Nonlinear balanced truncation: Computing energy functions and model reduction

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Nonlinear control-affine model reduction

We are interested in high-dimensional nonlinear systems:

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)) + \mathbf{g}(\mathbf{x})\mathbf{u}(t), \qquad \mathbf{y}(t) = \mathbf{h}(\mathbf{x}(t)),$$

with states $\mathbf{x} \in \mathbb{R}^n$, controls $\mathbf{u} \in \mathbb{R}^m$, nonlinearity $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^n$, outputs $\mathbf{y} \in \mathbb{R}^p$.

- For the large-scale systems of interest, i.e., semi-discretized PDEs, and differential algebraic equations (DAEs), $n \gg 1,000$.
- We assume invertible $\mathbf{E}$ matrices, and present the methods for $\mathbf{E} = \mathbf{I}$, which can be obtained with a suitable change of variables (see numerical examples).

Goal of control-affine nonlinear model reduction:

Find a low-dimensional coordinate transformation $\mathbf{x} \approx \Phi(\mathbf{z}_r)$, $\mathbf{z}_r \in \mathbb{R}^r$ and derive a reduced-order model (ROM)

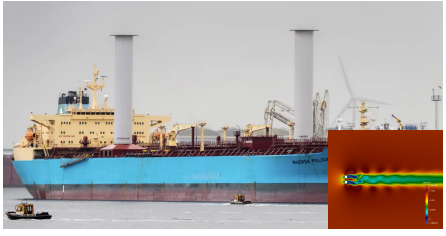
$$\dot{\mathbf{z}}_r(t) = \mathbf{f}_r(\mathbf{z}_r(t)) + \mathbf{g}_r(\mathbf{z}_r)\mathbf{u}(t), \qquad \mathbf{y}_r(t) = \mathbf{h}_r(\mathbf{z}_r(t)),$$

with reduced states $\mathbf{z}_r \in \mathbb{R}^r$ with $r \ll n$, such that $\|\mathbf{x} - \Phi(\mathbf{z}_r)\|_{\mathcal{X}}$ or $\|\mathbf{y} - \mathbf{y}_r\|_{\mathcal{X}}$ are small (in some norm $\|\cdot\|_{\mathcal{X}}$), and where the system has favorable control theoretic properties.

Motivation: control-oriented model reduction

For input-driven and controlled systems, taking into account the effects of the inputs & controls in the model reduction process is paramount.

- **Trajectory-based methods** (proper orthogonal decomposition, reduced basis method, dynamic mode decomposition, ...) require carefully choosing representative forcing functions/initial conditions.
- **System-theoretic methods** use the underlying transfer function ($\mathcal{H}_2$, $\mathcal{H}_\infty$, Loewner), moments thereof, or system energies (balanced truncation) to find appropriate subspaces for projection.



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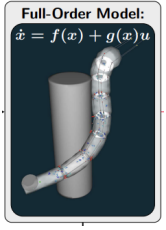
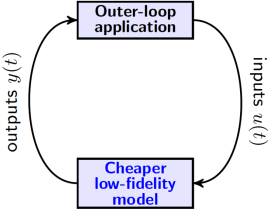


Soft robots



generic control system

In these next two hours, we will discuss:

1. Various energy functions for nonlinear systems

2. Scalable computation of energy functions via polynomial approximations and tensor calculus[1]

3. Simultaneous balance-and-reduce strategy: ROMs on nonlinear balanced manifolds[2]

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[1] K./Gugercin/Borggaard, *Nonlinear Balanced Truncation: Part 1—Computing Energy Functions, arxiv:2209.07645*

[2] K./Gugercin/Borggaard, *Nonlinear Balanced Truncation: Part 2—Model Reduction on Manifolds, arXiv:2302.02036*

Part 1:
Energy functions for nonlinear systems

Controllers and energy functions for nonlinear systems

Theorem ([Lukes, 1969])

Consider a control-affine nonlinear dynamical system and a quadratic cost (or energy)

$$\widehat{\mathcal{E}}(\mathbf{x}_0, \mathbf{u}) = \frac{1}{2}\int_0^\infty \mathbf{x}(t)^\top \mathbf{Q}\mathbf{x}(t) + \mathbf{u}(t)^\top \mathbf{R}\mathbf{u}(t)\mathrm{d}t, \qquad \mathbf{Q}, \mathbf{R} \succ \mathbf{0}.$$

Let the following assumptions hold: (1) there is a neighborhood Ω of the origin where $\mathbf{f} \in C^2(\Omega)$; $\mathbf{f}(\mathbf{0}) = \mathbf{0}$; (2) the pair $\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\mathbf{0}), \mathbf{g}(\mathbf{0})\right)$ is stabilizable; (3) the nonlinear system is stabilizable on Ω, so there exists a stabilizing controller so that the closed-loop system is asymptotically stable on Ω. Then there exists a unique solution $\mathbf{u}^*(\mathbf{x})$ to the HJB equation

$$0 = \min_{\mathbf{u}} \left\{ \mathbf{x}(t)^\top \mathbf{Q}\mathbf{x}(t) + \mathbf{u}(t)^\top \mathbf{R}\mathbf{u}(t) + \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}} \left[\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u}\right] \right\}$$

where $\mathcal{E}(\mathbf{x}) = \min_{\mathbf{u}} \widehat{\mathcal{E}}(\mathbf{x}, \mathbf{u})$ and the unique continuously differentiable minimizer for the optimal feedback control $\mathbf{u}^*(\mathbf{x})$ is

$$\mathbf{u}^*(\mathbf{x}) = -\mathbf{R}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}}.$$

Moreover, if $\mathbf{f}(\mathbf{x})$ is analytic, so are $\mathbf{u}^*(\mathbf{x})$ and $\mathcal{E}(\mathbf{x})$.

Controllers and energy functions for nonlinear systems ctd

Inserting the optimal control $\mathbf{u}^*(\mathbf{x}) = -\mathbf{R}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}}$ into the HJB equation we obtain

$$0 = \mathbf{x}(t)^\top \mathbf{Q}\mathbf{x}(t) + \mathbf{u}(t)^\top \mathbf{R}\mathbf{u}(t) + \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}} \left[\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x}) \left(-\mathbf{R}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}}\right)\right]$$

which after reorganizing becomes

$$0 = \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{R}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial \mathcal{E}(\mathbf{x})}{\partial \mathbf{x}} + \mathbf{x}(t)^\top \mathbf{Q}\mathbf{x}(t) + \mathbf{u}(t)^\top \mathbf{R}\mathbf{u}(t)$$

- The HJB equation is therefore a necessary and sufficient condition to the optimal control problem

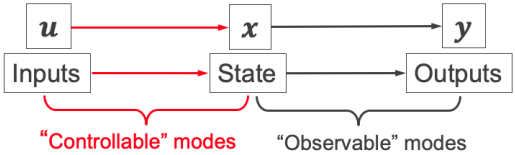
$$\begin{aligned} &\min_u \widehat{\mathcal{E}}(\mathbf{x}_0, \mathbf{u}) \\ &\text{s.t.} \qquad \dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)) + \mathbf{g}(\mathbf{x})\mathbf{u}(t), \qquad \mathbf{x}_0 = \mathbf{x}(0) \end{aligned}$$

- Analytic solutions: since we assume polynomial dynamics going forward, $\mathbf{f}(\mathbf{x})$ is analytic, so we know that we can search for Taylor series of $\mathbf{u}^*(\mathbf{x})$ and $\mathcal{E}(\mathbf{x})$.

Energy functions for LTI systems

Consider a linear time-invariant system:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)$$
$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t)$$



The energy to reach $\mathbf{x}_0$ from zero, and the observability energy associated with state $\mathbf{x}_0$, can be defined as

$$\mathcal{E}_c(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2(-\infty,0] \\ \mathbf{x}(-\infty)=\mathbf{0} \\ \mathbf{x}(0)=\mathbf{x}_0}} \frac{1}{2}\int_{-\infty}^{0} \|\mathbf{u}(t)\|^2 \mathrm{d}t, \qquad \mathcal{E}_o(\mathbf{x}_0) := \frac{1}{2}\int_{0}^{\infty} \|\mathbf{y}(t)\|^2 \mathrm{d}t$$

It can be shown that they are **quadratic functions of the state**:

$$\mathcal{E}_c(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^\top \mathbf{P}^{-1}\mathbf{x}_0, \qquad \mathcal{E}_o(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^\top \mathbf{Q}\mathbf{x}_0,$$

where *controllability (observability) Gramians* $\mathbf{P}, \mathbf{Q}$ are solutions to the Lyapunov equations:

$$\mathbf{A}\mathbf{P} + \mathbf{P}\mathbf{A}^\top + \mathbf{B}\mathbf{B}^\top = \mathbf{0}, \qquad \mathbf{A}^\top\mathbf{Q} + \mathbf{Q}\mathbf{A} + \mathbf{C}^\top\mathbf{C} = \mathbf{0}.$$

What does this have to do with model reduction?

Let us decompose the (symmetric positive definite) controllability Gramian using the SVD:

$$\mathbf{P} = \mathbf{W}\mathbf{\Sigma}\mathbf{W}^\top, \qquad \mathbf{W}^\top\mathbf{W} = \mathbf{I}_n, \quad \mathbf{\Sigma} = \mathrm{diag}(\sigma_1, ..., \sigma_n).$$

The energy to reach a state $\mathbf{x}_0 = \mathbf{w}_i$ (a column of $\mathbf{W}$) from $\mathbf{x}(-\infty) = \mathbf{0}$ is:

$$\mathcal{E}_c(\mathbf{w}_i) = \mathbf{w}_i^\top \mathbf{P}^{-1}\mathbf{w}_i = \mathbf{w}_i^\top \mathbf{W}\mathbf{\Sigma}^{-1}\mathbf{W}^\top\mathbf{w}_i = \frac{1}{\sigma_i},$$

so the energy to reach $\mathbf{w}_i$ is given by $\frac{1}{\sigma_i}$. This leads us to make two observations:

1. "Easy" to reach states correspond to large σ_i.

2. "Hard" to reach states correspond to small σ_i.

What does this have to do with model reduction?

Similar observations can be made for the observability Gramian. Let us decompose the observability Gramian using its SVD:

$$\mathbf{Q} = \mathbf{V}\mathbf{S}\mathbf{V}^\top, \mathbf{V}^\top\mathbf{V} = \mathbf{I}, \qquad \mathbf{V}^\top\mathbf{V} = \mathbf{I}_n, \quad \mathbf{\Sigma} = \mathrm{diag}(\sigma_1, ..., \sigma_n)$$

The output energy that is generated by $\mathbf{x}_0 = \mathbf{v}_i$ (the observability energy) is

$$\mathcal{E}_o(\mathbf{v}_i) = \mathbf{v}_i^\top \mathbf{V}\mathbf{\Sigma}\mathbf{V}^\top \mathbf{v}_i = \sigma_i.$$

We can make similar observations:

1. The eigenvectors corresponding to large σ_i are easy to observe.
2. The eigenvectors corresponding to small σ_i are hard to observe.

Balanced truncation model reduction

We want to find a coordinate system (i.e., a state-space transformation) where states are easy to reach and easy to observe. [Moore, 1981] pioneered balanced truncation for LTI systems:

- A **linear transformation** $\mathbf{x} = \mathbf{T}\mathbf{z}$ simultaneously diagonalizes $\mathbf{P}, \mathbf{Q}$.
- Truncating the balanced high-dimensional model yields a **balanced ROM with states that are easy to reach and easy to control**.

Model reduction for nonlinear systems via energy functions

Energy-function-based approaches

- [Scherpen, 1993] introduced the concept of nonlinear balancing via energy functions for (locally) stable, open-loop nonlinear systems.
- HJB balancing [Scherpen and Van der Schaft, 1994], $\mathcal{H}_\infty$ balancing [Scherpen, 1996]
- [Newman and Krishnaprasad, 2000] : controllability energy function is related to the stationary density p_∞ of a Markov process; suggest to solve Fokker-Planck equations
- Symbolic computing toolbox: [Krener, 2008]
- [Fujimoto and Tsubakino, 2008] use Taylor series for open-loop controllability and observability energy functions ($n = 4$)
- Interpretation from a Hankel singular value perspective: [Fujimoto and Scherpen, 2010]
- Machine-learning for balancing transformation based on RKHS [Bouvrie and Hamzi, 2017]

Gramian-based approaches (linear transformation $\Rightarrow$ quadratic energy function)

- Empirical Gramians for nonlinear systems [Lall et al., 2002]
- Algebraic Gramians for local balancing [Gray and Verriest, 2006, Benner and Goyal, 2017, Kramer and Willcox, 2019].

Nonlinear open-loop observability & controllability energy fcts.

For *stable* nonlinear systems controllability and observability energy functions are fully nonlinear, and can be defined [Scherpen, 1993] as

$$\mathcal{E}_c(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2(-\infty,0] \\ \mathbf{x}(-\infty)=\mathbf{0} \\ \mathbf{x}(0)=\mathbf{x}_0}} \frac{1}{2}\int_{-\infty}^{0} \|\mathbf{u}(t)\|^2 \mathrm{d}t, \qquad \mathcal{E}_o(\mathbf{x}_0) := \frac{1}{2}\int_{0}^{\infty} \|\mathbf{y}(t)\|^2 \mathrm{d}t$$

- $\mathcal{E}_c(\mathbf{x}_0)$: minimum energy to steer system from $\mathbf{x}(-\infty)=\mathbf{0}$ to $\mathbf{x}(0)=\mathbf{x}_0$.
- $\mathcal{E}_o(\mathbf{x}_0)$: output energy generated by $\mathbf{x}_0 \neq 0$ and $\mathbf{u}(t)\equiv\mathbf{0}$.

Energy functions are solutions to Hamilton-Jacobi equations:

$$\begin{aligned} 0 =& \frac{\partial \mathcal{E}_o(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) + \frac{1}{2}\mathbf{h}(\mathbf{x})^\top \mathbf{h}(\mathbf{x}), \\ 0 =& \frac{\partial \mathcal{E}_c(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) + \frac{1}{2}\frac{\partial \mathcal{E}_c(\mathbf{x})}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_c(\mathbf{x})}{\partial \mathbf{x}}. \end{aligned}$$

- $\mathcal{E}_o$ exists if $\mathbf{f}$ is asymptotically stable in a neighborhood of the origin
- $\mathcal{E}_c$ exists if $-\left(\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_c(\mathbf{x})}{\partial \mathbf{x}}\right)$ is asympt. stable in a neighborhood of origin.

HJB-balancing energy functions

HJB balancing [Scherpen and Van der Schaft, 1994] (applicable to unstable systems) defines the *past* and *future energy function* as

$$\mathcal{E}^-(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2(-\infty,0]\\ \mathbf{x}(-\infty)=\mathbf{0}\\ \mathbf{x}(0)=\mathbf{x}_0}} \frac{1}{2}\int_{-\infty}^{0} \|\mathbf{y}(t)\|^2 + \|\mathbf{u}(t)\|^2 \mathrm{d}t$$

$$\mathcal{E}^+(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2[0,\infty)\\ \mathbf{x}(0)=\mathbf{x}_0\\ \mathbf{x}(\infty)=\mathbf{0}}} \frac{1}{2}\int_{0}^{\infty} \|\mathbf{y}(t)\|^2 + \|\mathbf{u}(t)\|^2 \mathrm{d}t$$

and they are solutions to the Hamilton-Jacobi-Bellman equation

$$0 = \frac{\partial \mathcal{E}^-(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) + \frac{1}{2}\frac{\partial \mathcal{E}^-(\mathbf{x})}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}^-(\mathbf{x})}{\partial \mathbf{x}} - \frac{1}{2}\mathbf{h}(\mathbf{x})^\top \mathbf{h}(\mathbf{x})$$

$$0 = \frac{\partial \mathcal{E}^+(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{1}{2}\frac{\partial \mathcal{E}^+(\mathbf{x})}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}^+(\mathbf{x})}{\partial \mathbf{x}} + \frac{1}{2}\mathbf{h}(\mathbf{x})^\top \mathbf{h}(\mathbf{x}).$$

Note: LQG-balancing [Verriest, 1981, Jonckheere and Silverman, 1983] and HJB-balancing are identical concepts for linear systems.

$\mathcal{H}_\infty$ energy functions

Definition [Scherpen, 1996]

For a nonlinear system, the $\mathcal{H}_\infty$ past energy in the state $\mathbf{x}_0$ is defined for $0 < \gamma \neq 1$ as

$$\mathcal{E}_\gamma^-(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2(-\infty,0] \\ \mathbf{x}(-\infty)=\mathbf{0},\ \mathbf{x}(0)=\mathbf{x}_0}} \frac{1}{2}\int_{-\infty}^{0} (1-\gamma^{-2})\|\mathbf{y}(t)\|^2 + \|\mathbf{u}(t)\|^2 \mathrm{d}t$$

and the $\mathcal{H}_\infty$ future energy in the state $\mathbf{x}_0$ is defined for $\gamma > 1$ as

$$\mathcal{E}_\gamma^+(\mathbf{x}_0) := \min_{\substack{\mathbf{u}\in L_2[0,\infty) \\ \mathbf{x}(0)=\mathbf{x}_0,\ \mathbf{x}(\infty)=\mathbf{0}}} \frac{1}{2}\int_{0}^{\infty} \|\mathbf{y}(t)\|^2 + \left(\frac{1}{1-\gamma^{-2}}\right)\|\mathbf{u}(t)\|^2 \mathrm{d}t$$

and for $0 < \gamma < 1$ as

$$\mathcal{E}_\gamma^+(\mathbf{x}_0) := \max_{\substack{\mathbf{u}\in L_2[0,\infty) \\ \mathbf{x}(0)=\mathbf{x}_0,\ \mathbf{x}(\infty)=\mathbf{0}}} \frac{1}{2}\int_{0}^{\infty} \|\mathbf{y}(t)\|^2 + \left(\frac{1}{1-\gamma^{-2}}\right)\|\mathbf{u}(t)\|^2 \mathrm{d}t.$$

Hamilton-Jacobi equations for $\mathcal{H}_\infty$ balancing

Theorem [Scherpen, 1996, Thm 5.2]

Assume that the HJB equation

$$0 = \frac{\partial \mathcal{E}_\gamma^-(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) + \frac{1}{2}\frac{\partial \mathcal{E}_\gamma^-}{\partial \mathbf{x}}(\mathbf{x})\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_\gamma^-(\mathbf{x})}{\partial \mathbf{x}} - \frac{1}{2}(1-\gamma^{-2})\mathbf{h}(\mathbf{x})^\top \mathbf{h}(\mathbf{x})$$

has a solution with $\mathcal{E}_\gamma^-(\mathbf{0}) = 0$ that also satisfies that $-\left(\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_\gamma^-(\mathbf{x})}{\partial \mathbf{x}}\right)$ is asymptotically stable. Then this solution is the past energy function $\mathcal{E}_\gamma^-(\mathbf{x})$. Furthermore, assume that the HJB equation

$$0 = \frac{\partial \mathcal{E}_\gamma^+(\mathbf{x})}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{1}{2}(1-\gamma^{-2})\frac{\partial \mathcal{E}_\gamma^+(\mathbf{x})}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_\gamma^+}{\partial \mathbf{x}}(\mathbf{x}) + \frac{1}{2}\mathbf{h}(\mathbf{x})^\top \mathbf{h}(\mathbf{x})$$

has a solution with $\mathcal{E}_\gamma^+(\mathbf{0}) = 0$ which satisfies that $\left(\mathbf{f}(\mathbf{x}) - (1-\gamma^{-2})\mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \frac{\partial^\top \mathcal{E}_\gamma^+}{\partial \mathbf{x}}(\mathbf{x})\right)$ is asymptotically stable. Then this solution is the future energy function.

Observations

1. For $\gamma = \sqrt{1/2}$ the past and future energy functions are identical:

$$\mathcal{E}^-_{\gamma=\frac{1}{\sqrt{2}}}(\mathbf{x}) = \mathcal{E}^+_{\gamma=\frac{1}{\sqrt{2}}}(\mathbf{x}).$$

2. The $\mathcal{H}_\infty$ energy functions are related to HJB balancing as [Scherpen, 1996]

$$\lim_{\gamma\to\infty} \mathcal{E}^-_\gamma(\mathbf{x}) = \mathcal{E}^-(\mathbf{x}). \qquad \lim_{\gamma\to\infty} \mathcal{E}^+_\gamma(\mathbf{x}) = \mathcal{E}^+(\mathbf{x}).$$

3. Under certain technical conditions we also have that the $\mathcal{H}_\infty$ energy functions approach the standard open-loop balancing energy functions:

$$\lim_{\gamma\to 1} \mathcal{E}^+_\gamma(\mathbf{x}) = \mathcal{E}_o(\mathbf{x}), \qquad \lim_{\gamma\to 1} \mathcal{E}^-_\gamma(\mathbf{x}) = \mathcal{E}_c(\mathbf{x}).$$

4. For an LTI system, $\mathcal{E}^-_\gamma(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}^\top \mathbf{Y}_\infty^{-1}\mathbf{x}$ and $\mathcal{E}^+_\gamma(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}^\top \mathbf{X}_\infty \mathbf{x}$, where $\mathbf{Y}_\infty,\ \mathbf{X}_\infty$ are the usual stabilizing positive definite solutions to the $\mathcal{H}_\infty$ AREs

$$\mathbf{A}\mathbf{Y}_\infty + \mathbf{Y}_\infty\mathbf{A}^\top + \mathbf{B}\mathbf{B}^\top - (1-\gamma^{-2})\mathbf{Y}_\infty\mathbf{C}^\top\mathbf{C}\mathbf{Y}_\infty = \mathbf{0},$$
$$\mathbf{A}^\top\mathbf{X}_\infty + \mathbf{X}_\infty\mathbf{A} + \mathbf{C}^\top\mathbf{C} - (1-\gamma^{-2})\mathbf{X}_\infty\mathbf{B}\mathbf{B}^\top\mathbf{X}_\infty = \mathbf{0}.$$

Example: One-dimensional quadratic dynamical system

Consider the equation

$$\dot{x}(t) = ax(t) + \mathrm{n}x(t)^2 + bu(t), \qquad y(t) = cx(t).$$

With $\eta = 1 - \gamma^{-2}$ the HJB equation is

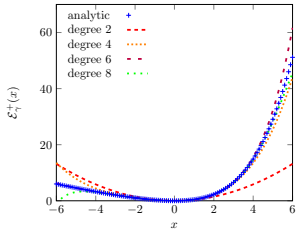
$$0 = \frac{\mathrm{d}\,\mathcal{E}_\gamma^+}{\mathrm{d}\,x}(x)[ax + \mathrm{n}x^2] - \frac{1}{2}b^2\eta\left(\frac{\mathrm{d}\,\mathcal{E}_\gamma^+}{\mathrm{d}\,x}(x)\right)^2 + \frac{1}{2}c^2x^2,$$

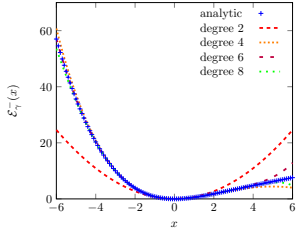
with analytical solution

$$\mathcal{E}_\gamma^+(x) = \frac{1}{b^2\eta}\left(\mp\frac{ab^2c^2\eta\sqrt{x^2((a+\mathrm{n}x)^2+b^2c^2\eta)}\log\left(\sqrt{(a+\mathrm{n}x)^2+b^2c^2\eta}+a+\mathrm{n}x\right)}{2n^2x\sqrt{(a+\mathrm{n}x)^2+b^2c^2\eta}}\right.$$
$$\left.\pm\frac{\sqrt{x^2((a+\mathrm{n}x)^2+b^2c^2\eta)}\left(\frac{(a+\mathrm{n}x)^2}{3\mathrm{n}}-\frac{a(a+\mathrm{n}x)}{2\mathrm{n}}+\frac{b^2c^2\eta}{3n}\right)}{\mathrm{n}x}+\frac{ax^2}{2}+\frac{\mathrm{n}x^3}{3}\right)$$

Figure: energy functions, $a = -2$, $b = 2$, $\mathrm{n} = 1, c = 2, \gamma = \sqrt{2}$.

Need higher degree terms to approximate energy functions!



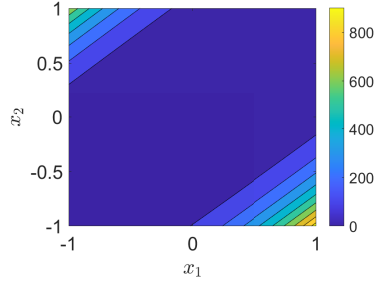


Two-dimensional example

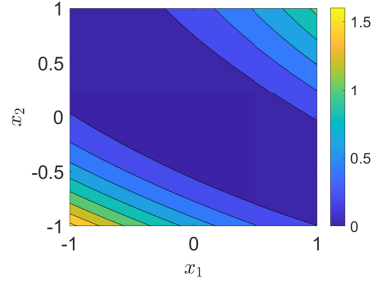
We modify the 2d nonlinear example from [Kawano and Scherpen, 2016, IV.C] :

$$\dot{\mathbf{x}} = \begin{bmatrix} -1 & 1 \\ 0 & -1 \end{bmatrix} \mathbf{x} + \begin{bmatrix} -x_2^2 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} \mathbf{u}, \qquad \mathbf{y} = [1\ 1]\mathbf{x}$$

- Plot for polynomial approximations with $d = 4$ for energy functions, and $\eta = 0.1$ ($\gamma \approx 1.054$) and
- Quadratic approximations again would not be sufficient (higher order terms needed)



$\mathcal{E}_\gamma^-(\mathbf{x})$



$\mathcal{E}_\gamma^+(\mathbf{x})$

Worksheet: Assume LTI system and obtain HJB solution

Part 2:
Computing energy functions via polynomial approximations

Notation and setting

- **Polynomial nonlinear systems** for scalability:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \sum_{k=2}^{\ell} \mathbf{F}_k \mathbf{x}^{\textcircled{k}}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t).$$

  For now, assume quadratic nonlinear system ($\ell = 2$ and $\mathbf{F}_2 = \mathbf{F}$);

- Define k-term Kronecker product of $\mathbf{x}$:

$$\mathbf{x}^{\textcircled{k}} := \underbrace{\mathbf{x} \otimes \ldots \otimes \mathbf{x}}_{k \text{ times}}.$$

- Define the *d-way Lyapunov matrix*/special *Kronecker sum*:

$$\mathcal{L}_d(\mathbf{A}) := \underbrace{\mathbf{A} \otimes \ldots \otimes \mathbf{I}}_{d \text{ times}} + \cdots + \underbrace{\mathbf{I} \otimes \ldots \otimes \mathbf{A}}_{d \text{ times}}.$$

- Define $\eta := (1 - \gamma^{-2})$ and note that $\eta \in (-\infty, 1)$ since $\gamma > 0$.

Symmetry considerations

For convenience and to ensure a unique representation of the coefficients, we impose symmetry of our coefficients in all monomial terms in the energy functions.

Definition (Symmetric Coefficients)

A monomial term with real coefficients $\mathbf{w}_d^\top \mathbf{x}^{\textcircled{d}}$ has *symmetric coefficients* if it satisfies

$$\mathbf{w}_d^\top (\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \cdots \otimes \mathbf{a}_d) = \mathbf{w}_d^\top (\mathbf{a}_{i_1} \otimes \mathbf{a}_{i_2} \otimes \cdots \otimes \mathbf{a}_{i_d}),$$

where the indices $\{i_k\}_{k=1}^d$ are any permutation of $1, \ldots, d$.

- This definition generalizes the definition of symmetry from matrices to tensors. For example,

$$\mathbf{w}_2^\top (\mathbf{a} \otimes \mathbf{b}) = \mathbf{w}_2^\top (\mathbf{b} \otimes \mathbf{a}) \quad \forall \mathbf{a}, \mathbf{b} \quad \Leftrightarrow \quad (\mathbf{a}^\top \otimes \mathbf{b}^\top)\mathbf{w}_2 = (\mathbf{b}^\top \otimes \mathbf{a}^\top)\mathbf{w}_2.$$

  Hence, using $\mathbf{w}_2 = \text{vec}(\mathbf{W}_2)$, we have $\mathbf{b}^\top \mathbf{W}_2 \mathbf{a} = \mathbf{a}^\top \mathbf{W}_2 \mathbf{b}$. Since these are real scalars, this implies $\mathbf{W}_2 = \mathbf{W}_2^\top$.

Symmetry considerations

We also remark that any polynomial can be uniquely written in Kronecker product form with symmetric coefficients. For example,

$$c_1 x_1^2 + c_2 x_1 x_2 + c_3 x_2^2 = [x_1 \ x_2] \begin{bmatrix} c_1 & \frac{1}{2}c_2 \\ \frac{1}{2}c_2 & c_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} c_1 & \frac{1}{2}c_2 & \frac{1}{2}c_2 & c_3 \end{bmatrix} (\mathbf{x} \otimes \mathbf{x}) = \mathbf{F}\mathbf{x}^{\textcircled{2}}.$$

The same set of quadratic terms would be realized with the coefficient matrices corresponding to either $[c_1 \ c_2 \ 0 \ c_3]$ or $[c_1 \ 0 \ c_2 \ c_3]$. However, the requirement of symmetry leads to a unique representation.

- We assume that each row of the coefficient matrices $\mathbf{F}_k$ in the FOM is symmetric as defined above, and that the polynomial representations of the energy functions and controls share this symmetric representation.
- Our algorithms are designed to ensure symmetry in the computed coefficients.

Expansion of future energy function

We approximate the future energy function as

$$\mathcal{E}_\gamma^+(\mathbf{x}) \approx \frac{1}{2}\left(\mathbf{w}_2^\top \mathbf{x}^{②} + \mathbf{w}_3^\top \mathbf{x}^{③} + \ldots + \mathbf{w}_d^\top \mathbf{x}^{ⓓ}\right) = \frac{1}{2}\left(\mathbf{w}_2^\top + \tilde{\mathbf{w}}_3^\top(\mathbf{x}) + \ldots + \tilde{\mathbf{w}}_d^\top(\mathbf{x})\right)\mathbf{x}^{②}.$$

Theorem (K./Gugercin/Borggaard/Balicki '22)

Let $\gamma > \gamma_0 > 0$, (can be computed), $\eta = 1 - \gamma^{-2}$. Let the future energy $\mathcal{E}_\gamma^+(\mathbf{x})$ for the quadratic nonlinear system ($\ell = 2$ and $\mathbf{F}_2 = \mathbf{F}$) be expanded with coefficients $\mathbf{w}_i, i = 2, \ldots, d$. Then, $\mathbf{w}_2 = vec(\mathbf{W}_2)$ where $\mathbf{W}_2$ is the s.p.d. solution to the $\mathcal{H}_\infty$ Riccati equation

$$\mathbf{0} = \mathbf{A}^\top \mathbf{W}_2 + \mathbf{W}_2 \mathbf{A} + \mathbf{C}^\top \mathbf{C} - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top \mathbf{W}_2.$$

For $2 < k \leq d$, let $\tilde{\mathbf{w}}_k \in \mathbb{R}^{n^k}$ solve the linear system

$$\mathcal{L}_k(\mathbf{A}^\top - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top)\tilde{\mathbf{w}}_k = -\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{w}_{k-1} + \frac{\eta}{4} \sum_{\substack{i,j>2 \\ i+j=k+2}} ij \ \mathrm{vec}(\mathbf{W}_i^\top \mathbf{B}\mathbf{B}^\top \mathbf{W}_j).$$

Then, the coefficient vector $\mathbf{w}_k = \mathrm{vec}(\mathbf{W}_k) \in \mathbb{R}^{n^k}$ is obtained by symmetrizing $\tilde{\mathbf{w}}_k$.

Proof idea

From the polynomial energy function it follows that

$$\begin{aligned}\frac{\partial \mathcal{E}_\gamma^+(\mathbf{x})}{\partial \mathbf{x}} =& \frac{1}{2}\left(\mathbf{w}_2^\top(\mathbf{I}\otimes\mathbf{x}) + \mathbf{w}_2^\top(\mathbf{x}\otimes\mathbf{I})\right.\\ &+\mathbf{w}_3^\top(\mathbf{I}\otimes\mathbf{x}\otimes\mathbf{x}) + \mathbf{w}_3^\top(\mathbf{x}\otimes\mathbf{I}\otimes\mathbf{x}) + \mathbf{w}_3^\top(\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{I})\\ &+\mathbf{w}_4^\top(\mathbf{I}\otimes\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{x}) + \mathbf{w}_4^\top(\mathbf{x}\otimes\mathbf{I}\otimes\mathbf{x}\otimes\mathbf{x}) + \mathbf{w}_4^\top(\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{I}\otimes\mathbf{x}) + \mathbf{w}_4^\top(\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{I})\\ &\left.+\cdots\right).\end{aligned}$$

Given $\mathbf{g}(\mathbf{x}) = \mathbf{B}$, $\mathbf{h}(\mathbf{x}) = \mathbf{C}\mathbf{x}$, $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{F}(\mathbf{x}\otimes\mathbf{x})$ the HBJ reads as

$$0 = \frac{\partial \mathcal{E}_\gamma^+(\mathbf{x})}{\partial \mathbf{x}}(\mathbf{A}\mathbf{x} + \mathbf{F}(\mathbf{x}\otimes\mathbf{x})) - \frac{1}{2}(1-\gamma^{-2})\frac{\partial \mathcal{E}_\gamma^+(\mathbf{x})}{\partial \mathbf{x}}\mathbf{B}\mathbf{B}^\top\frac{\partial^\top \mathcal{E}_\gamma^+}{\partial \mathbf{x}}(\mathbf{x}) + \frac{1}{2}\mathbf{x}^\top\mathbf{C}^\top\mathbf{C}\mathbf{x},$$

- We now collect terms by degree of $\mathbf{x}$, starting with quadratic, to cubic, to higher-order.
- We can pull out $\mathbf{x}^{\textcircled{k}}$'s etc and set terms inside to zero (similar to what you did for the LTI into HJB example)

Expansion of past energy function

We approximate the past energy function as

$$\mathcal{E}_\gamma^-(\mathbf{x}) \approx \frac{1}{2}\left(\mathbf{v}_2^\top \mathbf{x}^{②} + \mathbf{v}_3^\top \mathbf{x}^{③} + \cdots \mathbf{v}_d^\top \mathbf{x}^{ⓓ}\right).$$

Theorem (K./Gugercin/Borggaard/Balicki '22)

Let $\gamma > \gamma_0 > 0$, (can be computed), $\eta = 1 - \gamma^{-2}$. Let the past energy function $\mathcal{E}_\gamma^-(\mathbf{x})$ for the quadratic nonlinear system ($\ell = 2$ and $\mathbf{F}_2 = \mathbf{F}$) be expanded as above with the coefficients $\mathbf{v}_i, i = 2, 3, \ldots, d$. Then, $\mathbf{v}_2 = \mathrm{vec}(\mathbf{V}_2)$ where $\mathbf{V}_2$ is the symmetric positive definite solution to the $\mathcal{H}_\infty$ Riccati equation

$$\mathbf{0} = \mathbf{A}^\top \mathbf{V}_2 + \mathbf{V}_2 \mathbf{A} - \eta \mathbf{C}^\top \mathbf{C} + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top \mathbf{V}_2.$$

For $2 < k \leq d$, let let $\tilde{\mathbf{v}}_k \in \mathbb{R}^{n^k}$ solve the linear system

$$\mathcal{L}_k(\mathbf{A}^\top + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top)\tilde{\mathbf{v}}_k = -\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{v}_{k-1} - \frac{1}{4} \sum_{\substack{i,j>2 \\ i+j=k+2}} ij \ \mathrm{vec}(\mathbf{V}_i^\top \mathbf{B}\mathbf{B}^\top \mathbf{V}_j).$$

Then, the coefficient vector $\mathbf{v}_k = \mathrm{vec}(\mathbf{V}_k) \in \mathbb{R}^{n^k}$ is obtained by the symmetrizing $\tilde{\mathbf{v}}_k$.

Algorithm for Energy Function Approximation

Algorithm 1 Computing HJB energy function approximations: $\mathcal{E}_\gamma^-(\mathbf{x})$ and $\mathcal{E}_\gamma^+(\mathbf{x})$.

Input: System matrices $\mathbf{A}, \mathbf{F}, \mathbf{B}, \mathbf{C}$; polynomial degree d; constant $\gamma > \gamma_0 > 0$, $\gamma \neq 1$.

Output: Coefficients $\{\mathbf{v}_i\}_{i=2}^d$ of the past energy and $\{\mathbf{w}_i\}_{i=2}^d$ of the future energy functions.

1: Set $\eta = (1 - \gamma^{-2})$.

2: Solve the $\mathcal{H}_\infty$ Riccati equations

$$\mathbf{0} = \mathbf{A}^\top \mathbf{V}_2 + \mathbf{V}_2 \mathbf{A} - \eta \mathbf{C}^\top \mathbf{C} + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top \mathbf{V}_2,$$
$$\mathbf{0} = \mathbf{A}^\top \mathbf{W}_2 + \mathbf{W}_2 \mathbf{A} + \mathbf{C}^\top \mathbf{C} - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top \mathbf{W}_2$$

and set $\mathbf{v}_2 = \mathrm{vec}(\mathbf{V}_2)$ and $\mathbf{w}_2 = \mathrm{vec}(\mathbf{W}_2)$.

3: **For** $k = 3, 4, \ldots, d$: Solve the systems for $\tilde{\mathbf{v}}_d$ and $\tilde{\mathbf{w}}_d$:

$$\mathcal{L}_k(\mathbf{A}^\top + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top)\tilde{\mathbf{v}}_k = -\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{v}_{k-1} - \frac{1}{4} \sum_{\substack{i,j>2 \\ i+j=k+2}} ij \ \mathrm{vec}(\mathbf{V}_i^\top \mathbf{B}\mathbf{B}^\top \mathbf{V}_j)$$

$$\mathcal{L}_k(\mathbf{A}^\top - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top)\tilde{\mathbf{w}}_k = -\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{w}_{k-1} + \frac{\eta}{4} \sum_{\substack{i,j>2 \\ i+j=k+2}} ij \ \mathrm{vec}(\mathbf{W}_i^\top \mathbf{B}\mathbf{B}^\top \mathbf{W}_j)$$

4: Symmetrize $\tilde{\mathbf{w}}_k$ and $\tilde{\mathbf{v}}_k$ to obtain $\mathbf{w}_k$ and $\mathbf{v}_k$.

Solvability of the coefficient systems

Theorem [Thm 8, K./Gugerin/Borggaard/Balicki]

Let $\gamma > \gamma_0 \geq 0$ hold so that the $\mathcal{H}_\infty$ ARE is solvable and $\eta = 1 - \gamma^{-2}$. Then, for any $k = 1, \ldots, d$ the matrices $\mathcal{L}_k(\mathbf{A}^\top - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top)$ and $\mathcal{L}_k(\mathbf{A}^\top + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top)$ are invertible, thus the coefficients $\mathbf{w}_i$ and $\mathbf{v}_i$ are uniquely determined.

Proof idea: A result from [Horn et al., 1994] states that for any $\mathbf{M} \in \mathbb{R}^{n \times n}$ the spectrum

$$\Lambda\left(\mathcal{L}_k(\mathbf{M})\right) = \left\{ \sum_{i \in \mathcal{P}_k} \lambda_i : \lambda_i \in \Lambda(\mathbf{M}) \right\},$$

where $\mathcal{P}_k$ denotes the set of all possible selection of k-indices from the set $\{1, 2, \ldots, n\}$. Since $\mathbf{W}_2$ is the unique stabilizing solution of the $\mathcal{H}_\infty$ Riccati equation, $\mathbf{M} = \mathbf{A}^\top - \eta \mathbf{W}_2 \mathbf{B}\mathbf{B}^\top$ has all eigenvalues in the open left-half plane. Therefore, all eigenvalues of $\mathcal{L}_k(\mathbf{M})$ are contained in the open left-half plane as well, thus $\mathcal{L}_k(\mathbf{M})$ is invertible and the $\tilde{\mathbf{w}}_k$ can be uniquely determined. For the second statement, we use that

$$\mathbf{A}^\top + \mathbf{V}_2 \mathbf{B}\mathbf{B}^\top = -\mathbf{V}_2 \mathbf{A} \mathbf{V}_2^{-1} + \eta \mathbf{C}^\top \mathbf{C} \mathbf{V}_2^{-1}.$$

and use similar arguments.

Solving Tensor Systems Efficiently

- For some $\mathbf{b}$, the kth-order polynomial terms require solving linear systems of the form

$$\mathcal{L}_k(\mathbf{A}^\top + \mathbf{V}_2\mathbf{B}\mathbf{B}^\top)\tilde{\mathbf{v}}_k = \mathbf{b},$$

  which grow exponentially in k and polynomially in n.

- We leverage the k-way Bartels-Stewart algorithm in [Borggaard and Zietsman, 2021]. By first performing a Schur factorization[3] of $\mathbf{A}^\top + \mathbf{V}_2\mathbf{B}\mathbf{B}^\top = \mathbf{U}\mathbf{T}\mathbf{U}^*$ and defining a matrix $\mathbf{U}^{\textcircled{k}} = \mathbf{U} \otimes \mathbf{U} \otimes \cdots \otimes \mathbf{U} \in \mathbb{R}^{n^k \times n^k}$, we convert the above linear system to

$$[\mathbf{U}^{\textcircled{k}}]^* \mathcal{L}_k(\mathbf{A}^\top + \mathbf{V}_2\mathbf{B}\mathbf{B}^\top)[\mathbf{U}^{\textcircled{k}}]\hat{\mathbf{v}}_k = \hat{\mathbf{b}}, \quad \text{where} \quad \hat{\mathbf{v}}_k = [\mathbf{U}^{\textcircled{k}}]^*\tilde{\mathbf{v}}_k, \hat{\mathbf{b}} = [\mathbf{U}^{\textcircled{k}}]^*\mathbf{b}.$$

- Resulting system $\mathcal{L}_k(\mathbf{T})\hat{\mathbf{v}}_k = \hat{\mathbf{b}}$ is upper triangular and can be solved by a block backsubstitution procedure requiring n^{k-1} linear system solutions of size n.
- From here, we can compute the solution $\tilde{\mathbf{v}}_k = \mathbf{U}^{\textcircled{k}}\hat{\mathbf{v}}_k$.
- **Overall computational cost of solving k-th order system is $O(n^{k+1})$.**

[3] Note: Schur decomposition of $\mathbf{A}$ okay for medium-scale problems to avoid performing any operation in n^k-dim. space. For large-scale problems: iterative methods to exploit tensor structure such as the Krylov methods [Kressner and Tobler, 2010] or low-rank ADI type methods [Benner and Saak, 2013].

Total Cost of Solving for Coefficients

- Next, we have a look at the right-hand side of the linear systems:

$$\mathbf{b} = -\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{v}_{k-1} - \frac{1}{4} \sum_{\substack{i,j>2 \\ i+j=k+2}} ij \ \text{vec}(\mathbf{V}_i^\top \mathbf{B}\mathbf{B}^\top \mathbf{V}_j)$$

- We efficiently compute products $\mathcal{L}_{k-1}(\mathbf{F}^\top)\mathbf{v}_{k-1}$ in $O(kn^k)$; a direct product of the $n^{2k} \times n^k$ matrix times a vector would require $O(n^{3k})$ operations.
- Cost of forming the summation terms is dominated by multiplying the stored matrices $\mathbf{V}_i^\top \mathbf{B}$ and $\mathbf{B}^\top \mathbf{V}_j$. The cost of forming the summation terms are $O(kmn^k)$.
- We perform a final step to impose symmetry.
- **In sum, the computational complexity of computing a dth order approximation of the energy functions is (for $n > dm$):**

$$O(n^{d+1}) \qquad \text{(vs } O(n^{3d}) \text{ for naive implementation)}$$

Numerical Results: Burgers' equation

We consider the one-dimensional Burgers' equation

$$z_t(x,t) = \epsilon z_{xx}(x,t) - \frac{1}{2}\left(z^2(x,t)\right)_x + \sum_{j=1}^{m} b_j^m(x)u_j(t),$$

$$y_i(t) = \int_{\chi_{[(i-1)/p,\, i/p]}} z(x,t)\mathrm{d}x, \qquad i = 1,\ldots,p,$$

- periodic BCs $z(0,t) = z(1,t)$ and $z_x(0,t) = z_x(1,t)$
- IC: $z(\cdot,0) = z_0(\cdot) \in H_0^1(0,1)$
- $\epsilon = 0.001$ to make the nonlinearity significant.
- $p = 4$ outputs: spatial averages
- $m = 4$ controls/inputs with $b_j^m(x) = \chi_{[(j-1)/m,\, j/m]}(x)$.

The discretized system has the form

$$\widetilde{\mathbf{E}}\dot{\mathbf{z}} = \widetilde{\mathbf{A}}\mathbf{z} + \widetilde{\mathbf{N}}_2\left(\mathbf{z}\otimes\mathbf{z}\right) + \widetilde{\mathbf{B}}\mathbf{u}$$
$$\mathbf{y} = \widetilde{\mathbf{C}}\mathbf{z},$$

A change of variables $\mathbf{x} = \widetilde{\mathbf{E}}^{1/2}\mathbf{z}$ and redefining $\mathbf{A} = \mathbf{S}^{-1}\widetilde{\mathbf{A}}\mathbf{S}^{-1}$, $\mathbf{B} = \mathbf{S}^{-1}\widetilde{\mathbf{B}}$, $\mathbf{C} = \widetilde{\mathbf{C}}\mathbf{S}^{-1}$, $\widetilde{\mathbf{N}}_2 = \mathbf{N}_2(\mathbf{S}^{-1}\otimes\mathbf{S}^{-1})$ leads to a system with $\mathbf{E} = \mathbf{I}$.

Burgers' equation: Computing the energy functions

$d = 3$, **convergence w.r.t** n.

n	n^3	CPU sec	$\mathcal{E}_3^+(\mathbf{z}_0)$
8	5.1200e+02	2.96e-02	1.144557e-06
16	4.0960e+03	1.08e-02	1.116244e-06
32	3.2768e+04	5.96e-02	1.093503e-06
64	2.6214e+05	4.40e-01	1.099870e-06
128	2.0972e+06	4.29e+00	1.097715e-06
256	1.6777e+07	5.48e+01	1.095300e-06
512	1.3422e+08	6.63e+02	1.096322e-06
1024	1.0737e+09	7.93e+03	1.096093e-06

$n = 8$ **approximation w.r.t.** d.

d	$\mathcal{E}_d^-(\mathbf{z}_0)$	$\mathcal{E}_d^+(\mathbf{z}_0)$
2	3.161325e-05	1.146135e-06
3	2.731740e-05	1.144557e-06
4	2.370917e-05	1.144783e-06
5	2.593642e-05	1.144792e-06
6	2.662942e-05	1.144791e-06
7	2.519892e-05	1.144791e-06
8	2.538956e-05	1.144791e-06

Observations

- Convergence of the energy function as n increases (set gain $\eta = 0.9$ for HJB equation)
- Flop-count analysis predicts computational cost with growth of $O(n^4)$ (since $d = 3$), but CPU times scale as $O(n^{2.84})$. For $d = 4$ case, we find growth of $O(n^{3.57})$. This suggests that CPU time scales more like $O(n^d)$ for our problem sizes.
- First time where a high-resolution approximation of the cubic term in the energy function
- For $n = 1024$, this requires solving linear systems of size 10^9, which, through an efficient BLAS-3 level implementation can be performed in less than 5h CPU time.

Numerical Results: Kuramoto-Sivashinsky equation

Consider the domain $x \in (0, 1)$ and $t > 0$, and

$$z_t(x,t) = -\epsilon z_{xx}(x,t) - \epsilon^2 z_{xxxx}(x,t) - \epsilon(z(x,t)^2)_x + \sum_{j=1}^{m} b_j^m(x) u_j(t)$$

- periodic BCs $z(0,t) = z(1,t)$ and $z_x(0,t) = z_x(1,t)$
- same control input functions b_j^m and observation as for Burgers's equation
- $m = 5$ (five controls) and $p = 2$ (two outputs), and here choosing $\eta = 0.1$
- parameter $\epsilon = 1/13.0291^2$, which is known to exhibit heteroclinic cycles in the open-loop system
- IC: $z(x,0) = z_0(x) = \frac{0.01}{\sqrt{\epsilon}} \sin(4\pi x)$

Table: $d = 3$, convergence w.r.t n.

n	n^3	CPU sec	$\mathcal{E}_3^+(\mathbf{z}_0)$
16	4.0960e+03	1.20e-02	4.369195e+00
32	3.2768e+04	8.44e-02	5.099752e+00
64	2.6214e+05	5.54e-01	4.793412e+00
128	2.0972e+06	9.14e+00	4.732940e+00
256	1.6777e+07	1.37e+02	4.811878e+00
512	1.3422e+08	1.70e+03	4.827930e+00
1024	1.0737e+09	2.04e+04	4.807904e+00

Table: $n = 16$ approximation w.r.t. d.

d	$\mathcal{E}_d^+(\mathbf{z}_0)$	CPU sec
2	4.3690773e+00	6.81e-03
3	4.3691951e+00	9.88e-03
4	4.3469410e+00	1.37e-01
5	4.3467633e+00	2.40e+00
6	4.3467610e+00	4.39e+01

Part 3:
Simultaneous Balance-and-Reduce Model Reduction on Manifolds

Balancing an LTI system

Recall, that to get the quadratic energy functions, we had to solve the Lyapunov equations:

$$\mathbf{AP} + \mathbf{PA}^\top + \mathbf{BB}^\top = \mathbf{0}, \qquad \mathbf{A}^\top\mathbf{Q} + \mathbf{QA} + \mathbf{C}^\top\mathbf{C} = \mathbf{0}.$$

Definition (Balanced system)

An asymptotically stable LTI system is *balanced* if $\mathbf{P} = \mathbf{Q} = \mathbf{\Sigma} = \text{diag}(\sigma_1, ..., \sigma_n)$.

Theorem (Balancing transformation)

Let $[\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}]$ be asymptotically stable, controllable and observable. Let $\mathbf{P} = \mathbf{RR}^\top$, $\mathbf{Q} = \mathbf{LL}^\top$ be the Cholesky factorizations and $\mathbf{L}^\top\mathbf{R} = \mathbf{U\Sigma V}^\top$ and let

$$\mathbf{T} = \mathbf{RV\Sigma}^{-\frac{1}{2}}, \qquad \mathbf{T}^{-1} = \mathbf{\Sigma}^{-\frac{1}{2}}\mathbf{U}^\top\mathbf{L}^\top.$$

Then $[\widetilde{\mathbf{A}}, \widetilde{\mathbf{B}}, \widetilde{\mathbf{C}}, \widetilde{\mathbf{D}}] = [\mathbf{T}^{-1}\mathbf{AT}, \mathbf{T}^{-1}\mathbf{B}, \mathbf{CT}, \mathbf{D}]$ is a balanced LTI system.

The controllability and observability energy functions of the balanced systems are then:

$$\mathcal{E}_c(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^\top\mathbf{\Sigma}^{-1}\mathbf{x}_0, \qquad \mathcal{E}_o(\mathbf{x}_0) = \frac{1}{2}\mathbf{x}_0^\top\mathbf{\Sigma}\mathbf{x}_0.$$

Claim to fame: A few key results

Since the states of the balanced system are now ordered by observability/controllability properties, we delete the states that are not relevant, i.e., $\widetilde{\mathbf{x}} = [x_1, x_2, \ldots, x_r]$, with $r \ll n$ is the reduced state.

Theorem (Stability and minimality)

Let $[\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}]$ be an asymptotially stable and minimal system. Let the balanced ROM be $[\mathbf{A}_r, \mathbf{B}_r, \mathbf{C}_r, \mathbf{D}_r]$ where $\sigma_r > \sigma_{r+1}$ for the Hankel singular values $\sigma_i, i = 1, \ldots, n$. Then, the ROM is asymptotically stable, minimal and balanced with Gramians $\mathbf{P}_r = \mathbf{Q}_r = \mathrm{diag}(\sigma_1, \ldots, \sigma_r) =: \mathbf{\Sigma}_r$.

Theorem (Error bound)

Let $[\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}]$ be asymptotically stable and balanced with controllability Gramian and observability Gramian $\mathbf{P} = \mathbf{Q} = \mathrm{diag}(\sigma_1 \mathbf{I}_{s_1}, \sigma_2 \mathbf{I}_{s_2}, \ldots, \sigma_k \mathbf{I}_{s_k})$($\sigma$ could be repeated), where $\sigma_1 > \sigma_2 > \ldots > \sigma_k \geqslant \mathbf{0}$. Let $[\mathbf{A}_r, \mathbf{B}_r, \mathbf{C}_r, \mathbf{D}_r]$ be the balanced ROM with $r = s_1 + s_2 + \ldots + s_l$ for some $l \leq k$. Then, we have:

$$||\mathbf{G} - \mathbf{G}_r||_{\mathcal{H}_\infty} \leqslant \sum_{j=l+1}^{k} 2\sigma_j.$$

Key "Ingredients" for balancing of nonlinear systems

Let's now consider a **quadratic nonlinear systems** again:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{F}\mathbf{x}^{②}(t) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t).$$

The key ingredients for nonlinear balancing are:

1. Energy functions: controllability/observability; past/future; HJB energy functions ($\Rightarrow$ Part 1 & 2)
2. A nonlinear transformation $\mathbf{x} = \Phi(\mathbf{z})$ (instead of $\mathbf{x} = \mathbf{T}\mathbf{z}$) that "diagonalizes" the energy
3. Singular value (functions) $\sigma_i(z_i)$ to decide on which states to truncate (instead of constant SVs for LTI)
4. A definition of the nonlinearly balanced ROM

Input-normal/output-diagonal balancing

We have computed polynomial expansions of the past and future energy functions of the form

$$\mathcal{E}_\gamma^-(\mathbf{x}) \approx \frac{1}{2}\left(\mathbf{v}_2^\top \mathbf{x}^{②} + \mathbf{v}_3^\top \mathbf{x}^{③} + \cdots \mathbf{v}_d^\top \mathbf{x}^{ⓓ}\right) \quad \text{and} \quad \mathcal{E}_\gamma^+(\mathbf{x}) \approx \frac{1}{2}\left(\mathbf{w}_2^\top \mathbf{x}^{②} + \mathbf{w}_3^\top \mathbf{x}^{③} + \ldots + \mathbf{w}_d^\top \mathbf{x}^{ⓓ}\right)$$

Theorem [Fujimoto and Scherpen, 2010, Thm. 2]

Suppose the Jacobian linearization of the nonlinear system is controllable, observable, and asymptotically stable. Then there is a neighborhood $\mathcal{W}$ of the origin and a coordinate transformation $\mathbf{x} = \Phi(\mathbf{z})$ on $\mathcal{W}$ with $\mathbf{z} = [z_1, z_2, \ldots, z_n]$ such that the energy functions have **input-normal** form:

$$\mathcal{E}_\gamma^-(\Phi(\mathbf{z})) = \frac{1}{2}\sum_{i=1}^{n} z_i^2, \qquad \mathcal{E}_\gamma^+(\Phi(\mathbf{z})) = \frac{1}{2}\sum_{i=1}^{n} \xi_i^2(z_i) z_i^2.$$

We assume that the state transformation is analytic, so

$$\mathbf{x} = \Phi(\mathbf{z}) = \mathbf{T}_1\mathbf{z} + \mathbf{T}_2\mathbf{z}^{②} + \ldots + \mathbf{T}_k\mathbf{z}^{ⓚ}$$

where $\mathbf{T}_k \in \mathbb{R}^{n \times n^k}$ are the polynomial coefficients and $\mathbf{T}_1$ is nonsingular.

Computation of tensors for transformation

Theorem (K./Gugercin/Borggaard/ '23)

Let $\mathbf{W}_2 = \mathbf{L}\mathbf{L}^\top$ and $\mathbf{V}_2 = \mathbf{R}\mathbf{R}^\top$. Compute the singular value decomposition of $\mathbf{L}^\top\mathbf{R}^{-\top} = \mathcal{U}\mathbf{\Xi}\mathcal{V}^\top$. The linear transformation $\mathbf{T}_1$ and its inverse $\mathbf{T}_1^{-1}$ are given by

$$\mathbf{T}_1 = \mathbf{R}^{-\top}\mathcal{V}, \qquad \mathbf{T}_1^{-1} = \mathbf{\Xi}^{-1}\mathcal{U}^\top\mathbf{L}^\top$$

and they satisfy $\mathbf{T}_1^{-1}\mathbf{V}_2^{-1}\mathbf{W}_2\mathbf{T}_1 = \mathbf{\Xi}^2 = \mathrm{diag}(\xi_1^2(0), \ldots, \xi_n^2(0))$. The higher-order tensors are

$$\mathbf{T}_2 = -\frac{1}{2}\mathbf{T}_1 \ \mathrm{unvec}([\mathbf{T}_1^{③}]^\top \mathbf{v}_3)^\top$$

$$\mathbf{T}_k = -\frac{1}{2}\mathbf{T}_1 \mathrm{unvec}\left(\mathbf{M}_k\right)^\top, \ \text{where} \quad \mathbf{M}_k = \sum_{\substack{i,j>1 \\ i+j=k+1}} \mathrm{vec}\left(\mathbf{T}_j^\top \mathbf{V}_2 \mathbf{T}_i\right) + \sum_{i=3}^{k+1} \mathcal{T}_{i,k+1}^\top \mathbf{v}_i$$

Here, unique tensor products with m terms and and n^l columns are denoted as

$$\mathcal{T}_{m,l} := \sum_{\sum i_j = l} \mathbf{T}_{i_1} \otimes \cdots \otimes \mathbf{T}_{i_m} \in \mathbb{R}^{n^m \times n^l}, \quad i_j \geq 1 \text{ for each } j = 1, \ldots, m,$$

Computation of singular value functions

The state-dependent singular value functions are approximated as

$$\xi_i(z_i) = \xi_i(0) + c_i^{(1)} z_i + c_i^{(2)} z_i^2 + \ldots + c_i^{(\ell)} z_i^\ell, \qquad i = 1, 2, \ldots, n.$$

Define the coefficients of the kth order terms as $\mathbf{c}_k := [c_1^{(k)},\ c_2^{(k)}, \ldots, c_n^{(k)}]^\top$, so that the vector of singular value functions of the input-normal form is

$$\xi(\mathbf{z}) = \boldsymbol{\Xi} \cdot \mathbf{1} + \operatorname{diag}(\mathbf{c}_1)\mathbf{z} + \ldots + \operatorname{diag}(\mathbf{c}_\ell)\mathbf{z}^\ell,$$

Since the transformation matrices $\mathbf{T}_1, \ldots, \mathbf{T}_k$ are already computed, we use the equation

$$\mathcal{E}_\gamma^+(\Phi(\mathbf{z})) = \frac{1}{2} \sum_{i=1}^{n} \xi_i^2(z_i) z_i^2$$

and insert the approximations to obtain

$$\mathbf{z}^\top \mathbf{T}_1^\top \mathbf{W}_2 \mathbf{T}_1 \mathbf{z} + 2\mathbf{z}^\top \mathbf{T}_1^\top \mathbf{W}_2 \Phi^h(\mathbf{z}) + \Phi^h(\mathbf{z})^\top \mathbf{W}_2 \Phi^h(\mathbf{z}) + 2\mathcal{E}_o^h(\Phi(\mathbf{z})) = \sum_{i=1}^{n} z_i^2 \left(\xi_i^2(0) + 2\xi_i(0)\xi_i^h(z_i) + \xi_i^h(z_i)^2 \right).$$

Coefficients of Singular Value Functions

Theorem (K./Gugercin/Borggaard/ '23)

Let $\mathbf{z} = [z_1, z_2, \ldots, z_n]^\top$ be the transformed state and $\mathbf{c}_k = [c_1^{(k)},\ c_2^{(k)}, \ldots, c_n^{(k)}]^\top$ be the vector of n coefficients of the kth order terms. Then,

$$\mathbf{c}_1 = \mathbf{\Xi}^{-1} \left(\text{vec}(\mathbf{T}_2^\top \mathbf{W}_2 \mathbf{T}_1)^\top + \frac{1}{2} \mathbf{w}_3^\top \mathbf{T}_1^{③} \right)_{\mathcal{I}_1}$$

for the indices $\mathcal{I}_1 = \{j \mid j = (i-1)(n^2+n) + i,\ i = 1, \ldots, n\}$. For $k \geq 1$ we obtain

$$\mathbf{c}_k = \frac{1}{2} \mathbf{\Xi}^{-1} \left[\left(\sum_{\substack{i,j \geq 1 \\ i+j=k+2}} \text{vec}\left(\mathbf{T}_j^\top \mathbf{W}_2^\top \mathbf{T}_i \right)^\top + \sum_{i=3}^{k+2} \mathbf{w}_i^\top \mathcal{T}_{i,k+2} \right)_{\mathcal{I}_k} - \sum_{i+j=k} \mathbf{c}_i \odot \mathbf{c}_j \right]$$

where $\mathcal{I}_k$ is the index set $\mathcal{I}_k = \{j \mid j = (i-1) \sum_{l=1}^{k+1} n^l + i,\ i = 1, \ldots, n\}$, and $\odot$ denotes the Hadamard product.

Comparison to the linear case

For LTI systems:

- $\mathbf{T}_i = \mathbf{0}$ for $i \geq 2$ so we recover the usual linear state transformation $\Phi(\mathbf{z}) = \mathbf{T}_1 \mathbf{z}$
- The energy functions are quadratic: $\mathcal{E}_\gamma^-(\mathbf{x}) = \frac{1}{2}\mathbf{v}_2^\top \mathbf{z}^{②}$, and hence $\mathbf{v}_i = \mathbf{0}$ for $i \geq 3$.
- The singular value functions are constant; our algorithm indeed produces $\mathbf{c}_i = \mathbf{0}$ for $i \geq 1$.
- In sum, for LTI, **the energy functions are quadratic, the transformation linear, and the singular value functions constant**.

However, this cascade of degrees does not hold for the general nonlinear case.

- Assume the energy function is exactly cubic, i.e., $\mathcal{E}_\gamma^-(\mathbf{x}) = \frac{1}{2}(\mathbf{v}_2^\top \mathbf{z}^{②} + \mathbf{v}_3^\top \mathbf{z}^{③})$.
- We can still compute $\mathbf{T}_k, k \geq 3$ as $\mathbf{T}_3 \neq \mathbf{0}$ and consequently $\mathbf{T}_k$ is nonzero.
- Similarly the $\mathbf{c}_i$ coefficients can be nonzero.

Thus the degree of the energy function has, in general, no direct impact on the degree of the transformation and singular value functions.

Fully balanced system

- Transformation $\Phi(\mathbf{z})$ brought system in input-normal/output-diagonal form
- Want input-output balanced form, where the singular values appear in both the controllability and observability energy functions.

Theorem [Fujimoto and Scherpen, 2010, Thm. 9]

Suppose that the Jacobian linearization of the nonlinear system is controllable, observable, and asymptotically stable. Then there is a neighborhood $\mathcal{W}$ of the origin and a coordinate transformation $\mathbf{x} = \bar{\Phi}(\bar{\mathbf{z}})$ on $\mathcal{W}$ converting the energy functions into the form

$$\mathcal{E}_c(\bar{\Phi}(\bar{\mathbf{z}})) = \frac{1}{2}\sum_{i=1}^{n} \frac{\bar{z}_i^2}{\sigma_i(\bar{z}_i)}, \qquad \mathcal{E}_o(\bar{\Phi}(\bar{\mathbf{z}})) = \frac{1}{2}\sum_{i=1}^{n} \sigma_i(\bar{z}_i)\bar{z}_i^2.$$

Moreover, if $\mathcal{W} = \mathbb{R}^n$, then the Hankel norm of the nonlinear system is given by

$$\|\Sigma\|_{\mathrm{H}} := \sup_{\mathbf{u}\in L_2(0,\infty), \mathbf{u}\neq\mathbf{0}} \frac{\|\mathcal{H}(\mathbf{u})\|}{\|\mathbf{u}\|} = \sup_{\bar{z}_1} \sigma_1(\bar{z}_1),$$

where $\mathcal{H}$ is the Hankel operator for the nonlinear system.

Balanced high-dimensional model

The nonlinear transformation that brings the dynamical system into a fully balanced coordinate system is

$$\mathbf{x} = \bar{\Phi}(\bar{\mathbf{z}}) = \mathbf{T}_1\mathbf{z} + \mathbf{T}_2\mathbf{z}^{\textcircled{2}} + \cdots + \mathbf{T}_k\mathbf{z}^{\textcircled{k}}$$
$$z_i = \bar{z}_i / \sqrt{\sigma_i(\bar{z}_i)}.$$

The dynamical system when transformed with the input-output balancing transformation $\mathbf{x} = \Phi(\bar{\mathbf{z}})$ (or alternatively the input-normal transform) is

$$\bar{\mathbf{J}}(\bar{\mathbf{z}})\dot{\bar{\mathbf{z}}} = \mathbf{f}(\bar{\Phi}(\bar{\mathbf{z}})) + \mathbf{g}(\bar{\Phi}(\bar{\mathbf{z}}))\mathbf{u},$$

where the Jacobian $\mathbf{J}(\bar{\mathbf{z}}) \in \mathbb{R}^{n\times n}$ of the state-space transformation is given by

$$\bar{\mathbf{J}}(\bar{\mathbf{z}}) := \frac{\mathrm{d}\bar{\Phi}(\bar{\mathbf{z}})}{\mathrm{d}\bar{\mathbf{z}}} = \mathbf{T}_1 + 2\mathbf{T}_2(\bar{\mathbf{z}} \otimes \mathbf{I}) + 3\mathbf{T}_3(\bar{\mathbf{z}} \otimes \bar{\mathbf{z}} \otimes \mathbf{I}) + \ldots$$

which can be computed explicitly without numerical approximation.

How to determine the ROM dimension?

- To determine the reduced dimension r of the ROM, we look for a significant gap in the $\mathcal{H}_\infty$ singular value functions, i.e., we look for the reduced dimension r such that

$$\max_{\bar{z}_r} \sigma_r(\bar{z}_r) \gg \max_{\bar{z}_{r+1}} \sigma_{r+1}(\bar{z}_{r+1})$$

  at a minimum we require that '$>$' holds in a neighborhood of the origin.

- This indicates that the state components $\bar{z}_1, \bar{z}_2, \ldots, \bar{z}_r$ are more important in terms of the past and future energy functions $\mathcal{E}_\gamma^-$ and $\mathcal{E}_\gamma^+$ than the states $\bar{z}_{r+1}, \bar{z}_{r+2}, \ldots, \bar{z}_n$. We therefore set

$$\bar{z}_{r+1} = \bar{z}_{r+2} = \ldots = \bar{z}_n = 0$$

  in the balanced coordinates.

- Define the reduced state vector as

$$\bar{\mathbf{z}}_r = \mathbf{\Psi}_r^\top \; \bar{\mathbf{z}} = [\bar{z}_1, \bar{z}_2, \ldots \bar{z}_r]^\top, \quad \mathbf{\Psi}_r = [\mathbf{I}_r, \; \mathbf{0}]^\top \in \mathbb{R}^{n \times r}.$$

Balanced ROM

The balance-then-reduce strategy suggested in [Scherpen, 1993, Scherpen, 1996] first computes the full balancing transformation, and then truncates the resulting fully balanced system. Applying this to the FOM yields

$$\begin{aligned}\dot{\bar{\mathbf{z}}}_r &= \underbrace{\boldsymbol{\Psi}_r^\top [\bar{\mathbf{J}}([\bar{\mathbf{z}}_r, \mathbf{0}])]^{-1} \mathbf{f}(\bar{\Phi}([\bar{\mathbf{z}}_r, \mathbf{0}]))}_{=:\mathbf{f}_r(\bar{\mathbf{z}}_r)} + \underbrace{\boldsymbol{\Psi}_r^\top [\bar{\mathbf{J}}([\bar{\mathbf{z}}_r, \mathbf{0}])]^{-1} \mathbf{g}(\bar{\Phi}([\bar{\mathbf{z}}_r, \mathbf{0}]))}_{=:\mathbf{g}_r(\bar{\mathbf{z}}_r)} \mathbf{u}, \\ \mathbf{y}_r &= \underbrace{\mathbf{h}(\bar{\Phi}([\bar{\mathbf{z}}_r, \mathbf{0}]))}_{=:\mathbf{h}_r(\bar{\mathbf{z}}_r)}.\end{aligned}$$

The high-dimensional state is reconstructed as $\mathbf{x} \approx \bar{\Phi}([\bar{\mathbf{z}}_r, \mathbf{0}])$.

Two problems with this approach:

1. Simulating the ROM is computationally expensive
2. The transformation is ill-conditioned due to the need to invert **all** Hankel singular values (in analogy to the linear case)

Simultaneous balancing and reduction

Goal: compute the truncated versions of the linear transformations and higher-order tensors $\mathbf{T}_i$ directly without computing the full-order quantities.

Proposition (K./Gugercin/Borggaard/ '23)

Consider a nonlinear dynamical system and define the embedding $\Phi_r : \mathbb{R}^r \mapsto \mathbb{R}^n$ via

$$\mathbf{x} \approx \Phi_r(\bar{\mathbf{z}}_r) := \mathbf{T}_{1,r}\bar{\mathbf{z}}_r + \mathbf{T}_{2,r}\bar{\mathbf{z}}_r^{②} + \cdots + \mathbf{T}_{k,r}\bar{\mathbf{z}}_r^{ⓚ},$$

with $\mathbf{T}_{k,r} \in \mathbb{R}^{n \times r^k}$ and where $\bar{\mathbf{z}}_r \in \mathbb{R}^r$ is the reduced state. Then, the reduced Jacobian can be computed analytically via

$$\mathbf{J}_r(\bar{\mathbf{z}}_r) := \frac{\mathrm{d}\Phi_r(\bar{\mathbf{z}}_r)}{\mathrm{d}\bar{\mathbf{z}}_r} = \mathbf{T}_{1,r} + 2\mathbf{T}_{2,r}(\bar{\mathbf{z}}_r \otimes \mathbf{I}) + 3\mathbf{T}_{3,r}(\bar{\mathbf{z}}_r \otimes \bar{\mathbf{z}}_r \otimes \mathbf{I}) + \cdots \in \mathbb{R}^{n \times r}.$$

so that the nonlinear ROM with $\mathbf{z}_r \in \mathbb{R}^r$ is

$$\dot{\bar{\mathbf{z}}}_r = \underbrace{\mathbf{J}_r(\bar{\mathbf{z}}_r)^\dagger \mathbf{f}(\Phi_r(\bar{\mathbf{z}}_r))}_{=:\mathbf{f}_r(\bar{\mathbf{z}}_r)} + \underbrace{\mathbf{J}_r(\bar{\mathbf{z}}_r)^\dagger \mathbf{g}(\Phi_r(\bar{\mathbf{z}}_r))}_{=:\mathbf{g}_r(\bar{\mathbf{z}}_r)}\mathbf{u} \qquad \mathbf{y}_r = \underbrace{\mathbf{h}(\Phi_r(\bar{\mathbf{z}}_r))}_{=:\mathbf{h}_r(\bar{\mathbf{z}}_r)}.$$

How to compute the reduced coefficient matrices $\mathbf{T}_{i,r}$?

Truncated (approximate) balanced transformation (K./Gugercin/Borggaard/ '22)

Let $\mathbf{v}_i, \mathbf{w}_i$ be the polynomial coefficients for the energy functions. Let $\mathbf{R}, \mathbf{L}$ be their Cholesky factors, i.e., $\mathbf{V}_2 = \mathbf{R}\mathbf{R}^\top$ and $\mathbf{W}_2 = \mathbf{L}\mathbf{L}^\top$. Let $\mathbf{L}^\top\mathbf{R}^{-\top} = \mathcal{U}\Xi\mathcal{V}^\top$ be the SVD and define

$$\mathcal{U}_r = \mathcal{U}(:, 1:r), \quad \Xi_r = \Xi(1:r, 1:r), \quad \mathcal{V}_r = \mathcal{V}(:, 1:r).$$

Then, the coefficient matrices of the nonlinear embedding $\Phi_r : \mathbb{R}^r \mapsto \mathbb{R}^n$ are

$$\begin{aligned}
\mathbf{T}_{1,r} &= \mathbf{R}^{-\top}\mathcal{V}_r \in \mathbb{R}^{n\times r},\\
\mathbf{T}_{1,r}^\dagger &= \Xi_r^{-1}\mathcal{U}_r^\top\mathbf{L}^\top \in \mathbb{R}^{r\times n}, \text{ (left inverse)}\\
\mathbf{T}_{2,r} &= -\frac{1}{2}\mathbf{T}_{1,r}\ \text{unvec}\left([\mathbf{T}_{1,r}^{③}]^\top\mathbf{v}_3\right)^\top \in \mathbb{R}^{n\times r^2},\\
\mathbf{T}_{k,r} &= -\frac{1}{2}\mathbf{T}_{1,r}\text{unvec}\left(\sum_{\substack{i,j>1\\ i+j=k+1}} \text{vec}\left(\mathbf{T}_{j,r}^\top\mathbf{V}_2\mathbf{T}_{i,r}\right) + \sum_{i=3}^{k+1}\mathcal{T}_{i,k+1}^\top\mathbf{v}_i\right)^\top \in \mathbb{R}^{n\times r^k}.
\end{aligned}$$

Complete balancing algorithm

Algorithm 2 Computation of nonlinear input-output $\mathcal{H}_\infty$-balanced ROM.

Input: Constant $\gamma > \gamma_0 \geq 0$, $\gamma \neq 1$; polynomial degrees $d > k > \ell$; reduced model order r

Output: Input-output nonlinear $\mathcal{H}_\infty$-balanced ROM

1: Obtain a polynomial representation (or approximation) of the past and future energy functions $\mathcal{E}_\gamma^-(\mathbf{x})$ and $\mathcal{E}_\gamma^+(\mathbf{x})$, i.e., coefficients $\{\mathbf{v}_i\}_{i=2}^d$ and $\{\mathbf{w}_i\}_{i=2}^d$.

2: Compute the truncated polynomial coefficient matrices $\{\mathbf{T}_{i,r}\}_{i=1}^k$ for $\mathbf{x} \approx \Phi_r(\bar{\mathbf{z}}_r)$ from Algorithm 1.

3: Symmetrize the coefficients $\{\mathbf{T}_{i,r}\}_{i=1}^r$

4: Assemble the nonlinear ROM functions $\mathbf{f}_r(\bar{\mathbf{z}}_r), \mathbf{g}_r(\bar{\mathbf{z}}_r), \mathbf{h}_r(\bar{\mathbf{z}}_r)$ with the explicit Jacobian.

Nonlinear Manifold ROM approximation

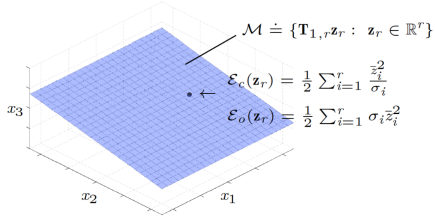
The described nonlinear balanced truncation approach is in essence a model reduction approach on the r-dimensional polynomially nonlinear manifold

$$\mathcal{M} = \left\{ \Phi(\bar{\mathbf{z}}_r) = \mathbf{T}_{1,r}\bar{\mathbf{z}}_r + \mathbf{T}_{2,r}\bar{\mathbf{z}}_r^{②} + \cdots + \mathbf{T}_{k,r}\bar{\mathbf{z}}_r^{ⓚ} \right\}.$$

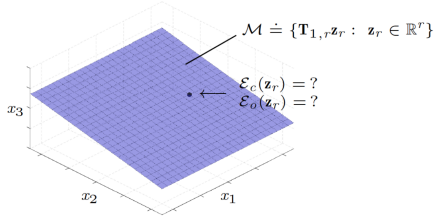
Recent work in NL-ROM on manifolds:

- Autoencoder ROM (fully nonlinear) in [Lee and Carlberg, 2020]
- Quadratic manifolds: use $\mathbf{x} \approx \mathbf{V}\mathbf{z}_r + \bar{\mathbf{V}}(\mathbf{z}_r \otimes \mathbf{z}_r)$ for intrusive [Jain et al., 2017, Barnett and Farhat, 2022] and nonintrusive [Geelen et al., 2022] ROMS.
- Reduced manifold ROM via autoencoder and propagation via feed-forward network, which approximates the ROM, [Fresca et al., 2021]
- Symplectic manifolds for Hamiltonian sysems: [Buchfink et al., 2021]
- Survey of methods to break Kolmogorov n-width problem [Peherstorfer, 2022]
- ...

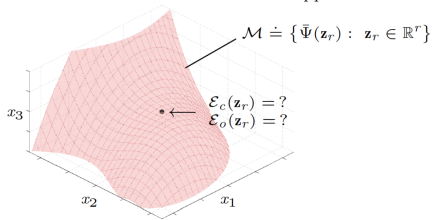
Linear subspace approximation (LTI)



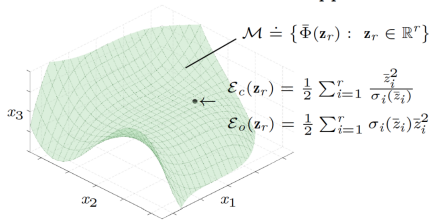
Linear subspace approximation (nonlinear model)



General nonlinear manifold approximation



Nonlinear balanced manifold approximation



Numerical Results: Burgers' equation

We consider the one-dimensional Burgers' equation

$$z_t(x,t) = \epsilon z_{xx}(x,t) - \frac{1}{2}\left(z^2(x,t)\right)_x + \sum_{j=1}^{m} b_j^m(x)u_j(t),$$

$$y_i(t) = \int_{\chi_{[(i-1)/p,\, i/p]}} z(x,t)\mathrm{d}x, \qquad i = 1,\ldots,p,$$

- periodic BCs $z(0,t) = z(1,t)$ and $z_x(0,t) = z_x(1,t)$
- IC: $z(\cdot,0) = z_0(\cdot) \in H_0^1(0,1)$
- $\epsilon = 0.001$ to make the nonlinearity significant.
- $p = 4$ outputs: spatial averages
- $m = 4$ controls/inputs with $b_j^m(x) = \chi_{[(j-1)/m,\, j/m]}(x)$.

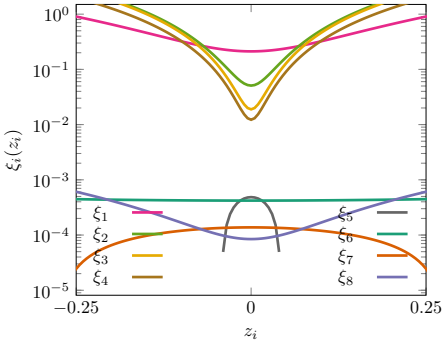
The discretized system has the form

$$\widetilde{\mathbf{E}}\dot{\mathbf{z}} = \widetilde{\mathbf{A}}\mathbf{z} + \widetilde{\mathbf{N}}_2\left(\mathbf{z}\otimes\mathbf{z}\right) + \widetilde{\mathbf{B}}\mathbf{u}$$
$$\mathbf{y} = \widetilde{\mathbf{C}}\mathbf{z},$$

A change of variables $\mathbf{x} = \widetilde{\mathbf{E}}^{1/2}\mathbf{z}$ and redefining $\mathbf{A} = \mathbf{S}^{-1}\widetilde{\mathbf{A}}\mathbf{S}^{-1}$, $\mathbf{B} = \mathbf{S}^{-1}\widetilde{\mathbf{B}}$, $\mathbf{C} = \widetilde{\mathbf{C}}\mathbf{S}^{-1}$, $\widetilde{\mathbf{N}}_2 = \mathbf{N}_2(\mathbf{S}^{-1}\otimes\mathbf{S}^{-1})$ leads to a system with $\mathbf{E} = \mathbf{I}$.

Numerical Results

Singular value functions



- $n = 16$ for FOM model
- Quartic energy functions
- Cubic transformation tensors $\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3$
- Quadratic singular value functions

Relative output error

$$e(r) = \frac{\left(\int_0^{10} |y(t) - y_r(t)|^2 \ \mathrm{d}t\right)^{1/2}}{\left(\int_0^{10} |y(t)|^2 \ \mathrm{d}t\right)^{1/2}}$$

r	$k = 1$	$k = 3$	$k = 5$
1	0.0714831	0.0714814	0.0713882
2	0.0036861	0.0036778	0.0031076
3	0.0026888	0.0026784	0.0026665
4	0.0024333	0.0024288	0.0024238
5	0.0024095	0.0024032	0.0023853

- Errors decay monotonely w.r.t r and k.
- Linear model transformation, however, already very good in this example.

Review and conclusion

We suggested several new computational and modeling choices for balanced nonlinear ROMs:

1. Scalable computation ($n = 1,024$) of a family ($\mathcal{H}_\infty$, HJB, open-loop) energy function approximations $\mathcal{E}_\gamma^-(\mathbf{x}), \mathcal{E}_\gamma^+(\mathbf{x})$
2. Scalable computation of singular value functions $\sigma_i(z_i)$
3. Nonlinear simultaneous balance-and-reduce state transformation $\mathbf{x} \approx \Phi_r(\bar{\mathbf{z}}_r)$
4. Projection of nonlinear model with nonlinear basis (speed up still needed)
5. Two semi-discretized PDE examples (first time use for PDEs)

Outlook and ongoing work:

1. Nonlinear ROMs still have to be made efficient ((D)EIM, other approximations)
2. Addition of polynomial drift/input/output terms in dynamical system (See Linus Balicki's and Nick Corbin's talk)
3. Other approximation techniques: Sum-of-squares (Hamza Adjerid's talk)
4. More efficient solvers: Low-rank, iterative, ...
5. Controllers based on these energy functions
6. Structured systems (DAEs, (port-) Hamiltonians, etc.

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