MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Rank-optimal approximations of higher-order tensors for low-dimensional space-time Galerkin approximations of parameter dependent dynamical systems

Manuel Baumann, Peter Benner, Jan Heiland

October 14, 2015

MoRePaS 2015, Trieste

1^{st} Ingredient

Generalized Measurements

$$Y_{gen} := \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix},$$

cf. $\quad Y_{POD} := \begin{bmatrix} y_1(t_1) & \dots & y_1(t_s) \\ \vdots & \ddots & \vdots \\ y_n(t_1) & \dots & y_n(t_s) \end{bmatrix}$

– the snapshot matrix known from POD.

2^{nd} Ingredient

POD in space and time

- A truncated SVD of $Y_{gen}M_S^{-1/2}$ gives an *optimal* basis for the
  $\rightarrow$ **space discretization**

- A truncated SVD of $M_S^{-1}Y_{gen}^{\mathsf{T}}M_y^{-1}$ gives an *optimal* basis for the
  $\rightarrow$ **time discretization**

3rd Ingredient

Parameter as third dimension

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \ddots & \vdots \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_0}$$

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & & \\ \vdots & & \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_1}$$

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & & \\ \vdots & & \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_2}$$

$\rightarrow$ Use higher-order SVD for optimal space, time, and parameter bases

Application

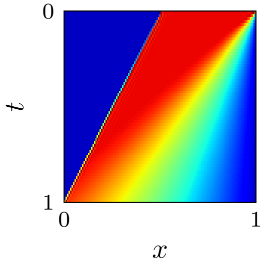
- consider Burgers equation

$$\partial_t z(t,x) + \partial_x\big(\frac{1}{2}z(t,x)^2 - \mu\partial_x z(t,x)\big) = 0,$$

- use a Finite Element discretization and a Runge Kutta scheme to assemble the generalized measurements (snapshots) for some parameter values
- use a higher order SVD to identify optimal low-dimensional bases for space and time discretizations
- use these bases for a low-dimensional space-time Galerkin discretization

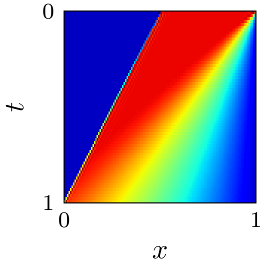
$\rightarrow$ the reduced model

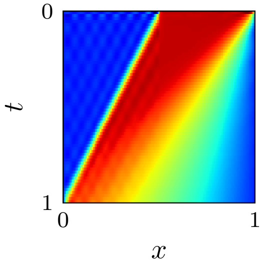
Some Pictures



- instead of conducting full simulation at a new parameter value

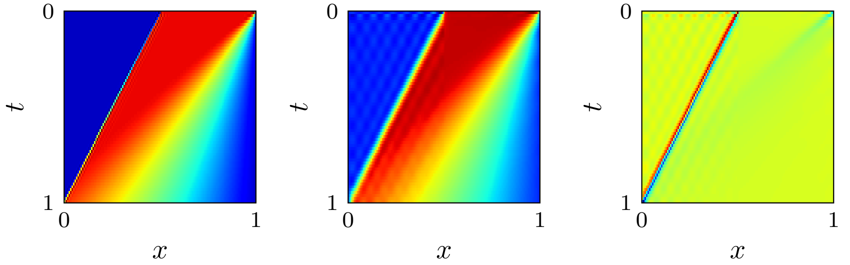
Some Pictures





- instead of conducting full simulation at a new parameter value
- solve a small nonlinear algebraic equation system

Some Pictures



- instead of conducting full simulation at a new parameter value
- solve a small nonlinear algebraic equation system
- and obtain satisfactory approximations

MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG

CSC COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

A generalized POD space-time Galerkin scheme for parameter dependent dynamical systems

Manuel Baumann[1], Peter Benner[2], Jan Heiland[2]

[1]Delft Institute of Applied Mathematics, Delft, The Netherlands
[2]Max Planck Institute for Dynamics of Complex Technical Systems, Computational Methods in Systems and Control Theory, Magdeburg, Germany

Exemplary Setup

We consider a parameter μ-dependent PDE

$$\dot{v}(t,x) = \mathcal{F}(v(t,x);\mu), \quad \text{on } (0,T)\times\Omega, \quad v(0,\cdot) = v_0 \in \mathcal{V}$$

and a finite element discretization with the *FEM* space $Y = \operatorname{span}\{\nu_1,\dots,\nu_q\}$ that leads to

$$M_Y\dot{y}(t) = f(y(t);\mu) \quad \text{on } (0,T), \quad y(0) = y(0) \in \mathbb{R}^q,$$

where M_Y is the mass matrix of Y.

Generalized Measurements and POD modes

Fix a $\mu = \mu_0$. Let $S = \operatorname{span}\{\psi_1,\dots,\psi_s\} \subset L^2(0,T)$ and consider the generalized measurement matrix

$$Y_{gen} := \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}, \quad \text{cf.} \quad Y_{POD} := \begin{bmatrix} y_1(t_1) & \dots & y_1(t_s) \\ \vdots & \ddots & \vdots \\ y_q(t_1) & \dots & y_q(t_s) \end{bmatrix}$$

– the snapshot matrix known from POD.

Generalized spatial POD modes

From the measurement matrix Y_{gen}, we can obtain an optimal (in the sense of Lemma 1) reduced basis $\{\hat{\nu}_1,\dots,\hat{\nu}_q\}$ for a space discretization via

$$\hat{\nu}_j := V_j^T \begin{bmatrix} \nu_1 \\ \vdots \\ \nu_q \end{bmatrix},$$

where V_j is the j-th leading singular vector of $Y_{gen}M_S^{-1/2}$.

Generalized time POD modes

With the same arguments we can obtain an optimal reduced basis $\{\hat{\psi}_1,\cdots,\hat{\psi}_s\}$ for the time discretization via

$$\hat{\psi}_k := U_k^T \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_s \end{bmatrix},$$

where V_j is the j-th leading singular vector of $M_S^{-1}Y_{gen}^T M_Y^{1/2}$.

Adding the parameter dependency

A discretization of the parameter domain with p degrees of freedom adds another dimension to the generalized measurement matrix turning it into a tensor $\mathbf{Y} \in \mathbb{R}^{q\times s\times p}$.

$$\begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_0} \quad \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_1} \quad \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_2}$$

Then, optimal bases are obtained via a *higher-order SVD*, i.e. via SVDs of tensor unfoldings with respect to the space dimension

$$\mathbf{Y}^{(\nu)} := \left[\begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_0} \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_1} \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_1,\psi_s\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_q,\psi_1\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_2} \right],$$

and with respect to the time dimension

$$\mathbf{Y}^{(\psi)} := \left[\begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_q,\psi_1\rangle_S \\ \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots \\ \langle y_1,\psi_s\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_0} \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_q,\psi_1\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_1,\psi_s\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_1} \begin{bmatrix} \langle y_1,\psi_1\rangle_S & \dots & \langle y_q,\psi_1\rangle_S \\ \vdots & \ddots & \vdots \\ \langle y_1,\psi_s\rangle_S & \dots & \langle y_q,\psi_s\rangle_S \end{bmatrix}_{\mu=\mu_2} \right],$$

respectively, cf. Lemma 1.

References

[1] M. Baumann, J. Heiland, and M. Schmidt, *Discrete input/output maps and their relation to proper orthogonal decomposition*, in Numerical Algebra, Matrix Theory, Differential-Algebraic Equations and Control Theory, P. Benner, M. Bollhfer, D. Kressner, C. Mehl, and T. Stykel, eds., Springer International Publishing, 2015, pp. 585–608.

[2] L. De Lathauwer, B. De Moor, and J. Vandewalle, *A multilinear singular value decomposition*, SIAM J. Matrix Anal. Appl., 21 (2000), pp. 1253–1278.

[3] S. Volkwein and S. Weiland, *An algorithm for Galerkin projections in both time and spatial coordinates*, Proc. 17th MTNS, (2006).

The basic theory

L^2 projections onto the measurements

Lemma 1 *The $L^2(0,T)$-orthogonal projection $\tilde{y}(t)$ of the state vector $y(t)$ onto the space spanned by the measurements is given as*

$$\tilde{y}(t) = Y_{gen}M_S^{-1}\psi(t),$$

where $\psi := [\psi_1,\dots,\psi_s]^T$, and where $[M_S]_{ij} := \langle\psi_i,\psi_j\rangle_S$.
The generalized POD basis can be computed via a (truncated) SVD of

$$Y_{gen}M_S^{-1/2}.$$

Higher order SVDs

For a third-order tensor like $\mathbf{Y} \in \mathbb{R}^{q\times s\times p}$ there exists a HOSVD

$$\mathbf{Y} = \mathbf{C} \times_1 U^{(\psi)} \times_2 U^{(\nu)} \times_3 U^{(\mu)}, \tag{1}$$

with the *core tensor* $\mathbf{C} \in \mathbb{R}^{q\times s\times p}$ satisfying some orthogonality properties and with unitary matrices $U^{(\psi)} \in \mathbb{R}^{s\times s}$, $U^{(\nu)} \in \mathbb{R}^{q\times q}$, and $U^{(\mu)} \in \mathbb{R}^{p\times p}$. Here, $\times_1,\dots,\times_3$ denote tensor-matrix multiplications. We define a *matrix unfolding* $\hat{\mathbf{Y}}^{(\psi)} \in \mathbb{R}^{s\times qp}$ of the tensor $\hat{\mathbf{Y}}$ via putting all elements belonging to $\psi_1,\psi_2,\dots,\psi_s$ into one respective row. Similarly, we define the unfoldings $\mathbf{Y}^{(\nu)} \in \mathbb{R}^{q\times ps}$ and $\mathbf{Y}^{(\mu)} \in \mathbb{R}^{p\times sq}$. Then we can calculate $U^{(\psi)}$, $U^{(\nu)}$ and $U^{(\mu)}$ in (1) by means of three SVDs like $\mathbf{Y}^{(\psi)} = U^{(\psi)}\Sigma^{(\psi)}(W^{(\psi)})^T$, with $\Sigma^{(\psi)}$ diagonal with entries $\sigma_1^{(\psi)} \geq \sigma_2^{(\psi)} \geq \dots \sigma_s^{(\psi)} \geq 0$ and $W^{(\psi)}$ column-wise orthonormal. The $\sigma_i^{(\psi)}$ are the *n-mode singular values* of the tensor $\mathbf{Y}$.

From these SVDs, we derive an approximation $\hat{\mathbf{Y}} \in \mathbb{R}^{q\times s\times p}$ of $\mathbf{Y}$ by discarding the smallest n-mode singular values. i.e. by setting the corresponding parts of $\mathbf{C}$ to zero. Then we have

$$\|\mathbf{Y} - \hat{\mathbf{Y}}\|_F^2 \leq \sum_{i=\hat{s}+1}^{s}\sigma_i^{(\psi)} + \sum_{k=\hat{q}+1}^{q}\sigma_k^{(\nu)} + \sum_{l=\hat{p}+1}^{p}\sigma_l^{(\mu)},$$

see [2].

Numerical tests

We consider the Burgers equation with the viscosity parameter μ

$$\partial_t z(t,x) + \partial_x\left(\frac{1}{2}z(t,x)^2 - \mu\partial_x z(t,x)\right) = 0, \tag{2}$$

with the spatial coordinate $x \in (0,1)$, the time variable $t \in (0,1]$, completed by zero Dirichlet boundary conditions and a step function as initial conditions as illustrated in Fig. 1(a).

Assembling the measurement matrices

The spatial discretization is done through piecewise linear finite elements on an equidistant grid of q nodes. For fixed choices of μ, the solution trajectories are obtained via a Runge-Kutta solver and then tested against the basis functions of a $S \in L^2(0,1)$ chosen as the span of s equidistantly distributed linear hat functions.

Test setups

We use the parameter values $\mu_0 = 10^{-2}$, $\mu_1 = 3\cdot10^{-3}$, $\mu_2 = 10^{-3}$ to set up the measurement tensor $\mathbf{Y}$ and to compute the space and time POD modes. These POD modes are then used in a space-time Galerkin scheme for Equation (2). Thus the solution of the reduced model is obtained via the solution of a nonlinear equation system with $s\times q$ degrees of freedom. As the error measure, we use the space time L^2 difference between a solution of the full and the reduced model.

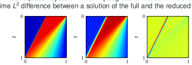


Figure 1: Burger setup for $\mu = 3\cdot10^{-3}$: The full solution, the reduced solution and the approximation error.

Space vs. time resolution We set the overall number of POD modes to $K := q + s$ and consider various space time resolutions $q = f\cdot K$ and $s = (1-f)\cdot K$, for $f \in [0.2, 0.8]$. Examining the time-space approximation vs. f, one sees that $f = 0.5$, e.g., $q = s =$ seems the best choice over the whole parameter range, cf. Figure 2(a).

Approximation error vs. parameter We investigate the error for reduced systems of order $K = \{20,30,40\}$ in a parameter range within and slightly outside the trainings set, see Figure 2(b).

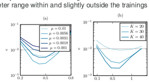


Figure 2: (a) the error for various numbers of f. (b): the error in the reduced model over the parameter range for various K.