MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Application of Physics-Informed Neural Networks in Nonlinear Systems Identification and Parameter Estimation

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SINDy Algorithm

SINDy algorithm identifies nonlinear dynamical systems from data, based on the assumption that many systems have relatively few active terms in the dynamics $\dot{x}(t) = f\big(x(t)\big)$.

- SINDy uses sparse regression to identify **active terms** out of a **library** of candidate linear and nonlinear model terms.

1. **Measuring** m snapshots of the state x in time and arrange them into a data matrix

$$X = [x_1 \ x_2 \ \cdots \ x_m]^T$$

2. **Computing the library** of D candidate nonlinear functions $\Theta(X) \in \mathbb{R}^{m \times D}$

$$\Theta(X) = [1 \ X \ X^2 \ \cdots X^d \ \cdots \ sin(X) \ \cdots]$$

3. **Computing time derivatives** of the state $X_t = [\dot{x}_1 \ \dot{x}_2 \ \ldots \ \dot{x}_m]$ and solving $X_t = \Theta(X)\Xi$

Extension to PDEs

Least Squares minimization:

$$\Xi = \arg\min_{\hat{\Xi}} \frac{1}{2} \|U_t - \Theta(U)\hat{\Xi}\|_2^2 + R(\hat{\Xi})$$

where, $R(\Xi)$ is a **regularizer to promote sparsity**

Examples:

- Sequentially Thresholded Least-Squares **(STLS)**, $R(\Xi) = \lambda \|\Xi\|_0$
- Sequentially thresholded ridge regression **(STRidge)**, $R(\Xi) = \lambda_1 \|\Xi\|_0 + \lambda_2 \|\Xi\|_2$

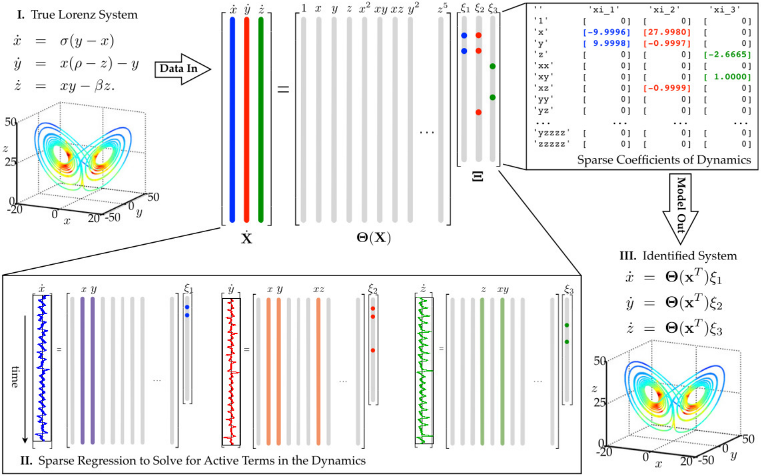
$\| \cdot \|_0$ stands for total number of non-zero elements in a vector

- For **PDEs** Similar to original SINDy with the **library including partial derivatives** if we have $u_t = \mathcal{G}(u), \; x \in \Omega, t \in [0, T]$

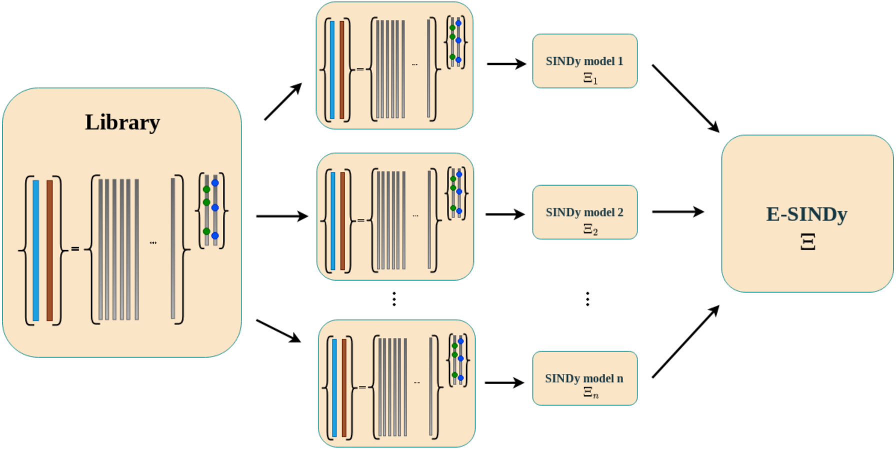
$$\Theta(U) = [1 \; U \; U^2 \; \cdots, \; U_x \; \cdots \; UU_x \; \cdots]$$

SINDy Algorithm

∗ Picture taken from the original paper



Ensemble-SINDy



iNeural-SINDy: **Integrating schemes and neural networks assisted SINDy approach**

SINDy **drawbacks:**

- Sensitivity to accurate derivative information
- Sensitivity to noisy data

Our solution:

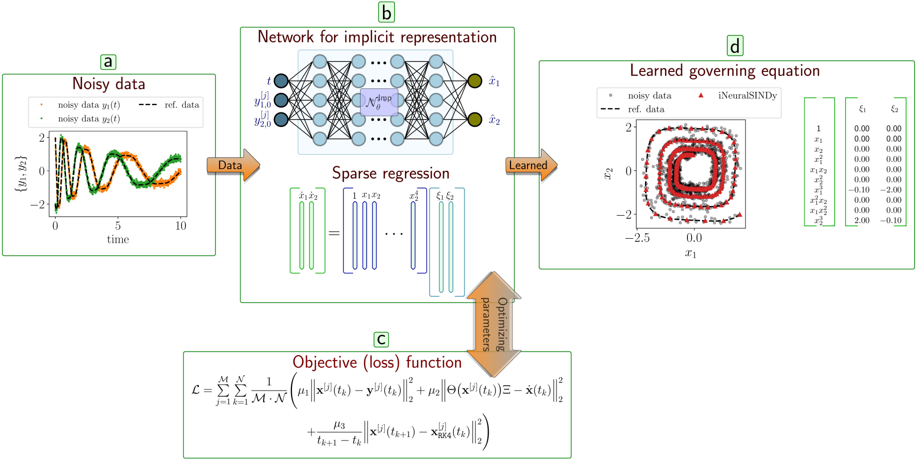
- Using *Deep Neural Network* (DNN) and *integration scheme*

$$\mathcal{L} = \mu_1 \mathcal{L}_{\texttt{MSE}} + \mu_2 \mathcal{L}_{\texttt{deri}} + \mu_3 \mathcal{L}_{\texttt{RK4}}, \quad \mu_1, \mu_2, \mu_3 \in [0,1], \tag{1}$$

$$\mathcal{L}_{\texttt{MSE}} = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \left\| x(t_k) - y(t_k) \right\|_2^2, \quad \mathcal{L}_{\texttt{deri}} = \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \left\| \dot{x}(t_k) - \Theta\big(x(t_k)\big)\Xi \right\|_2^2, \tag{2}$$

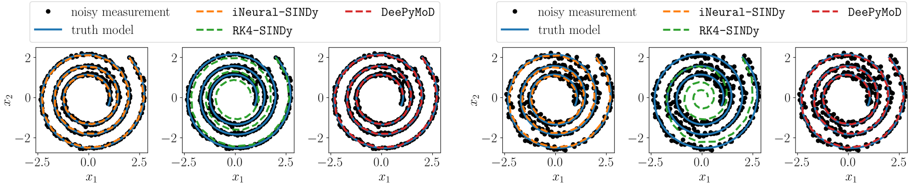
$$\mathcal{L}_{\texttt{RK4}} = \frac{1}{h} \frac{1}{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \left\| x(t_k) - \mathcal{F}_{\texttt{RK4}}\Big(\Theta\big(x(t_k)\big)\Xi, x(t_k), h_k\Big) \right\|_2^2. \tag{3}$$

iNeural-SINDy



Two-dimensional damped oscillators:

$$\begin{aligned}\dot{x}_1(t) &= -0.1x_1(t) + 2.0x_2(t)\\ \dot{x}_2(t) &= -2.0x_1(t) - 0.1x_2(t).\end{aligned} \tag{4}$$



(a) noise 0.04 (b) noise 0.08

PINN

In PINN we focus on computing data-driven solutions to partial differential equations of the general form

$$u_t + \mathcal{G}(u) = 0,\ x \in \Omega, t \in [0, T], \tag{5}$$

$\mathcal{G}(\cdot)$ is a nonlinear differential operator, and Ω is a subset of $\mathbb{R}^D$.
We define $g(t, x)$ to be given by the left-hand-side of equation (5); i.e.

$$g := u_t + \mathcal{G}(u) \tag{6}$$

as usual we would like to approximate $u(t, x)$ by a DNN. This assumption along with (6) result in a *physics informed neural network* $g(t, x)$.

The shared parameters between the neural networks $u(t,x)$ and $g(t,x)$ can be learned by minimizing the mean squared error loss

$$\mathtt{MSE} = \mathtt{MSE}_u + \mathtt{MSE}_g, \tag{7}$$

where

$$\mathtt{MSE}_u = \frac{1}{\mathcal{N}_u}\sum_{i=1}^{\mathcal{N}_u}\left|u(t_u^i, x_u^i) - u^i\right|^2, \mathtt{MSE}_g = \frac{1}{\mathcal{N}_g}\sum_{i=1}^{\mathcal{N}_g}\left|g(t_g^i, x_g^i)\right|. \tag{8}$$

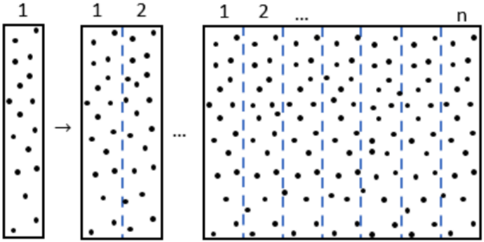
and if we want o solve the PDE then we need also boundary condition, and accordingly its corresponding loss $\mathtt{MSE}_b$.

$$\mathtt{MSE}_b = \frac{1}{\mathcal{N}_b}\sum_{i=1}^{\mathcal{N}_b}\left|u(t_u^b, x_u^b) - u^b\right|^2 \tag{9}$$

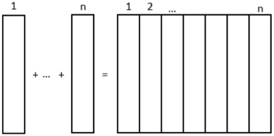
Improved PINN

Some strategies to improve the accuracy of the PINN:

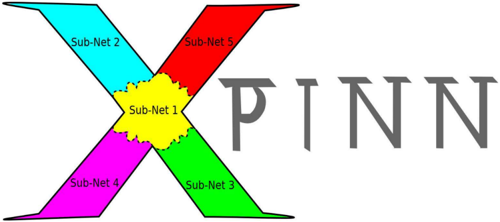
- Adding weights in the loss function
- Mini-batching strategy to improve convergence
- Adaptive time-sampling



- Time-marching



- Extended PINN(XPINN)

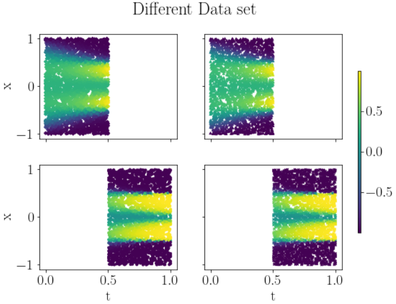


Allen-Cahn equation:

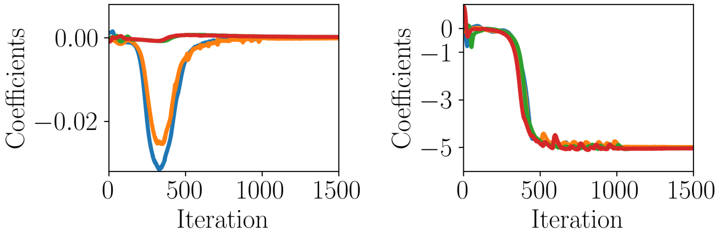
$$u_t - 0.0001u_{xx} + 5u^3 - 5u = 0, \quad x \in [-1, 1], \ t \in [0, 1]$$

Simulation setup for **ensemble** `XPINN`:

- 2 subdomains each having 2 ensemble, using 5% of data set
- DNN structure of each ensemble: $2 * 128 * 128 * 128 * 1$
- Fixing the library terms



Ensembled XPINN



Estimated Coefficients:

$$\text{first: } \begin{bmatrix} 2.0689e-04 \\ -5.0332e+00 \end{bmatrix}, \text{ second: } \begin{bmatrix} -1.3232e-04 \\ -4.9878e+00 \end{bmatrix}$$

$$\text{third: } \begin{bmatrix} 2.0832e-04 \\ -5.0352e+00 \end{bmatrix}, \text{ forth: } \begin{bmatrix} 1.2654e-05 \\ -4.9930e+00 \end{bmatrix}$$

- Greedy Samples computed via `Q-DEIM` algorithm

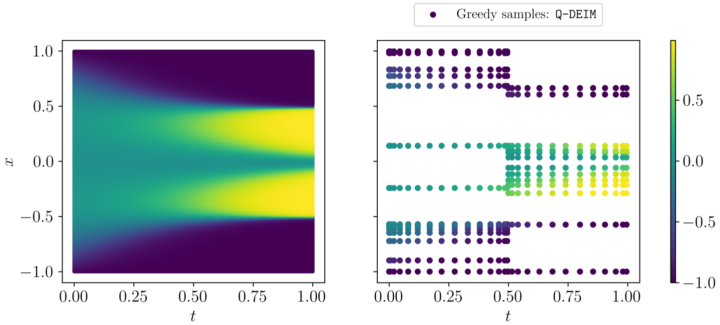
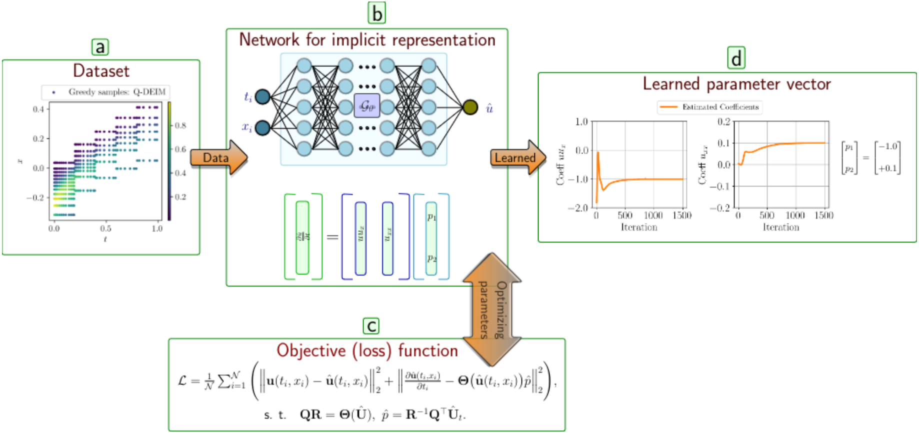


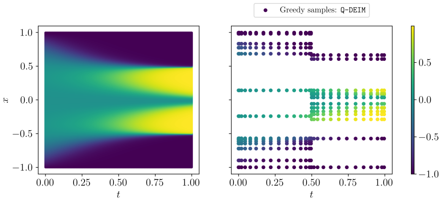
Figure: (left) Entire dataset ; (right) Greedy samples by for Allen-Cahn equation

GS-PINN

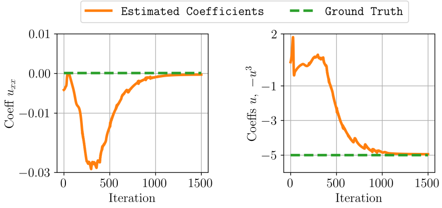

a
Dataset
Greedy samples: Q-DEIM
b
Network for implicit representation
Data
Learned
d
Learned parameter vector
Estimated Coefficients
Iteration
Iteration
Optimizing parameters
c
Objective (loss) function
$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}\left(\left\|\mathbf{u}(t_i,x_i) - \hat{\mathbf{u}}(t_i,x_i)\right\|_2^2 + \left\|\frac{\partial \hat{\mathbf{u}}(t_i,x_i)}{\partial t_i} - \mathbf{\Theta}(\hat{\mathbf{u}}(t_i,x_i))\hat{p}\right\|_2^2\right),$
s. t. $\mathbf{QR} = \mathbf{\Theta}(\hat{\mathbf{U}}),\ \hat{p} = \mathbf{R}^{-1}\mathbf{Q}^\top\hat{\mathbf{U}}_t.$

COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

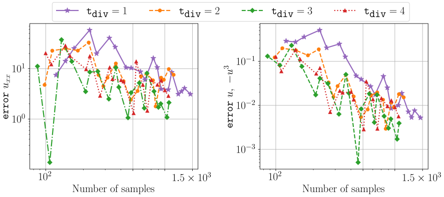
Allen-Cahn



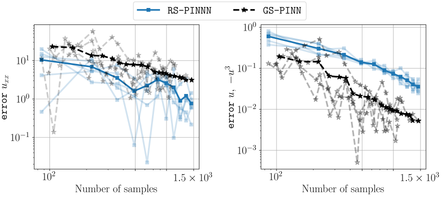
(a) greedy samples



(b) coefficients

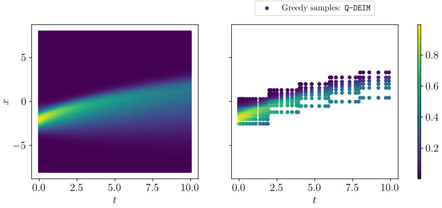


(c) different configuration

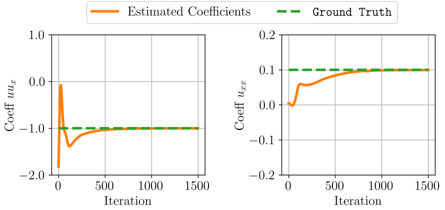


(d) comparison

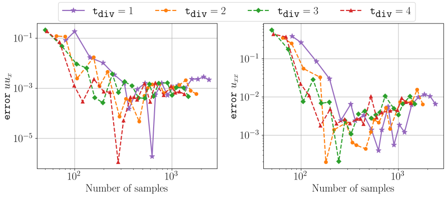
Burgers'



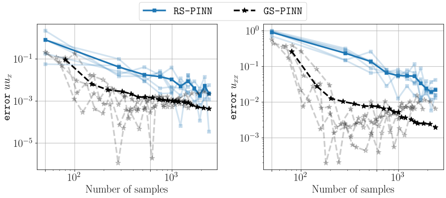
(a) greedy samples



(b) coefficients



(c) different configuration



(d) comparison