Generalized Stability Guaranteed Quadratic Embeddings for Nonlinear Dynamics

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Joint work with
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Igor Pontes Duff (Max Planck Institute, Magdeburg)

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initiative for applied artificial intelligence

MAX-PLANCK-INSTITUT FÜR DYNAMIK KOMPLEXER TECHNISCHER SYSTEME MAGDEBURG

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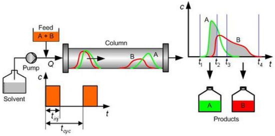

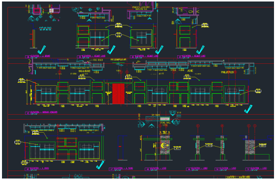

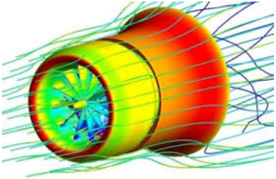

Dynamic models are important to

- analyze transient behavior under operating conditions
- control design
- parameter optimization
- long-time horizon prediction

Objective

Problem set-up

- Construct a mathematical model

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- The more information about the process is known, the more we can make learning efficient.

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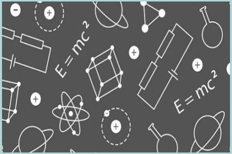
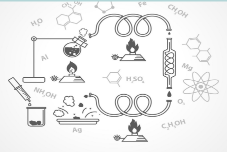
Key sources of information



Physical laws

Domain knowledge



Collected data

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  describing dynamics of the process.
- Neural network-based approaches: recurrent neural networks and long short time memory networks
- The more information about the process is known, the more we can make learning efficient.
- For efficient engineering study, e.g., parameter optimization, control, we want the model to be as simple as possible.

Koopman Operator and DMD

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  - ⇝ Many tools for optimal/feedback control, optimization, and prediction

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- Given data $\mathbf{x}(t_i)$ and its derivative $\dot{\mathbf{x}}(t_i)$, a linear model can be determined by solving

$$\min_{\mathbf{A}} \|\dot{\mathbf{X}} - \mathbf{A}\mathbf{X}\|,$$

  where $\dot{\mathbf{X}} = [\dot{\mathbf{x}}(t_1), \ldots, \dot{\mathbf{x}}(t_n)]$ and $\mathbf{X} = [\mathbf{x}(t_1), \ldots, \mathbf{x}(t_n)]$

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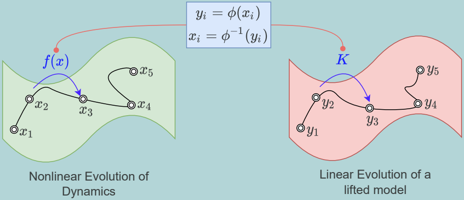
- Often referred to as Dynamic Mode Decomposition, or Operator Inference
- Once linear models are learned and verified, we can deploy for engineering studies
- However, challenges are:
  - Cannot measure the full state $\mathbf{x} \rightsquigarrow$ partial measurements
  - The world is nonlinear, thus learning a linear model may not be sufficient to characterize complex dynamic behavior

Koopman Operator and DMD

Koopman Operator in Nutshell [Koopman 1931]

A nonlinear dynamical system $\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t))$ can be written as a linear system in a infinite dimensional Hilbert space.



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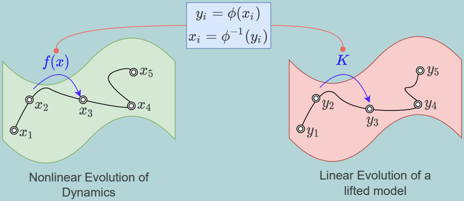

Extended DMD [Williams et al. 2015]

- An aim is to approximate infinite dimensional Koopman linear operator via a finite dimensional one.

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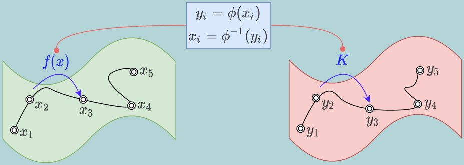

Nonlinear Evolution of Dynamics

Linear Evolution of a lifted model

Extended DMD [Williams et al. 2015]

- An aim is to approximate infinite dimensional Koopman linear operator via a finite dimensional one.
- For this, often hand-design observables are needed, which are
    - challenging, and gives an approximation.

Koopman Operator and DMD

Example 1 [Lusch et al. '18]

- Consider nonlinear system.

$$\begin{bmatrix} \dot{\mathbf{x}}_1(t) \\ \dot{\mathbf{x}}_2(t) \end{bmatrix} = \begin{bmatrix} -\mathbf{x}_1 \\ \mathbf{x}_2 - \mathbf{x}_1^2 \end{bmatrix}.$$

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- Introduce a variable $\mathbf{x}_3 := \mathbf{x}_1^2$. This gives $\dot{\mathbf{x}}_3 = 2\cdot\dot{\mathbf{x}}_1\mathbf{x}_1 = -2\cdot\mathbf{x}_1^2 = -2\cdot\mathbf{x}_3$.

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Example 2

- Consider a simple pendulum model:

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- For this example, we do not have an exact linear representation due to continuum spectrum.

Our Ideal Goal

- Seek to rewrite a nonlinear system to a common structure and in finite dimension
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- Key ingredient is lifting; the optimization problem in a higher-dimensional using auxiliary variables (can think of observables in Koopman theory).
- Similar ideas have been developed for learning dynamical systems.

Quadratic Lifting-Principle for Dynamical Systems

Lifted Nonlinear Dynamical Models to Quadratic Systems using Lifting Principle

- Consider a nonlinear system of the generic form:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}),$$

where $\mathbf{x} \in \mathbb{R}^n$, and the function $\mathbf{f}(\cdot)$ is assumed to be smooth enough.

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- Then, there exists a lifting mapping $\mathcal{L} : \mathbb{R}^n \to \mathbb{R}^m$, and its inverse mapping $\mathcal{L}^\sharp : \mathbb{R}^m \to \mathbb{R}^n$, resulting in

$$\dot{\mathbf{y}}(t) = \mathbf{A}\mathbf{y} + \mathbf{H}\left(\mathbf{y}(t) \otimes \mathbf{y}(t)\right) + \mathbf{B}$$

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- For model reduction for nonlinear systems [Gu 2009/2011, Benner/Breiten 2015, Kramer/Willcox 2022].

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- For model reduction for nonlinear systems [Gu 2009/2011, Benner/Breiten 2015, Kramer/Willcox 2022].
- Lifting in data-driven setting [Qian et al. 2019].

An illustration

- Consider a simple pendulum model:

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- Let us define lifted coordinates (observables) and an inverse transformation:

$$\mathcal{L} : \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \begin{bmatrix} x_1 \\ x_2 \\ \sin(x_2) \\ \cos(x_2) \end{bmatrix} =: \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}, \qquad \mathcal{L}^\sharp : \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} \mapsto \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \equiv \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

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- Consequently, we can write the dynamics in the variables y_i as a quadratic system:

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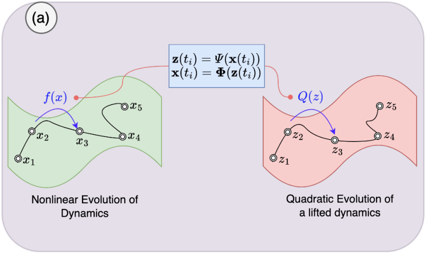
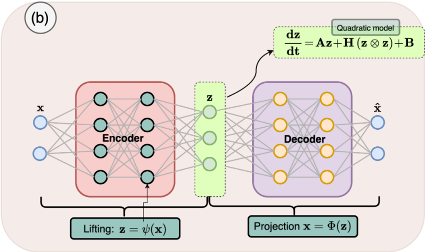
- Note that the inverse mapping is linear, and even continuous spectrum models can be easily written using appropriate observables.

- Using observables—inspired by *Lifting-principle*—we can write nonlinear systems as quadratic systems which are
  - finite dimensional
  - given nonlinear systems, lifted observables are easy to determine





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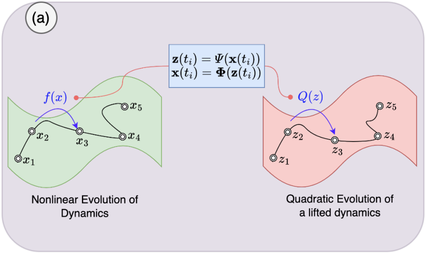

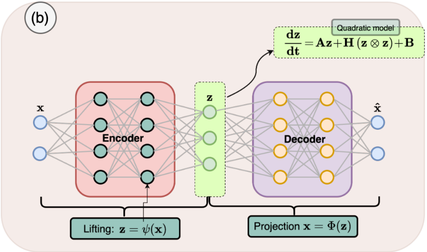

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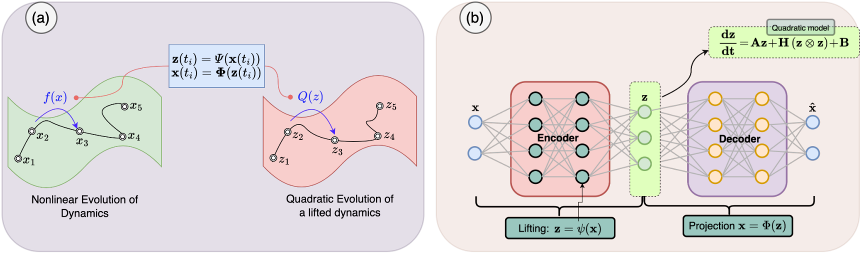

- For given nonlinear dynamical models, we can determine suitable observables.
- However, our goal itself is to learn dynamical models from data.

Lifting-Principle for Dynamical Systems

Problem Statement **(G./Benner 2024)**

Given data $\{\mathbf{x}(t_1), \ldots, \mathbf{x}(t_\mathcal{N})\}$ and derivative information $\{\dot{\mathbf{x}}(t_1), \ldots, \dot{\mathbf{x}}(t_\mathcal{N})\}$, we seek to identify

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- Observables $\mathbf{z} := \psi(\mathbf{x})$ such that

$$\dot{\mathbf{z}}(t) = \mathbf{A}\mathbf{z}(t) + \mathbf{H}\left(\mathbf{z}(t) \otimes \mathbf{z}(t)\right) + \mathbf{B} =: \mathcal{Q}(\mathbf{z}),$$
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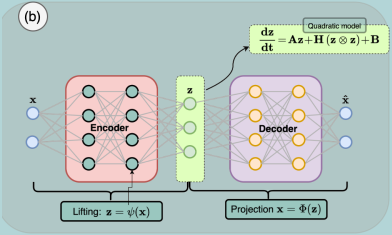

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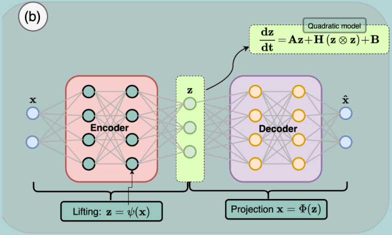
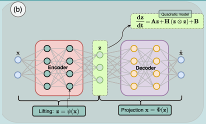
- Since we do not have any prior information, we learn $\psi(\cdot)$ using a neural network.
- We learn parameters of neural networks $\psi(\cdot)$ and $\phi(\cdot)$, and the system matrices $\{\mathbf{A}, \mathbf{H}, \mathbf{B}\}$ simultaneously.



Naive Loss for Training (G./Benner 2024)

- Auto-encoder type loss:



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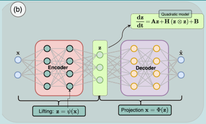

- Derivative loss for $\dot{\mathbf{x}}$:

$$\dot{\mathbf{x}} = \nabla_{\mathbf{z}}\Phi(\mathbf{z})\dot{\mathbf{z}} = \nabla_{\mathbf{z}}\Phi(\mathbf{z})\left(\mathbf{A}\mathbf{z} + \mathbf{H}\left(\mathbf{z}\otimes\mathbf{z}\right) + \mathbf{B}\right).$$

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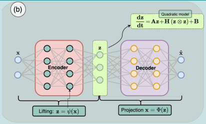

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Naive Loss for Training (G./Benner 2024)

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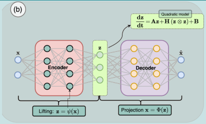

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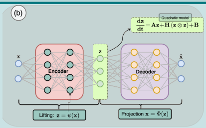

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Lifting-Principle for Dynamical Systems

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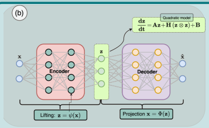

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– These are continuous dynamical systems; thus, in the formulation none of the properties are included.

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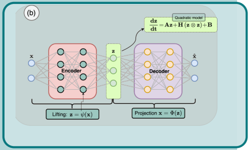

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Stability of linear systems

A linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$ is asymptotically stable if and only if all the eigenvalues of $\mathbf{A}$ lie in left-half plane strictly. This implies, $\lim_{t\to\infty} \mathbf{x}(t) = 0$.

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- Given data $\dot{\mathbf{X}}$ and $\mathbf{X}$, a linear model can be inferred by solving

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Stable matrix parameterization [Gillis/Sharma '17]

Any stable matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ can be parameterized as follows:

$$\mathbf{A} = (\mathbf{J} - \mathbf{R})\mathbf{Q},$$

where $\mathbf{J} = -\mathbf{J}^\top$, $\mathbf{R} = \mathbf{R}^\top \succ 0$, and $\mathbf{Q} = \mathbf{Q}^\top \succ 0$.

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Inference of Linear Stable Systems

Linear stable inference [G./Pontes/Benner '22]

- An inference problem for linear systems, ensuring stability

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- We solve these optimization problems using gradient descent.

- Recall, for inference of quadratic systems, we require to solve

$$\min_{\mathbf{A},\mathbf{H},\mathbf{B}} \left\| \dot{\mathbf{X}} - \mathbf{A}\mathbf{X} - \mathbf{H}\mathbf{X}^{\otimes} - \mathbf{B} \right\|,$$

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Local stability of quadratic systems

- Consider a quadratic system, $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{H}(\mathbf{x} \otimes \mathbf{x})$. If $\Lambda(\mathbf{A}) \subset \mathbb{C}^{-}$, then the system is locally asymptotically stable. This implies, $\lim_{t\to\infty} \mathbf{x}(t) = 0$ if $\mathbf{x}(0) \in \mathcal{B}(0, r)$.
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Inference of locally stable quadratic systems [Sawant et al. '23, G./Pontes/Benner '23]

- We, thus, require to solve the following constraints:

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- We already know how to parameterize stable matrices, i.e., $\mathbf{A} = (\mathbf{J} - \mathbf{R})\mathbf{Q}$.

Globally Asymptotically Stable Quadratic Systems

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Energy preserving quadratic nonlinearity **e.g., [Lorenz '63, Schlegel/Noack '15]**

- A quadratic non-linearity $\mathbf{H}(\mathbf{x} \otimes \mathbf{x})$ is said to be energy preserving if $\mathbf{x}^\top \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) = 0$ for all $\mathbf{x}$.
- Such non-linearity naturally appears, e.g., in flow problems (Navier-Stokes equations).

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How to parameterize energy-preserving nonlinearity [G./Pontes/Benner '23]

If the matrix $\mathbf{H} \in \mathbb{R}^{n \times n}$ is of the following form:

$$\mathbf{H} = \left[\mathbf{H}_1, \dots, \mathbf{H}_n\right],$$

where $\mathbf{H}_i = -\mathbf{H}_i^\top$, then $\mathbf{x}^\top \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) = 0$, or the non-linearity is energy preserving.

Lifting-Principle for Dynamical Systems

Stability-Enforced Loss for Training (G./Benner 2024)

- Auto-encoder type loss:

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Illustrative Examples

Pendulum example

- Governing equation is

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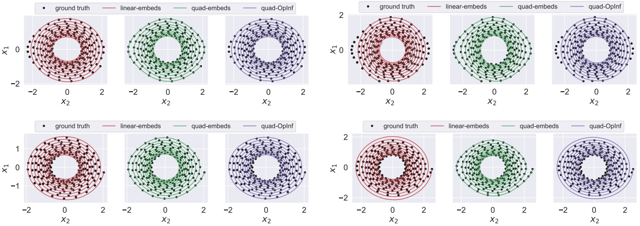

Figure: Nonlinear pendulum example: A comparison of the trajectories.

Illustrative Examples

Pendulum example

- Governing equation is

$$\begin{bmatrix}\dot{\mathbf{x}}_1(t)\\ \dot{\mathbf{x}}_2(t)\end{bmatrix} = \begin{bmatrix}-\sin(\mathbf{x}_2(t)) - 0.025\mathbf{x}_1(t)\\ \mathbf{x}_1(t)\end{bmatrix},$$

- The data are collected for time interval $[0, 25]s$ for 50 random initial conditions with $\{\mathbf{x}_1, \mathbf{x}_2\} \in [-3, 3]$.
- We learn 3-dimensional quadratic model ($\equiv 3$ observables).
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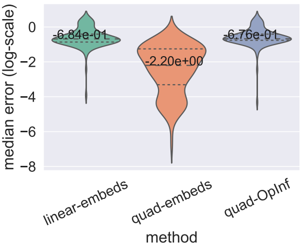

Dissipative Lotka-Volterra example

- Governing equation is

$$\begin{bmatrix}\dot{\mathbf{q}}(t)\\ \dot{\mathbf{p}}(t)\end{bmatrix} = \begin{bmatrix}-e^{\mathbf{p}} - 0.05 \cdot \mathbf{q} + 1\\ e^{\mathbf{q}} - 0.05 \cdot \mathbf{p} - 2\end{bmatrix},$$

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Illustrative Examples

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Illustrative Examples

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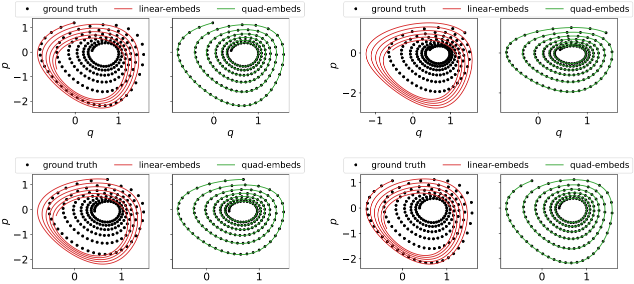

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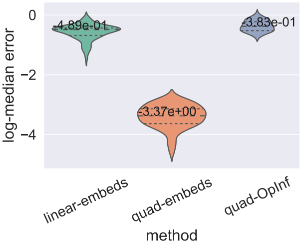

Figure: Dissipative Lotka-Volterra example: A comparison of the trajectories

A High-dimensional Example: Nonlinear Burgers' Equations

- Governing equations:

$$
\begin{aligned}
&u_t + uu_x + u^3 u_x = u_{xx}, \quad \text{with} \quad x \in (0,1) \text{ and } t \in (0,T),\\
&u(0,\cdot) = 0, \quad \text{and } u(1,\cdot) = 0,\\
&u(x,0) = 10 \cdot \sin(\pi x \cdot f) x(1-x),
\end{aligned}
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Numerical Examples

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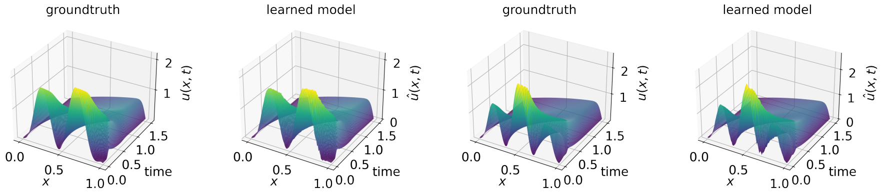

Figure: Burgers' equation: A comparison of the solutions.

Contribution

- Discussed Lifting-principle for nonlinear dynamical systems

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Thank you for your attention!!

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