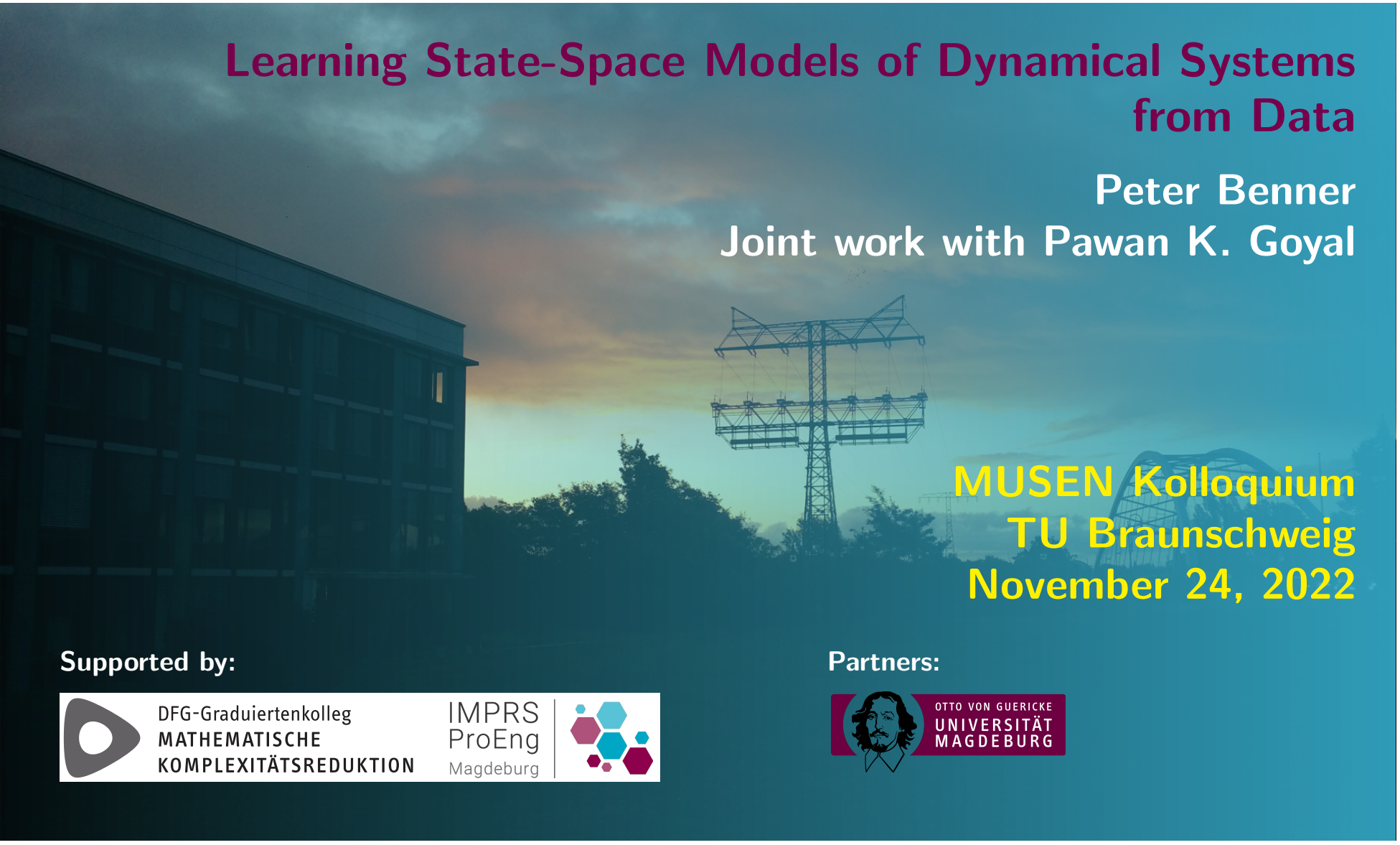

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Learning State-Space Models of Dynamical Systems from Data

Peter Benner

Joint work with Pawan K. Goyal

MUSEN Kolloquium
TU Braunschweig
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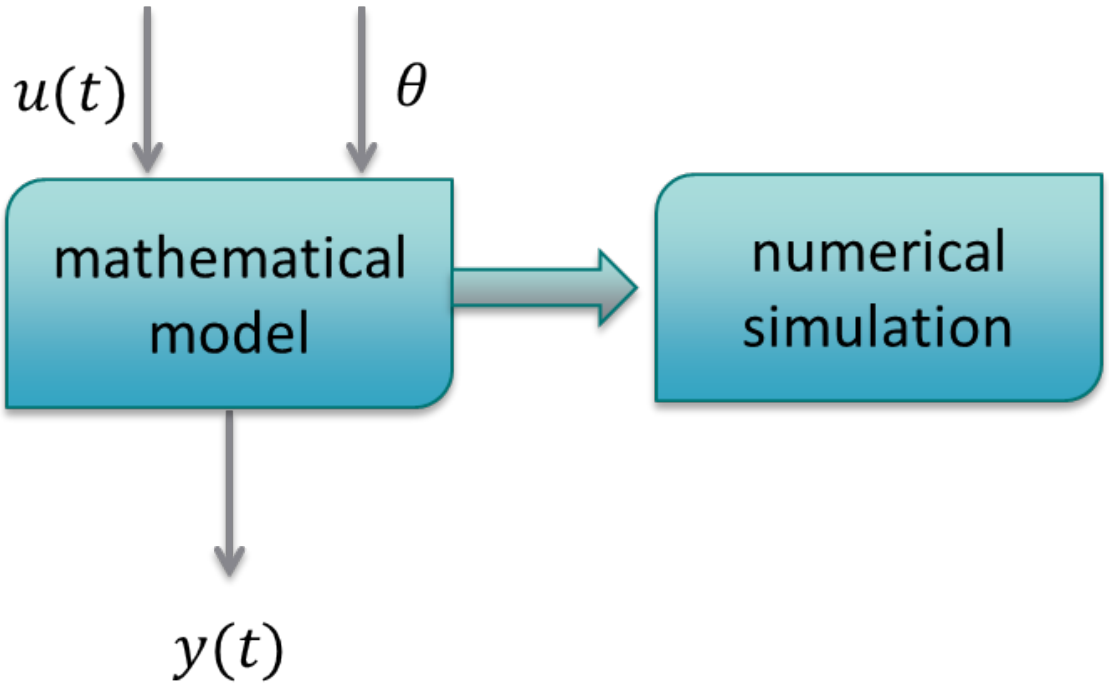
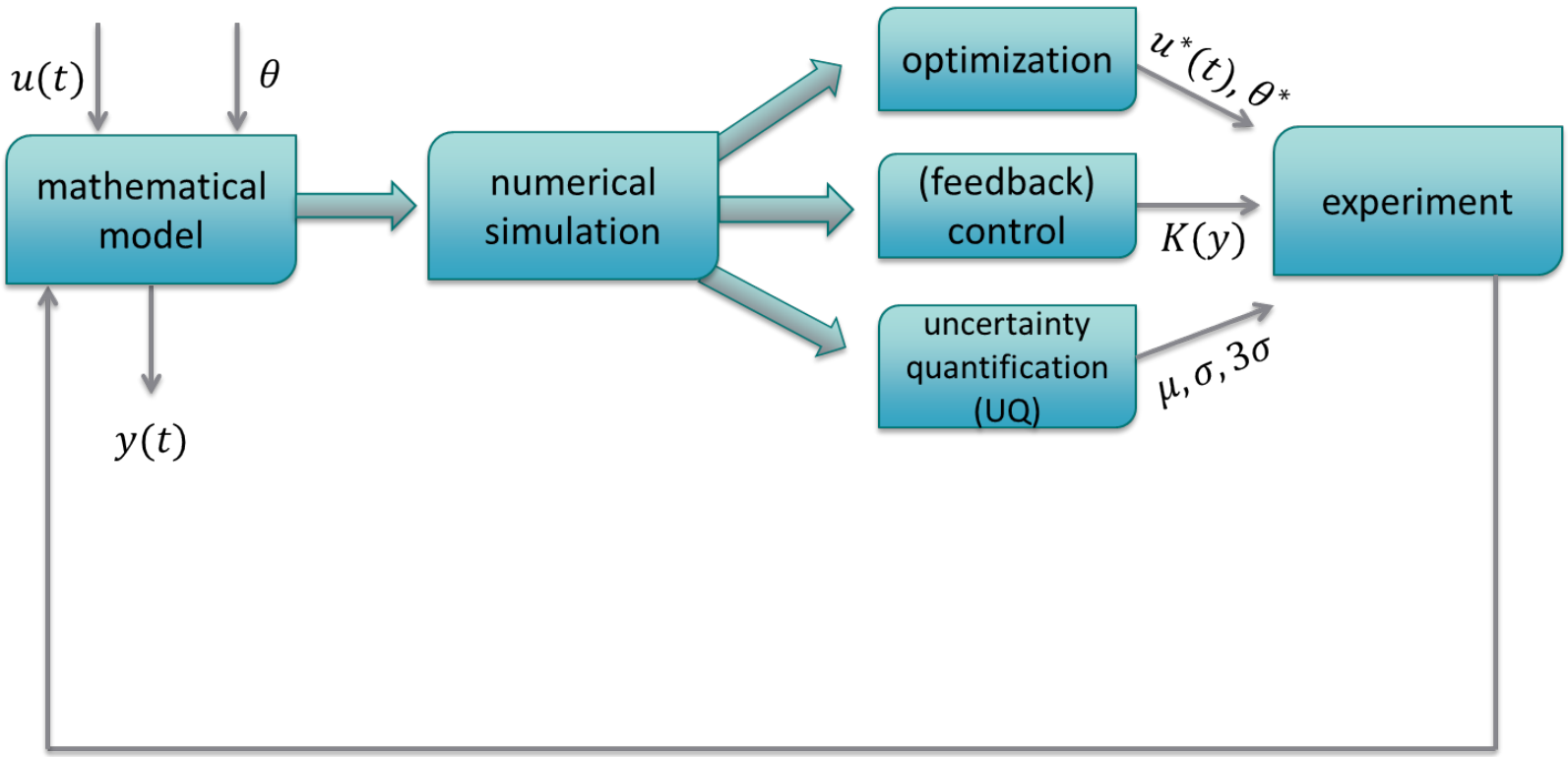

$u(t)$
θ
mathematical model
numerical simulation
$y(t)$

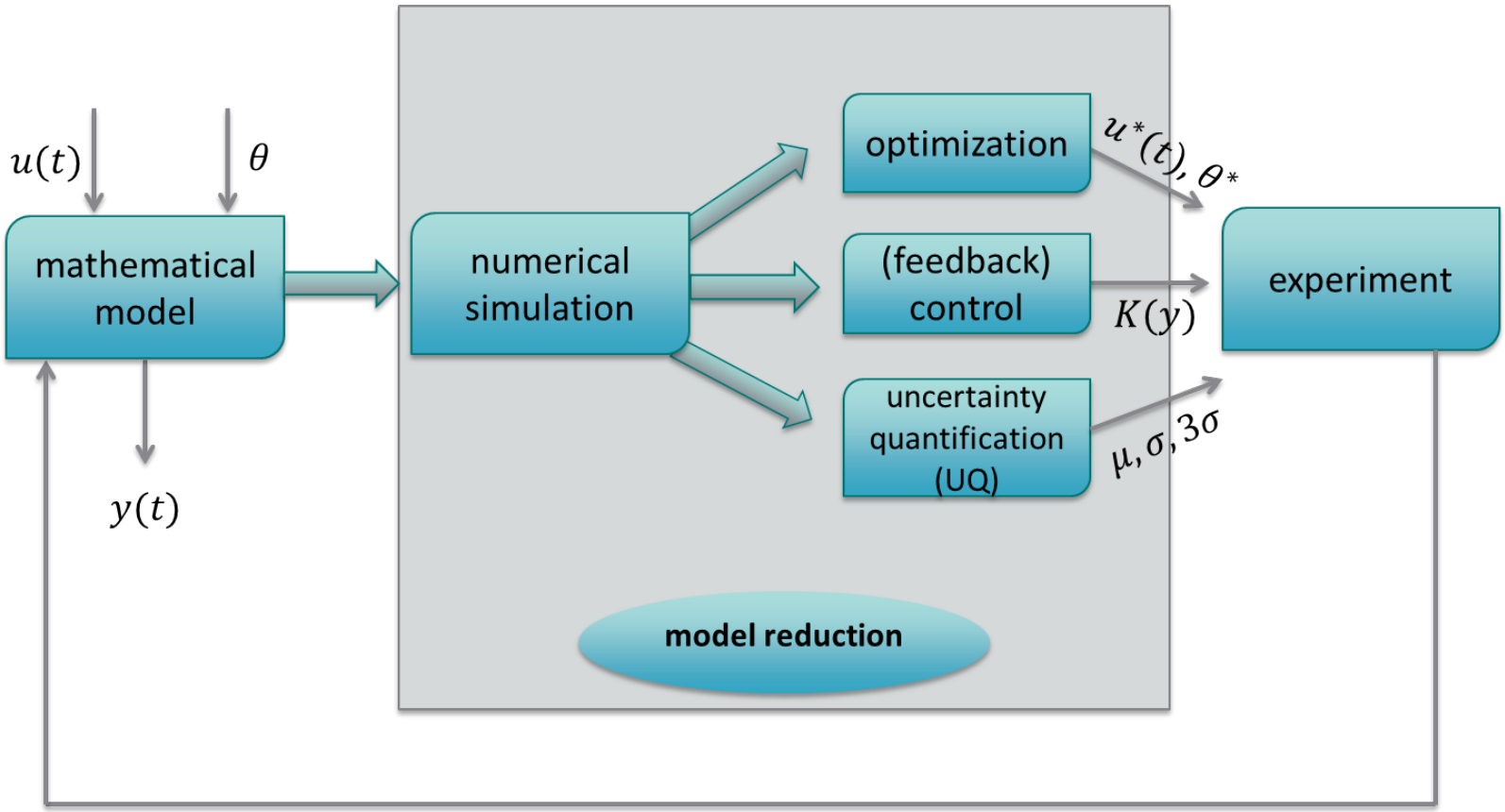
A Process Chain in Computational Sciences and Engineering (CSE)

Optimization, Control, and Uncertainty Quantification



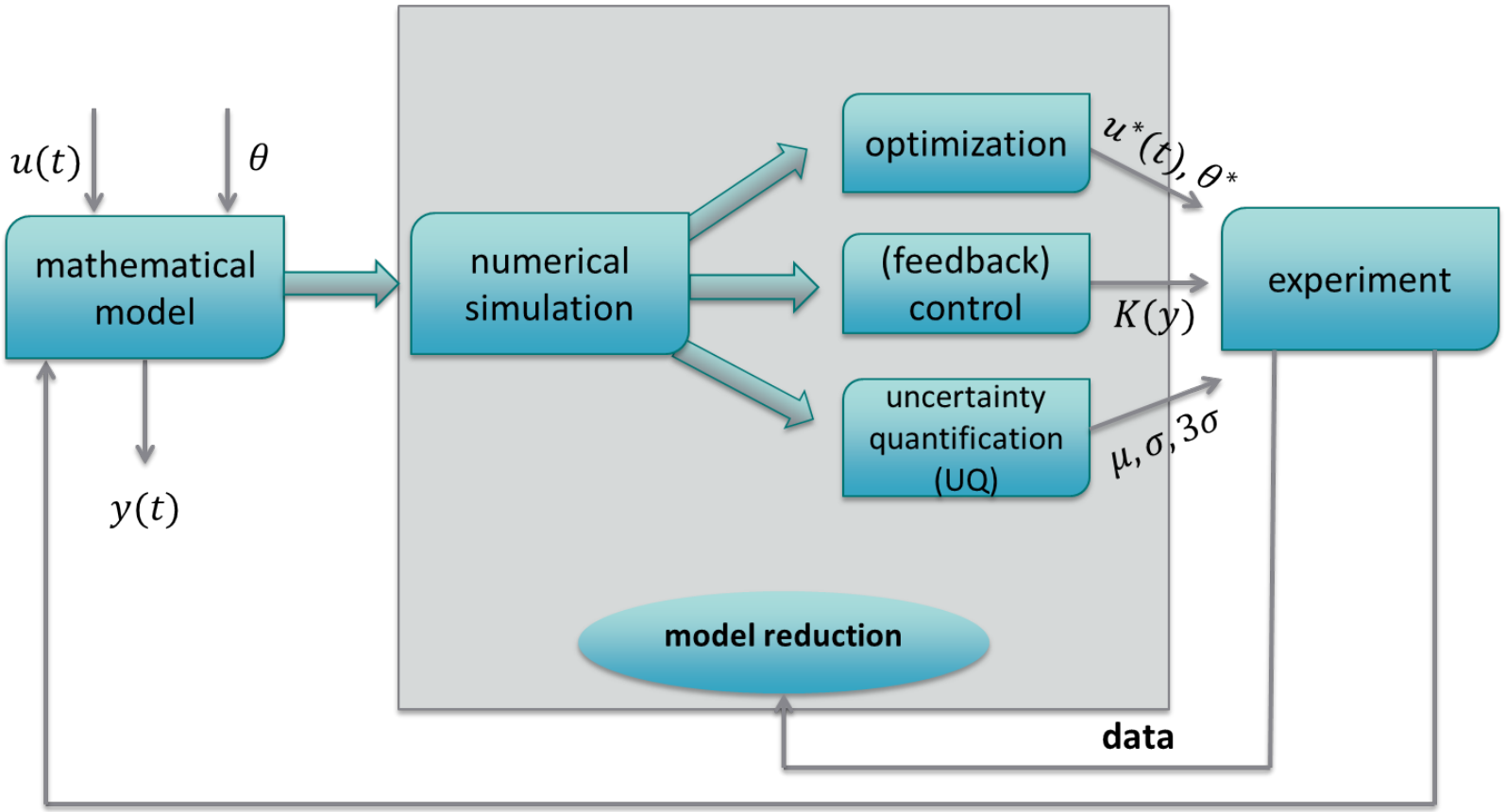
A Process Chain in Computational Sciences and Engineering (CSE)

Model Order Reduction (MOR)



A Process Chain in Computational Sciences and Engineering (CSE)

Data-Driven Sciences



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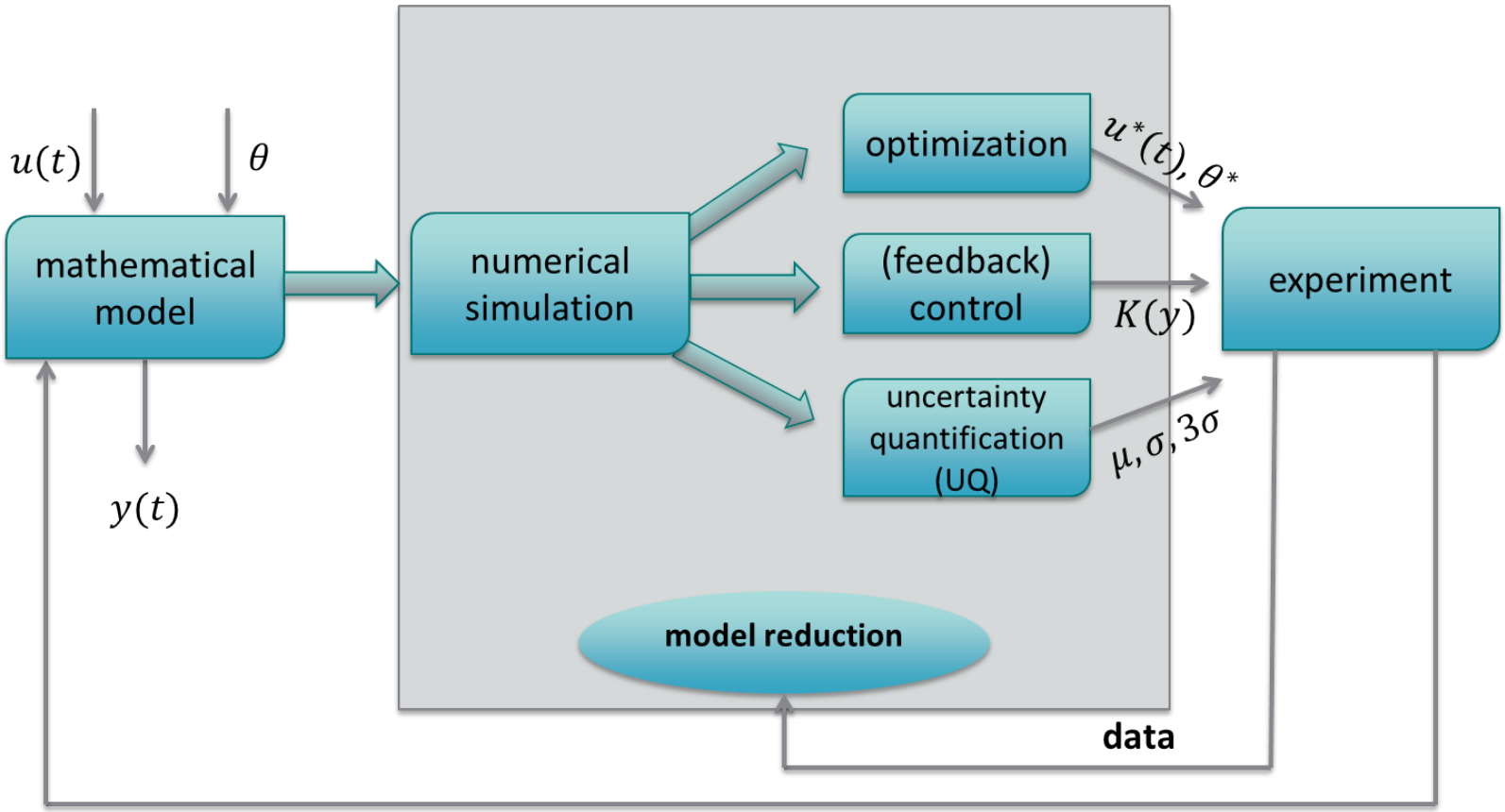

Goal: *Use all acquired knowledge about the model during the CSE process chain in the design of the reduced-order model, including experimental data.*

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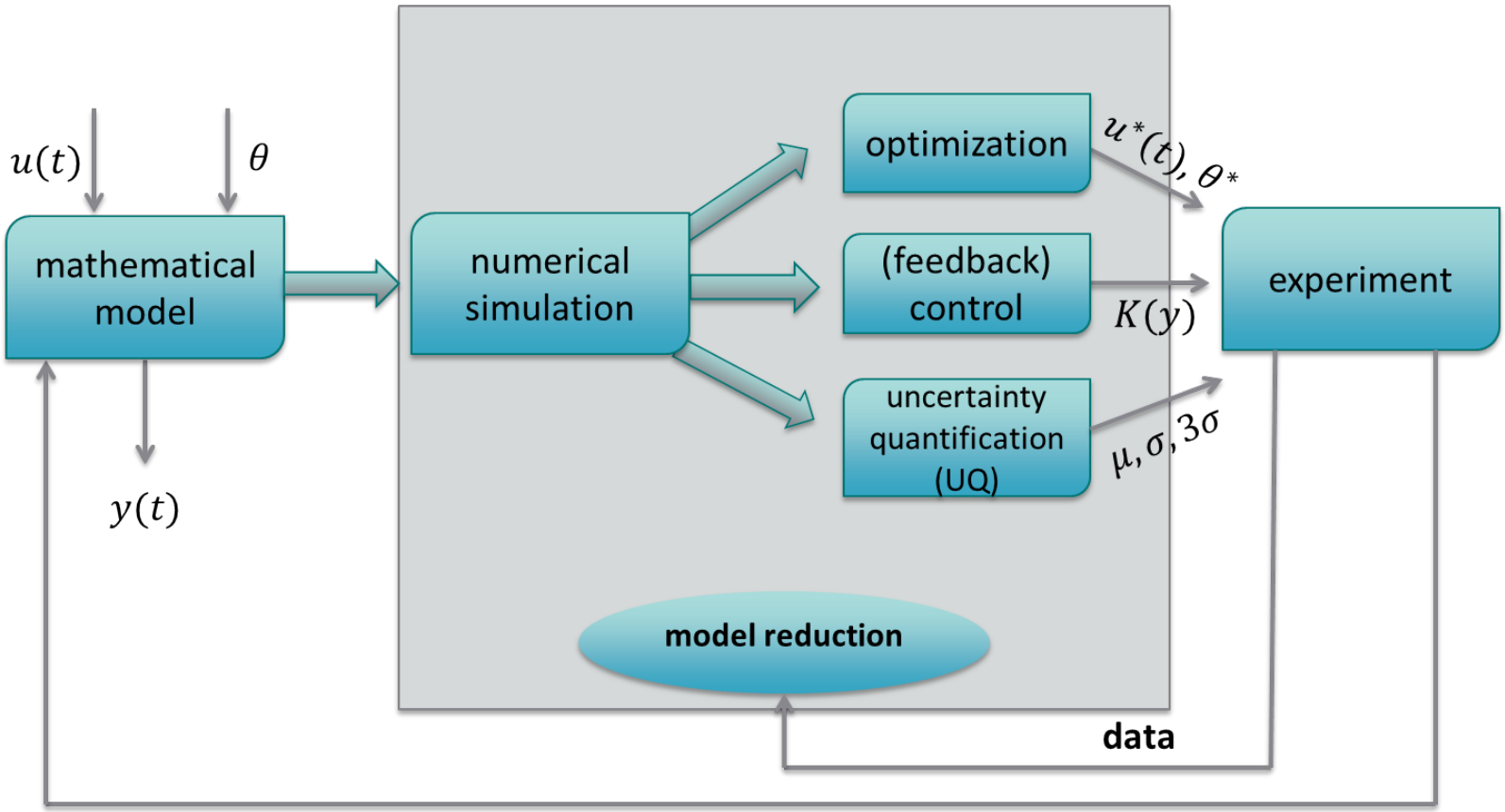

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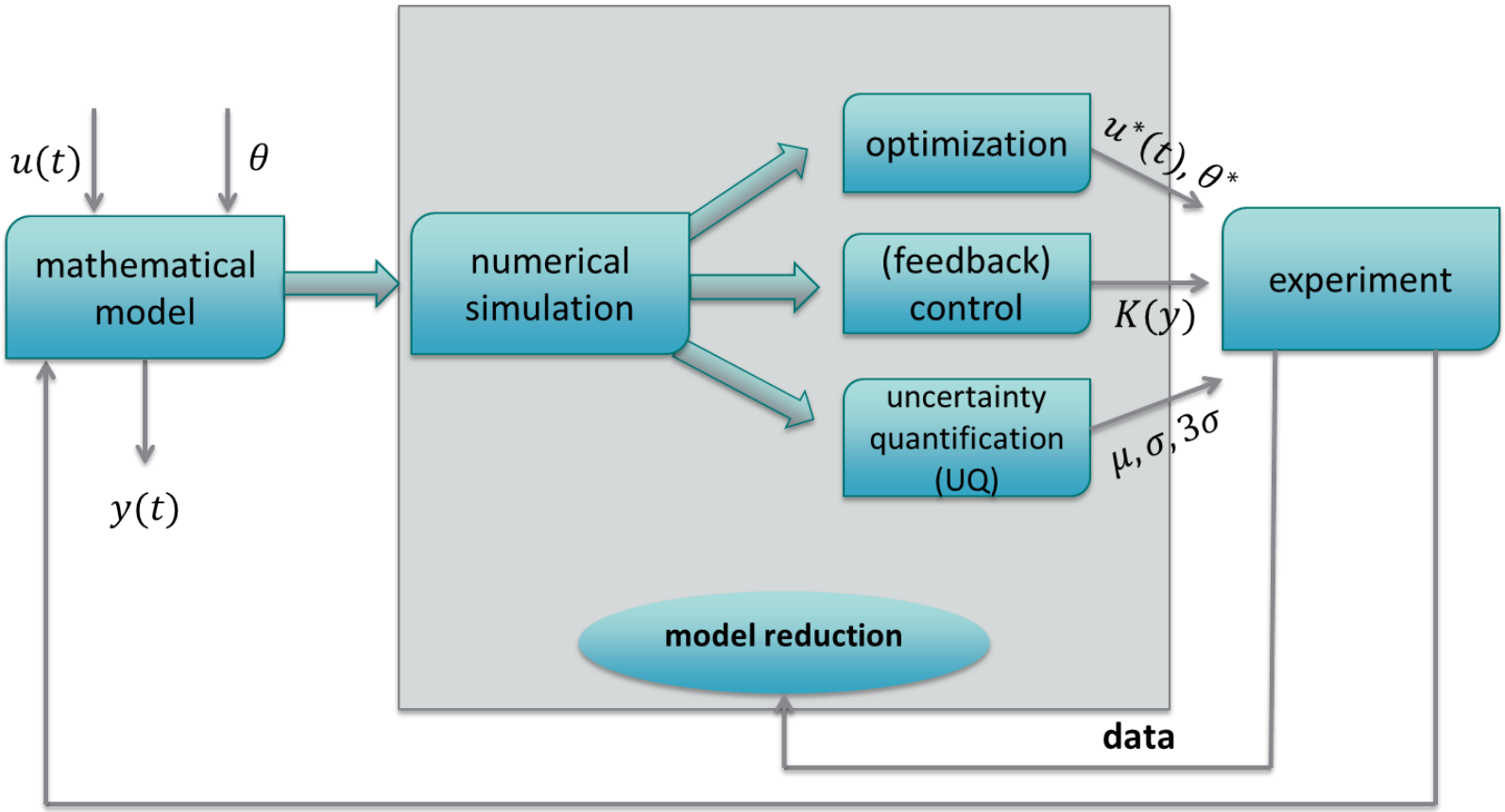

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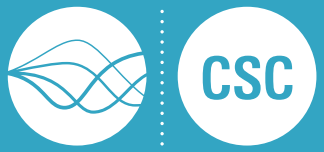
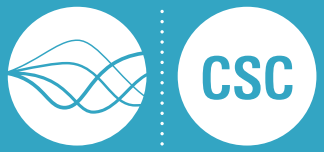
or in AI/ML idiom: Learning a dynamical (compact) model from data.



Outline

1. Model Order Reduction of Dynamical Systems
2. Data-driven/-enhanced Model Reduction
3. Koopman Operator and DMD
4. Lifting Principle for Dynamical Systems



Outline

Original System

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

- states $x(t) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
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Reduced-Order Model (ROM)

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Goals:

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

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

Original System

$$\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t), \\ y(t) = Cx(t) + Du(t). \end{cases}$$

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Model Order Reduction of Linear Systems

Model Reduction Schematically

$$E\,\dot{x}(t) = A\,x(t) + B\,u(t)$$

$$y(t) = C\,x(t) + D\,u(t)$$

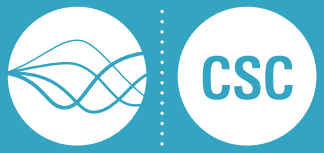
MOR

$$\hat{E}\,\dot{\hat{x}}(t) = \hat{A}\,\hat{x}(t) + \hat{B}\,u(t)$$

$$\hat{y}(t) = \hat{C}\,\hat{x}(t) + \hat{D}\,u(t)$$

- $E, A \in \mathbb{R}^{n\times n}$
- $B \in \mathbb{R}^{n\times m}$
- $C \in \mathbb{R}^{p\times n}$
- $D \in \mathbb{R}^{p\times m}$

- $\hat{E}, \hat{A} \in \mathbb{R}^{r\times r}$
- $\hat{B} \in \mathbb{R}^{r\times m}$
- $\hat{C} \in \mathbb{R}^{p\times r}$
- $\hat{D} \in \mathbb{R}^{p\times m}$



MOR Methods Based on Projection

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Then, with $\hat{x} = W^T x$, we obtain $x \approx V\hat{x} = VW^T x =: \tilde{x}$ so that

$$||x - \tilde{x}|| = ||x - V\hat{x}||.$$

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For linear systems ($E = I_n$ for simplicity), the reduced-order model is

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- The state equation residual satisfies $\dot{\tilde{x}} - A\tilde{x} - Bu \perp \mathcal{W}$, since

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Extends to nonlinear systems with some effort:

$$\begin{aligned} \dot{\hat{x}} &= W^T f(t, V\hat{x}, u), \\ \hat{y} &= g(t, V\hat{x}, u). \end{aligned}$$

Needs hyperreduction if the cost for evaluation of the functions $W^T f, g$ is not reduced!

MOR Methods Based on Projection

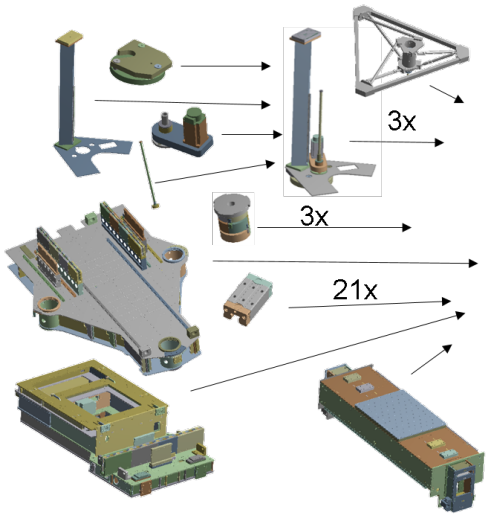
Classes of Projection-based MOR Methods

1. Modal Truncation
2. Rational Interpolation / Moment Matching
   (Padé-Approximation and (rational) Krylov Subspace Methods)
3. Balanced Truncation
4. Proper Orthogonal Decomposition (POD) / Principal Component Analysis (PCA)
5. Reduced Basis Method
6. ...

MOR Methods Based on Projection

Example: Thermal model of experimental machine tool MAX

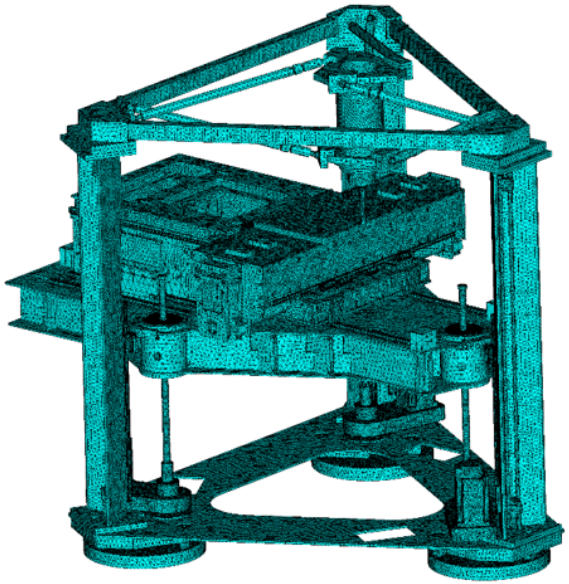
50 subassemblies



CAD model

$\overset{FEM}{\rightsquigarrow}$

FE-Model: 1.2M DOFs



MAX: Results considering an inhomogeneous initial condition $T_0 \neq 0$

Results by Julia Vettermann (MilT/TU Chemnitz)

FE-coupled

method	red. order tol 10^{-3}	t_{red}
2phase	196	6.5h
BTX0	174	4.5h

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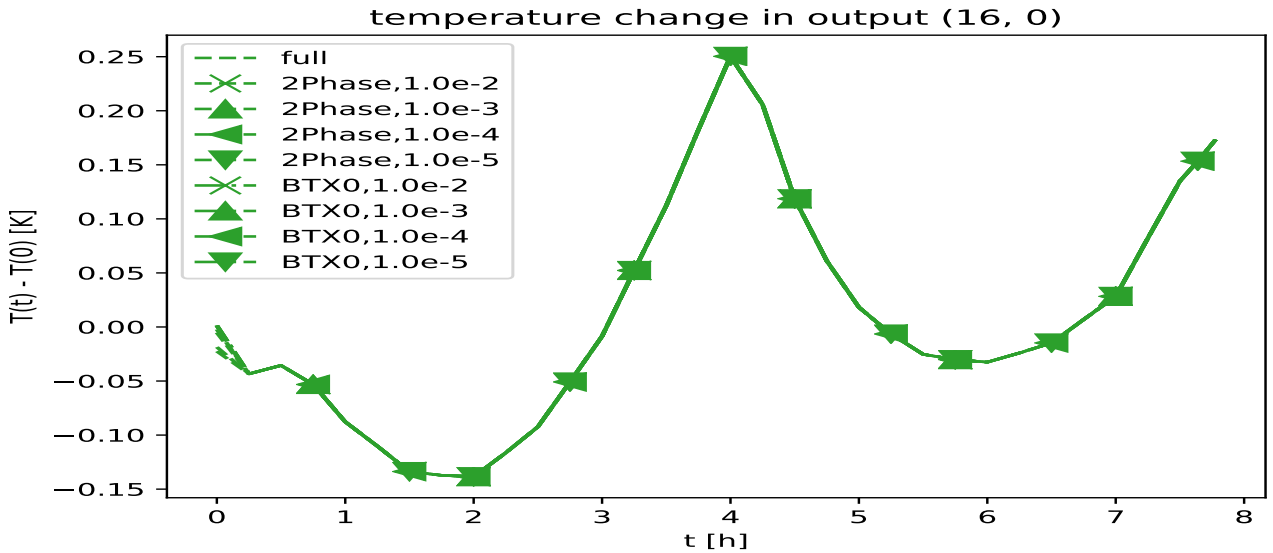
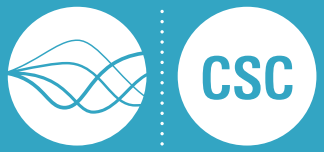
→ *Required storage for reduced matrices just 1MB!*
→ *Simulation speed-up factors range from* ≈ 8–$2,000$.



Vettermann, J., Sauerzapf, S., Naumann, A., Beitelschmidt, M., Herzog, R., Benner, P., Saak, J. (2021): Model order reduction methods for coupled machine tool models. MM Science Journal, pp. 4652–4659.



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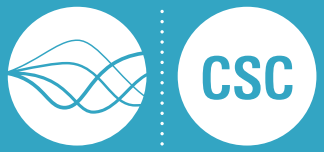
$\rightsquigarrow$ **non-intrusive MOR**

$=$ *LEARNING (compact, surrogate) MODELS FROM DATA!*



Outline

1. Model Order Reduction of Dynamical Systems

2. Data-driven/-enhanced Model Reduction
   - A few Remarks on System Identification and DNNs
   - DMD in a Nutshell
   - Operator Inference

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4. Lifting Principle for Dynamical Systems

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Black box Σ: the only information we can get is either

- time domain data / times series: $u_k \approx u(t_k)$ and $x_k \approx x(t_k)$ or $y_k \approx y(t_k)$, or

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- Operator inference (OpInf): time domain [Peherstorfer/Willcox 2016; Kramer, Qian, B., Goyal,...]

A few Remarks on System Identification and DNNs

- System identification tries to infer discrete linear time-invariant (LTI) systems

$$x_{k+1} = Ax_k + Bu_k + Kw_k,$$
$$y_k = Cx_k + Du_k + v_k.$$

from input-output data, given as time series $(u_0, y_0), (u_1, y_1), \ldots, (u_K, y_K)$, where v_k, w_k are uncorrelated Gaussian white noise processes.

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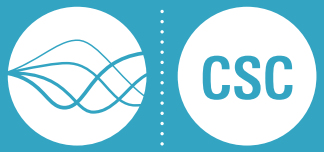

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- Continuous-time system can be identified, e.g., by "inverse" Euler method.
- Many extensions to nonlinear systems, imposing certain structural assumptions, including artificial neural networks...

A few Remarks on System Identification and DNNs

A paper from 1990...

4 IEEE TRANSACTIONS ON NEURAL NETWORKS, VOL. 1, NO. 1, MARCH 1990

Identification and Control of Dynamical Systems Using Neural Networks

KUMPATI S. NARENDRA FELLOW, IEEE, AND KANNAN PARTHASARATHY

Abstract—**The paper demonstrates that neural networks can be used effectively for the identification and control of nonlinear dynamical systems. The emphasis of the paper is on models for both identification and control. Static and dynamic back-propagation methods for the adjustment of parameters are discussed. In the models that are introduced, multilayer and recurrent networks are interconnected in novel configurations and hence there is a real need to study them in a unified fashion. Simulation results reveal that the identification and adaptive control schemes suggested are practically feasible. Basic concepts and definitions are introduced throughout the paper, and theoretical questions which have to be addressed are also described.**

are well known for such systems [1]. In this paper our interest is in the identification and control of nonlinear dynamic plants using neural networks. Since very few results exist in nonlinear systems theory which can be directly applied, considerable care has to be exercised in the statement of the problems, the choice of the identifier and controller structures, as well as the generation of adaptive laws for the adjustment of the parameters.

Two classes of neural networks which have received considerable attention in the area of artificial neural net-

Narendra, K.S., Parthasarathy, K. (1990): Identification and control of dynamical systems using neural networks. IEEE Transactions on Neural Networks 1(1):4–27.

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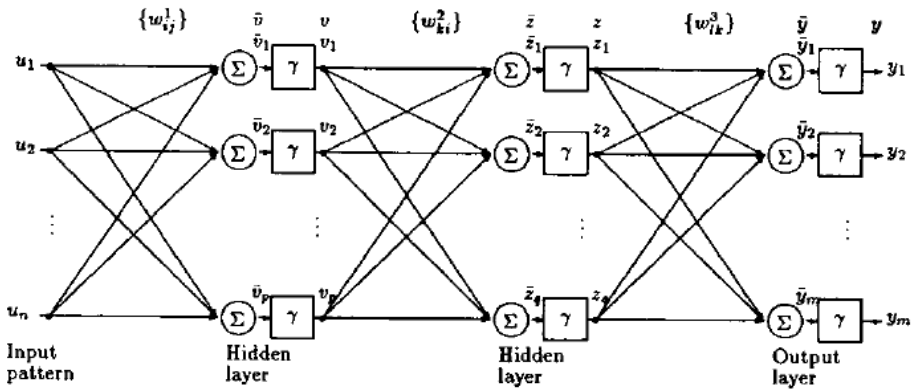

Fig. 2. A three layer neural network.

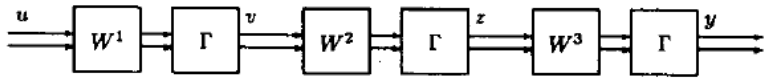

Fig. 3. A block diagram representation of a three layer network.

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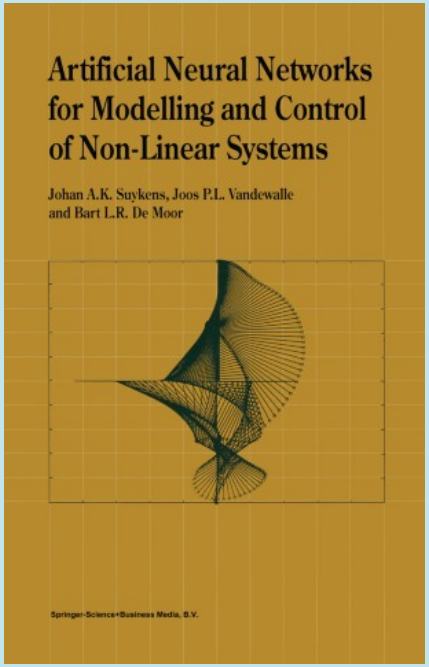

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Suykens, J.A.K., Vandewalle, J.P.L., de Moor, B.L. (1996): Artificial Neural Networks for Modelling and Control of Non-Linear Systems. Springer US.

DMD in a Nutshell

Basic Framework

Given a smooth dynamical system

$$\dot{x}(t) = f(x(t)), \quad x(0) = x_0 \in \mathbb{R}^n.$$

Take snapshots $x_k := x(t_k)$ on grid $t_k := kh$ for $k = 0, 1, \ldots, K$ and fixed $h > 0$ (using simulation software, or measurements from real life experiment $\rightsquigarrow$ nonintrusive!), and find "best possible" A_* such that

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Motivation: Koopman theory

- $\exists$ a linear, infinite-dimensional operator describing the evolution of $f(x(\cdot))$ in an appropriate function space setting.
- Can be considered as lifting of a finite-dimensional, nonlinear problem to a infinite-dimensional, linear problem.

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Basic DMD Algorithm

Set $X_0 := [\, x_0, x_1, \ldots, x_{K-1} \,] \in \mathbb{R}^{n \times K}$, $X_1 := [\, x_1, x_2, \ldots, x_K \,] \in \mathbb{R}^{n \times K}$ and note that $X_1 = AX_0$ is desired $\rightsquigarrow$ over-/underdetermined linear system, solved by linear least-squares problem (regression):

$$A_* := \arg\min_{A \in \mathbb{R}^{n \times n}} \|X_1 - AX_0\|_F + \beta \|A\|_q$$

with a potential regularization term choosing $\beta > 0$, $q = 0, 1, 2$.

Computation usually via singular value decomposition (SVD), many variants.

DMD in a Nutshell

DMD with Inputs and Outputs

Given a smooth control system

$$\dot{x}(t) = f(x(t), u(t)), \quad x(0) = x_0 \in \mathbb{R}^n, \qquad y(t) = g(x(t), u(t)),$$

with control $u(t) \in \mathbb{R}^m$ and output $y(t) \in \mathbb{R}^p$.

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Take state, control, and output snapshots

$$x_k := x(t_k), \quad u_k := u(t_k), \quad y_k := y(t_k), \qquad k = 0, 1, \ldots, K$$

(using simulation software, or measurements from real life experiment $\rightsquigarrow$ nonintrusive!), and find "best possible" discrete-time LTI system such that

$$x_{k+1} \approx A_* x_k + B_* u_k, \qquad y_k \approx C_* x_k + D_* u_k.$$

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Basic ioDMD Algorithm ($\equiv$ N4SID)

Let $\mathbb{S} := \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times m} \times \mathbb{R}^{p\times n} \times \mathbb{R}^{p\times m}$. Set X_0, X_1 as before and

$$U_0 := [\, u_0, u_1, \ldots, u_{K-1} \,] \in \mathbb{R}^{m\times K}, \qquad Y_0 := [\, y_0, y_1, \ldots, y_{K-1} \,] \in \mathbb{R}^{p\times K}.$$

Solve the linear least-squares problem (regression):

$$(A_*, B_*, C_*, D_*) := \arg\min_{(A,B,C,D)\in\mathbb{S}} \left\| \begin{bmatrix} X_1 \\ Y_0 \end{bmatrix} - \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} X_0 \\ U_0 \end{bmatrix} \right\|_F + \beta \| [\, A\, B\, C\, D \,] \|_q$$

with a potential regularization term choosing $\beta > 0$, $q = 0, 1, 2$.

DMD in a Nutshell

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Operator Inference

Reduced-order / compressive DMD

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$$\hat{A}_* := \arg\min_{\hat{A} \in \mathbb{R}^{r \times r}} \|\hat{X}_1 - \hat{A}\hat{X}_0\|_F + \beta \|\hat{A}\|_q.$$

Can be combined with ioDMD to obtain reduced-order LTI system.

Operator Inference

Basic Algorithm

Basic idea: apply compressive ioDMD in continuous-time setting,

$$\dot{x}(t) = f(x(t), u(t)), \quad x(0) = x_0 \in \mathbb{R}^n,$$

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$$\dot{\hat{x}}(t) = \hat{A}\hat{x}(t) + \hat{H}\left(\hat{x}(t) \otimes \hat{x}(t)\right) + \hat{B}u(t),$$

where $P \otimes Q := [p_{ij}Q]_{ij}$ denotes the Kronecker (tensor) product, from data

$$X := [\, x_0, x_1, \ldots, x_K \,] \in \mathbb{R}^{n \times (K+1)}, \quad U := [\, u_0, u_1, \ldots, u_K \,] \in \mathbb{R}^{m \times (K+1)}.$$

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  $$\dot{\hat{X}} := [\, \dot{x}(0), \dot{x}(t_1), \ldots, \dot{x}(t_K) \,] \approx [\, f(x_0, u_0), f(x_1, u_1), \ldots, f(x_K, u_K) \,] \in \mathbb{R}^{n\times(K+1)},$$

  otherwise, approximate time-derivatives by finite differences $\rightsquigarrow \dot{\hat{X}}$.

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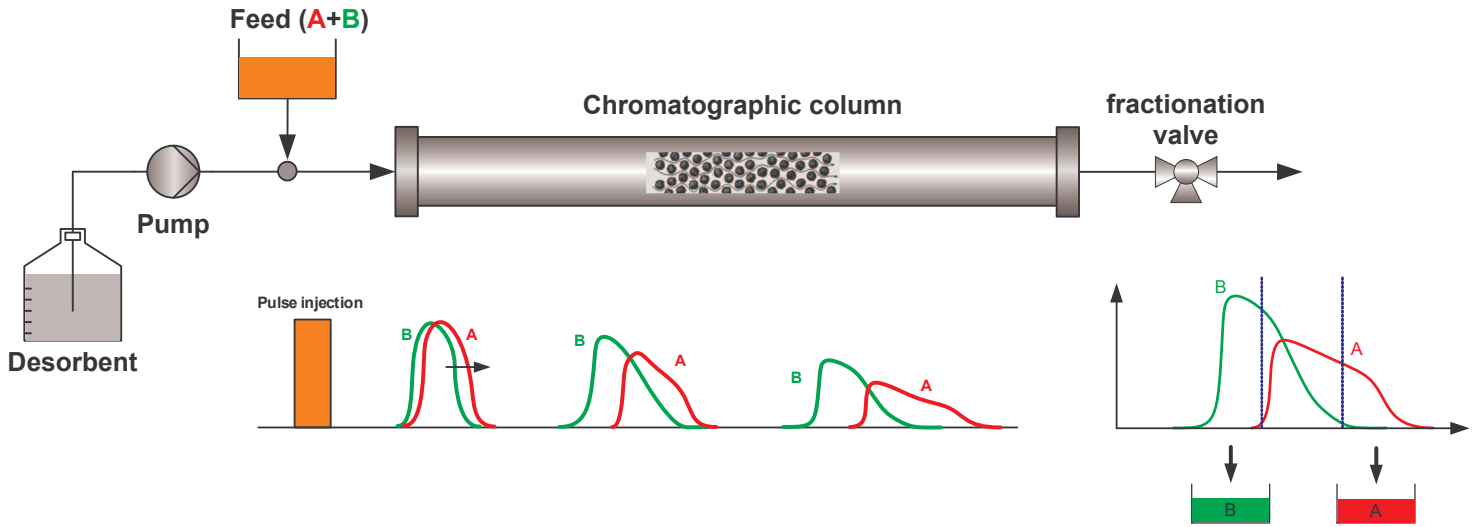
  otherwise, approximate time-derivatives by finite differences $\rightsquigarrow \dot{\hat{X}}$.
- Solve the linear least-squares problem (regression):

  $$(\hat{A}_*, \hat{H}_*, \hat{B}_*) := \arg\min_{(\hat{A},\hat{H},\hat{B})} \left\| \dot{\hat{X}} - \begin{bmatrix} \hat{A} & \hat{H} & \hat{B} \end{bmatrix} \begin{bmatrix} \hat{X} \\ \widehat{X^2} \\ U \end{bmatrix} \right\|_F + \beta \left\| \begin{bmatrix} \hat{A}\,\hat{H}\,\hat{B} \end{bmatrix} \right\|_q$$

  with potential regularization as before and $\widehat{X^2} := [x_0 \otimes x_0, \ldots, x_K \otimes x_K]$.

Operator Inference: Numerical Examples

Batch Chromatography: A Chemical Separation Process



- The dynamics of a batch chromatography column can be described by the coupled PDE system of advection-diffusion type:

$$\frac{\partial c_i}{\partial t} + \frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t} + \frac{\partial c_i}{\partial x} - \frac{1}{\mathrm{Pe}}\frac{\partial^2 c_i}{\partial x^2} = 0,$$
$$\frac{\partial q_i}{\partial t} = \kappa_i \left(q_i^{Eq} - q_i\right).$$

- It is a coupled PDE; thus, the coupling structure is desired to be preserved in learned ROM
- This is achieved by block diagonal projection, thereby not mixing separate physical quantities.

Operator Inference: Numerical Examples

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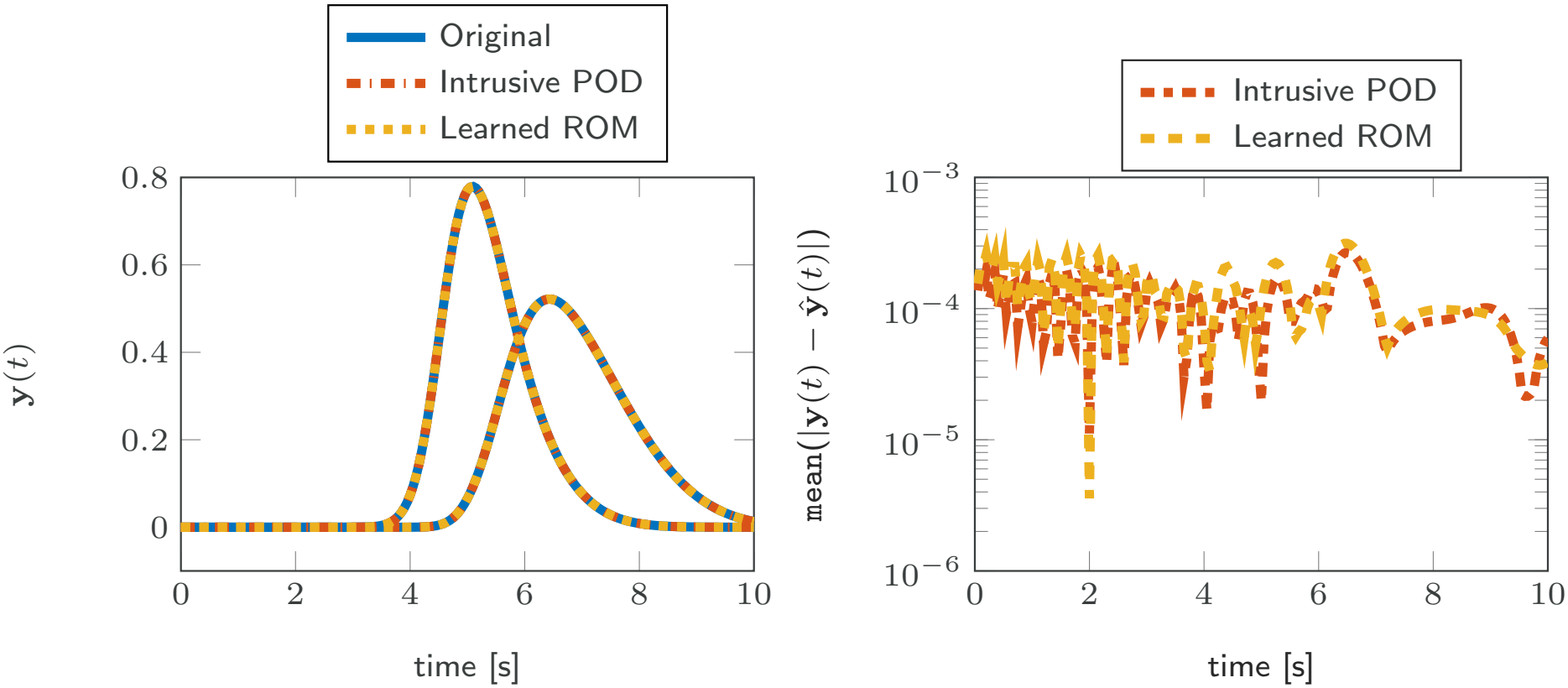

Figure: Batch chromatography example: A comparison of the POD intrusive model with the learned model of order $r = 4 \times 22$, where $n = 1600$ and $\mathrm{Pe} = 2000$.

Operator Inference: Numerical Examples

Parameterized Shallow Water Equations

- Parameterized shallow water equations are given by [Yildiz et al '21]

$$\begin{aligned}
\frac{\partial}{\partial t}\tilde{u} &= -h_x + \sin\theta\ \tilde{v} - \tilde{u}\tilde{u}_x - \tilde{v}\tilde{u}_y + \delta\cos\theta(h\tilde{u})_x - \frac{3}{8}\left(\delta\cos\theta\right)^2(h^2)_x,\\
\frac{\partial}{\partial t}\tilde{v} &= -h_y + \sin\theta\ \tilde{u} + \frac{1}{2}\delta\sin\theta\cos\theta\ h - \tilde{u}\tilde{v}_x - \tilde{v}\tilde{v}_y\\
&\qquad + \delta\cos\theta\left((h\tilde{u})_y + \frac{1}{2}h\left(\tilde{v}_x - \tilde{u}_y\right)\right) - \frac{3}{8}\left(\delta\cos\theta\right)^2(h^2)_y,\\
\frac{\partial}{\partial t}h &= -(h\tilde{u})_x - (h\tilde{v})_y + \frac{1}{2}\delta\cos\theta(h^2)_x.
\end{aligned}$$

- Parameterized by the latitude θ.
- $\tilde{\mathbf{u}} =: (\tilde{u}; \tilde{v})$ is the canonical velocity.
- h is the height field.
- We collect the training data for 5 different parameter realizations θ in $\left[\frac{\pi}{6}, \frac{\pi}{3}\right]$.
- Infer a reduced parametric model directly from data of order $r = 75$.

Operator Inference: Numerical Examples

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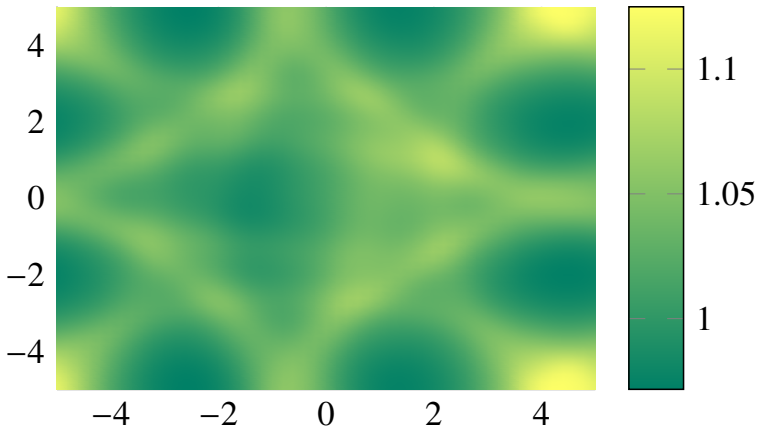
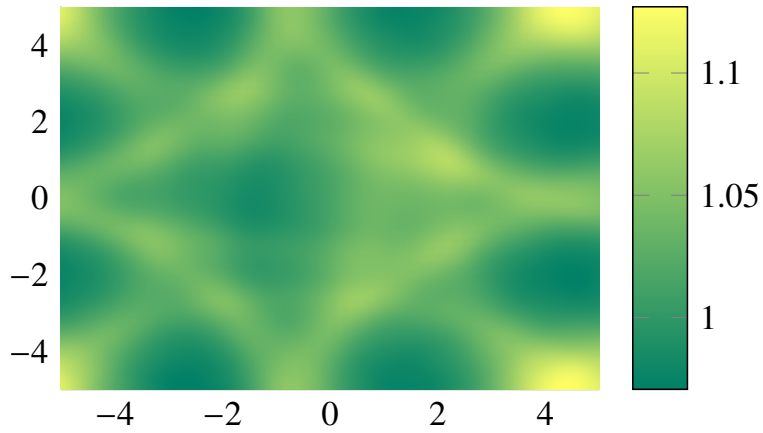
- Comparison of the height field for the parameter $\theta = \frac{5\pi}{24}$:



(a) FOM

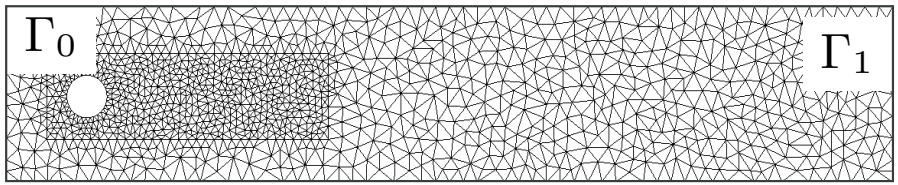


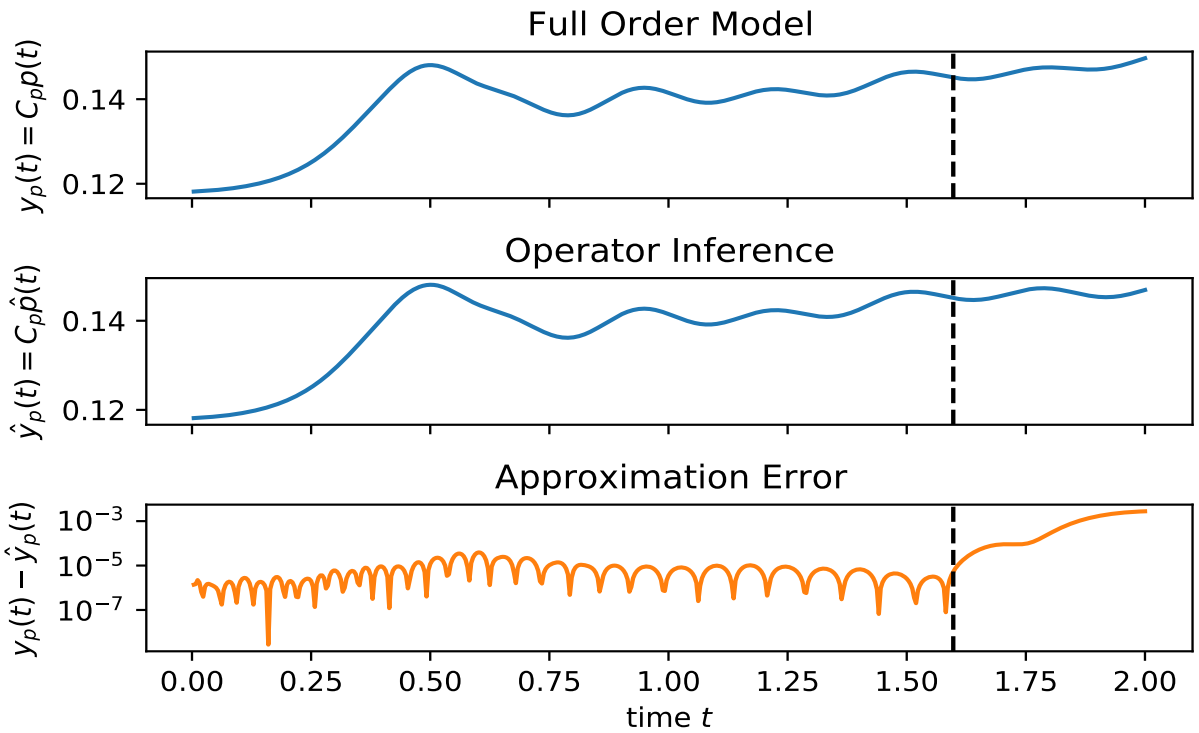
(b) Learned parametric model

Operator Inference: Numerical Examples

Navier-Stokes Equations

Tailored operator inference for incompressible Navier-Stokes equations, by heeding incompressibility condition. [B./Goyal/Heiland/Pontes '22]





Operator Inference

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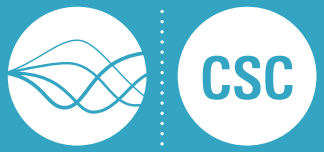
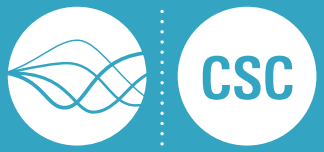
Conclusions — Part I

- DMD and operator inference (OpInf) are regression-based powerful methods to infer linear and certain nonlinear dynamical systems from data.
- Both look simple, but the devil is in the details.
- Choice of good observables? (Learning to learn?)
- Statistical aspects are not too well understood: impact of noise in the data on inferred models?
- Recent work combines OpInf with neural networks to solve nonlinear identification problems **($\rightsquigarrow$ Part II).**
- Error bounds for non-intrusive MOR not well developed yet, but theoretic results indicate that the OpInf model asymptotically (when increasing the number of snapshots) yields the POD model. Then, intrusive MOR error bounds can be applied.



Outline

1. Model Order Reduction of Dynamical Systems
2. Data-driven/-enhanced Model Reduction
3. Koopman Operator and DMD
4. Lifting Principle for Dynamical Systems



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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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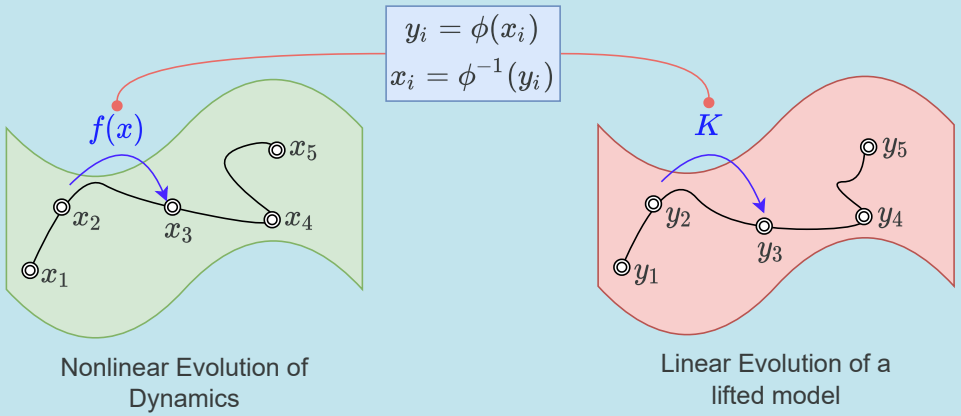
- Often referred to (in a simplistic view) as Dynamic Mode Decomposition or Operator Inference.
- Once a linear model is learned and verified, it can be deployed for control and design tasks.
- However, several challenges remain:
  - Often, one cannot measure the full state $\mathbf{x}$ ⇝ partial measurements!
  - Real-world processes are often nonlinear, thus learning a linear model may not be sufficient to characterize complex dynamic behavior.

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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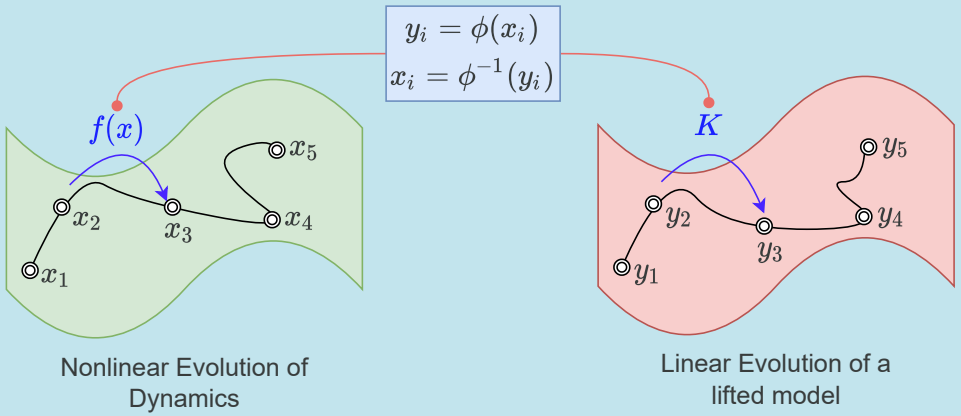

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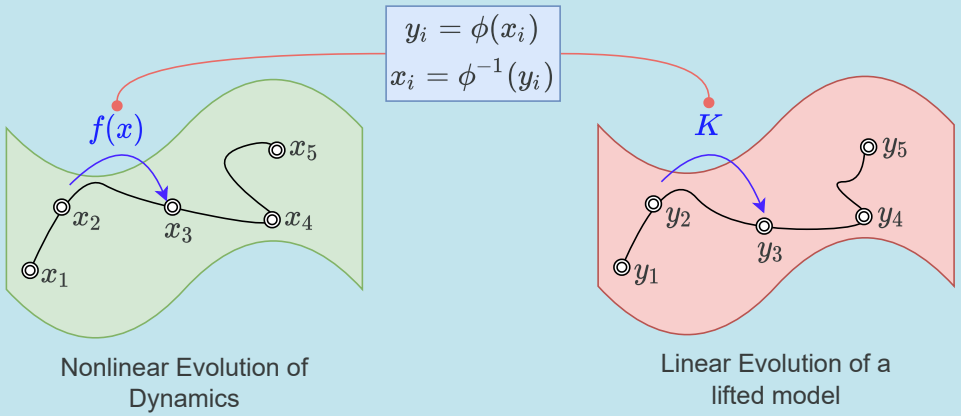

Extended DMD [Williams et al. 2015]

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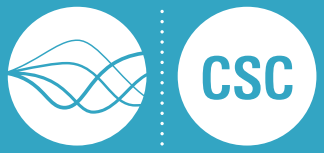
- For this, often hand-design observables are needed,
  - but challenging design decisions need to be taken, and it still is an approximation.



Our "Holy Grail"

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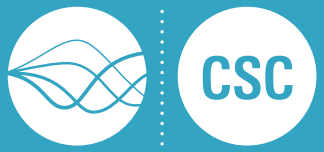

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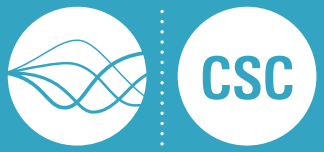

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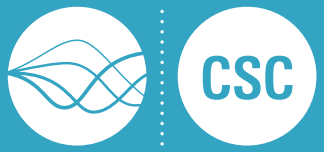
Lifting Principle



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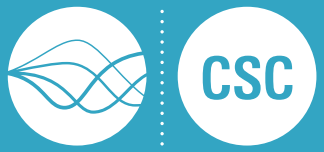

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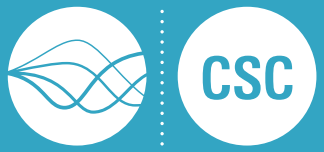

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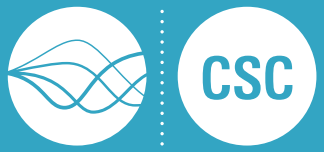
- This ideas has been further developed for learning dynamical systems.



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

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

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

  where $\mathbf{y}(t) = \mathcal{L}(\mathbf{x}(t))$ and $\mathcal{L}^\sharp\left(\mathbf{y}(t)\right) = \mathbf{x}(t)$.

- Such a lifting concept was first developed by [Savageau/Voit 1987] for control purposes.
- Also used for model reduction for nonlinear systems [Gu 2009, B./Breiten 2015].

Lifting Principle for Dynamical Systems

Lifted Nonlinear Dynamical Models 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.

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

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- Also used for model reduction for nonlinear systems [Gu 2009, B./Breiten 2015].
- Recently, it has become popular using terminology Lift and Learn by Willcox, Peherstorfer, Qian, Krämer, ... [Qian et al. 2019].

Lifting Principle for Dynamical Systems

An illustration

- Consider the simple pendulum model:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -\sin(x_2) \\ x_1 \end{bmatrix}.$$

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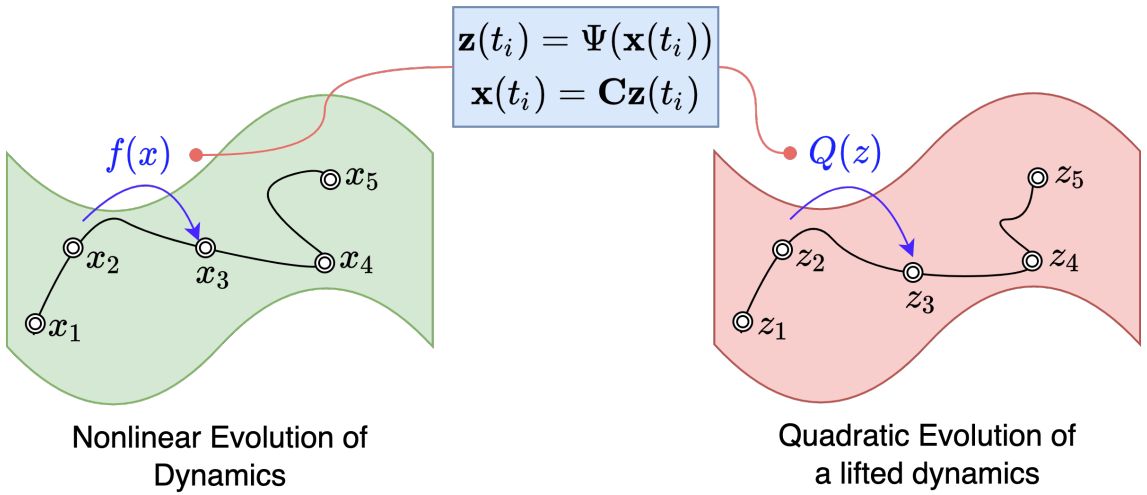
- Note that the inverse mapping is indeed linear.

Lifting Principle for Dynamical Systems

- Using observables—inspired by *lifting principle*—we can write nonlinear systems as quadratic systems
  - which are finite dimensional
  - for which we can reconstruct full-state using a linear projection (restriction) of observables.
  - so that for a given nonlinear system, lifted observables are easy to determine.



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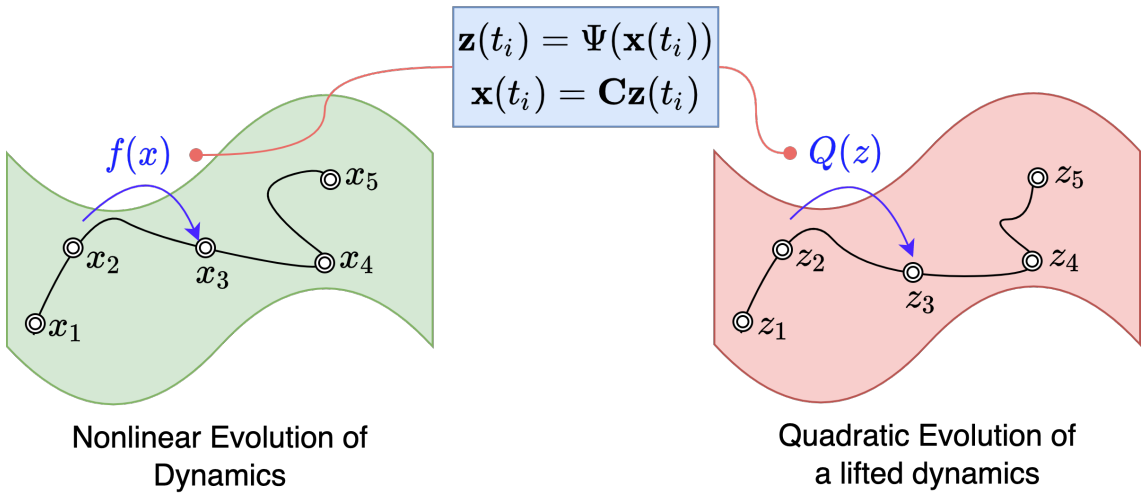

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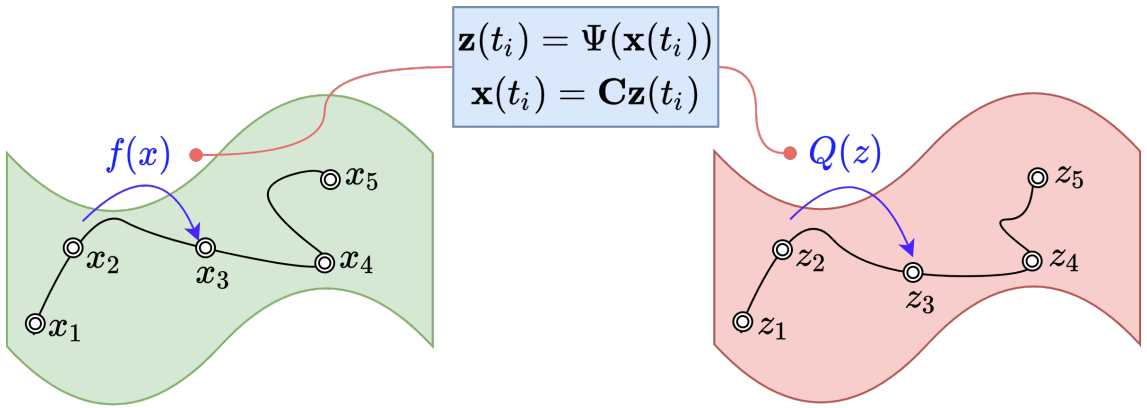

- For given nonlinear dynamical models, we can determine suitable observables.
- However, our goal itself is to learn dynamical models from data.

Lifting Principle for Dynamical Systems

Problem Statement (for fast decay of Kolmogorov n-width) **(Goyal/Benner 2022)**

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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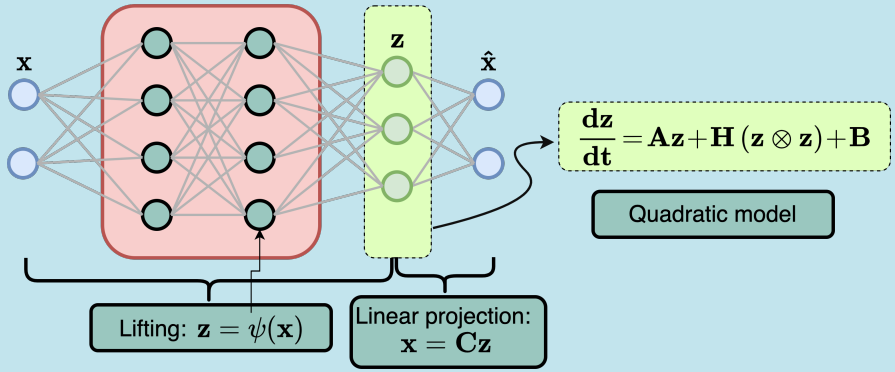

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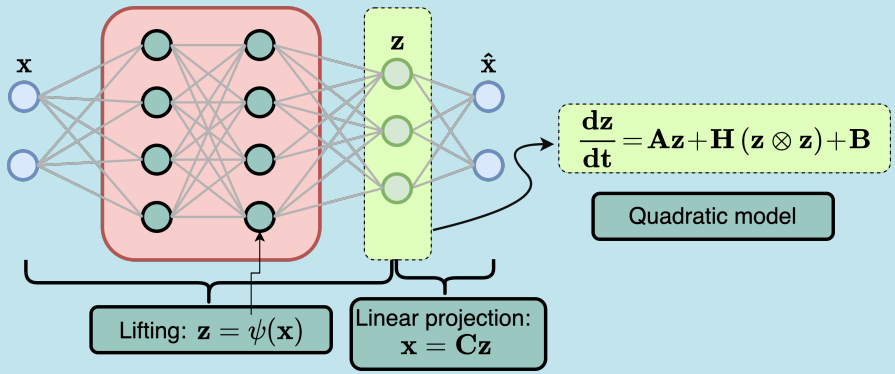
- We learn parameters of neural network $\psi(\cdot)$ and the system matrices $\{\mathbf{A}, \mathbf{H}, \mathbf{B}, \mathbf{C}\}$ simultaneously.



Loss function (Goyal/B. 2022)

- Compute $\dot{\mathbf{z}}$ using $\dot{\mathbf{x}}$ by the chain rule:

$$\mathcal{L}_{\dot{\mathbf{z}}\dot{\mathbf{x}}} = \| \left(\nabla_{\mathbf{x}} \mathbf{z}\right) \dot{\mathbf{x}} - \mathcal{Q}(\mathbf{z}) \|$$

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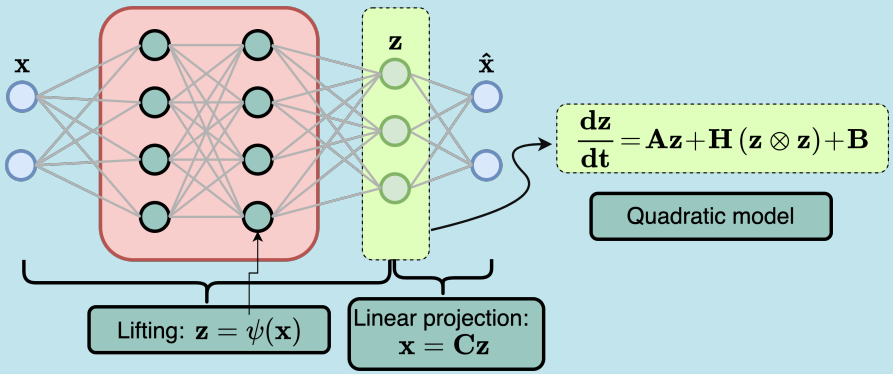

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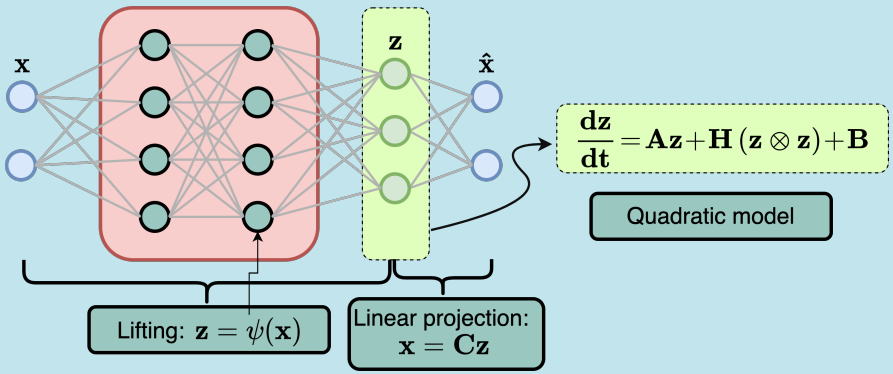

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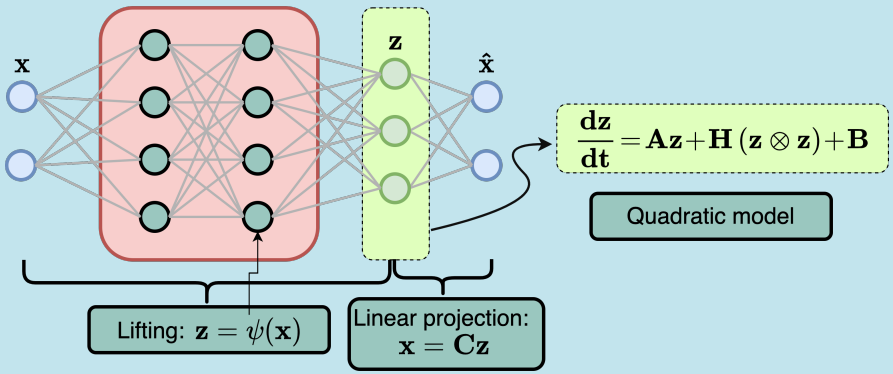

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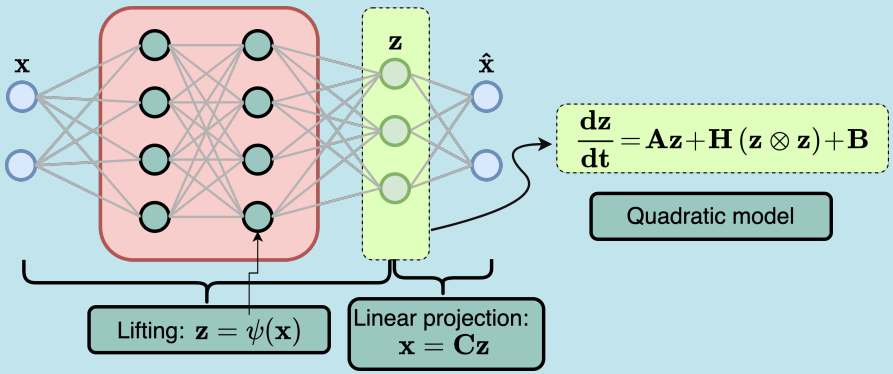

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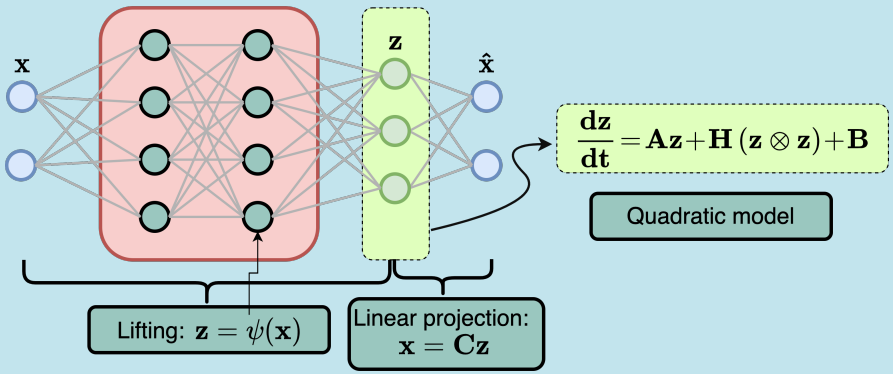

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- Note that once we have all these parameters, we need encoder (neural network) only to get initial condition for $\mathbf{z}$.
- The rest of the model is very classical state-space quadratic model
  $\rightsquigarrow$ can be used for engineering design.

Numerical Examples

Lambda–Omega reaction–diffusion example

- The governing equations are

$$u_t = (1 - (u^2 + v^2))u + \beta(u^2 + v^2)v + d_1(u_{xx} + u_{yy}),$$
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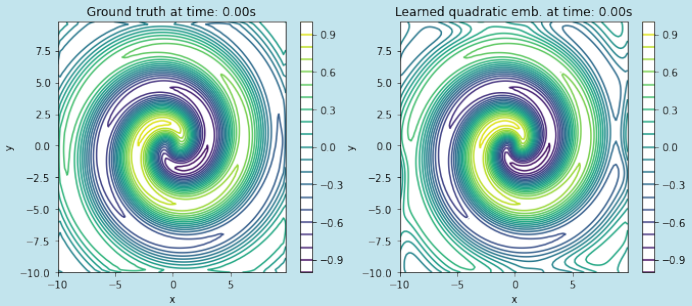
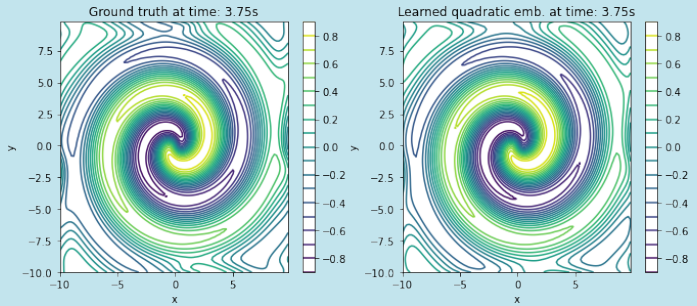
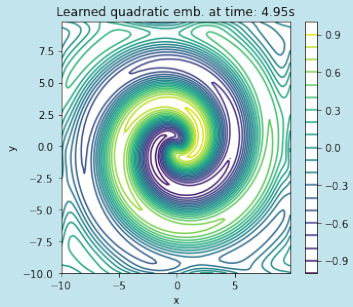


training



testing truth known



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Challenges and Possible Solutions

1. Recall that we have a linear projection from $\mathbf{z} \mapsto \mathbf{x}$. It works good only if we have a fast decay of singular values of our high-dimensional data
   - However, there is no suitable low-dimensional linear subspace for advection-dominant problems.
     - ⇝ Slow decay of Komologov n-width.
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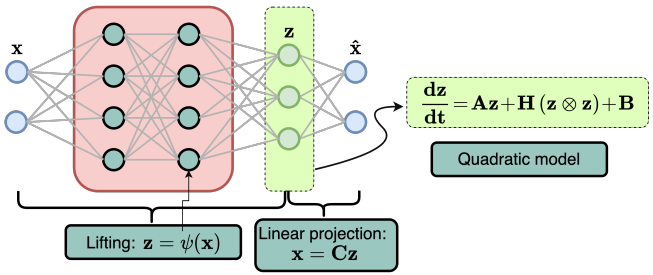

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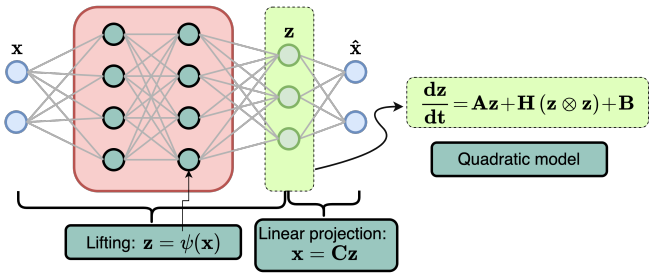
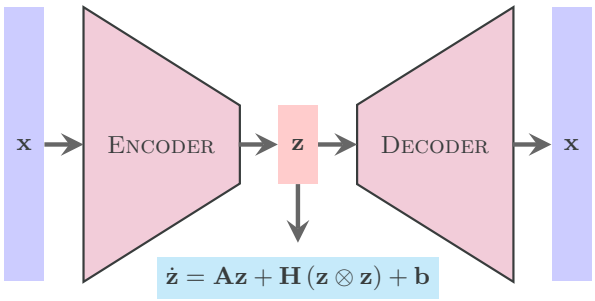
Remedy: Use a nonlinear decoder using neural networks (e.g., convolutional NNs for structured data)





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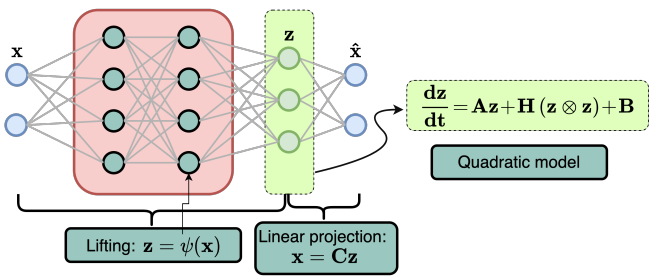
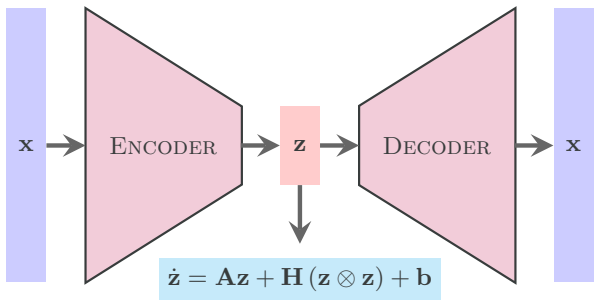
2. Moreover, to train networks, we need to determine derivative of output w.r.t. inputs.
   - If $\dim(\mathbf{x})$ is large, then derivative computations using, e.g., `autograd` become computationally very expensive.





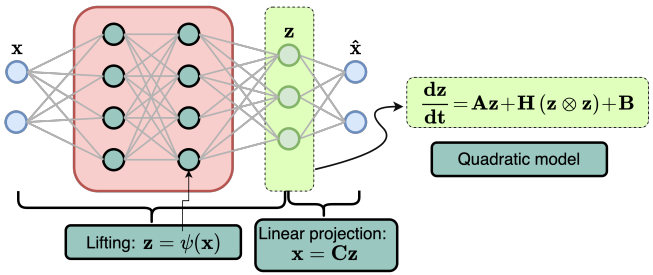
Challenges and Possible Solutions

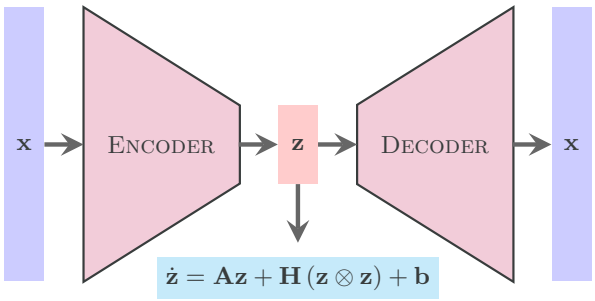
1. Recall that we have a linear projection from $\mathbf{z} \mapsto \mathbf{x}$. It works good only if we have a fast decay of singular values of our high-dimensional data
   - However, there is no suitable low-dimensional linear subspace for advection-dominant problems.
     - ⇝ Slow decay of Komologov n-width.
     - ⇝ Need a large-dimensional $\mathbf{z}$, meaning engineering studies can still be intractable.

   Remedy: Use a nonlinear decoder using neural networks (e.g., convolutional NNs for structured data)

2. Moreover, to train networks, we need to determine derivative of output w.r.t. inputs.
   - If $\dim(\mathbf{x})$ is large, then derivative computations using, e.g., `autograd` become computationally very expensive.

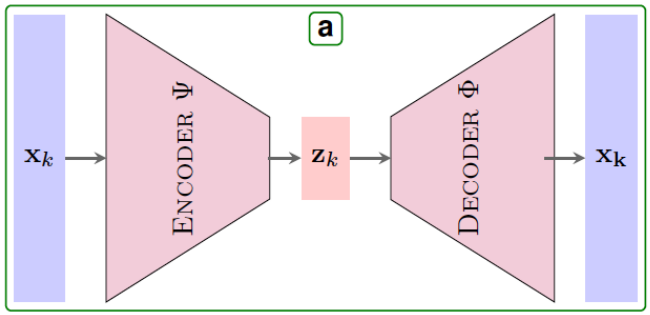
   Remedy: Embed a numerical integrator





Numerical Integrator and Low-dimensional Quadratic-embeddings

- Combining all, we have



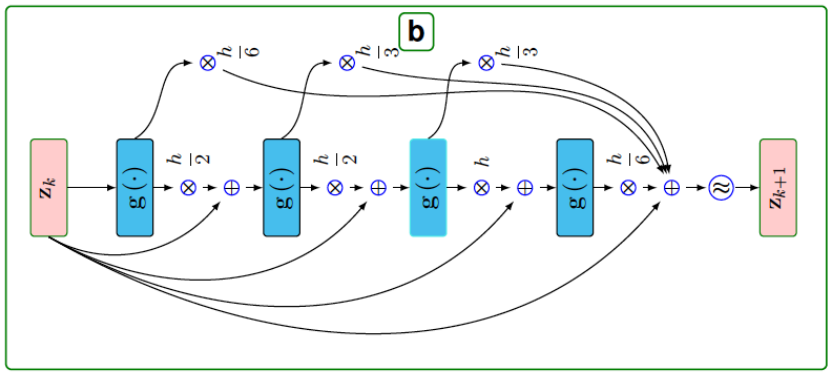
Encoding: $\mathbf{z}_k = \Psi(\mathbf{x}_k)$

Decoding: $\mathbf{x}_k = \Phi(\mathbf{z}_k)$

Runge-Kutta Constraint:

$\mathbf{z}_{k+1} \approx \Pi_{\mathsf{RK4}}(\mathbf{z}_k)$

$\mathbf{g}(\mathbf{z}) := \mathbf{A}\mathbf{z} + \mathbf{H}(\mathbf{z} \otimes \mathbf{z}) + \mathbf{b}$



- We focus on a Runge-Kutta scheme, but any integrator including adaptive ones can be utilized using Neural ODEs. [Chen et al. 2018]
- Once such an architecture is framed, we can learn encoder, decoder, and a quadratic model.

Numerical Example
Tubular Reactor Model

- One dimensional model with a single reaction, describing dynamics of the species concentration $\psi(x,t)$ and temperature $\theta(x,t)$ via

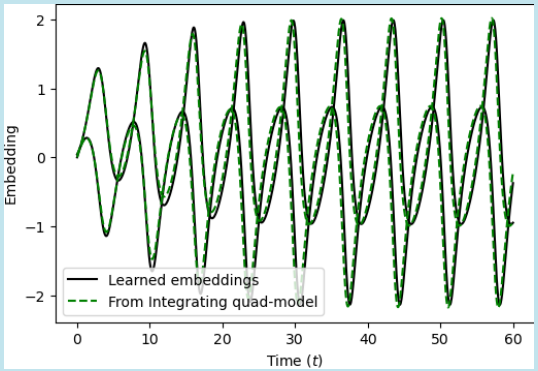
$$\begin{aligned}\frac{\partial \psi}{\partial t} &= \frac{1}{\mathrm{Pe}}\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial \psi}{\partial x} - \mathcal{D}\mathcal{F}(\psi,\theta;\gamma),\\ \frac{\partial \theta}{\partial t} &= \frac{1}{\mathrm{Pe}}\frac{\partial^2 \theta}{\partial x^2} - \frac{\partial \theta}{\partial x} - \beta(\theta-\theta_{\mathsf{ref}}) + \mathcal{B}\mathcal{D}\mathcal{F}(\psi,\theta;\gamma),\end{aligned}$$

  with spatial variable $x \in (0,1)$, time $t > 0$ and Arrhenius reaction term

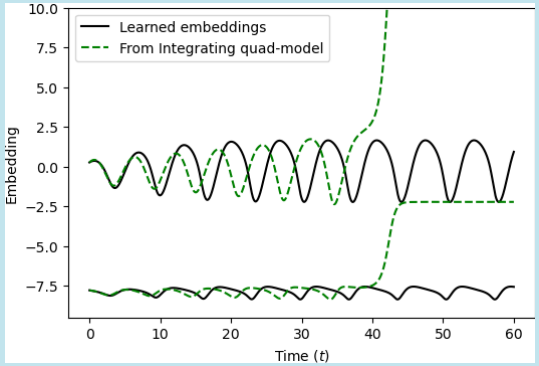
$$\mathcal{F}(\psi,\theta;\gamma) = \psi \exp\left(\gamma - \frac{\gamma}{\theta}\right).$$

- Collect snapshots in time $\mathbf{T} = [0,10]$.
- We learn 2-dimensional embeddings using convolutional autoencoder.
- For comparison, we also compute a 2-dimensional model using POD projection (classical OpInf).

Numerical Example
Tubular Reactor Model

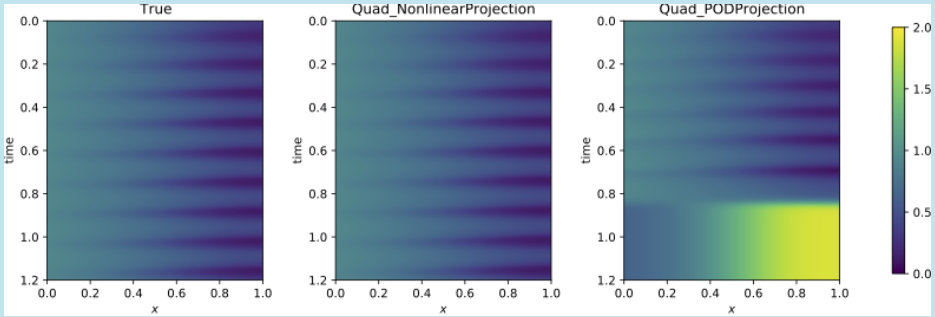


(a) convolutional autoencoder

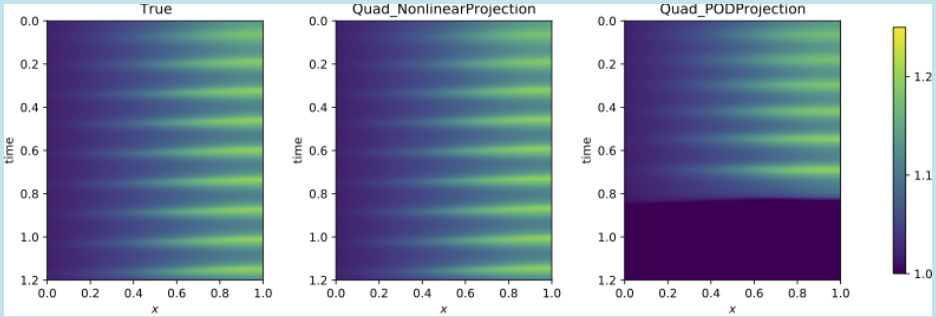


(b) POD

Figure: 2-dimensional embeddings.



(a) Concentration on the full-grid.



(b) Temperature on the full-grid.

Figure: Comparison of the convolutional autoencoders and POD-based approaches.

Numerical Example
2D Burgers equation

- Governing equation:

$$\frac{\partial u(x,t)}{\partial t} + \left(\frac{1}{2}, \frac{1}{2}\right)^\top \cdot \nabla u(x,t)^2 = 0 \quad \forall (x,t) \in \Omega \times [0,T].$$

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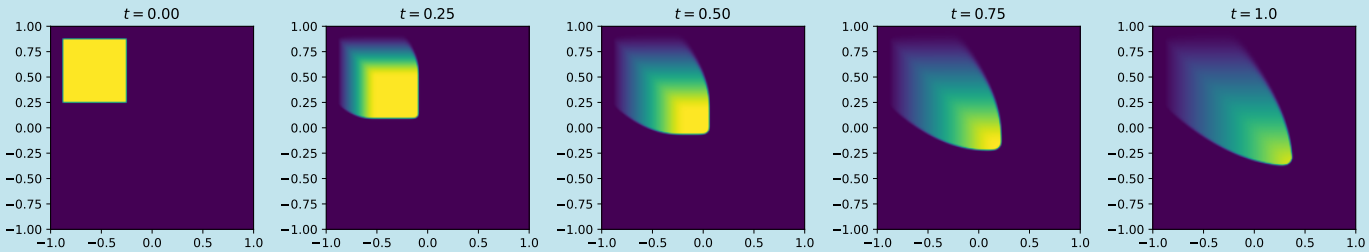

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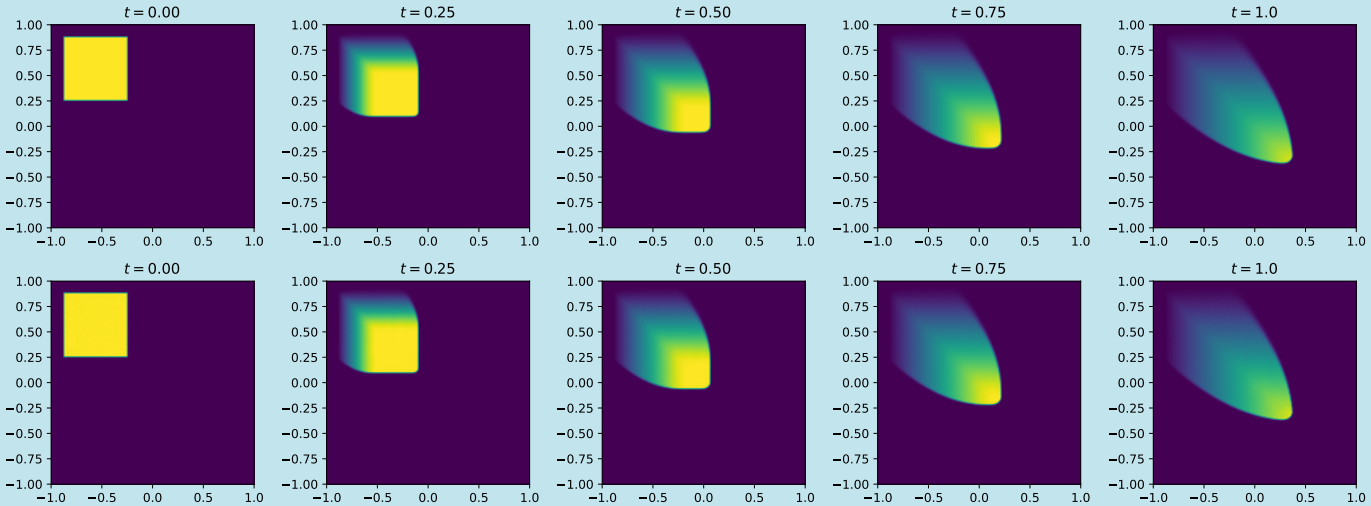

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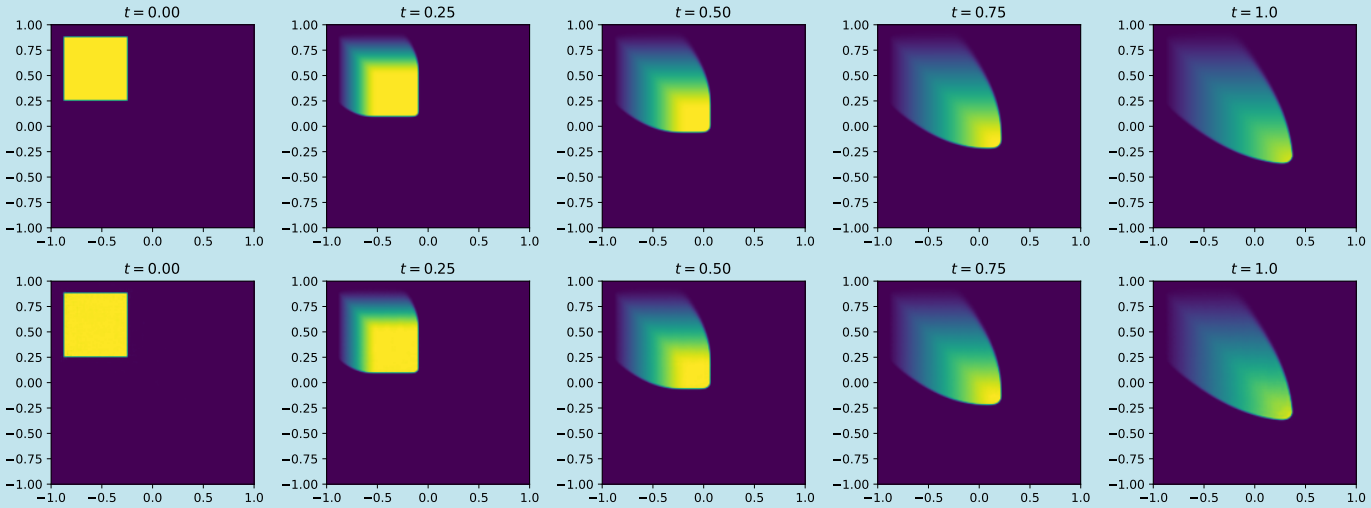

- Note that for rich dynamics,we may need to increase the dimension of the quadratic embeddings.

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Thank you for your attention!!

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