UNIVERSITY OF CAMBRIDGE

Neural Relational Inference for Interacting Systems

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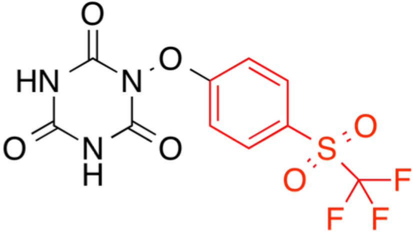
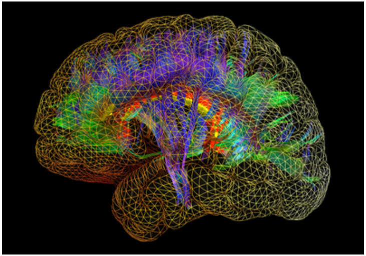
Introduction

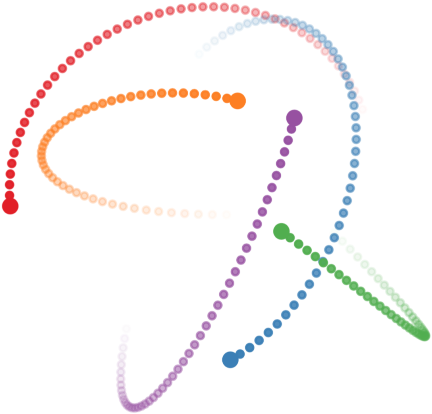
- In this talk, I will survey the recently published **Neural Relational Inference** model (Kipf, Fetaya *et al.*, ICML 2018).
- This model enables the **discovery and exploitation of latent interactions between objects**, through the synergy of *graph convolutional networks* and *variational autoencoders*.
- Exciting results + avenues for further work!

Graphs are **everywhere**!





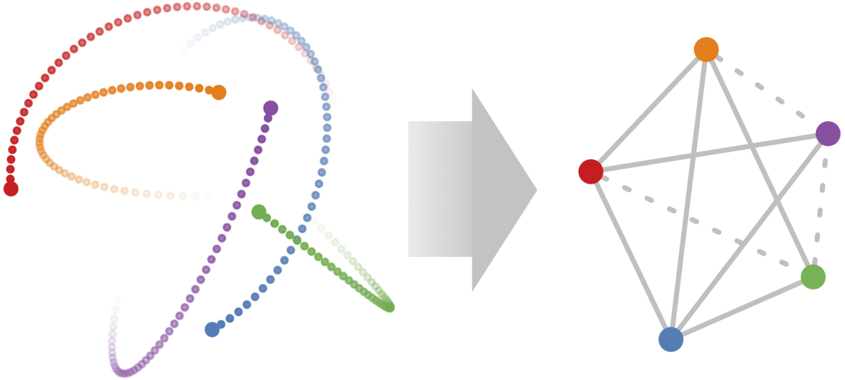
. . . but can we always *see* them?



Relational inference

- Virtually all graph convolutional techniques require a graph to be *provided* as input!
- However, often we will only have access to *node features*...
- Approaches such as *Relational Networks* (Santoro *et al.*, 2017), or *VAIN* (Hoshen, 2017) circumvent this by assuming a **complete graph** (i.e. all-pairs interactions).
- But most interaction graphs have properties (such as *sparsity*) that we may wish to explicitly demand!
- Furthermore, we may wish to *identify* and *decouple* different **types of interaction**.

Our task for today

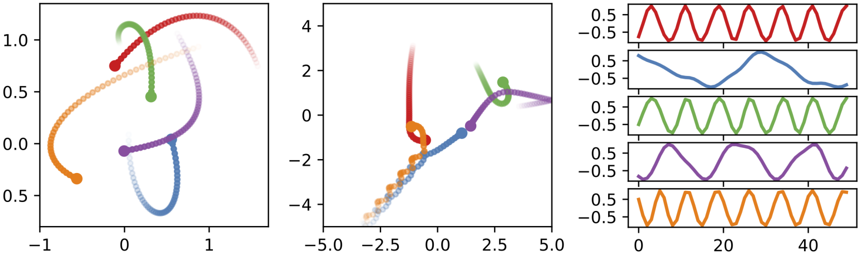


Observed dynamics

Interaction graph

Motivation: predicting *trajectories*

- **Input:** Trajectories (e.g. coordinates) $\vec{x}_i^{\leq t}$ for each particle i.
- **Output:** Future trajectories $\vec{x}_i^{>t}$ for each particle i.



Springs (2D) Charged (2D) Kuramoto (1D)

- The interaction graph between particles will be a *byproduct*!

Simple baseline #1: RNN

- Let $\vec{x}^t$ denote the coordinates of all particles at time t:

$$\vec{x}^t = \left[\vec{x}_1^t, \vec{x}_2^t, \ldots, \vec{x}_n^t\right]$$

- We can now define a recurrent neural network (e.g. LSTM or GRU) to operate on this sequential input:

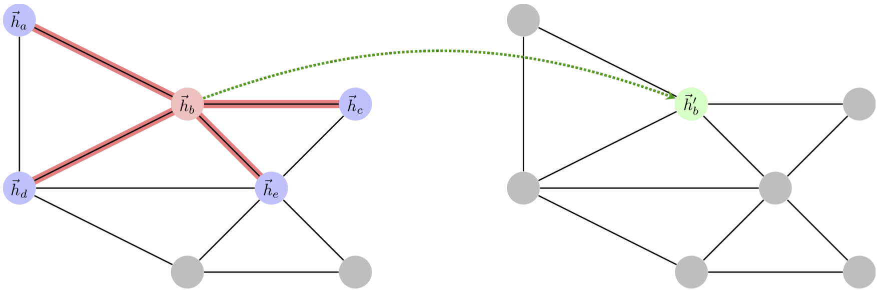
$$\vec{h}^t = RNN(\vec{h}^{t-1}, \vec{x}^t)$$

- From its hidden states, we can predict the future timesteps:

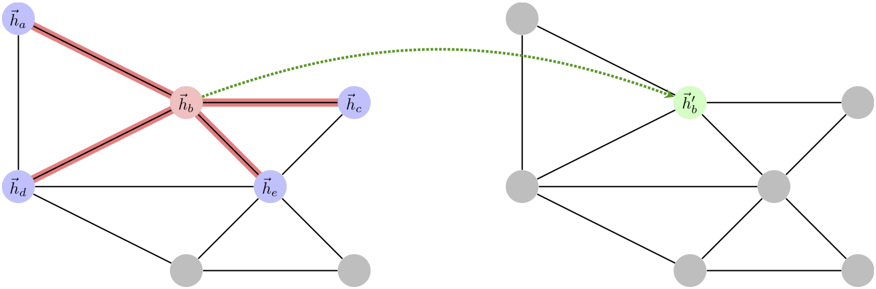
$$\vec{x}^{t+1} = f(\vec{h}^{t+1})$$

where f is an MLP.

Graph convolutional network



Graph convolutional network



In a nutshell, obtain higher-level representations of a node i by leveraging its *neighbourhood*, $\mathcal{N}_i$!

$$\vec{h}_i^{\ell+1} = g^\ell(\vec{h}_a^\ell, \vec{h}_b^\ell, \vec{h}_c^\ell, \dots) \ \ (a, b, c, \dots \in \mathcal{N}_i)$$

where g^ℓ is the ℓ-th *graph convolutional layer*.

The MPNN framework

- The NRI model leverages a graph convolutional layer inspired by *message-passing neural networks* (Gilmer *et al.*, 2017).

The MPNN framework

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- First, compute *edge messages*, $\vec{h}^{\ell}_{i\to j}$, for each edge $i \to j$ in the graph. Apply a simple MLP, f_e^{ℓ}, over the features of i and j:

$$\vec{h}^{\ell}_{i\to j} = f_e^{\ell}(\vec{h}^{\ell}_i, \vec{h}^{\ell}_j)$$

The MPNN framework

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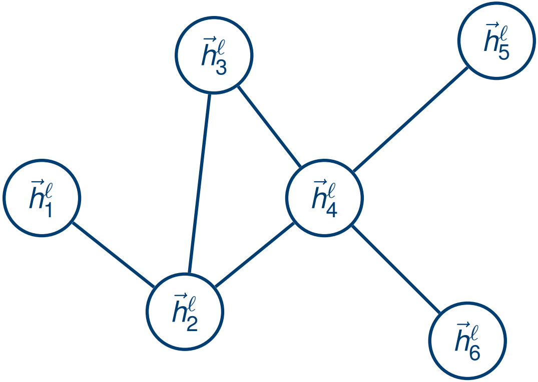
- First, compute *edge messages*, $\vec{h}^{\ell}_{i\rightarrow j}$, for each edge $i \rightarrow j$ in the graph. Apply a simple MLP, f^{ℓ}_{e}, over the features of i and j:

$$\vec{h}^{\ell}_{i\rightarrow j} = f^{\ell}_{e}(\vec{h}^{\ell}_{i}, \vec{h}^{\ell}_{j})$$

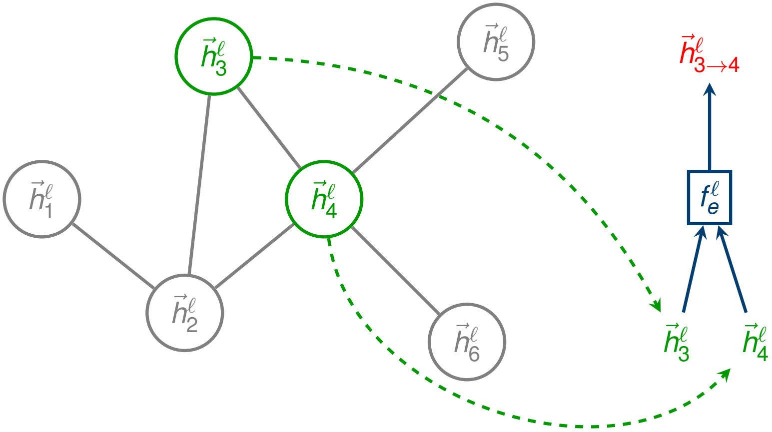
- Then, aggregate all messages entering a node j to obtain the next-level features, $\vec{h}^{\ell+1}_{j}$. Apply a simple MLP, f^{ℓ}_{v}, over the summed messages.

$$\vec{h}^{\ell+1}_{j} = f^{\ell}_{v}\left(\sum_{j\in\mathcal{N}_i} \vec{h}^{\ell}_{i\rightarrow j}\right)$$

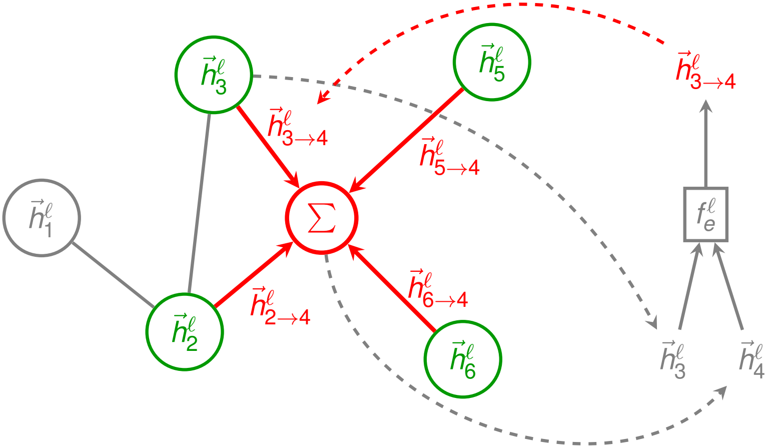
MPNN: initial setup



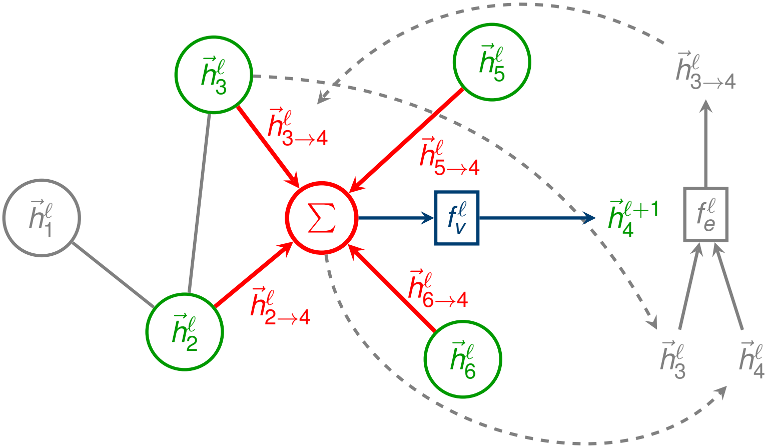
MPNN, computing messages



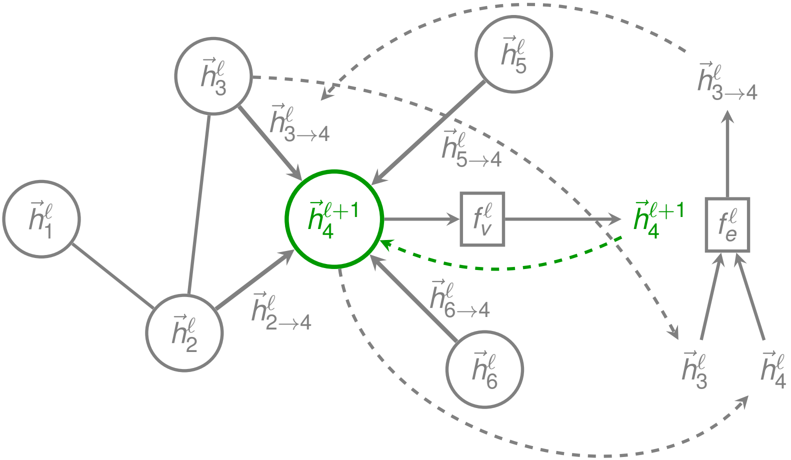
MPNN, aggregating messages



MPNN, computing node features



MPNN, next-level features



Simple baseline #2: Complete graph

- As another baseline approach, we may use this kind of layer to predict trajectories using a complete graph (assume all pairs of nodes interact).
- The equations of the baseline become equivalent to:

$$\vec{h}^t_{i\to j} = f_e(\vec{x}^t_i, \vec{x}^t_j)$$

$$\vec{x}^{t+1}_j = f_v\left(\sum_{i\neq j} \vec{h}^t_{i\to j}\right)$$

with a few kinks, specific to the trajectory predicting task…

Simple baseline #2: Complete graph

- First, to simplify the job of the network, have it only predict *changes in position*:

$$\vec{h}^t_{i\to j} = f_e(\vec{x}^t_i, \vec{x}^t_j)$$

$$\vec{x}^{t+1}_j = \boxed{\vec{x}^t_j} + f_v\left(\sum_{i\neq j} \vec{h}^t_{i\to j}\right)$$

Simple baseline #2: Complete graph

- Also, *explicitly model uncertainty*; will be useful for the variational framework later on.

$$\vec{h}^t_{i\to j} = f_e(\vec{x}^t_i, \vec{x}^t_j)$$

$$\boxed{\vec{\mu}^{t+1}_j} = \vec{x}^t_j + f_v\left(\sum_{i\neq j} \vec{h}^t_{i\to j}\right)$$

$$\boxed{\vec{x}^{t+1}_j \sim \mathcal{N}(\vec{\mu}^{t+1}_j, \sigma^2\mathbf{I})}$$

Simple baseline #2: Complete graph, *with GRU*

- The model thus far assumed the *Markov property* (i.e. that $\vec{x}^{t+1}$ depends fully on $\vec{x}^{t}$). This is OK for physics, but if necessary, we can alleviate the constraint by using a recurrent update:

$$\vec{h}^t_{i\rightarrow j} = f_e(\vec{x}^t_i, \vec{x}^t_j)$$

$$\boxed{\vec{h}^{t+1}_j = GRU\left(\left[\vec{x}^t_j, \sum_{i\neq j} \vec{h}^t_{i\rightarrow j}\right], \vec{h}^t_j\right)}$$

$$\vec{\mu}^{t+1}_j = \vec{x}^t_j + f_v \boxed{\left(\vec{h}^{t+1}_j\right)}$$

$$\vec{x}^{t+1}_j \sim \mathcal{N}(\vec{\mu}^{t+1}_j, \sigma^2\mathbf{I})$$

Interaction graph

- This baseline can be improved if we specify an explicit *interaction graph*. Initially, assume there are K edge types (with one type reserved for “no edge”).
- Then, define a binary tensor $\mathbf{z} \in \mathbb{R}^{V \times V \times K}$ such that z_{ijk} denotes whether the edge $i \rightarrow j$ is of the k-th type.
- Assume an edge cannot have more than one type, i.e., $\vec{z}_{ij}$ is one-hot.

Leveraging the interaction graph

- Now this graph can be exploited—define a separate MLP f_e^k for each edge type. For the Markov decoder:

$$\vec{h}_{i \to j}^t = f_e(\vec{x}_i^t, \vec{x}_j^t)$$

$$\vec{\mu}_j^{t+1} = \vec{x}_j^t + f_v\left(\sum_{i \neq j} \vec{h}_{i \to j}^t\right)$$

$$\vec{x}_j^{t+1} \sim \mathcal{N}(\vec{\mu}_j^{t+1}, \sigma^2 \mathbf{I})$$

The NRI *decoder*

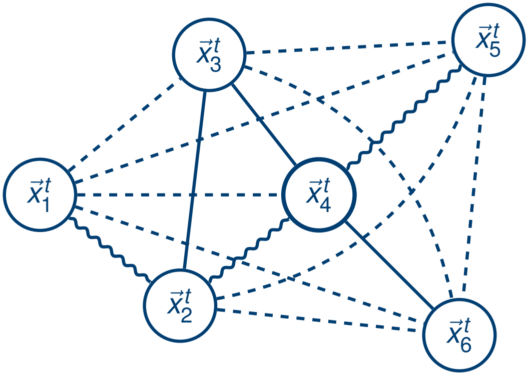
- Now this graph can be exploited—define a separate MLP f_e^k for each edge type. For the Markov decoder:

$$\vec{h}_{i\to j}^t = \boxed{\sum_k z_{ijk} f_e^k(\vec{x}_i^t, \vec{x}_j^t)}$$

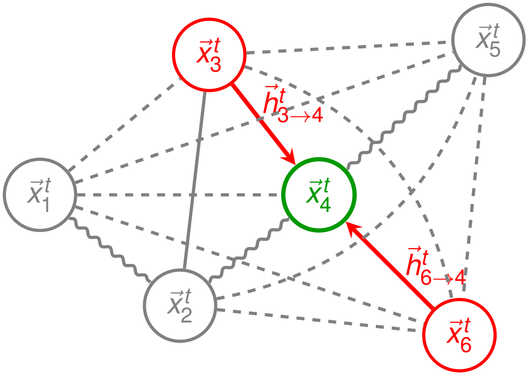
$$\vec{\mu}_j^{t+1} = \vec{x}_j^t + f_v\left(\sum_{i\neq j} \vec{h}_{i\to j}^t\right)$$

$$\vec{x}_j^{t+1} \sim \mathcal{N}(\vec{\mu}_j^{t+1}, \sigma^2\mathbf{I})$$

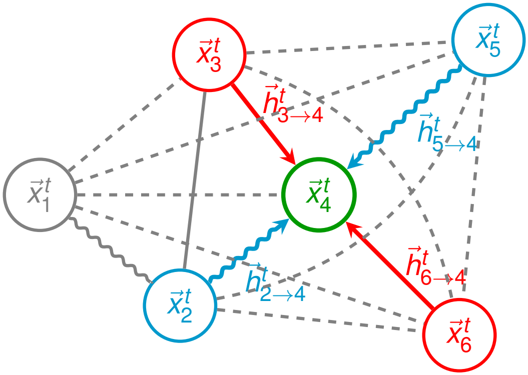
The NRI *decoder*



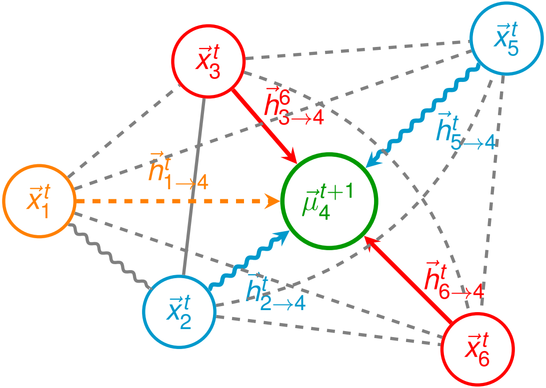
The NRI *decoder*, computing messages. . .



The NRI *decoder*, computing messages. . .



The NRI *decoder*, computing messages. . .



Latent graph inference

- We are still tasked with discovering the entries of the tensor **z.**
- **Idea:** Use MPNNs over a complete graph once more—then classify edge types based on the edge messages $\vec{h}_{i\rightarrow j}$.
- This time, *stack two layers*—so that edges can be derived based on global interactions!
  - $\vec{h}^1_{i\rightarrow j}$ will only depend on $\vec{x}_i$ and $\vec{x}_j$;
  - $\vec{h}^2_{i\rightarrow j}$ will depend on all the nodes in the graph.

The NRI *encoder*

- In equation form:

$$
\begin{aligned}
\vec{h}_j^1 &= f(\vec{x}_j) \\
\vec{h}_{i\to j}^1 &= f_e^1(\vec{h}_i^1, \vec{h}_j^1) \\
\vec{h}_j^2 &= f_v^1\left(\sum_{i\neq j} \vec{h}_{i\to j}^1\right) \\
\vec{h}_{i\to j}^2 &= f_e^2(\vec{h}_i^2, \vec{h}_j^2) \\
z_{ij} &\sim Categorical(softmax(\vec{h}_{i\to j}^2))
\end{aligned}
$$

where f is an embedding, and f_e^1, f_v^1 and f_e^2 are MLPs.

The variational setup

- The encoder gives us the probability distribution $q(\mathbf{z}|\vec{x})$, and the decoder gives us the probability distribution $p(\vec{x}|\mathbf{z})$.
- Combine learning the two in a VAE-style framework by maximising the evidence lower bound (ELBO):

$$\mathcal{L} = \underbrace{\mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\vec{x})}[\log p(\vec{x}|\mathbf{z})]}_{\text{Reconstruction accuracy}} - \underbrace{D_{KL}(q(\mathbf{z}|\vec{x})\|p(\mathbf{z}))}_{\text{Regularisation}}$$

- The prior $p(\mathbf{z})$ can encode desirable properties of the latent graph. **Sparsity** is enforced by setting the probability of "no edge" to be higher than the other types.

Backpropagating through the sampling

- The operation of selecting z_{ij} is a *discrete* decision—therefore, we cannot directly propagate gradients through it.
- Can use the **Gumbel softmax** trick to circumvent this:

$$\vec{z}_{ij} = softmax((\vec{h}^2_{i\to j} + \vec{g})/\tau)$$

  where $g_k \sim Gumbel(0, 1)$ and τ is a temperature parameter (converges to one-hot when $\tau \to 0$).
- This is a *continuous approximation* to the discrete distribution—and gradients can be propagated through it.

Avoiding degenerate decoders

- Optimising the ELBO directly would involve only *single-step* predictions (predicting $\vec{x}^{t+1}$ from $\vec{x}^{t}$). This can often be nicely approximated by ignoring relational structure altogether!

- To enforce robust decoders, predict many steps at once! Every M steps, feed back the ground-truth input.

Avoiding degenerate decoders, *cont'd*

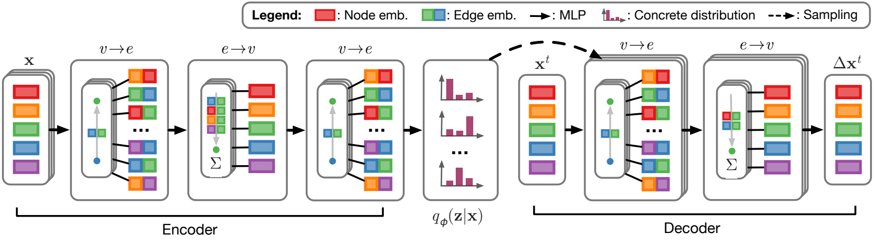
$$
\begin{aligned}
\vec{\mu}_j^2 &= decode(\vec{x}_j^1) \\
\vec{\mu}_j^3 &= decode(\vec{\mu}_j^2) \\
\vec{\mu}_j^4 &= decode(\vec{\mu}_j^3) \\
&\vdots \\
\vec{\mu}_j^{M+1} &= decode(\vec{\mu}_j^M) \\
\vec{\mu}_j^{M+2} &= decode(\vec{x}_j^{M+1}) \\
\vec{\mu}_j^{M+3} &= decode(\vec{\mu}_j^{M+2}) \\
&\vdots
\end{aligned}
$$

Putting it all together

For a given training trajectory, $\vec{x}$, of length T:

1. Compute $q(\mathbf{z}|\vec{x})$ using the encoder.
2. Sample $\vec{z}_{ij}$ from $q(\mathbf{z}|\vec{x})$ using the Gumbel softmax trick.
3. Execute the decoder to obtain $\vec{\mu}^t$ for $t \in \{2, 3, \ldots, T\}$.
4. Compute the reconstruction error (of $\vec{\mu}^t$ against $\vec{x}^t$) and KL-divergence (of $q(\mathbf{z}|\vec{x})$ against the prior $p(\mathbf{z})$).
5. Optimise the ELBO using gradient descent.

The NRI architecture



Physics simulations: latent graph discovery

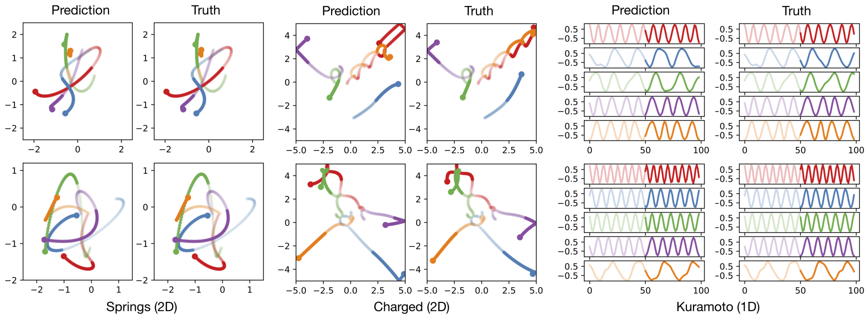
Model	Springs	Charged	Kuramoto
	5 objects		
Corr. (path)	52.4$\pm$0.0	55.8$\pm$0.0	62.8$\pm$0.0
Corr. (LSTM)	52.7$\pm$0.9	54.2$\pm$2.0	54.4$\pm$0.5
NRI (sim.)	**99.8**$\pm$0.0	59.6$\pm$0.8	–
NRI (learned)	**99.9**$\pm$0.0	**82.1**$\pm$0.6	**96.0**$\pm$0.1
Supervised	99.9$\pm$0.0	95.0$\pm$0.3	99.7$\pm$0.0
	10 objects		
Corr. (path)	50.4$\pm$0.0	51.4$\pm$0.0	59.3$\pm$0.0
Corr. (LSTM)	54.9$\pm$1.0	52.7$\pm$0.2	56.2$\pm$0.7
NRI (sim.)	**98.2**$\pm$0.0	53.7$\pm$0.8	–
NRI (learned)	**98.4**$\pm$0.0	**70.8**$\pm$0.4	**75.7**$\pm$0.3
Supervised	98.8$\pm$0.0	94.6$\pm$0.2	97.1$\pm$0.1

Physics simulations: trajectory prediction

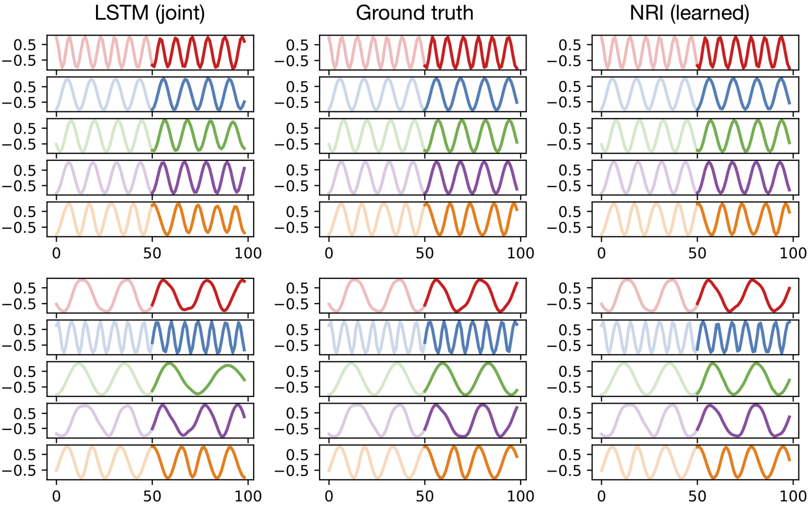
	Springs			Charged			Kuramoto		
Prediction steps	1	10	20	1	10	20	1	10	20
Static	7.93e-5	7.59e-3	2.82e-2	5.09e-3	2.26e-2	5.42e-2	5.75e-2	3.79e-1	3.39e-1
LSTM (single)	2.27e-6	4.69e-4	4.90e-3	2.71e-3	7.05e-3	1.65e-2	7.81e-4	3.80e-2	8.08e-2
LSTM (joint)	4.13e-8	2.19e-5	7.02e-4	1.68e-3	6.45e-3	1.49e-2	**3.44e-4**	**1.29e-2**	4.74e-2
NRI (full graph)	1.66e-5	1.64e-3	6.31e-3	**1.09e-3**	3.78e-3	9.24e-3	2.15e-2	5.19e-2	8.96e-2
NRI (learned)	**3.12e-8**	**3.29e-6**	**2.13e-5**	**1.05e-3**	**3.21e-3**	**7.06e-3**	1.40e-2	2.01e-2	**3.26e-2**
NRI (true graph)	1.69e-11	1.32e-9	7.06e-6	1.04e-3	3.03e-3	5.71e-3	1.35e-2	1.54e-2	2.19e-2

It might seem as if the LSTM outperforms the NRI on Kuramoto!
Qualitative analysis may show otherwise...

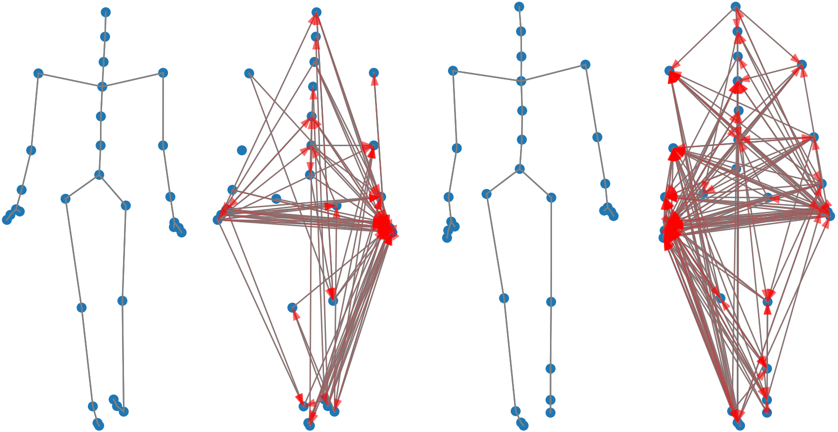
Physics simulations: qualitative results



Physics simulations: qualitative results

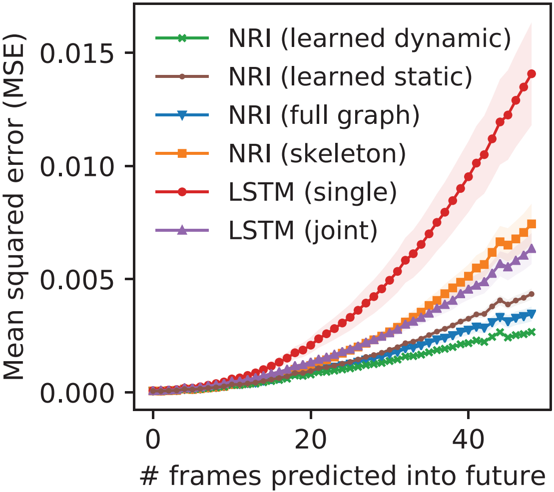


Motion capture

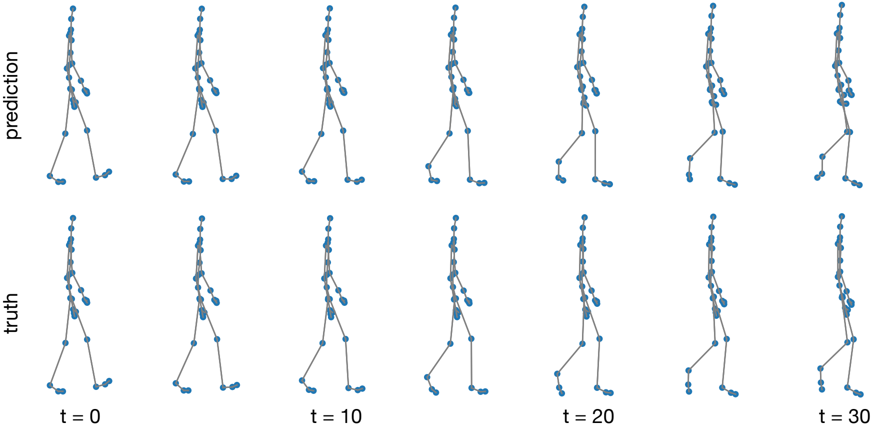


The graph is now **dynamic**! Re-evaluate at every decoding step.

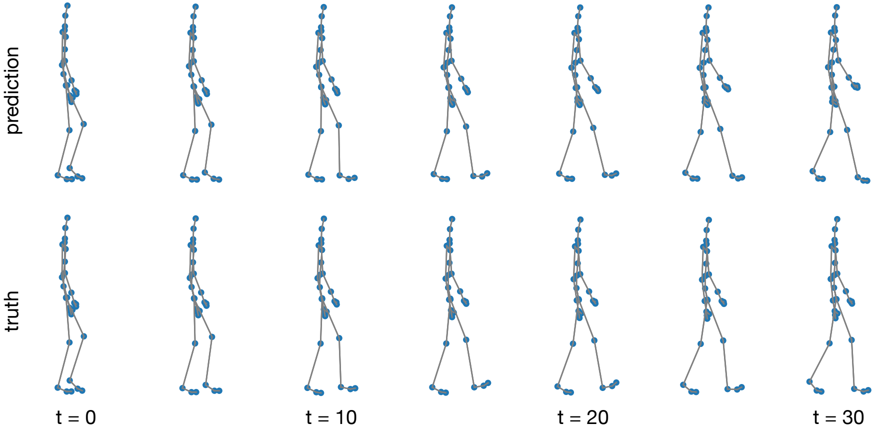
Motion capture: trajectory prediction



Motion capture: qualitative results



Motion capture: qualitative results



Concluding remarks

- The NRI is an extremely versatile model for inferring latent interaction graphs from pointwise trajectories.
- Latent graph discovery is still in its early phases of development—plentiful improvements possible!
- **Limitation:** *does not scale to large graphs!* $O(V^2)$ memory requirements, and computing edge messages makes subsampling cumbersome.
- Should not be required—most real-world graphs are sparse! But techniques we have thus far need to start with complete graph, and gradually discover sparsity...

Thank you!

Questions?

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http://www.cst.cam.ac.uk/~pv273/