EECE 571F: Deep Learning with Structures

Lecture 6: Autoregressive Models II (Graphs)

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University of British Columbia

Winter, Term 1, 2023

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: Message Passing & Graph Convolution GNNs
  - Group Equivariant Deep Learning

- Probabilistic Deep Learning

  - Auto-regressive models, Large Language Models (LLMs)
  - Variational Auto-Encoders (VAEs) and Generative Adversarial Networks (GANs)
  - Energy based models (EBMs)
  - Diffusion/Score based models

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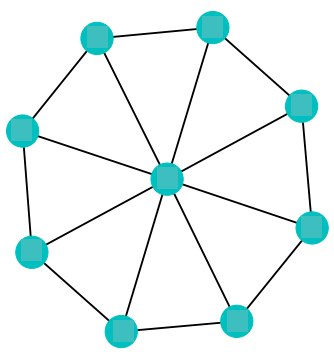
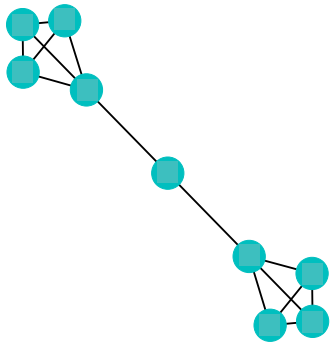
Deep Generative Models of Graphs

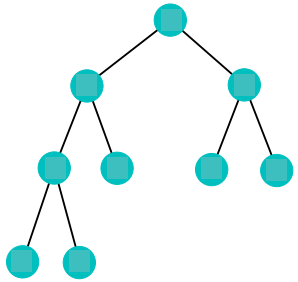
G



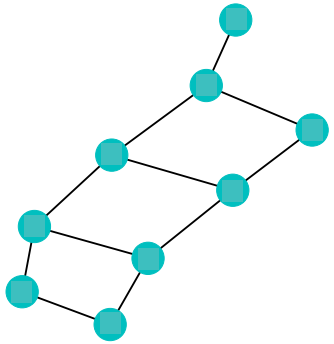
Wheel



Barbell



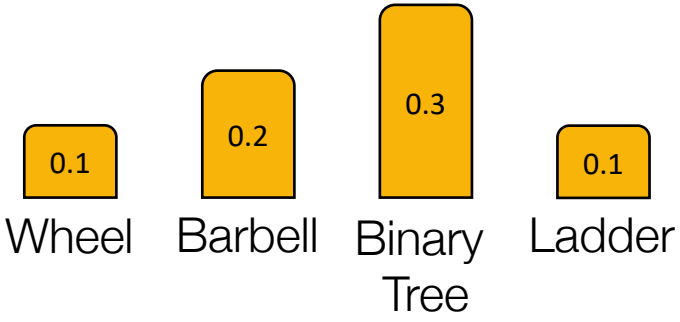
Binary Tree



Ladder

.....

$P(G)$



.....

$G \sim P(G)$

Applications

Drug discovery, e.g. molecules [1]

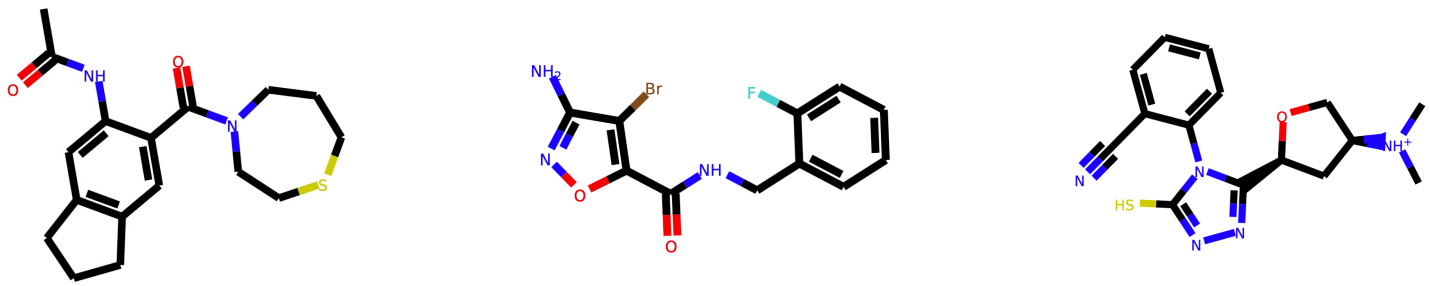


Image Credit: [1]

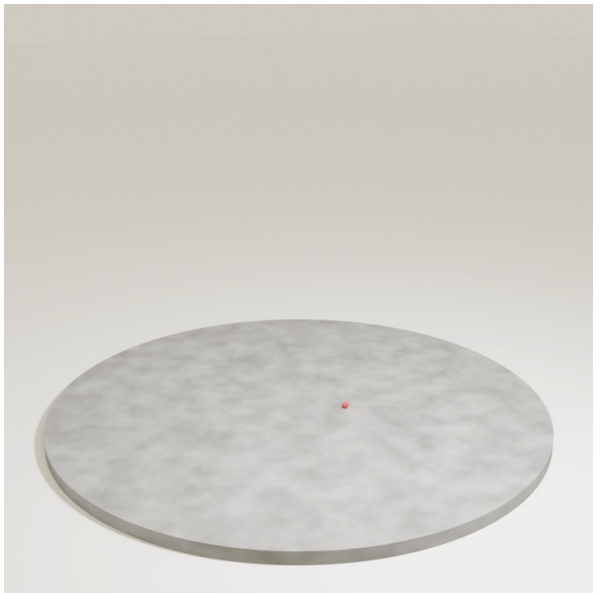
Applications

Urban planning, e.g. road layout [2]

Image Credit: [2]

Applications

Graphics, e.g., 3D objects [3]



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Autoregressive Models for Graphs

Let us start with an intuitive generation process:

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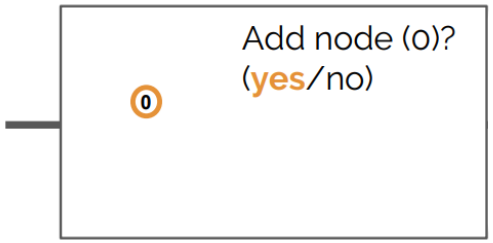

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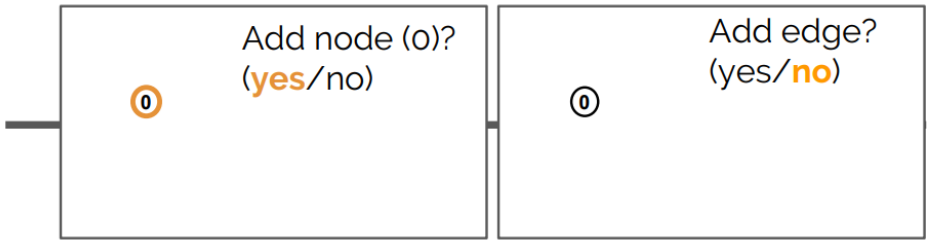

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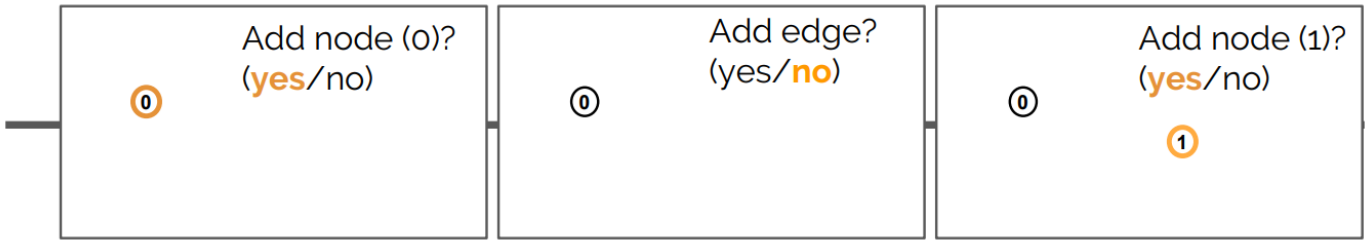

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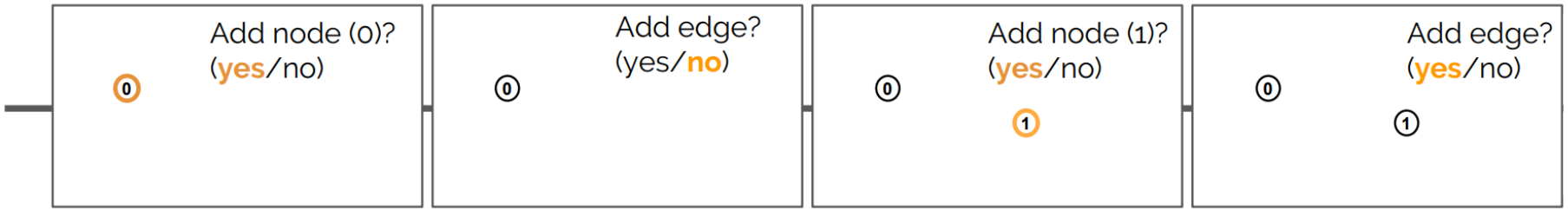

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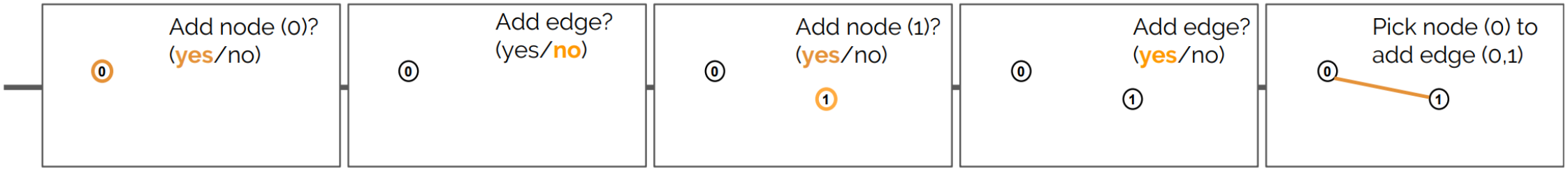

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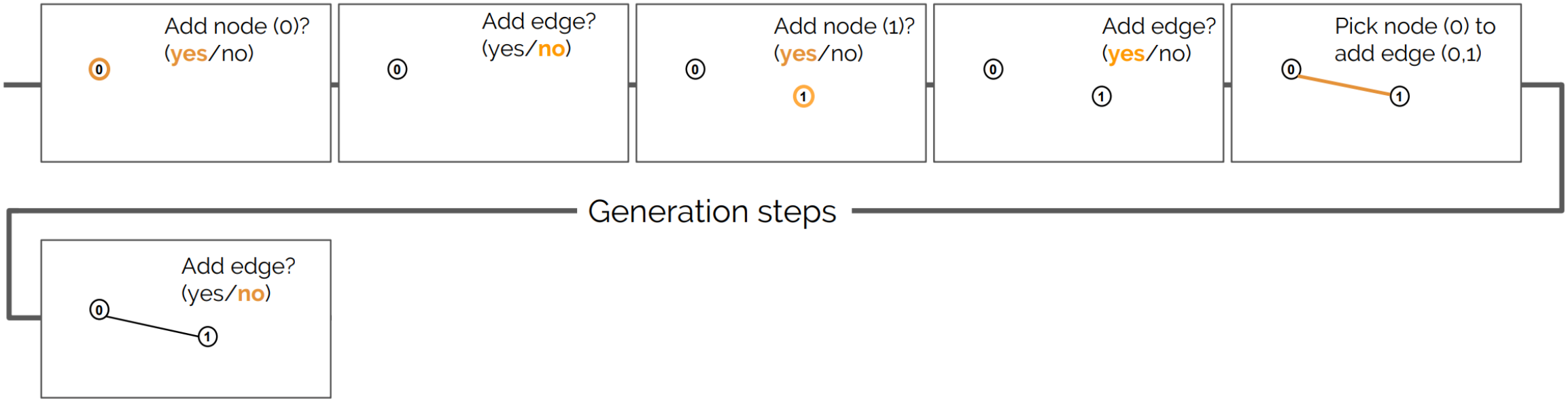

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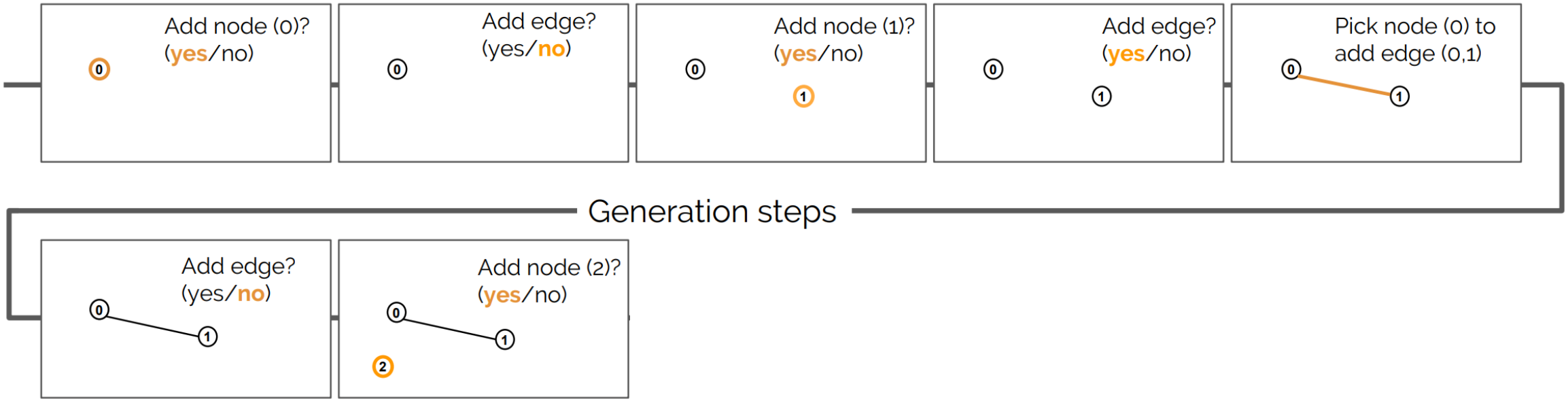

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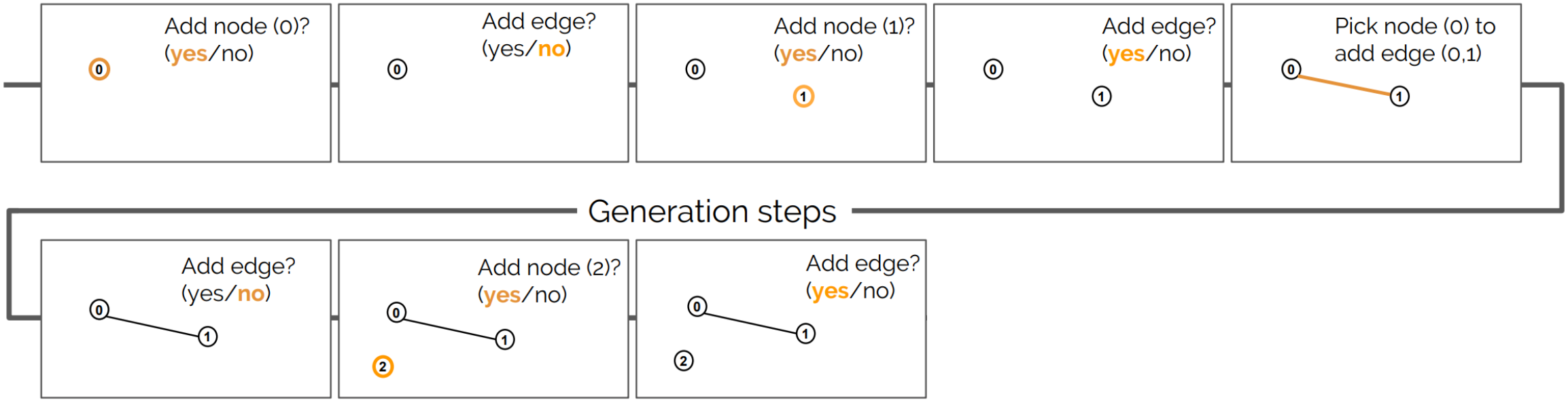

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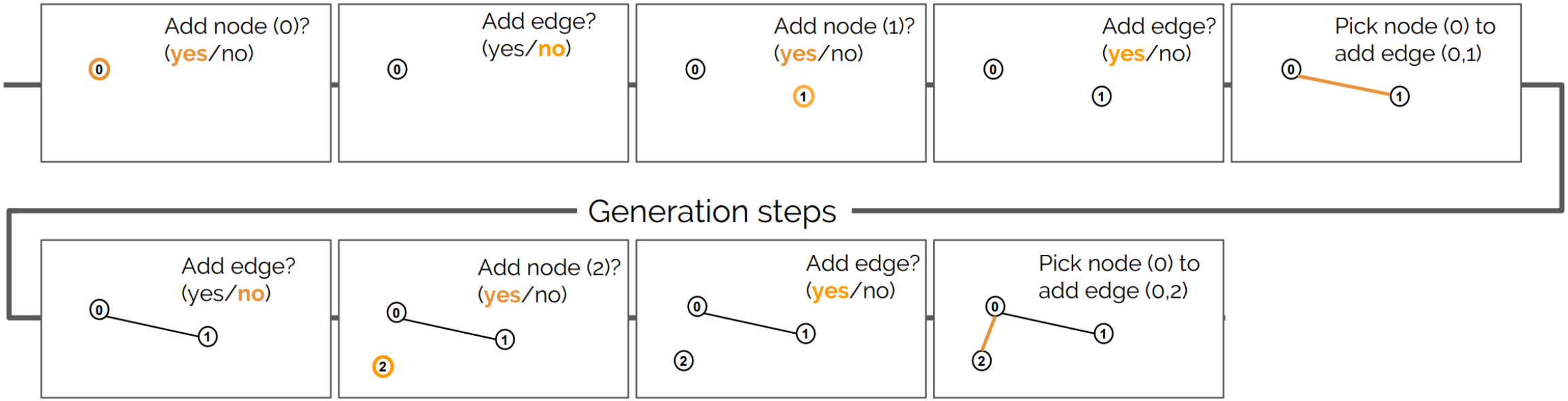

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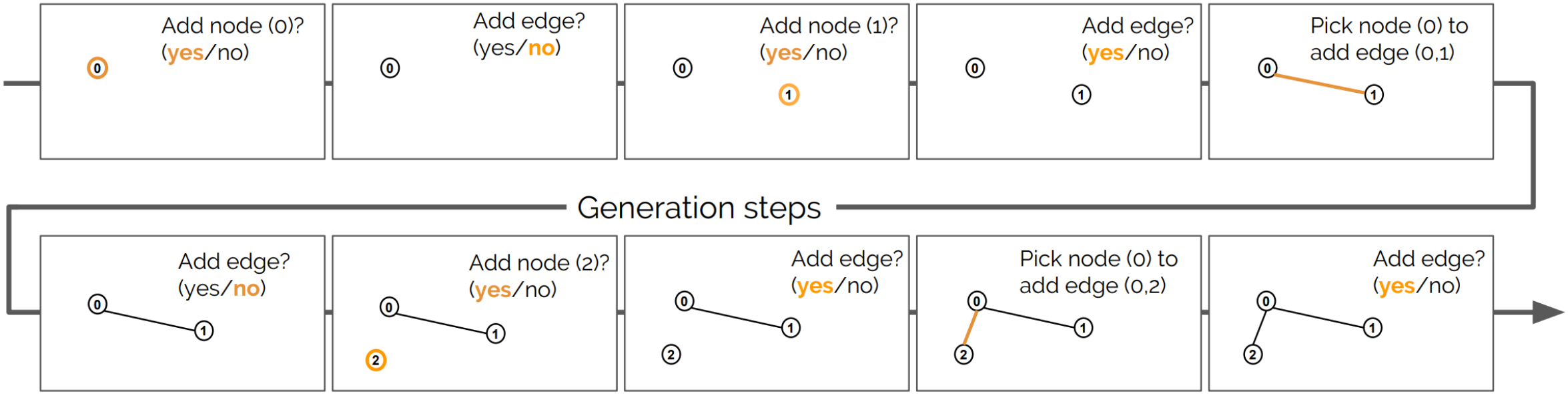

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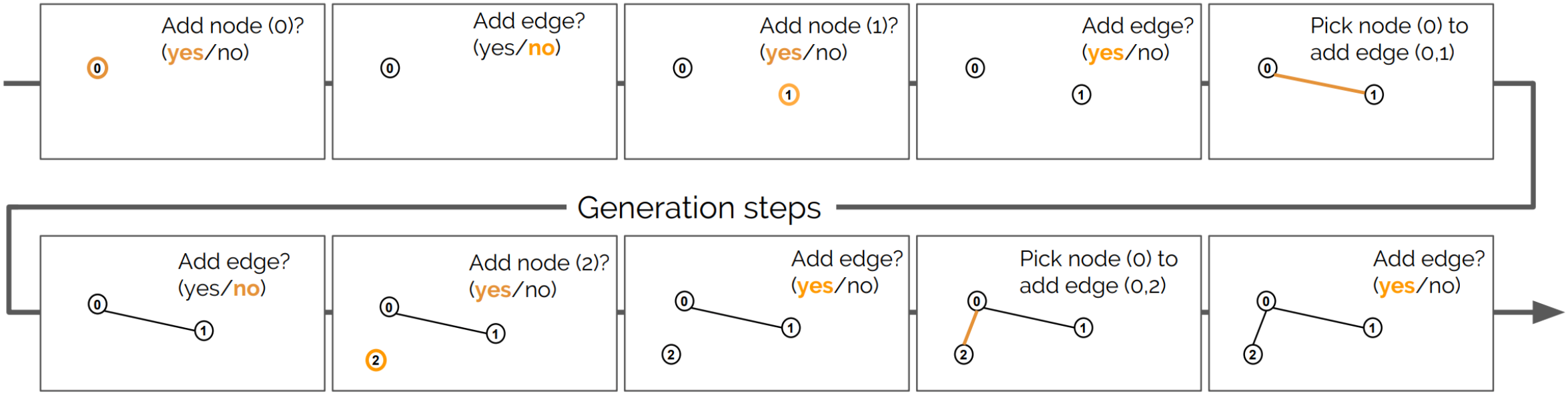

- *Graph Generation = Sequential Decision Making!*

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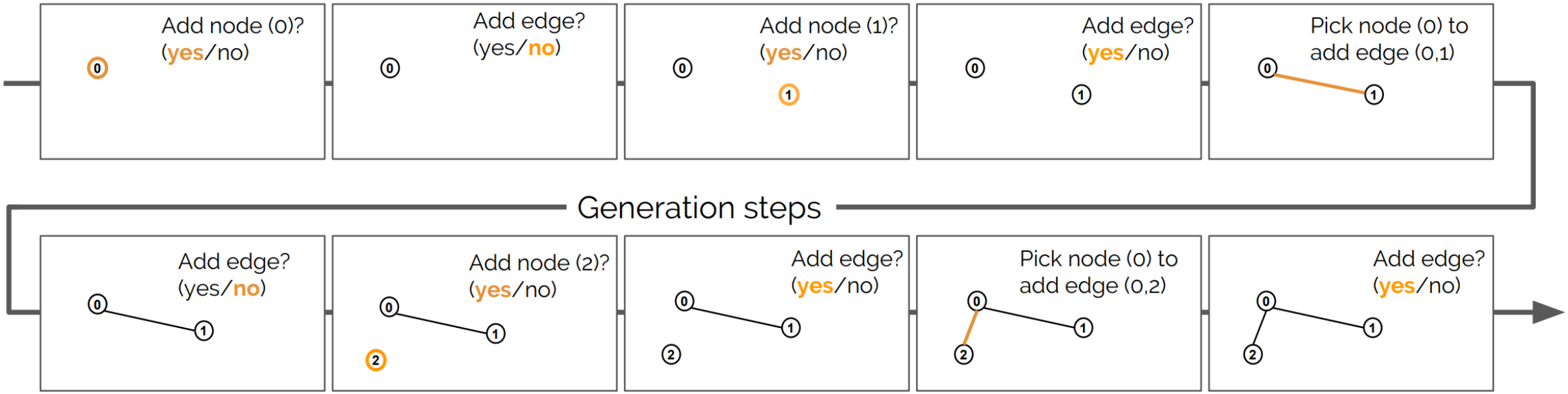

- *Graph Generation = Sequential Decision Making!*
- *We can sequentially generate a graph conditioning on the previously generated (sub)graph!*

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Autoregressive Models for Graphs

GNN-RNN-based Autoregressive Model [4]

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GNN-RNN-based Autoregressive Model [4]

At each step, decisions are:

- Add Node: *stop or +1 node*
- Add Edge: *stop or +1 edge*
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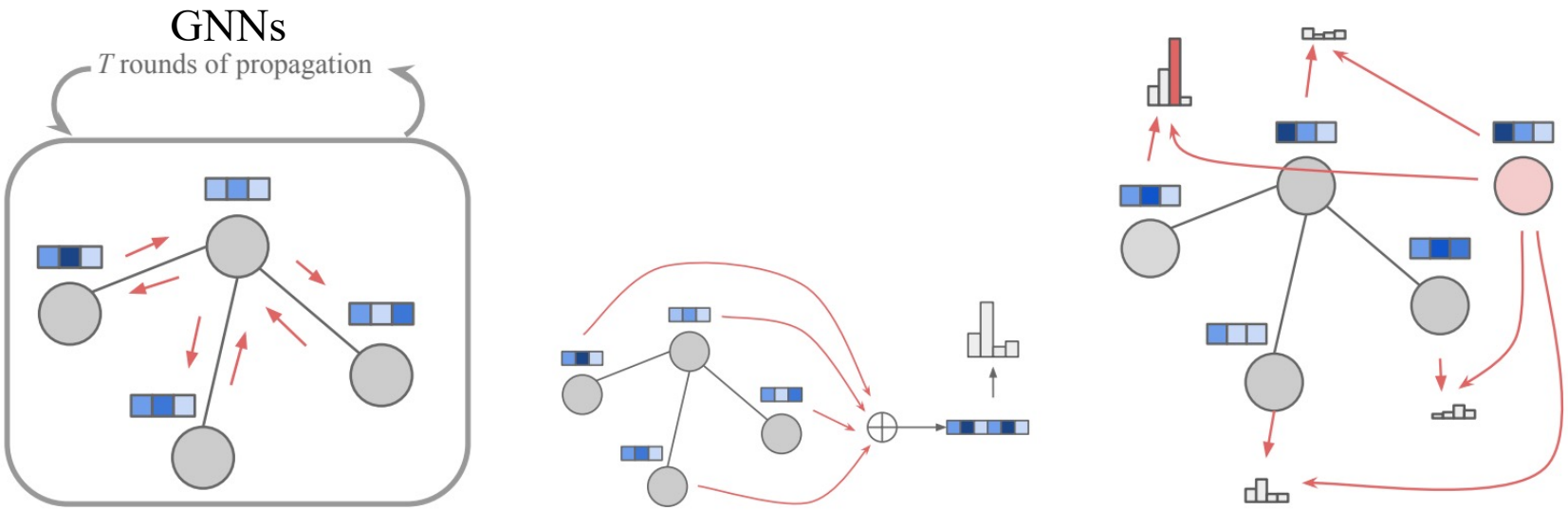

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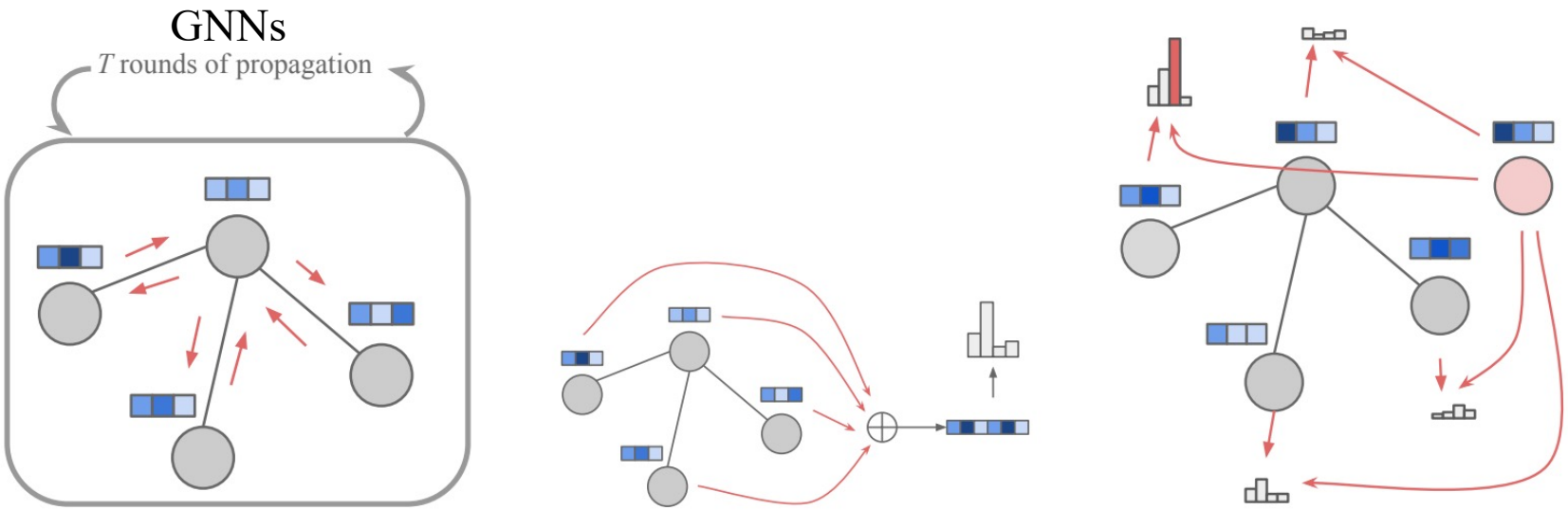
$$\mathbf{h}_V^{(T)} = \text{prop}^{(T)}(\mathbf{h}_V, G)$$
$$\mathbf{h}_G = R(\mathbf{h}_V^{(T)}, G)$$
$$f_{addnode}(G) = \text{softmax}(f_{an}(\mathbf{h}_G))$$
$$f_{addedge}(G, v) = \sigma(f_{ae}(\mathbf{h}_G, \mathbf{h}_v^{(T)}))$$
$$s_u = f_s(\mathbf{h}_u^{(T)}, \mathbf{h}_v^{(T)}), \quad \forall u \in V$$
$$f_{nodes}(G, v) = \text{softmax}(\mathbf{s})$$



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Recurrent Neural Network

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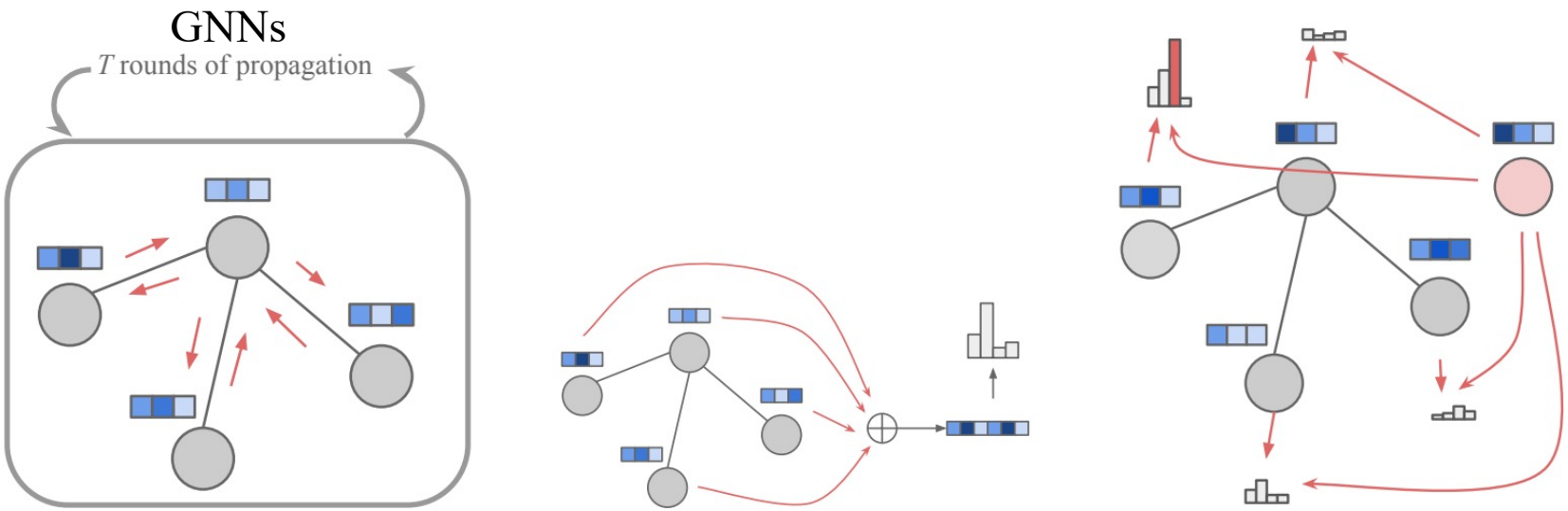

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Learning via Back Propagation Through Time (BPTT)

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Pros:

- Autoregressive models can capture the dependencies among nodes/edges
- Enable the usage of GNNs and RNNs for graph generation

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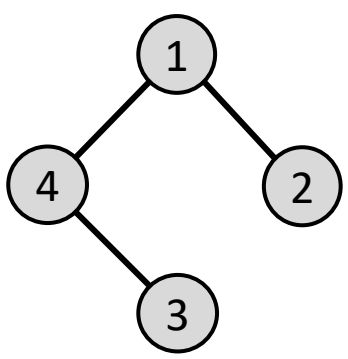
- Enable the usage of GNNs and RNNs for graph generation

Cons:

- The likelihood is permutation-dependent
- Generating a medium-sized graph requires a lot of generation/unrolling steps
- Learning long-unrolled RNNs with BPTT is hard

Autoregressive Models for Graphs

RNN-based Autoregressive Model, GraphRNN [5]

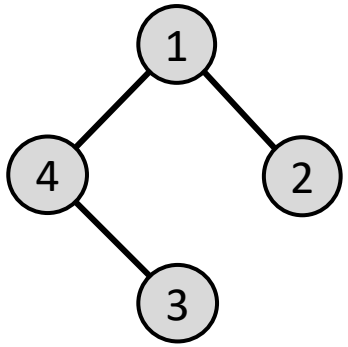


	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

Autoregressive Models for Graphs

RNN-based Autoregressive Model, GraphRNN [5]

$$S_i^\pi = (A_{1,i}^\pi, ..., A_{i-1,i}^\pi)^T, \forall i \in \{2, ..., n\}$$



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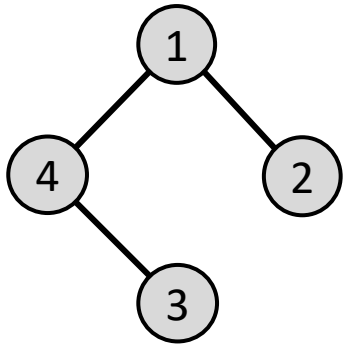

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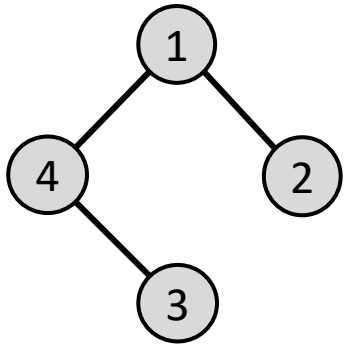

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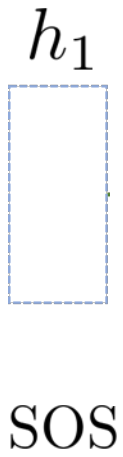

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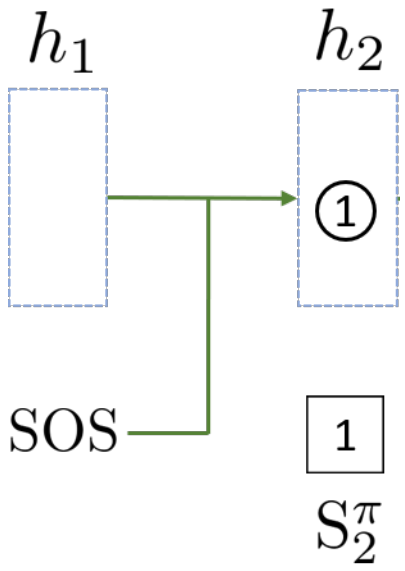

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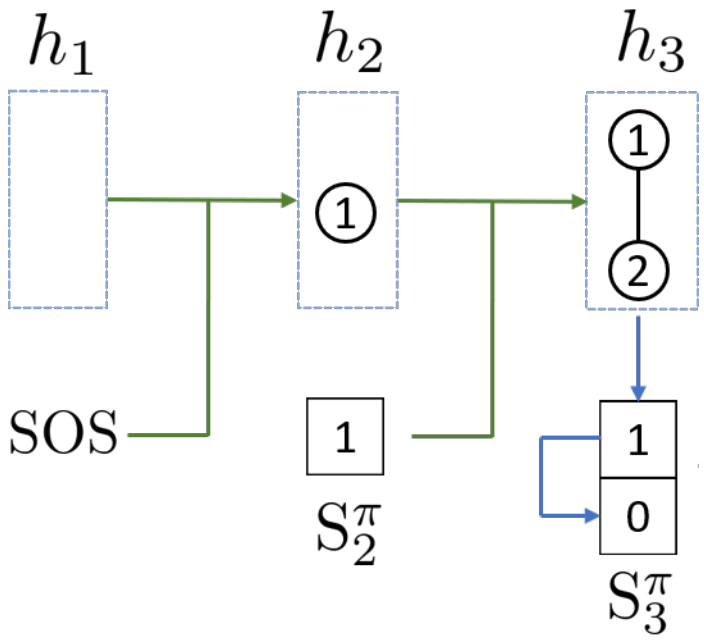

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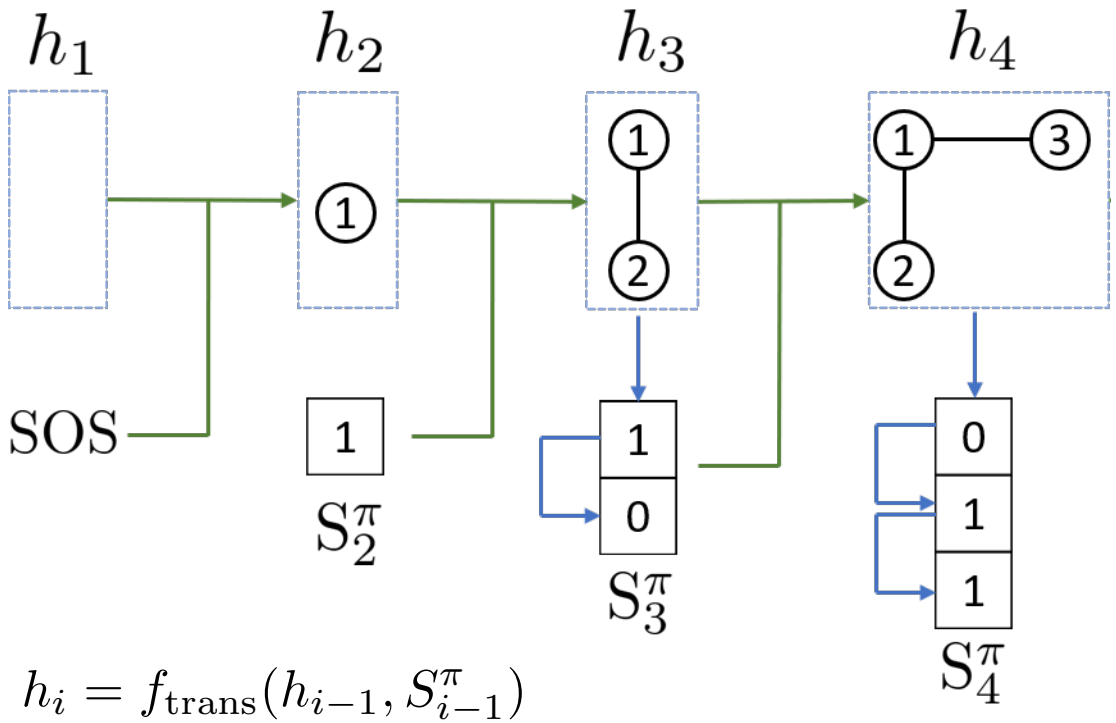

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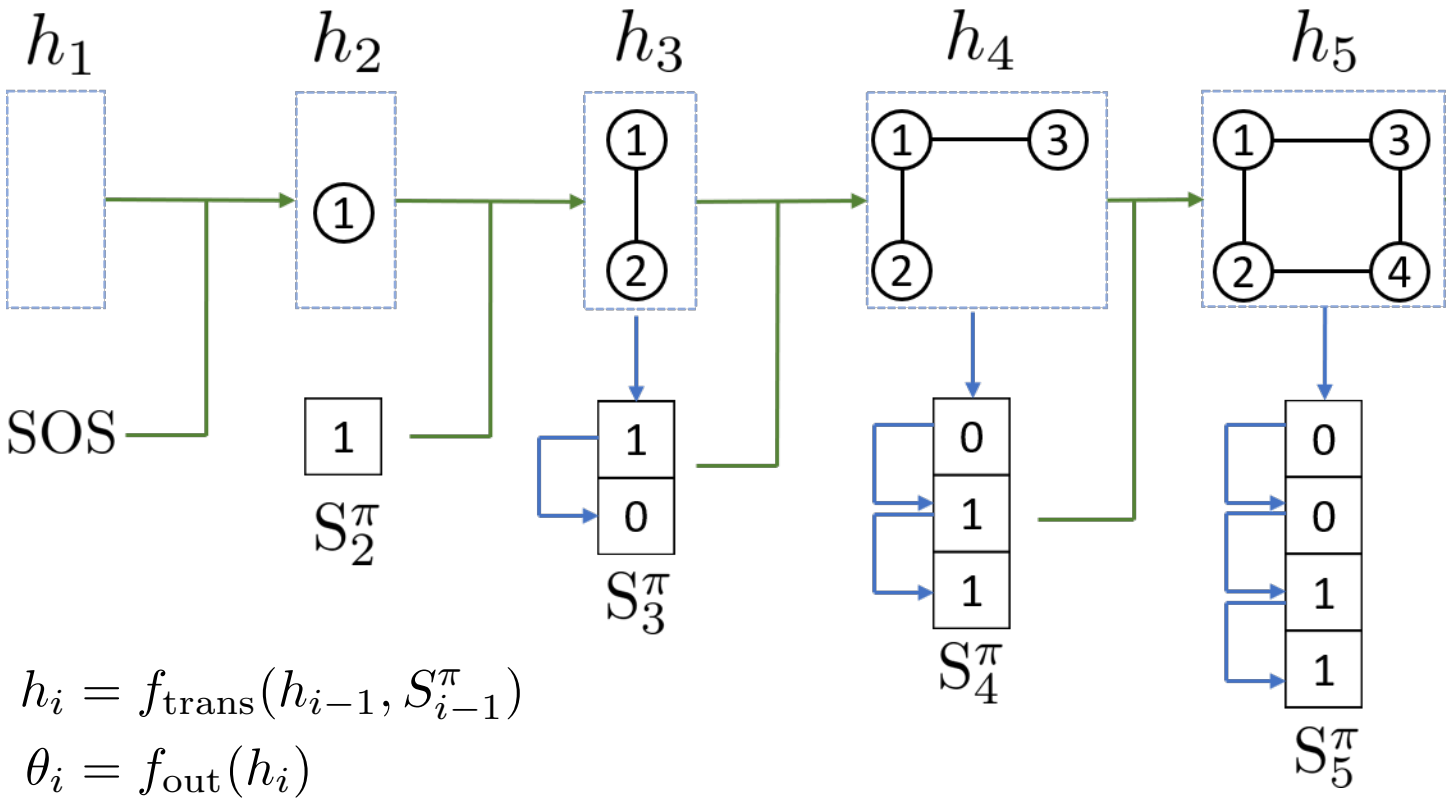

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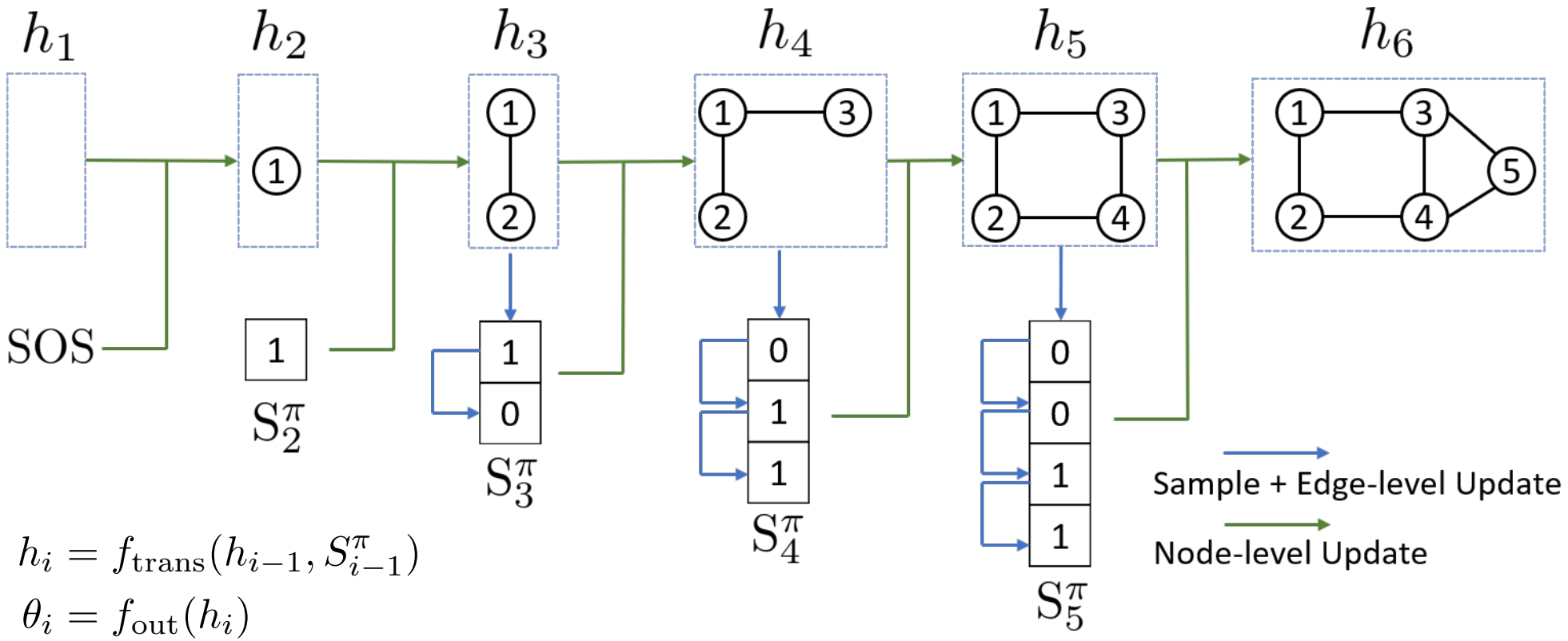

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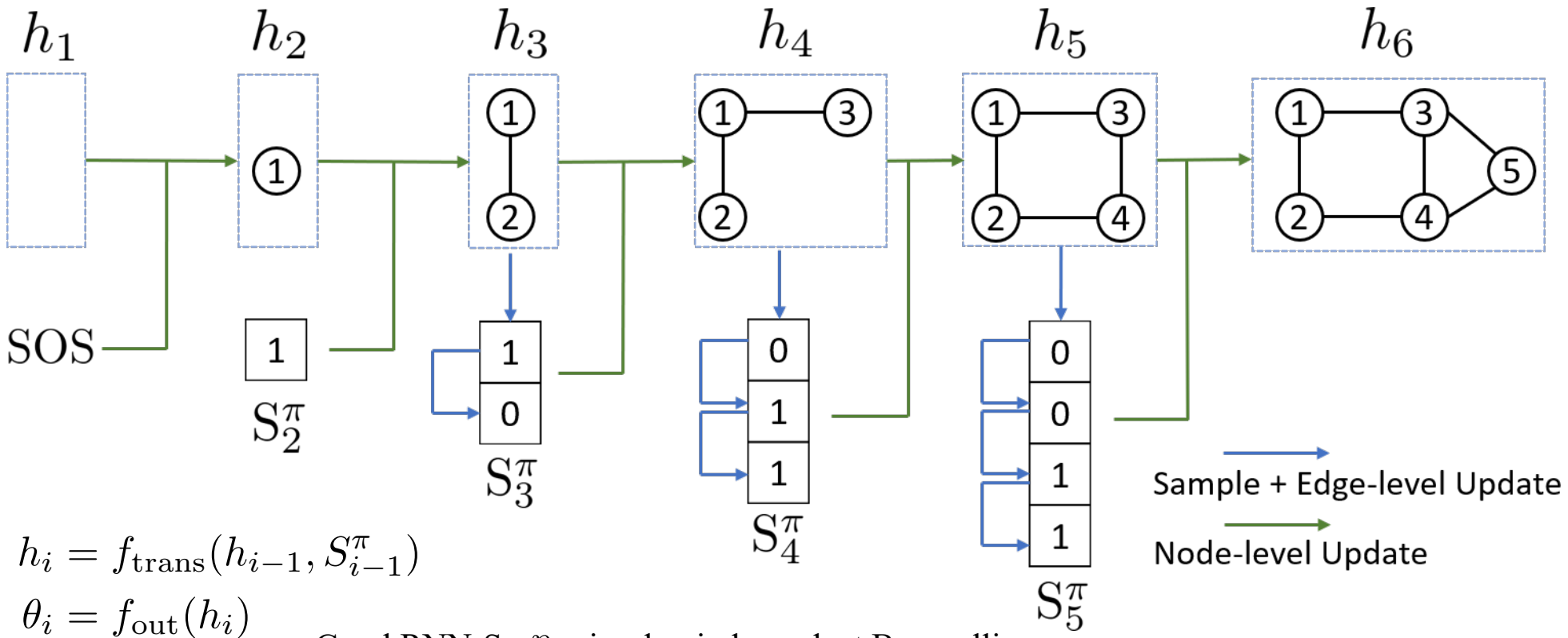

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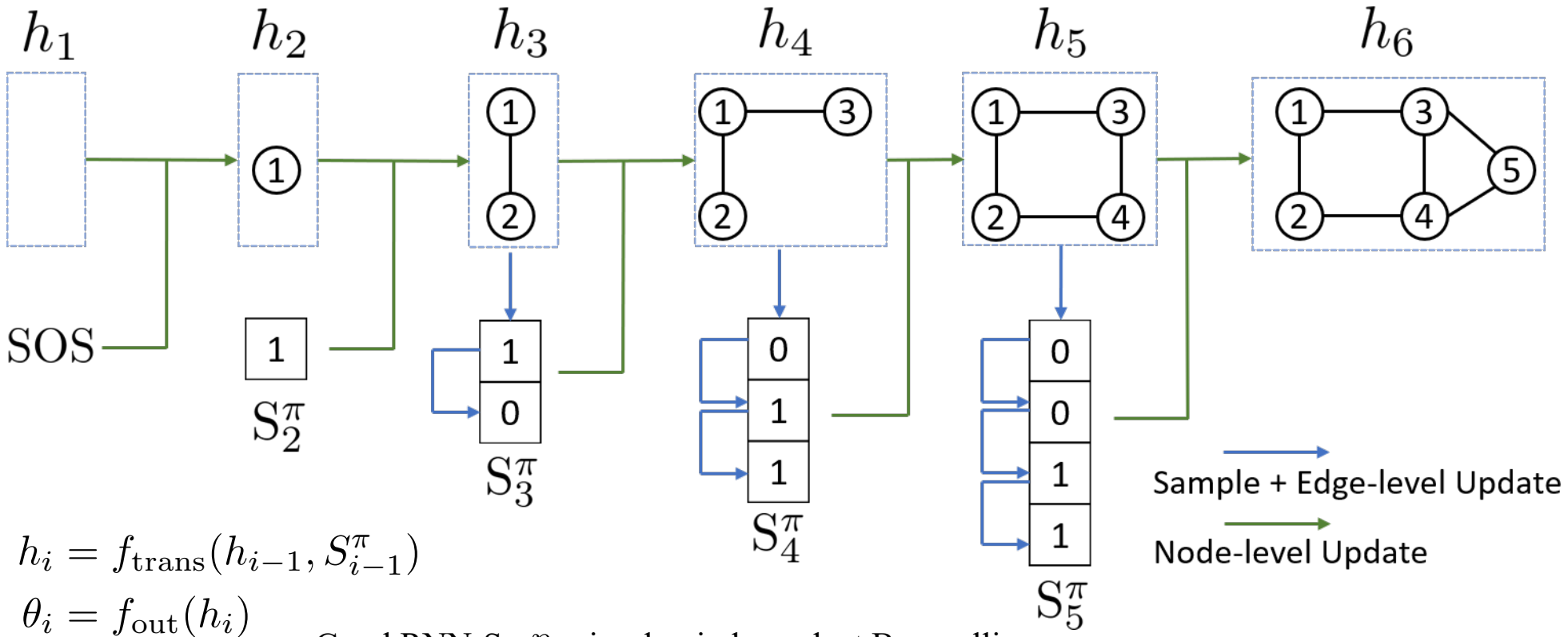

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GraphRNN-S: p_{θ_i} is edge-independent Bernoulli

GraphRNN: $p_{\theta_i}(S_i^\pi | S_{<i}^\pi) = \prod_{j=1}^{i-1} p_{\theta_i}(S_{i,j}^\pi | S_{i,<j}^\pi, S_{<i}^\pi)$

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Autoregressive Models for Graphs

RNN-based Autoregressive Model, GraphRNN [5]

$$\max_{\theta} \quad \log p_\theta(G) = \log \left(\sum_{\pi} p_\theta(G, \pi) \right)$$

$$p_\theta(G) = \sum_{\pi} p_\theta(G, \pi) = \mathbb{E}_{q(\pi|G)} \left[\frac{p_\theta(G, \pi)}{q(\pi|G)} \right]$$

$$\max_{\theta} \quad \log \left(\sum_{\pi \sim q(\pi|G)} \left[\frac{p_\theta(G, \pi)}{q(\pi|G)} \right] \right)$$

Learning via Back Propagation Through Time (BPTT)

Autoregressive Models for Graphs

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What are their relationship?

$$G, \pi, S^{\pi}$$

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BFS ordering with random starting node!

$$\max_{\theta} \quad \log \left(\sum_{\pi \sim q(\pi|G)} \left[\frac{p_\theta(G, \pi)}{q(\pi|G)} \right] \right)$$

Learning via Back Propagation Through Time (BPTT)

Autoregressive Models for Graphs

RNN-based Autoregressive Model, GraphRNN [5]

Pros:

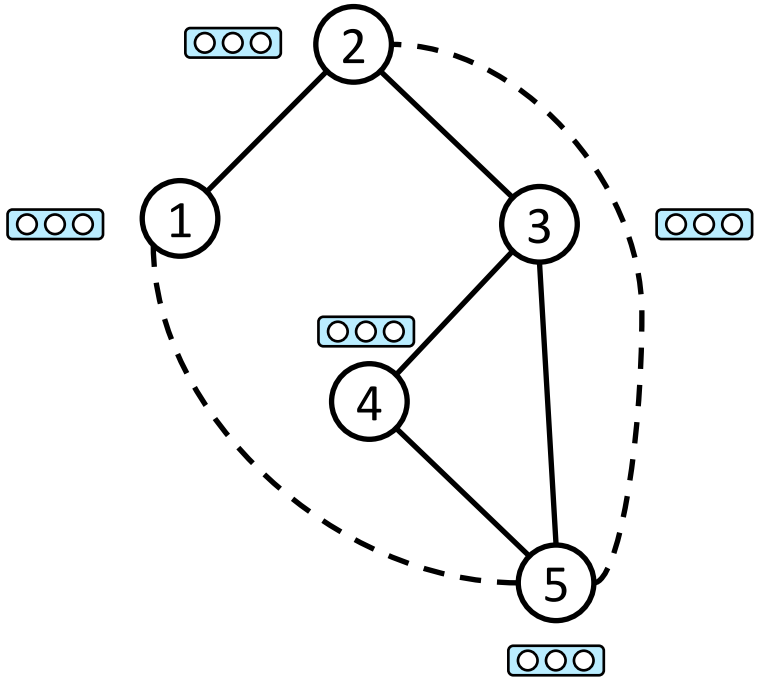
- Autoregressive models can capture the dependencies among nodes/edges
- Enable the usage of RNNs for graph generation
- It could generate one row (i.e., multiple edges) of adjacency matrix at one step

Cons:

- The likelihood is permutation-dependent
- Generating a medium-sized graph could still require many generation/unrolling steps
- Learning long-unrolled RNNs with BPTT is hard

Autoregressive Models for Graphs

GNN-based Autoregressive Model, GRAN [6]



Autoregressive Models for Graphs

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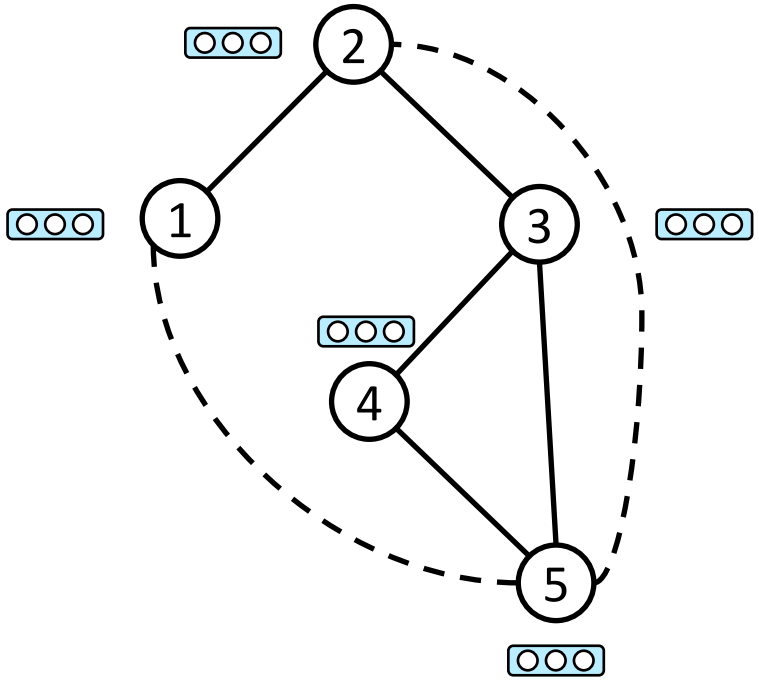

- Sequential Order Bias

  More serious in RNNs [5] than GNNs [4] (permutation invariant), e.g., 5 often links to 3,4 rather than 1,2

Autoregressive Models for Graphs

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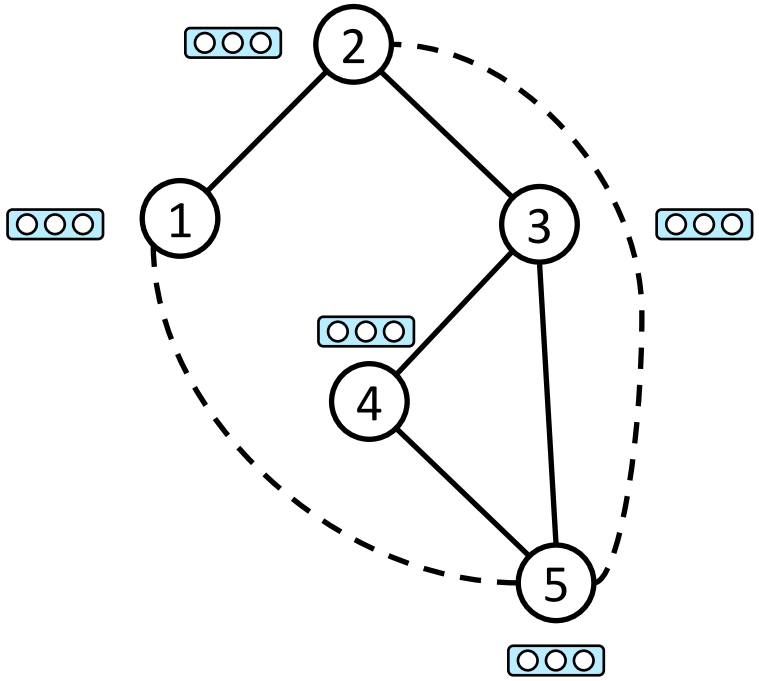


- Sequential Order Bias

  More serious in RNNs [5] than GNNs [4] (permutation invariant), e.g., 5 often links to 3,4 rather than 1,2

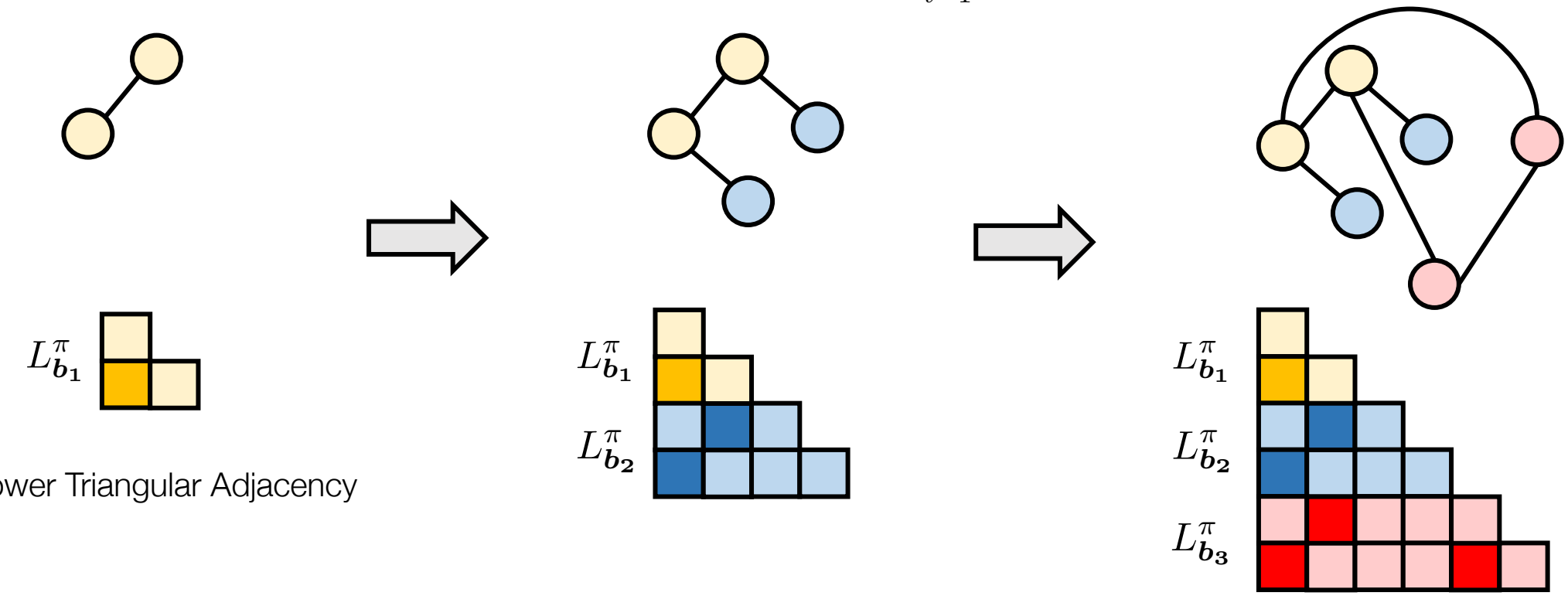
- Training Inefficiency

  Training RNNs via BPTT [4,5] is impractical for moderately large graphs (~1k)

Autoregressive Models for Graphs

GNN-based Autoregressive Model, GRAN [6]

$$p(L^{\pi}) = \prod_{t=1}^{T} p(L^{\pi}_{\boldsymbol{b_t}} | L^{\pi}_{\boldsymbol{b_1}}, \cdots, L^{\pi}_{\boldsymbol{b_{t-1}}})$$

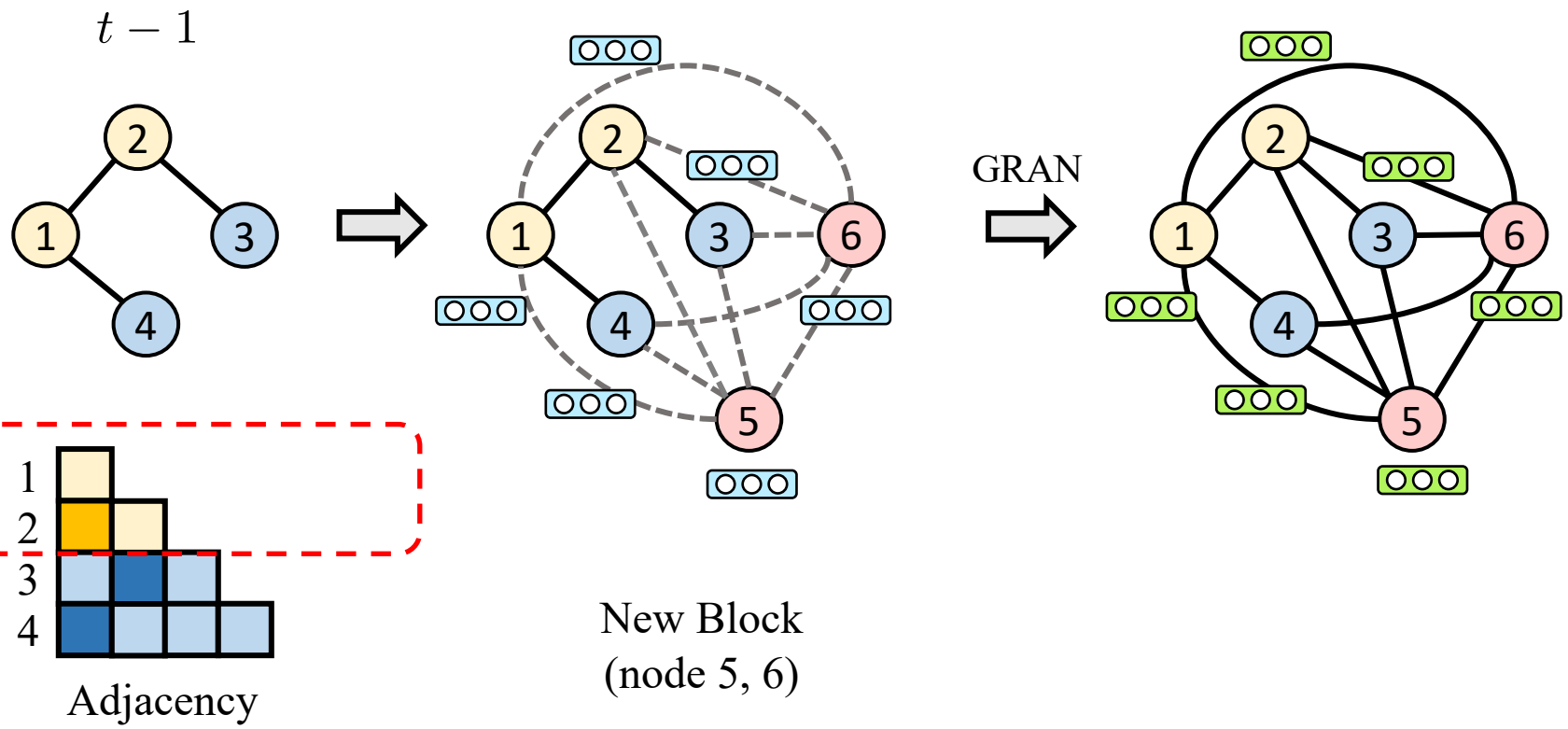


Lower Triangular Adjacency

- Sequential Order Bias — Graph Neural Network + Attention!
- Training Inefficiency — Block Generation + Parallel Training!

Autoregressive Models for Graphs

GNN-based Autoregressive Model, GRAN [6]



$$m_{ij}^t = f(h_i^t - h_j^t)$$
$$\tilde{h}_i^t = [h_i^t, x_i]$$
$$a_{ij}^t = \text{Sigmoid}\left(g(\tilde{h}_i^t - \tilde{h}_j^t)\right)$$
$$h_i^{t+1} = \text{GRU}(h_i^t, \sum_{j \in \mathcal{N}(i)} a_{ij}^t m_{ij}^t)$$

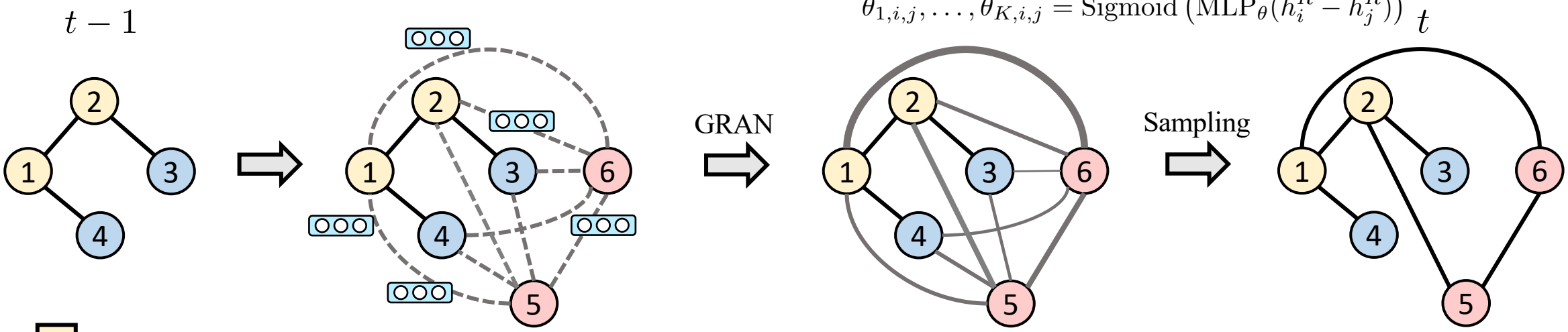
Autoregressive Models for Graphs

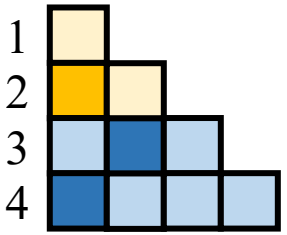
GNN-based Autoregressive Model, GRAN [6]

$$p(L_{\boldsymbol{b_t}}^{\pi}|L_{\boldsymbol{b_1}}^{\pi},...,L_{\boldsymbol{b_{t-1}}}^{\pi}) = \sum_{k=1}^{K} \alpha_k \prod_{i \in \boldsymbol{b_t}} \prod_{1 \le j \le i} \theta_{k,i,j},$$

$$\alpha_1, \ldots, \alpha_K = \text{Softmax}\left(\sum\nolimits_{i \in \boldsymbol{b_t}, 1 \le j \le i} \text{MLP}_{\alpha}(h_i^R - h_j^R)\right),$$

$$\theta_{1,i,j}, \ldots, \theta_{K,i,j} = \text{Sigmoid}\left(\text{MLP}_{\theta}(h_i^R - h_j^R)\right)$$

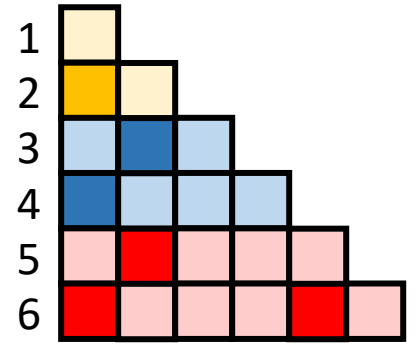




Adjacency

New Block
(node 5, 6)

Distribution over ***dashed edges***



Parallel Subgraph Training!

Autoregressive Models for Graphs

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Parallel Subgraph Learning via Back Propagation. No BPTT !

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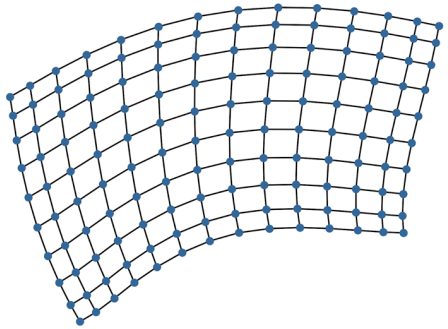
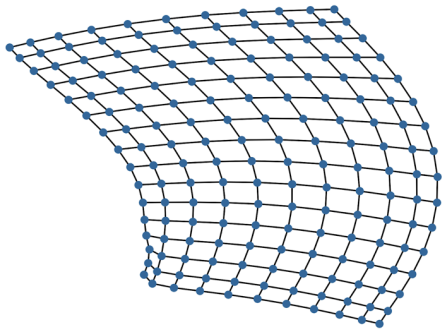
- BFS ordering starting from the largest degree node
- DFS ordering starting from the largest degree node
- K-core descending ordering
- Node degree ascending ordering
- Node degree descending ordering

Parallel Subgraph Learning via Back Propagation. No BPTT !

Random Grid Graphs

Train



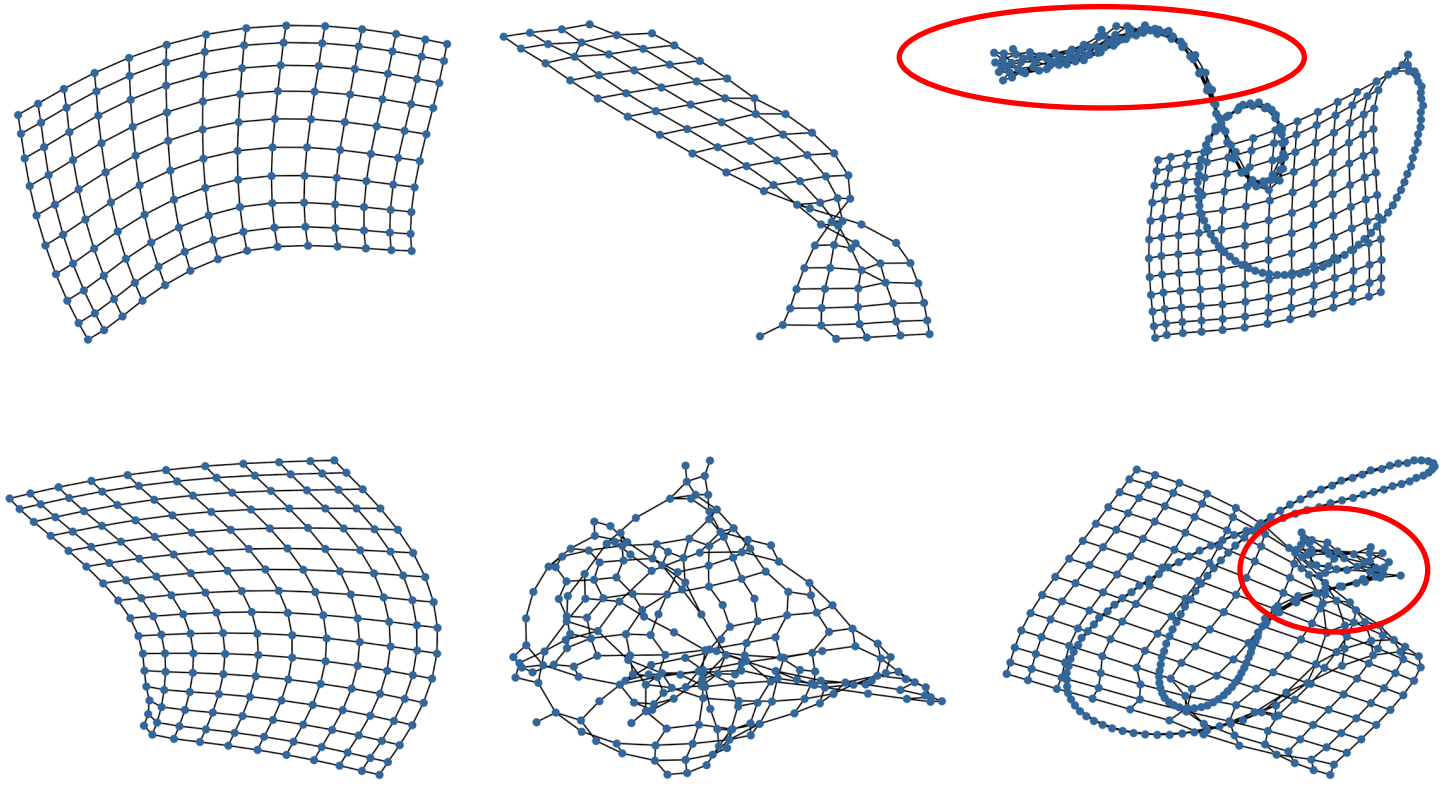


Random Grid Graphs

Train

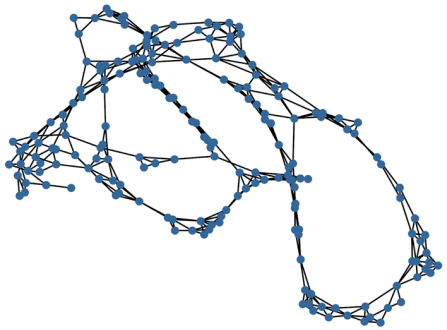
Graph VAE

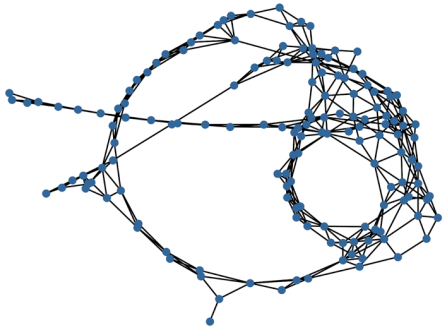
Graph RNN



Protein Graphs

Train





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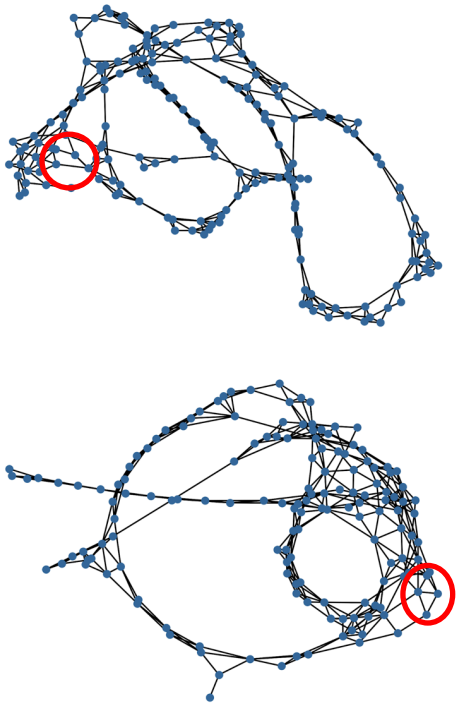
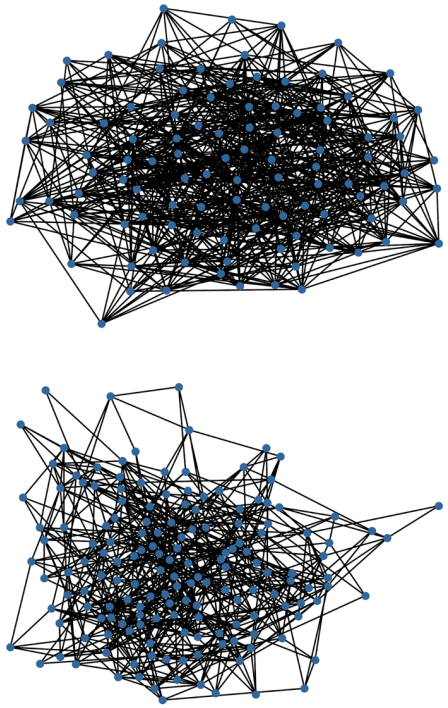
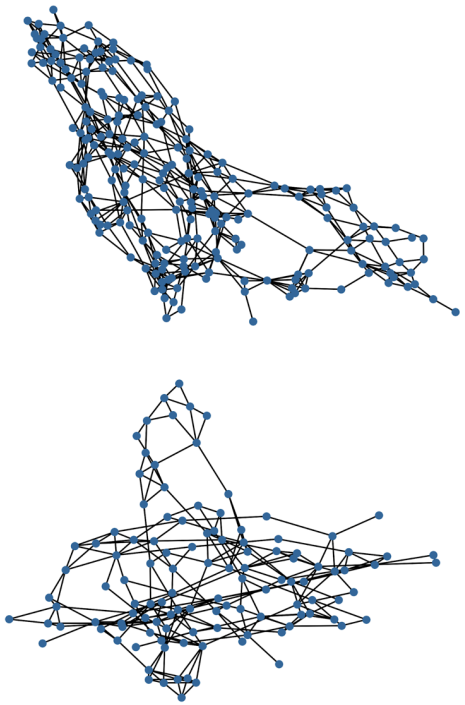


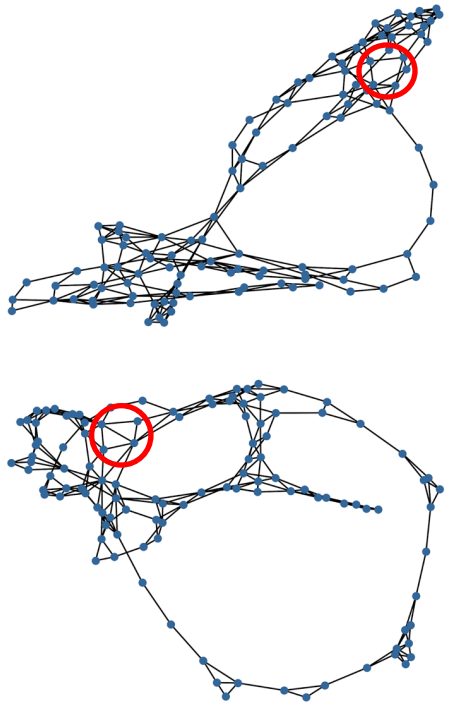
Graph VAE



Graph RNN



Ours



Protein Graphs

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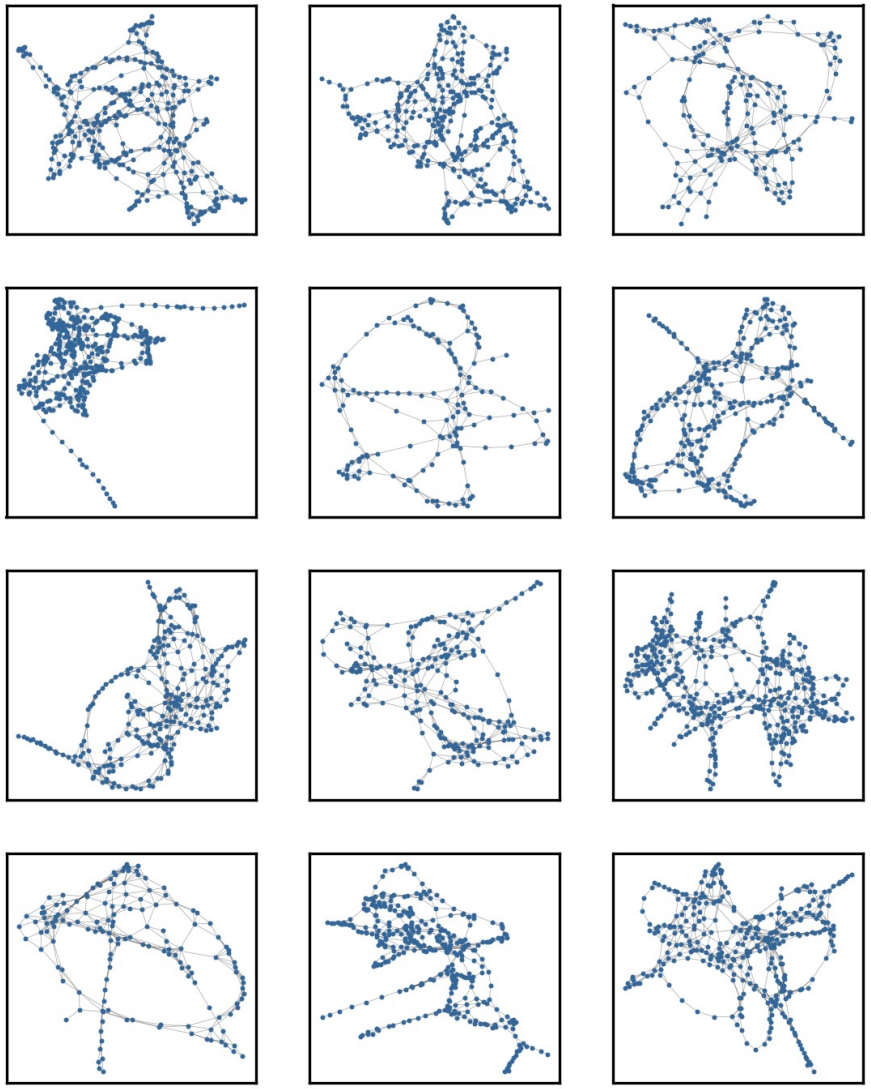

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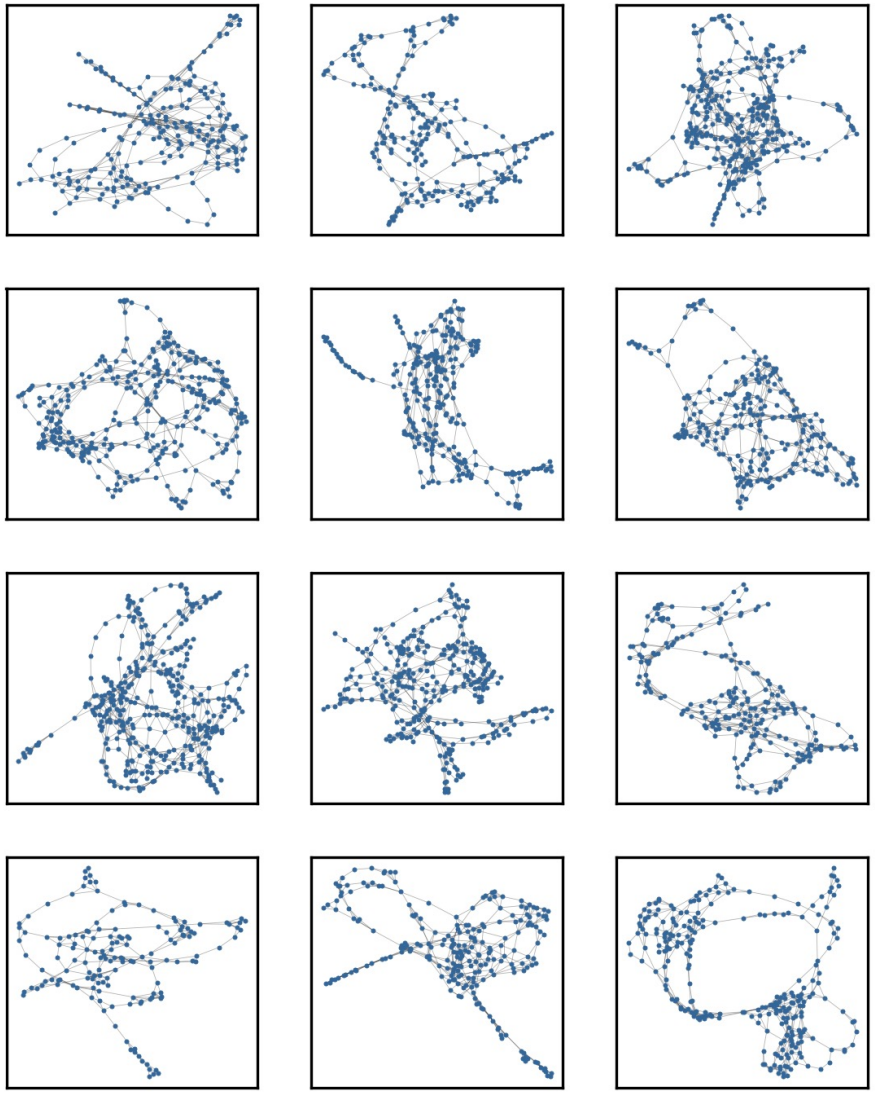
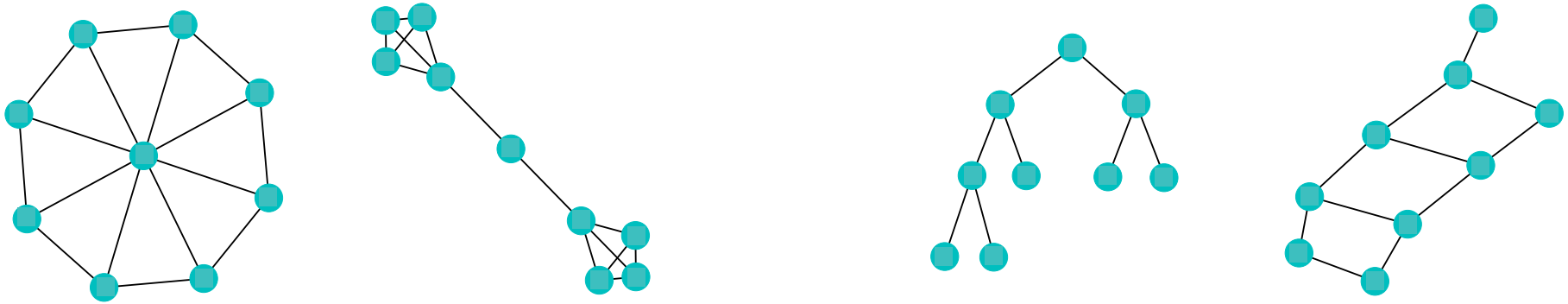


Quantitative Evaluation



Observation

Generation

Maximum Mean Discrepancy (MMD) between two distributions of graph statistics

$$\text{MMD}(P, Q) = \sup_{f \in \mathcal{F}} \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{Y \sim Q}[f(Y)]$$

- Degree distribution
- Clustering Coefficients
- # 4-node orbits
- Spectrum

Protein Graphs

train/dev/test graphs = 734/183/184
Max: # nodes = 500, # edges = 1575
Mean: # nodes = 258, # edges = 646

Models	Degree	Clustering Coeff.	Orbits	Spectrum
Erdős-Rényi	0.0564	1.00	1.54	0.0913
GraphVAE	0.480	0.0714	0.740	0.110
GraphRNN-S	0.0402	**0.0479**	0.230	0.210
GraphRNN	0.0106	0.140	0.880	0.0188
Ours	**0.00198**	0.0486	**0.130**	**0.00513**

*For all metrics, the lower the better

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Questions?