EECE 571F: Deep Learning with Structures

Lecture 12: Learning Latent Graph Structures

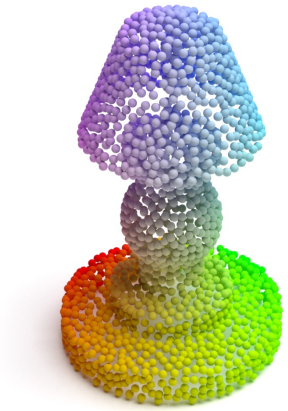
Renjie Liao

University of British Columbia

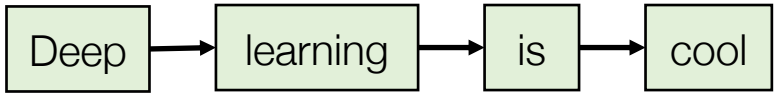
Winter, Term 2, 2021/22

Course Scope

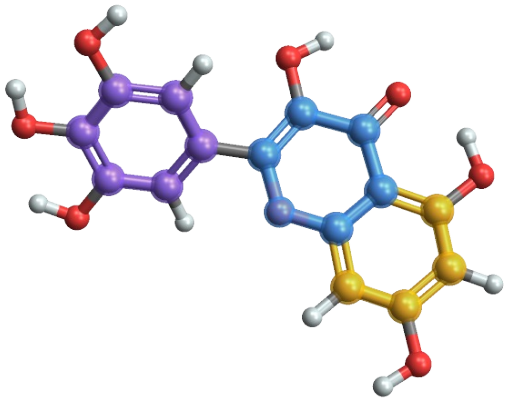
- Supervised Learning with Observable Structures
- Unsupervised / Self-supervised Learning with Observable Structures
- **Supervised Learning with Latent Structures**



Points/Sets



Lists/Sequences



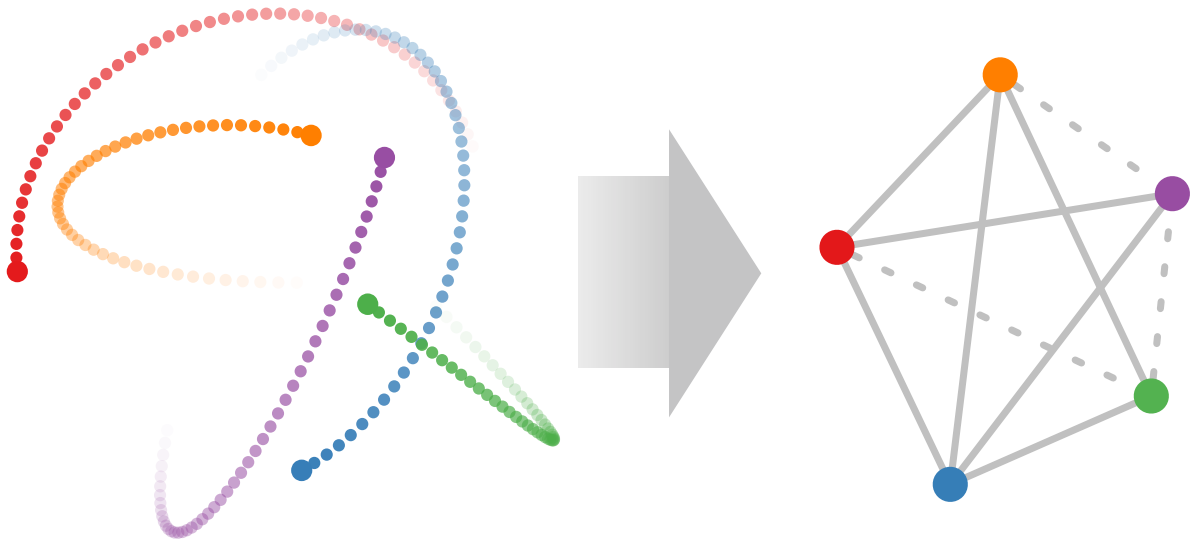
Graphs

Image Credit: https://github.com/AnTao97/PointCloudDatasets
https://www.wolfram.com/language/12/molecular-structure-and-computation/molecule-graphs.html.en?product=mathematica

Contents

Neural Relational Inference

Suppose we observe dynamics of particles, we are interested in inferring the latent interaction graph



Observed dynamics

Interaction graph

Image Credit: [1]

Neural Relational Inference

Suppose we observe dynamics of particles, we are interested in inferring the latent interaction graph

It arises in dynamic systems from physics, biology, sports, transportation, etc.

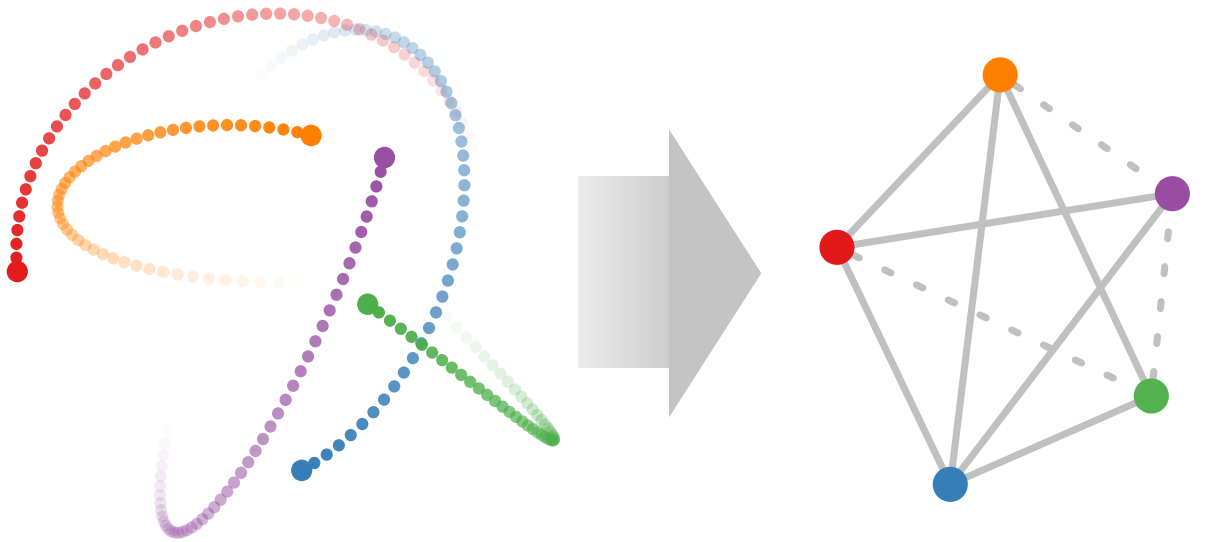


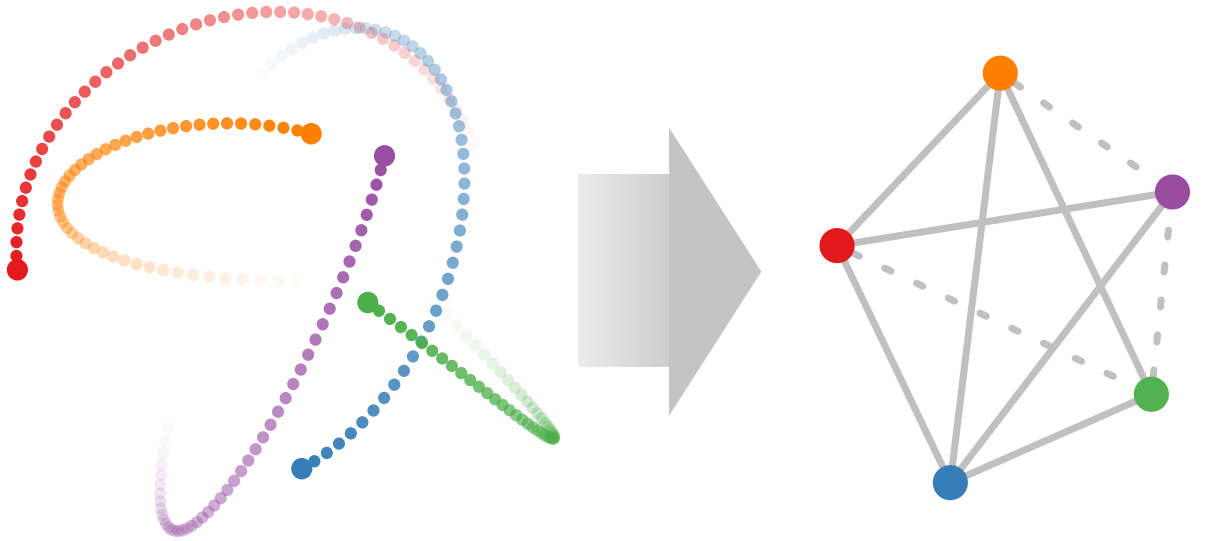
Image Credit: [1]

Neural Relational Inference

Let us formalize the problem:

We have N particles (nodes) $\mathcal{V} = \{v_1, ..., v_N\}$

At time t, the feature is $\mathbf{x}^t = \{\mathbf{x}_1^t, ..., \mathbf{x}_N^t\}$



Observed dynamics

Interaction graph

Image Credit: [1]

Neural Relational Inference

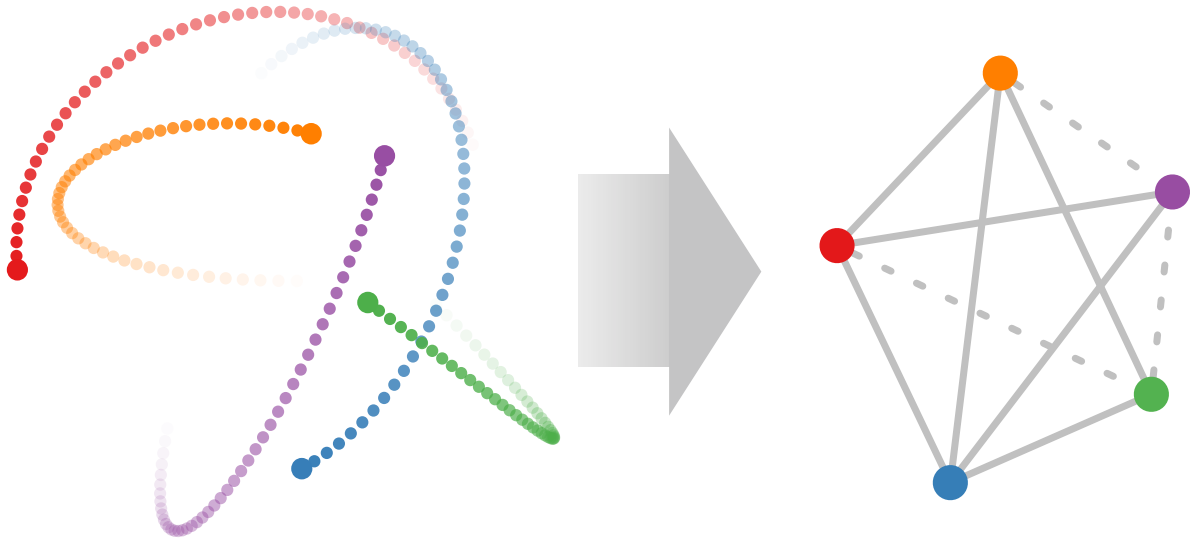
Let us formalize the problem:

We have N particles (nodes) $\mathcal{V} = \{v_1, ..., v_N\}$

At time t, the feature is $\mathbf{x}^t = \{\mathbf{x}_1^t, ..., \mathbf{x}_N^t\}$

For all nodes, we have N trajectories

$$\mathbf{x} = (\mathbf{x}^1, ..., \mathbf{x}^T)$$



Observed dynamics

Interaction graph

Image Credit: [1]

Neural Relational Inference

Let us formalize the problem:

We have N particles (nodes) $\mathcal{V} = \{v_1, ..., v_N\}$

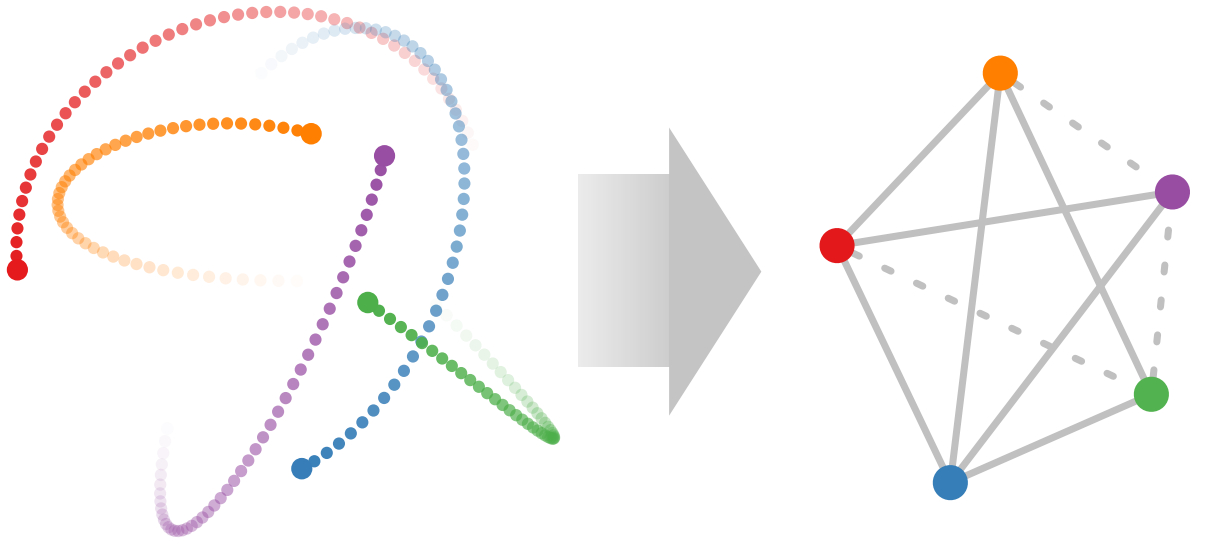
At time t, the feature is $\mathbf{x}^t = \{\mathbf{x}_1^t, ..., \mathbf{x}_N^t\}$

For all nodes, we have N trajectories

$$\mathbf{x} = (\mathbf{x}^1, ..., \mathbf{x}^T)$$

For any pair of node (v_i, v_j) , we introduce

a discrete latent variable $\mathbf{z}_{ij}$ to model interaction



Observed dynamics

Interaction graph

Image Credit: [1]

Neural Relational Inference

Let us formalize the problem:

We have N particles (nodes) $\mathcal{V} = \{v_1, ..., v_N\}$

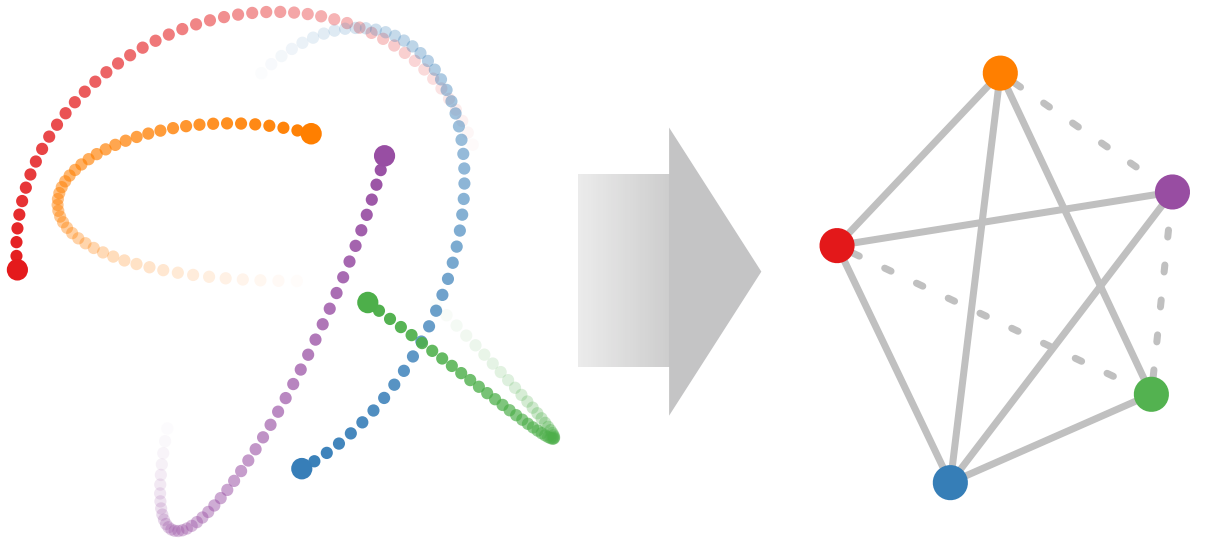
At time t, the feature is $\mathbf{x}^t = \{\mathbf{x}_1^t, ..., \mathbf{x}_N^t\}$

For all nodes, we have N trajectories

$$\mathbf{x} = (\mathbf{x}^1, ..., \mathbf{x}^T)$$

For any pair of node (v_i, v_j) , we introduce

a discrete latent variable $\mathbf{z}_{ij}$ to model interaction



Observed dynamics

Interaction graph

Our goal is to infer the set of all latent variables , which forms the latent graph!

Image Credit: [1]

Neural Relational Inference

We use VAEs as the probabilistic framework

Neural Relational Inference

We use VAEs as the probabilistic framework

- Encoder $q_\phi(\mathbf{z}|\mathbf{x})$
- Decoder $p_\theta(\mathbf{x}|\mathbf{z})$
- Prior $p(\mathbf{z})$

Neural Relational Inference

We use VAEs as the probabilistic framework

- Encoder $q_\phi(\mathbf{z}|\mathbf{x})$
- Decoder $p_\theta(\mathbf{x}|\mathbf{z})$
- Prior $p(\mathbf{z})$
- Learning the model by maximizing the ELBO

$$\mathcal{L} = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathrm{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})]$$

Neural Relational Inference

We use VAEs as the probabilistic framework

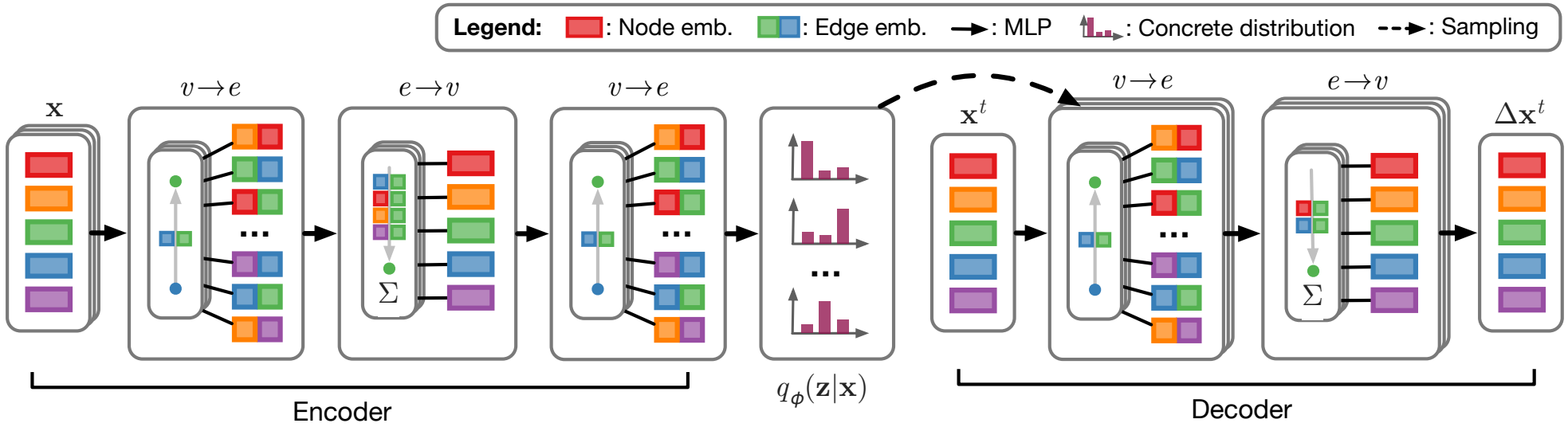


Image Credit: [1]

Neural Relational Inference

Encoder: A GNN applied to a fully connected graph

$$q_\phi(\mathbf{z}|\mathbf{x}) = \prod_{ij} q_\phi(\mathbf{z}_{ij}|\mathbf{x})$$

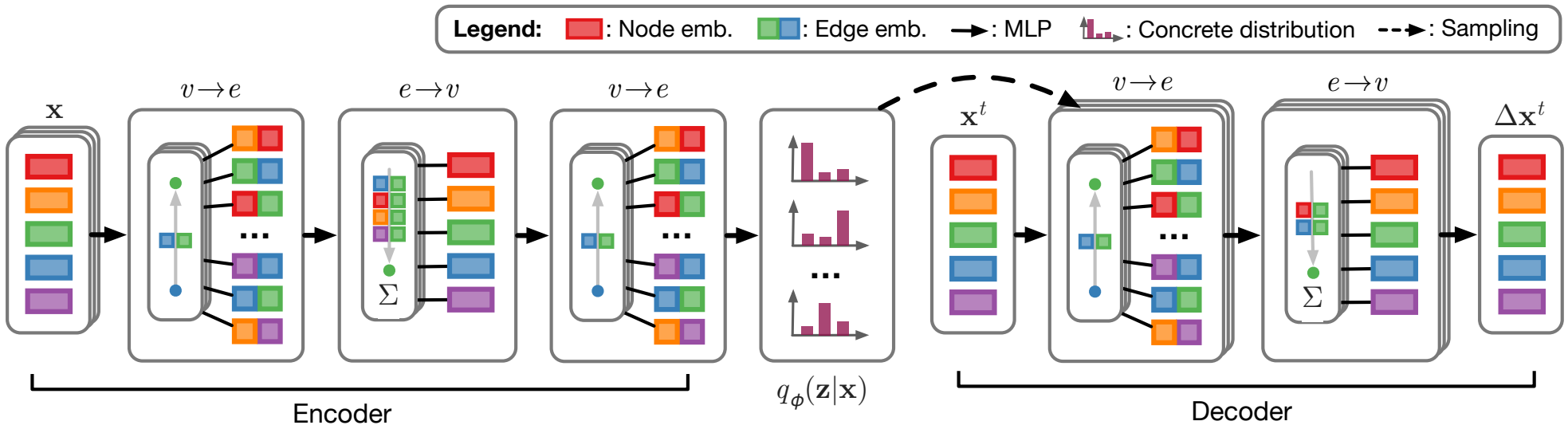
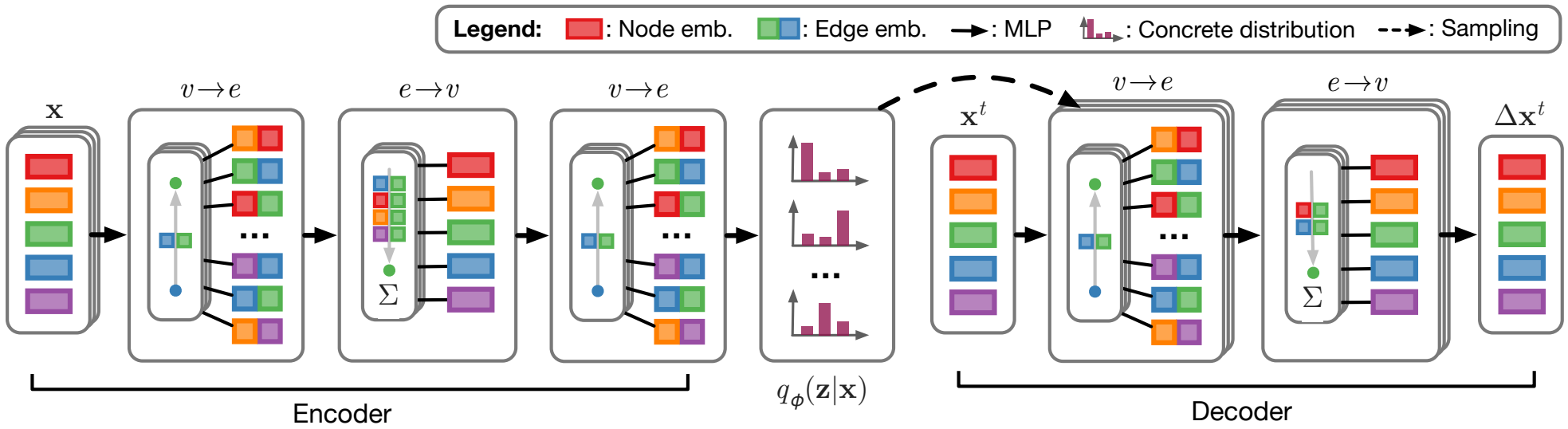


Image Credit: [1]

Neural Relational Inference

Encoder: A GNN applied to a fully connected graph

$$q_\phi(\mathbf{z}|\mathbf{x}) = \prod_{ij} q_\phi(\mathbf{z}_{ij}|\mathbf{x})$$



$$\mathbf{h}_j^1 = f_{\text{emb}}(\mathbf{x}_j)$$

Node to Edge $v \to e$: $\mathbf{h}_{(i,j)}^1 = f_e^1([\mathbf{h}_i^1, \mathbf{h}_j^1])$

Edge to Node $e \to v$: $\mathbf{h}_j^2 = f_v^1(\sum_{i \neq j} \mathbf{h}_{(i,j)}^1)$

Node to Edge $v \to e$: $\mathbf{h}_{(i,j)}^2 = f_e^2([\mathbf{h}_i^2, \mathbf{h}_j^2])$

Readout $q_\phi(\mathbf{z}_{ij}|\mathbf{x}) = \text{softmax}(\mathbf{h}_{(i,j)}^2)$

Image Credit: [1]

Neural Relational Inference

Decoder: A GNN applied to the sampled graph

$$p_\theta(\mathbf{x}|\mathbf{z}) = \prod_{t=1}^{T} p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z})$$

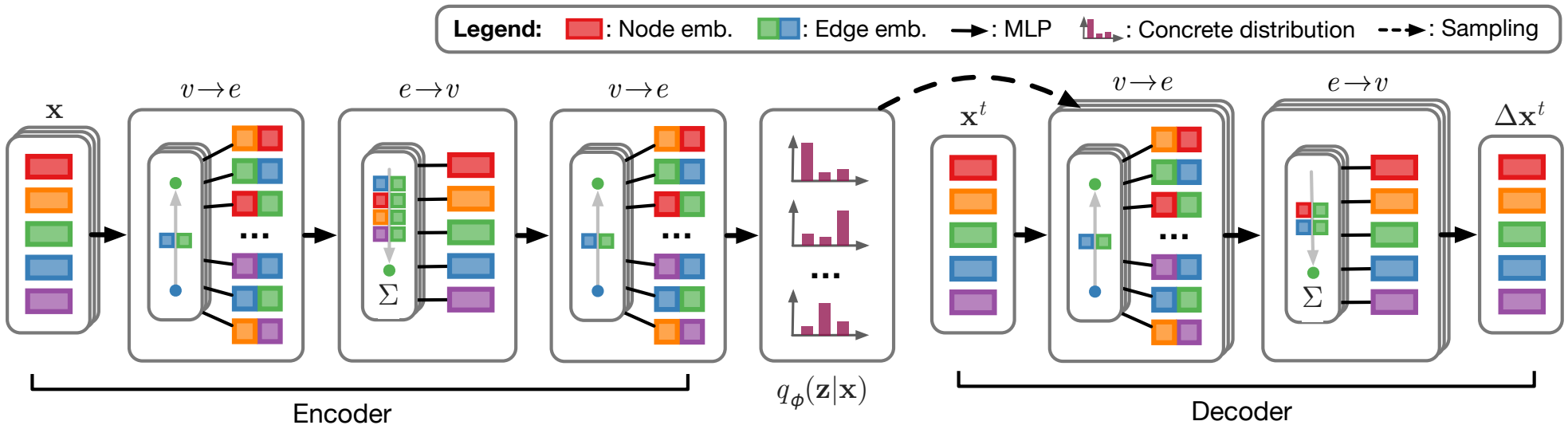
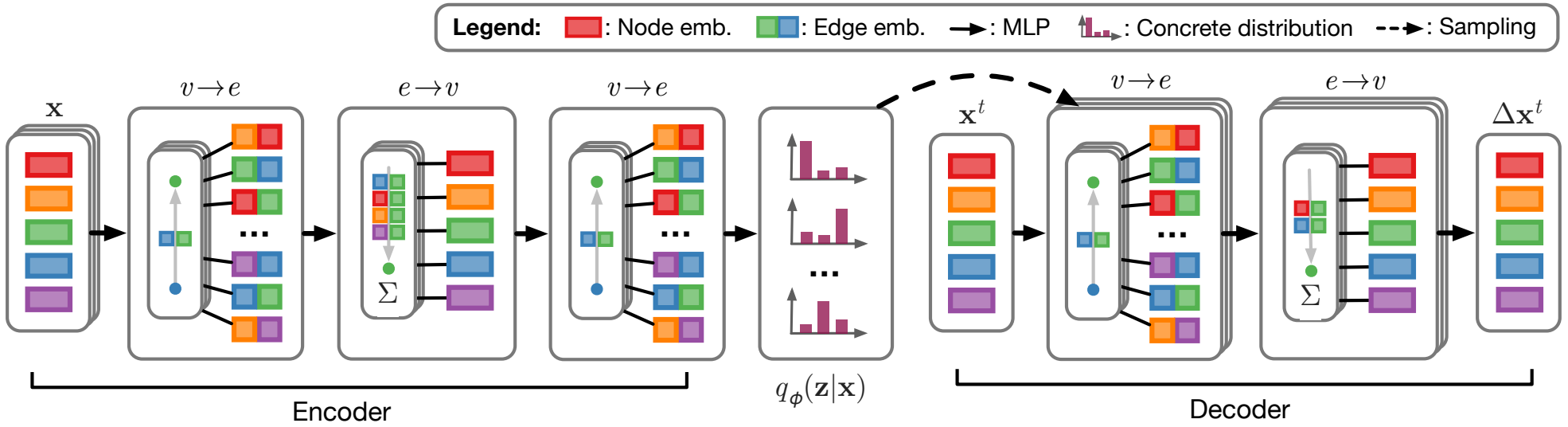


Image Credit: [1]

Neural Relational Inference

Decoder: A GNN applied to the sampled graph

$$p_\theta(\mathbf{x}|\mathbf{z}) = \prod_{t=1}^{T} p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z})$$



Option I: Markovian

$$p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z}) = p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, \mathbf{z})$$

Node to Edge $v \to e$:

$$\tilde{\mathbf{h}}_{(i,j)}^t = \sum_k z_{ij,k} \tilde{f}_e^k([\mathbf{x}_i^t, \mathbf{x}_j^t])$$

Edge to Node $e \to v$:

$$\boldsymbol{\mu}_j^{t+1} = \mathbf{x}_j^t + \tilde{f}_v(\textstyle\sum_{i \neq j} \tilde{\mathbf{h}}_{(i,j)}^t)$$

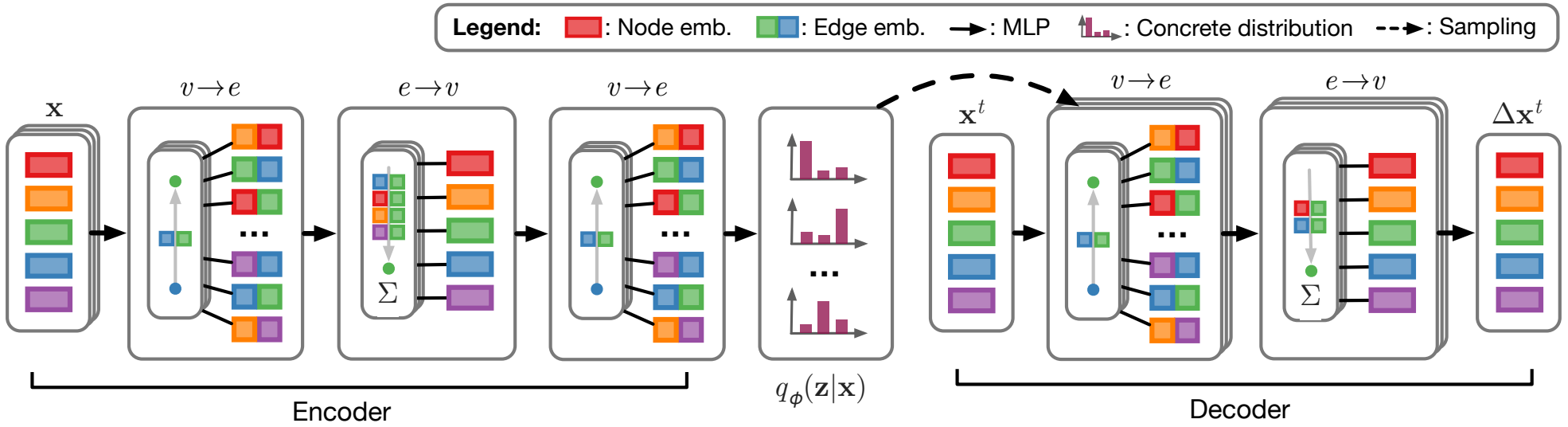
$$p(\mathbf{x}_j^{t+1}|\mathbf{x}^t, \mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_j^{t+1}, \sigma^2 \mathbf{I})$$

Image Credit: [1]

Neural Relational Inference

Decoder: A GNN applied to the sampled graph

$$p_\theta(\mathbf{x}|\mathbf{z}) = \prod_{t=1}^{T} p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z})$$



Option II: Auto-Regressive

Node to Edge $\quad v \to e: \quad \tilde{\mathbf{h}}^t_{(i,j)} = \sum_k z_{ij,k} \tilde{f}^k_e([\tilde{\mathbf{h}}^t_i, \tilde{\mathbf{h}}^t_j])$

Edge to Node $\quad e \to v: \quad \mathrm{MSG}^t_j = \sum_{i \neq j} \tilde{\mathbf{h}}^t_{(i,j)}$

$$\tilde{\mathbf{h}}^{t+1}_j = \mathrm{GRU}([\mathrm{MSG}^t_j, \mathbf{x}^t_j], \tilde{\mathbf{h}}^t_j)$$

$$\boldsymbol{\mu}^{t+1}_j = \mathbf{x}^t_j + f_{\text{out}}(\tilde{\mathbf{h}}^{t+1}_j)$$

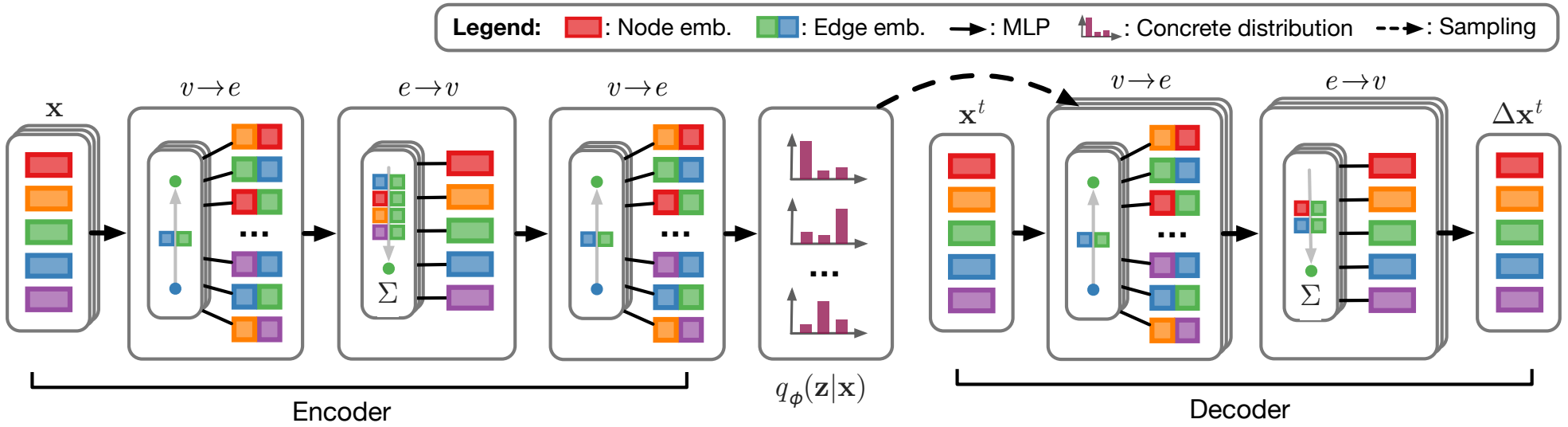
$$p(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}^{t+1}, \sigma^2\mathbf{I})$$

Image Credit: [1]

Neural Relational Inference

Decoder: A GNN applied to the sampled graph

$$p_\theta(\mathbf{x}|\mathbf{z}) = \prod_{t=1}^{T} p_\theta(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z})$$



Option II: Auto-Regressive

To avoid degenerated decoder:

- One message network per edge type
- Predict multiple futures

Node to Edge $v \to e: \quad \tilde{\mathbf{h}}^t_{(i,j)} = \sum_k z_{ij,k} \tilde{f}^k_e([\tilde{\mathbf{h}}^t_i, \tilde{\mathbf{h}}^t_j])$

Edge to Node $e \to v: \quad \mathrm{MSG}^t_j = \sum_{i \neq j} \tilde{\mathbf{h}}^t_{(i,j)}$

$$\tilde{\mathbf{h}}^{t+1}_j = \mathrm{GRU}([\mathrm{MSG}^t_j, \mathbf{x}^t_j], \tilde{\mathbf{h}}^t_j)$$

$$\boldsymbol{\mu}^{t+1}_j = \mathbf{x}^t_j + f_{\text{out}}(\tilde{\mathbf{h}}^{t+1}_j)$$

$$p(\mathbf{x}^{t+1}|\mathbf{x}^t, ..., \mathbf{x}^1, \mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}^{t+1}, \sigma^2\mathbf{I})$$

Image Credit: [1]

Neural Relational Inference

Prior: Independent uniform distributions over edge types

$$p_\theta(\mathbf{z}) = \prod_{i \neq j} p_\theta(\mathbf{z}_{ij})$$

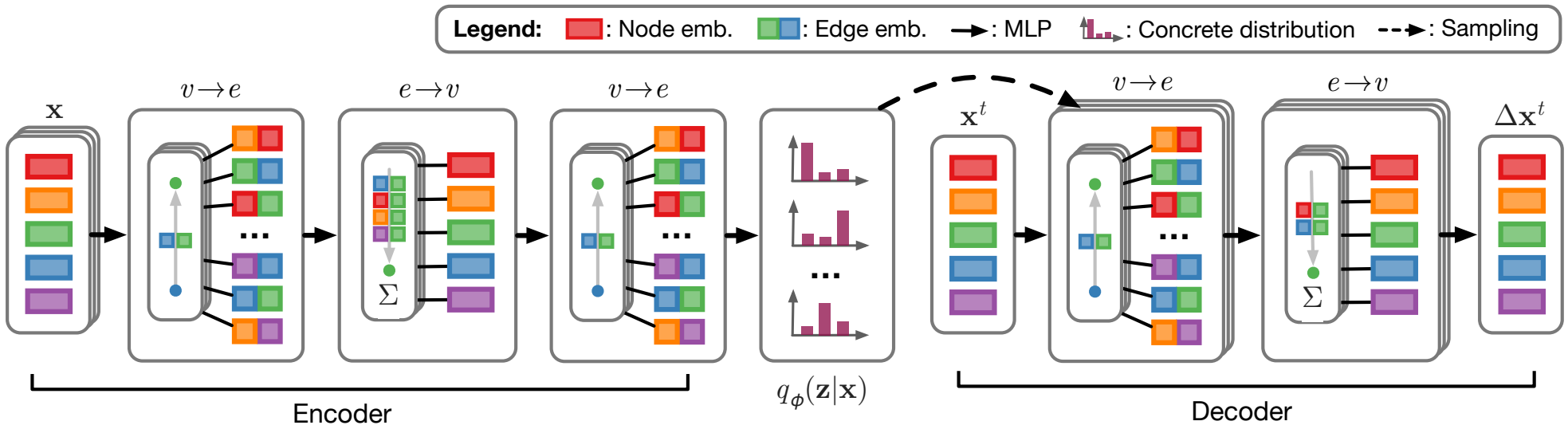
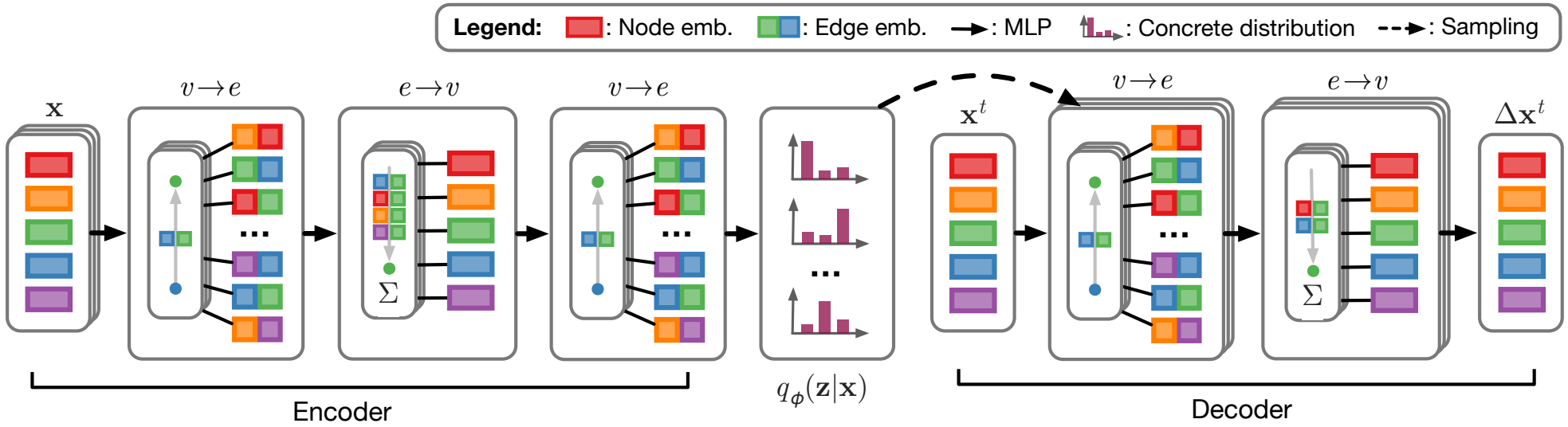


Image Credit: [1]

Neural Relational Inference

Learning VAE

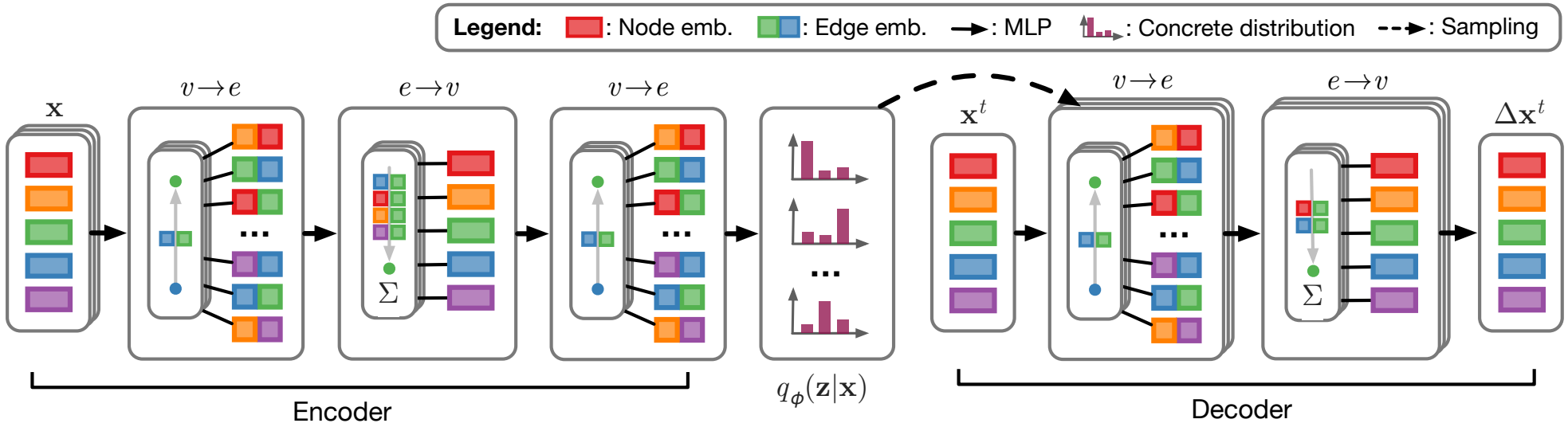


Sampling discrete latent variables

Image Credit: [1]

Neural Relational Inference

Learning VAE



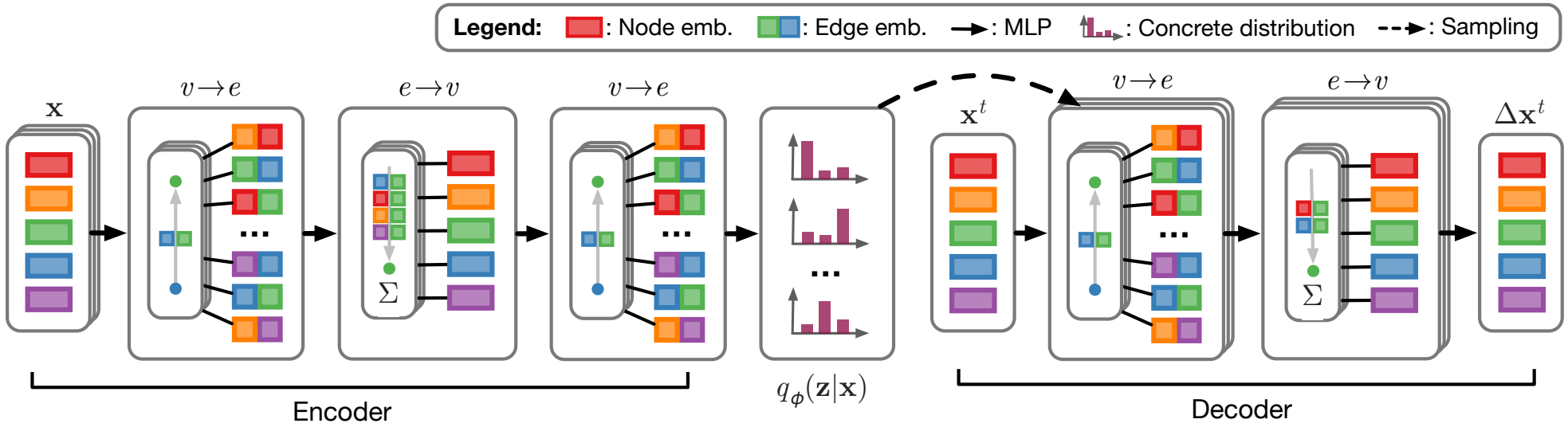
Sampling discrete latent variables

- Score function estimator (REINFORCE)
- Gumbel-Softmax / Concrete (Relaxation + Reparameterization)

Image Credit: [1]

Neural Relational Inference

Learning VAE



Sampling discrete latent variables

- Score function estimator (REINFORCE)
- **Gumbel-Softmax / Concrete (Relaxation + Reparameterization)**

Image Credit: [1]

Neural Relational Inference

Predicting the walking motion

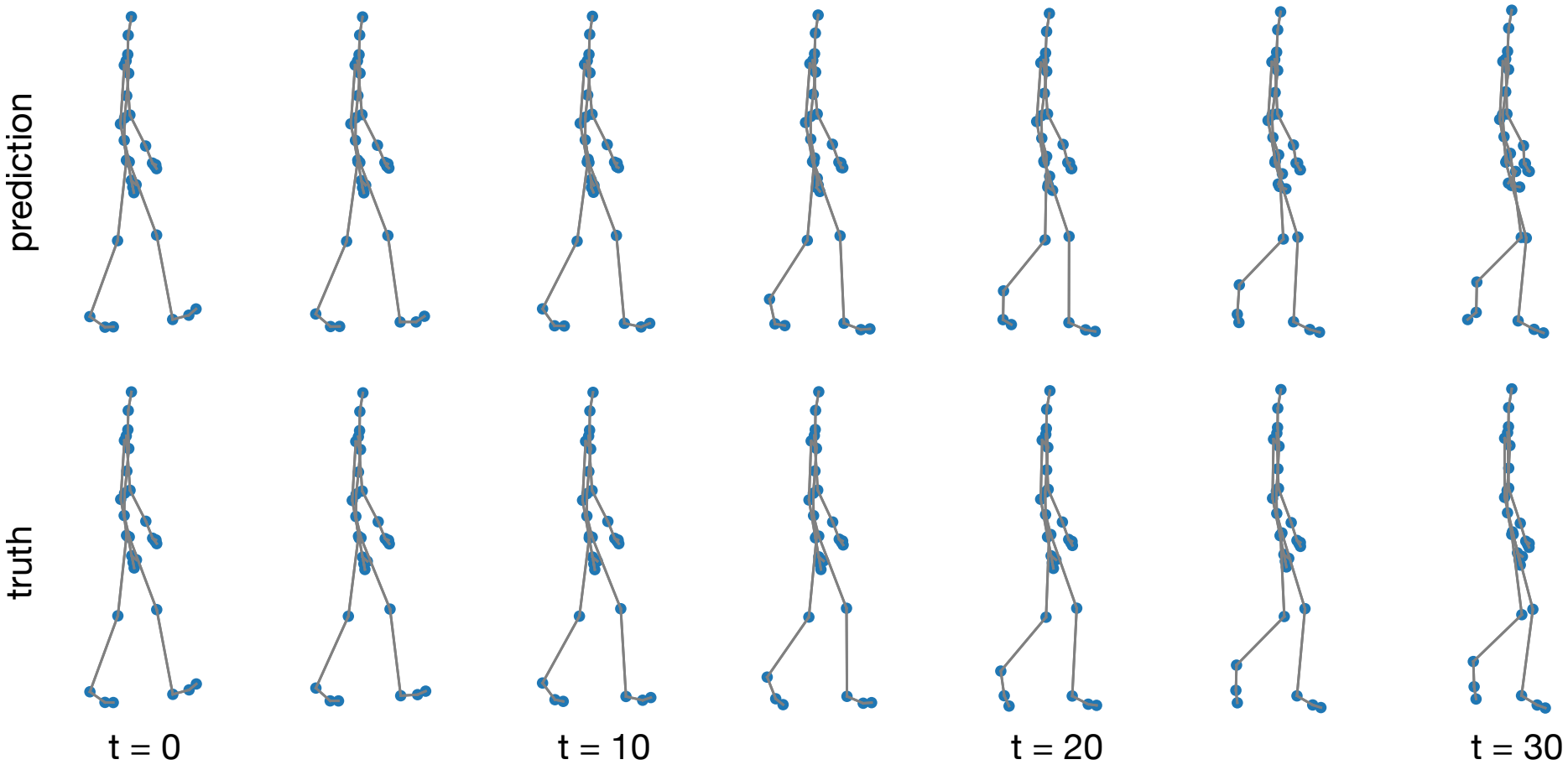
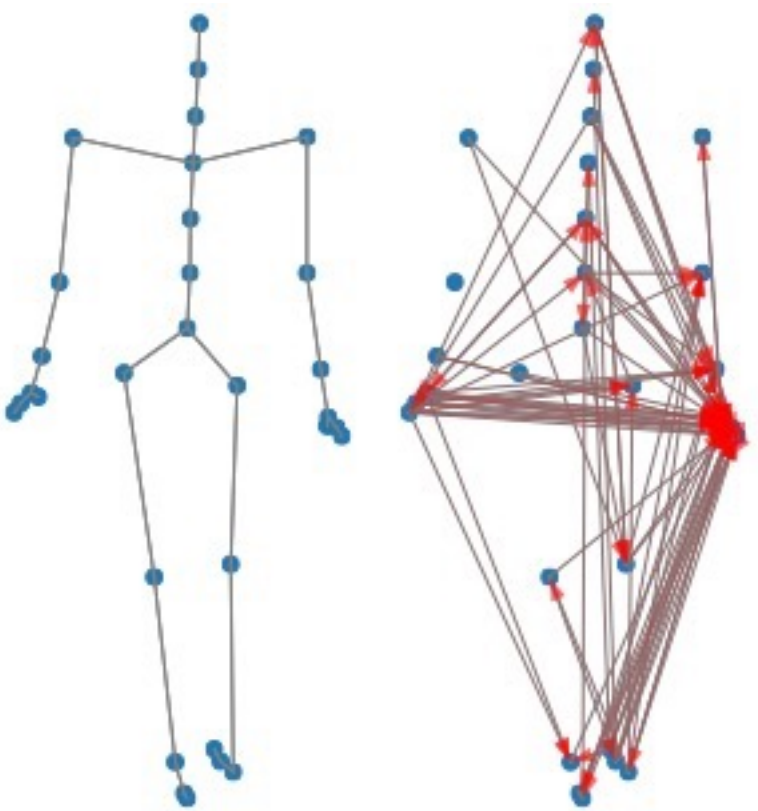


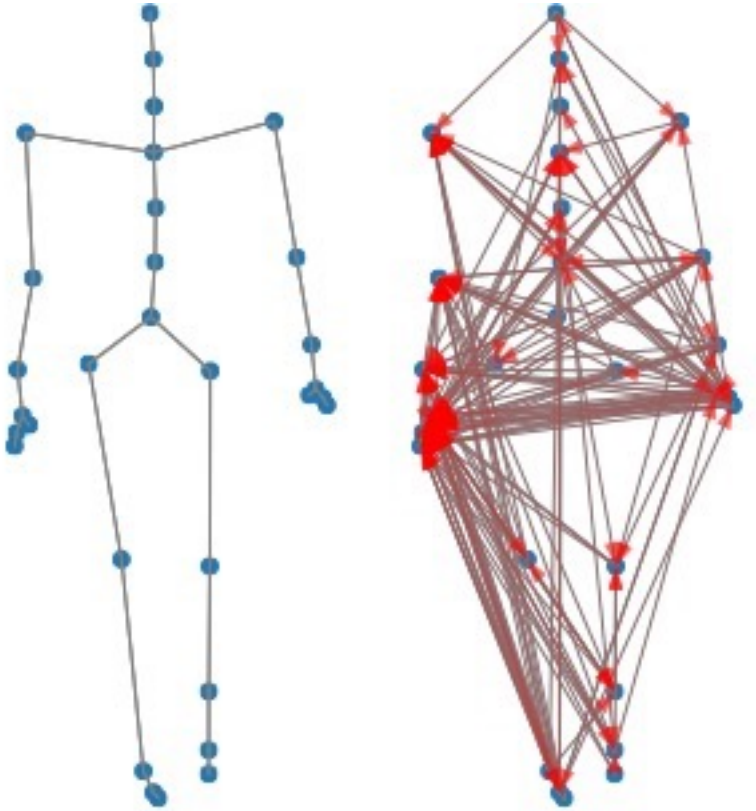
Image Credit: [1]

Neural Relational Inference

Learned latent graphs



Right hand focus



Left hand focus

Image Credit: [1]

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

- Transductive vs. Inductive

  Transductive: *reasoning from observed, specific (training) cases to specific (test) cases*

  Inductive: *reasoning from observed training cases to general rules, which are then applied to the test cases*

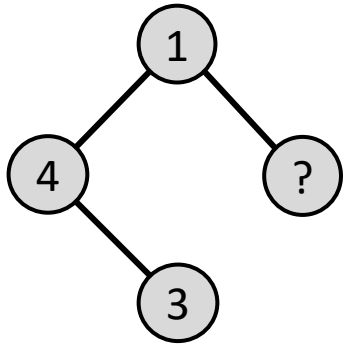
Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

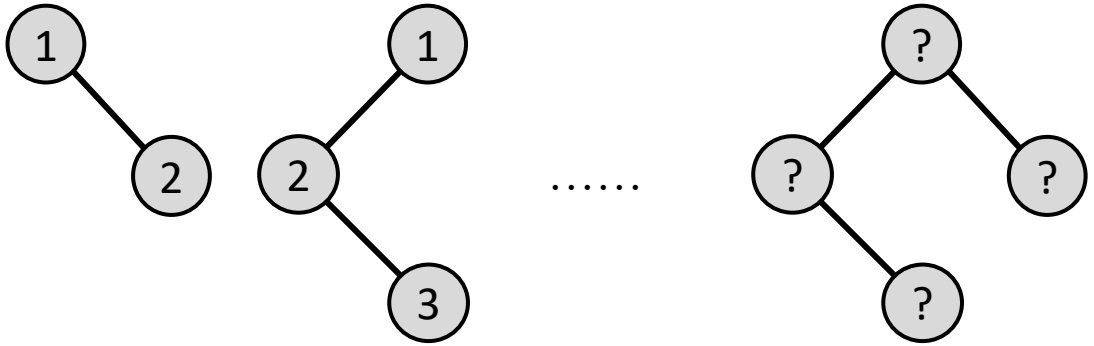
- Transductive vs. Inductive

  Transductive: *reasoning from observed, specific (training) cases to specific (test) cases*

  Inductive: *reasoning from observed training cases to general rules, which are then applied to the test cases*



Transductive



Inductive

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Can we learn a latent graph and then apply GNNs?

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Can we learn a latent graph and then apply GNNs?

One can formulate a bi-level optimization problem [2]:

$$\begin{aligned} \min_{A} \quad & \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v) \\ \text{s.t.} \quad & w_A = \arg\min_{w} \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w) \end{aligned}$$

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Can we learn a latent graph and then apply GNNs?

One can formulate a bi-level optimization problem [2]:

$$\min_{A} \quad \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v)$$

Outer level/loop

$$\text{s.t.} \quad w_A = \arg\min_{w} \quad \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Can we learn a latent graph and then apply GNNs?

One can formulate a bi-level optimization problem [2]:

$$\min_{A} \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v)$$

Outer level/loop

$$\text{s.t.} \quad w_A = \arg\min_{w} \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

Inner level/loop

Learning Discrete Structures for GNNs

Suppose we are given a single graph and want to perform (transductive) node classification

Suppose the graph is incomplete or even completely missing

Can we learn a latent graph and then apply GNNs?

One can formulate a bi-level optimization problem [2]:

$$\min_{A} \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v)$$

Outer level/loop

$$\text{s.t.} \quad w_A = \arg\min_{w} \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

Inner level/loop

w_A is a function (parameterized by the optimization algorithm) of A !

Learning Discrete Structures for GNNs

One can formulate a bi-level optimization problem [2]:

$$\begin{aligned} \min_{A} \quad & \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v) \\ \text{s.t.} \quad & w_A = \arg\min_{w} \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w) \end{aligned}$$

This problem is a hard mixed-integer programming problem!

Learning Discrete Structures for GNNs

One can formulate a bi-level optimization problem [2]:

$$\begin{aligned} \min_{A} \quad & \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v) \\ \text{s.t.} \quad & w_A = \arg\min_{w} \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w) \end{aligned}$$

This problem is a hard mixed-integer programming problem!

We can relax it (introducing edge-independent Bernoulli distribution):

$$\begin{aligned} \min_{\theta} \quad & \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[\sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v) \right] \\ \text{s.t.} \quad & w_\theta = \arg\min_{w} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[\sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w) \right] \end{aligned}$$

Learning Discrete Structures for GNNs

One can formulate a bi-level optimization problem [2]:

$$\min_{A} \quad \sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v)$$

$$\text{s.t.} \quad w_A = \arg\min_{w} \quad \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

This problem is a hard mixed-integer programming problem!

We can relax it (introducing edge-independent Bernoulli distribution):

$$\min_{\theta} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[\sum_{v \in V_{\texttt{Val}}} \ell(f_{w_A}(X, A)_v, y_v) \right]$$

We can unroll SGD for a few steps!

$$\text{s.t.} \quad w_\theta = \arg\min_{w} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[\sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w) \right]$$

Learning Discrete Structures for GNNs

Denoting the outer objective as $$F(w, A) = \sum_{v \in V_{\texttt{Val}}} \ell(f_w(X, A)_v, y_v)$$

Denoting the inner objective as $$L(w, A) = \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

Learning Discrete Structures for GNNs

Denoting the outer objective as $$F(w, A) = \sum_{v \in V_{\texttt{Val}}} \ell(f_w(X, A)_v, y_v)$$

Denoting the inner objective as $$L(w, A) = \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

The bi-level optimization is simplified as

$$\begin{aligned} \min_{\theta} \quad & \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[F(w_\theta, A) \right] \\ \text{s.t.} \quad & w_\theta = \arg\min_{w} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[L(w, A) \right] \end{aligned}$$

Learning Discrete Structures for GNNs

Denoting the outer objective as $$F(w, A) = \sum_{v \in V_{\texttt{Val}}} \ell(f_w(X, A)_v, y_v)$$

Denoting the inner objective as $$L(w, A) = \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

The bi-level optimization is simplified as

$$\begin{aligned} \min_{\theta} \quad & \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[F(w_\theta, A) \right] \\ \text{s.t.} \quad & w_\theta = \arg\min_{w} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[L(w, A) \right] \end{aligned}$$

For Inner optimization, we unroll SGD as $$w_{\theta,t+1} = w_{\theta,t} - \gamma_t \nabla L(w_{\theta,t}, A_t)$$

Learning Discrete Structures for GNNs

Denoting the outer objective as $$F(w, A) = \sum_{v \in V_{\texttt{Val}}} \ell(f_w(X, A)_v, y_v)$$

Denoting the inner objective as $$L(w, A) = \sum_{v \in V_{\texttt{Train}}} \ell(f_w(X, A)_v, y_v) + \Omega(w)$$

The bi-level optimization is simplified as

$$\begin{aligned} \min_{\theta} \quad & \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[F(w_\theta, A) \right] \\ \text{s.t.} \quad & w_\theta = \arg\min_{w} \quad \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[L(w, A) \right] \end{aligned}$$

For Inner optimization, we unroll SGD as $$w_{\theta,t+1} = w_{\theta,t} - \gamma_t \nabla L(w_{\theta,t}, A_t)$$

The (hyper) gradient is

$$\nabla_\theta \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[F(w_{\theta,T}, A) \right] = \mathbb{E}_{A \sim \mathrm{Ber}(\theta)} \left[\frac{\partial F(w_{\theta,T}, A)}{\partial w_{\theta,T}} \frac{\partial w_{\theta,T}}{\partial \theta} + \frac{\partial F(w_{\theta,T}, A)}{\partial A} \frac{\partial A}{\partial \theta} \right]$$

Learning Discrete Structures for GNNs

The (hyper) gradient is

$$\nabla_\theta \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[F(w_{\theta,T}, A)\right] = \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[\frac{\partial F(w_{\theta,T}, A)}{\partial w_{\theta,T}}\frac{\partial w_{\theta,T}}{\partial \theta} + \frac{\partial F(w_{\theta,T}, A)}{\partial A}\frac{\partial A}{\partial \theta}\right]$$

Learning Discrete Structures for GNNs

The (hyper) gradient is

$$\nabla_\theta \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[F(w_{\theta,T}, A)\right] = \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[\frac{\partial F(w_{\theta,T}, A)}{\partial w_{\theta,T}}\frac{\partial w_{\theta,T}}{\partial \theta} + \frac{\partial F(w_{\theta,T}, A)}{\partial A}\frac{\partial A}{\partial \theta}\right]$$

A is discrete samples drawn from edge-independent Bernoulli distribution

Since it is non-differentiable, we use straight-through estimator [2]

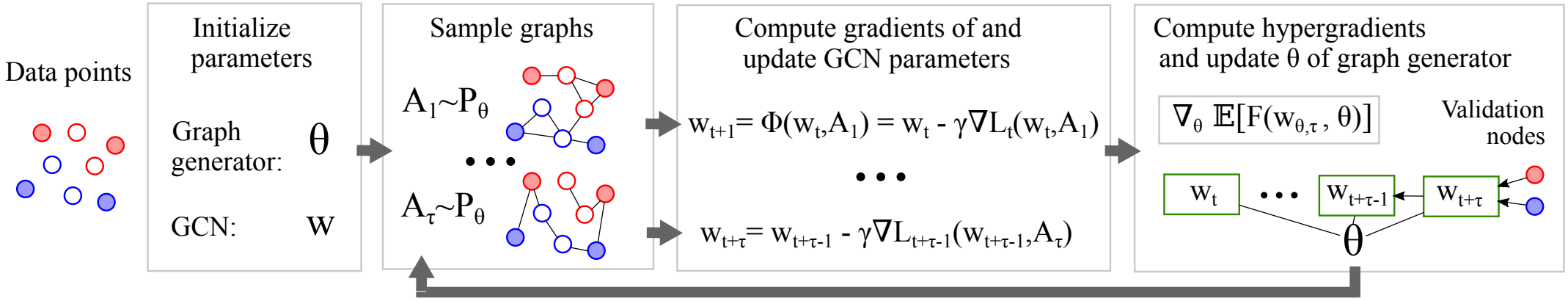
Learning Discrete Structures for GNNs

The (hyper) gradient is

$$\nabla_\theta \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[F(w_{\theta,T}, A)\right] = \mathbb{E}_{A\sim \mathrm{Ber}(\theta)}\left[\frac{\partial F(w_{\theta,T}, A)}{\partial w_{\theta,T}}\frac{\partial w_{\theta,T}}{\partial \theta} + \frac{\partial F(w_{\theta,T}, A)}{\partial A}\frac{\partial A}{\partial \theta}\right]$$

A is discrete samples drawn from edge-independent Bernoulli distribution

Since it is non-differentiable, we use straight-through estimator [2]



Learning Discrete Structures for GNNs

Transductive Classification:

	Wine	Cancer	Digits	Citeseer	Cora	20news	FMA
LogReg	92.1 (1.3)	**93.3 (0.5)**	85.5 (1.5)	62.2 (0.0)	60.8 (0.0)	42.7 (1.7)	37.3 (0.7)
Linear SVM	93.9 (1.6)	**90.6 (4.5)**	87.1 (1.8)	58.3 (0.0)	58.9 (0.0)	40.3 (1.4)	35.7 (1.5)
RBF SVM	**94.1 (2.9)**	**91.7 (3.1)**	86.9 (3.2)	60.2 (0.0)	59.7 (0.0)	41.0 (1.1)	**38.3 (1.0)**
RF	93.7 (1.6)	**92.1 (1.7)**	83.1 (2.6)	60.7 (0.7)	58.7 (0.4)	40.0 (1.1)	**37.9 (0.6)**
FFNN	89.7 (1.9)	**92.9 (1.2)**	36.3 (10.3)	56.7 (1.7)	56.1 (1.6)	38.6 (1.4)	33.2 (1.3)
LP	89.8 (3.7)	76.6 (0.5)	**91.9 (3.1)**	23.2 (6.7)	37.8 (0.2)	35.3 (0.9)	14.1 (2.1)
ManiReg	90.5 (0.1)	81.8 (0.1)	83.9 (0.1)	67.7 (1.6)	62.3 (0.9)	**46.6 (1.5)**	34.2 (1.1)
SemiEmb	91.9 (0.1)	89.7 (0.1)	**90.9 (0.1)**	68.1 (0.1)	63.1 (0.1)	**46.9 (0.1)**	34.1 (1.9)
Sparse-GCN	63.5 (6.6)	72.5 (2.9)	13.4 (1.5)	33.1 (0.9)	30.6 (2.1)	24.7 (1.2)	23.4 (1.4)
Dense-GCN	90.6 (2.8)	90.5 (2.7)	35.6 (21.8)	58.4 (1.1)	59.1 (0.6)	40.1 (1.5)	34.5 (0.9)
RBF-GCN	90.6 (2.3)	**92.6 (2.2)**	70.8 (5.5)	58.1 (1.2)	57.1 (1.9)	39.3 (1.4)	33.7 (1.4)
kNN-GCN	93.2 (3.1)	**93.8 (1.4)**	**91.3 (0.5)**	68.3 (1.3)	66.5 (0.4)	41.3 (0.6)	**37.8 (0.9)**
kNN-LDS (dense)	**97.5 (1.2)**	**94.9 (0.5)**	**92.1 (0.7)**	**70.9 (1.3)**	**70.9 (1.1)**	**45.6 (2.2)**	**38.6 (0.6)**
kNN-LDS	**97.3 (0.4)**	**94.4 (1.9)**	**92.5 (0.7)**	**71.5 (1.1)**	**71.5 (0.8)**	**46.4 (1.6)**	**39.7 (1.4)**

Conclusions

Summary:

- Neural Relational Inference

  Amortized inference, thus being applicable to inductive and transductive setting

  Use Edge-Independent Categorical and Gumbel-Softmax to learn latent graphs

Conclusions

Summary:

- Neural Relational Inference

  Amortized inference, thus being applicable to inductive and transductive setting

  Use Edge-Independent Categorical and Gumbel-Softmax to learn latent graphs

- Learning Latent Graphs via Bi-level Optimization

  Learn a single latent graph, thus being inapplicable to inductive setting

  Use Edge-Independent Bernoulli and Straight-Through to learn latent graphs

Open Questions

- Can we use more expressive generative models over graphs? E.g., deep auto-regressive models?

- For bi-level optimization, it may be beneficial to run inner SGD until convergence. Can we still efficiently learn the latent graph in this case?

  Yes, Implicit Differentiation [3, 4]!

References

[1] Kipf, T., Fetaya, E., Wang, K.C., Welling, M. and Zemel, R., 2018, July. Neural relational inference for interacting systems. In International Conference on Machine Learning (pp. 2688-2697). PMLR.

[2] Franceschi, L., Niepert, M., Pontil, M. and He, X., 2019, May. Learning discrete structures for graph neural networks. In International conference on machine learning (pp. 1972-1982). PMLR.

[3] Liao, R., Xiong, Y., Fetaya, E., Zhang, L., Yoon, K., Pitkow, X., Urtasun, R. and Zemel, R., 2018, July. Reviving and improving recurrent back-propagation. In International Conference on Machine Learning (pp. 3082-3091). PMLR.

[4] Bai, S., Kolter, J.Z. and Koltun, V., 2019. Deep equilibrium models. Advances in Neural Information Processing Systems, 32.

Questions?