Roto-translated Local Coordinate Frames For Interacting Dynamical Systems

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Geometric Deep Learning Study Visit, 2 June 2022

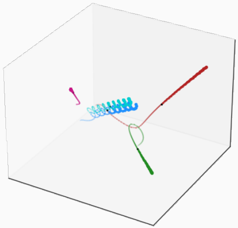
UNIVERSITY OF AMSTERDAM

BMW GROUP THE NEXT 100 YEARS

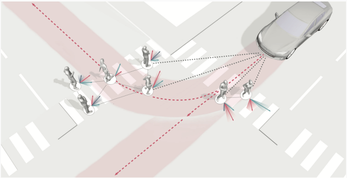
Rolls-Royce Motor Cars Limited

Interacting systems are everywhere

- Colliding particles
- N-body systems
- Molecules
- Motion capture
- Traffic scenes



3D Charged particles [6]



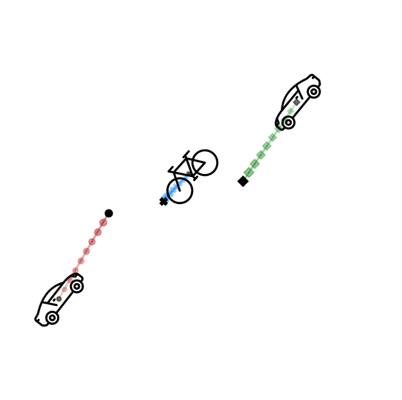
Traffic scene [8]

[6] Thomas Kipf†, Ethan Fetaya†, et al. "Neural relational inference for interacting systems". In: *ICML*. 2018

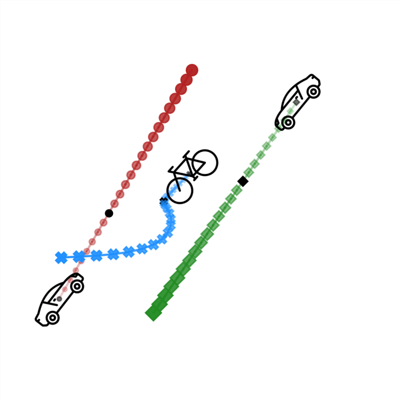
[8] Tim Salzmann†, Boris Ivanovic†, et al. "Trajectron++: Dynamically-Feasible Trajectory Forecasting With Heterogeneous Data". In: *ECCV*. 2020

Future forecasting

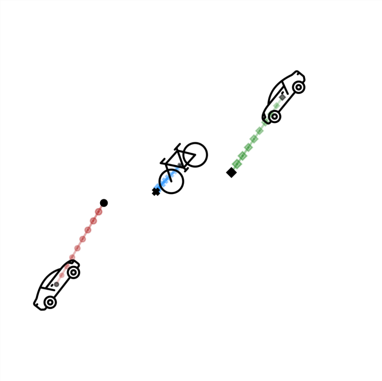
Past

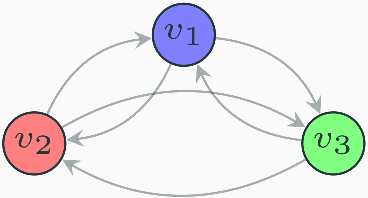


Future



Geometric graphs





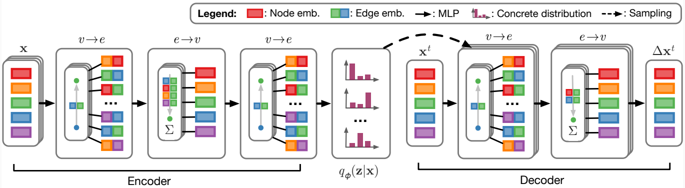
Geometric graph

$$\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{X})$$

$$\mathcal{V} = \{v_i\}_{i=1}^{N}, \quad \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$$

$$\mathbf{X} = \left\{ \begin{pmatrix} \mathbf{p}_i, & \text{position} \\ \mathbf{u}_i, & \text{velocity} \end{pmatrix} \right\}_{i=1}^{N}$$

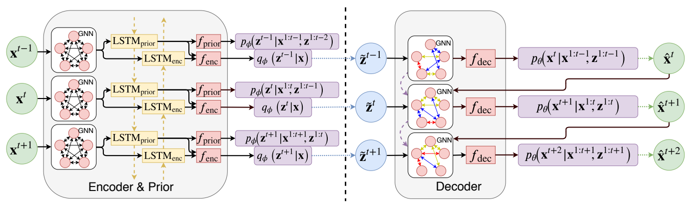
Related work - Neural Relational Inference [6]



- Explicitly infer graph structure over latent edge types
- Simultaneously learn the dynamical system

[5] Diederik P Kingma and Max Welling. "Auto-encoding variational bayes". In: *ICLR*. 2014
[6] Thomas Kipf†, Ethan Fetaya†, et al. "Neural relational inference for interacting systems". In: *ICML*. 2018

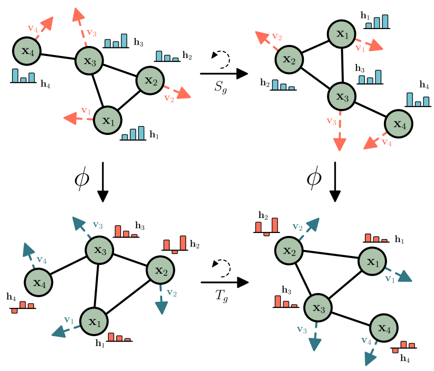
Related work - Dynamic Neural Relational Inference [4]



- Dynamic relations through time
- Sequential approximate posterior based on past states

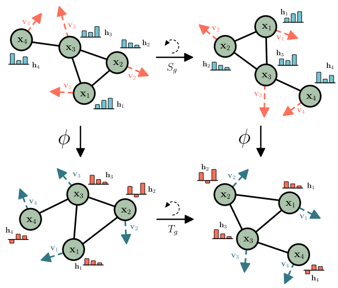
[4] Colin Graber and Alexander G Schwing. “Dynamic Neural Relational Inference”. In: *CVPR*. 2020

Related work - E(n) Equivariant Graph Networks [9]



- Leverage rotation equivariant relative positions and invariant euclidean distances

[9] Víctor Garcia Satorras, Emiel Hoogeboom, and Max Welling. "E(n) Equivariant Graph Neural Networks". In: *ICML*. 2021



$$\mathbf{m}_{j,i} = \phi_e\left(\mathbf{h}_i^l, \mathbf{h}_j^l, \boxed{\left\|\mathbf{p}_j^l - \mathbf{p}_i^l\right\|_2^2}\right)$$

$$\mathbf{p}_i^{l+1} = \mathbf{p}_i^l + \frac{1}{|\mathcal{N}(i)|}\sum_{j\in\mathcal{N}(i)} \boxed{\left(\mathbf{p}_j^l - \mathbf{p}_i^l\right)} \cdot \phi_x(\mathbf{m}_{j,i})$$

$$\mathbf{m}_i = \sum_{j\in\mathcal{N}(i)} \mathbf{m}_{j,i}$$

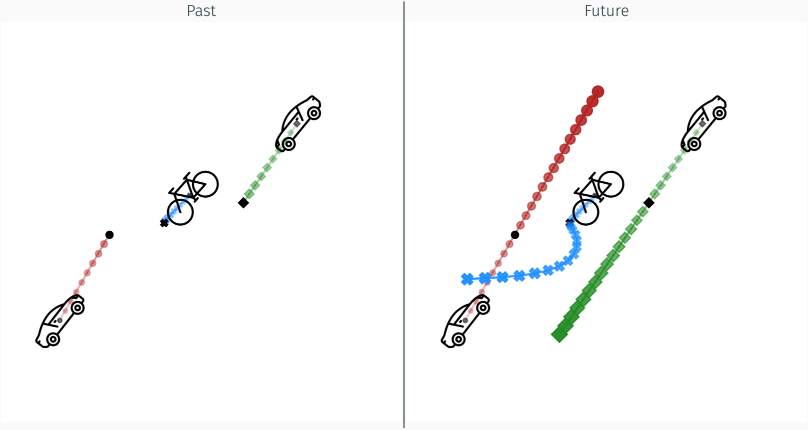
$$\mathbf{h}_i^{l+1} = \phi_h\left(\mathbf{h}_i^l, \mathbf{m}_i\right)$$

- Leverage rotation equivariant relative positions and invariant euclidean distances

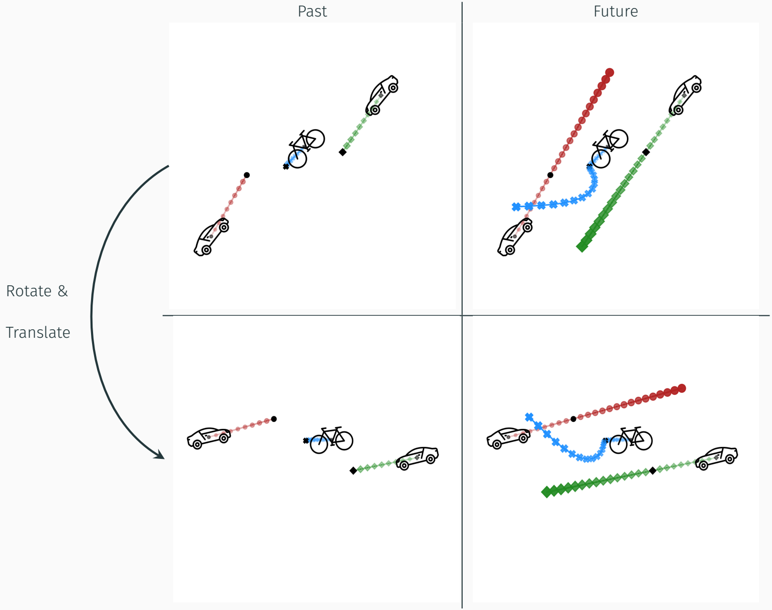
[9] Víctor Garcia Satorras, Emiel Hoogeboom, and Max Welling. “E(n) Equivariant Graph Neural Networks”. In: *ICML*. 2021

Motivation

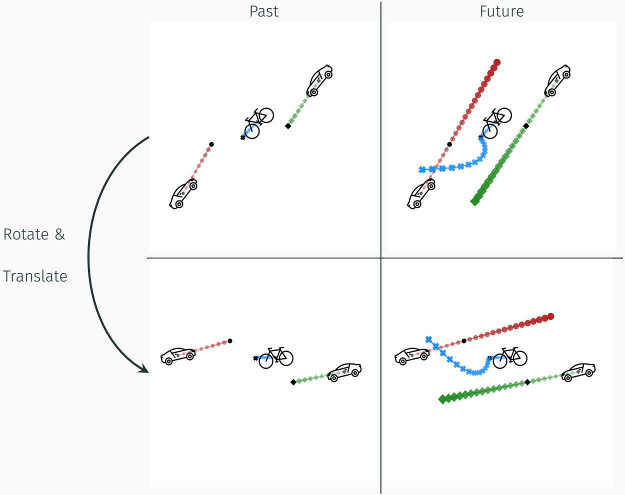
What happens when we rotate/translate the inputs?



Motivation



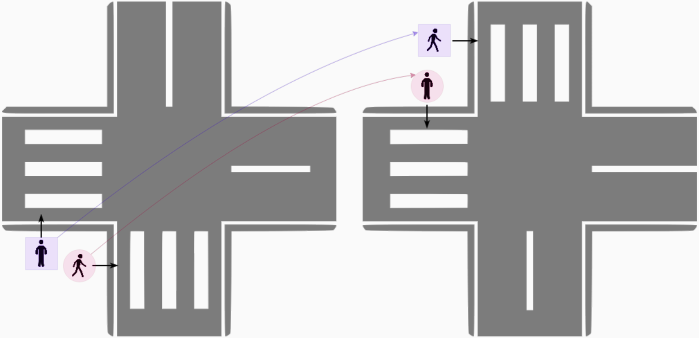
Motivation



Roto-translation equivariance

Dynamics do not change under rotations and translations

Motivation



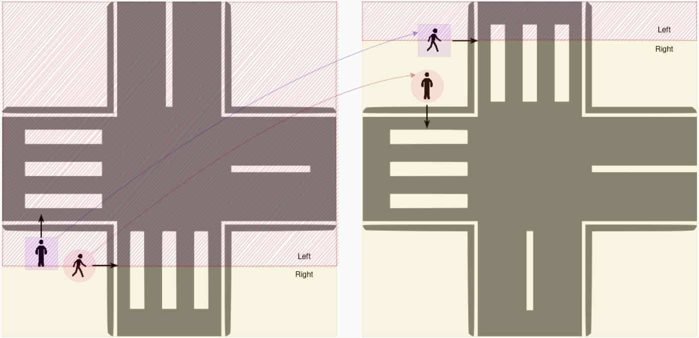
Ego-centric perspective

Objects operate in ego-centric and asymmetric views of the world

Global coordinate frames

Graphs embedded in arbitrary global coordinate frames

Motivation



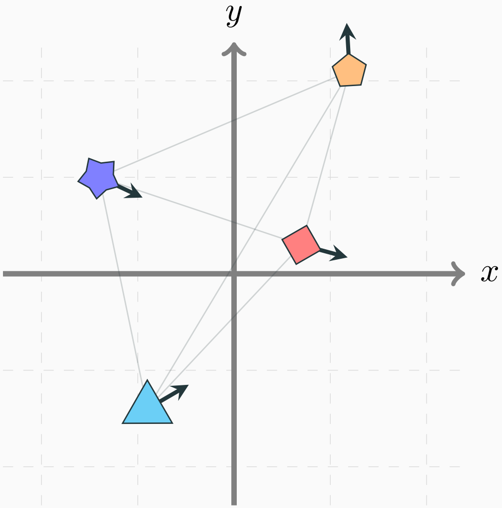
Ego-centric perspective

Objects operate in ego-centric and asymmetric views of the world

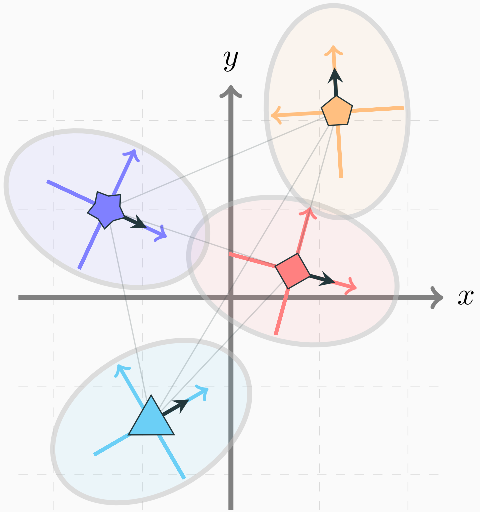
Global coordinate frames

Graphs embedded in arbitrary global coordinate frames

Local coordinate frames (LoCS)



Local coordinate frames (LoCS)



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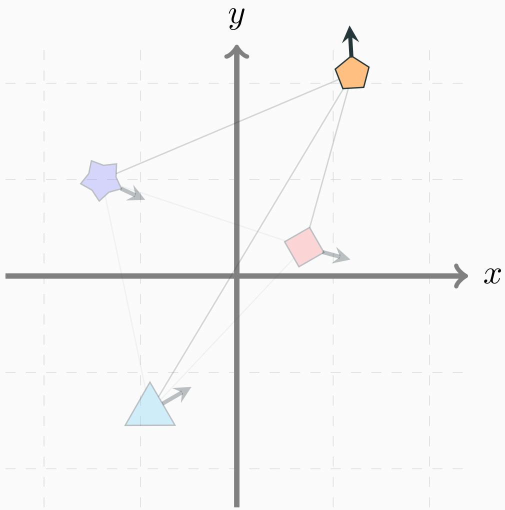

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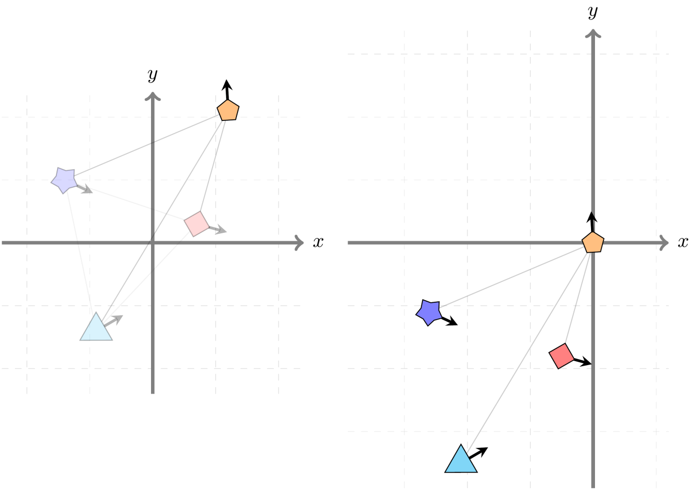

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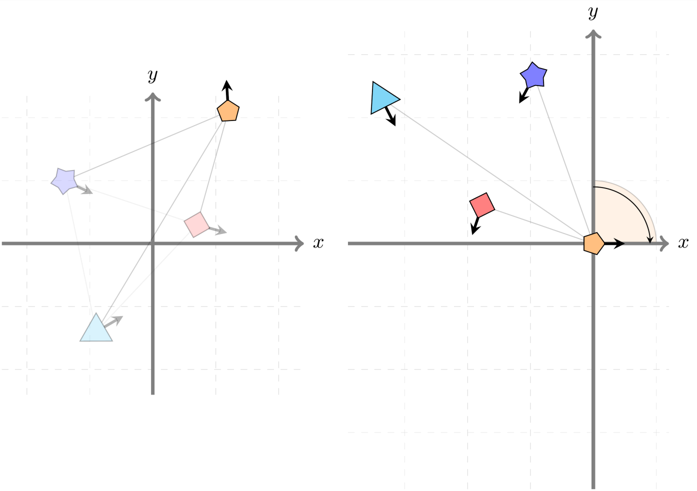

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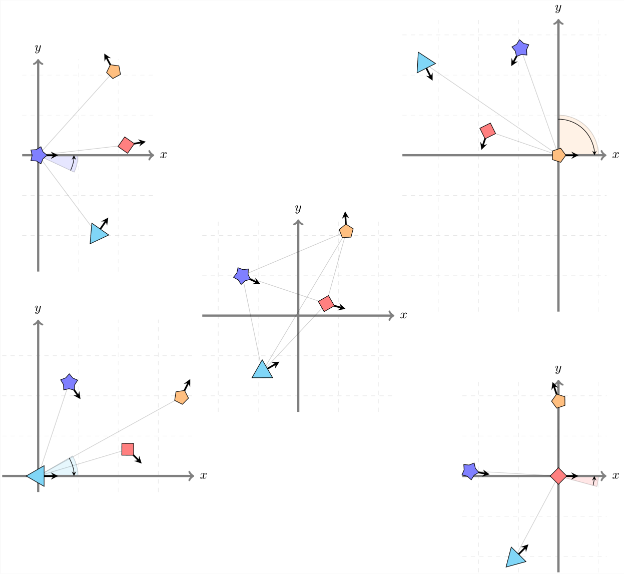


Local coordinate frames (LoCS)

Node states

$$\mathbf{x}_j^t = \left\{ \begin{array}{ll} \mathbf{p}_j^t, & \text{position} \\ \mathbf{u}_j^t, & \text{velocity} \end{array} \right\}$$

$$\mathbf{v}_j^t = \left\{ \begin{array}{lr} \mathbf{p}_j^t, & \text{position} \\ \mathbf{u}_j^t, & \text{velocity} \\ \boldsymbol{\omega}_j^t, & \text{orientation} \end{array} \right\}$$

Relative positions $\qquad \mathbf{r}_{j,i}^t = \mathbf{p}_j^t - \mathbf{p}_i^t$

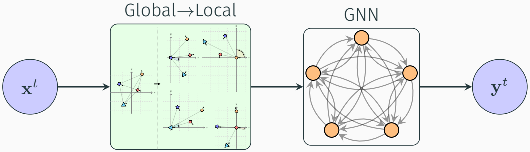
Rotation matrix $\qquad \mathbf{Q}_i^t = \mathbf{Q}\left(\boldsymbol{\omega}_i^t\right)$

Local state $\qquad \mathbf{v}_{j|i}^t = \begin{pmatrix} \mathbf{Q}_i^{t\top} \cdot \mathbf{r}_{j,i}^t \\ \mathbf{Q}_i^{t\top} \cdot \boldsymbol{\omega}_j^t \\ \mathbf{Q}_i^{t\top} \cdot \mathbf{u}_j^t \end{pmatrix}$

Graph Networks in local coordinate frames

Node states

$$\mathbf{x}_j^t = \left(\mathbf{p}_j^t, \mathbf{u}_j^t\right) \qquad \mathbf{v}_j^t = \left(\mathbf{p}_j^t, \mathbf{u}_j^t, \boldsymbol{\omega}_j^t\right)$$



Invariant GNN

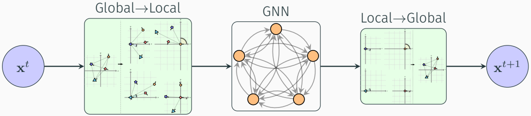
$$\mathbf{v}_{j|i}^t = \textsc{Global2Local}\left(\mathbf{v}_j^t, \mathbf{v}_i^t\right)$$

$$\mathbf{y}_{i|i}^t = \mathrm{GNN}\left(\mathbf{v}_{i|i}^t, \left\{\mathbf{v}_{j|i}^t\right\}_{j \in \mathcal{N}(i)}\right)$$

Graph Networks in local coordinate frames

Node states

$$\mathbf{x}_j^t = \left(\mathbf{p}_j^t, \mathbf{u}_j^t\right) \qquad \mathbf{v}_j^t = \left(\mathbf{p}_j^t, \mathbf{u}_j^t, \boldsymbol{\omega}_j^t\right)$$



Equivariant GNN

$$\mathbf{v}_{j|i}^t = \textsc{Global2Local}\left(\mathbf{v}_j^t, \mathbf{v}_i^t\right)$$

$$\boldsymbol{\Delta}\mathbf{x}_{i|i}^{t+1} = \mathrm{GNN}\left(\mathbf{v}_{i|i}^t, \left\{\mathbf{v}_{j|i}^t\right\}_{j\in\mathcal{N}(i)}\right)$$

$$\boldsymbol{\Delta}\mathbf{x}_i^{t+1} = \textsc{Local2Global}\left(\boldsymbol{\Delta}\mathbf{x}_{i|i}^{t+1}\right)$$

$$\mathbf{x}_i^{t+1} = \mathbf{x}_i^t + \boldsymbol{\Delta}\mathbf{x}_i^{t+1}$$

Graph network formulation

$$
\begin{aligned}
\mathbf{h}_{j,i} &= f_e\big(\big[\mathbf{v}_{j|i}, \mathbf{v}_{i|i}\big]\big) \\
\mathbf{h}_i &= f_v\left(g_v\big(\mathbf{v}_{i|i}\big) + \frac{1}{|\mathcal{N}(i)|}\sum_{j\in\mathcal{N}(i)} \mathbf{h}_{j,i}\right)
\end{aligned}
$$

Local coordinate frames as Neural relational inference models

[5] Diederik P Kingma and Max Welling. “Auto-encoding variational bayes”. In: *ICLR*. 2014
[6] Thomas Kipf†, Ethan Fetaya†, et al. “Neural relational inference for interacting systems”. In: *ICML*. 2018
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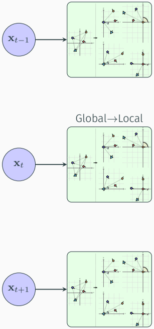

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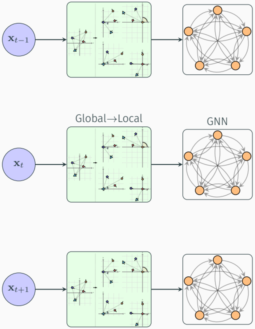

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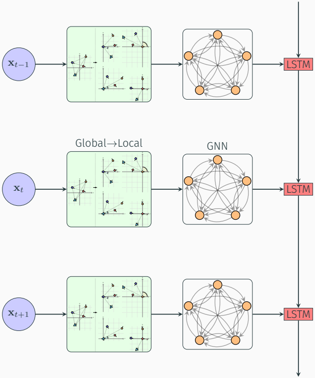

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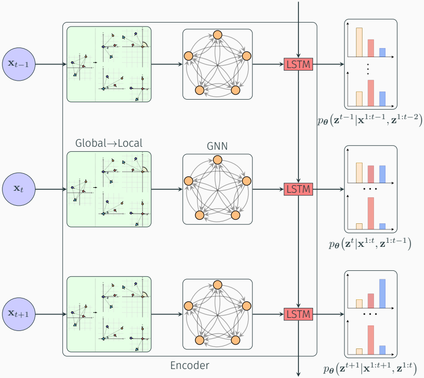

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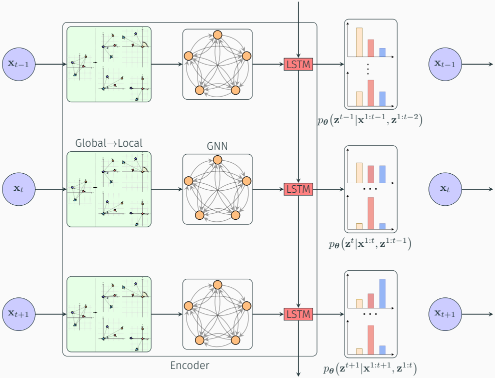

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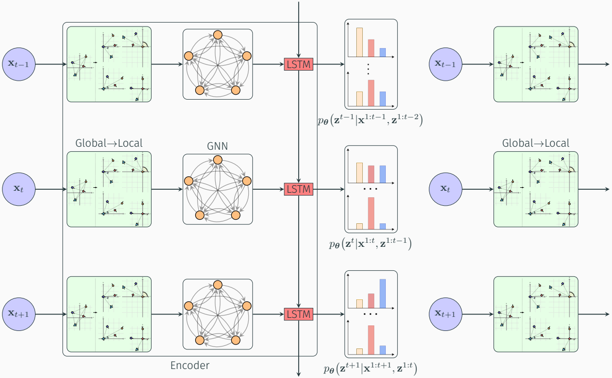

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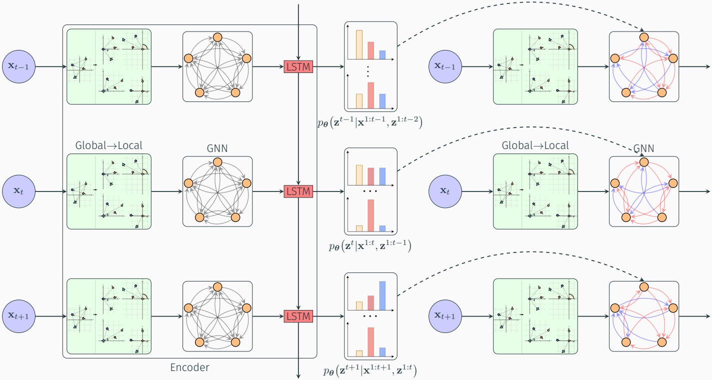

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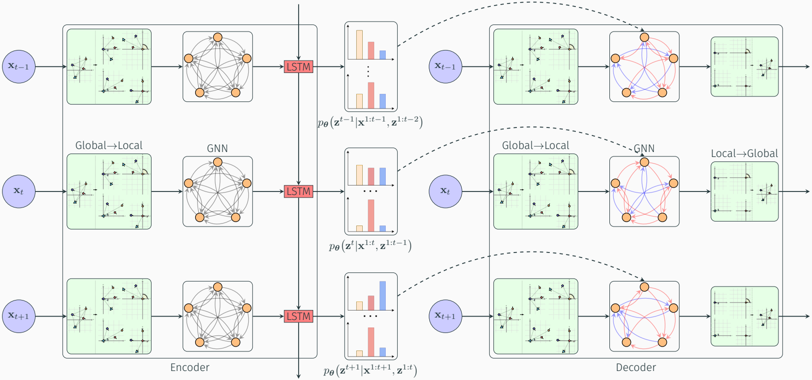

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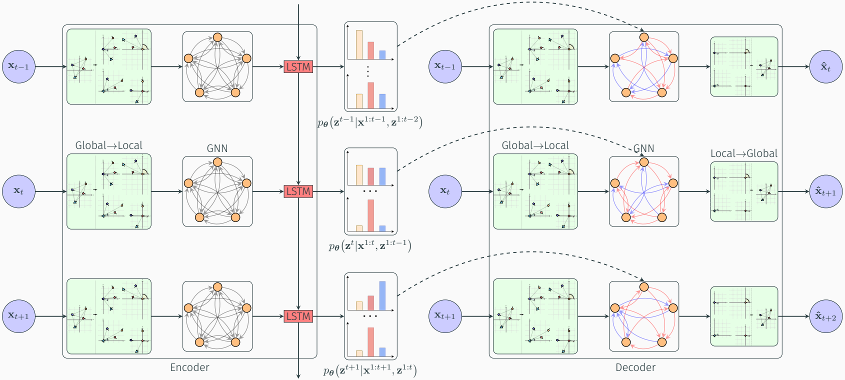

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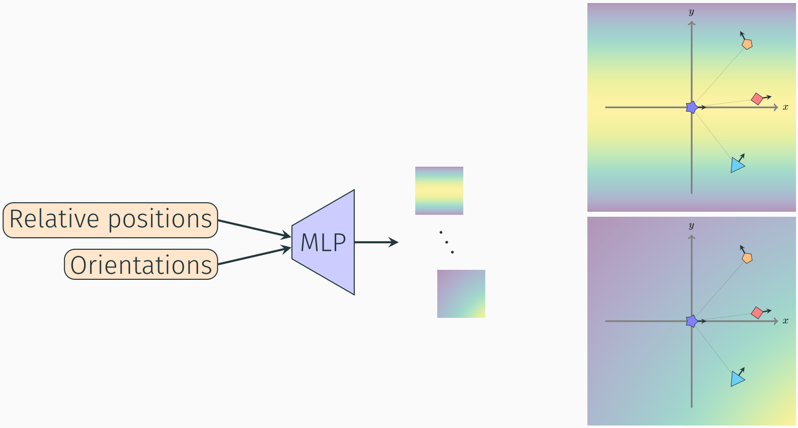
Anisotropic continuous filtering in local coordinate frames

Directionality in graphs $\Longrightarrow$ Anisotropic filtering



Experiments

Synthetic [1]

- 2D, repulsive forces

InD [1]

- Traffic scenes, 2D, social interactions

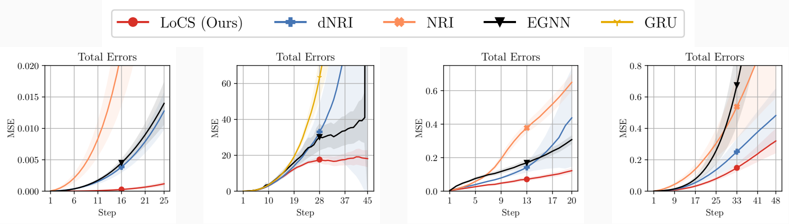
Charged particles [6]

- 3D, electrostatic forces

CMU Motion capture [3]

- 3D, subject #35, walking trajectories

Results



(a) Synthetic [4] (b) Traffic scenes, inD [1] (c) Charged particles [6] (d) Motion Capture [3]

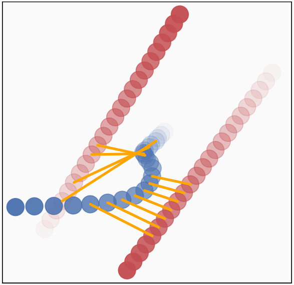
[4] Colin Graber and Alexander G Schwing. "Dynamic Neural Relational Inference". In: *CVPR*. 2020

[1] Julian Bock et al. "The inD dataset: A drone dataset of naturalistic road user trajectories at german intersections". In: *2020 IEEE Intelligent Vehicles Symposium (IV)*. 2020

[6] Thomas Kipf†, Ethan Fetaya†, et al. "Neural relational inference for interacting systems". In: *ICML*. 2018

[3] CMU. *Carnegie-Mellon Motion Capture Database*. 2003. URL: http://mocap.cs.cmu.edu

Results - Synthetic Dataset



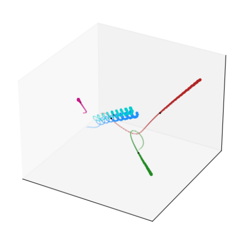
Relation prediction F1 score on synthetic dataset

Method	NRI	dNRI	LoCS
F1	26.5	60.8	88.9

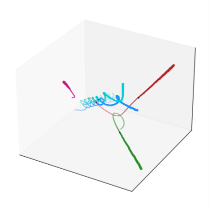
[6] Thomas Kipf†, Ethan Fetaya†, et al. "Neural relational inference for interacting systems". In: *ICML*. 2018
[4] Colin Graber and Alexander G Schwing. "Dynamic Neural Relational Inference". In: *CVPR*. 2020

Qualitative results - charged particles

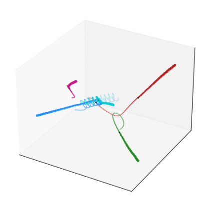
Groundtruth



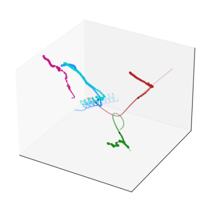
LoCS (Ours)



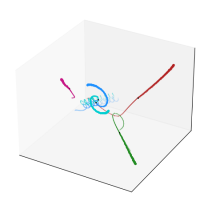
dNRI [4]



NRI [6]



EGNN [9]



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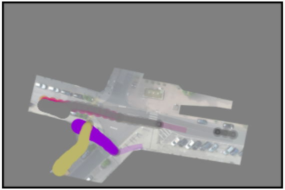
Qualitative results - inD

Groundtruth



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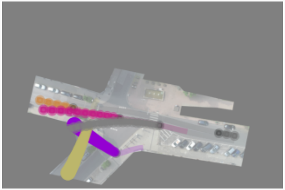
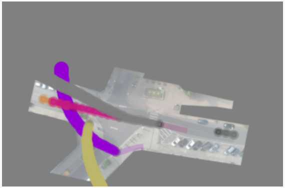
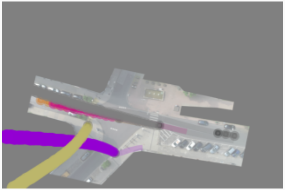


dNRI [4]



EGNN [9]



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Conclusion

- Local coordinate frames for all objects
- Invariance/equivariance to global roto-translations
- Anisotropic continuous filters in local coordinate frames
- Demonstrate effectiveness on a range of 2D/3D settings

- Paper: https://arxiv.org/abs/2110.14961
- Source code: https://github.com/mkofinas/locs

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