{\ell}(t) + (\mathbf{\Psi}^{\text{POD}})^{T} \mathbf{\Psi}^{\text{DEIM}} \mathbf{f}(t, \mathbf{y}^{\text{DEIM}}) \\ \mathbf{y}^{\ell}(0) = \mathbf{y}_{0}^{\ell}. \end{cases}$$

low-rank approximation of the nonlinear term.

Error Estimation

$$\|\mathbf{f} - \mathbf{f}^{ extsf{DEIM}}\|_2 \leq c \|(\mathbf{I} - \mathbf{U}\mathbf{U}^{ op})f\|_2, \quad c = \|(\mathbf{S}^{ op}\mathbf{U})^{-1}\|_2$$

with different performances depending on the matrix S.

Introduction to DMD

DMD is an equation-free, data-driven method capable of providing accurate model for complex system, and short-time future estimates of such a systems.

It traces its origins to pioneering work of **Bernard Koopman** in 1931. Koopman theory is a dynamical systems tool that provides information about a nonlinear dynamical system via an associated infinite-dimensional linear system.

DMD method was proposed as a data-driven algorithm for modeling complex flows as a special case of Koopman theory. (Brunton, Kutz, Mezic, Noack, Rowley, Schmid, Tu, ...)

Dynamic Mode Decomposition

Dynamic Mode Decomposition

Suppose we have a dynamical system and compute snapshots $\{(y(t_0), \ldots, y(t_m))\}$ and two sets of data

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}(t_0) & \mathbf{y}(t_1) & \cdots & \mathbf{y}(t_{m-1}) \\ | & | & | & | \end{bmatrix}, \quad \mathbf{Y}' = \begin{bmatrix} \mathbf{y}(t_1) & \mathbf{y}(t_2) & \cdots & \mathbf{y}(t_m) \\ | & | & | & | & | \end{bmatrix}$$

with $\mathbf{y}(t_j)$ an initial condition of the dynamical system and $\mathbf{y}(t_{j+1})$ its corresponding output $\Rightarrow \mathbf{Y}' = \mathbf{A}_{\mathbf{Y}}\mathbf{Y}$ with $\mathbf{A}_{\mathbf{Y}} \in \mathbb{R}^{n \times n}$ unknown.

The DMD modes are eigenvectors of

$${\sf A_y} = {\sf Y}'{\sf Y}^\dagger$$

where † denotes the Moore-Penrose pseudoinverse.

Dynamic Mode Decomposition

- **A**_y is a finite dimensional approximation of the Koopman operator for a linear observable.
- The definition of DMD produces a regression procedure whereby the data snapshots in time are used to produce the **best-fit linear** dynamical system for the data Y.

The DMD procedure constructs the proxy, approximate linear evolution

$$\frac{d\tilde{\mathbf{y}}}{dt} = \mathbf{A}_{\mathbf{y}}\tilde{\mathbf{y}}$$

with $\tilde{\mathbf{y}}(0) = \tilde{\mathbf{y}}_0$ and whose solution is: $\tilde{\mathbf{y}}(t) = \sum_{i=1}^n b_i \psi_i \exp(\omega_i t)$, ψ_i and ω_i are the eigenfunctions and eigenvalues of the matrix $\mathbf{A}_{\mathbf{y}}$.

SOLUTION

DMD circumvents the eigendecomposition of A_y by considering a rank-reduced representation in terms of a POD-projected matrix \tilde{A}_y .

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Dynamic Mode Decomposition

DMD algorithm

Require: Snapshots $\{\mathbf{y}(t_0), \ldots, \mathbf{y}(t_m)\},\$

- 1: Set $\mathbf{Y} = [\mathbf{y}(t_0), \dots, \mathbf{y}(t_{m-1})]$ and $\mathbf{Y}' = [\mathbf{y}(t_1), \dots, \mathbf{y}(t_m)]$,
- 2: Compute the (reduced) SVD of $\mathbf{Y}, \mathbf{Y} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{T}$
- 3: Define $\tilde{A}_{\mathbf{y}} := \mathbf{U}^* \mathbf{Y}' \mathbf{V} \mathbf{\Sigma}^{-1}$
- 4: Compute eigenvalues and eigenvectors of $\tilde{A}_{V}W = W\Lambda$.
- 5: Set $\Psi^{\text{DMD}} = \mathbf{Y}' \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{W}$

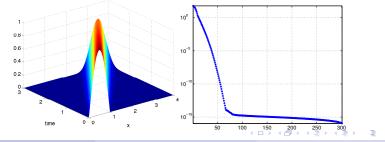
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Example: DMD-Galerkin approximation

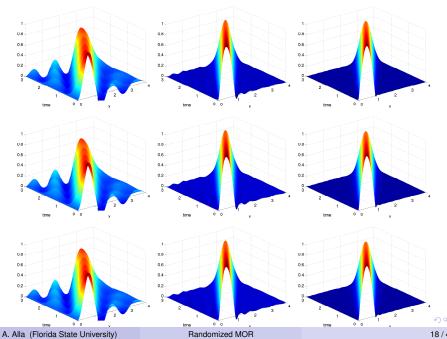
$$egin{aligned} y_t(x,t) + y_x(x,t) &= 0 & (x,t) \in [0,4] imes [0,3], \ y(x,0) &= y_0(x) & x \in [0,4], \ y(0,t) &= 0 = y(4,t) & t \in [0,T], \end{aligned}$$

where $y_0(x) = \sin(\pi x)$ if $0 \le x \le 1$ and 0 elsewhere.

DMD Ansatz: $\mathbf{y}(t) \approx \mathbf{\Psi}^{\text{DMD}} \mathbf{y}^{\text{DMD}}(t)$.



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Example: DMD-Galerkin approximation

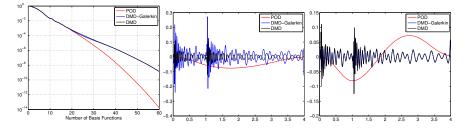


Figure: Error analysis with respect to the Frobenius norm (left), first mode (middle), second mode (right).

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POD-DMD method

MAIN IDEA

The evaluation of the nonlinearity is the **most expensive** part in model order reduction. We aim faster approximation of the nonlinear term.

We need snapshots!

- { $\mathbf{y}(t_0), \ldots, \mathbf{y}(t_m)$ }, to compute the POD basis functions,
- { $\mathbf{f}(t_0, \mathbf{y}(t_0)), \dots, \mathbf{f}(t_m, \mathbf{y}(t_m))$ } to compute the DMD basis functions.

POD-DMD method (NO EVALUATION OF THE NONLINEARITY) (A., Kutz, 2016)

$$\begin{cases} \mathbf{M}^{\ell} \dot{\mathbf{y}}^{\ell}(t) = \mathbf{A}^{\ell} \mathbf{y}^{\ell}(t) + (\mathbf{\Psi}^{\text{POD}})^{T} \mathbf{\Psi}^{\text{DMD}} diag(e^{\omega^{\text{DMD}}t}) \mathbf{b}, \\ \mathbf{y}^{\ell}(0) = \mathbf{y}_{\mathbf{0}}^{\ell}. \end{cases}$$

$$\begin{aligned} y_t - \theta \Delta y + \mu (y - y^3) &= 0 \qquad (x, t) \in \Omega \times [0, T], \\ y(x, 0) &= y_0(x) \quad x \in \Omega, \\ y(\cdot, t) &= 0 \qquad x \in \partial \Omega, t \in [0, T], \end{aligned}$$

Parameters:

$$\Omega = [0, 1] \times [0, 1], T = 3,$$

 $y_0(x) = 0.1$ if $0.1 \le x_1 x_2 \le 0.6$ and 0 elsewhere.

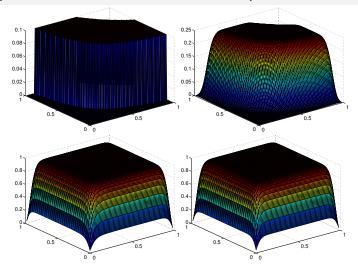


Figure: Solution at time $t = \{0, 0.1\}$ (top) and $t = \{1.5, 3\}$ (bottom)

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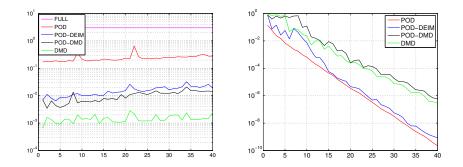


Figure: CPU-time online stage (left) and Relative Error wrt Frobenius norm. Number of POD modes and DEIM/DMD points are the same

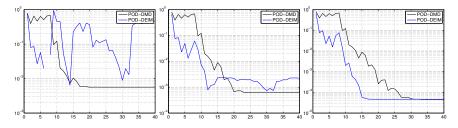
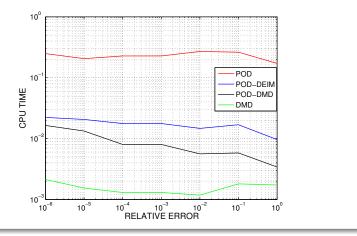


Figure: Relative Error for 5 POD basis functions (left), 10 POD basis (middle), 15 POD basis (right)

A fair comparison



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- Compressed Model Order Reduction Techniques
- Compressed POD
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Numerical Tests

Randomized SVD (Haiko, Martinsson, Tropp, 2011)

Computational Costs for $\mathbf{Y} \in \mathbb{R}^{m \times n}$:

- SVD: *O*(*mn*²)
- Randomized SVD: $O(mn\ell)$,

First Steps:

- Choose desired target rank $\ell \ll \{m, n\}$,
- Create a random (gaussian) sampling matrix $\Omega \in \mathbb{R}^{n \times \ell}$,
- Sampled matrix $\mathbf{X} \in \mathbb{R}^{n \times \ell}$ is computed as: $\mathbf{X} = \mathbf{Y} \Omega$.

Remarks:

- If the matrix Y has exact rank ℓ, then the sampled matrix X spans, with high probability, a basis for the column space.
- In practice, it is favorable to *slightly oversample* ℓ = ℓ + p, were p denotes the number of additional samples.

Randomized SVD

Second Steps: Obtain low-rank SVD from a compressed matrix

- Compute $\mathbf{X} = \mathbf{QR}, \mathbf{Q} \in \mathbb{R}^{n \times \ell}$ orthonormal,
- **Y** is projected into this low-dimensional space $\mathbf{B} \in \mathbb{R}^{\ell \times m}$:

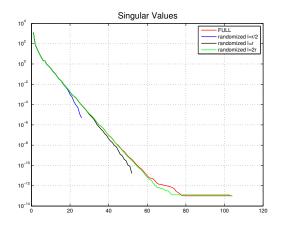
 $\mathbf{B} = \mathbf{Q}^{\mathsf{T}}\mathbf{Y},$

Compute the (cheap) SVD B = ÛΣV^T,
Set U = QÛ

Remark: if ℓ is large enough:

 $\begin{aligned} \mathbf{Y} &\approx \mathbf{Q} \mathbf{Q}^{\mathsf{T}} \mathbf{Y} \\ &\approx \mathbf{Q} \mathbf{B} \\ &\approx \mathbf{Q} \tilde{\boldsymbol{U}} \boldsymbol{\Sigma} \mathbf{V}^{\mathcal{T}} \\ &\approx \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{\mathcal{T}} \end{aligned}$

Randomized SVD



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How to use RSVD in model reduction?

Model order reduction techniques:

- are based on snapshots of the dynamical system.
- SVD decomposition of the snapshots matrix provides a low-dimension projector operator that allows one to obtain surrogate models.
- WARNING: SVD may be computationally expensive to reduced the offline cost of the method.

IDEA:

Compute basis functions from a few spatially incoherent measurements (not from the full set of measurements)

Compressed POD

Compressed POD

- we collect the snapshot set,
- we solve the POD optimization problem,
- optimality conditions provide eigenvalue problems,
- RSVD computes compressed POD basis functions in a significantly faster way.

Algorithm

- **Require:** Snapshot Matrix $\mathbf{Y} \in \mathbb{R}^{n \times m}$, ℓ number of basis functions., *p* number of measurements.
 - 1: Compute the Randomized SVD $[\mathbf{U}, \mathbf{\Sigma}, \mathbf{V}] = rsvd(\mathbf{Y}, p)$
 - 2: Set $\Psi_i = U_i$ for $i = 1, ..., \ell$.

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Compressed POD

Error (d rank of Y, p number of samples)

$$\mathbb{E}\left(\sum_{j=1}^{m} \alpha_j \left\| \mathbf{y}(t_j) - \sum_{i=1}^{\ell} \langle \mathbf{y}(t_j), \psi_i \rangle \psi_i \right\|^2\right) = \left(1 + \sqrt{\frac{\ell}{p-1}}\right) \sigma_{\ell+1}^2 + \frac{\sqrt{\ell+p}}{p} \sum_{j=\ell+1}^{d} \sigma_j^2.$$

Remarks:

- we consider the expectation value of the error
- error depends on the computation of the set of snapshots and *p*,
- if the singular values of **Y** decay rapidly a few samples drives the error close to the theoretically minimum value.
- if the singular values do not decay rapidly we can lose accuracy.
- we suppose Y ∈ ℝ^{m×n}, such that m ≈ n (eigenvalue problem is also expensive)

Compressive DMD (Brunton, Proctor, Kutz, 2015)

GOAL:

Compute DMD and apply as Galerkin projection method.

Algorithm

- **Require:** Snapshots $\{\mathbf{y}(t_0), \ldots, \mathbf{y}(t_m)\}, \mathbf{C} \in \mathbb{R}^{p \times m}$
 - 1: Set $\mathbf{Y} = [\mathbf{y}(t_0), \dots, \mathbf{y}(t_{m-1})]$ and $Y' = [\mathbf{y}(t_1), \dots, \mathbf{y}(t_m)]$,

2:
$$X = CY, X' = CY$$

- 3: Compute the SVD of **X**, $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{T}$
- 4: Define $\tilde{\mathbf{A}}_{\mathbf{x}} := \mathbf{U}^* \mathbf{Y}' \mathbf{V} \mathbf{\Sigma}^{-1}$
- 5: Compute eigenvalues and eigenvectors of $\tilde{A}_x W = W \Lambda$.
- 6: Set $\Psi^{\text{DMD}} = \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{W}$

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Numerical Tests

Test 1: Semi-Linear Parabolic Equation

$$\begin{aligned} y_t - \theta \Delta y + \mu (y - y^3) &= 0 \qquad (x, t) \in \Omega \times [0, T], \\ y(x, 0) &= y_0(x) \quad x \in \Omega, \\ y(\cdot, t) &= 0 \qquad x \in \partial \Omega, t \in [0, T], \end{aligned}$$

Parameters:

$$\Omega = [0, 1] \times [0, 1], T = 3,$$

 $y_0(x) = 0.1$ if $0.1 \le x_1 x_2 \le 0.6$ and 0 elsewhere.

Test 1: Semi-Linear Parabolic Equation

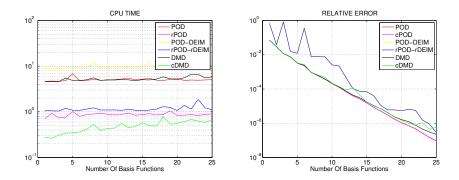


Figure: CPU-time online stage (left) and Relative Error wrt Frobenius norm. Number of POD modes and DEIM/DMD points are the same

Test 1: Semi-Linear Parabolic Equation

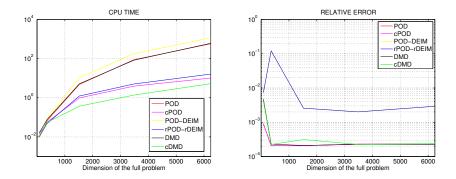


Figure: CPU-time online stage (left) and Relative Error wrt Frobenius norm. Number of POD modes and DEIM/DMD points are the same

Test 2: Parametric Elliptic Equation

$$\begin{aligned} -\Delta u(x,y) + s(u(x,y);\mu) &= f(x,y) \qquad (x,y) \in \Omega \\ u(x,y) &= 0 \qquad (x,y) \in \partial \Omega \end{aligned}$$

Parameters:

$$\Omega = [0, 1] \times [0, 1], \mu = (\mu_1, \mu_2) \in \mathcal{D} = [0.01, 10]^2$$

$$s(u,\mu) = \frac{\mu_1}{\mu_2}(e^{\mu_2 u} - 1), \quad f(x,y) = 100\sin(2\pi x)\sin(2\pi y).$$

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Numerical Tests

Test 2: Parametric Elliptic Equations

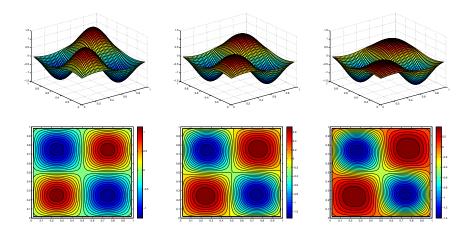


Figure: Test 2: Solution of problem for different parametric configurations (top) and countour lines (bottom)

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Test 2: Parametric Elliptic Equations

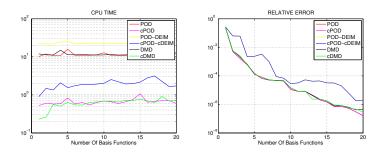


Figure: Test 2: CPU-time of the offline-online stages (left) and Relative Error in Frobenius norm (right). We compare the following methods: POD (red), cPOD (magenta), POD-DEIM (yellow), cPOD-cDEIM (blue, DMD (black), cDMD (green). Number of model are always the same for all the methods.

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Conclusions

- Model order reduction is a successful technique that projects nonlinear high dimensional dynamical systems and PDEs into low dimensional surrogate models
- Compressed (randomized) techniques are a promising approach to circumventing expensive offline stages in model order reduction.
- DMD works successfully in a Galerkin projection framework

Thank you for your attention

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