ODE indentification Without time label

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1 Method

- 1. Using Clustering Method to segment data into short trajectories with initial condition and determined time length.
- 2. Using Neural Network $y_{\theta}(t)$ to learn the solution function y(t) of ODEs $\frac{dy}{dt} = f(y, t)$ via Sliced Wasserstein Loss.
- 3. Using STRidge Regression Method (or PINN Inverse method) to identify the hidden dynamic system of $y_{\theta}(t)$.

1.1 PINN Augmented

Here we introduce an additional loss to enforce regularity of Neural Network $y_{\theta}(t)$ in step2.

- 1. After Sliced Wasserstein Loss smaller than threshold, Training a Representation source $f_{\phi}(\boldsymbol{y},t)$ using PINN as inverse problem.
- 2. Add regularity loss $L_{\text{reg}} = \left\| \frac{d\boldsymbol{y}_{\theta}}{dt} \boldsymbol{f}_{\phi}(\boldsymbol{y}_{\theta}, \{t_{j}\}_{j=1}^{N_{\text{reg}}}) \right\|_{2}^{2}$ in training stage and train $\{\theta, \phi\}$ at the same time.

1.2 Alternating Direction Optimization

By using delayed updated, we can introduce Alternating Direction Optimization in our task:

- 1. After Sliced Wasserstein Loss smaller than threshold, Training a Representation source $f_{\phi}(y,t)$ using STRidge Regression.
- 2. Add regularity loss $L_{\text{reg}} = \left\| \frac{d\mathbf{y}_{\theta}}{dt} \mathbf{f}_{\phi}(\mathbf{y}_{\theta}, \{t_j\}_{j=1}^{N_{\text{reg}}}) \right\|_{2}^{2}$ in training stage and only train $\{\theta\}$ at training stage.
- 3. Update ϕ every Iter_{reg} time.

1.3 Shooting Method

After learning with ADO or PINN, we obtain high-quality initial guess of Representation $f_{\phi}(y, t)$. We can use shooting method to obtain parameters with higher accuracy by introducing forward information.

2 Experiment

In our experiment , noise level means the gaussian noise of observation with sigma = noise leval * L_{∞} norm of data.

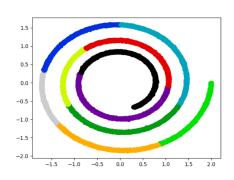
2.1 Low Dimensional Experiment

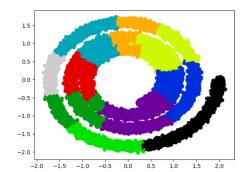
2.1.1 Linear2D

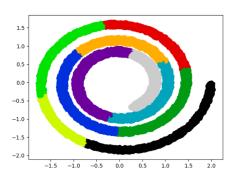
$$\frac{d}{\mathrm{dt}} \left[\begin{array}{c} q \\ p \end{array} \right] \! = \! \left[\begin{array}{cc} -0.1 & 2 \\ -2 & -0.1 \end{array} \right] \! \left[\begin{array}{c} q \\ p \end{array} \right]$$

Setting:

Validate num	Т	Initial	Particle	Cluster
2500	10	[2.0,0.0]	50000	10







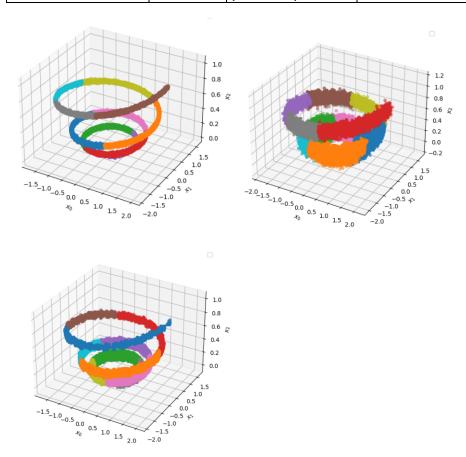
	MAE(Parameters)	MAE(Traj)	MAE(Time)
0%Noise	0.01/0.1 and $1.99/2$	0.8%	0.65%
1%Noise	0.02/0.1 and $1.95/2$	1.2%	1%
5%Noise	0.03/0.1 and $1.95/2$	1.7%	3.%

2.1.2 Linear3D

$$\frac{d}{dt} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -0.1 & -2 & 0 \\ 2 & -0.1 & 0 \\ 0 & 0 & -0.3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$
(1)

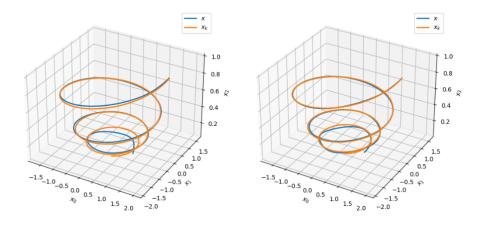
Setting:

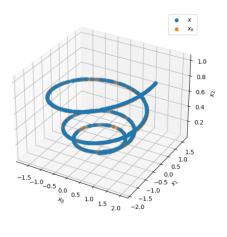
Validate num	${ m T}$	Initial	Particle	Cluster	
2500	10	[2.0,0.0,1.0]	50000	10	



	MAE(Parameters)	MAE(Traj)	MAE(Time)
0%Noise	$0.01/0.1 \ 1.99/2 \ 0.02/0.3$	0.6%	1.1%
1%Noise	0.02/0.1 and $1.97/2$ $0.03/0.3$	1.8%	2.1%
5%Noise	0.02/0.1 and $1.94/2$ $0.04/0.3$	2.3%	2.9%

Before ADO(1500 epoch) and After ADO(3000epoch) and shooting

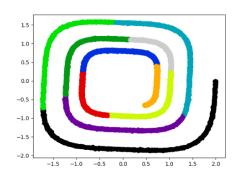


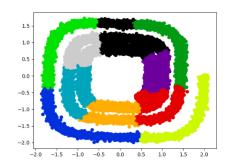


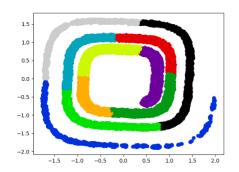
2.1.3 Cubic2D

$$\frac{d}{\mathrm{dt}} \begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} -0.1 & 2 \\ -2 & -0.1 \end{bmatrix} \begin{bmatrix} q^3 \\ p^3 \end{bmatrix}$$

Validate num	T	Initial	Particle	Cluster
2500	10	[2.0,0.0]	50000	10







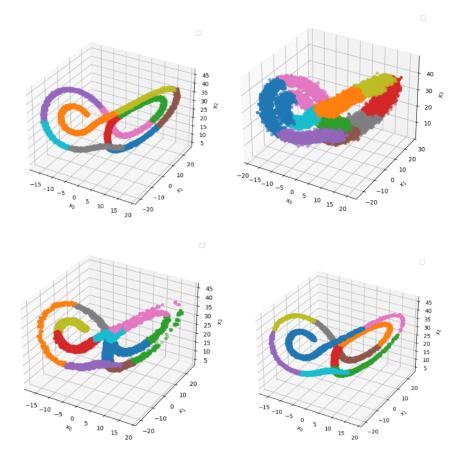
	MAE(Parameters)	MAE(Traj)	MAE(Time)
0%Noise	$0.02/0.1 \ 1.98/2$	1.%	1.2%
1%Noise	0.02/0.1 and $1.98/2$	2.2%	2.2%
5%Noise	0.03/0.1 and $1.95/2$	2.8%	3.1%

2.1.4 Lorentz

$$\dot{x} = \sigma(y - x)
\dot{y} = x(\rho - z) - y
\dot{z} = xy - \beta z$$
(2)

Setting:

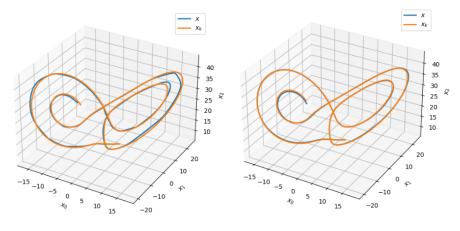
Validate num	Τ	Initial	Particle	Cluster	Parameter
2500	3	[10,-10,20]	50000	10	$\sigma = 10, \beta = \frac{8}{3}, \rho = 28$



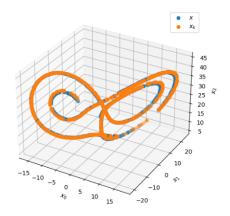
	MAE(Parameters)	MAE(Traj)	MAE(Time)
0%Noise	$0.5/10\ 0.07/1\ 0.15/2.6\ 0.93/28$	2.%	1.3%
1%Noise	1./10 0.09/1 0.13/2.6 1./28	3.1%	2.1%
5%Noise	1.3/10 0.12/1 0.2/2.6 1.3/28	4.6%	6.% 15%

Analysis

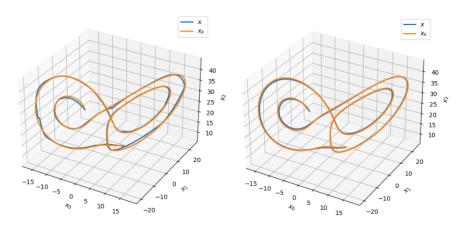
Before ADO (Pretrain 12000epoch) and After ADO (2000epoch)



ODE inference



Data with noise: (Pretrain 12000epoch) and After ADO (4000epoch)

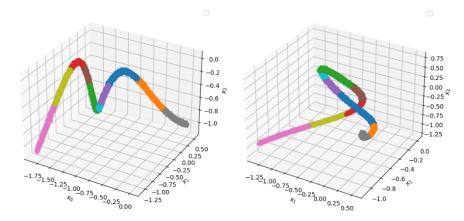


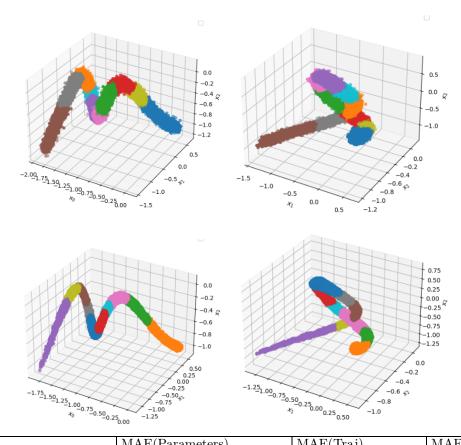
2.2 High Dimensional Experiment

2.2.1 HH model 4D

$$\begin{split} \frac{d}{dt}\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} &= \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \\ \frac{d}{dt}\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} &= \begin{pmatrix} -q_1 - 2q_1q_2 \\ -q_2 - q_1^2 + q_2^2 \end{pmatrix} \end{split}$$

Validate num	Τ	Initial	Particle	Cluster
2500	5	[0,0.5,-1.0,0]	50000	10





	MAE(Parameters)	MAE(Traj)	MAE(Time)
0%Noise	0.03/1	1.2%	1.%
1%Noise	0.035/1	2.1%	2.4%
5%Noise	0.08/1	4.9%	5.2%