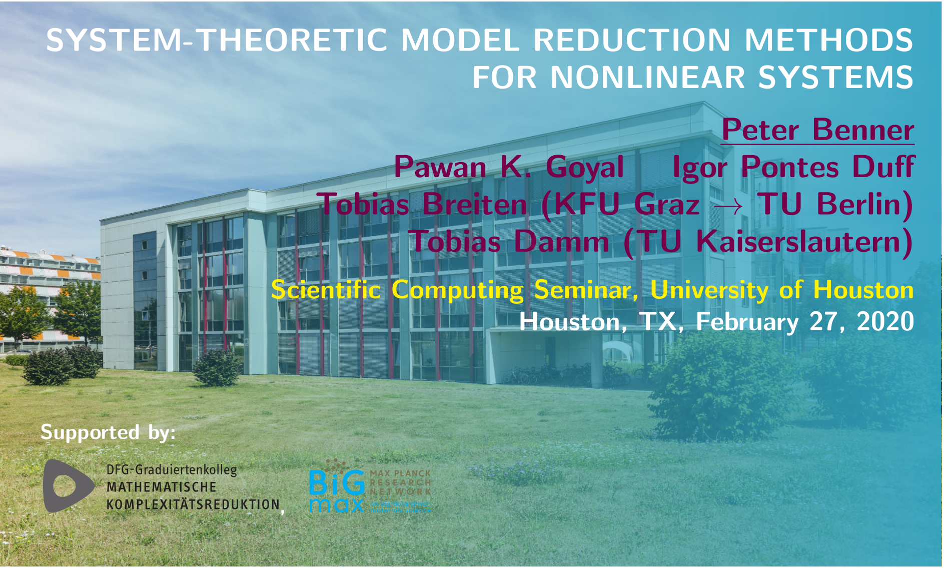
MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY



SYSTEM-THEORETIC MODEL REDUCTION METHODS FOR NONLINEAR SYSTEMS

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BiG max MAX PLANCK RESEARCH NETWORK

The Max Planck **Society**

- is dedicated to fundamental research;
- operates 86 institutes — 81 in Germany, 2 in Italy (Rome, Florence), 1 each in The Netherlands, Luxembourg, US;
- has $\sim$ 24,000 employees;
- had 18 Nobel Laureates since 1948.

The Max Planck Institute (MPI) in Magdeburg

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"The first MPI in engineering. . . "

- founded 1998
- 4 departments (directors)
- 9 research groups
- budget $\sim$ 15 Mio. EUR
- $\sim$ 230 employees
- $\sim$ 160 scientific staff
- research areas:
  - biotechnology
  - chemical engineering
  - process engineering
  - energy conversion
  - applied math
  - HPC

Overview

Outline

Nonlinear Control Systems

$$\Sigma : \begin{cases} E\dot{x}(t) = f(t, x(t), u(t)), & Ex(t_0) = Ex_0, \\ y(t) = g(t, x(t), u(t)), \end{cases}$$

with

- (generalized) states $x(t) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t) \in \mathbb{R}^q$.

If E singular $\rightsquigarrow$ descriptor system. Here, $E = I_n$ for simplicity.

Original System ($E = I_n$)

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Goals:

$\|y - \hat{y}\| < \text{tolerance} \cdot \|u\|$ for all admissible input signals.

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Reduced-Order Model (ROM)

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- states $\hat{x}(t) \in \mathbb{R}^r$, $r \ll n$,
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Model Reduction for Control Systems

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Goals:

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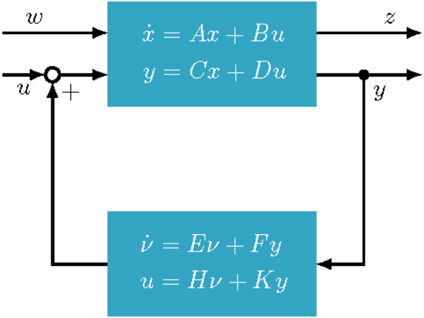
Secondary goal: reconstruct approximation of x from $\hat{x}$.

Feedback Controllers

A feedback controller (dynamic compensator) is a linear system of order N, where

- input $=$ output of plant,
- output $=$ input of plant.

Modern (LQG-/$\mathcal{H}_2$-/$\mathcal{H}_\infty$-) control design: $N \geq n$.



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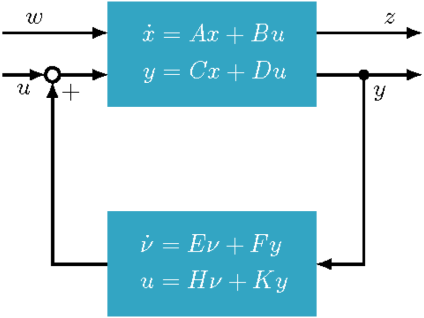

Practical controllers require small N ($N \sim 10$, say) due to

- real-time constraints,
- increasing fragility for larger N.

Application Areas
(Optimal) Control

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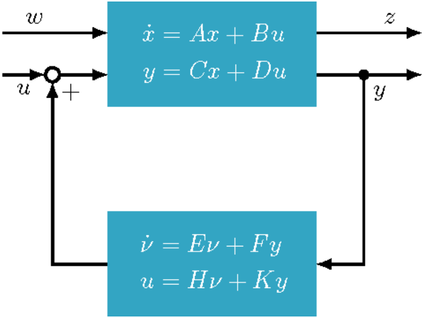

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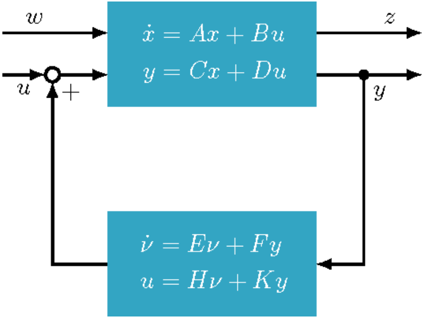

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Standard MOR techniques in systems and control: balanced truncation and related methods.

- Progressive miniaturization: **Moore's Law** states that the number of on-chip transistors doubled each 12/18 months.

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Application Areas
Micro Electronics/Circuit Simulation

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- Verification of VLSI/ULSI chip design requires high number of simulations for different input signals.
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- Linear systems in micro electronics occur through modified nodal analysis (MNA) for RLC networks, e.g., when
  - decoupling large linear subcircuits,
  - modeling transmission lines (interconnect, powergrid), parasitic effects,
  - modeling pin packages in VLSI chips,
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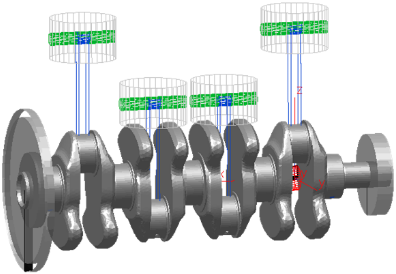
Standard MOR techniques in circuit simulation: Krylov subspace / Padé approximation / rational interpolation methods — not discussed in this talk!



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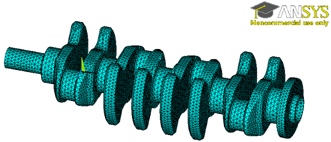
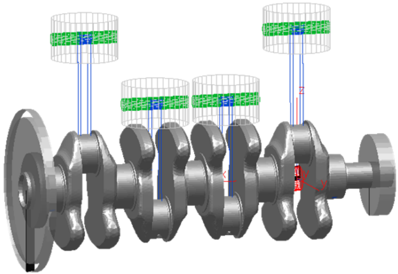


- Resolving complex 3D geometries $\Rightarrow$ millions of degrees of freedom.
- Analysis of elastic deformations requires many simulation runs for varying external forces.

Application Areas

Structural Mechanics / Finite Element Modeling



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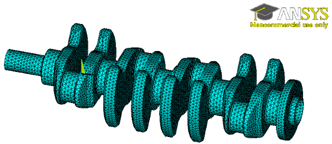

- Resolving complex 3D geometries $\Rightarrow$ millions of degrees of freedom.
- Analysis of elastic deformations requires many simulation runs for varying external forces.

Standard MOR techniques in structural mechanics: modal truncation, combined with Guyan reduction (static condensation) $\rightsquigarrow$ Craig-Bampton method — not discussed in this talk!

Control-Affine (Autonomous) Systems

$$\begin{aligned}
\dot{x}(t) &= f(t,x,u) = \mathcal{A}(x(t)) + \mathcal{B}(x(t))u(t), \quad \mathcal{A} : \mathbb{R}^n \to \mathbb{R}^n,\ \mathcal{B} : \mathbb{R}^n \to \mathbb{R}^{n\times m}, \\
y(t) &= g(t,x,u) = \mathcal{C}(x(t)) + \mathcal{D}(x(t))u(t), \quad \mathcal{C} : \mathbb{R}^n \to \mathbb{R}^q,\ \mathcal{D} : \mathbb{R}^n \to \mathbb{R}^{q\times m}.
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System Classes

Control-Affine (Autonomous) Systems

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Linear, Time-Invariant (LTI) Systems

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\begin{aligned}
\dot{x}(t) &= f(t,x,u) &&= Ax(t) + Bu(t), \qquad A \in \mathbb{R}^{n\times n},\ B \in \mathbb{R}^{n\times m},\\
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Bilinear Systems

$$\begin{aligned}
\dot{x}(t) &= f(t,x,u) = Ax(t) + \sum_{i=1}^{m} u_i(t)A_i x(t) + Bu(t), \quad A, A_i \in \mathbb{R}^{n\times n},\ B \in \mathbb{R}^{n\times m},\\
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Quadratic-Bilinear (QB) Systems

$$\begin{aligned}\dot{x}(t) &= f(t,x,u) = Ax(t) + H\,(x(t) \otimes x(t)) + \textstyle\sum_{i=1}^{m} u_i(t)A_i x(t) + Bu(t),\\ &\qquad A, A_i \in \mathbb{R}^{n\times n},\ H \in \mathbb{R}^{n\times n^2},\ B \in \mathbb{R}^{n\times m},\\ y(t) &= g(t,x,u) = Cx(t) + Du(t), \qquad C \in \mathbb{R}^{q\times n},\ D \in \mathbb{R}^{q\times m}.\end{aligned}$$

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Polynomial Systems

$$
\begin{aligned}
\dot{x}(t) &= f(t,x,u) = Ax(t) + \sum_{j=2}^{n_p} H_j\left(\otimes^j x(t)\right) + \sum_{j=2}^{n_p}\sum_{k=1}^{m} A_j^k \left(\otimes^j x(t)\right) u_k(t) + Bu(t), \\
&\qquad\qquad H_j, A_j^k \text{ of "appropriate size"}, \\
y(t) &= g(t,x,u) = Cx(t) + Du(t), \qquad C \in \mathbb{R}^{q\times n},\ D \in \mathbb{R}^{q\times m}.
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Written in control-affine form:

$$\begin{aligned} \mathcal{A}(x) &:= Ax + H\left(x\otimes x\right), & \mathcal{B}(x) &:= [A_1,\ldots,A_m]\left(I_m \otimes x\right) + B \\ \mathcal{C}(x) &:= Cx, & \mathcal{D}(x) &:= D. \end{aligned}$$

Consider smooth nonlinear, control-affine system with $m = 1$:

$$\begin{aligned} \dot{x} &= \mathcal{A}(x) + Bu \qquad \text{with } \mathcal{A}(0) = 0, \\ y &= Cx + Du. \end{aligned}$$

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Instead of truncating Taylor expansion, Carleman (bi)linearization takes into account K higher order terms (h.o.t.) by introducing new variables:

$$x^{(k)} := x \underbrace{\otimes \;\cdots\; \otimes}_{(k-1)\ \text{times}} x, \qquad k = 1, \ldots, K.$$

Here: $K = 2$, i.e., $z := x^{(2)} = x \otimes x$.

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$$\dot{z} = \dot{x} \otimes x + x \otimes \dot{x} = (Ax + Hz + \ldots + Bu) \otimes x + x \otimes (Ax + Hz + \ldots + Bu).$$

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Ignoring h.o.t. $\Longrightarrow$ bilinear system with state $x^{\otimes} := \left[x^T, z^T\right]^T \in \mathbb{R}^{n+n^2}$:

$$\begin{aligned} \frac{d}{dt} x^{\otimes} &= \begin{bmatrix} A & H \\ 0 & A \otimes I_n + I_n \otimes A \end{bmatrix} x^{\otimes} + \begin{bmatrix} 0 & 0 \\ B \otimes I_n + I_n \otimes B & 0 \end{bmatrix} (x^{\otimes}) u + \begin{bmatrix} B \\ 0 \end{bmatrix} u, \\ y^{\otimes} &= \begin{bmatrix} C & 0 \end{bmatrix} x^{\otimes} + Du. \end{aligned}$$

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Remark

Bilinear systems directly occur, e.g., in biological systems, PDE control problems with mixed boundary conditions, "control via coefficients", networked control systems, ...

QB systems can be obtained as approximation (by truncating Taylor expansion) to weakly nonlinear systems [PHILLIPS '03].

C. Gu. QLMOR: A Projection-Based Nonlinear Model Order Reduction Approach Using Quadratic-Linear Representation of Nonlinear Systems. IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, 30(9):1307–1320, 2011.

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J. R. Phillips. Projection-based approaches for model reduction of weakly nonlinear time-varying systems. IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, 22(2):171–187, 2003.

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But **exact representation** of smooth nonlinear systems possible:

Theorem [Gu '09/'11]

Assume that the state equation of a nonlinear system 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 uni-variable rational, exponential, logarithmic, trigonometric or root functions, respectively. Then, by iteratively taking derivatives and adding algebraic equations, respectively, the nonlinear system can be transformed into a QB(DAE) system.

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Theorem [GU '09/'11]

Assume that the state equation of a nonlinear system 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 uni-variable rational, exponential, logarithmic, trigonometric or root functions, respectively. Then, by iteratively taking derivatives and adding algebraic equations, respectively, the nonlinear system can be transformed into a QB(DAE) system.

Alternatively, polynomial-bilinear system can be obtained using iterated Lie brackets [GU '11].

C. Gu. QLMOR: A Projection-Based Nonlinear Model Order Reduction Approach Using Quadratic-Linear Representation of Nonlinear Systems. IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, 30(9):1307–1320, 2011.

L. Feng, X. Zeng, C. Chiang, D. Zhou, and Q. Fang. Direct nonlinear order reduction with variational analysis. In: Proceedings of DATE 2004, pp. 1316–1321.

J. R. Phillips. Projection-based approaches for model reduction of weakly nonlinear time-varying systems. IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, 22(2):171–187, 2003.

Idea borrowed from non-convex optimization:

- **Lift to higher dimensions using** $const. \cdot n$ **additional variables,**
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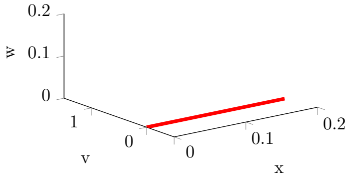
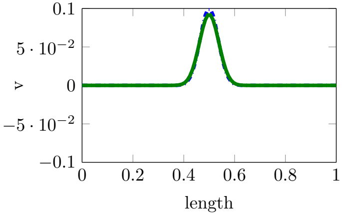
FitzHugh-Nagumo model



- Model describes activation and de-activation of neurons.
- Contains a cubic nonlinearity, which can be transformed to QB form.

Sine-Gordon equation



- Applications in biomedical studies, mechanical transmission lines, etc.
- Contains sin function, which can also be rewritten into QB form.

Definition

The Laplace transform of a time domain function $f \in L_{1,\mathrm{loc}}$ with $\mathrm{dom}\,(f) = \mathbb{R}_0^+$ is

$$\mathcal{L} : f \mapsto F, \quad F(s) := \mathcal{L}\{f(t)\}(s) := \int_0^\infty e^{-st} f(t)\, dt, \quad s \in \mathbb{C}.$$

F is a function in the (Laplace or) frequency domain.

Note: With $\Re s = 0$ and $\Im s \geq 0$, $\omega := \Im s$ takes the role of a frequency (in [rad/s], i.e., $\omega = 2\pi\nu$ with ν measured in [Hz]).

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Note: for ease of notation, in the following we will use lower-case letters for both, a function and its Laplace transform!

Linear Systems in Frequency Domain

Application of Laplace transform $(x(t) \mapsto x(s),\ \dot{x}(t) \mapsto sx(s) - x(0))$ to linear system

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t) + Du(t)$$

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Model reduction in frequency domain: Fast evaluation of mapping $u \rightarrow y$.

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$\Longrightarrow$ I/O-relation in frequency domain:

$$y(s) = \Big(\underbrace{C(sI_n - A)^{-1}B + D}_{=:G(s)} \Big) u(s).$$

$G(s)$ is the **transfer function** of Σ.

Model reduction in frequency domain: Fast evaluation of mapping $u \rightarrow y$.

Formulating model reduction in frequency domain

Approximate the dynamical system

$$\begin{aligned} \dot{x} &= Ax + Bu, \qquad A \in \mathbb{R}^{n\times n},\ B \in \mathbb{R}^{n\times m}, \\ y &= Cx + Du, \qquad C \in \mathbb{R}^{q\times n},\ D \in \mathbb{R}^{q\times m}, \end{aligned}$$

by reduced-order system

$$\begin{aligned} \dot{\hat{x}} &= \hat{A}\hat{x} + \hat{B}u, \quad \hat{A} \in \mathbb{R}^{r\times r},\ \hat{B} \in \mathbb{R}^{r\times m}, \\ \hat{y} &= \hat{C}\hat{x} + \hat{D}u, \quad \hat{C} \in \mathbb{R}^{q\times r},\ \hat{D} \in \mathbb{R}^{q\times m} \end{aligned}$$

of order $r \ll n$, such that

$$\|y - \hat{y}\| = \left\|Gu - \hat{G}u\right\| \leq \left\|G - \hat{G}\right\| \cdot \|u\| < \text{tolerance} \cdot \|u\| .$$

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$\Longrightarrow$ Approximation problem: $\displaystyle \min_{\text{order}\,(\hat{G})\leq r} \left\|G - \hat{G}\right\|.$

Outline

Basic concept

- System Σ : $\begin{cases} \dot{x}(t) = Ax(t) + Bu(t), \\ y(t) = Cx(t), \end{cases}$ with A stable, i.e., $\Lambda(A) \subset \mathbb{C}^-$,

  is balanced, if system Gramians, i.e., 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 $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

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Balanced Truncation for Linear Systems

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

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

Motivation:

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

$$\mathcal{H} : L_2(-\infty, 0) \mapsto L_2(0, \infty) : u_- \mapsto y_+.$$

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Minimum energy to reach x_0 in balanced coordinates:

$$\inf_{\substack{u \in L_2(-\infty,0] \\ x(0)=x_0}} \int_{-\infty}^{0} u(t)^T u(t)\, dt = x_0^T P^{-1} x_0 = \sum_{j=1}^{n} \frac{1}{\sigma_j} x_{0,j}^2$$

Balanced Truncation for Linear Systems

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Energy contained in the system if $x(0) = x_0$ and $u(t) \equiv 0$ in balanced coordinates:

$$\|y\|_2^2 = \int_0^{\infty} y(t)^T y(t)\, dt = x_0^T Q x_0 = \sum_{j=1}^{n} \sigma_j x_{0,j}^2$$

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In balanced coordinates, energy transfer from u_- to y_+ is

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"engineer's point of view"

$\Longrightarrow$ Truncate states corresponding to "small" HSVs

Properties

- Reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$.

Balanced Truncation for Linear Systems

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

$$\|y - \hat{y}\|_2 \leq \|G - \hat{G}\|_{\mathcal{H}_\infty} \|u\|_2 \leq \left(2 \sum\nolimits_{k=r+1}^{n} \sigma_k\right) \|u\|_2 \,,$$

where $\|G\|_{\mathcal{H}_\infty} := \sup_{u \in \mathcal{L}_2 \setminus \{0\}} \frac{\|Gu\|_2}{\|u\|_2} = \sup_{\omega \in \mathbb{R}} \sigma_{\max}(G(\jmath\omega))$.

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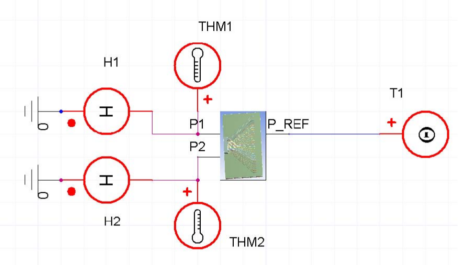
Practical implementation

- Rather than solving Lyapunov equations for P, Q (n^2 unknowns!), find $S, R \in \mathbb{R}^{n \times s}$ with $s \ll n$ such that $P \approx SS^T$, $Q \approx RR^T$.
- Reduced-order model directly obtained via small-scale ($s \times s$) SVD of $R^T S$!
- No $\mathcal{O}(n^3)$ or $\mathcal{O}(n^2)$ computations necessary!

- SIMPLORER® test circuit with 2 transistors.



- Conservative thermic sub-system in SIMPLORER:
  voltage $\rightsquigarrow$ temperature, current $\rightsquigarrow$ heat flow.
- Original model: $n = 270.593$, $m = q = 2 \Rightarrow$
  Computing time (on Intel Xeon dualcore 3GHz, 1 Thread):
  - Main computational cost for set-up data $\approx 22min$.
  - Computation of reduced models from set-up data: 44–49sec. ($r = 20$–70).
  - Bode plot (MATLAB on Intel Core i7, 2,67GHz, 12GB):
    7.5h for original system , $<$ 1min for reduced system.

Numerical Example

Electro-Thermic Simulation of Integrated Circuit (IC) [Source: Evgenii Rudnyi, CADFEM GmbH]

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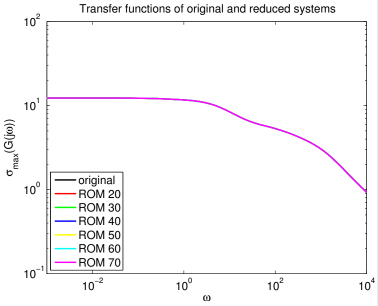
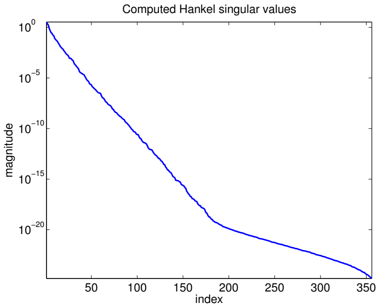
Bode Plot (Amplitude)



Hankel Singular Values



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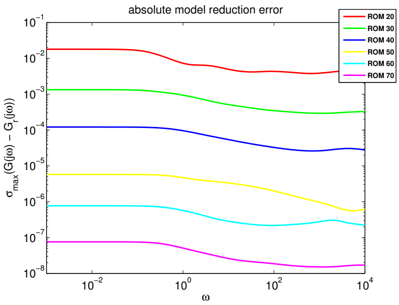
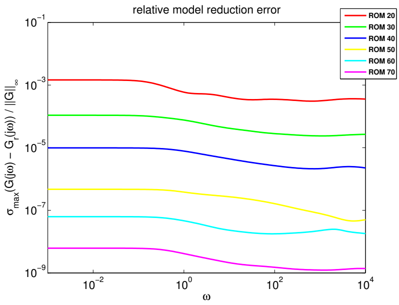
Absolute Error



Relative Error



Balanced Truncation for Bilinear Systems

The concept of balanced truncation can be generalized to the class of bilinear systems, where we need the solutions of the Lyapunov-plus-positive equations:

$$AP + PA^T + \sum_{i=1}^{m} A_i P A_i^T + BB^T = 0,$$

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- If unique solutions $P = P^T \geq 0$, $Q = Q^T \geq 0$ exist, these can be used in balancing procedure like for linear systems, with

$$\hat{A} := W^T A V, \quad \hat{A}_i = W^T A_i V, \quad \hat{B} := W^T B, \quad \hat{C} := CV.$$

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- "Twice-the-trail-of-the-HSVs" error bound does not hold [B./Damm 2014].

Balanced Truncation for Bilinear Systems

The concept of balanced truncation can be generalized to the class of bilinear systems, where we need the solutions of the Lyapunov-plus-positive equations:

$$AP + PA^T + \sum_{i=1}^{m} A_i P A_i^T + BB^T = 0,$$

$$A^T Q + QA^T + \sum_{i=1}^{m} A_i^T Q A_i + C^T C = 0.$$

- If unique solutions $P = P^T \geq 0$, $Q = Q^T \geq 0$ exist, these can be used in balancing procedure like for linear systems, with

  $$\hat{A} := W^T AV, \quad \hat{A}_i = W^T A_i V, \quad \hat{B} := W^T B, \quad \hat{C} := CV.$$

  See [Al-Baiyat/Bettayeb 1993, B./Damm 2011] for details.
- Stability preservation [B./Damm/Redmann/Rodriguez Cruz 2016].
- These equations also appear for stochastic control systems, see [B./Damm 2011].
- "Twice-the-trail-of-the-HSVs" error bound does not hold [B./Damm 2014].
- Alternative Gramians based on linear matrix inequalities investigated by [Redmann 2018], yield H_∞ error bound based on truncated characteristic values, but hard to compute for large-scale systems!

$$AX + XA^T + \sum_{i=1}^{m} A_i X A_i^T + BB^T = 0. \qquad (1)$$

- Need a positive semi-definite symmetric solution X.

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$$\left(I_n \otimes A + A \otimes I_n + \sum_{i=1}^{m} A_i \otimes A_i \right) \operatorname{vec}(X) = -\operatorname{vec}(BB^T).$$

  Sufficient condition for unique solvability: smallness of A_i (related to stability radius of A). $\rightsquigarrow$ **bounded-input bounded-output (BIBO) stability** of bilinear systems.

  This will be assumed from here on, hence: existence and uniqueness of positive semi-definite solution $X = X^T$.

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- Want: solution methods for large scale problems, i.e., only matrix-matrix multiplication with A, A_j, solves with (shifted) A allowed!
- Requires to compute data-sparse approximation to generally dense X; here: $X \approx ZZ^T$ with $Z \in \mathbb{R}^{n \times n_Z}$, $n_Z \ll n$!

Theorem **[B./Breiten 2012]**

Assume existence and uniqueness with stable A and $A_j = U_j V_j^T$, with $U_j, V_j \in \mathbb{R}^{n \times r_j}$. Set $r = \sum_{j=1}^m r_j$.
Then the solution X of

$$AX + XA^T + \sum_{j=1}^{m} A_j X A_j^T + BB^T = 0$$

can be approximated by X_k of rank $(2k+1)(m+r)$, with an error satisfying

$$\|X - X_k\|_2 \lesssim \exp(-\sqrt{k}).$$

- Generalized Alternating Directions Iteration (ADI) method.
    1. Computing square solution matrix ($\sim n^2$ unknowns) [Damm 2008].
    2. Computing low-rank factors of solutions ($\sim n$ unknowns) [B./Breiten 2013].

- Generalized Extended (or Rational) Krylov Subspace Method (EKSM/RKSM) [B./Breiten 2013].

- Tensorized versions of standard Krylov subspace methods, e.g., PCG, PBiCGStab [Kressner/Tobler 2011, B./Breiten 2013].

- Inexact stationary (fix point) iteration [Shank/Simoncini/Szyld 2016].

Consider bilinear control systems:

$$\Sigma : \quad \begin{cases} \dot{x}(t) = Ax(t) + \sum_{i=1}^{m} A_i x(t) u_i(t) + Bu(t), \\ y(t) = Cx(t), \quad x(0) = x_0, \end{cases}$$

where $A, A_i \in \mathbb{R}^{n \times n},\ B \in \mathbb{R}^{n \times m},\ C \in \mathbb{R}^{q \times n}$.

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Key Observation **[B./Breiten 2011]**

Consider parameters as additional inputs, a linear parametric system

$$\dot{x}(t) = Ax(t) + \sum_{i=1}^{m_p} a_i(p) A_i x(t) + B_0 u_0(t), \quad y(t) = Cx(t)$$

with $B_0 \in \mathbb{R}^{n\times m_0}$ can be interpreted as bilinear system:

$$u(t) := \begin{bmatrix} a_1(p) & \dots & a_{m_p}(p) & u_0(t) \end{bmatrix}^T,$$

$$B := \begin{bmatrix} \mathbf{0} & \dots & \mathbf{0} & B_0 \end{bmatrix} \in \mathbb{R}^{n\times m}, \quad m = m_p + m_0.$$

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Consequence

Model order reduction techniques for bilinear systems can be applied to linear parametric systems!

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Alternative: $\mathcal{H}_2$-optimal rational interpolation/bilinear IRKA [B./Breiten 2012, B./Bruns 2015, Flagg/Gugercin 2015].

Application to Parametric MOR

Fast Simulation of Cyclic Voltammogramms [Feng/Koziol/Rudnyi/Korvink 2006]

$$E\dot{x}(t) = (A + p_1(t)A_1 + p_2(t)A_2)x(t) + B,$$
$$y(t) = Cx(t), \quad x(0) = x_0 \neq 0,$$

- Rewrite as system with zero initial condition,
- FE model: $n = 16,912, \; m = 3, \; q = 1,$
- $p_j \in [0, 10^9]$ time-varying voltage functions,
- transfer function $G(i\omega, p_1, p_2)$,
- reduced system dimension $r = 67$,
- $\max\limits_{\substack{\omega\in\{\omega_{min},\dots,\omega_{max}\}\\ p_j\in\{p_{min},\dots,p_{max}\}}} \frac{\|G-\hat{G}\|_2}{\|G\|_2} < 6 \cdot 10^{-4},$
- evaluation times: FOM 4.5h, ROM 38s $\rightsquigarrow$ speed-up factor ≈ 426.

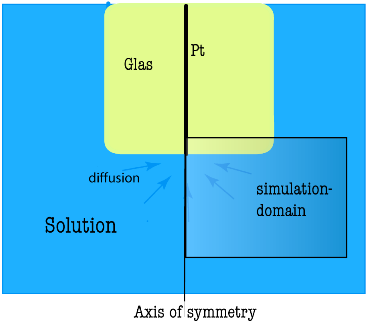
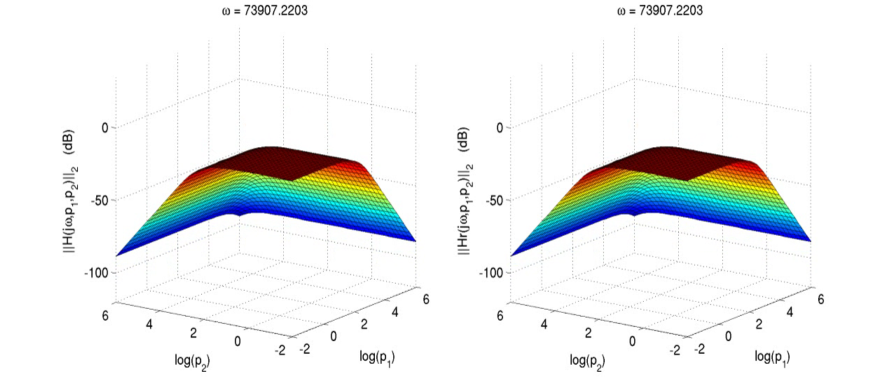


Figure: [Feng et al. 2006]

Original. . . **and reduced-order model.**



Outline

- Nonlinear balancing based on energy functionals [Scherpen '93, Gray/Mesko '96].

Definition [Scherpen '93, Gray/Mesko '96]

The reachability energy functional, $L_c(x_0)$, and observability energy functional, $L_o(x_0)$ of a system are given as:

$$L_c(x_0) = \inf_{\substack{u \in L_2(-\infty,0] \\ x(-\infty)=0,\ x(0)=x_0}} \frac{1}{2} \int_{-\infty}^{0} \|u(t)\|^2 dt, \qquad L_o(x_0) = \frac{1}{2} \int_{0}^{\infty} \|y(t)\|^2 dt.$$

Disadvantage: energy functionals are the solutions of nonlinear Hamilton-Jacobi equations which are hardly solvable for large-scale systems.

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- Empirical Gramians/frequency-domain POD [Lall et al '99, Willcox/Peraire '02].

Example: controllability Gramian from time domain data (snapshots)

1. Define reachability Gramian of the system

$$P = \int_0^\infty x(t)x(t)^T dt, \quad \text{where } x(t) \text{ solves } \dot{x} = f(x, \delta),\ x(0) = x_0.$$

2. Use time-domain integrator to produce snapshots $x_k \approx x(t_k)$, $k = 1, \ldots, K$.
3. Approximate $P \approx \sum_{k=0}^{K} w_k x_k x_k^T$ with positive weights w_k.
4. Analogously for observability Gramian.
5. Compute balancing transformation and apply it to nonlinear system.

Disadvantage: Depends on chosen training input (e.g., $\delta(t_0)$) like other POD approaches.

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- $\rightsquigarrow$ **Goal:** computationally efficient and input-independent method!

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- For recent developments on empirical Gramians, see [Himpe '18].

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- For bilinear systems, such local bounds were derived in [B./Damm 2011] using the solutions to the Lyapunov-plus-positive equations:

$$AP + PA^T + \sum_{i=1}^m A_i P A_i^T + BB^T = 0,$$
$$A^T Q + QA^T + \sum_{i=1}^m A_i^T Q A_i + C^T C = 0.$$

  (If their solutions exist, they define reachability and observability Gramians of BIBO stable bilinear system.)
- **Here we aim at determining algebraic Gramians for QB (and polynomial) systems, which**
  - **provide bounds for the energy functionals of QB systems,**
  - **generalize the Gramians of linear and bilinear systems, and**
  - **allow us to find the states that are hard to control as well as hard to observe in an efficient and reliable way.**

- Consider input $\rightarrow$ state map of QB system ($m = 1,\ N \equiv A_1$):

$$\dot{x}(t) = Ax(t) + Hx(t) \otimes x(t) + Nx(t)u(t) + Bu(t), \qquad x(0) = 0.$$

- Integration yields

$$x(t) = \int_0^t e^{A\sigma_1} Bu(t-\sigma_1)d\sigma_1 + \int_0^t e^{A\sigma_1} Nx(t-\sigma_1)u(t-\sigma_1)d\sigma_1 + \int_0^t e^{A\sigma_1} Hx(t-\sigma_1) \otimes x(t-\sigma_1)d\sigma_1$$

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$$= \int_0^t e^{A\sigma_1} Bu(t-\sigma_1)d\sigma_1 + \int_0^t \int_0^{t-\sigma_1} e^{A\sigma_1} Ne^{A\sigma_2} Bu(t-\sigma_1)u(t-\sigma_1-\sigma_2)d\sigma_1 d\sigma_2$$

$$+ \int_0^t \int_0^{t-\sigma_1} \int_0^{t-\sigma_1} e^{A\sigma_1} H(e^{A\sigma_2}B \otimes e^{A\sigma_3}B)u(t-\sigma_1-\sigma_2)u(t-\sigma_1-\sigma_3)d\sigma_1 d\sigma_2 d\sigma_3 + \ldots$$

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&\qquad + \int_0^t e^{A\sigma_1} Hx(t-\sigma_1) \otimes x(t-\sigma_1)d\sigma_1 \\
&= \int_0^t e^{A\sigma_1} Bu(t-\sigma_1)d\sigma_1 + \int_0^t \int_0^{t-\sigma_1} e^{A\sigma_1} Ne^{A\sigma_2} Bu(t-\sigma_1)u(t-\sigma_1-\sigma_2)d\sigma_1 d\sigma_2 \\
&\quad + \int_0^t \int_0^{t-\sigma_1} \int_0^{t-\sigma_1} e^{A\sigma_1} H(e^{A\sigma_2} B \otimes e^{A\sigma_3} B)u(t-\sigma_1-\sigma_2)u(t-\sigma_1-\sigma_3)d\sigma_1 d\sigma_2 d\sigma_3 + \ldots
\end{aligned}$$

- By iteratively inserting expressions for $x(t - \bullet)$, we obtain the **Volterra series expansion** for the QB system. [Rugh '81]

Using the *Volterra kernels*, we can define the controllability mappings

$$\Pi_1(t_1) := e^{At_1}B, \qquad \Pi_2(t_1, t_2) := e^{At_1}N\Pi_1(t_2),$$
$$\Pi_3(t_1, t_2, t_3) := e^{At_1}[H(\Pi_1(t_2) \otimes \Pi_1(t_3)), N\Pi_2(t_1, t_2)], \ldots$$

and a candidate for a new Gramian:

$$P := \sum_{k=1}^{\infty} P_k, \qquad \text{where} \quad P_k = \int_0^{\infty} \cdots \int_0^{\infty} \Pi_k(t_1, \ldots, t_k)\Pi_k(t_1, \ldots, t_k)^T \, dt_1 \ldots dt_k.$$

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Theorem [B./Goyal '16]

If it exists, the new controllability Gramian P for QB (MIMO) systems with stable A solves the **quadratic Lyapunov equation**

$$AP + PA^T + \sum_{k=1}^{m} A_k P A_k^T + H(P\otimes P)H^T + BB^T = 0.$$

Note: $H = 0 \rightsquigarrow$ "bilinear reachability Gramian"; if additionally, all $A_k = 0 \rightsquigarrow$ linear one.

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- This allows to define dual systems for QB systems:

$$
\begin{aligned}
\dot{x}(t) &= Ax(t) + Hx(t) \otimes x(t) + \sum_{k=1}^{m} A_k x(t) u_k(t) + Bu(t), && x(0) = 0,\\
\dot{x}_d(t) &= -A^T x_d(t) - H^{(2)} x(t) \otimes x_d(t) - \sum_{k=1}^{m} A_k^T x_d(t) u_k(t) - C^T u_d(t), && x_d(\infty) = 0,\\
y_d(t) &= B^T x_d(t),
\end{aligned}
$$

where $H^{(2)}$ is the mode-2 matricization of the QB Hessian.

- Writing down the Volterra series for the dual system $\rightsquigarrow$ observability mapping.

- This provides the observability Gramian Q for the QB system. It solves

$$A^T Q + QA + \sum_{k=1}^{m} A_k^T Q A_k + H^{(2)}(P \otimes Q) \left(H^{(2)}\right)^T + C^T C = 0.$$

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Remarks:

- Observability Gramian depends on controllability Gramian!
- For $H = 0$, obtain "bilinear observability Gramian", and if also all $A_k = 0$, the linear one.

Bounding the energy functionals:

Lemma [B./Goyal '17]

In a neighborhood of the stable equilibrium, $B_\varepsilon(0)$,

$$L_c(x_0) \geq \frac{1}{2} x_0^T P^{-1} x_0, \qquad L_o(x_0) \leq \frac{1}{2} x_0^T Q x_0, \qquad x_0 \in B_\varepsilon(0),$$

for "small signals" and x_0 pointing in unit directions.

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for "small signals" and x_0 pointing in unit directions.

Another interpretation of Gramians in terms of energy functionals

1. If the system is to be steered from 0 to x_0, where $x_0 \notin \text{range}(P)$, then $L_c(x_0) = \infty$ for all feasible input functions u.
2. If the system is (locally) controllable and $x_0 \in \ker(Q)$, then $L_o(x_0) = 0$.

Illustration using a scalar system

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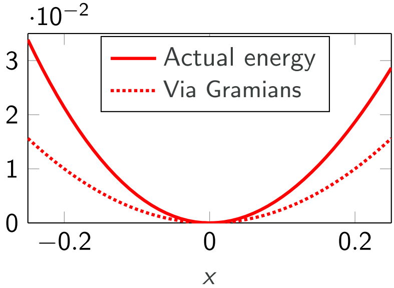
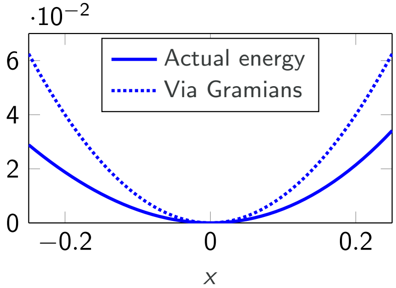


(a) Input energy lower bound.



(b) Output energy upper bound.

Figure: Comparison of energy functionals for $-a = b = c = 2, h = 1, n = 0$.

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[DAMM '08]

- To overcome this issue, we propose truncated Gramians for QB systems.

Definition (Truncated Gramians) [B./GOYAL '16]

The truncated Gramians $P_{\mathcal{T}}$ and $Q_{\mathcal{T}}$ for QB systems satisfy

$$AP_{\mathcal{T}} + P_{\mathcal{T}}A^T = -BB^T - \sum_{k=1}^{m} A_k P_l A_k^T - H(P_l \otimes P_l)H^T,$$

$$A^T Q_{\mathcal{T}} + Q_{\mathcal{T}}A = -C^T C - \sum_{k=1}^{m} A_k^T Q_l A_k - H^{(2)}(P_l \otimes Q_l)(H^{(2)})^T,$$

where

$$AP_l + P_l A^T = -BB^T \quad \text{and} \quad A^T Q_l + Q_l A = -C^T C.$$

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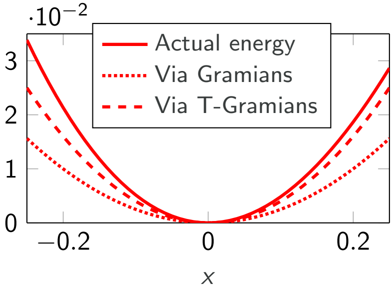

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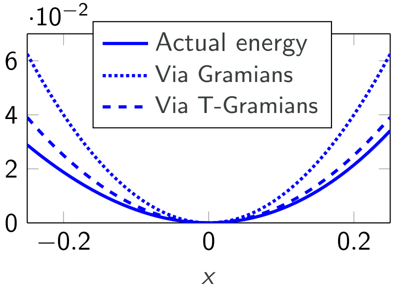

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- $\sigma_i(P \cdot Q) > \sigma_i(P_{\mathcal{T}} \cdot Q_{\mathcal{T}}) \Rightarrow$ obtain smaller order of reduced system if truncation is done at the same cutoff threshold.
- Most importantly, we need solutions of only four standard Lyapunov equations.
- Interpretation of controllability/observability of the system via T-Gramians:
  - If the system is to be steered from 0 to x_0, where $x_0 \notin \text{range}(P_{\mathcal{T}})$, then $L_c(x_0) = \infty$.
  - If the system is controllable and $x_0 \in \ker(Q_{\mathcal{T}})$, then $L_o(x_0) = 0$.

Balanced Truncation Algorithm

Algorithm 1 Balanced Truncation MOR for QB Systems (Truncated Gramians).

1: **Input:** A, H, A_k, B, C.

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5: **Output:** reduced-order matrices:

$$\hat{A} = \mathcal{W}^T A\mathcal{V}, \quad \hat{H} = \mathcal{W}^T H(\mathcal{V} \otimes \mathcal{V}), \quad \hat{A}_k = \mathcal{W}^T A_k \mathcal{V},$$
$$\hat{B} = \mathcal{W}^T B, \quad \hat{C} = C\mathcal{V}.$$

Remark: There are efficient ways to compute $\hat{H}$, avoiding the explicit computation of $\mathcal{V} \otimes \mathcal{V}$. [B./Breiten '15, B./Goyal/Gugercin '18]

$$
\begin{aligned}
v_t + v^3 &= v_{xx} + v, && (0, L) \times (0, T),\\
v(0,.) &= u(t), && (0, T),\\
v_x(L,.) &= 0, && (0, T),\\
v(x,0) &= v_0(x), && (0, L).
\end{aligned}
$$

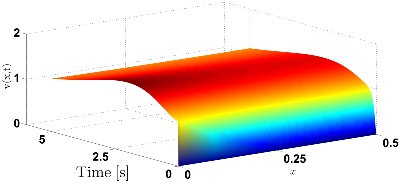

Figure: Chafee-Infante equation.

- Cubic nonlinearity that can be rewritten into QB form. [B./Breiten '15']

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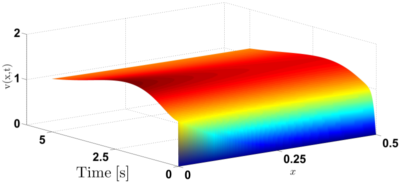

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- The transformed QB system is of order $n = 1,000$.
- The output of interest is the response at right boundary at $x = L$.

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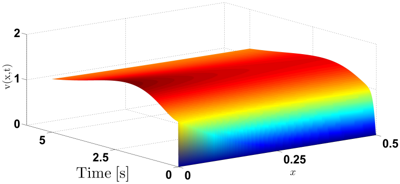


Figure: Chafee-Infante equation.

- Cubic nonlinearity that can be rewritten into QB form. [B./Breiten '15']
- The transformed QB system is of order $n = 1,000$.
- The output of interest is the response at right boundary at $x = L$.
- We determine the reduced-order system of order $r = 10$.

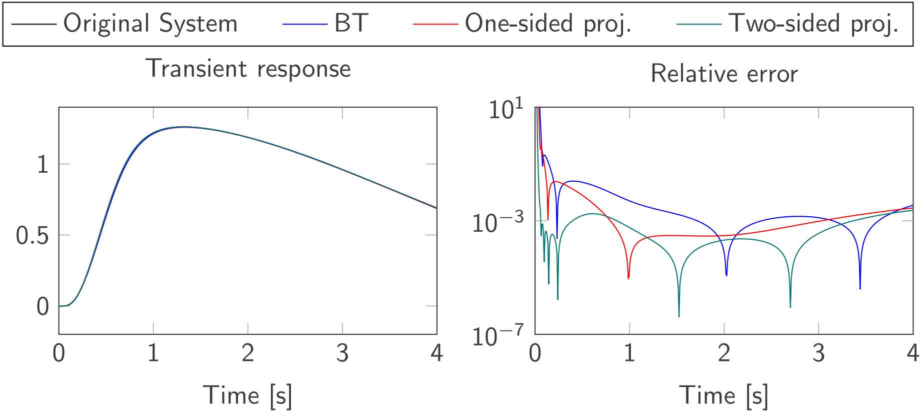


Figure: Boundary control for a control input $u(t) = 5t\,\exp(-t)$.

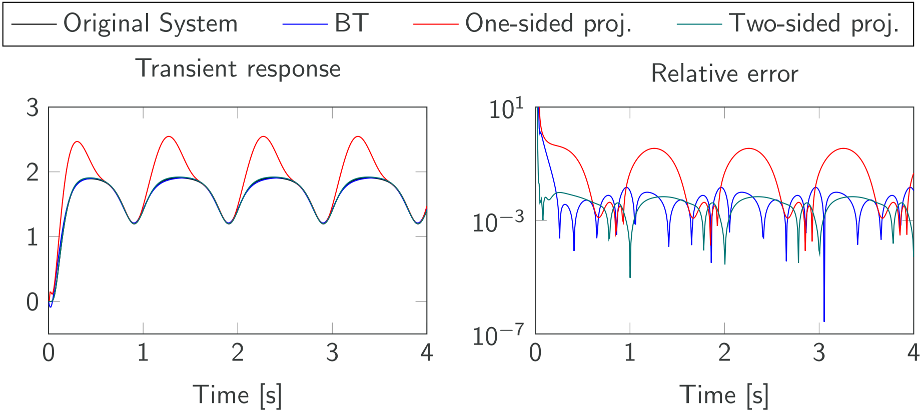


Figure: Boundary control for a control input $u(t) = 25(1 + \sin(2\pi t))/2$.

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

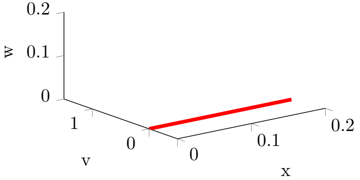
with a nonlinear function

$$f(v(x,t)) = v(v-0.1)(1-v).$$

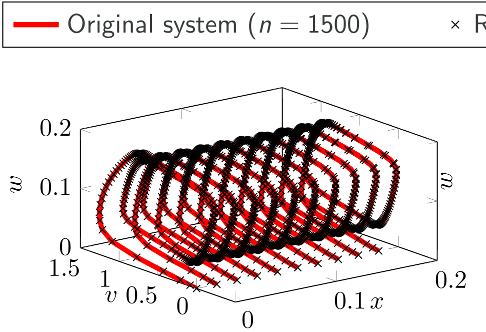
The boundary conditions are as follows:

$$v_x(0,t) = i_0(t), \quad v_x(L,t) = 0, \quad t \geq 0,$$

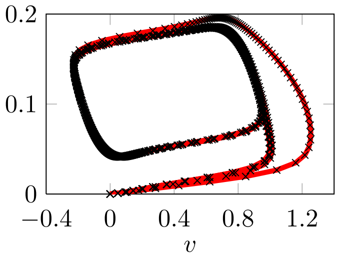
where $\epsilon = 0.015,\ h = 0.5,\ \gamma = 2,\ q = 0.05,$
$L = 0.2.$



- Input $i_0(t) = 5 \cdot 10^4 t^3 \exp(-15t)$ serves as actuator.



(a) Limit-cycles at various x.



(b) Projection onto the v−w plane.

Figure: Comparison of the limit-cycles obtained via the original and reduced-order (BT) systems. The reduced-order systems constructed by moment-matching methods were unstable.

Outline

Polynomial Control Systems

Now, consider the class of **polynomial control (PC) Systems**:

$$\boxed{\begin{aligned}\dot{x}(t) &= Ax(t) + \sum_{j=2}^{n_p} H_j \left(\otimes^j x(t)\right) + \sum_{j=2}^{n_p} \sum_{k=1}^{m} N_j^k \left(\otimes^j x(t)\right) u_k(t) + Bu(t),\\ y(t) &= Cx(t), \quad x(0) = 0,\end{aligned}}$$

where

- n_p is the degree of the polynomial part of the system,
- $x(t) \in \mathbb{R}^n$, $\otimes^j x(t) = \underbrace{x(t) \otimes \cdots \otimes x(t)}_{j\text{-times}}$,
- $u(t) \in \mathbb{R}^m$, and $y(t) \in \mathbb{R}^p$, $n \gg m, p$.
- $A \in \mathbb{R}^{n \times n}$, $H_j, N_j^k \in \mathbb{R}^{n \times n^j}$, $B \in \mathbb{R}^{n \times m}$ and $C \in \mathbb{R}^{p \times n}$.
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Examples: FitzHugh-Nagumo and Chafee-Infante equations lead to cubic control systems; cubic-quintic Allen-Cahn equation to quintic control system.

Expanding the response of the PC system into a Volterra series representation and following the same ideas as in the QB case, we define the reachability Gramian as

$$\boxed{P = \sum_{k=1}^{\infty} \int_0^{\infty} \cdots \int_0^{\infty} \bar{P}_k(t_1, \ldots, t_k) \bar{P}_k(t_1, \ldots, t_k)^T dt_1 \ldots dt_k,}$$

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where $\bar{P}_1(t_1) = e^{At_1} B, \quad \bar{P}_2(t_1, t_2) = \sum_{k=1}^{m} e^{At_1} N_1^k e^{At_2} B,$

$\bar{P}_3(t_1, t_2, t_3) = e^{At_1} H_2 e^{At_2} B \otimes e^{At_3} B, \ldots$ are the kernels of the Volterra series.

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Theorem

The reachability Gramian **P** of a PC system solves the polynomial Lyapunov equation

$$AP + PA^T + BB^T + \sum_{j=2}^{n_p} H_j \left(\otimes^j P \right) H_j^T + \sum_{j=2}^{n_p} \sum_{k=1}^{m} N_j^k \left(\otimes^j P \right) \left(N_j^k \right)^T = 0.$$

The Observability Gramian is defined as follows

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- First, we write the adjoint system as [Fujimoto et. al. '02]

$$\boxed{\begin{aligned}
&\dot{x}(t) = Ax(t) + \sum_{j=2}^{n_p} H_j x_j^{\otimes}(t) + \sum_{j=1}^{n_p}\sum_{k=1}^{m} N_j^k x_j^{\otimes}(t) u_k(t) + Bu(t),\\
&\dot{x_d}(t) = -A^T x_d(t) - \sum_{j=2}^{n_p} H_j^{(2)} x_{d,j}^{\otimes}(t) - \sum_{j=1}^{n_p}\sum_{k=1}^{m} \left(N_j^{k,(2)}\right) x_{d,j}^{\otimes}(t) u_{d,k}(t) - C^T u_d(t), \quad x_d(\infty) = 0,\\
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y_d(t) &= B^T x_d(t).
\end{aligned}$$

- Then, by taking the kernel of Volterra series, one has

Theorem

Let **P** be the reachability Gramian. Then, the observability Gramian **Q** of a PC system solves the polynomial Lyapunov equation

$$A^T Q + QA + C^T C + \sum_{j=2}^{n_p} H_j^{(2)} \left(\otimes^{j-1} P \otimes Q\right) \left(H_j^{(2)}\right)^T + \sum_{j=2}^{n_p}\sum_{k=1}^{m} N_j^{k,(2)} \left(\otimes^{j-1} P \otimes Q\right) \left(N_j^{k,(2)}\right)^T = 0.$$

Truncated Gramians

- Polynomial Lyapunov equations are very expensive to solve.
- As for QB systems, we thus propose truncated Gramians that only involve a finite number of kernels.

$$\boxed{P_{\mathcal{T}} = \sum_{k=1}^{n_p+1} \int_0^\infty \cdots \int_0^\infty \bar{P}_k(t_1,\ldots,t_k)\bar{P}_k(t_1,\ldots,t_k)^T dt_1 \ldots dt_k,}$$

Truncated Gramians

The reachability truncated Gramian solves

$$AP_{\mathcal{T}} + P_{\mathcal{T}}A^T + BB^T + \sum_{j=2}^{n_p} H_j \otimes^j P_l H_j^T + \sum_{j=2}^{n_p}\sum_{k=1}^{m} N_j^k \otimes^j P_l \left(N_j^k\right)^T = 0.$$

where $AP_l + P_lA^T + BB^T = 0$

- Advantage: Only need to solve a finite number of (linear) Lyapunov equations.

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

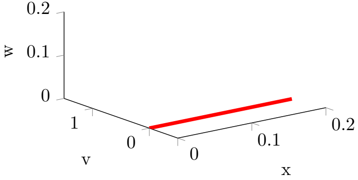
with a nonlinear function

$$f(v(x,t)) = v(v-0.1)(1-v).$$

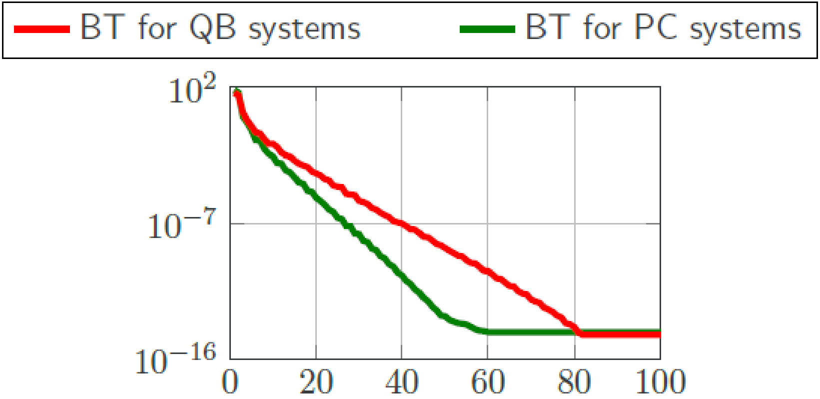
The boundary conditions are as follows:

$$v_x(0,t) = i_0(t), \quad v_x(L,t) = 0, \quad t \geq 0,$$

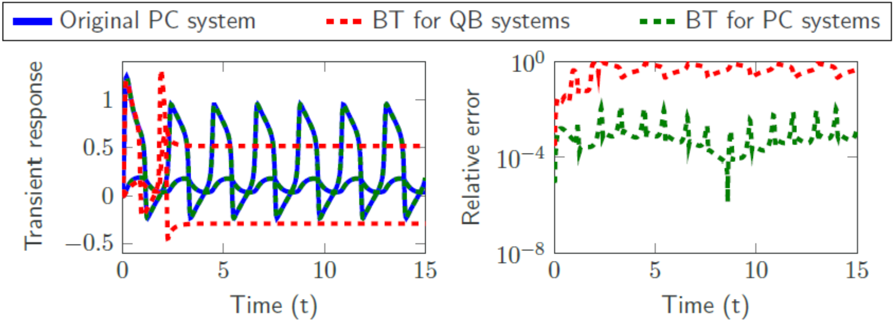
where $\epsilon = 0.015,\ h = 0.5,\ \gamma = 2,\ q = 0.05,\ L = 0.2.$



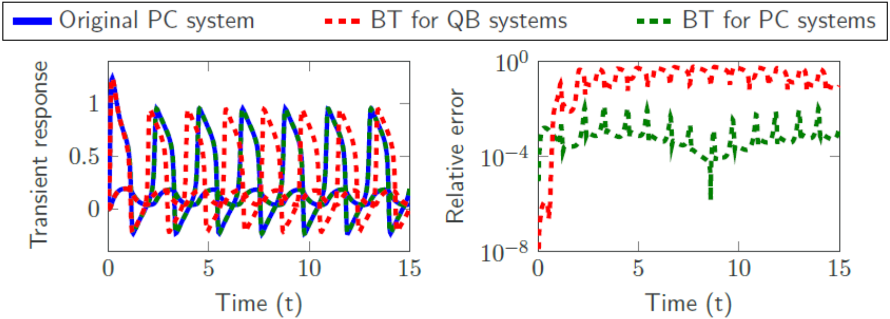
- After discretization we obtain a PC system with cubic nonlinearity of order $n_{pc} = 600$. [B./Breiten '15]
- The transformed quadratic-bilinear (QB) system is of order $n_{qb} = 900$.
- The outputs of interest $v(0,t), w(0,t)$ are the responses at the left boundary at $x = 0$.
- We compare balanced truncation for PC and QB systems.



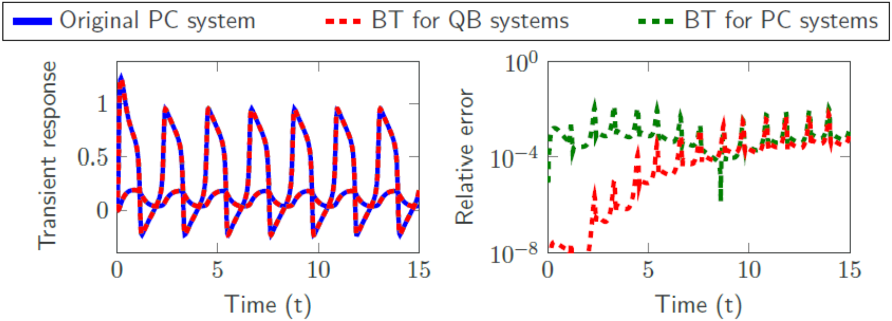
- Decay singular values for PC systems is faster $\Rightarrow$ smaller reduced order model!



- Original PC system of order 600. Original QB system of order 900.
- Reduced PC system of order 10. Reduced QB system of order 10.



- Original PC system of order 600. Original QB system of order 900.
- Reduced PC system of order 10. Reduced QB system of order 30.



- Original PC system of order 600. Original QB system of order 900.
- Reduced PC system of order 10. Reduced QB system of order 43.

Conclusions

- BT extended to bilinear, QB, and polynomial systems.
- Local Lyapunov stability is preserved.
- As of yet, only weak motivation by bounding energy functionals.
- No error bounds in terms of "Hankel" singular values.
- Computationally efficient (as compared to nonlinear balancing), and input independent.
- **To do:**
  - improve efficiency of Lyapunov solvers with many right-hand sides further;
  - error bound;
  - conditions for existence of new QB Gramians;
  - extension to descriptor systems;
  - time-limited versions.

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