Moving Frontiers in Model Reduction Using Numerical Linear Algebra

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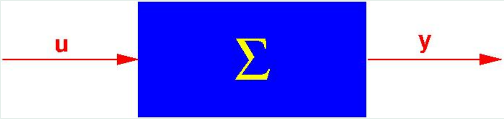
Outline

Dynamical Systems

$$\Sigma(p): \begin{cases} 0 &= f(t, x(t), \partial_t x(t), \partial_{tt} x(t), u(t), p), \quad x(t_0) = x_0, & \text{(a)} \\ y(t) &= g(t, x(t), \partial_t x(t), u(t), p) & \text{(b)} \end{cases}$$

with

- (generalized) states $x(t) \equiv x(t;p) \in \mathcal{X}$,
- inputs $u(t) \in \mathcal{U}$,
- outputs $y(t) \equiv y(t;p) \in \mathcal{Y}$, (b) is called output equation,
- $p \in \mathbb{R}^d$ is a parameter vector.



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(a) may represent

- system of ordinary differential equations (ODEs);
- system of differential-algebraic equations (DAEs);
- system of partial differential equations (PDEs);
- a mixture thereof.

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Introduction to Model Order Reduction

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Main idea

Replace differential equation by low-order one while preserving input-output behavior as well as important system invariants and physical properties!

Original System

$$\Sigma(p) : \begin{cases} E(x,p)\dot{x} = f(t,x,u,p), \\ y = g(t,x,u,p). \end{cases}$$

- states $x(t;p) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
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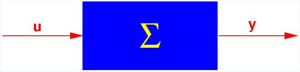

Reduced-Order System

$$\widehat{\Sigma}(p) : \begin{cases} \hat{E}(\hat{x},p)\dot{\hat{x}} = \widehat{f}(t,\hat{x},u,p), \\ \hat{y} = \widehat{g}(t,\hat{x},u,p). \end{cases}$$

- states $\hat{x}(t;p) \in \mathbb{R}^r$, $r \ll n$
- inputs $u(t) \in \mathbb{R}^m$,
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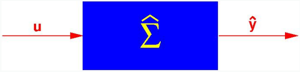

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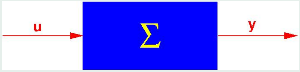

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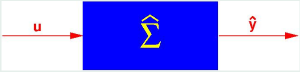

Large-Scale Linear Systems

Linear, time-invariant (LTI) systems

$$\Sigma : \begin{cases} \dot{x}(t) &= Ax + Bu, \qquad A \in \mathbb{R}^{n\times n}, \quad B \in \mathbb{R}^{n\times m}, \\ y(t) &= Cx + Du, \qquad C \in \mathbb{R}^{q\times n}, \quad D \in \mathbb{R}^{q\times m}. \end{cases}$$

(A, B, C, D) is a realization of Σ (nonunique).
Laplace transform: state-space → frequency domain yields transfer function of Σ:

$$Y(s) = \underbrace{\left(C(sI_n - A)^{-1}B + D\right)}_{=:G(s)} U(s).$$

Goal: find $\hat{A} \in \mathbb{R}^{r\times r}, \hat{B} \in \mathbb{R}^{r\times q}, \hat{C} \in \mathbb{R}^{q\times r}, D \in \mathbb{R}^{q\times m}$ such that

$$\begin{aligned} \|G - \hat{G}\| &= \|(C(sI_n - A)^{-1}B + D) - (\hat{C}(sI_r - \hat{A})^{-1}\hat{B} + \hat{D})\| < \mathrm{tol} \\ &\Rightarrow \|y - \hat{y}\| \leq \mathrm{tol}\|u\|. \end{aligned}$$

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Model order reduction by projection

Galerkin or Petrov-Galerkin-type projection of state-space onto low-dimensional subspace $\mathcal{V}$ along $\mathcal{W}$: assume $x \approx VW^T x =: \tilde{x}$, where

$$\mathrm{range}\,(V) = \mathcal{V}, \quad \mathrm{range}\,(W) = \mathcal{W}, \quad W^T V = I_r.$$

Then, with $\hat{x} = W^T x$, we obtain $x \approx V\hat{x}$ and

$$\hat{A} = W^T AV, \quad \hat{B} = W^T B, \quad \hat{C} = CV, \quad \hat{D} = D.$$

where $V_c W_c^T$ projects onto $\mathcal{V}_c$, the complement of $\mathcal{V}$.

Idea (for simplicity, $E = I_n$)

- A system Σ, realized by (A, B, C, D), is called balanced, if solutions P, Q of the Lyapunov equations

$$AP + PA^T + BB^T = 0, \qquad A^TQ + QA + C^TC = 0,$$

satisfy: $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

- $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- Compute balanced realization of the system via state-space transformation

$$\mathcal{T} : (A, B, C, D) \mapsto (TAT^{-1}, TB, CT^{-1}, D) = \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix}, D \right)$$

- Truncation $\rightsquigarrow (\hat{A}, \hat{B}, \hat{C}, \hat{D}) = (A_{11}, B_1, C_1, D)$.

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Motivation:

HSV are system invariants: they are preserved under $\mathcal{T}$ and determine the energy transfer given by the Hankel map

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In balanced coordinates ... energy transfer from u_- to y_+:

$$E := \sup_{\substack{u \in L_2(-\infty,0] \\ x(0)=x_0}} \frac{\int_0^\infty y(t)^T y(t)\, dt}{\int_{-\infty}^0 u(t)^T u(t)\, dt} = \frac{1}{\|x_0\|_2} \sum_{j=1}^n \sigma_j^2 x_{0,j}^2$$

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$\Longrightarrow$ Truncate states corresponding to “small” HSVs

$\Longrightarrow$ analogy to best approximation via SVD, therefore balancing-related methods are sometimes called SVD methods.

Implementation: SR Method

1. Compute (Cholesky) factors of the solutions of the Lyapunov equations,
$$P = S^T S, \quad Q = R^T R.$$
2. Compute SVD
$$SR^T = [\, U_1,\ U_2 \,] \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}.$$
3. Set
$$W = R^T V_1 \Sigma_1^{-1/2}, \qquad V = S^T U_1 \Sigma_1^{-1/2}.$$
4. Reduced model is $(W^T AV, W^T B, CV, D)$.

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Properties:

- Reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$.
- Adaptive choice of r via computable error bound:

$$\|y - \hat{y}\|_2 \leq \left(2 \sum\nolimits_{k=r+1}^{n} \sigma_k\right) \|u\|_2.$$

- General misconception:
  complexity $\mathcal{O}(n^3)$ – true for several implementations (e.g., MATLAB, SLICOT, MorLAB).

But: recent developments in Numerical Linear Algebra yield matrix equation solvers with sparse linear systems complexity!

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Solving Large-Scale Lyapunov Equations

General form for $A, W = W^T \in \mathbb{R}^{n\times n}$ given and $P \in \mathbb{R}^{n\times n}$ unknown:

$$0 \quad = \quad \mathcal{L}(Q) := A^T Q + QA + W.$$

In large scale applications from semi-discretized control problems for PDEs,

- $n = 10^3 - 10^6$ ($\Longrightarrow$ $10^6 - 10^{12}$ unknowns!),
- A has sparse representation ($A = -M^{-1}K$ for FEM),
- W low-rank with $W \in \{BB^T, C^TC\}$, where $B \in \mathbb{R}^{n\times m}$, $m \ll n$, $\quad C \in \mathbb{R}^{q\times n}$, $p \ll n$.
- Standard (Schur decomposition-based) $\mathcal{O}(n^3)$ methods are not applicable!

- For $A \in \mathbb{R}^{n \times n}$ stable, $B \in \mathbb{R}^{n \times m}$ ($w \ll n$), consider Lyapunov equation

$$AX + XA^T = -BB^T.$$

- ADI Iteration: [Wachspress 1988]

$$\begin{aligned}(A + p_k I)X_{(k-1)/2} &= -BB^T - X_{k-1}(A^T - p_k I)\\ (A + \overline{p_k} I){X_k}^T &= -BB^T - X_{(k-1)/2}(A^T - \overline{p_k} I)\end{aligned}$$

with parameters $p_k \in \mathbb{C}^-$ and $p_{k+1} = \overline{p_k}$ if $p_k \notin \mathbb{R}$.

- For $X_0 = 0$ and proper choice of p_k: $\lim_{k \to \infty} X_k = X$ (super)linearly.
- Re-formulation using $X_k = Y_k Y_k^T$ yields iteration for Y_k...

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Factored ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$.

Setting $X_k = Y_k Y_k^T$, some algebraic manipulations $\Longrightarrow$

Algorithm [Penzl '97/'00, Li/White '99/'02, B. 04, B./Li/Penzl '99/'08]

$$V_1 \leftarrow \sqrt{-2\mathrm{Re}\,(p_1)}(A + p_1 I)^{-1}B, \qquad Y_1 \leftarrow V_1$$

FOR $j = 2, 3, \ldots$

$$V_k \leftarrow \sqrt{\frac{\mathrm{Re}\,(p_k)}{\mathrm{Re}\,(p_{k-1})}}\left(V_{k-1} - (p_k + \overline{p_{k-1}})(A + p_k I)^{-1}V_{k-1}\right)$$

$$Y_k \leftarrow \left[\begin{array}{cc} Y_{k-1} & V_k \end{array}\right]$$

$$Y_k \leftarrow \mathrm{rrlq}(Y_k, \tau) \qquad \text{% column compression}$$

At convergence, $Y_{k_{\max}} Y_{k_{\max}}^T \approx X$, where

$$Y_{k_{\max}} = \left[\begin{array}{ccc} V_1 & \ldots & V_{k_{\max}} \end{array}\right], \quad V_k = \Big[\;\Big] \in \mathbb{C}^{n \times m}.$$

Note: Implementation in real arithmetic possible by combining two steps.

Factored Galerkin-ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$

Projection-based methods for Lyapunov equations with $A + A^T < 0$:

1. Compute orthonormal basis $\mathrm{range}(Z)$, $Z \in \mathbb{R}^{n \times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, $\dim \mathcal{Z} = r$.
2. Set $\hat{A} := Z^T A Z$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
4. Use $X \approx Z\hat{X}Z^T$.

Examples:

- Krylov subspace methods, i.e., for $m = 1$:

$$\mathcal{Z} = \mathcal{K}(A, B, r) = \mathrm{span}\{B, AB, A^2B, \ldots, A^{r-1}B\}$$

[Jaimoukha/Kasenally '94, Jbilou '02–'08].

- K-PIK [Simoncini '07],

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Examples:

- ADI subspace [B./R.-C. Li/Truhar '08]:

$$\mathcal{Z} = \mathrm{colspan}\left[\ V_1, \quad \ldots, \quad V_r\ \right].$$

Note: ADI subspace is rational Krylov subspace [J.-R. Li/White '02].

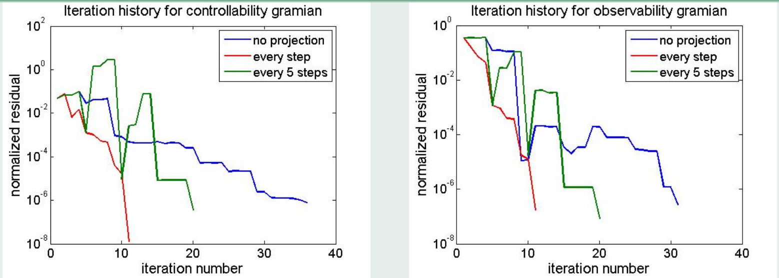
Factored Galerkin-ADI Iteration

Numerical example

FEM semi-discretized control problem for parabolic PDE:

- optimal cooling of rail profiles,
- $n = 20,209, \ m = 7, \ p = 6.$

Good ADI shifts



CPU times: 80s (projection every 5th ADI step) vs. 94s (no projection).

Computations by Jens Saak.

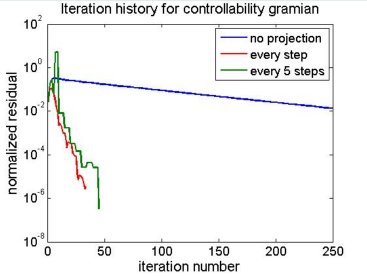
Factored Galerkin-ADI Iteration

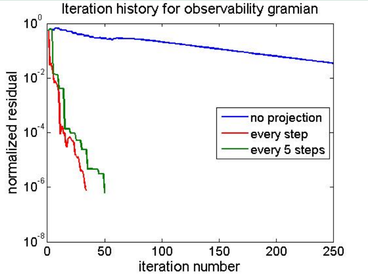
Numerical example

FEM semi-discretized control problem for parabolic PDE:

- optimal cooling of rail profiles,
- $n = 20,209$, $m = 7$, $p = 6$.

Bad ADI shifts





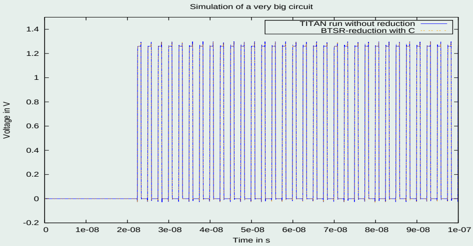
CPU times: 368s (projection every 5th ADI step) vs. 1207s (no projection).

Computations by Jens Saak.

Application in Microelectronics: VLSI Design

Balanced Truncation was implemented in circuit simulator TITAN (Qimonda AG, Infineon Technologies).

TITAN simulation results for industrial circuit:
14,677 resistors, 15,404 capacitors, 14 voltage sources, 4,800 MOSFETs.
14 linear subcircuits of varying order extracted and reduced.



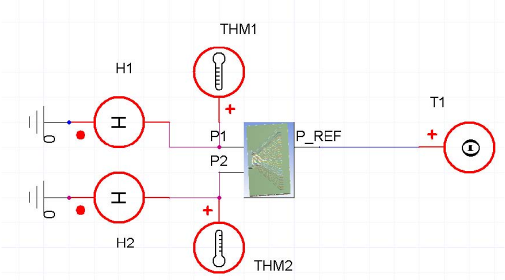
[GÜNZEL, Diplomarbeit '08; B. '08]

Supported by BMBF network *SyreNe* (includes Qimonda, Infineon, NEC), EU Marie Curie grant *O-Moore-Nice!* (includes NXP), industry grants.

Balanced Truncation

Sample applications: electro-thermic simulation of integrated circuit (IC) [Source: Evgenii Rudnyi, CADFEM GmbH]

- Test circuit in Simplorer® with 2 transistors.
- Conservative thermic sub-system in Simplorer: voltage ⇝ heat, current ⇝ heat flux.
- Original model: $n = 270.593$, $m = p = 2$ ⇒
  Computing times (CMESS on Intel Xeon dualcore 3GHz, 1 Thread):
  - Solution of Lyapunov equations: ≈ 22*min*.
    (420/356 columns in solution factors),
  - Computation of ROMs: 44sec. ($r = 20$) — 49sec. ($r = 70$).
  - Bode diagram (MATLAB on Intel Core i7, 2,67GHz, 12GB):
    using original system 7.5h, with reduced system < 1min.



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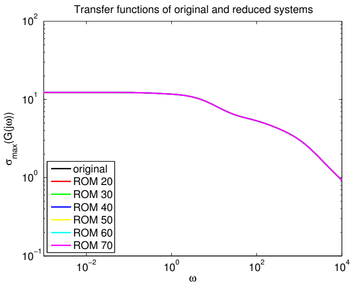
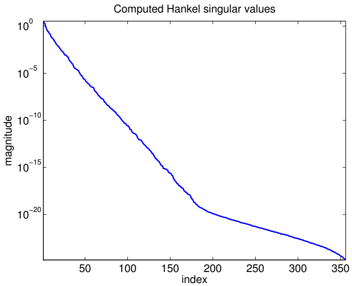
Bode Diagram (Amplitude)



Hankel Singular Values



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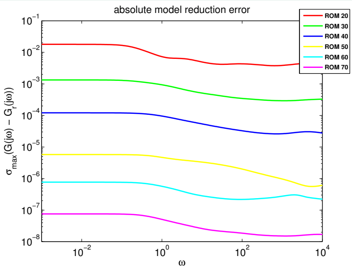
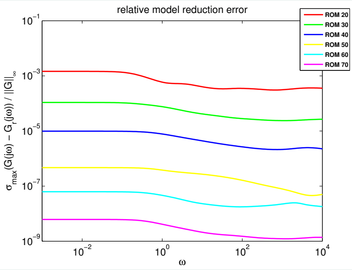
Absolute Error



Relative Error



Bilinear control system of the form

$$\dot{x} = Ax + \sum_{j=1}^{k} N_j x u_j + Bu, \quad y = Cx,$$

arise, e.g., in

- control of PDEs with mixed boundary conditions,
- approximation of nonlinear systems using Carleman bilinearization.

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- approximation of nonlinear systems using Carleman bilinearization.

The solutions of the generalized Lyapunov equations

$$AP + PA^T + \sum_{j=1}^{k} N_j P N_j^T = -BB^T, \quad A^T Q + QA + \sum_{j=1}^{k} N_j^T Q N_j = -C^T C$$

possess certain properties of the reachability and observability Gramians of linear systems, generalized Hankel singular values can be defined, and model reduction analogous to Balanced Truncation can be based upon them [Al-Baiyat/Bettaye '93].

Energy functionals [Gray/Mesko, IFAC 1998]

$$E_c(x_0) = \min_{\substack{u\in L^2(-\infty,0)\\ x(-\infty,u)=0,x(0,u)=x_0}} \|u\|_{L^2}^2 \quad \overset{?}{\geq} \quad x_0^T P^{-1} x_0$$

$$E_o(x_0) = \max_{u\in L^2(0,\infty),\|u\|_{L^2}\leq 1} \|y(\cdot,x_0,u)\|_{L^2}^2 \quad \overset{?}{\leq} \quad x_0^T Q x_0$$

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$$E_o(x_0) = \max_{u \in L^2(0,\infty),\, \|u\|_{L^2} \leq 1} \|y(\cdot, x_0, u)\|_{L^2}^2 \overset{?}{\leq} x_0^T Q x_0$$

$$\left.\begin{matrix} x_0^T P x_0 \\ x_0^T Q x_0 \end{matrix}\right\} \text{small} \overset{?}{\Rightarrow} \text{state } x_0 \text{ hard} \left\{\begin{matrix} \text{to reach} \\ \text{to observe} \end{matrix}\right.$$

Theorem ($k = 1$ for simplicity)

Let $AP + PA^T + NPN^T + BB^T = 0$.

If $P \geq 0$ then $\operatorname{im} P$ is invariant w.r.t. $\dot{x} = Ax + Nxu + Bu$.

In particular: ker P is unreachable from 0.

Analogously for (un)observability.

Theorem ($k=1$ for simplicity)

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If $P \geq 0$ then im P is invariant w.r.t. $\dot{x} = Ax + Nxu + Bu$.
In particular: ker P is unreachable from 0.

Proof: Let $v \in \ker P$. Then $\quad 0 = v^T \left(NPN^T + BB^T\right) v$

- $\Rightarrow$ $B^T v = 0$ and $PN^T v = 0$
- $\Rightarrow$ $N^T \ker P \subset \ker P \subset \ker B^T$
- $\Rightarrow$ $PA^T v = 0$, i.e. $A^T \ker P \subset \ker P$.

If $x(t) \in \operatorname{im} P = (\ker P)^\perp$ for some t, then

$$\dot{x}(t)^T v = x(t)^T \underbrace{A^T v}_{\in \ker P} + u(t) x(t)^T \underbrace{N^T v}_{\in \ker P} + u(t)^T \underbrace{B^T v}_{=0} = 0$$

Hence $\dot{x}(t) \in \operatorname{im} P$, implying invariance.

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Let $AP + PA^T + NPN^T + BB^T = 0$.

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In particular: $\ker P$ is unreachable from 0.

Consequence:

If $\|Px_1\|$ is small, then x_1 should be almost unreachable.

How can this be quantified?

Given factorizations $P = LL^T$, $L^T QL = U\Sigma^2 U^T$,
the transformation $T = LU\Sigma^{-1/2}$ is balancing: the equivalent system

$$\widetilde{A} = T^{-1}AT\ , \quad \widetilde{N}_j = T^{-1}N_jT\ , \quad \widetilde{B} = T^{-1}B\ , \quad \widetilde{C} = CT\ .$$

satisfies $\widetilde{P} = \widetilde{Q} = \mathrm{diag}\,(\sigma_1, \dots, \sigma_n)$.
If the small Hankel singular values $\sigma_{r+1}, \dots, \sigma_n$ vanish: state negligible!(?)

Projection on $\mathbb{R}^r$, $(r \overset{!}{\ll} n)$.

Partition: $T = [T_1, T_2]$, $T^{-1} = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix}$.

Truncation:
$$\begin{aligned} \widetilde{A}^{(r)} &= S_1AT_1 & \widetilde{N}_j^{(r)} &= S_1N_jT_1 \\ \widetilde{B}^{(r)} &= S_1B & \widetilde{C}^{(r)} &= CT_1 \end{aligned}$$

Reduced model:

$$\dot{\tilde{x}}_r = \widetilde{A}^{(r)}\tilde{x}_r + \sum_{j=1}^{m} \widetilde{N}_j^{(r)}\tilde{x}_r u_j + \widetilde{B}^{(r)}u \qquad \tilde{y} = \widetilde{C}^{(r)}\tilde{x}_r\ .$$

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Nonlinear control system (SISO):

$$\dot{v}(t) = f\left(v(t)\right) + g\left(v(t)\right) u(t),$$
$$y(t) = c^T v(t), \quad v(0) = 0, \; f(0) = 0$$

where $f, g : \mathbb{R}^N \to \mathbb{R}^N$ are nonlinear and analytic in v.

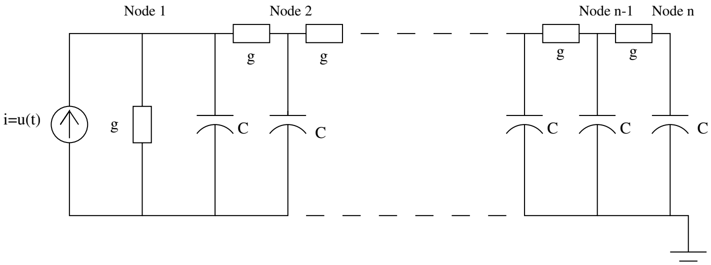
$$f(v) \approx A_1 v + \frac{1}{2} A_2 v \otimes v, \quad g(v) \approx B_0 + B_1 v$$

with $B_0 \in \mathbb{R}^N, \; A_1, B_1 \in \mathbb{R}^{N \times N}, \; A_2 \in \mathbb{R}^{N \times N^2}$,

$$x = \begin{bmatrix} v \\ v \otimes v \end{bmatrix}, \; A = \begin{bmatrix} A_1 & \frac{1}{2} A_2 \\ 0 & A_1 \otimes I + I \otimes A_1 \end{bmatrix},$$

$$N = \begin{bmatrix} B_1 & 0 \\ B_0 \otimes I + I \otimes B_0 & 0 \end{bmatrix}, \; B = \begin{bmatrix} B_0 \\ 0 \end{bmatrix}, \; C = \begin{bmatrix} c^T & 0 \end{bmatrix}.$$

- Nonlinear RC circuit [Chen/White '00, Bai/Skoogh '06].
- Carleman bilinearization $\rightsquigarrow$ bilinear system with $n = 2,550$, $k = 1$.
- Compare bilinear Balanced Truncation with Krylov subspace method taken from [Bai/Skoogh '06].



$g(v) = \exp(40v) + v - 1,\ u(t) = \cos(t)$

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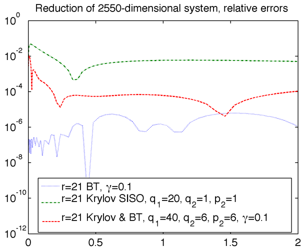
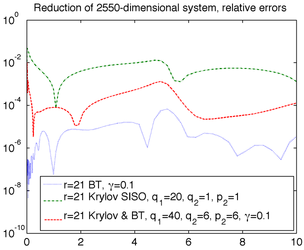


$u(t) = e^{-t}$



$u(t) = (\cos \frac{2\pi t}{10} + 1)/2$

[B./Damm '09]

Numerical Solution of Bilinear Lyapunov Equations

Bilinear balanced truncation both require solutions of

Bilinear Lyapunov Equation

$$AXE^T + EXA^T + NXN^T + BB^T = 0.$$

Naive attempt based on fixed-point iteration

$$X_{j+1} = -N^{-1}\left(AXE^T + EXA^T + BB^T\right)N^{-T}$$

not applicable as N often singular.

Current best available method: ADI-preconditioned Krylov subspace methods [Damm '08], using

$$\mathcal{L}_s^{-1}\left(\mathcal{L}(X) + \mathcal{P}(X) + BB^T\right) = 0,$$

where

- $\mathcal{L} : X \to AXE^T + EXA^T$ is the associated Lyapunov operator,
- $\mathcal{P} : X \to NXN^T$ is a positive operator,
- $\mathcal{L}_s^{-1}$ is a preconditioner, obtained by running a fixed (low) number s of ADI steps on the Lyapunov part.

Problem: equations beyond $n = 1,000$ hardly solvable as no version computing low-rank approximations to X is known yet!

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Computation of reduced-order model by projection

Given a linear (descriptor) system $E\dot{x} = Ax + Bu,\ y = Cx$ with transfer function $G(s) = C(sE - A)^{-1}B$, a reduced-order model is obtained using projection matrices $V, W \in \mathbb{R}^{n \times r}$ with $W^T V = I_r$ ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector) by computing

$$\hat{E} = W^T EV,\ \hat{A} = W^T AV,\ \hat{B} = W^T B,\ \hat{C} = CV.$$

Petrov-Galerkin-type (two-sided) projection: $W \neq V$,

Galerkin-type (one-sided) projection: $W = V$.

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Rational Interpolation/Moment-Matching

Choose V, W such that

$$G(s_j) = \hat{G}(s_j), \quad j = 1, \ldots, k,$$

and

$$\frac{d^i}{ds^i} G(s_j) = \frac{d^i}{ds^i} \hat{G}(s_j), \quad i = 1, \ldots, K_j, \quad j = 1, \ldots, k.$$

Theorem (simplified) [Grimme '97, Villemagne/Skelton '87]

If

$$\begin{aligned} \operatorname{span}\left\{(s_1 E - A)^{-1}B, \ldots, (s_k E - A)^{-1}B\right\} &\subset \operatorname{Ran}(V), \\ \operatorname{span}\left\{(s_1 E - A)^{-T}C^T, \ldots, (s_k E - A)^{-T}C^T\right\} &\subset \operatorname{Ran}(W), \end{aligned}$$

then

$$G(s_j) = \hat{G}(s_j), \quad \frac{d}{ds}G(s_j) = \frac{d}{ds}\hat{G}(s_j), \quad \text{for } j = 1, \ldots, k.$$

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then

$$G(s_j)=\hat{G}(s_j),\quad \frac{d}{ds}G(s_j)=\frac{d}{ds}\hat{G}(s_j),\quad \text{for } j=1,\ldots,k.$$

Remarks:

computation of V, W from rational Krylov subspaces, e.g.,

- dual rational Arnoldi/Lanczos [Grimme '97],
- Iterative Rational Krylov-Algo. [Antoulas/Beattie/Gugercin '07].

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Remarks:

using Galerkin/one-sided projection yields $G(s_j) = \hat{G}(s_j)$, but in general

$$\frac{d}{ds}G(s_j) \neq \frac{d}{ds}\hat{G}(s_j).$$

Theorem (simplified) [Grimme '97, Villemagne/Skelton '87]

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then

$$G(s_j) = \hat{G}(s_j), \quad \frac{d}{ds}G(s_j) = \frac{d}{ds}\hat{G}(s_j), \quad \text{for } j = 1, \ldots, k.$$

Remarks:

$k = 1$, standard Krylov subspace(s) of dimension $K \rightsquigarrow$ moment-matching methods/Padé approximation,

$$\frac{d^i}{ds^i}G(s_1) = \frac{d^i}{ds^i}\hat{G}(s_1), \quad i = 0, \ldots, K-1(+K).$$

Recall: bilinear system

$$\dot{x} = Ax + Nxu + Bu, \quad y = Cx,$$

For I/O-behavior, generalize concepts for linear systems by Volterra series

$$y(t) = \sum_{k=1}^{\infty} \int_0^t \int_0^{t_1} \dots \int_0^{t_{k-1}} h(t_1, t_2, \dots, t_k) u(t - t_1 - \dots - t_k) \cdots u(t - t_k) dt_k \dots dt_1$$

$$h(t_1, t_2, \dots, t_k) = c^T e^{At_k} N \cdots e^{At_2} N e^{At_1} b$$

$\rightarrow$ degree-k kernel

$\Updownarrow$ multivariable Laplace transform

$$H(s_1, s_2, \dots, s_k) = c^T (s_k I - A)^{-1} N \cdots (s_2 I - A)^{-1} N (s_1 I - A)^{-1} b$$

$\rightarrow$ k-th transfer function

$s_i = \xi_i^{-1}$:

$$\begin{aligned} H(s_1,\ldots,s_k) &= c^T(s_kI-A)^{-1}N\cdots(s_2I-A)^{-1}N(s_1I-A)^{-1}b \\ &= c^T(\xi_k^{-1}I-A)^{-1}N\cdots(\xi_2^{-1}I-A)^{-1}N(\xi_1^{-1}I-A)^{-1}b \\ &= c^T\xi_k(I-\xi_kA)^{-1}N\cdots\xi_2(I-\xi_2A)^{-1}N\xi_1(I-\xi_1A)^{-1}b \end{aligned}$$

for $\xi_i \to 0$ ($s_i \to \infty$) use Neumann expansion:

$$(I-\xi_iA)^{-1} = \sum_{l_i=0}^{\infty} \xi_i^{l_i}A^{l_i}$$

$$H(s_1,\ldots,s_k) = \sum_{l_k=1}^{\infty}\cdots\sum_{l_1=1}^{\infty} m(l_1,\ldots,l_k)s_1^{-l_1}\cdots s_k^{-l_k}$$

$$m(l_1,\ldots,l_k) = c^TA^{l_k-1}N\cdots A^{l_2-1}NA^{l_1-1}b$$

$\rightarrow$ high frequency multimoments

$s_i = \xi_i^{-1}$:

$$
\begin{aligned}
H(s_1, \ldots, s_k) &= c^T (s_k I - A)^{-1} N \cdots (s_2 I - A)^{-1} N (s_1 I - A)^{-1} b \\
&= c^T (\xi_k^{-1} I - A)^{-1} N \cdots (\xi_2^{-1} I - A)^{-1} N (\xi_1^{-1} I - A)^{-1} b \\
&= c^T \xi_k (I - \xi_k A)^{-1} N \cdots \xi_2 (I - \xi_2 A)^{-1} N \xi_1 (I - \xi_1 A)^{-1} b
\end{aligned}
$$

for $\xi_i \to 0$ ($s_i \to \infty$) use Neumann expansion:

$$
(I - \xi_i A)^{-1} = \sum_{l_i = 0}^{\infty} \xi_i^{l_i} A^{l_i}
$$

$$m(l_1) = c^T A^{l_1 - 1} b$$ Markov parameters

$$
\begin{aligned}
m(l_1, l_2) &= c^T A^{l_2 - 1} N A^{l_1 - 1} b \\
m(l_1, l_2, l_3) &= c^T A^{l_3 - 1} N A^{l_2 - 1} N A^{l_1 - 1} b \\
&\vdots
\end{aligned}
$$

Similar for $s_i \to \sigma_i \in \mathbb{C}$:

$$H(s_1, \ldots, s_k) = \sum_{l_k=1}^{\infty} \ldots \sum_{l_1=1}^{\infty} m(l_1, \ldots, l_k) s_1^{l_1-1} \cdots s_k^{l_k-1}$$

$$m(l_1, \ldots, l_k) = (-1)^k c^T (A - \sigma_k I)^{-l_k} N \cdots (A - \sigma_2 I)^{-l_2} N (A - \sigma_1 I)^{-l_1} b$$

special case $\sigma_i = 0$:

$$m(l_1, \ldots, l_k) = (-1)^k c^T A^{-l_k} N \cdots A^{-l_2} N A^{-l_1} b$$

$\to$ low frequency multimoments

Matching multi-moments:

- multimoments locally characterize input-output behaviour
- construct reduced system Σ that matches q^k multimoments of the first r subsystems of the original system

$$m(l_1, \ldots, l_k) \stackrel{!}{=} \hat{m}(l_1, \ldots, l_k), \quad k = 1, \ldots, r, \quad l_j = 1, \ldots, q$$

Construct reduced system by Petrov-Galerkin projection:

$$\hat{\Sigma} : \begin{cases} \dot{\hat{x}}(t) = \underbrace{W^T A V}_{\hat{A}} \hat{x}(t) + \underbrace{W^T N V}_{\hat{N}} \hat{x}(t) u(t) + \underbrace{W^T b}_{\hat{b}} u(t), \\ \hat{y}(t) = \underbrace{c^T V}_{\hat{c}^T} \hat{x}(t), \quad x(t) \approx V \hat{x}(t) \end{cases}$$

with $V, W \in \mathbb{R}^{n \times k}$, $W^T V = I$.

Use sequence of nested Krylov subspaces

$$\mathcal{K}_q(A, b) = span\left\{ b, Ab, \ldots, A^{q-1} b \right\}, \qquad A \in \mathbb{R}^{n \times n}, \ b \in \mathbb{R}^n$$

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Theorem

Let a bilinear SISO system Σ be given.

- $span\{V^{(1)}\} = \mathcal{K}_q(A, b)$,
- $span\{V^{(k)}\} = \mathcal{K}_q(A, NV^{(k-1)}), \quad k = 2, \ldots, r$
- $span\{V\} = span\left\{\bigcup_{k=1}^{r} span\{V^{(k)}\}\right\}$
- W arbitrary left inverse of V

$\rightarrow m(l_1, \ldots, l_k) = \hat{m}(l_1, \ldots, l_k),\ k = 1, \ldots, r,\ l_j = 1, \ldots, q$

Example:

$V^{(1)} = \mathcal{K}_{10}(A, b), \quad V^{(2)} = \mathcal{K}_4(A, NV^{(1)}_{[4]})$

$$c^T A^{l_1-1} b = \hat{c}^T \hat{A}^{l_1-1} \hat{b}, \qquad l_1 = 1, \ldots, 10$$

$$c^T A^{l_2-1} N A^{l_1-1} b = \hat{c}^T \hat{A}^{l_2-1} \hat{N} \hat{A}^{l_1-1} \hat{b}, \qquad l_1, l_2 = 1, \ldots, 4$$

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Multimoment-matching for different expansion points to cover broader frequency range:

Theorem

Let a bilinear SISO system Σ be given.

- $span\{V^{(1)}\} = \mathcal{K}_q((A-\sigma_1 I)^{-1}, (A-\sigma_1 I)^{-1}b)$,
- $span\{V^{(k)}\} = \mathcal{K}_q((A-\sigma_k I)^{-1}, (A-\sigma_k I)^{-1}NV^{(k-1)})$,
- $span\{V\} = span\left\{\bigcup_{k=1}^{r} span\{V^{(k)}\}\right\}$
- W arbitrary left inverse of V

$$\rightarrow m(l_1,\ldots,l_k) = \hat{m}(l_1,\ldots,l_k),\ k=1,\ldots,r,\ l_j = 1,\ldots,q$$

Special cases:

- $V^T V = I,\ W^T = V^T$

  $\rightarrow$ orthogonal projection

  $\rightarrow$ first approach, proposed by [Phillips '03], see also [B./Feng '07] for multi-moment matching proof.

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- $span\{V\} = span\left\{\bigcup_{k=1}^{r} span\{V^{(k)}\}\right\}$
- W arbitrary left inverse of V

$$\rightarrow m(l_1,\ldots,l_k) = \hat{m}(l_1,\ldots,l_k),\ k=1,\ldots,r,\ l_j=1,\ldots,q$$

Special cases:

- $V^TV = I,\ W^T = (V^TA^{-1}V)^{-1}V^TA^{-1}$

  $\rightarrow$ multiply state equation by A^{-1}, proposed by [Skoogh/Bai '06]

  $\rightarrow$ seems to yield better results for bilinearized systems.

Better choices for projection matrix W?

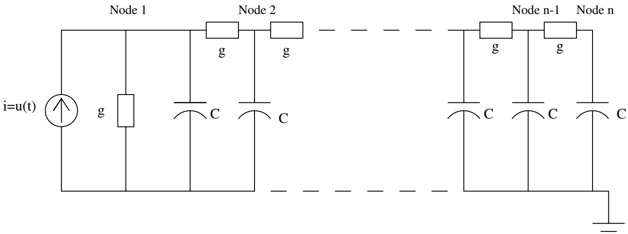
- $span\{W^{(1)}\} = \mathcal{K}_q(A^T, c)$,
- $span\{W^{(k)}\} = \mathcal{K}_q(A^T, N^T W^{(k-1)}), \quad k = 2, \dots, r$
- $span\{W\} = span\left\{\bigcup_{k=1}^{r} span\{W^{(k)}\}\right\}$

$$V^{(1)} = \mathcal{K}_6(A, b), \;\; W^{(1)} = \mathcal{K}_6(A^T, c)$$

$$m(l_1) = \hat{m}(l_1), l_1 = 1, \dots, 12, \;\; m(l_1, l_2) = \hat{m}(l_1, l_2), l_1, l_2 = 1, \dots, 6$$

$\longrightarrow$ significantly more multimoments are preserved.

$\longrightarrow$ Number of matched subsystems automatically doubles.



$v(t)$: node voltages $v_1(t), \ldots, v_N(t)$, $\quad N = 50 \rightarrow dim\ \Sigma = 2550$

$u(t)$: independent current source, $C = 1$, $g(v) = exp(40v) + v - 1$

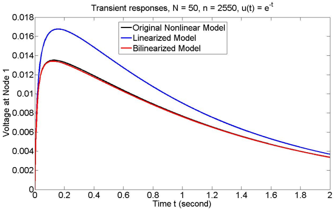
$y(t)$: voltage between node 1 and ground

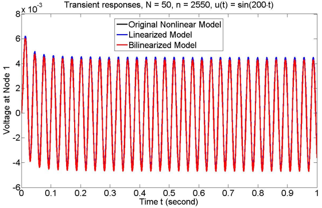
Projection subspaces:

- High frequency multimoments (∞):
  $V^{(1)} = \mathcal{K}_{19}(A, b)$,
  $V^{(2)} = \mathcal{K}_4(A, NV^{(1)}_{[4]})$
  $V = V^{(1)} \cup V^{(2)}, \quad V^T V = I$
- Low frequency multimoments ($\sigma_j = 0$):
  $V^{(1)} = \mathcal{K}_{19}(A^{-1}, A^{-1}b)$,
  $V^{(2)} = \mathcal{K}_4(A^{-1}, A^{-1}NV^{(1)}_{[4]})$
  $V = V^{(1)} \cup V^{(2)}, \quad V^T V = I$
- Multiple interpolation points ($\sigma_j = 0, 1, 10, 100, \infty$):
  e.g. $\sigma_j = 10$:
  $V^{(1)} = \mathcal{K}_{q_1}((A - 10 \cdot I)^{-1}, (A - 10 \cdot I)^{-1}b)$
  $V^{(2)} = \mathcal{K}_{q_2}((A - 10 \cdot I)^{-1}, (A - 10 \cdot I)^{-1}NV^{(1)}_{[p]})$

$\rightarrow$ First and second order multimoments are preserved.

Simulation results:





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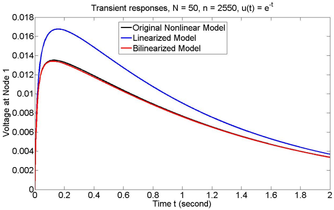

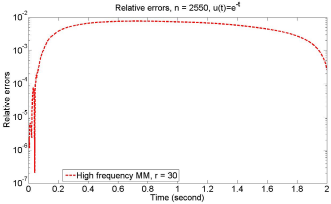

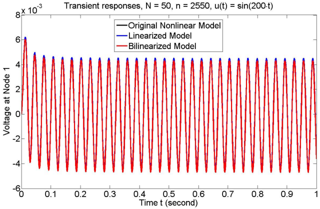

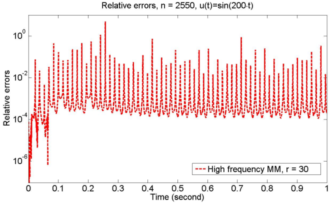

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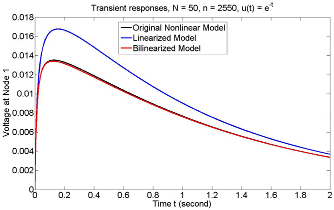

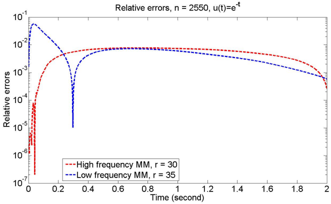

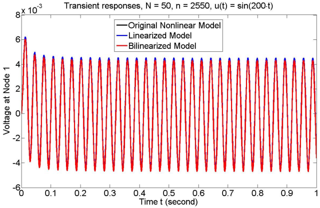

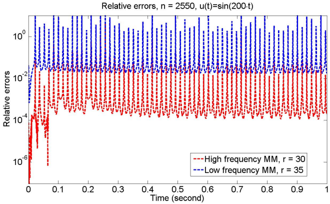

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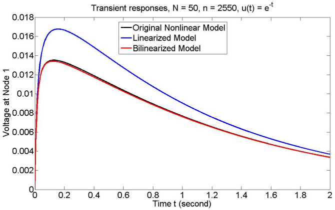

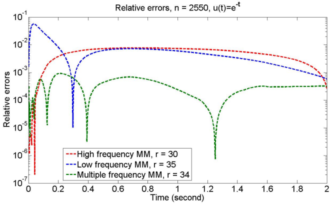

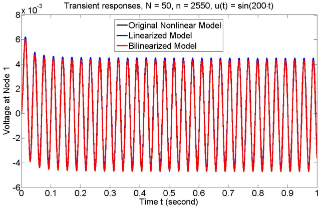

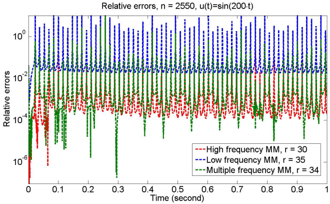

Moving Frontiers: Moment Matching for Quadratic-Bilinear Approximations

- Many nonlinear dynamics can be modeled by quadratic bilinear differential algebraic equations (QBDAEs), i.e.

$$\begin{aligned} E\dot{x} &= A_1 x + A_2 x \otimes x + Nxu + bu, \\ y &= cx, \end{aligned}$$

where $E, A_1, N \in \mathbb{R}^{n\times n}, A_2 \in \mathbb{R}^{n\times n^2}, b, c^T \in \mathbb{R}^n$.

- Combination of quadratic and bilinear control systems.
- Variational analysis allows characterization of input-output behavior via generalized transfer functions, e.g.

$$H_1(s) = c\underbrace{(sE - A_1)^{-1} b}_{G(s)},$$

$$H_2(s_1, s_2) = \frac{1}{2} c\left((s_1 + s_2) E - A_1\right)^{-1} \left[A_2(G(s_1) \otimes G(s_2) + G(s_2) \otimes G(s_1)) + N\left(G(s_1) + G(s_2)\right)\right]$$

Moving Frontiers: Moment Matching for Quadratic-Bilinear Approximations

Which systems can be transformed?

Theorem [Gu '09]

Assume that the state equation of a nonlinear system Σ is given by

$$\dot{x} = a_0 x + a_1 g_1(x) + \ldots + a_k g_k(x) + bu,$$

where $g_i(x) : \mathbb{R}^n \to \mathbb{R}^n$ are compositions of rational, exponential, logarithmic, trigonometric or root functions, respectively.
Then Σ can be transformed into a quadratic bilinear differential algebraic equation of dimension $N > n$.

- transformation is not unique
- original system has to be increased before reduction is possible
- minimal dimension N?

Example

- Consider the following two dimensional nonlinear control system:

$$\dot{x}_1 = \exp(-x_2) \cdot \sqrt{x_1^2 + 1},$$
$$\dot{x}_2 = \sin x_2 + u.$$

- Introduce useful new state variables, e.g.

$$x_3 := \exp(-x_2),\ x_4 := \sqrt{x_1^2 + 1},\ x_5 := \sin x_2,\ x_6 := \cos x_2.$$

- System can be replaced by a QBDAE of dimension 6:

$$\dot{x}_1 = x_3 \cdot x_4, \qquad \dot{x}_2 = x_5 + u,$$
$$\dot{x}_3 = -x_3 \cdot (x_5 + u), \qquad \dot{x}_4 = \frac{2 \cdot x_1 \cdot x_3 \cdot x_4}{2 \cdot x_4},$$
$$\dot{x}_5 = x_6 \cdot (x_5 + u), \qquad \dot{x}_6 = -x_5 \cdot (x_5 + u).$$

Multi-moment-Matching for QBDAEs

- Construct reduced order model by projection:

$$\hat{E} = Z^T E Z, \quad \hat{A}_1 = Z^T A_1 Z, \quad \hat{N} = Z^T N Z,$$
$$\hat{A}_2 = Z^T A_2 Z \otimes Z, \quad \hat{b} = Z^T b, \quad \hat{c} = cZ$$

- Approximate values and derivatives ("multi-moments") of transfer functions about an expansion point σ using Krylov spaces, e.g.

$$\begin{aligned}
\text{span}\{V\} &= \mathcal{K}_6\left(A_\sigma E, A_\sigma b\right) \\
\text{span}\{W_1\} &= \mathcal{K}_3\left(A_{2\sigma} E, A_{2\sigma}(A_2 V_1 \otimes V_1 - N_1 V_1)\right) \\
\text{span}\{W_2\} &= \mathcal{K}_2\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_2 \otimes V_1 + V_1 \otimes V_2) - N_1 V_2)\right) \\
\text{span}\{W_3\} &= \mathcal{K}_1\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_2 \otimes V_2 + V_2 \otimes V_2))\right) \\
\text{span}\{W_4\} &= \mathcal{K}_1\left(A_{2\sigma} E, A_{2\sigma}(A_2(V_3 \otimes V_1 + V_1 \otimes V_3) - N_1 V_3)\right),
\end{aligned}$$

with $A_\sigma = (A_1 - \sigma E)^{-1}$ and V_i denoting the i-*th* column of V
$\rightarrow$ derivatives match up to order 5 (H_1) and 2 (H_2), respectively.

Numerical Example

- FitzHugh-Nagumo system: simple model for neuron (de-)activation.

$$\begin{aligned} \epsilon v_t(x,t) &= \epsilon^2 v_{xx}(x,t) + f(v(x,t)) - w(x,t) + g, \\ w_t(x,t) &= hv(x,t) - \gamma w(x,t) + g, \end{aligned}$$

  with $f(v) = v(v - 0.1)(1 - v)$ and initial and boundary conditions

$$\begin{aligned} v(x,0) &= 0, & w(x,0) &= 0, & x &\in [0,1] \\ v_x(0,t) &= -i_0(t), & v_x(1,t) &= 0, & t &\geq 0, \end{aligned}$$

  where $\epsilon = 0.015, h = 0.5, \gamma = 2, g = 0.05, i_0(t) = 50000t^3 \exp(-15t)$

- parameter g handled as an additional input
- original state dimension $n = 2 \cdot 400$, QBDAE dimension $N = 3 \cdot 400$, reduced QBDAE dimension $r = 26$, chosen expansion point $\sigma = 1$

[B./Breiten 2010]

Numerical Example

2d Phase Space

[B./Breiten 2010]

Numerical Example

3d Phase Space

[B./Breiten 2010]

Conclusions and Outlook

Model reduction for nonlinear systems based on

- Carleman bilinearization and bilinear Balanced Truncation,
- QBDAE transformation and multi-moment matching

has high potential for many classes of nonlinear dynamical systems.

Current work:

- High dimensions can be dealt with using tensor product structures of coefficient matrices — already done for bilinear Krylov subspaces [Condon/Ivanov '07], for Gramian computation in progress [B./Damm].
- QBDAE is exact for many nonlinearities, e.g.
  - + reaction-diffusion systems and population balances;
  - + various PDEs with nonlinear convective terms $\mathbf{x}.\nabla\mathbf{x}$: *Burgers, Euler, Navier-Stokes, Kuramoto-Sivashinsky* eqns;

  hence, reduced-order model will have the same nonlinear structure.
- Enhance efficiency of QBDAE approach using tensor decomposition, low-rank and sparse approximations.

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Thank you for your attention!