

MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG



COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

Solving Quadratic Lyapunov Equations

Peter Benner

Steffen W. R. Werner (Virginia Tech) Pawan K. Goyal (appliedAl Initiative)

SIAM LA24 MS84 "Matrix and Kensor Equations in Action: Simulation, Model Reduction and Scientific Machine Learning" Paris, May 13–17, 2024

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Solving Quadratic Lyapunov Equations ... and why

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1. Motivation

- 2. Balanced Truncation for Nonlinear Systems
- 3. Numerical Methods



1. Motivation

Problem Setting Model Reduction for Control Systems System Classes Balanced Truncation for Linear Systems

- 2. Balanced Truncation for Nonlinear Systems
- 3. Numerical Methods



For $A, A_k \in \mathbb{R}^{n \times n}$, k = 1, ..., m, $B \in \mathbb{R}^{n \times m}$, $H \in \mathbb{R}^{n \times n^2}$, find symmetric positive semidefinite solution P of

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

=: $\mathcal{L}(P)$ + $\Pi(P)$ + $\mathcal{K}(P)$ + BB^T .

We assume A stable throughout, i.e. $\Lambda(A) \subset \mathbb{C}^-$, implying $\Lambda(\mathcal{L}) \subset \mathbb{C}^-$.



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We assume A stable throughout, i.e. $\Lambda(A) \subset \mathbb{C}^-$, implying $\Lambda(\mathcal{L}) \subset \mathbb{C}^-$.

Note:

- \mathcal{L} is the standard Lyapunov operator.
- For $A_k \equiv 0$, H = 0, we obtain a standard Lyapunov equation.
- $\bullet~\Pi, \mathcal{K}$ are nonnegative operators, i.e., they map spsd matrices to spsd matrices.
- $\mathcal{L} + \Pi$ is linear ("Lyapunov-plus-positive"/"bilinear Lyapunov"); \mathcal{K} is nonlinear.



Motivation Model Reduction for Control Systems

Nonlinear Control Systems

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

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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Reduced-Order Model (ROM)

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

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



Goal:

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



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Goal:

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



Control-Affine (Autonomous) Systems

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



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Linear, Time-Invariant (LTI) Systems

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



Control-Affine (Autonomous) Systems

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

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Bilinear Systems

$$\dot{x}(t) = f(t, x, u) = Ax(t) + \sum_{i=1}^{m} u_i(t)A_ix(t) + Bu(t), \quad A, A_i \in \mathbb{R}^{n \times n}, \ B \in \mathbb{R}^{n \times n}, y(t) = g(t, x, u) = Cx(t) + Du(t), \qquad C \in \mathbb{R}^{q \times n}, \ D \in \mathbb{R}^{q \times n}.$$



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Quadratic-Bilinear (QB) Systems

$$\dot{x}(t) = f(t, x, u) = Ax(t) + H(x(t) \otimes x(t)) + \sum_{i=1}^{m} u_i(t)A_ix(t) + Bu(t),$$

$$A, A_i \in \mathbb{R}^{n \times n}, \ H \in \mathbb{R}^{n \times n^2}, \ B \in \mathbb{R}^{n \times m},$$

$$y(t) = g(t, x, u) = Cx(t) + Du(t), \qquad C \in \mathbb{R}^{q \times n}, \ D \in \mathbb{R}^{q \times m}.$$



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

- 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.
- 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.



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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.

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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FitzHugh-Nagumo model

Sine-Gordon equation

- Model describes activation and de-activation of neurons.
- Contains a cubic nonlinearity, which can be transformed to QB form.
- Applications in biomedical studies, mechanical transmission lines, etc.
- Contains sin function, which can also be rewritten into QB form.



1



1

• System
$$\Sigma$$
:

$$\begin{cases}
\dot{x}(t) = Ax(t) + Bu(t), \\
y(t) = Cx(t), \\
\text{is balanced, if system Gramians, i.e., solutions } P, Q \text{ of the Lyapunov equations} \\
AP + PA^T + BB^T = 0, \quad A^TQ + QA + C^TC = 0, \\
\text{satisfy: } P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) \text{ with } \sigma_1 \ge \sigma_2 \ge \dots \ge \sigma_n > 0.
\end{cases}$$

• $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ .



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

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



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



Balanced Truncation for Linear Systems

Properties

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



Properties

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

$$\|y - \hat{y}\|_{2} \le \|G - \hat{G}\|_{\mathcal{H}_{\infty}} \|u\|_{2} \le \left(2\sum_{k=r+1}^{n} \sigma_{k}\right) \|u\|_{2}.$$



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Practical implementation

 Rather than solving Lyapunov equations for P, Q (n² unknowns!), find S, R ∈ ℝ^{n×s} with s ≪ n such that P ≈ SS^T, Q ≈ RR^T.
 Many algorithms: [Antoulas, Baur, B., Chu, Druskin, Hammarling, Fassbender, Freitag, Grasedyck, Gugercin, Jaimoukha, Knizherman, Köhler, Kressner, Kürschner, Li, Palitta, Penzl, Quintana-Ortí, Saad, Saak, Simoncini, Sorensen, Stykel, White, ...]



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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 $P \approx SS^T$, $Q \approx RR^T$. Many algorithms: [Antoulas, Baur, B., Chu, Druskin, Hammarling, Fassbender, Freitag, Grasedyck, Gugercin, Jaimoukha, Knizherman, Köhler, Kressner, Kürschner, Li, Palitta, Penzl, Quintana-Ortí, Saad, Saak, Simoncini, Sorensen, Stykel, White, ...]
- 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!



1. Motivation

- 2. Balanced Truncation for Nonlinear Systems Energy Functionals and Gramians Gramians for QB Systems
- 3. Numerical Methods

• 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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- Empirical Gramians/frequency-domain POD [LALL ET AL '99, WILLCOX/PERAIRE '02]. **Disadvantage:** Depends on chosen training input (e.g., $\delta(t_0)$) like other POD approaches.
- ~ Goal: computationally efficient and input-independent method!

- W. S. Gray and J. P. Mesko. Controllability and observability functions for model reduction of nonlinear systems. In Proc. of the Conf. on Information Sci. and Sys., pp. 1244–1249, 1996.
- S. Lall, J. Marsden, and S. Glavaški. A subspace approach to balanced truncation for model reduction of nonlinear control systems. INTERNATIONAL JOURNAL OF ROBUST AND NONLINEAR CONTROL, 12:519–535, 2002.
- 🗎 J. M. A. Scherpen. Balancing for nonlinear systems. SYSTEMS & CONTROL LETTERS, 21:143–153, 1993.
- 🖹 K. Willcox and J. Peraire, Balanced model reduction via the proper orthogonal decomposition. AIAA JOURNAL, 40:2323–2330, 2002.



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- For example, (locally) $L_c(x_0) \geq \frac{1}{2} x_0^T \tilde{P}^{-1} x_0$, where $\tilde{P} = \tilde{P}^T > 0$ [Gray/Mesko '96].
- For bilinear systems, such local bounds were derived in [B./DAMM '11] using the solutions to the Lyapunov-plus-positive equations:

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

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

(If their solutions exist, they define reachability and observability Gramians of BIBO stable bilinear system.)

• Efficient solution methods for Lyapunov-plus-positive equations are derived in [B./BREITEN '13, SHANK/SIMONCINI/SZYLD '16, KÜRSCHNER '17, ...].



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- Here we aim at determining algebraic Gramians for QB 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.



- Gramians for QB Systems Controllability Gramians
- 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

$$\begin{aligned} x(t) &= \int\limits_0^t e^{A\sigma_1} Bu(t-\sigma_1) d\sigma_1 + \int\limits_0^t e^{A\sigma_1} Nx(t-\sigma_1)u(t-\sigma_1) d\sigma_1 \\ &+ \int\limits_0^t e^{A\sigma_1} Hx(t-\sigma_1) \otimes x(t-\sigma_1) d\sigma_1 \end{aligned}$$

[RUGH '81]



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[RUGH '81]



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$$= \int_{0}^{t} e^{A\sigma_{1}} Bu(t-\sigma_{1}) d\sigma_{1} + \int_{0}^{t} \int_{0}^{t-\sigma_{1}} e^{A\sigma_{1}} Ne^{A\sigma_{2}} Bu(t-\sigma_{1})u(t-\sigma_{1}-\sigma_{2}) d\sigma_{1} d\sigma_{2} \\ &+ \int_{0}^{t} \int_{0}^{t-\sigma_{1}} \int_{0}^{t-\sigma_{1}} e^{A\sigma_{1}} H(e^{A\sigma_{2}} B \otimes e^{A\sigma_{3}} B)u(t-\sigma_{1}-\sigma_{2})u(t-\sigma_{1}-\sigma_{3}) d\sigma_{1} d\sigma_{2} d\sigma_{3} + \ldots \end{aligned}$$

 By iteratively inserting expressions for x(t − •), we obtain the Volterra series expansion for the QB system.



Using the Volterra kernels, we can define the controllability mappings

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

and a candidate for a new Gramian:

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



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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**

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

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



1. Motivation

2. Balanced Truncation for Nonlinear Systems

3. Numerical Methods

Truncated Gramians Fix point iterations Numerical Example



• Now, the main obstacle for using the new Gramians is the solution of the (quadratic) Lyapunov-type equations.



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- Fix point iteration scheme can be employed \rightsquigarrow next subsection.



- Now, the main obstacle for using the new Gramians is the solution of the (quadratic) Lyapunov-type equations.
- Fix point iteration scheme can be employed \rightsquigarrow next subsection.
- For model order reduction, we proposed truncated Gramians for QB systems.

Definition (Truncated Gramians)[B./GOYAL '16, B./GOYAL/REDMANN '17]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

$$AP_l + P_l A^T = -BB^T$$
 and $A^T Q_l + Q_l A = -C^T C.$







(a) Input energy lower bounds.

(b) Output energy upper bounds.

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



• $\sigma_i(P \cdot Q) > \sigma_i(P_T \cdot Q_T) \Rightarrow$ obtain smaller order of reduced system if truncation is done at the same cutoff threshold.



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- T-Gramians approximate energy functionals better than the actual Gramians.
- $\sigma_i(P \cdot Q) > \sigma_i(P_T \cdot Q_T) \Rightarrow$ 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 $x_0 \notin \operatorname{range}(P_{\mathcal{T}})$, then $L_c(x_0) = \infty$.
 - If the system is controllable and $x_0 \in \ker (Q_T)$, then $L_o(x_0) = 0$.



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



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Lyapunov iteration:

$$P_{0} = 0$$

$$\mathcal{L}(P_{j+1}) = AP_{j+1} + P_{j+1}A^{T}$$

$$= -BB^{T} - \sum_{k=1}^{m} A_{k}P_{j}A_{k}^{T} - H(P_{j} \otimes P_{j})H^{T}, \qquad j = 0, 1, \dots$$

Note: P_1 is reachability Gramian of associated linear-time invariant system.



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Numerical Methods Fix point iterations

Quadratic Lyapunov equation

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Conjecture: converges to the minimal spsd solution under certain stability assumptions.



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

Lyapunov-plus-positive iteration:

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 $(\mathcal{L} + \Pi)(P_{j+1}) = AP_{j+1} + P_{j+1}A^{T} + \sum_{k=1}^{m} A_{k}P_{j+1}A_{k}^{T}$
 $= -BB^{T} - H(P_{k} \otimes P_{j})H^{T}, \quad j = 0, 1, \dots$

Note: P_1 is reachability Gramian of associated bilinear system if it exists.



Numerical Methods Fix point iterations

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Toy data (homogeneous bilinear term)

$$A = \begin{bmatrix} -1 & 0 \\ 0 & -3 \end{bmatrix}, \ H = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{bmatrix}, \ B = \begin{bmatrix} 0 \\ 2 \end{bmatrix} \quad \rightsquigarrow \quad X = \begin{bmatrix} 0.3410 & 0 \\ 0 & 0.7522 \end{bmatrix}.$$



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- Extension of balanced truncation to asymptotically stable quadratic (and polynomial) systems leads to quadratic Lyapunov equations.
- Can be solved by fix point iteration or truncated series formula.
- Each step requires solution of standard Lyapunov equation; via sign function method or other Lyapunov solvers.
- Factorized versions possible \rightsquigarrow large-scale, sparse solvers can be employed, but controlling rank growth might be problematic.
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- Code will be available in upcoming MORLAB release, see https://www.mpi-magdeburg.mpg.de/projects/morlab.
- Acceleration of fix point iterations via vector extrapolation possible.
- Open problems: Existence of solutions, variety of solutions, convergence of fix point iterations.



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