# EECE 571F: Deep Learning with Structures

## Lecture 12: Learning Latent Graph Structures

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University of British Columbia

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# Course Scope

- Brief Intro to Deep Learning

- Geometric Deep Learning

    - Deep Learning Models for Sets and Sequences: Deep Sets & Transformers
    - Deep Learning Models for Graphs: Graph Convolution & Message Passing GNNs
    - Expressiveness & Generalizations of GNNs
    - Unsupervised/Self-supervised Graph Representation Learning

- Probabilistic Deep Learning

    - Deep Generative Models:
      Auto-regressive models, GANs, VAEs, Diffusion/Score based models
    - Discrete/Hybrid Latent Variable Models: RBMs, Latent Graph Models
    - Stochastic Gradient Estimation

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# Contents

Learning Latent Graphs for Deep Probabilistic Models

- Neural Relational Inference
- Learning Latent Graphs via Bi-level Optimization

# Neural Relational Inference

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

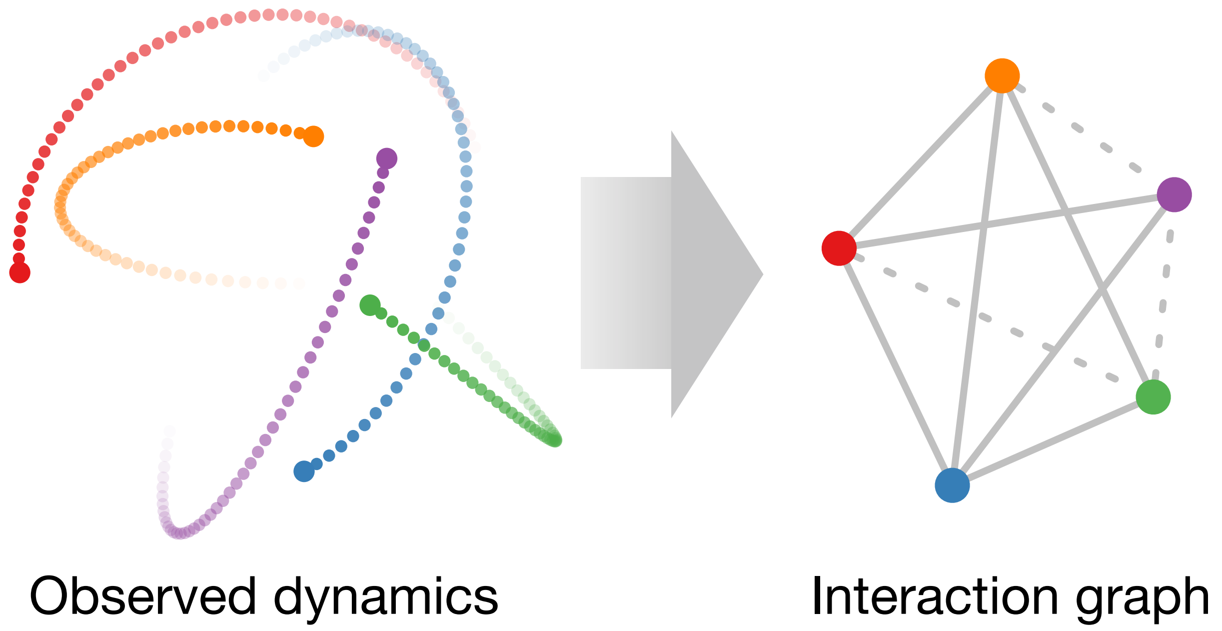
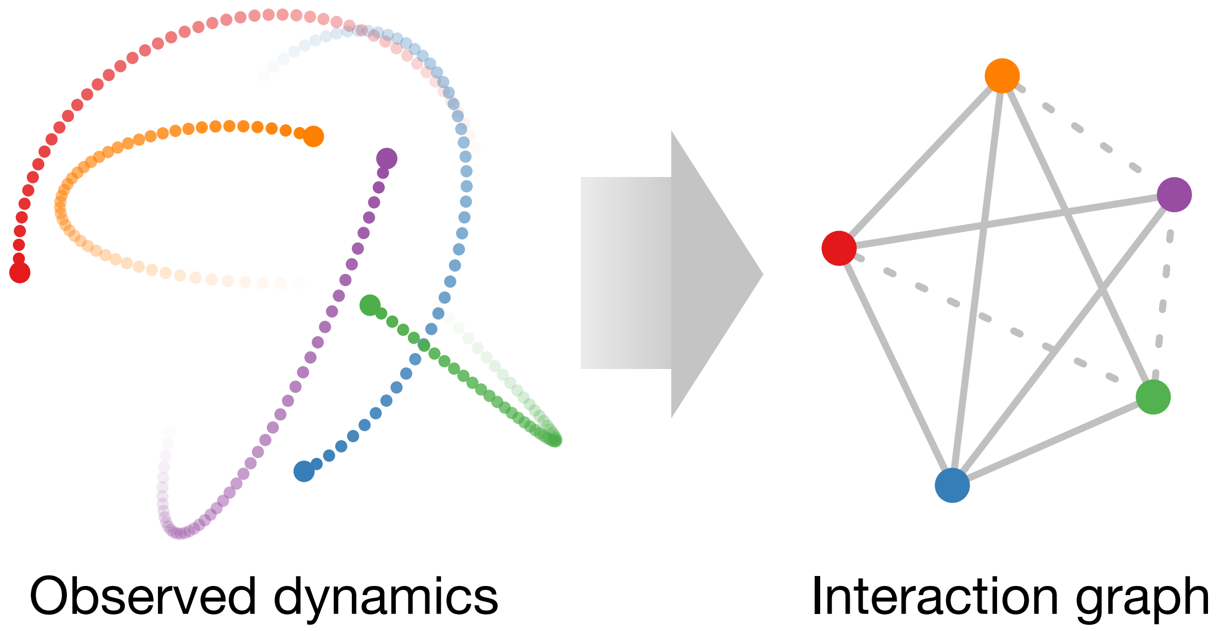



Image Credit: [1]

# 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.

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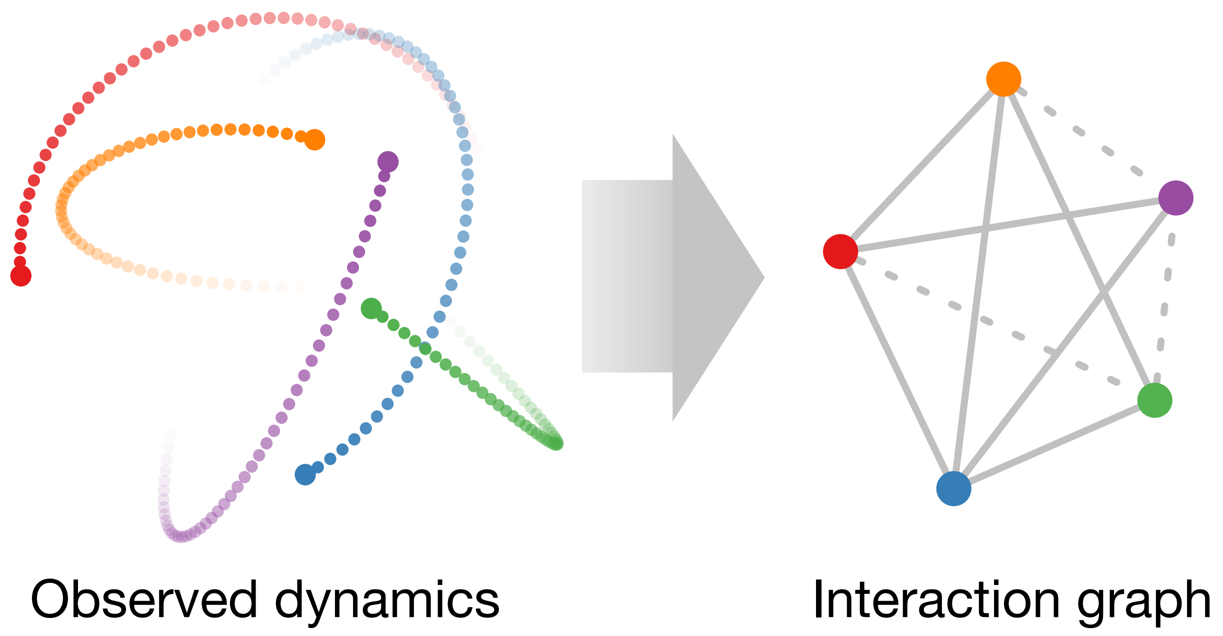
# Neural Relational Inference

Let us formalize the problem:

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

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

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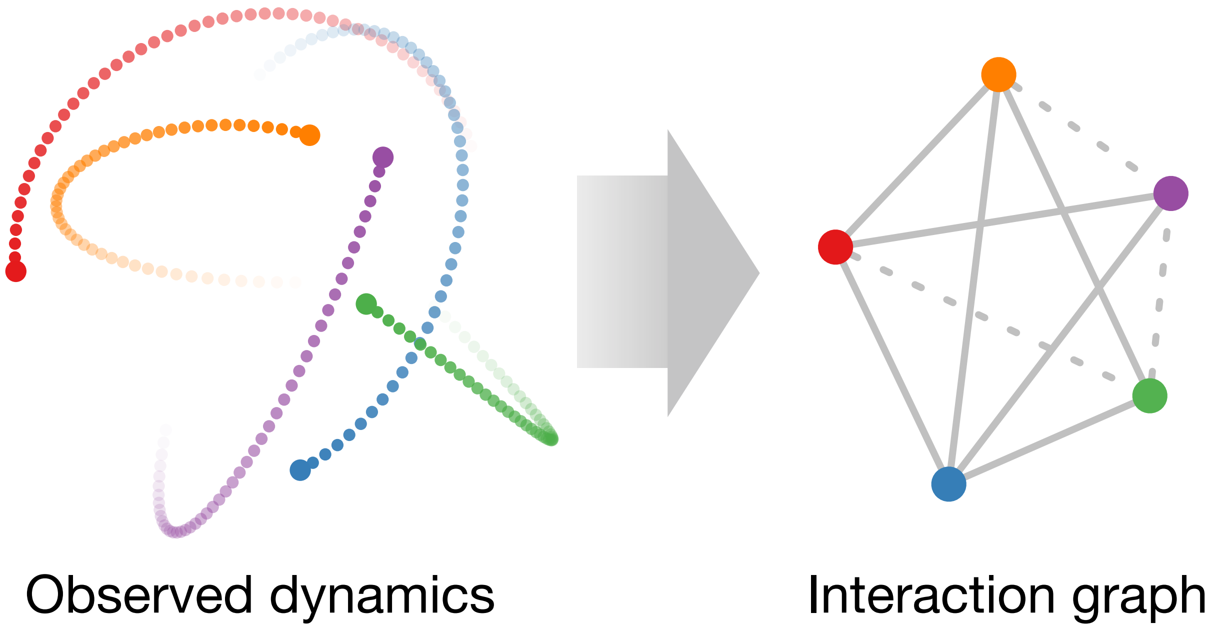
$$\mathbf{x} = (\mathbf{x}^1, ..., \mathbf{x}^T)$$

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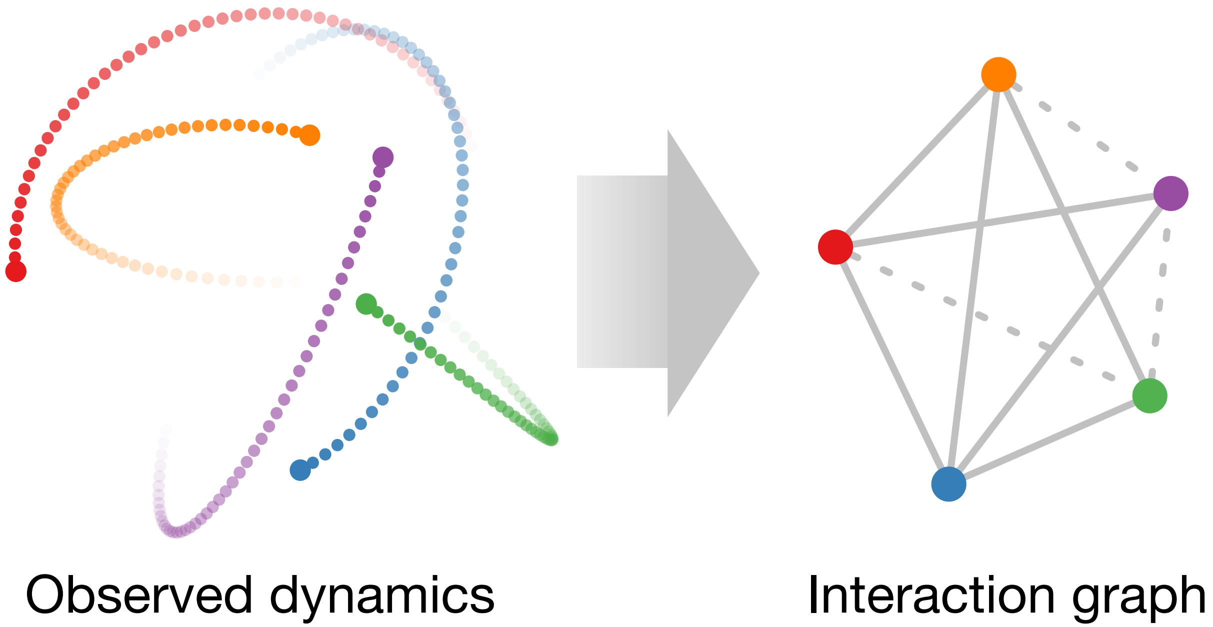
For any pair of node $(v_i, v_j)$ , we introduce

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

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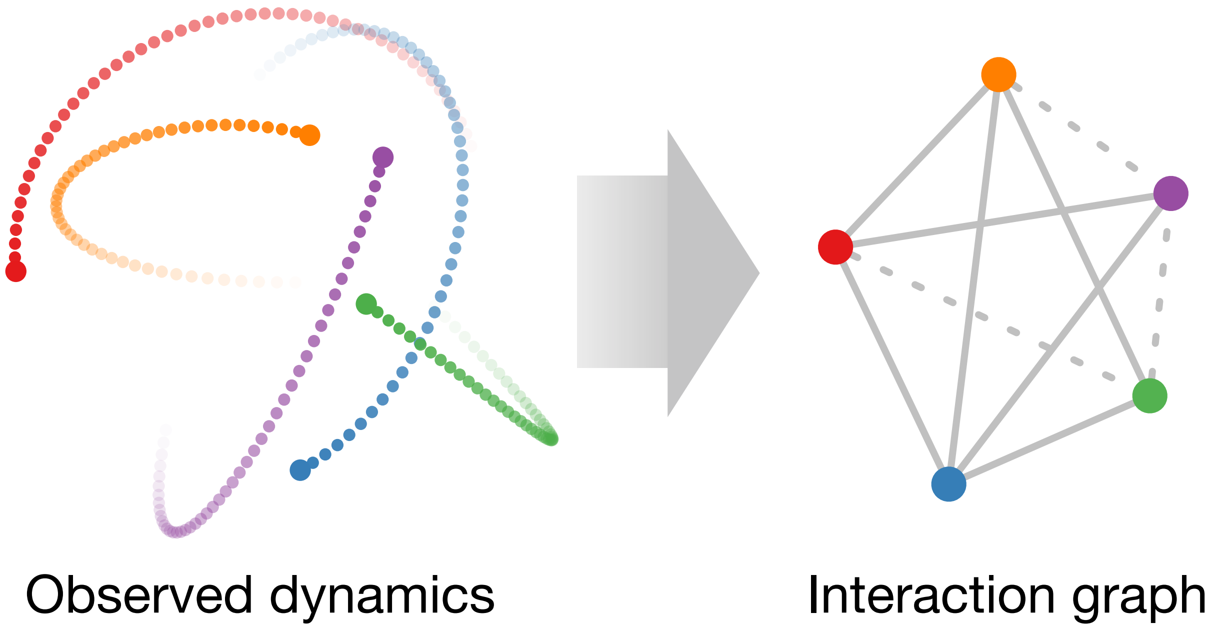


Our goal is to infer the set of all latent variables , which forms the latent graph!

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# Neural Relational Inference

We use VAEs as the probabilistic framework

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

# Neural Relational Inference

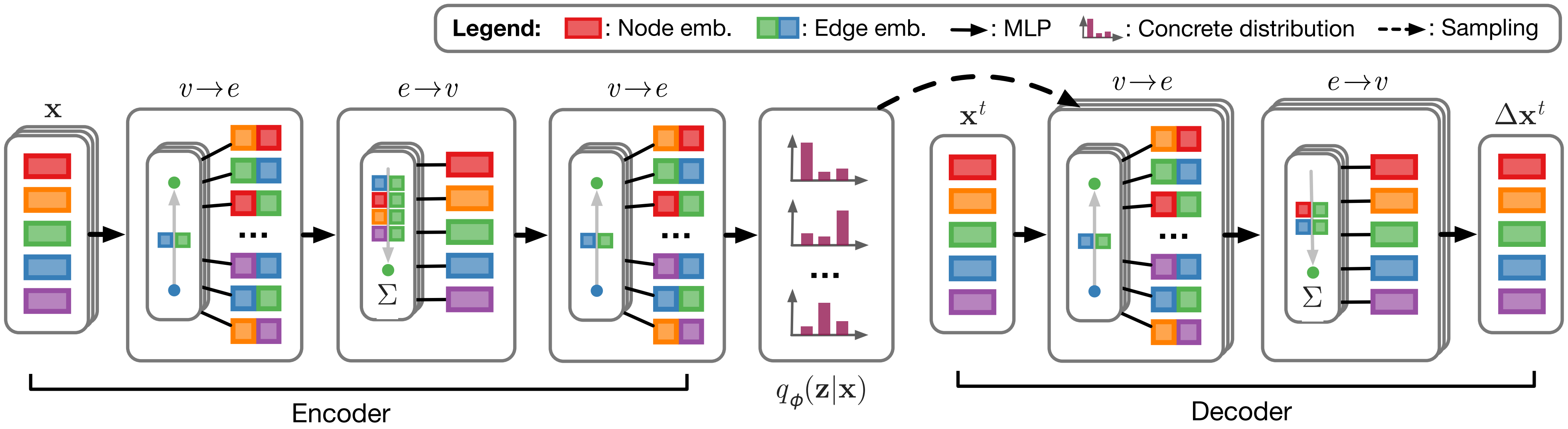
We use VAEs as the probabilistic framework

- 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

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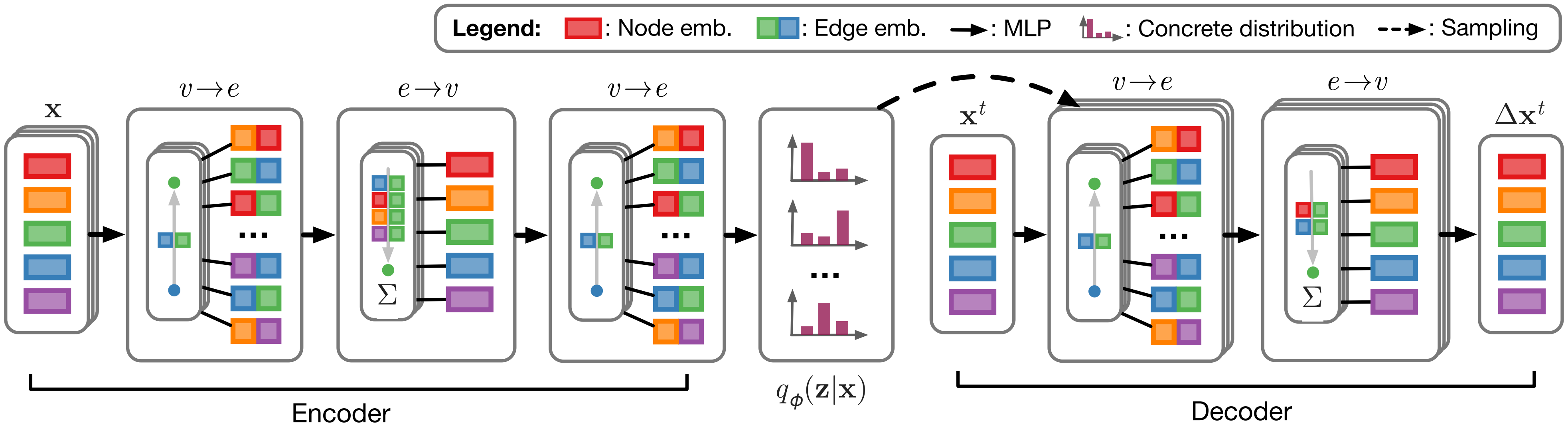
# Neural Relational Inference

Encoder: A GNN applied to a fully connected graph

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

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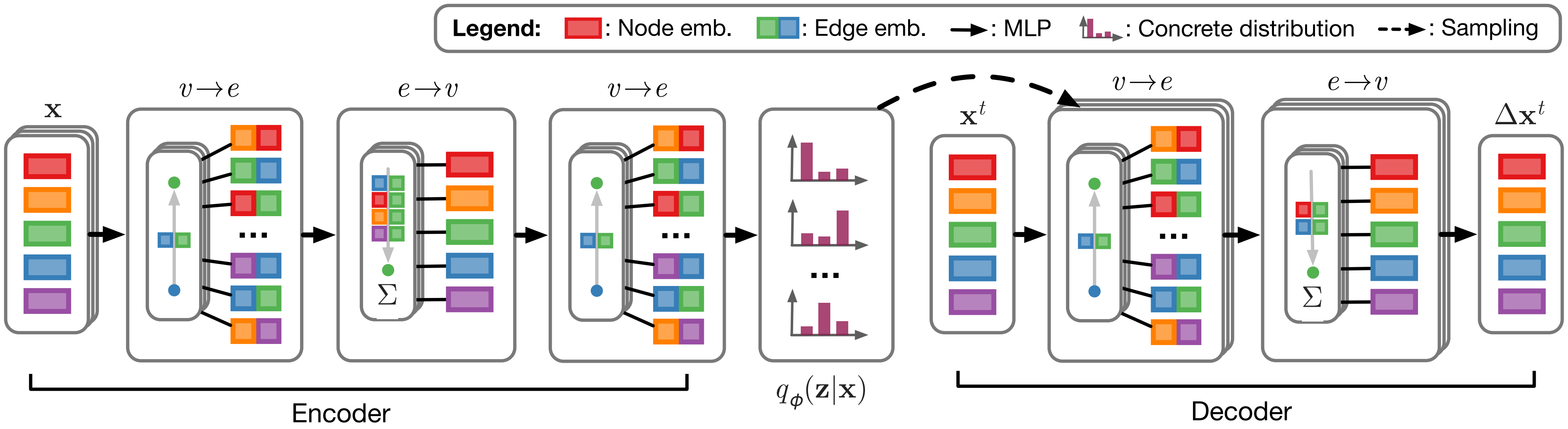



$$\mathbf{h}_j^1 = f_{\text{emb}}(\mathbf{x}_j)$$

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

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

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

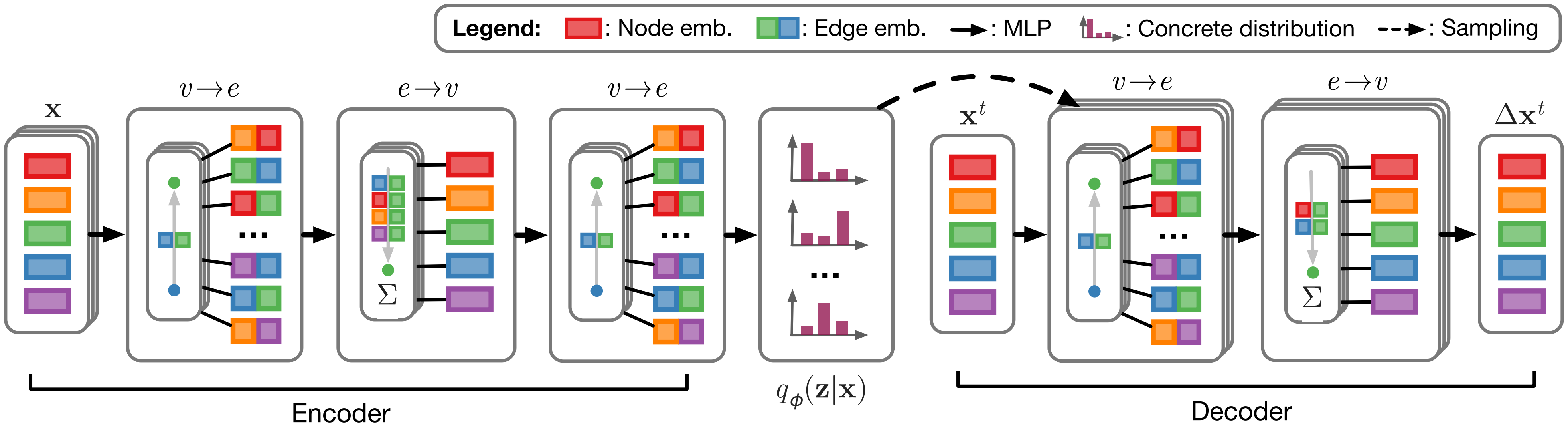
Readout $q_\phi(\mathbf{z}_{ij}|\mathbf{x}) = \text{softmax}(\mathbf{h}^2_{(i,j)})$

Image Credit: [1]

# Neural Relational Inference

Decoder: A GNN applied to the sampled graph

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

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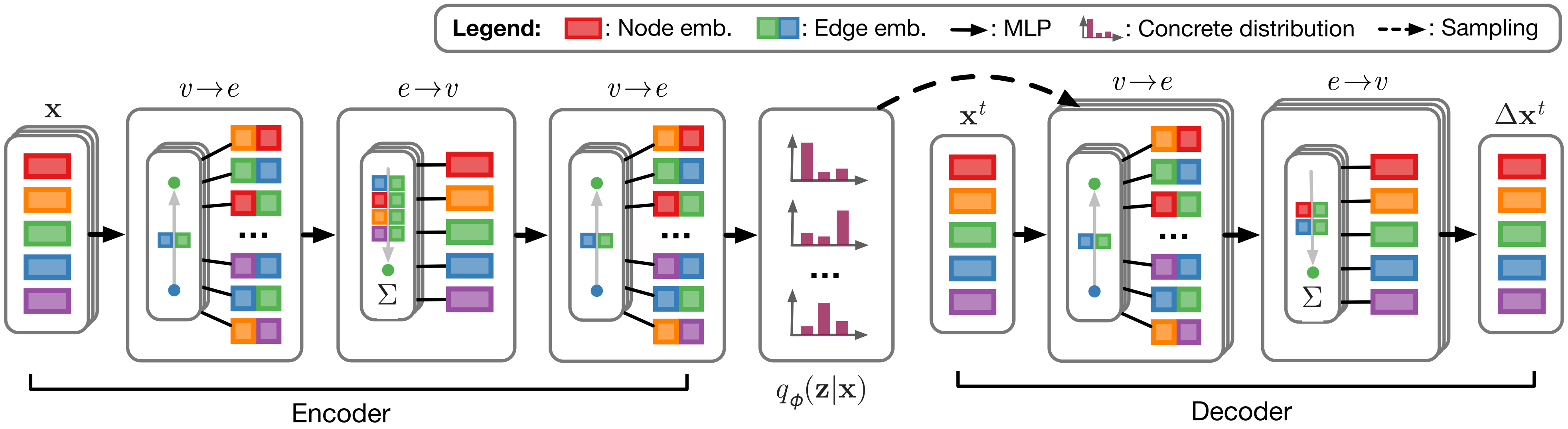


Option I: Markovian

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

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

Edge to Node $\quad e \to v: \quad \boldsymbol{\mu}^{t+1}_j = \mathbf{x}^t_j + \tilde{f}_v(\sum_{i \neq j} \tilde{\mathbf{h}}^t_{(i,j)})$

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

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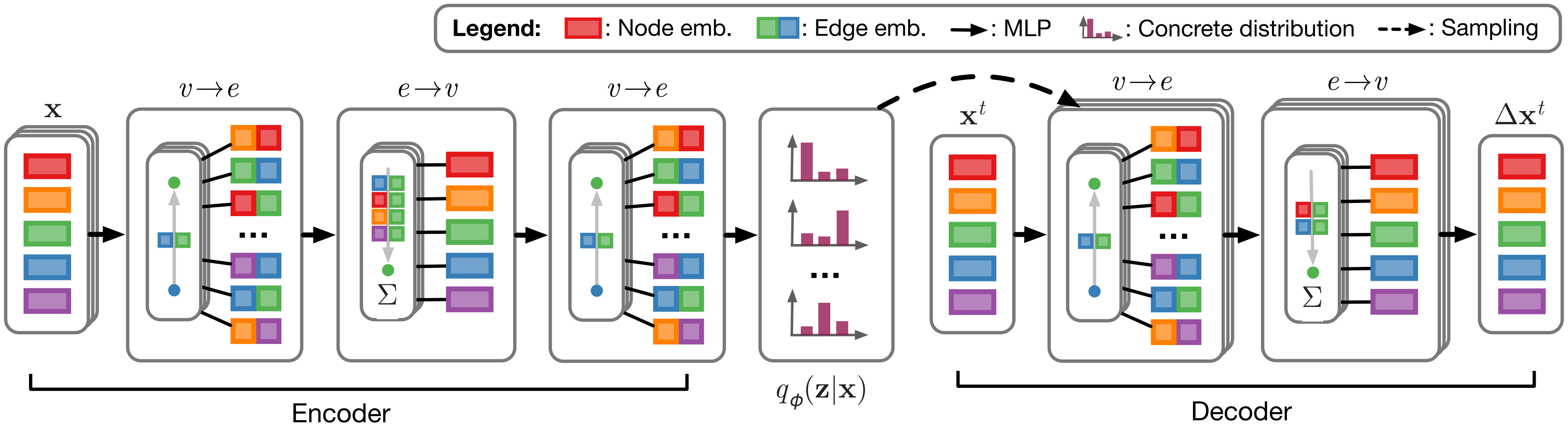


Option II: Auto-Regressive

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

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

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

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

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# Neural Relational Inference

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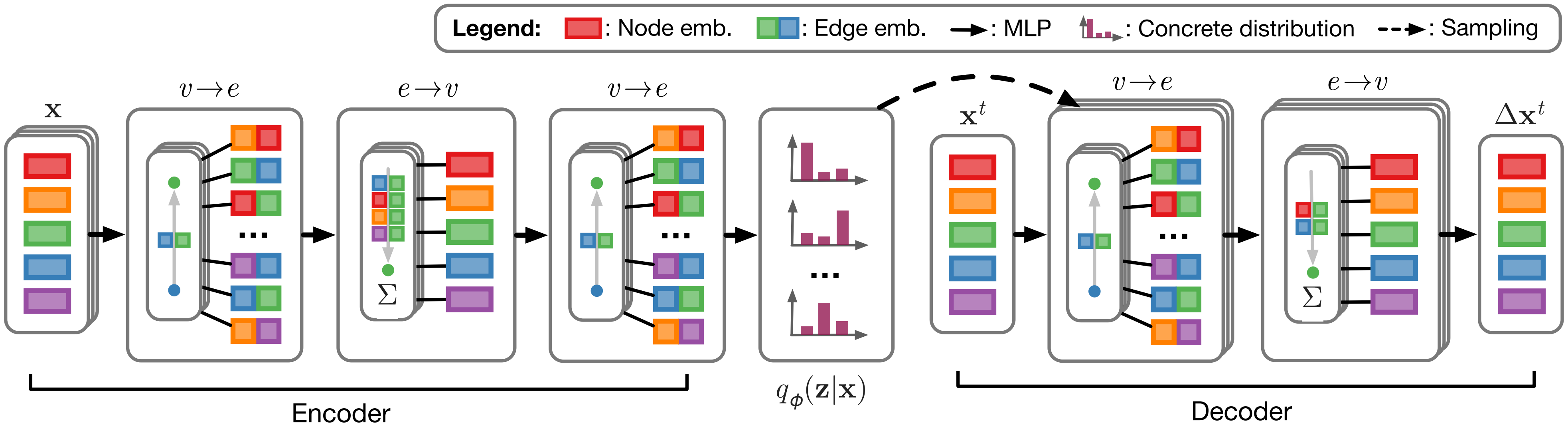


Option II: Auto-Regressive

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

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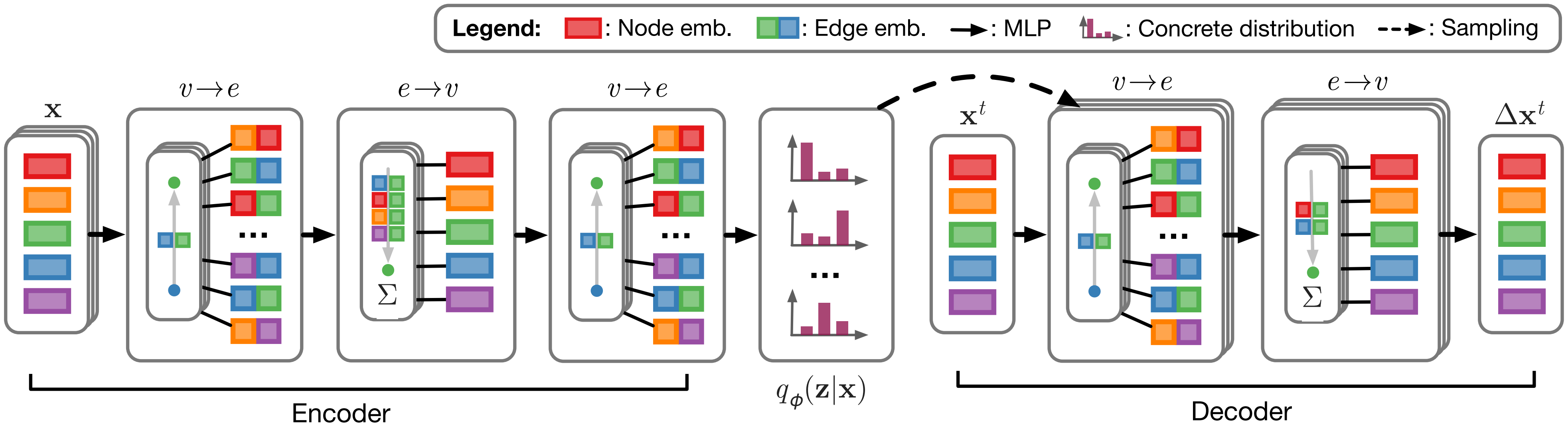
Image Credit: [1]

# Neural Relational Inference

Prior: Independent uniform distributions over edge types

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

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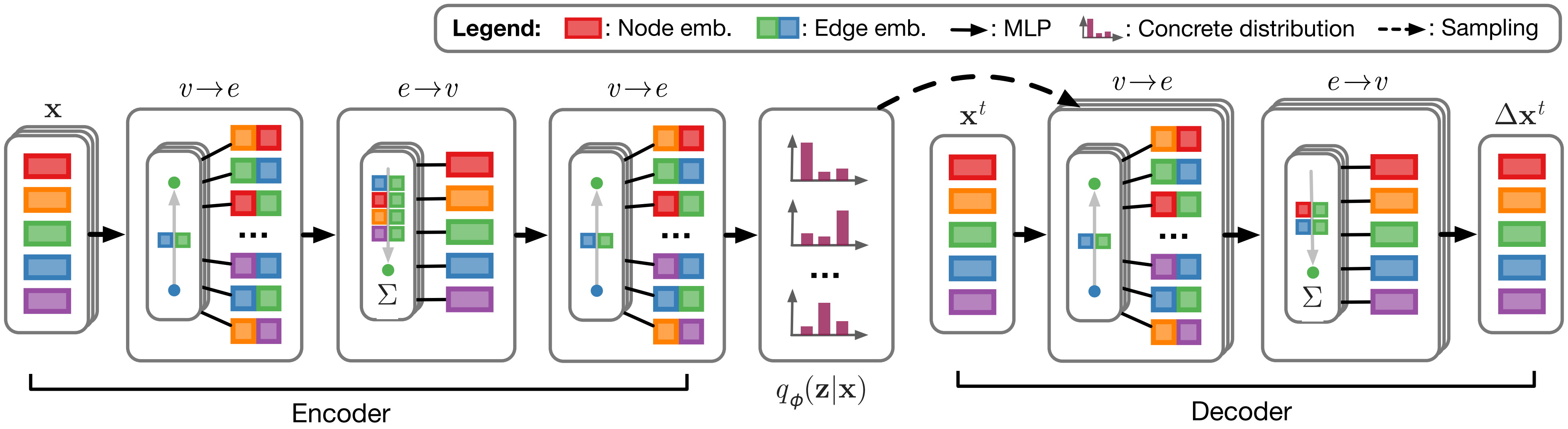
# Neural Relational Inference

Learning VAE




Sampling discrete latent variables

Image Credit: [1]

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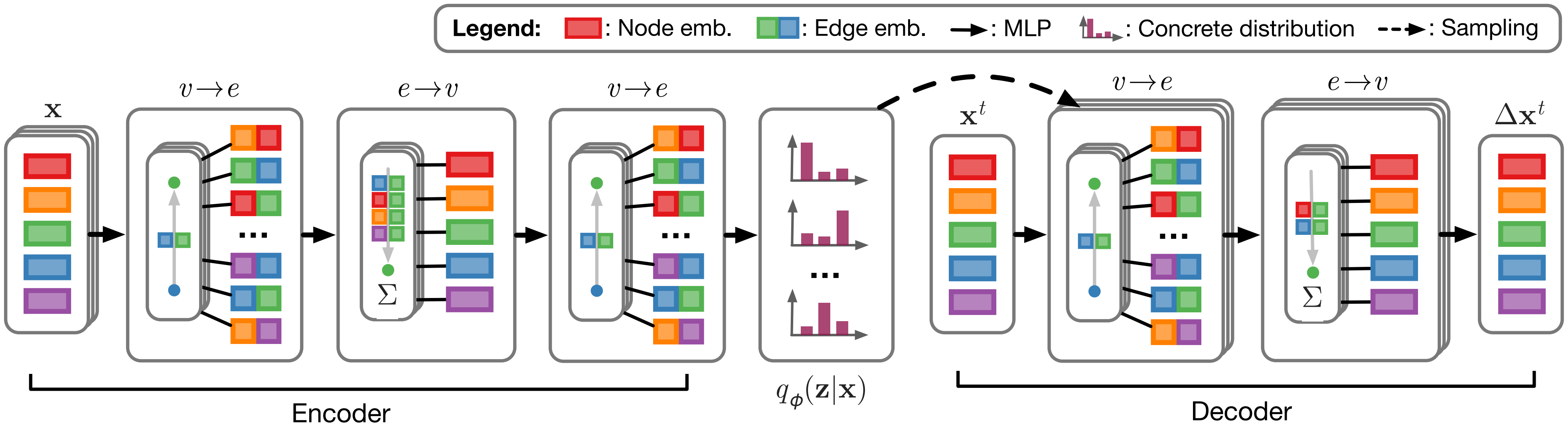


Sampling discrete latent variables

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

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# Neural Relational Inference

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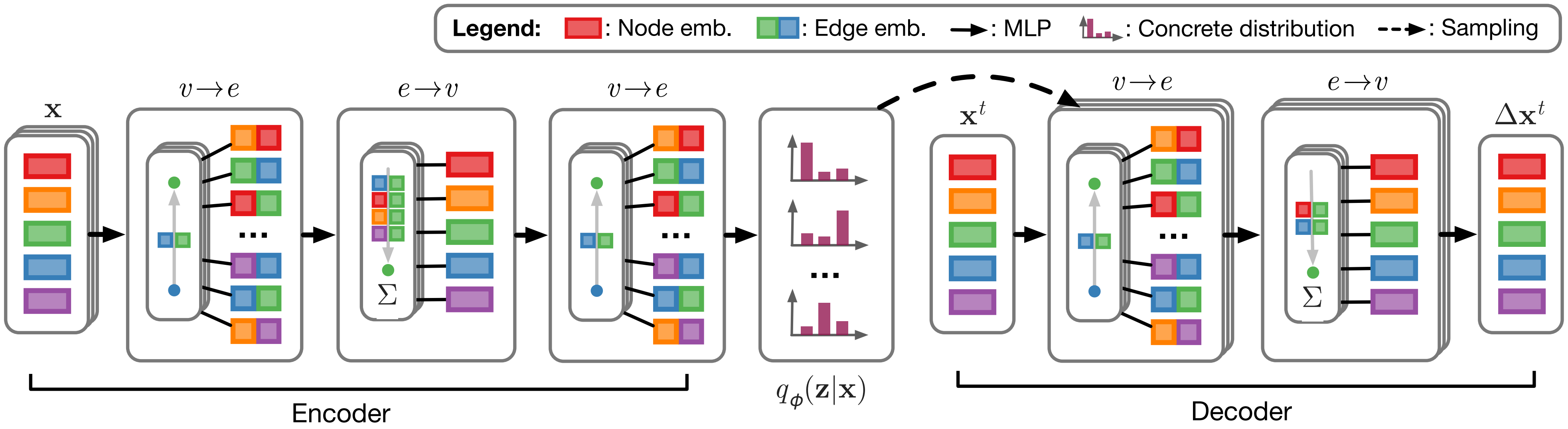


Sampling discrete latent variables

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- **Gumbel-Softmax / Concrete (Relaxation + Reparameterization)**

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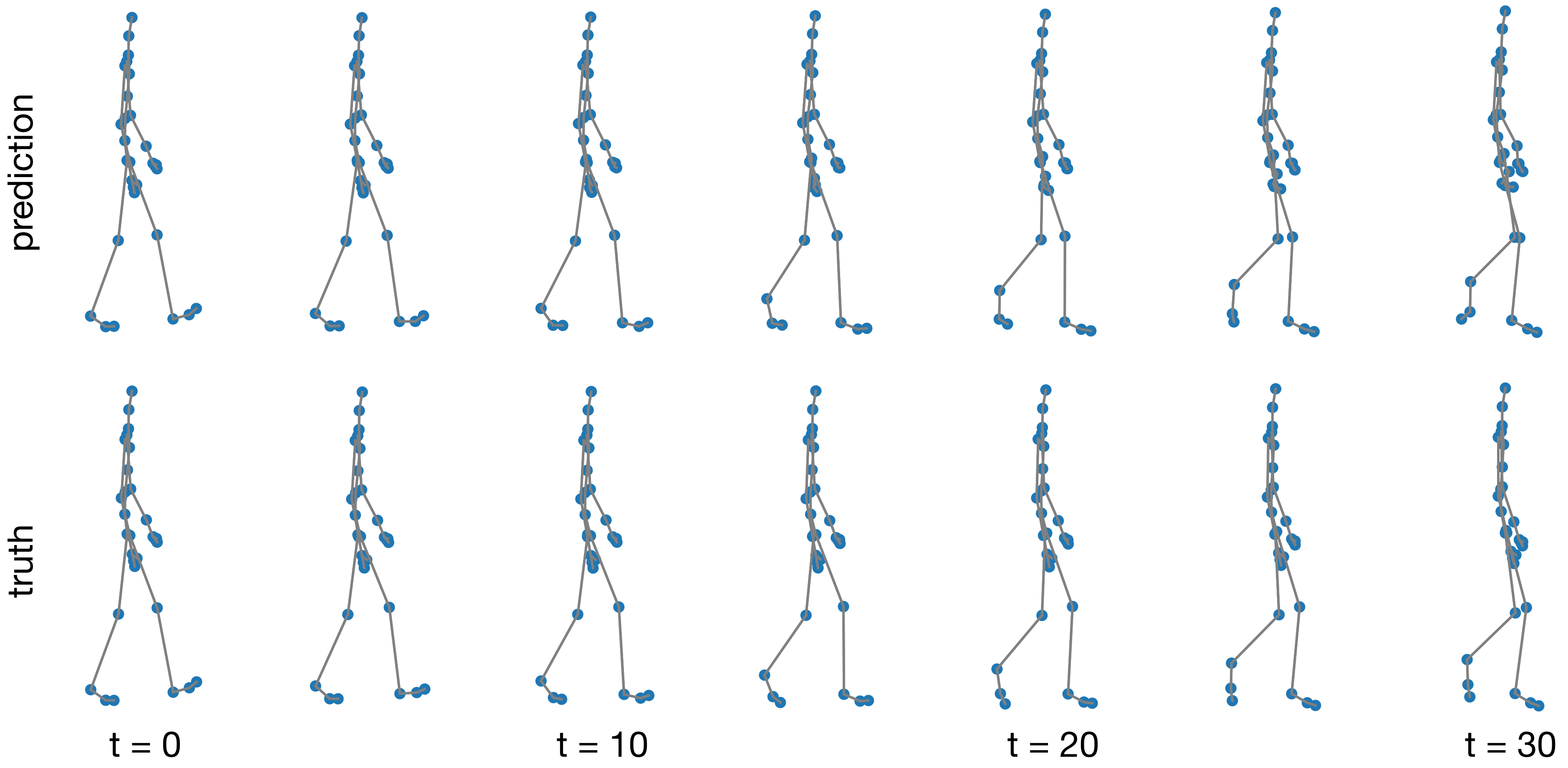
# Neural Relational Inference

Predicting the walking motion

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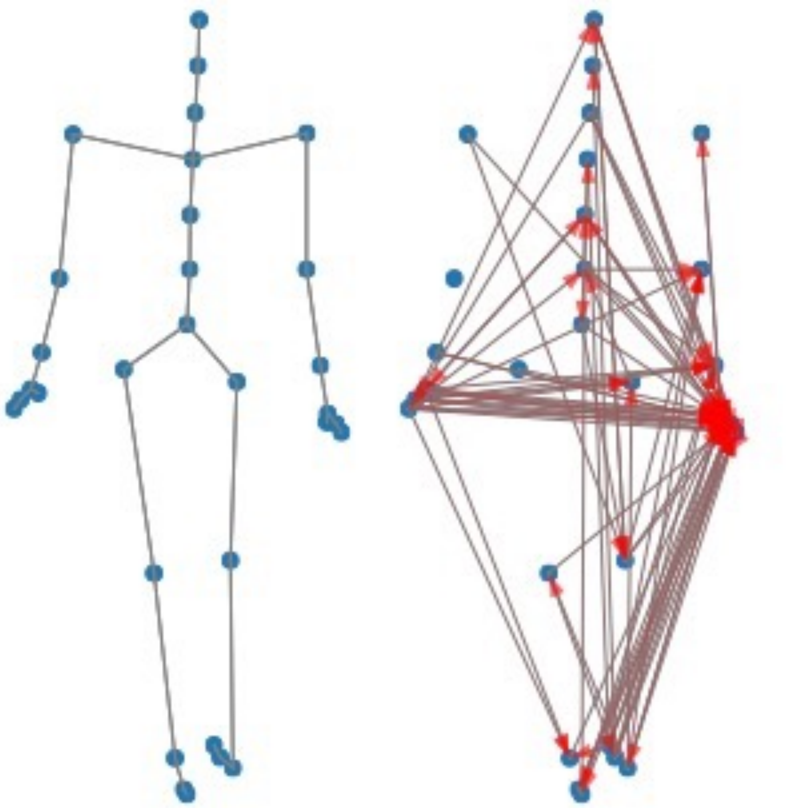
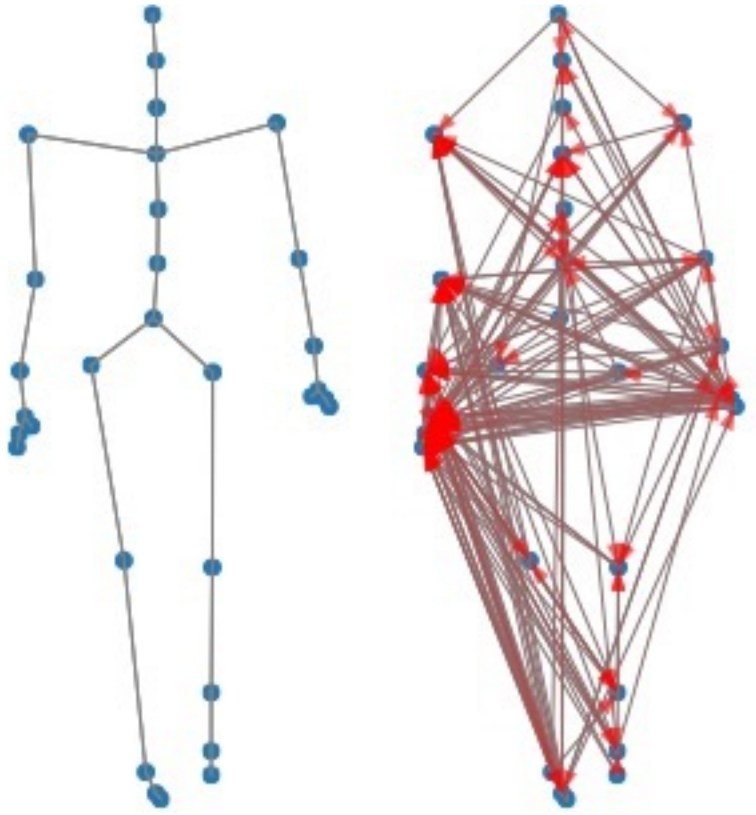
# Neural Relational Inference

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*

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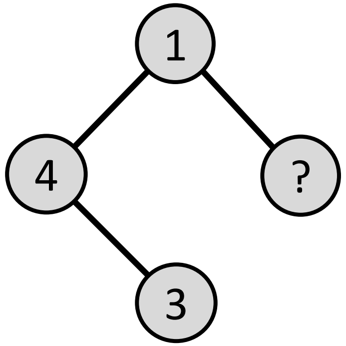
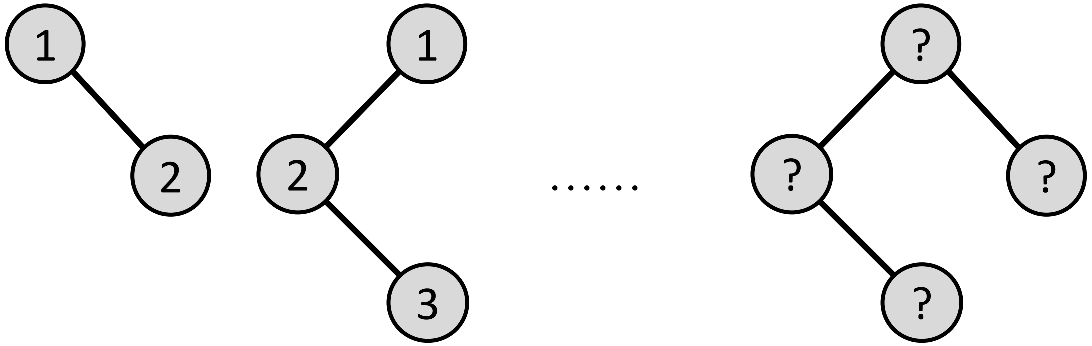



Transductive




Inductive

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

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

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Outer level/loop

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Inner level/loop

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

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This problem is a hard mixed-integer programming problem!

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

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

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

We can unroll SGD for a few steps!

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

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

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The bi-level optimization is simplified as

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

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

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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

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

# Learning Discrete Structures for GNNs

The (hyper) gradient is

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

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A is discrete samples drawn from edge-independent Bernoulli distribution

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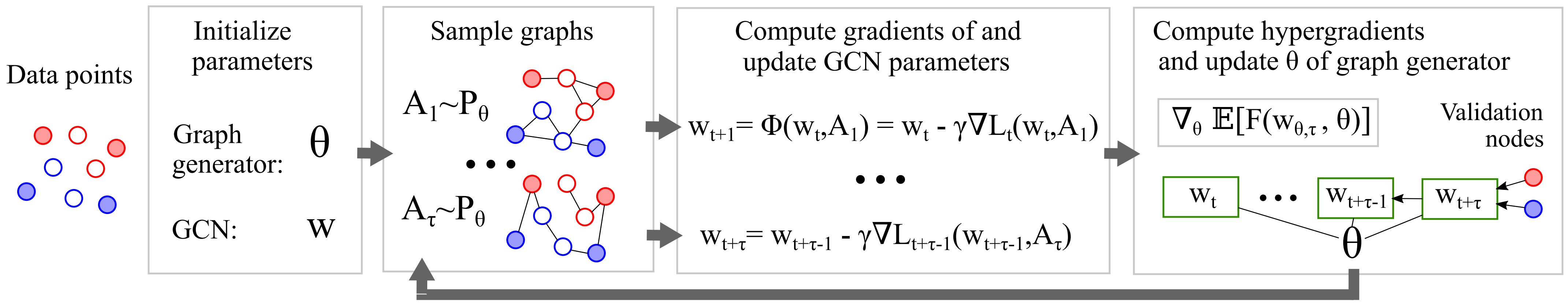

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Transductive Classification:

| | 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) |
| $k$NN-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)** |
| $k$NN-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)** |
| $k$NN-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

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[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.

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Questions?