CARE: Modeling Interacting Dynamics Under Temporal Environmental Variation

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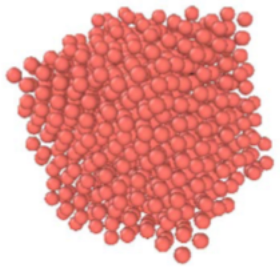
Interacting Systems are Dynamic in Nature

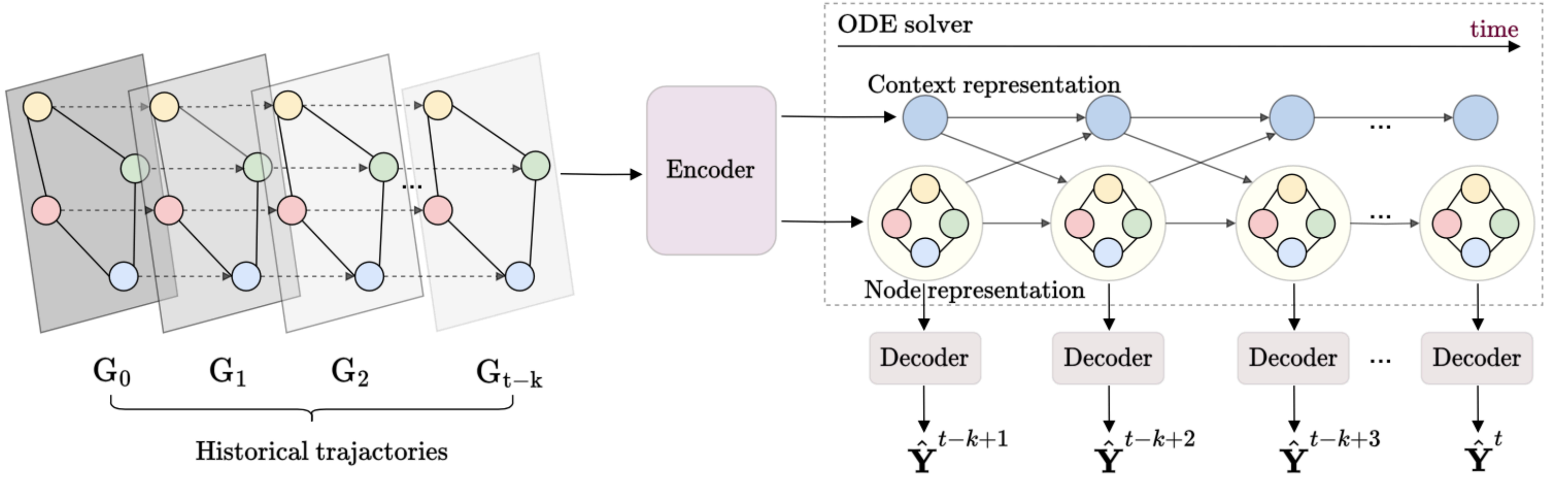
- In interacting systems, objects would interact with each other and demonstrate complicated behavior along the time.
- Example: Molecular dynamical system



Challenges: Changeable System Environment

- Example: Different temperatures and pressures
- Temporal environmental variation would indicate different data distributions over the time
- Continuous distribution variation is difficult to capture

Overall Framework



Probabilistic Model

Assumption 4.1. *(Independence-I) The context variable is independent of the sequences before the last observed timestamp, i.e.,* $P(\mathbf{c}^t|\mathbf{c}^{t-k}, G^{0:t}) = P(\mathbf{c}^t|\mathbf{c}^{t-k}, G^{t-k:t})$*, where* $t-k$ *is the last observed timestamp.*

Assumption 4.2. *(Independence-II) Given the current states and contexts, the future trajectories are independent of the previous trajectories and contexts, i.e.,* $P(\boldsymbol{Y}^{t-k:t+l}|G^{0:t-k}, \mathbf{c}^{0:t-k}) = P(\boldsymbol{Y}^{t-k:t-k+l}|G^{t-k}, \mathbf{c}^{t-k})$ *where* l *is the length of the prediction.*

$$\mathrm{P}\left(\boldsymbol{Y}^t \mid G^{0:t-1}\right) = \int \mathrm{P}\left(\boldsymbol{Y}^t \mid \boldsymbol{c}^{t-1}, G^{t-1}\right) \cdot \mathrm{P}\left(\boldsymbol{c}^{t-1} \mid \boldsymbol{c}^{t-k}, G^{t-k:t-1}\right) \cdot \mathrm{P}\left(\boldsymbol{c}^{t-k} \mid G^{0:t-k}\right) d\boldsymbol{c}^{t-1} d\boldsymbol{c}^{t-k}.$$

- Divide each training sequence into two parts, namely [0,t-k], (t-k,t]

Context Acquirement

- Construct a temporal graph connecting all the observations.

$$\boldsymbol{h}_i^{s,(l+1)} = \boldsymbol{h}_i^{s,(l)} + \sigma\left(\sum_{j^{s'} \in \mathcal{N}(i^s)} w^{(l)}(i^s, j^{s'})\boldsymbol{W}_{value}\boldsymbol{h}_j^{s',(l)}\right),$$

$$\boldsymbol{q}_i^s = \boldsymbol{h}_i^{s,(L)} + \mathrm{TE}(s), \quad \boldsymbol{u}_i^{t-k} = \frac{1}{t-k+1}\sum_{s=0}^{t-k}\sigma(\boldsymbol{W}_{sum}\boldsymbol{q}_i^s),$$

$$\beta_i^t = tanh\left(\left(\frac{1}{|V|}\sum_{i' \in V}\boldsymbol{u}_{i'}^{t-k}\right)\boldsymbol{W}_{context}\right) \cdot \boldsymbol{u}_i^{t-k}, \quad \boldsymbol{c}^{t-k} = \sum_{i \in V}\beta_i^t \boldsymbol{u}_i^{t-k},$$

Context-attended Graph ODE

- We then introduce coupled ODEs to model the dynamic evolution of node representations and the context variable. Specifically, the context variable can be inferred during the evolution of node representations, which in turn drives the evolution of the system.

$$\frac{d\boldsymbol{v}_i^s}{ds} = \Phi([\boldsymbol{v}_1^s, \cdots, \boldsymbol{v}_N^s, \boldsymbol{c}^s]) = \sigma\Big(\sum_{j\in\mathcal{N}^s(i)} \frac{\hat{\boldsymbol{A}}_{ij}^s}{\sqrt{\hat{D}_i^s \cdot \hat{D}_j^s}} \boldsymbol{v}_j^s \boldsymbol{W}_1 + \boldsymbol{c}^s \boldsymbol{W}_2\Big),$$

$$\frac{d\boldsymbol{c}^s}{ds} = \Phi^c(\mathrm{AGG}(\{\boldsymbol{v}_i^s\}_{i\in V}), \mathrm{AGG}(\{\frac{d\boldsymbol{v}_i^s}{ds}\}_{i\in V}), \boldsymbol{c}^s]),$$

Decoder and Optimization

- Generate the predictions:

$$[\hat{\boldsymbol{p}}_i^s, \hat{\boldsymbol{q}}_i^s] = \Phi^d(\boldsymbol{v}_i^s).$$

- Learning Objective:

$$\mathcal{L} = \sum_{s=t-k}^{t} ||\hat{\boldsymbol{Y}}^s - \boldsymbol{Y}^s|| + \eta(||\tilde{\boldsymbol{V}}^s - \boldsymbol{V}^s|| + ||\tilde{\boldsymbol{c}}^s - \boldsymbol{c}^s||),$$

Results

Table 1: The RMSE ($\times 10^{-2}$) results of the compared methods with the prediction lengths 1, 5, 10 and 20. v_x, v_y and v_z represent the velocity in the direction of each coordinate axis.

Prediction Length	+1			+5			+10			+20		
Variable	v_x	v_y	v_z	v_x	v_y	v_z	v_x	v_y	v_z	v_x	v_y	v_z
Lennard-Jones Potential												
LSTM	3.95	3.92	3.68	9.12	9.21	9.15	10.84	10.87	10.76	14.82	14.94	14.67
GNS	3.28	3.75	3.39	7.97	8.05	7.68	10.09	10.15	10.13	13.65	13.62	13.59
STGCN	2.91	3.08	2.95	5.06	5.17	5.11	6.89	6.90	6.93	9.31	9.32	9.44
MeshGraphNet	2.89	3.13	2.94	5.29	5.53	5.28	7.03	7.09	7.11	9.12	9.21	9.24
CG-ODE	1.79	2.05	1.71	3.47	3.92	3.38	5.46	5.99	5.36	9.03	9.26	8.92
TIE	1.62	1.98	1.47	3.25	3.90	3.15	5.24	5.82	5.17	8.24	8.34	8.47
Ours	**0.76**	**0.89**	**1.01**	**2.94**	**3.16**	**2.85**	**5.01**	**4.69**	**4.71**	**5.75**	**5.91**	**5.82**
3-body Stillinger-Weber Potential												
LSTM	17.11	17.14	17.18	23.64	23.69	23.60	25.46	25.42	25.48	28.44	28.45	28.44
GNS	15.39	15.27	15.33	22.14	22.19	22.17	25.29	25.36	25.31	27.18	27.15	27.14
STGCN	12.33	12.31	12.35	17.94	17.96	17.91	20.08	20.14	20.13	23.49	23.51	23.52
MeshGraphNet	12.16	12.10	12.13	18.33	18.38	18.34	20.65	20.62	20.71	23.62	23.54	23.61
CG-ODE	9.78	9.74	9.75	12.11	12.05	12.14	15.55	15.58	15.50	16.17	16.24	16.22
TIE	10.18	10.26	10.19	14.75	14.70	14.73	18.42	18.45	18.41	20.92	21.04	21.36
Ours	**4.21**	**4.29**	**4.18**	**9.74**	**9.79**	**9.71**	**13.65**	**13.71**	**13.57**	**15.30**	**15.39**	**15.35**

Results

Table 2: The RMSE results of the compared methods over different prediction lengths 1, 10, 20 and 50. v_x, v_y and p represent the velocity in different directions and the pressure field, respectively.

Prediction Length	+1			+10			+20			+50		
Variable	v_x	v_y	p	v_x	v_y	p	v_x	v_y	p	v_x	v_y	p
CylinderFlow												
LSTM	3.35	29.4	12.5	7.06	44.8	17.8	9.47	49.5	19.9	14.3	73.6	42.3
GNS	3.12	28.8	11.9	7.18	44.3	17.3	9.01	49.6	19.2	13.5	73.2	41.6
STGCN	2.68	26.7	11.0	5.47	42.1	16.9	6.72	45.6	18.4	9.15	68.7	40.0
MeshGraphNet	1.75	22.4	10.6	4.09	39.7	15.7	5.38	44.5	17.2	7.92	64.3	37.7
CG-ODE	1.05	20.4	8.51	3.44	36.8	13.6	4.15	38.5	17.1	5.14	61.2	32.3
TIE	1.22	20.8	8.94	3.75	35.2	13.0	4.62	40.6	16.0	5.87	59.5	32.1
Ours	**0.87**	**19.1**	**7.21**	**3.02**	**32.9**	**11.8**	**3.95**	**37.8**	**13.9**	**4.97**	**55.8**	**29.4**
Airfoil												
LSTM	7.49	7.73	1.92	8.86	9.02	3.78	10.8	11.0	4.71	14.9	15.7	4.96
GNS	6.95	7.14	1.69	8.20	8.34	3.34	10.2	10.5	3.98	14.2	14.1	4.11
STGCN	6.24	5.35	1.07	6.57	6.51	2.33	7.88	8.01	3.16	11.6	11.8	3.17
MeshGraphNet	4.72	4.68	0.50	5.89	5.74	1.23	6.32	6.48	1.85	9.03	9.12	2.08
CG-ODE	4.26	4.32	0.35	4.78	4.70	0.46	5.81	5.66	1.04	7.39	7.85	1.69
TIE	4.17	4.39	0.33	4.99	4.86	0.51	5.75	5.62	0.95	7.25	7.63	1.44
Ours	**3.51**	**4.11**	**0.19**	**3.86**	**3.75**	**0.34**	**4.16**	**4.12**	**0.45**	**6.74**	**6.82**	**0.81**

Thank You