MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Computational Learning of Dynamical Systems with Stability Constraints

Peter Benner

Joint work with Igor Pontes Duff
and Pawan K. Goyal (appliedAI Initiative, Heilbronn/Germany)

Computational Learning for Model Reduction
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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 $x(t) \in \mathbb{R}^n$,
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Model Order Reduction of Dynamical Systems

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

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

Model Order Reduction of Linear Systems
Linear Time-Invariant (LTI) Systems

Original System

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

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$$\widehat{\Sigma} : \begin{cases} \dot{\hat{x}}(t) = \widehat{A}\hat{x}(t) + \widehat{B}u(t), \\ \hat{y}(t) = \widehat{C}\hat{x}(t) + \widehat{D}u(t). \end{cases}$$

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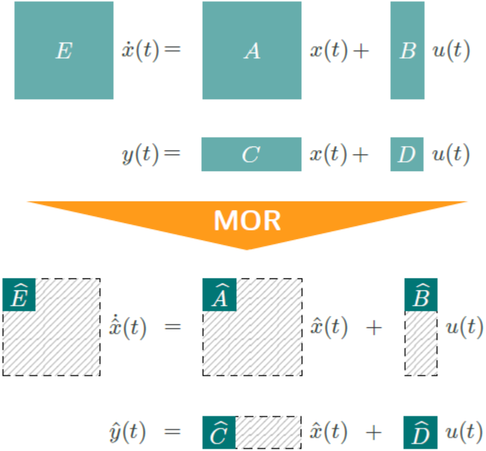

- $E, A \in \mathbb{R}^{n \times n}$
- $B \in \mathbb{R}^{n \times m}$
- $C \in \mathbb{R}^{p \times n}$
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From intrusive to non-intrusive MOR

Assumption: trajectory $x(t;u)$ is contained in low-dimensional subspace $\mathcal{V} \subset \mathbb{R}^n$.
Thus, use Galerkin or Petrov-Galerkin-type projection of state-space onto $\mathcal{V}$ (trial space) along complementary subspace $\mathcal{W}$ (test space), where

$$\operatorname{range}(V) = \mathcal{V}, \quad \operatorname{range}(W) = \mathcal{W}, \quad W^T V = I_r.$$

The **reduced-order (or surrogate) model** then is

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This is often impossible!

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

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Data-driven/-enhanced Model Reduction
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- Operator inference (OpInf): time domain [Kravtsov/Kondrashov/Ghil 2005, Peherstorfer/Willcox 2016; Kramer, Qian, Farcas, B., Goyal, Pontes Duff, Yildiz,...]

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$$\begin{aligned} x_{k+1} &= Ax_k + Bu_k + Kw_k, \\ y_k &= Cx_k + Du_k + v_k. \end{aligned}$$

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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 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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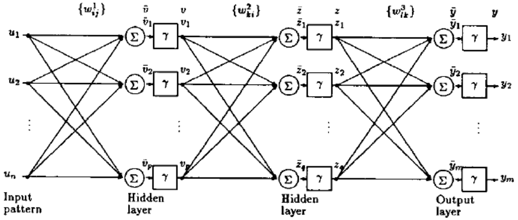

Fig. 2. A three layer neural network.

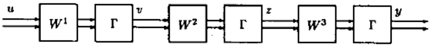

Fig. 3. A block diagram representation of a three layer network.

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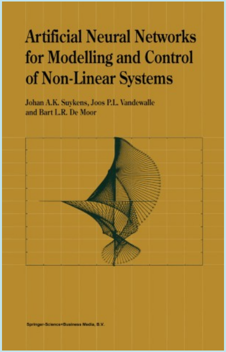

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Suykens, J.A.K., Vandewalle, J.P.L., de Moor, B.L. (1996): Artificial Neural Networks for Modelling and Control of Non-Linear Systems. Springer US.

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

$$A_* := \operatorname{argmin}_{A \in \mathbb{R}^{n \times n}} \|X_1 - AX_0\|_F^2 + \mathcal{R}(A)$$

with a potential regularization term $\mathcal{R}(A)$, e.g., Tikhonov regularization aka kernel ridge regression: $\mathcal{R}(A) = \beta \|A\|_F^2$.

Given a smooth control system

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

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

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

Given a smooth control system

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

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

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

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

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):

$$(A_*, B_*, C_*, D_*) := \operatorname{argmin}_{(A,B,C,D)\in\mathbb{S}} \left\| \begin{bmatrix} X_1 \\ Y_0 \end{bmatrix} - \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} X_0 \\ U_0 \end{bmatrix} \right\|_F^2 + \mathcal{R}(A, B, C, D)$$

with a potential regularization term $\mathcal{R}(A, B, C, D)$.

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

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

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- Compress snapshot matrix of time derivatives: if residuals $f(x_j, u_j)$ are available

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

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

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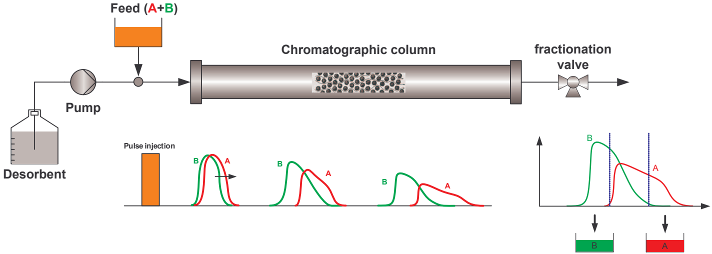
- Solve the regularized linear least-squares problem (regression):

  $$(\hat{A}_*, \hat{H}_*, \hat{B}_*) := \operatorname{argmin}_{(\hat{A}, \hat{H}, \hat{B})} \left\| \dot{\hat{X}} - \begin{bmatrix} \hat{A} & \hat{H} & \hat{B} \end{bmatrix} \begin{bmatrix} \hat{X} \\ \hat{X} * \hat{X} \\ U \end{bmatrix} \right\|_F^2 + \mathcal{R}(\hat{A}, \hat{H}, \hat{B})$$

  with the Khatri-Rao product $\hat{X} * \hat{X} := [\hat{x}_0 \otimes \hat{x}_0, \ldots, \hat{x}_K \otimes \hat{x}_K]$.



- 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.

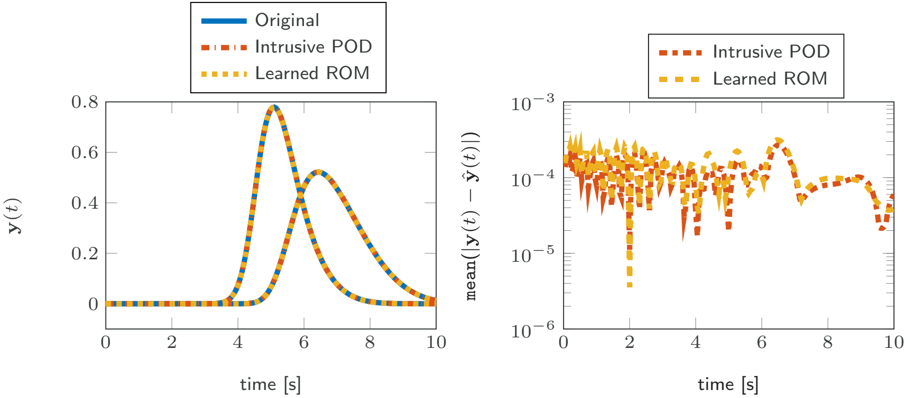


Figure: Batch chromatography example: A comparison of the POD intrusive model with the learned model of order $r = 4 \times 22$, where $n = 1600$ and $\mathrm{Pe} = 2000$.

- Parameterized shallow water equations are given by

$$\frac{\partial}{\partial t}\tilde{u} = -h_x + \sin\theta\ \tilde{v} - \tilde{u}\tilde{u}_x - \tilde{v}\tilde{u}_y + \delta\cos\theta(h\tilde{u})_x - \frac{3}{8}\left(\delta\cos\theta\right)^2\left(h^2\right)_x,$$

$$\frac{\partial}{\partial t}\tilde{v} = -h_y + \sin\theta\ \tilde{u} + \frac{1}{2}\delta\sin\theta\cos\theta\ h - \tilde{u}\tilde{v}_x - \tilde{v}\tilde{v}_y$$

$$+\,\delta\cos\theta\left((h\tilde{u})_y + \frac{1}{2}h\left(\tilde{v}_x - \tilde{u}_y\right)\right) - \frac{3}{8}\left(\delta\cos\theta\right)^2\left(h^2\right)_y,$$

$$\frac{\partial}{\partial t}h = -(h\tilde{u})_x - (h\tilde{v})_y + \frac{1}{2}\delta\cos\theta(h^2)_x.$$

- 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 $r = 75$.

Paramterized Operator Inference [Yildiz/Goyal/B./Karasözen 2021]

Numerical Example: Shallow Water Equations

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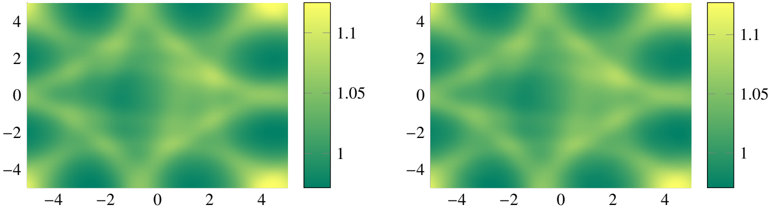
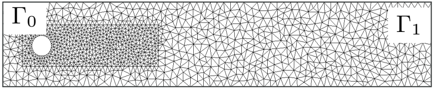
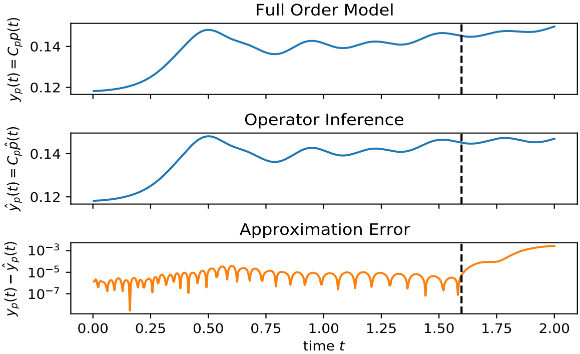
- Comparison of the height field for the parameter $\theta = \frac{5\pi}{24}$:



(a) FOM (b) Learned parametric model

Tailored operator inference for incompressible Navier-Stokes equations, by heeding incompressibility condition.





Problem: OpInf regression potentially yields unstable dynamics.
$\rightsquigarrow$ Even marginal instability can lead to unphysical simulation results.

Preserving Stability in Operator Inference

Problem: OpInf regression potentially yields unstable dynamics.
$\rightsquigarrow$ Even marginal instability can lead to unphysical simulation results.

Goal: infer systems with guaranteed stability.

Asymptotic (exponential, Lyapunov) stability of linear systems

$$\dot{x}(t) = Ax(t), \qquad x(0) = x_0,$$

can be explicitly parameterized:

Theorem (Gillis/Sharma 2017)

A matrix $A \in \mathbb{R}^{n \times n}$ is asymptotically stable (Hurwitz, Lyapunov stable) if and only if it can be represented as

$$A = (J - R)Q,$$

where $J = -J^T$ and $R = R^T$, $Q = Q^T$ are both positive definite.

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$\Longrightarrow$ **Stability-preserving OpInf for linear systems** [Goyal/Pontes Duff/B. 2023]:

$$(S_*, L_*, K_*) := \operatorname{argmin}_{\substack{L,K \text{ upper triangular} \\ \text{with positive diagonals}}} \left(\|\dot{X} - (S - S^T - L^T L) K^T K X\|_F^2 + \mathcal{R}(L, K, S) \right).$$

The matrix obtained from this nonlinear (regularized) least-squares problem,

$$A_* = \left(S_* - S_*^T - L_*^T L_* \right) K_*^T K_*,$$

is guaranteed to be stable due to [Gillis/Sharma 2017].

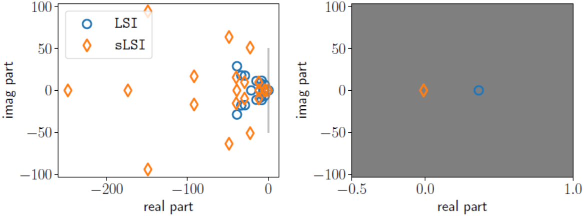
Related work by *Schwerdtner/Voigt*, *Unger*, ...

Consider 1D Burgers' equation for viscous flow

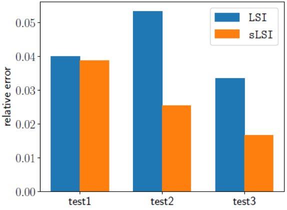
$$\begin{aligned} v_t + v v_x &= \nu v_{xx} \text{ in } (0,1)\times(0,T) \\ v_x(0,t) &= v_x(1,t) = 0, \\ v(x,0) &= v_0(x,\mu), \end{aligned}$$

discretized on uniform 1000×500 space-time grid for $17+3$ training+testing initial conditions.

Reduced-order model ($r = 21$) computed using standard ("LSI") and stabilized ("SLSI") OpInf applied to (POD)-projected data.
(Implementation using `PyTorch` and `Adam` optimizer for solving nonlinear regression problem.)



Eigenvalues of linearization



Errors for different initial conditions (test data)

Solving the OpInf regression problem

$$(A_*, H_*) := \operatorname{argmin}_{(A,H)} \left\| \dot{X} - \begin{bmatrix} A & H \end{bmatrix} \begin{bmatrix} X \\ X * X \end{bmatrix} \right\|_F^2 + \mathcal{R}(A\,H)$$

using the stability-constraint on A as just discussed leads to a nonlinear system with local Lyapunov stability, noting that the inferred $Q_* = K_*^T K_* > 0$ provides a quadratic Lyapunov function for the identified system [Goyal/Pontes Duff/B. 2023].

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We can achieve more for energy-preserving quadratic systems, i.e.,

$$H_{ijk} + H_{ikj} + H_{jik} + H_{jki} + H_{kij} + H_{kji} = 0 \quad \text{for all } i, j, k \in \{1, \dots, n\}.$$

Note: the latter is equivalent to $x^T H(x \otimes x) = 0$ for all $x \in \mathbb{R}^n$ [Schlegel/Noack 2015].

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Theorem (Goyal/Pontes Duff/B. 2023)

A locally Lyapunov stable quadratic system in $\mathbb{R}^n$

$$\dot{z} = Az + H(z \otimes z), \qquad A = (J - R)Q,\ J = -J^T,\ R = R^T > 0,\ Q = Q^T > 0,$$

is generalized energy-preserving w.r.t. Q, i.e., $x^T QH(x \otimes x) = 0$ for all x, if

$$H = [H_1 Q, \ldots, H_n Q], \quad \text{where} \quad H_j = -H_j^T, \quad j = 1, \ldots, n.$$

Moreover, $V(x) = \frac{1}{2} x^T Qx$ is a global Lyapunov function for the quadratic system.

Constrained OpInf problem for learning GAS systems [Goyal/Pontes Duff/B. 2023]

$$(A_*, H_*) := \operatorname{argmin}_{(A,H)} \left\| \dot{X} - \begin{bmatrix} A & H \end{bmatrix} \begin{bmatrix} X \\ X * X \end{bmatrix} \right\|_F^2 + \mathcal{R}(A\,H)$$

subject to the stability constraints

$$A = \left(S - S^T - L^T L\right) K^T K \quad \text{with } L, K \text{ upper triangular with positive diagonals}$$

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Implementation:

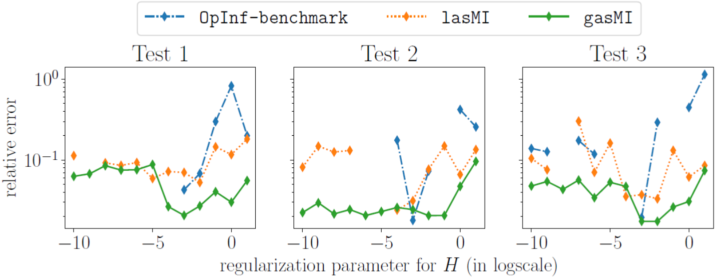
- Usually, as discussed before, the data are projected onto the leading r PCA modes for dimension reduction.
- Quite involved optimization problem, can be solved via stochastic gradient descent (Adam) and backpropagation (setting $Q = I_r$ may be necessary).
- We do not explicitly need derivative data by using a Neural ODE approach for noisy data [Goyal/B. 2023].

Consider again 1D Burgers' equation for viscous flow

$$\begin{aligned} v_t + v v_x &= \nu v_{xx} \text{ in } (0,1)\times(0,T) \\ v(0,t) &= v(1,t) = 0, \\ v(x,0) &= v_0(x,\mu), \end{aligned}$$

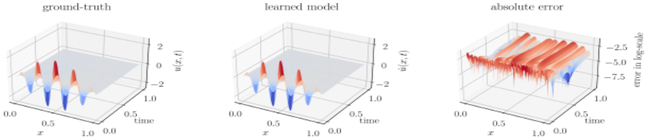
discretized on uniform 250×500 space-time grid for $17+3$ training+testing initial conditions and $\nu = 0.05$.

Reduced-order model ($r = 20$) computed using standard, locally stable (lasMI) and globally stable (gasMI) OpInf applied to (POD)-projected data.
(Implementation using `PyTorch` and `Adam` optimizer for solving nonlinear regression problem.)

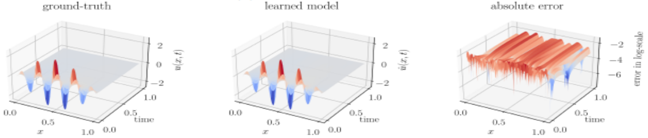


(missing data = blow-up in numerical simulation)

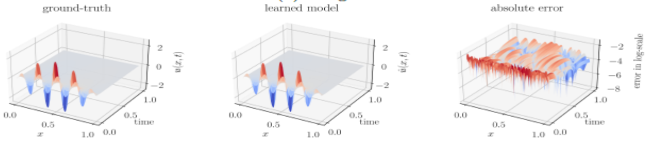
Consider again 1D Burgers' equation for viscous flow



(a) Using **opInf-benchmark**.



(b) Using **lasMI**.



(c) Using **gasMI**.

Full simulation for test initial condition (not seen during training)

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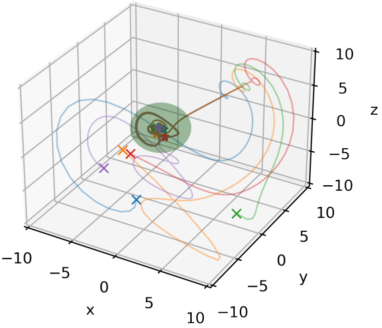

Figure: An illustration of nonlinear dynamics with attractor.

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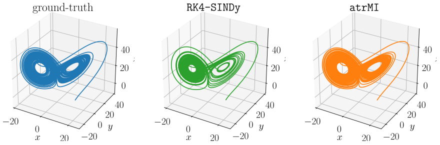
Inference of ATR quadratic systems [Goyal/Pontes Duff/B. 2023]

- It can be shown that for energy-preserving quadratic systems, an ATR system can be turned into a GAS system by translation $x(t) \to x(t) - y$
- We, thus, require to solve the following constraint problem:

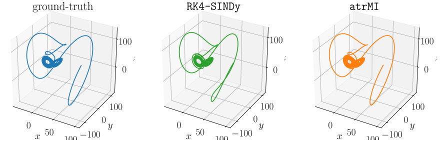
$$\min_{A,H,y} \left\| \dot{X} - A(X-y) - H\left((X-y) * (X-y)\right) \right\|$$

subject to $\Lambda(A) \in \mathbb{C}^-$ and H is energy preserving.

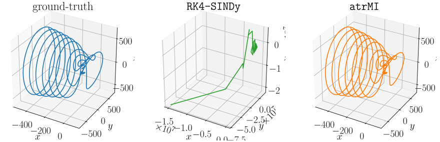
- Note that we do not know y a priori, it is learned from the data.



(a) For initial condition $[10, 10, -10]$.



(b) For initial condition $[100, -100, 100]$.



(c) For initial condition $[-500, 500, 500]$.

A comparison of the time-domain simulations of the learned models for testing initial conditions.

Conclusions

- Operator inference (OpInf) is a regression-based powerful method to infer linear and certain nonlinear dynamical systems from data, very similar to DMD in the linear case.
- Looks simple, but the devil is in the details.
- Stability constraints can be encoded explicitly in the regression problem for the model inference.
- For application to control problems, see MTNS2024 contribution by Pontes Duff [Pontes Duff/Goyal/B. 2024].
- The same approach can also be used to infer stable systems using sparse regression (SINDy).
- Recent work combines OpInf with neural networks to solve nonlinear parametric identification problems with stability guarantee (preprint coming out soon).
- Error bounds for non-intrusive MOR need to be further developed.
- Better solvers for special nonlinear regression problems needed!

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