Beyond Prediction: Graph Generative Models

Jiaxuan You

Assistant Professor at UIUC CDS

CS598: Deep Learning with Graphs, 2024 Fall

https://ulab-uiuc.github.io/CS598/

Recap: KG Reasoning with Box Embedding

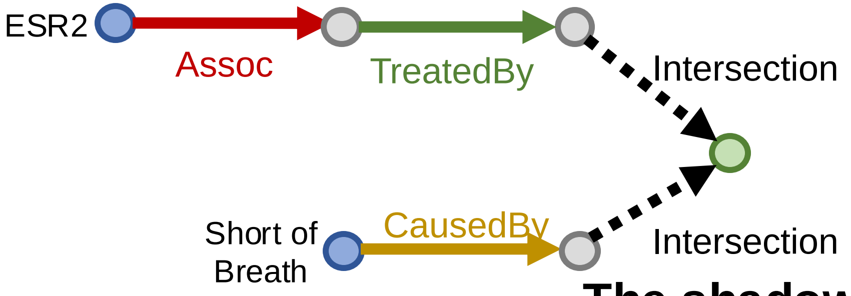
"What is the drug that causes Short of Breath and treats disease associated with protein ESR2?"

((e:ESR2, (r:Assoc, r:TreatedBy)), (e:Short of Breath, (r:CausedBy))

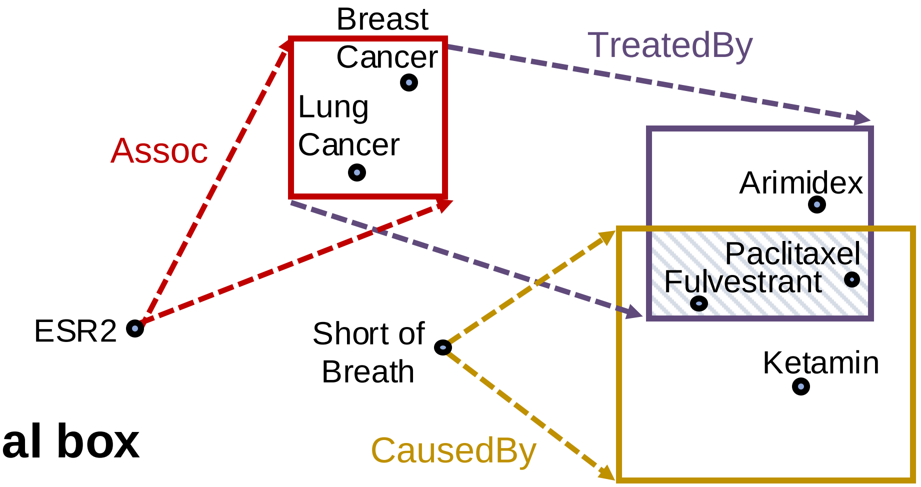
- **Use box intersection operator**

Query Plan

Embedding Space



The shadow box represents the final box embedding of the query



Motivation for Graph Generation

- So far, we have been **learning from graphs**
  - We assume the graphs are given

Image credit: Medium

Social Networks

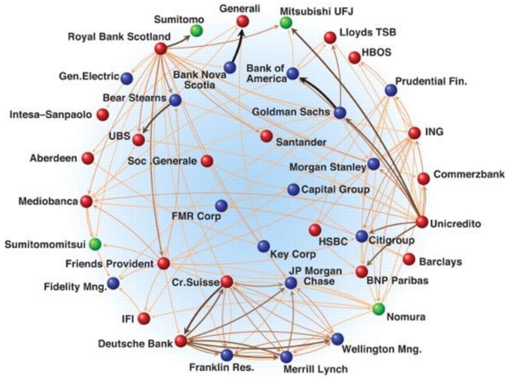


Image credit: Science

Economic Networks

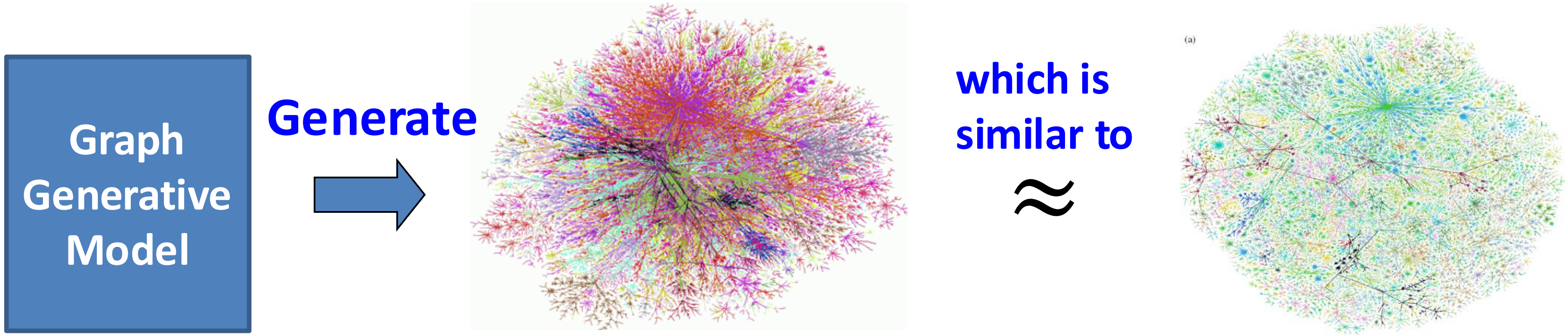
Image credit: Lumen Learning

Communication Networks

- **But how are these graphs generated?**

The Problem: Graph Generation

- We want to generate realistic graphs, using **graph generative models**



Graph Generative Model

Generate

which is similar to ≈

Synthetic graph

Real graph

- **Applications:**
  - **Drug discovery, material design**
  - **Social network modeling**

Why Do We Study Graph Generation

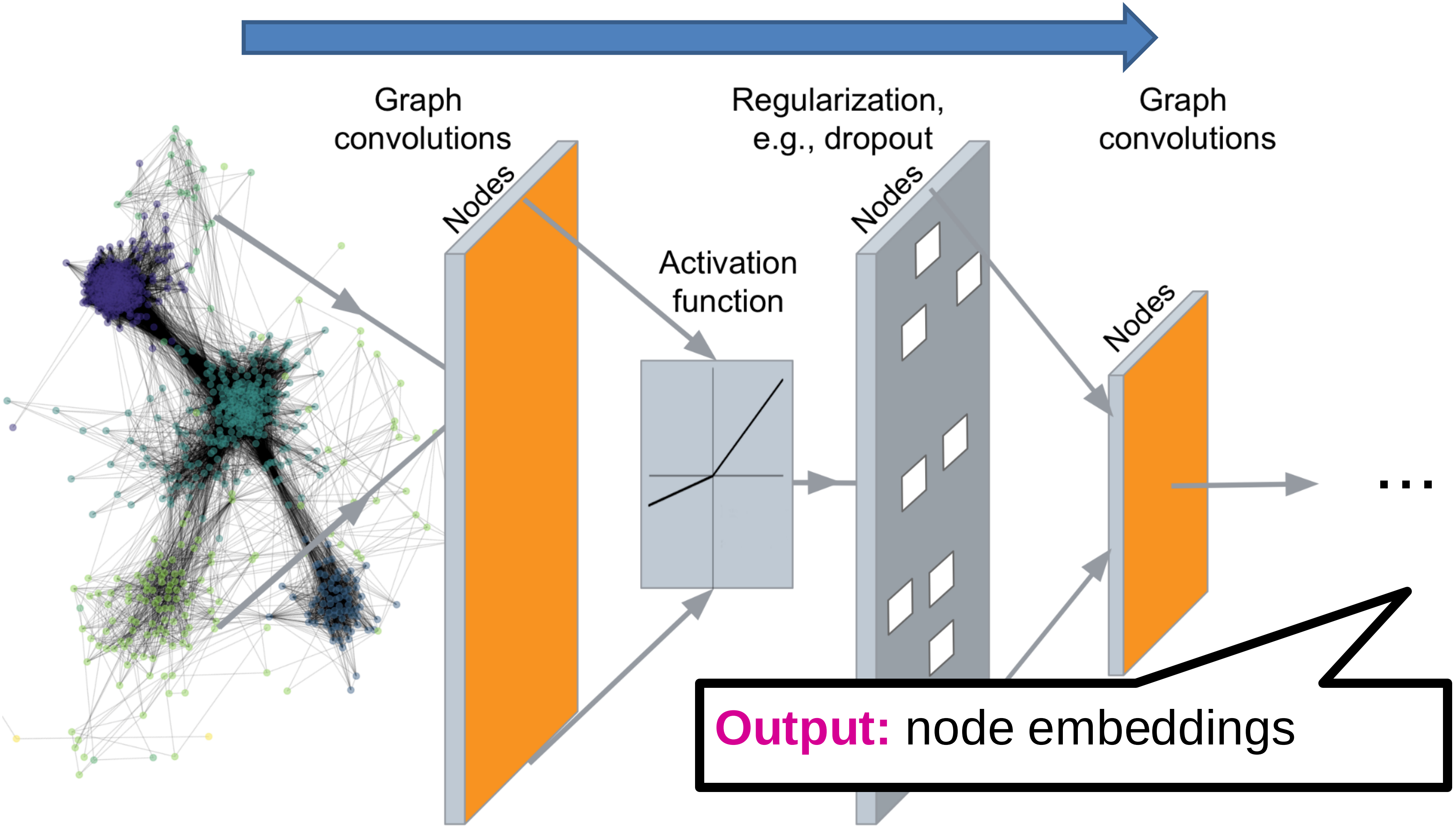
- **Insights** – We can understand the formulation of graphs
- **Predictions** – We can predict how will the graph further evolve
- **Simulations** – We can use the same process to general novel graph instances
- **Anomaly detection** - We can decide if a graph is normal / abnormal

- **In the Era of GenAI:**
  - A more flexible modality compared to sequences

History of Graph Generation

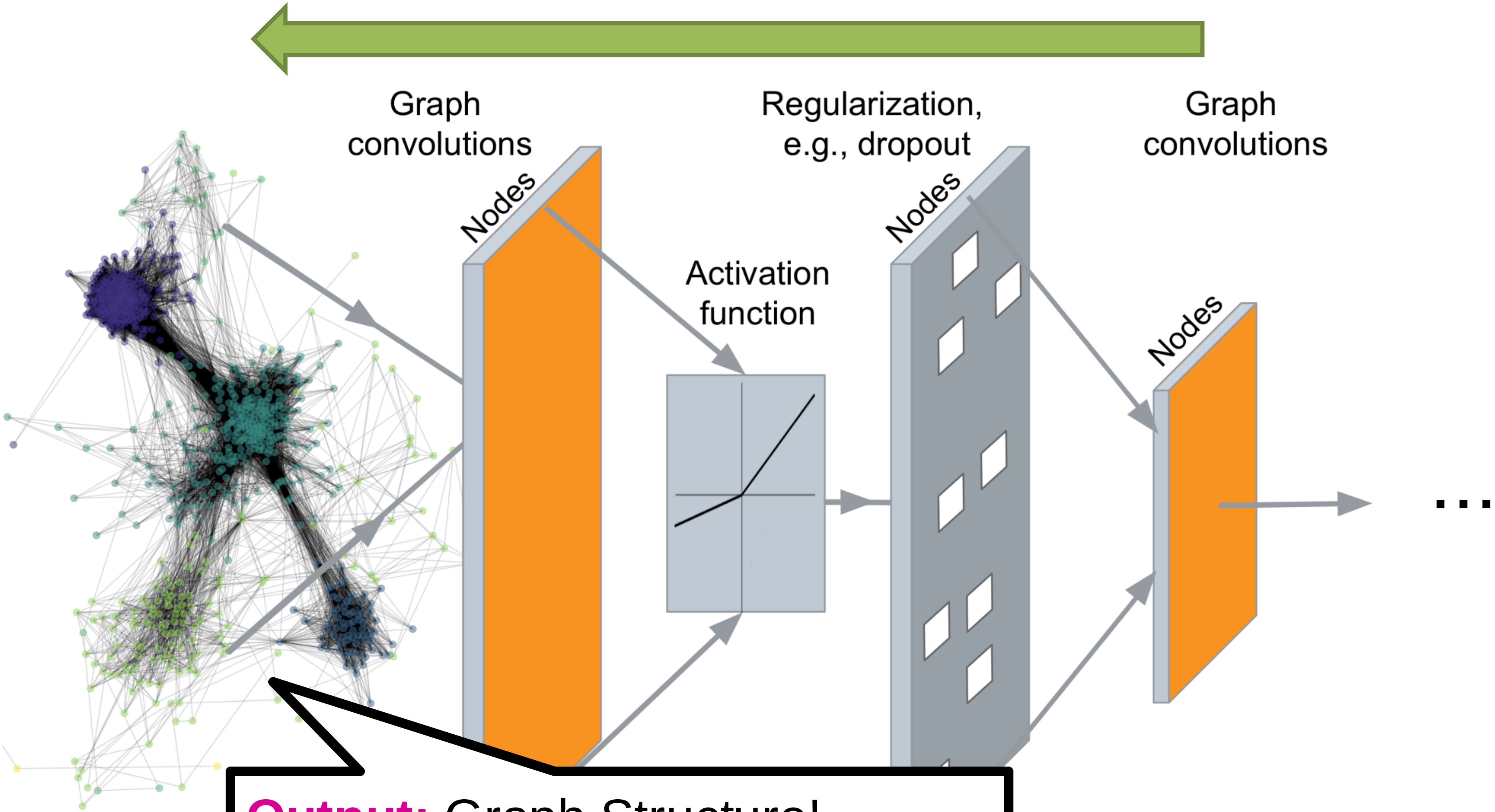
- **Step 1: Properties of real-world graphs**
  - A successful graph generative model should fit these properties
- **Step 2: Traditional graph generative models**
  - Each come with different assumptions on the graph formulation process
- **Step 3: Deep graph generative models**
  - Learn the graph formation process from the data
  - **Focus for this lecture!**

Previously: Deep Graph Encoders



Output: node embeddings

Today: Deep Graph Decoders



Output: Graph Structure!

Beyond Prediction: Graph Generative Models

Machine Learning for Graph Generation

Graph Generation Tasks

Task 1: Realistic graph generation

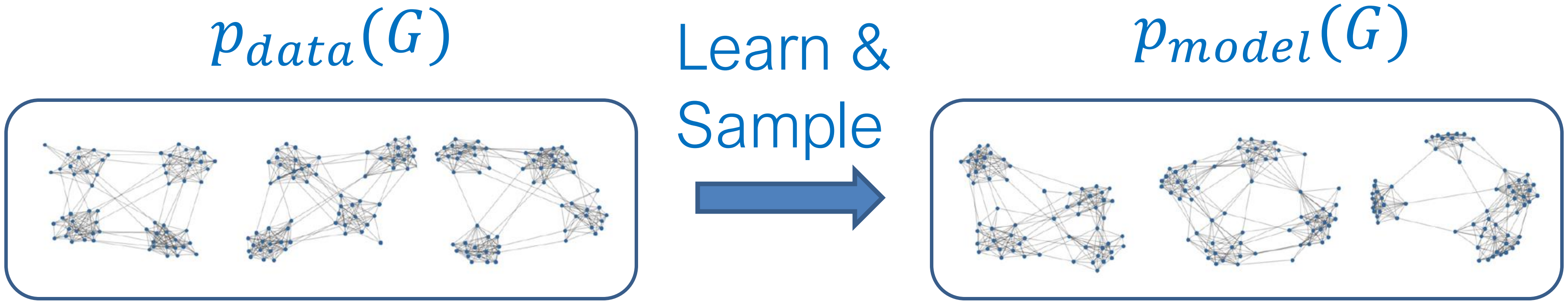
- Generate graphs that are **similar to a given set of graphs** **[Focus of this lecture]**

Task 2: Goal-directed graph generation

- Generate graphs that **optimize given objectives/constraints**
    - E.g., Drug molecule generation/optimization

Graph Generative Models

- **Given:** Graphs sampled from $p_{data}(G)$
- **Goal:**
  - Learn the distribution $p_{model}(G)$
  - Sample from $p_{model}(G)$



$p_{data}(G)$

Learn & Sample

$p_{model}(G)$

Generative Models Basics

- **Setup:**
  - Assume we want to learn a generative model from a set of data points (i.e., graphs) $\{\boldsymbol{x}_i\}$
    - $p_{data}(\boldsymbol{x})$ is the data distribution, which is never known to us, but we have sampled $\boldsymbol{x}_i \sim p_{data}(\boldsymbol{x})$
    - $p_{model}(\boldsymbol{x};\theta)$ is the model, parametrized by θ, that we use to approximate $p_{data}(\boldsymbol{x})$
- **Goal:**
  - **(1)** Make $p_{model}(\boldsymbol{x};\theta)$ close to $p_{data}(\boldsymbol{x})$ **(Density estimation)**
  - **(2)** Make sure we can sample from $p_{model}(\boldsymbol{x};\theta)$ **(Sampling)**
    - We need to generate examples (graphs) from $p_{model}(\boldsymbol{x};\theta)$

Generative Models Basics

(1) Make $\boldsymbol{p_{model}(x;\theta)}$ close to $\boldsymbol{p_{data}(x)}$

- **Key Principle**: **Maximum Likelihood**
- Fundamental approach to modeling distributions

$$\boldsymbol{\theta}^{*}=\arg\max_{\boldsymbol{\theta}}\mathbb{E}_{x\sim p_{\text{data}}}\log p_{\text{model}}(\boldsymbol{x}\mid\boldsymbol{\theta})$$

  - Find parameters θ^*, such that for observed data points $\boldsymbol{x}_i \sim p_{data}$ the $\sum_i \log p_{model}(\boldsymbol{x}_i; \theta^*)$ has the highest value, among all possible choices of θ
    - That is, find the model that is most likely to have generated the observed data x

Generative Models Basics

(2) Sample from $\boldsymbol{p_{model}(x;\theta)}$

- **Goal**: Sample from a complex distribution
- A common approach:
  - **(1)** Sample from a simple noise distribution

$$\boldsymbol{z}_i \sim N(0,1)$$

  - **(2)** Transform the noise z_i via $f(\cdot)$

$$\boldsymbol{x}_i = f(\boldsymbol{z}_i;\theta)$$

Then $\boldsymbol{x}_i$ follows a complex distribution

- **Q: How to design $\boldsymbol{f}(\cdot)$?**
- **A**: Use Deep Neural Networks and train it using the data we have!

Deep Generative Models

Auto-regressive models:

- $\boldsymbol{p_{model}(x;\theta)}$ is used for **both density estimation and sampling** (remember our two goals)
  - Other models like Variational Auto Encoders (VAEs), Generative Adversarial Nets (GANs) have 2 or more models, each playing one of the roles
- **Idea: Chain rule.** Joint distribution is a product of conditional distributions:

$$p_{model}(\boldsymbol{x};\theta) = \prod_{t=1}^{n} p_{model}(x_t | x_1, \dots, x_{t-1}; \theta)$$

- E.g., $\boldsymbol{x}$ is a vector, x_t is the t-th dimension;
  $\boldsymbol{x}$ is a sentence, x_t is the t-th word.
- **In our case:** x_t will be the t-th action (add node, add edge)

Beyond Prediction: Graph Generative Models

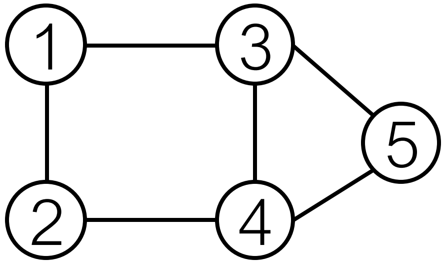
GraphRNN: Generating Realistic Graphs

GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models. J. You, R. Ying, X. Ren, W. L. Hamilton, J. ICML, 2018.

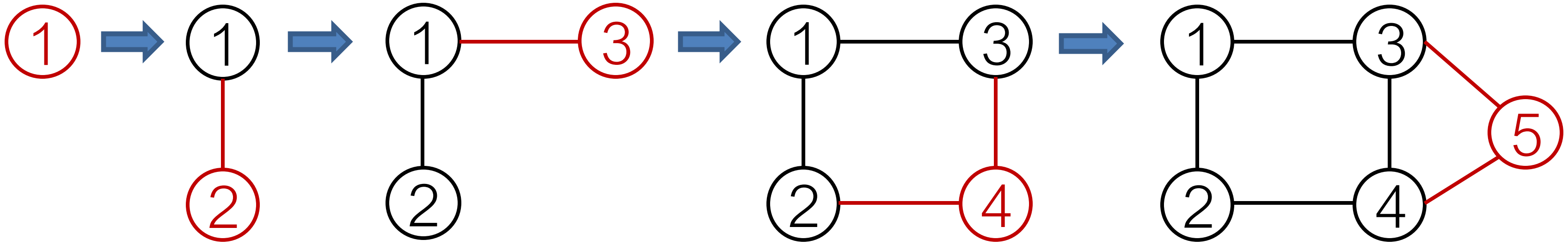
GraphRNN Idea

- **Generating graphs via sequentially adding nodes and edges**

Graph G

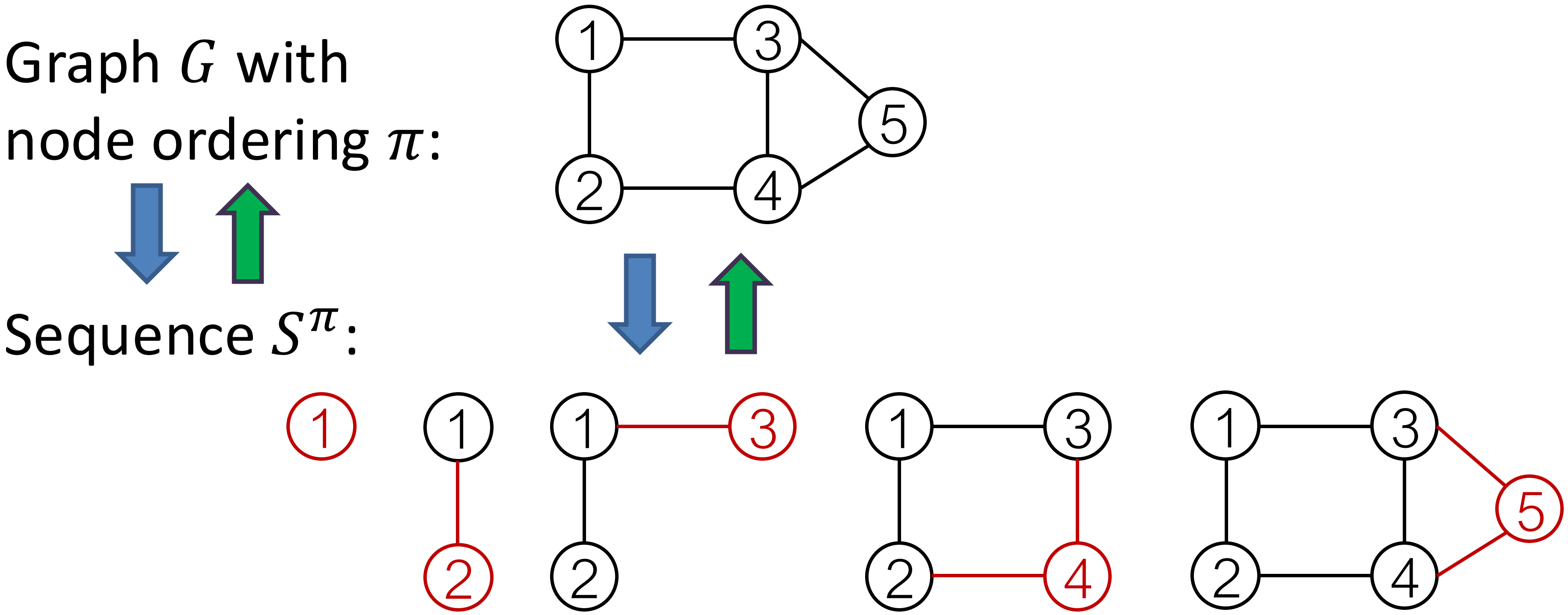


Generation process S^{π}



Model Graphs as Sequences

Graph G with node ordering π can be uniquely mapped into a sequence of node and edge additions S^{π}



Graph G with node ordering π:

Sequence S^{π}:

$$S^{\pi} = (\ S_1^{\pi}\ ,\ S_2^{\pi}\ ,\ S_3^{\pi}\ ,\ S_4^{\pi}\ ,\ S_5^{\pi}\ )$$

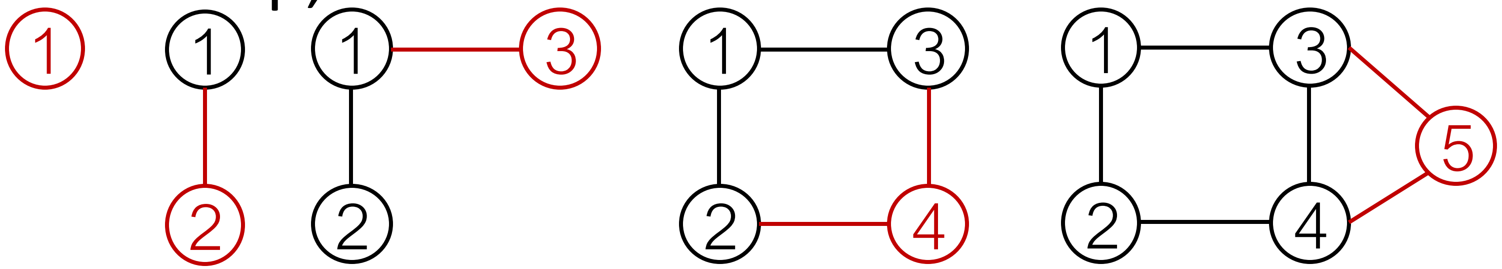
Model Graphs as Sequences

The sequence S^{π} has **two levels**

(S is a sequence of sequences**):**

- **Node-level:** add nodes, one at a time
- **Edge-level:** add edges between existing nodes

- **Node-level**: At each step, a new node is added



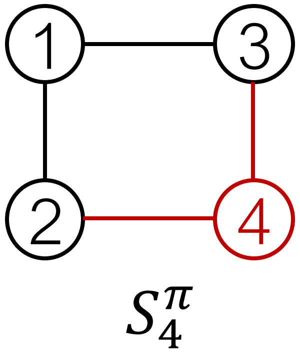
$$S^{\pi} = (\; S_1^{\pi} \; , S_2^{\pi} \; , \; S_3^{\pi} \; , \; S_4^{\pi} \; , \; S_5^{\pi} \;)$$

"Add node 1" ... "Add node 5"

Model Graphs as Sequences

The sequence S^{π} has **two levels:**

- Each Node-level step is an edge-level sequence
- **Edge-level**: At each step, add a new edge



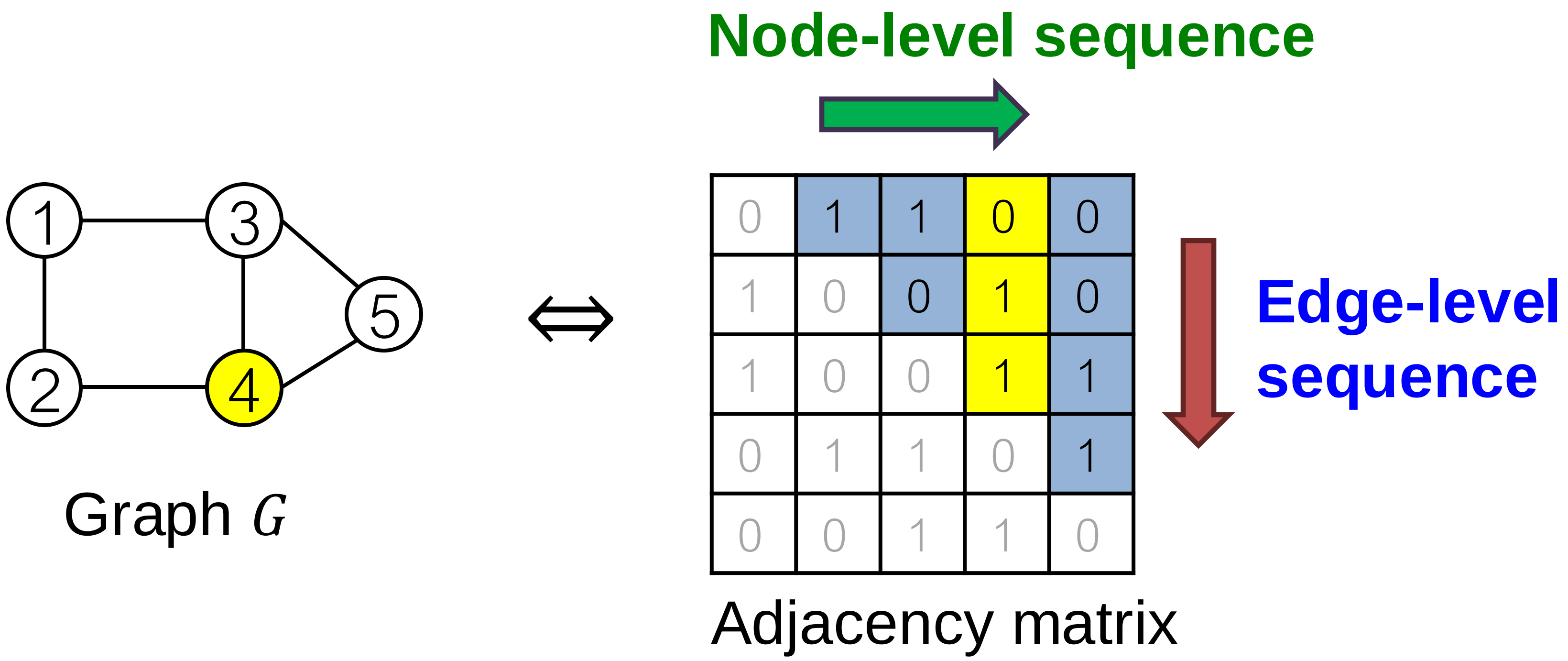
$$S_4^{\pi} = (\quad S_{4,1}^{\pi} \quad , \quad S_{4,2}^{\pi} \quad , \quad S_{4,3}^{\pi} \quad)$$

"Not connect 4, 1" "Connect 4, 2" "Connect 4, 3"

0 1 1

Model Graphs as Sequences

- **Summary: A graph + a node ordering = A sequence of sequences**
- Node ordering is randomly selected (we will come back to this)



Graph G

Node-level sequence

0	1	1	0	0
1	0	0	1	0
1	0	0	1	1
0	1	1	0	1
0	0	1	1	0

Edge-level sequence

Adjacency matrix

Model Graphs as Sequences

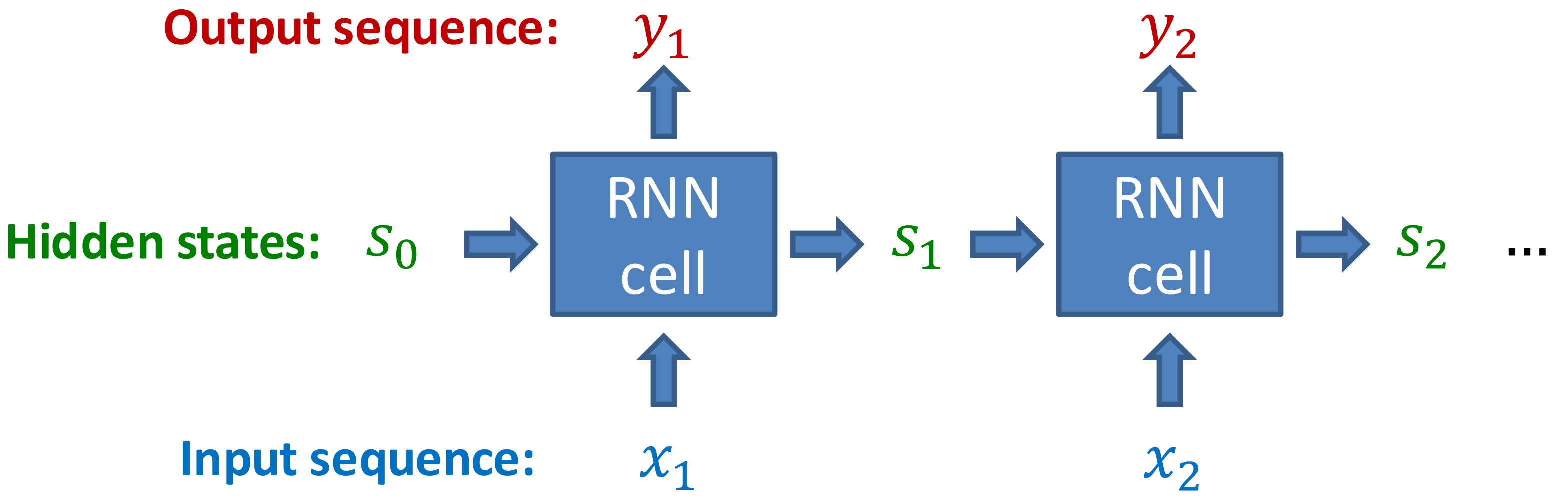
- **We have transformed graph generation problem into a sequence generation problem**

- **Need to model two processes:**
  - **1)** Generate a state for a new node (Node-level sequence)
  - **2)** Generate edges for the new node based on its state (Edge-level sequence)

- **Approach**: Use **Recurrent Neural Networks (RNNs)** to model these processes!

Background: Recurrent NNs

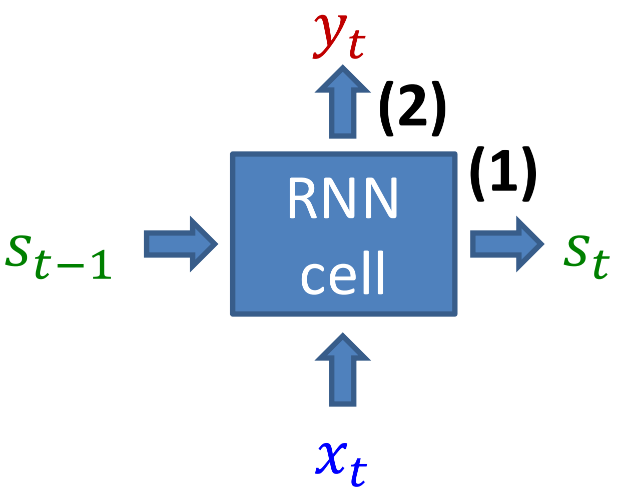
- RNNs are designed for **sequential data**
  - RNN sequentially takes **input sequence** to **update its hidden states**
  - The **hidden states** summarize all the information input to RNN
  - The update is conducted via **RNN cells**



Background: Recurrent NNs

- s_t: **State** of RNN after step t
- x_t: **Input** to RNN at step t
- y_t: **Output** of RNN at step t
- **RNN cell:** W, U, V: Trainable parameters

In our case s_t, x_t and y_t will be scalars (edge probabilities)



The RNN cell:

(1) Update hidden state:

$$s_t = \sigma(W \cdot x_t + U \cdot s_{t-1})$$

(2) Output prediction:

$$y_t = V \cdot s_t$$

- **More expressive cells:** GRU, LSTM, etc.

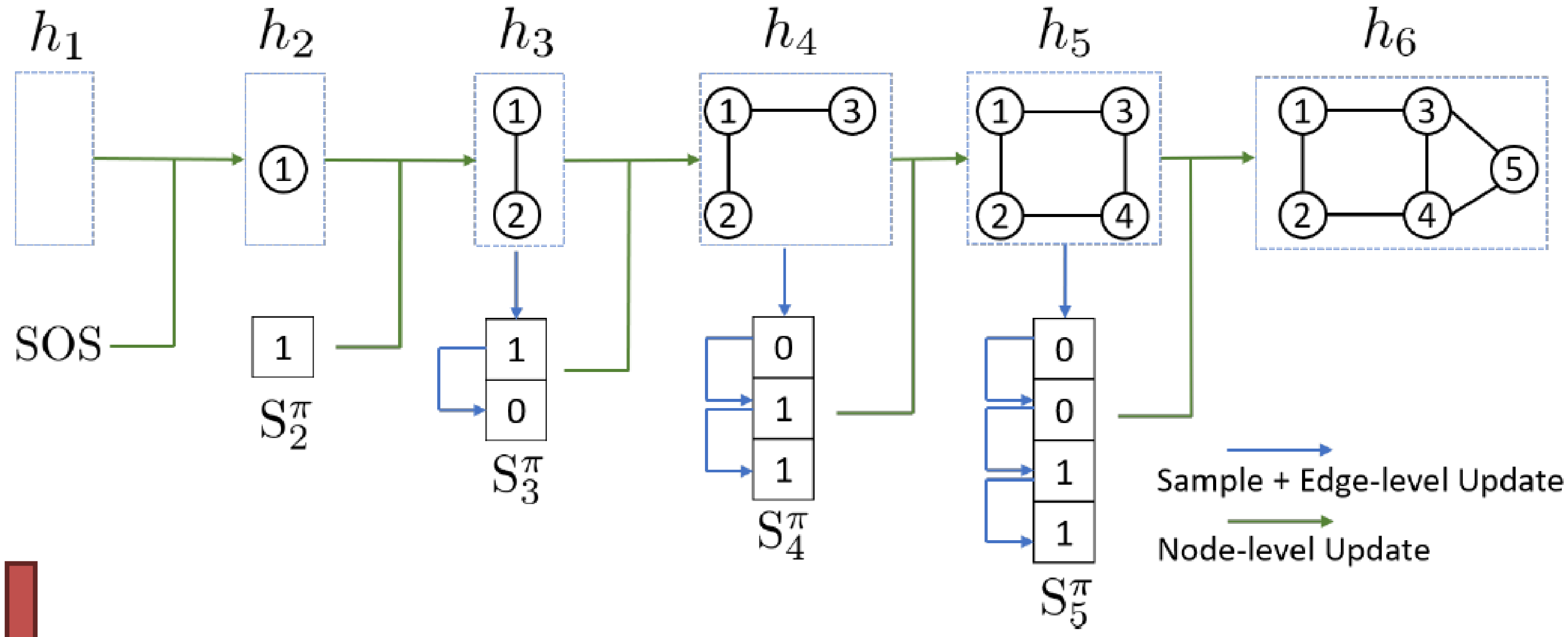
GraphRNN: Two levels of RNN

- **GraphRNN has a node-level RNN and an edge-level RNN**

- **Relationship between the two RNNs:**
  - Node-level RNN generates the initial state for edge-level RNN
  - Edge-level RNN sequentially predict if the new node will connect to each of the previous node

GraphRNN: Two levels of RNN

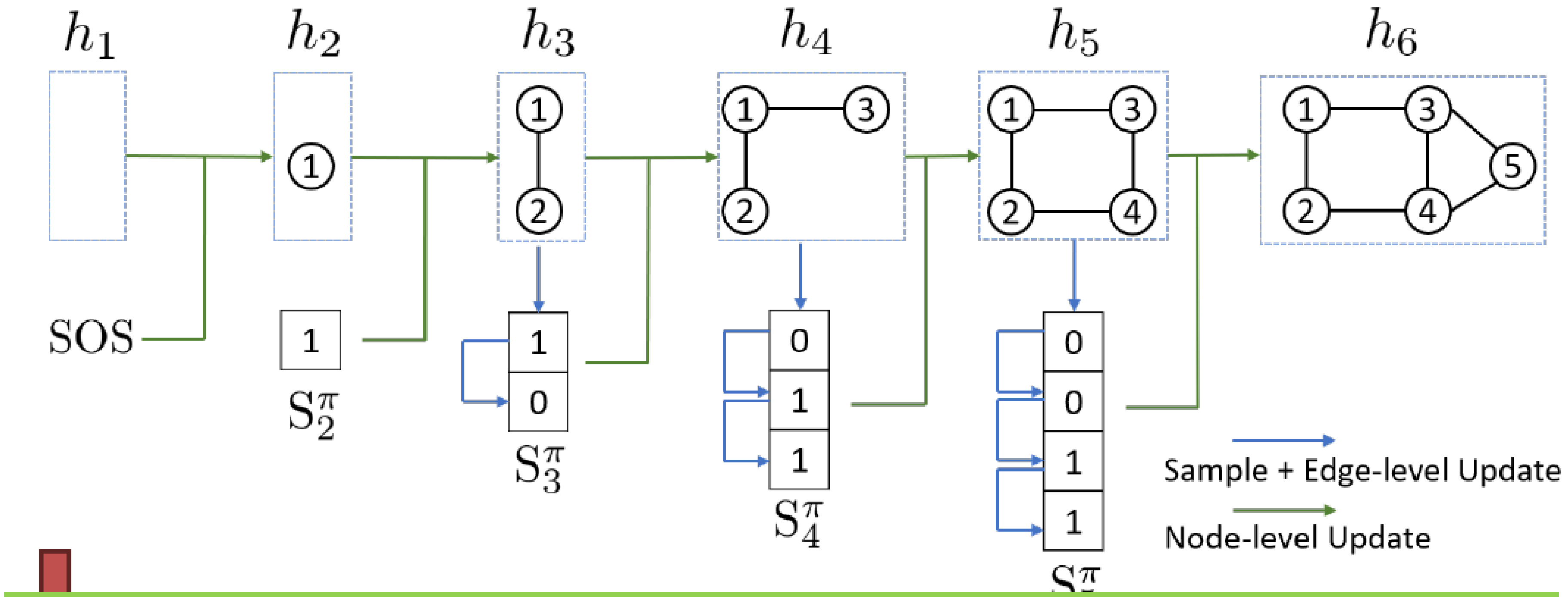
Node-level RNN generates the initial state for edge-level RNN



Edge-level RNN sequentially predict if the new node will connect to each of the previous node

GraphRNN: Two levels of RNN

Node-level RNN generates the initial state for edge-level RNN



Next: How to generate a sequence with RNN?

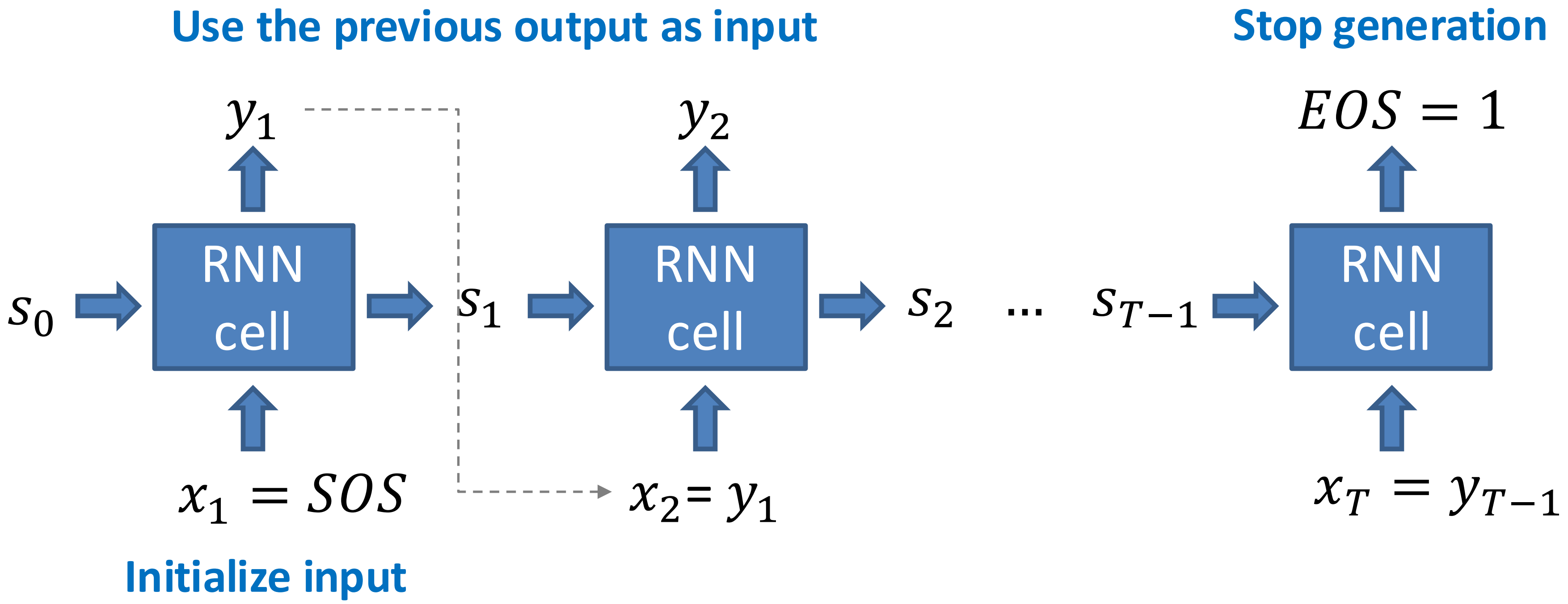
RNN for Sequence Generation

- **Q:** How to use RNN to generate sequences?
- **A:** Let $x_{t+1} = y_t$ (Use the previous output as input)

- **Q:** How to initialize the input sequence?
- **A:** Use **start of sequence token (SOS)** as the initial input
  - SOS is usually a vector with all zero/ones

- **Q:** When to stop generation?
- **A:** Use **end of sequence token (EOS)** as an **extra** RNN output
  - If output EOS=0, RNN will continue generation
  - If output EOS=1, RNN will stop generation

RNN for Sequence Generation

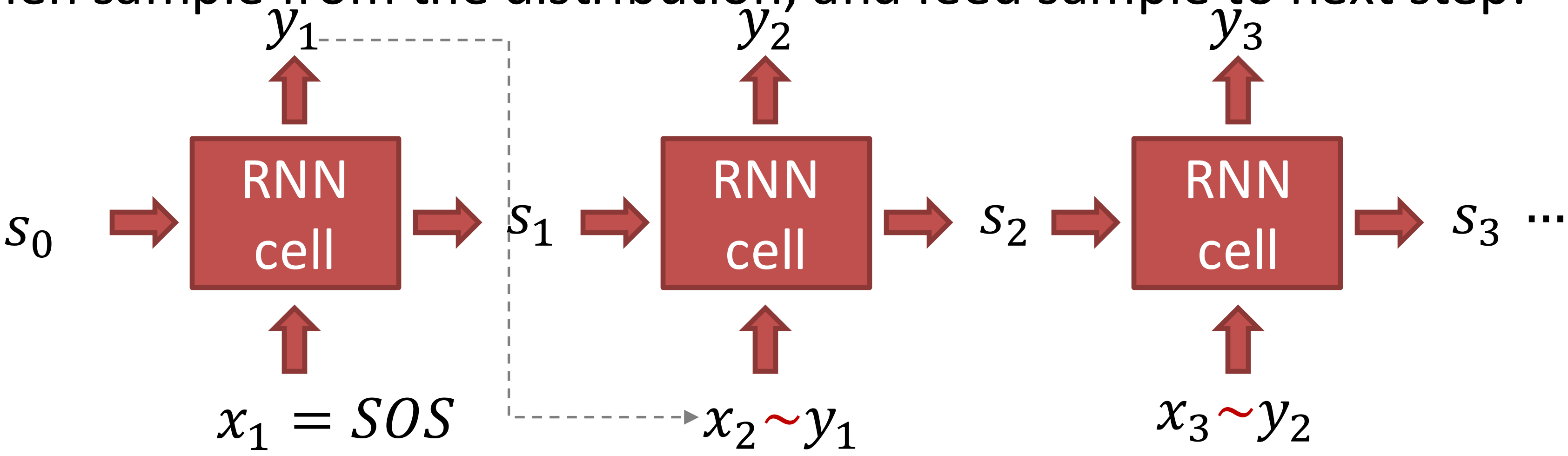


- This is good, but this model is **deterministic**

Building Edge-Level RNN

Consider the Edge-level RNN for now.

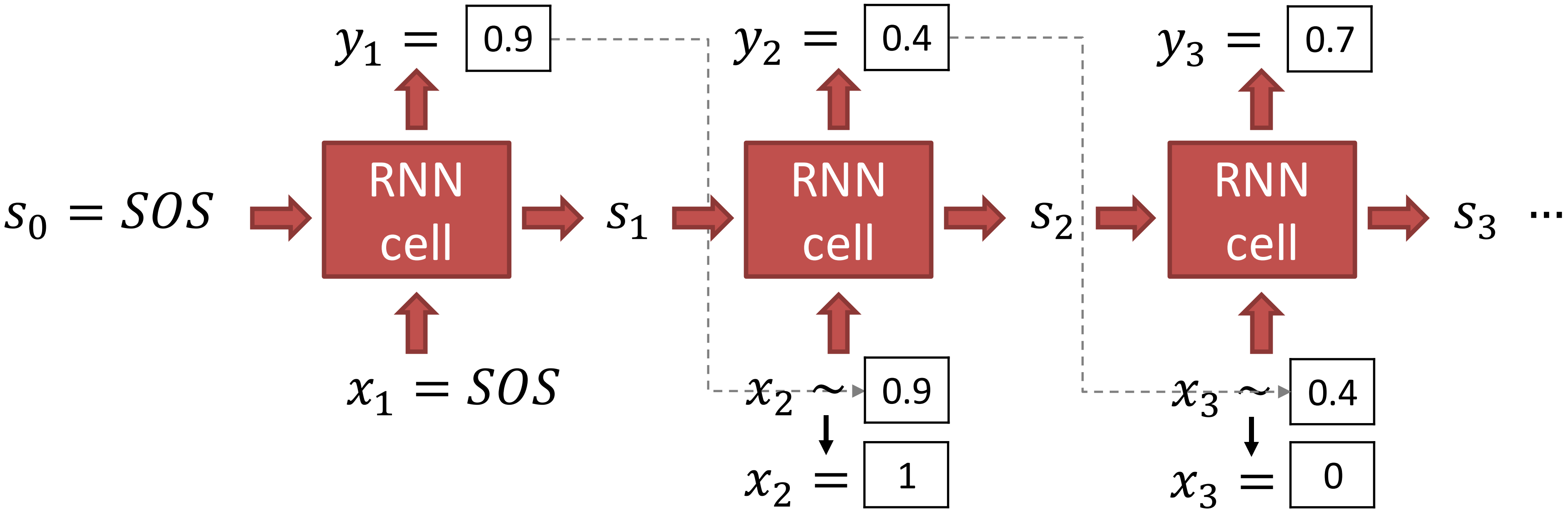
- **Our goal**: Model $\prod_{k=1}^{n} p_{model}(x_t|x_1, \ldots, x_{t-1}; \theta)$
- Let $y_t = p_{model}(x_t|x_1, \ldots, x_{t-1}; \theta)$
- Then we need to sample x_{t+1} from y_t: $x_{t+1} \sim y_t$
  - Each step of RNN outputs a **probability of a single edge**
  - We then sample from the distribution, and feed sample to next step:



Building Edge-Level RNN

Suppose we already have trained the edge-level RNN

- y_t is a **scalar**, following a **Bernoulli distribution**
- $\boxed{p}$ means value 1 has prob. p, value 0 has prob. $1 - p$

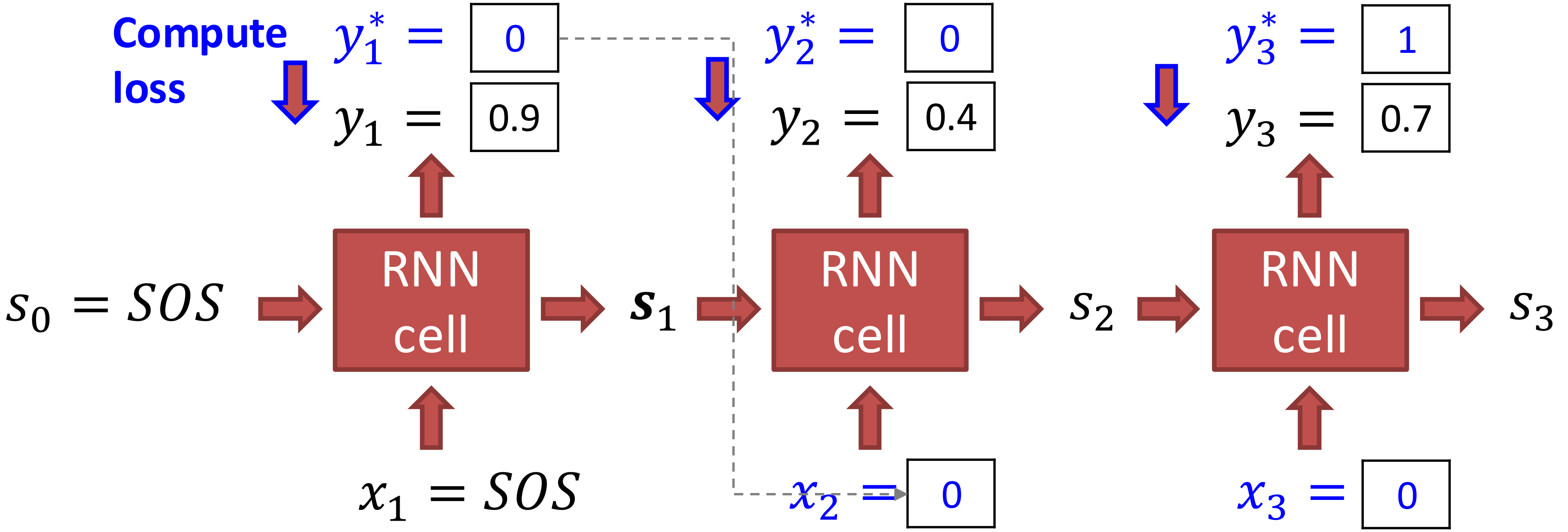


- **How do we use training data $x_1, x_2, \ldots, x_n$?**

Edge-Level RNN at Training Time

Training the model:

- We observe a sequence y^* of edges [0,0,1,…]
- **Principle**: **Teacher Forcing** -- Replace input and output by the real sequence



Edge-Level RNN at Training Time

- **Loss** L : **Binary cross entropy**
- **Minimize**:

$$L = -[y_1^* \log(y_1) + (1 - y_1^*) \log(1 - y_1)]$$

Compute loss ⬇

$$y_1^* = \boxed{0}$$

$$y_1 = \boxed{0.9}$$

- If $y_1^* = 1$, we minimize $-\log(y_1)$, making y_1 higher
- If $y_1^* = 0$, we minimize $-\log(1 - y_1)$, making y_1 lower
- This way, y_1 is fitting the data samples y_1^*
- **Reminder**: y_1 is computed by RNN, this loss will adjust RNN parameters accordingly, using back propagation!

Putting Things Together

- **Our Plan:**

(1) **Add a new node:** We run Node RNN for a step, and use it output to initialize Edge RNN

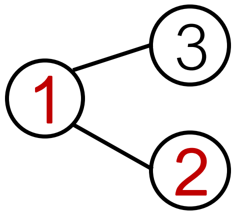
(2) **Add new edges for the new node:** We run Edge RNN to predict if the new node will connect to each of the previous node

(3) **Add another new node:** We use the last hidden state of Edge RNN to run Node RNN for another step

(4) **Stop graph generation:** If Edge RNN outputs EOS at step 1, we know no edges are connected to the new node. We stop the graph generation.

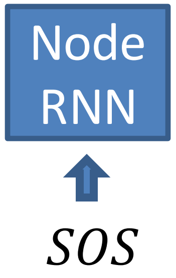
Put Things Together: Training

Assuming **Node 1** is in the graph
Now adding **Node 2**



0	1	1
1	0	0
1	0	0

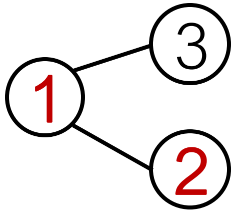
Observed graph



Start the node RNN

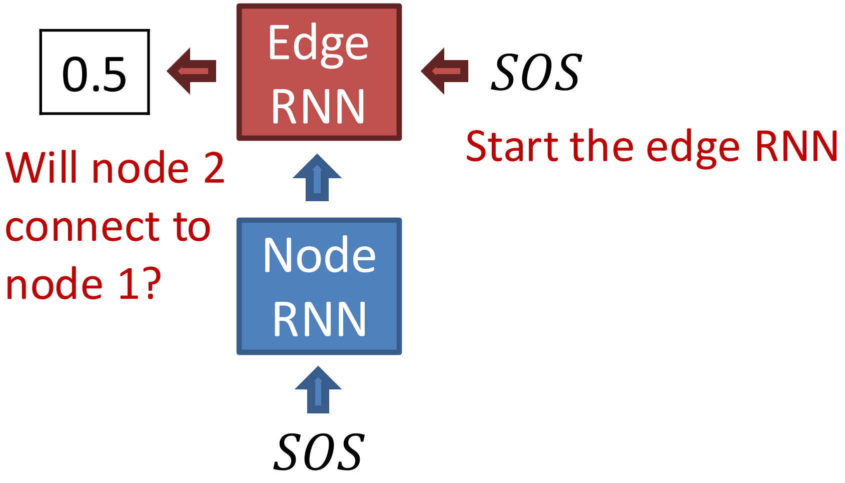
Put Things Together: Training

Edge RNN predicts how
Node 2 connects to **Node 1**



0	1	1
1	0	0
1	0	0

Observed graph

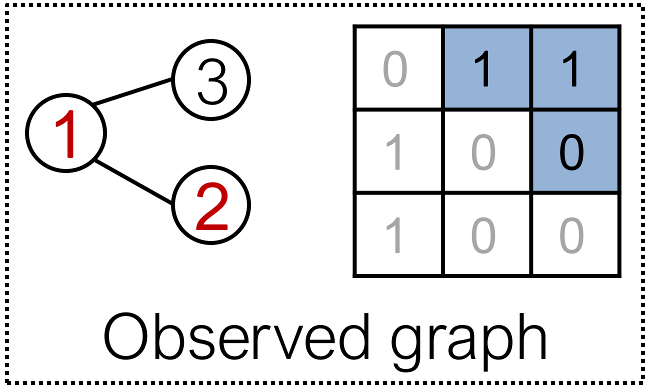


Start the edge RNN

Will node 2 connect to node 1?

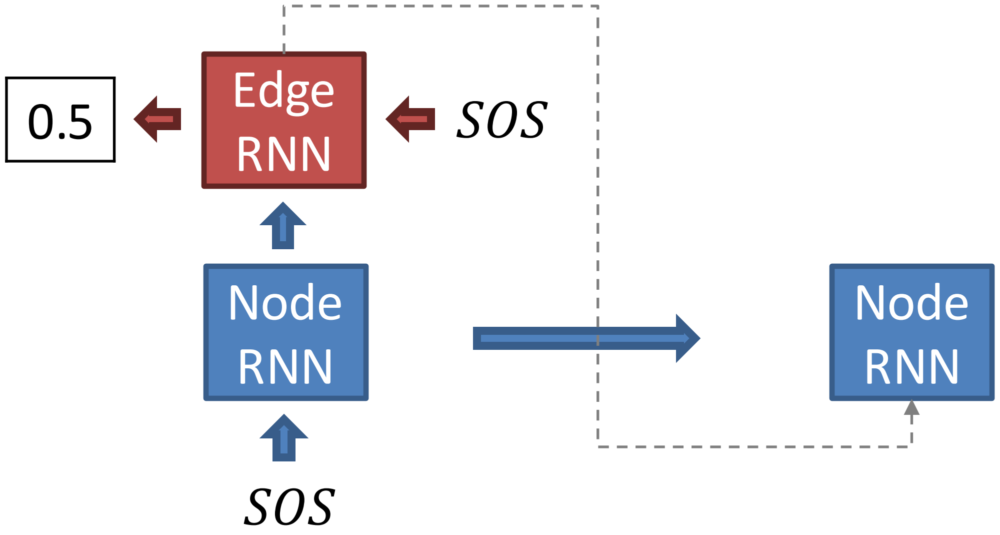
Put Things Together: Training

Update Node RNN using
Edge RNN's hidden state



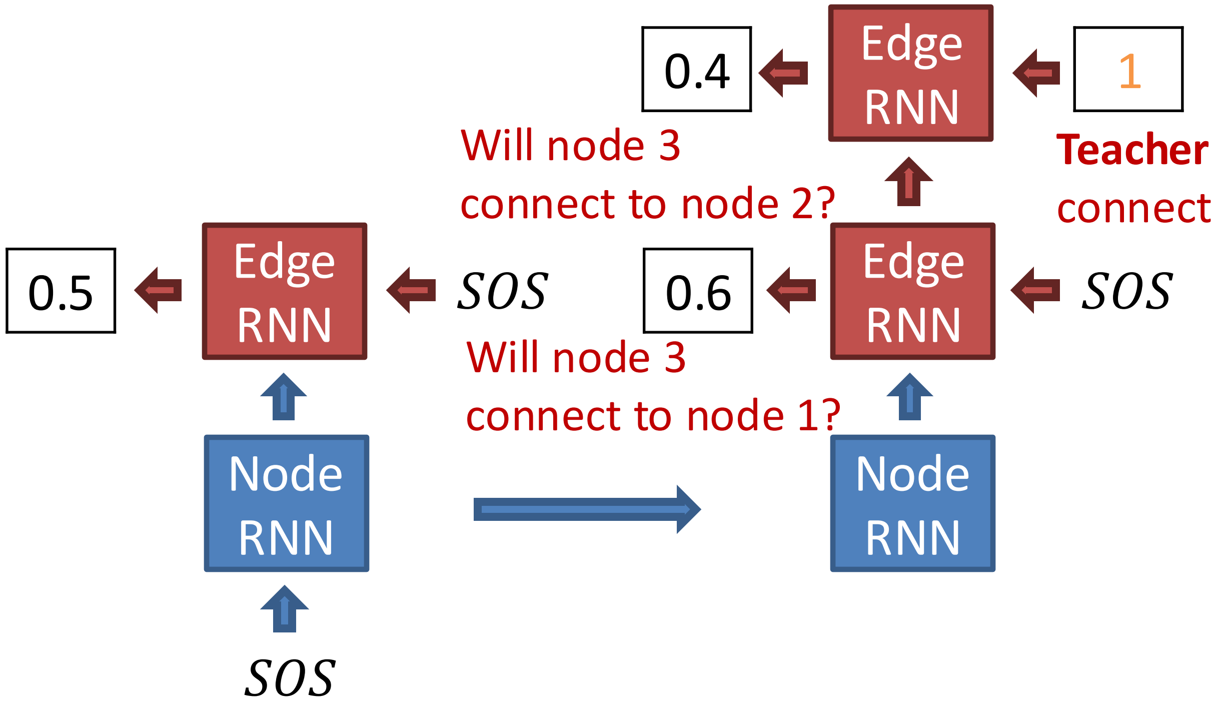
0	1	1
1	0	0
1	0	0

Observed graph



Put Things Together: Training

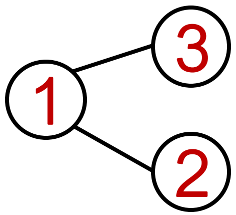
Edge RNN predicts how **Node 3** tries to connects to **Nodes 1, 2**



Will node 3 connect to node 2?

Will node 3 connect to node 1?

Teacher forcing: node 3 will connect to node 1

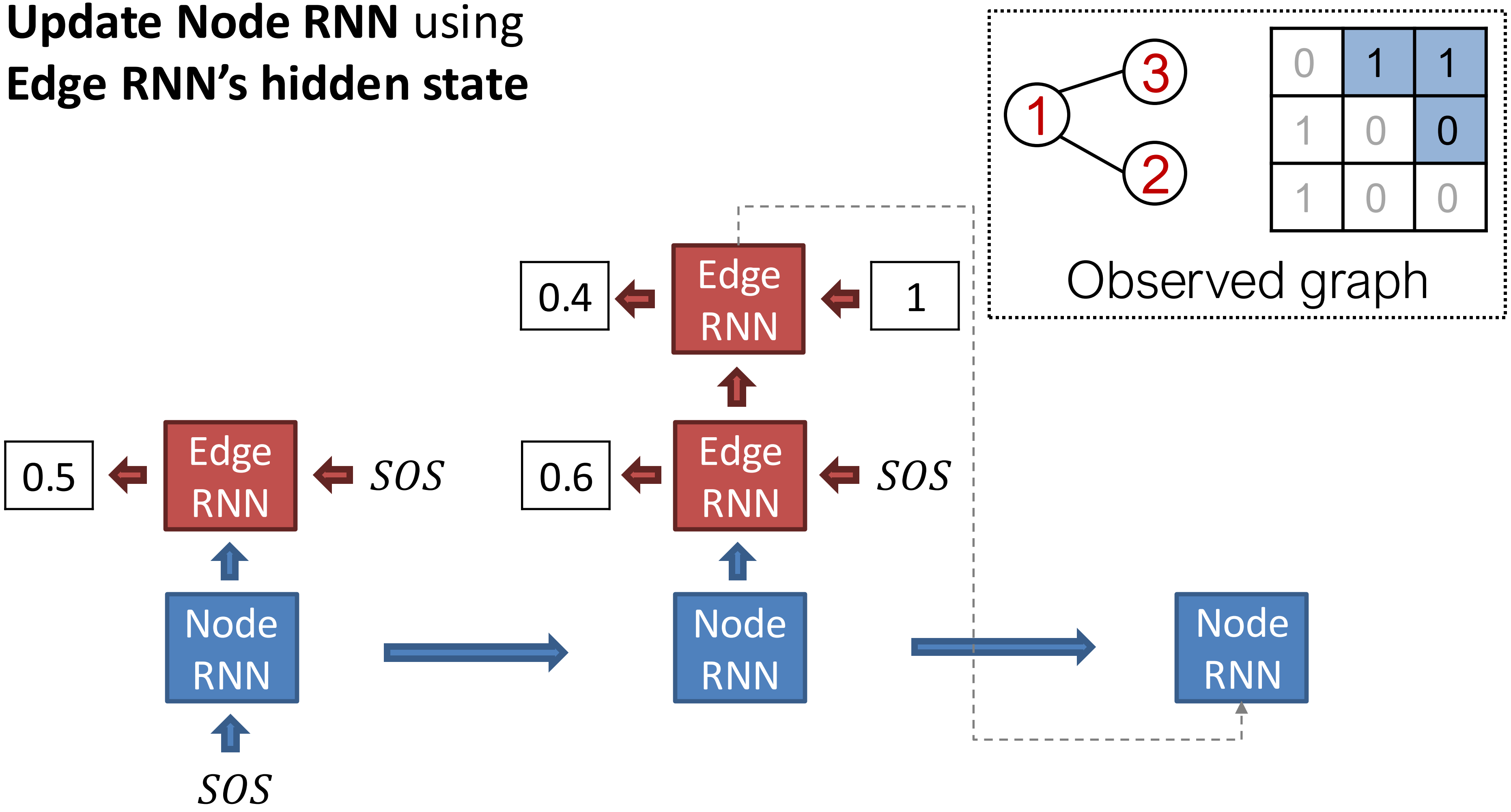


0	1	1
1	0	0
1	0	0

Observed graph

Put Things Together: Training

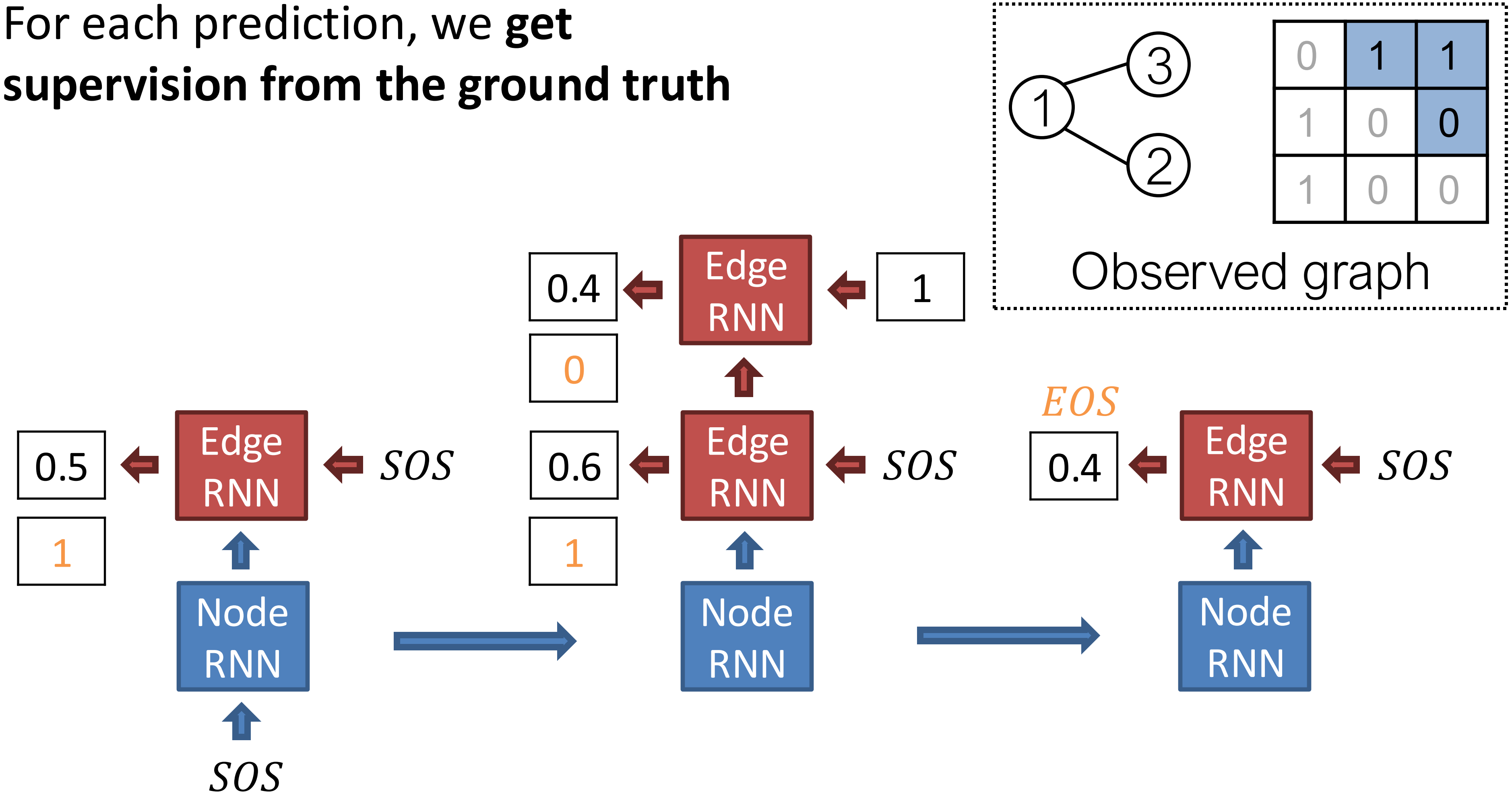
Update Node RNN using
Edge RNN's hidden state



0	1	1
1	0	0
1	0	0

Put Things Together: Training

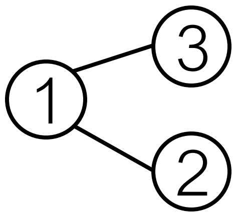
For each prediction, we **get supervision from the ground truth**



0	1	1
1	0	0
1	0	0

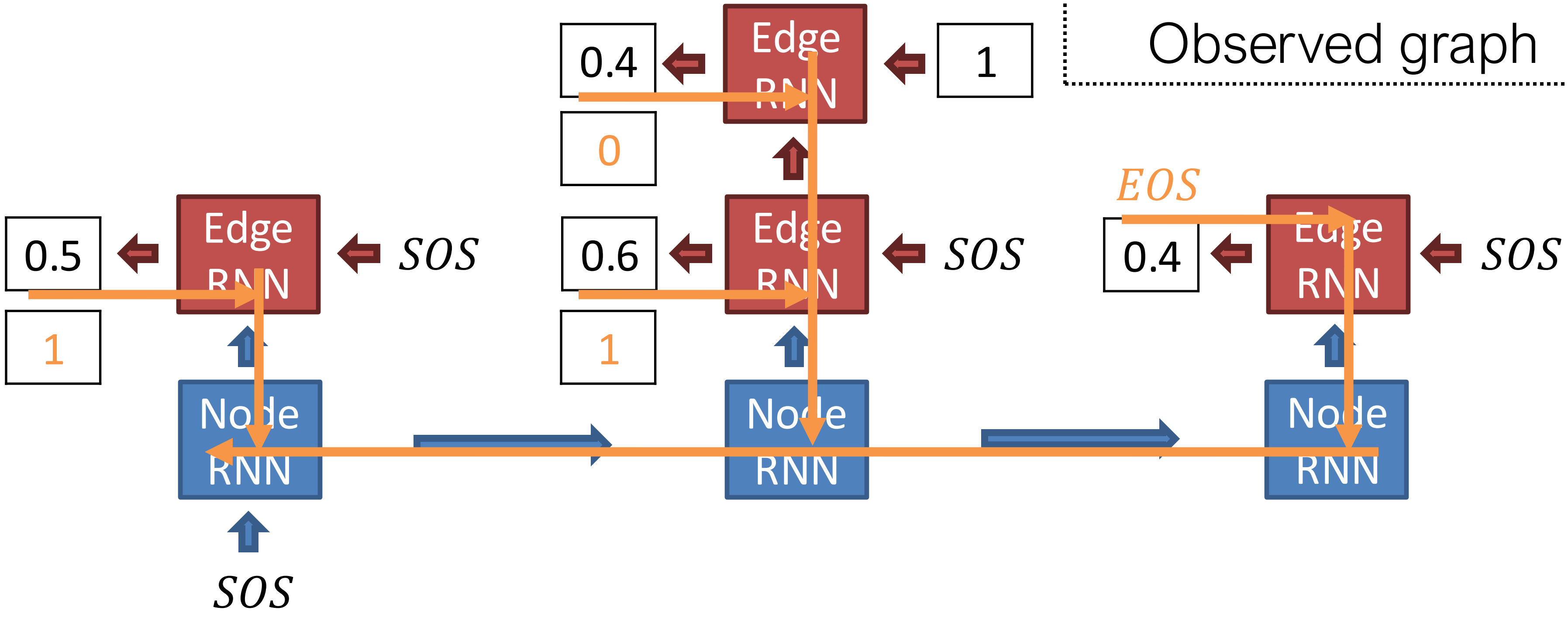
Put Things Together: Training

Backprop through time:
Gradients are **accumulated across time steps**



0	1	1
1	0	0
1	0	0

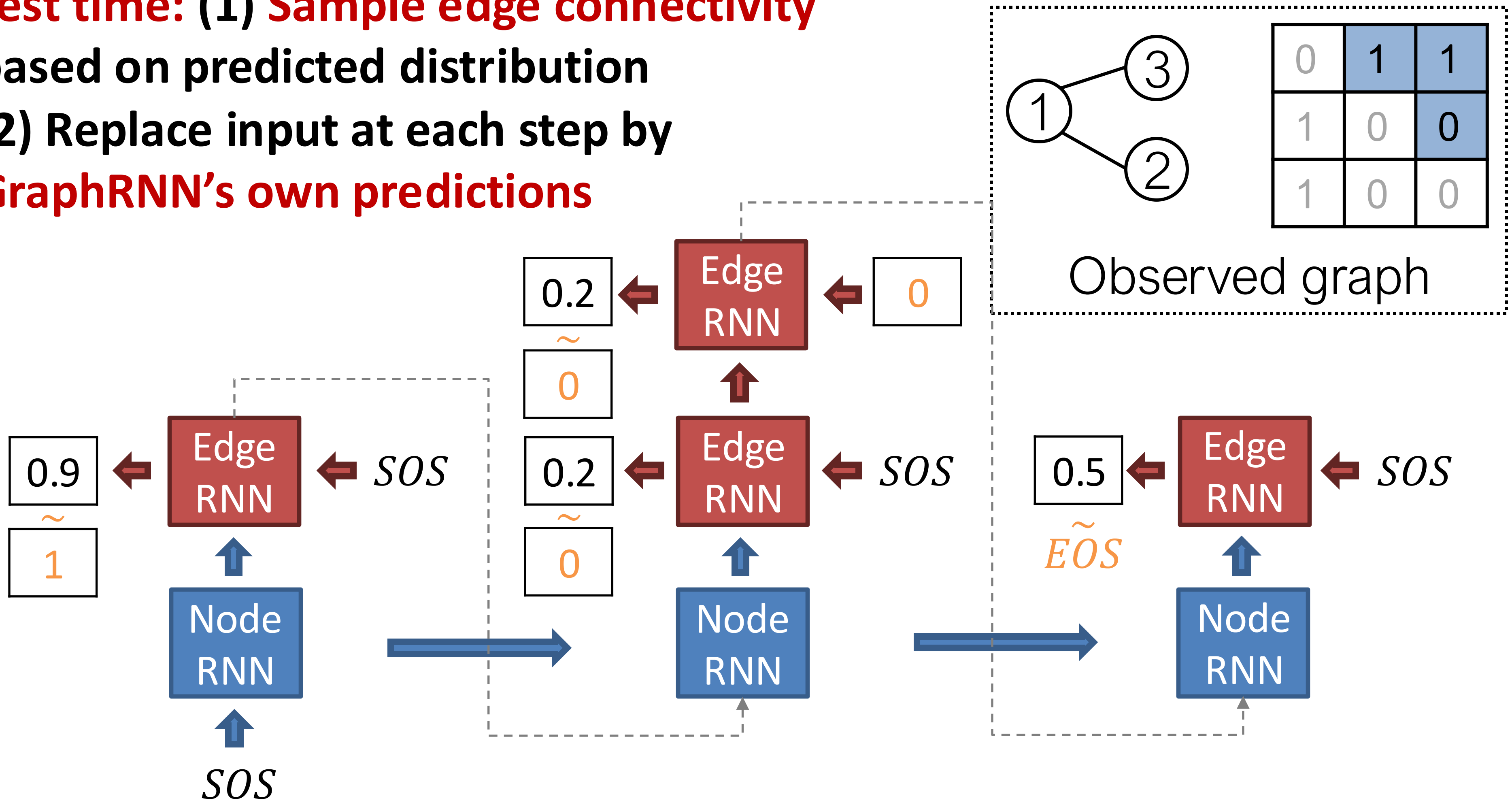
Observed graph



Put Things Together: Test

Test time: (1) Sample edge connectivity based on predicted distribution

(2) Replace input at each step by GraphRNN's own predictions

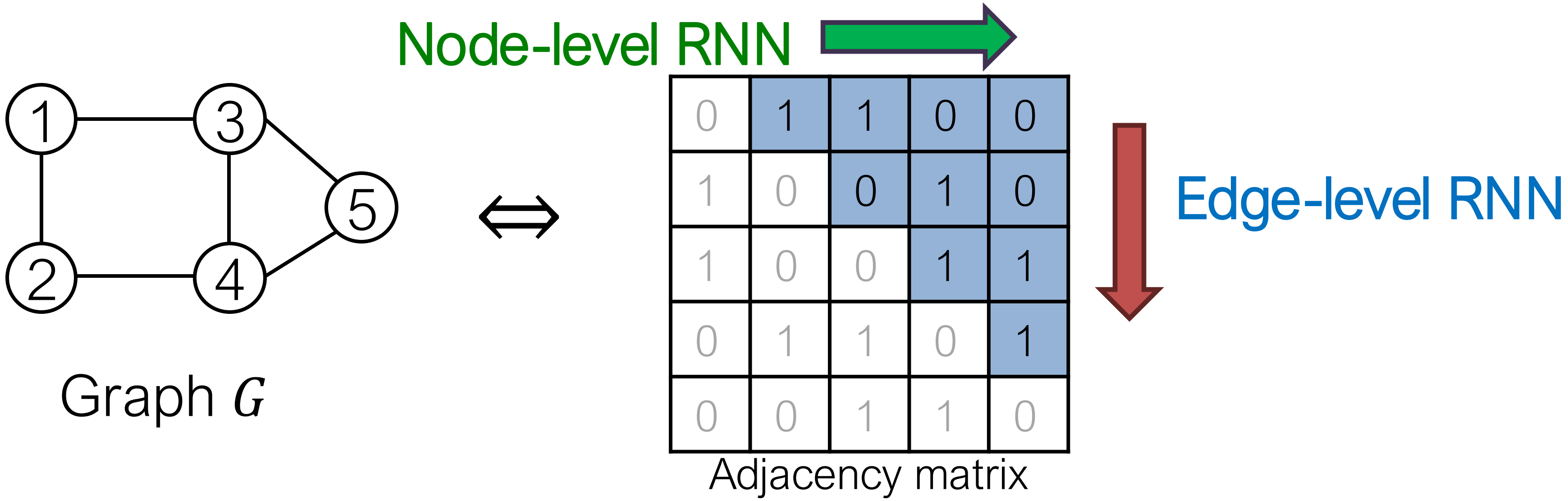


GraphRNN: Two levels of RNN

Quick Summary of GraphRNN:

- Generate a graph by generating a two-level sequence
- Use RNN to generate the sequences

- **Next**: Making GraphRNN tractable, proper evaluation



Node-level RNN

Edge-level RNN

0	1	1	0	0
1	0	0	1	0
1	0	0	1	1
0	1	1	0	1
0	0	1	1	0

Graph G

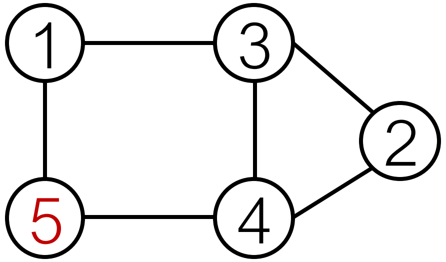
Adjacency matrix

Beyond Prediction: Graph Generative Models

Scaling Up and Evaluating Graph Generation

Issue: Tractability

- Any node can connect to any prior node
- Too many steps for edge generation
  - Need to generate full adjacency matrix
  - Complex too-long edge dependencies



Random node ordering:

Node 5 may connect to any/all previous nodes

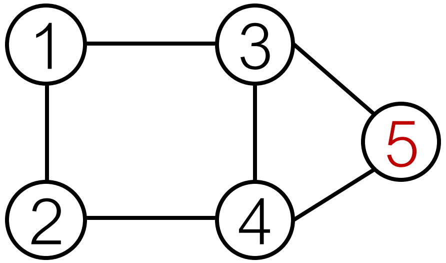
"Recipe" to generate the left graph:

- Add node 1
- Add node 2
- Add node 3
- Connect 3 with 2 and 1
- Add node 4
- …

How do we limit this complexity?

Solution: Tractability via BFS

- **Breadth-First Search node ordering**



BFS ordering

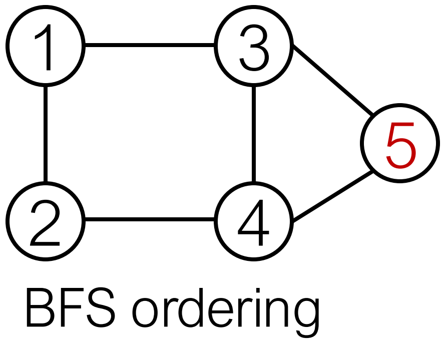
"Recipe" to generate the left graph:

- Add node 1
- Add node 2
- Connect 2 with 1
- Add node 3
- Connect 3 with 1
- Add node 4
- Connect 4 with 3 and 2

- **BFS node ordering:**
  - Since Node 4 doesn't connect to Node 1
  - We know all Node 1's neighbors have already been traversed
  - Therefore, Node 5 and the following nodes will never connect to node 1
  - We only need memory of 2 "steps" rather than $n - 1$ steps

Solution: Tractability via BFS

- **Breadth-First Search node ordering**



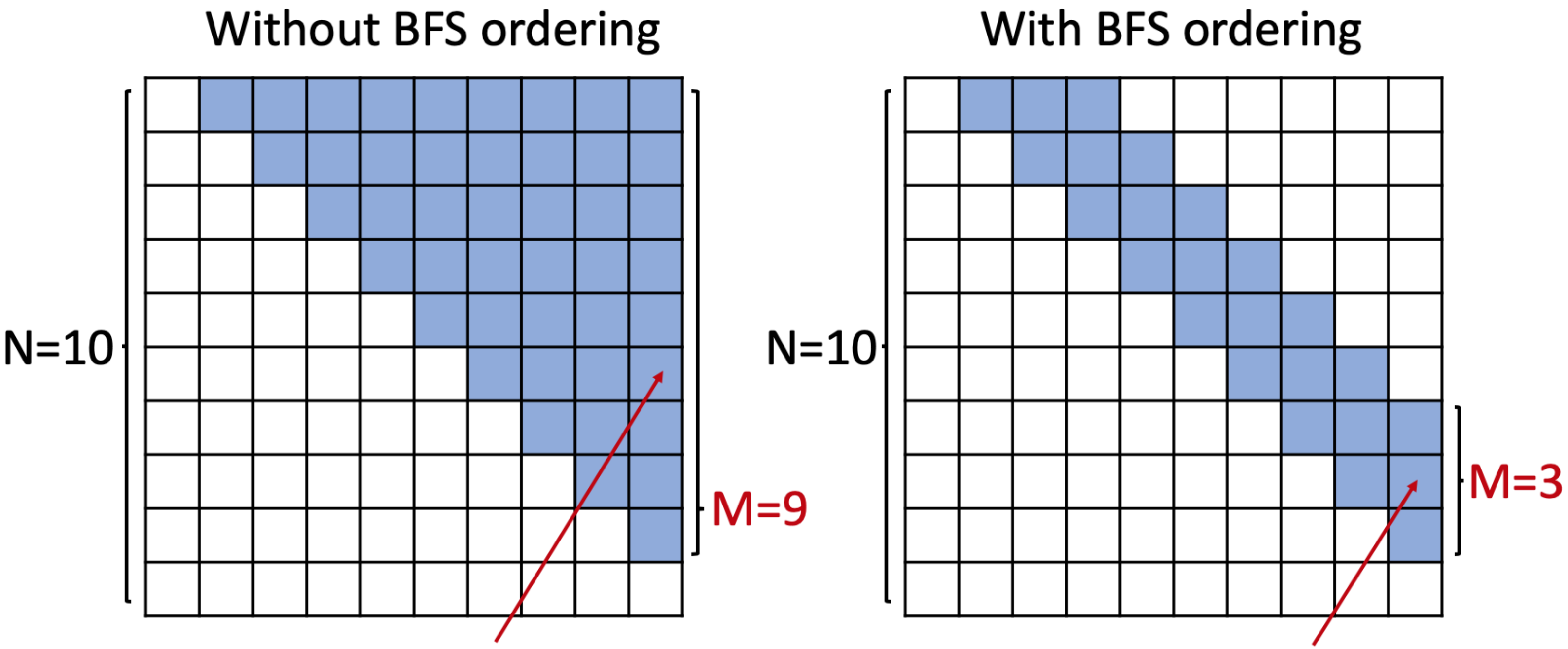
BFS node ordering: Node 5 will never connect to node 1 (only need memory of 2 “steps” rather than $n - 1$ steps)

- **Benefits:**
  - Reduce possible node orderings
    - From $O(n!)$ to number of distinct BFS orderings
  - Reduce steps for edge generation
    - Reducing number of previous nodes to look at

Solution: Tractability via BFS

- **BFS reduces the number of steps for edge generation**

Adjacency matrices


Without BFS ordering

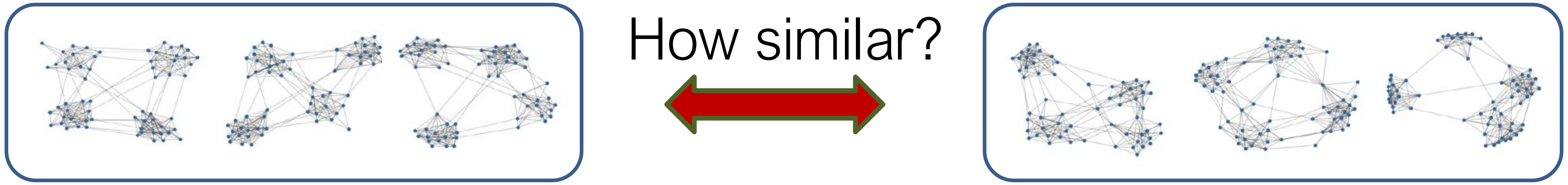
With BFS ordering

Connectivity with
All Previous nodes

Connectivity only with
nodes in the BFS frontier

Evaluating Generated Graphs

- **Task: Compare two sets of graphs**

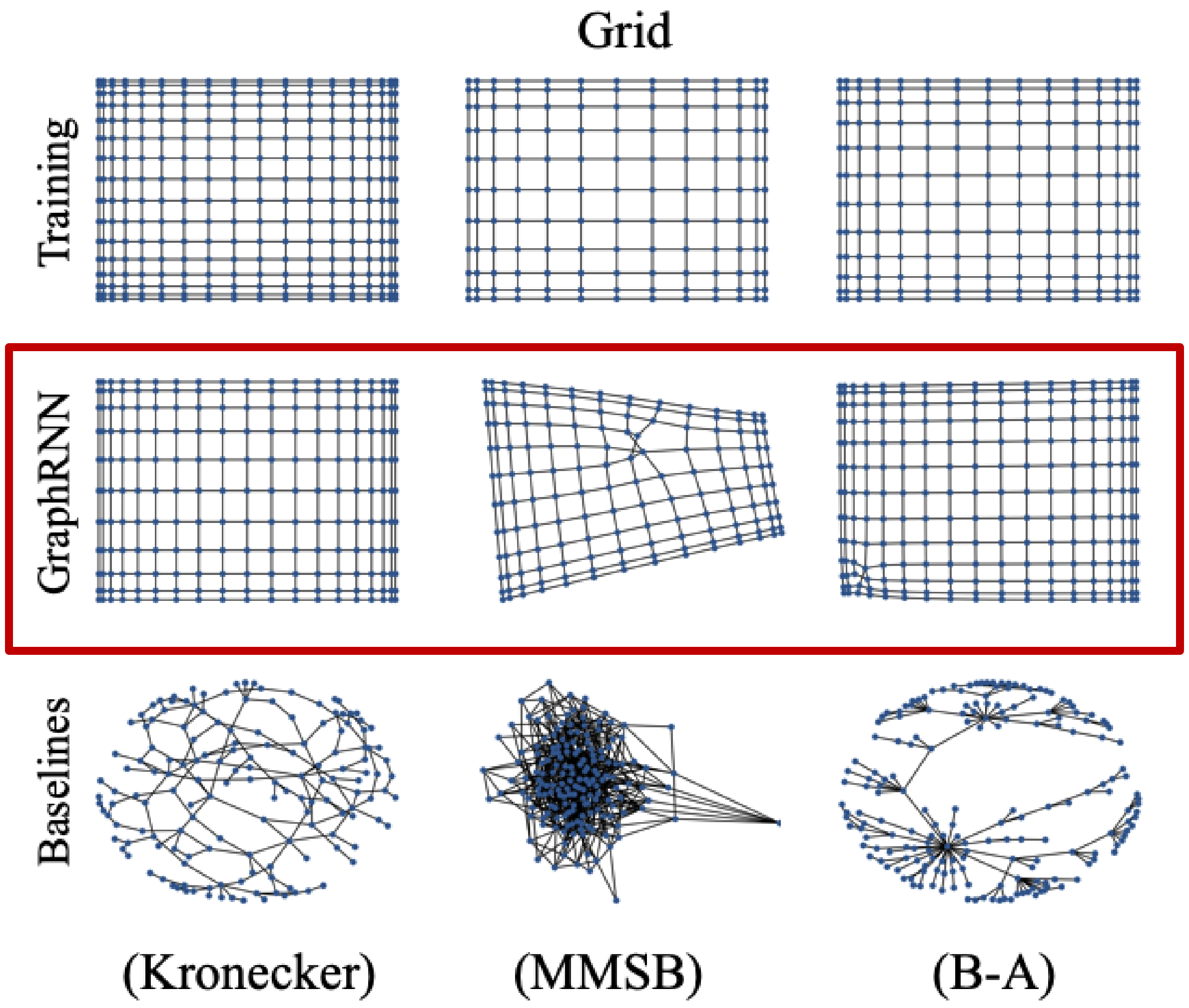


How similar?

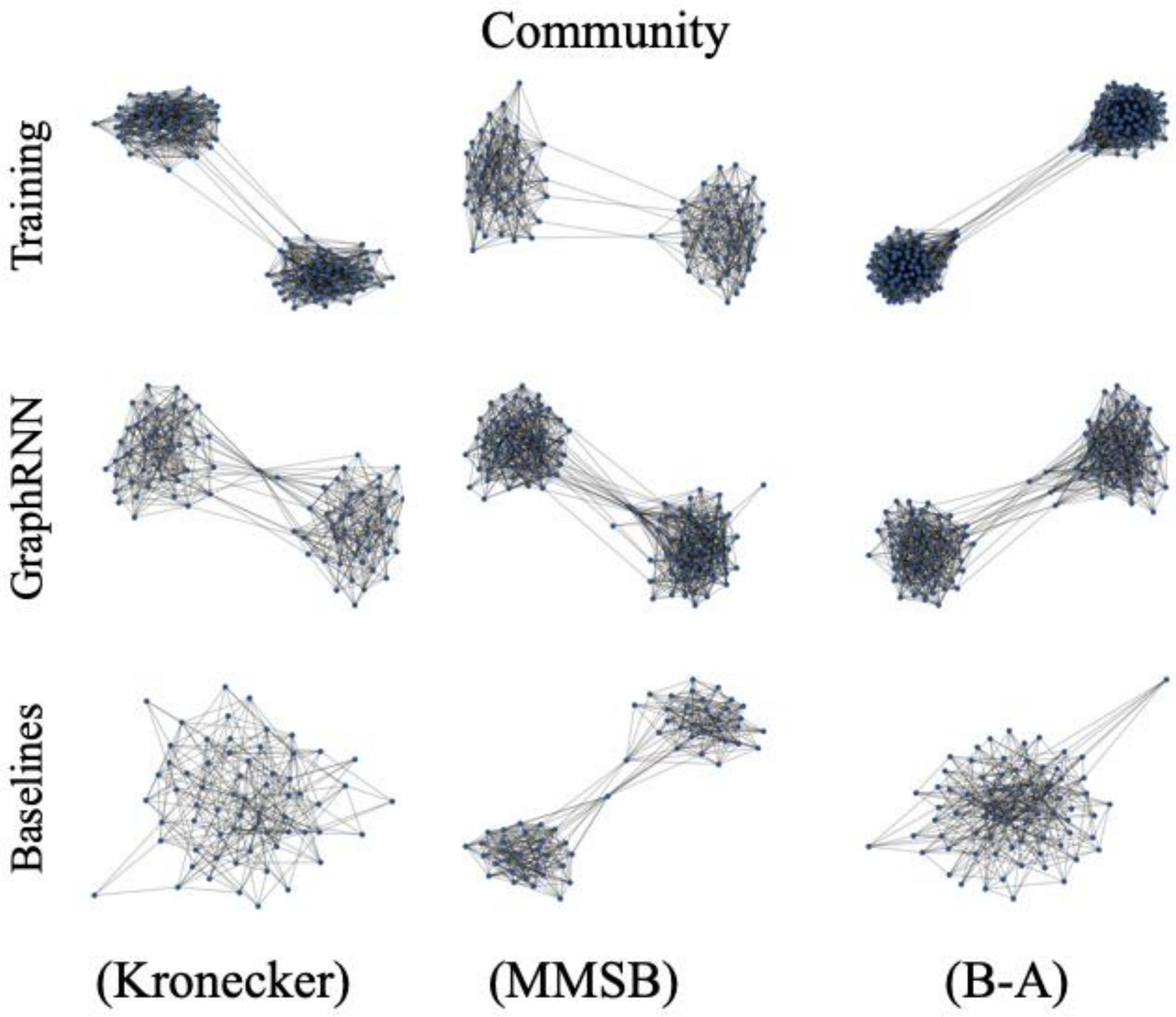
- **Goal:** Define similarity metrics for graphs

- **Solution**
  - **(1) Visual similarity**
  - **(2) Graph statistics similarity**

(1) Visual Similarity



(1) Visual Similarity

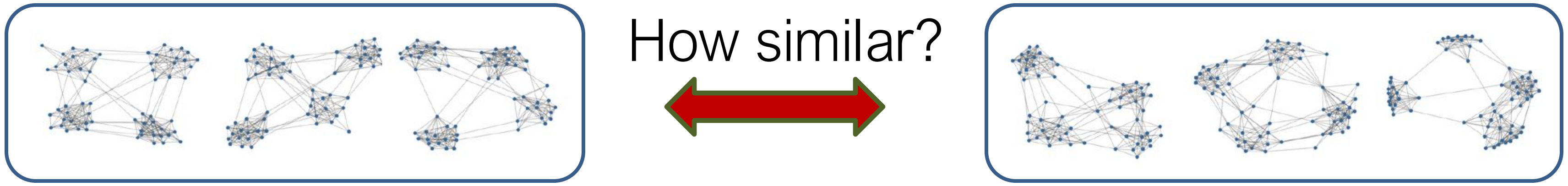


(2) Graph statistics similarity

- **Can we do more rigorous comparison?**
- **Issue:** Direct comparison between two graphs is hard (isomorphism test is NP)!
- **Solution:** Compare **graph statistics**!
- Typical Graph Statistics:
  - Degree distribution (Deg.)
  - Clustering coefficient distribution (Clus.)
  - Orbit count statistics (Orbit)
- **Note:** Each statistic is a probability distribution

(2) Graph statistics similarity

- **Issue:** want to compare sets of training graph statistics and generated graph statistics

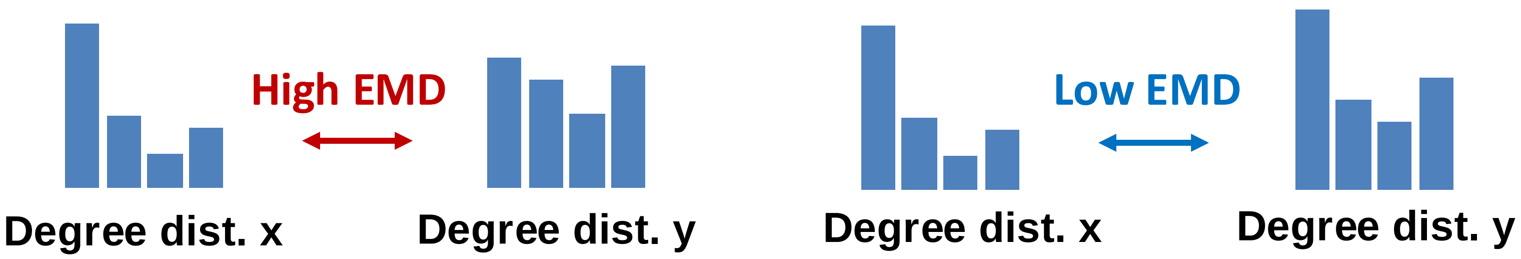


How similar?

- **Solution:**
- **Step 1:** How to compare two graph statistics
  - Earth Mover Distance (EMD)
- **Step 2:** How to compare sets of graph statistics
  - Maximum Mean Discrepancy (MMD) based on EMD

(2) Graph statistics similarity

- **Step 1: Earth Mover Distance (EMD)**
  - Compare **similarity between 2 distributions**
  - **Intuition:** Measure the minimum effort that **move earth from one pile to the other**



The EMD can be solved as the optimal flow and is found by solving this linear optimization problem.

$$\mathrm{WORK}(F, \mathbf{x}, \mathbf{y}) = \sum_{i=1}^{m} \sum_{j=1}^{n} f_{ij} d_{ij}$$

We want to find a flow F, with f_{ij} the flow between distributions x_i and y_j, that minimizes the overall cost. d_{ij} is the ground distance between x_i and y_j.

(2) Graph statistics similarity

- **Step 2: Maximum Mean Discrepancy (MMD)**
  - Idea of representing distances between distributions as distances between *mean embeddings* of feature

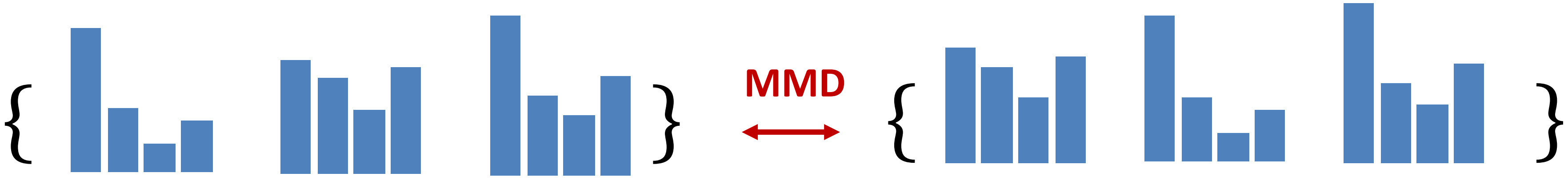
$$\mathrm{MMD}^2(p||q) = \mathbb{E}_{x,y\sim p}[k(x,y)] + \mathbb{E}_{x,y\sim q}[k(x,y)] \\ - 2\mathbb{E}_{x\sim p, y\sim q}[k(x,y)].$$

{2,3,5} **High MMD** ↔ {8,2,3] {2,3,5} **Low MMD** ↔ {5,4,2}

Similarity between set elements: L2 distance

(Each element is a scalar)

  - **Recall: We compare 2 sets of graph statistics (distributions)**

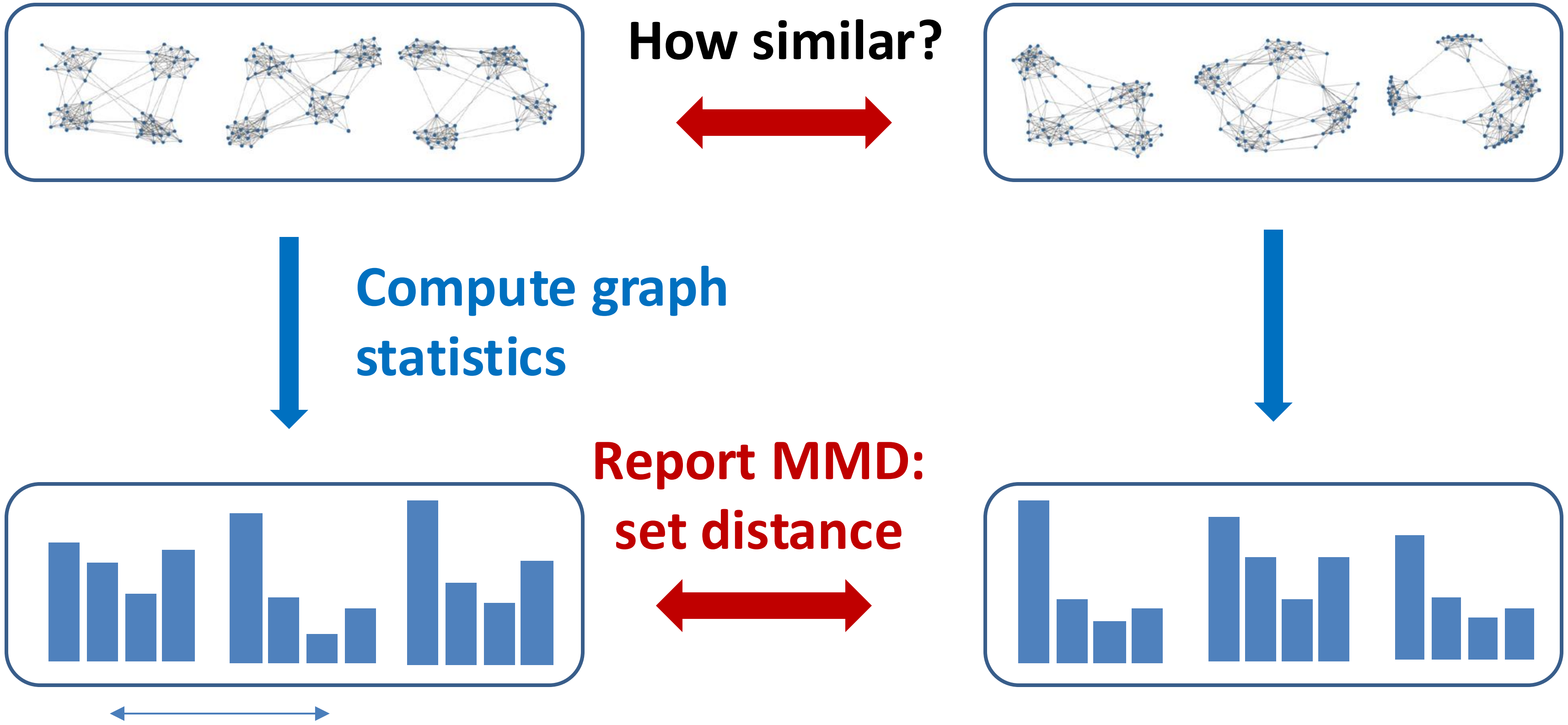


Similarity between set elements: EMD

(Each element is a distribution)

(2) Graph statistics similarity

- Putting things together



How similar?

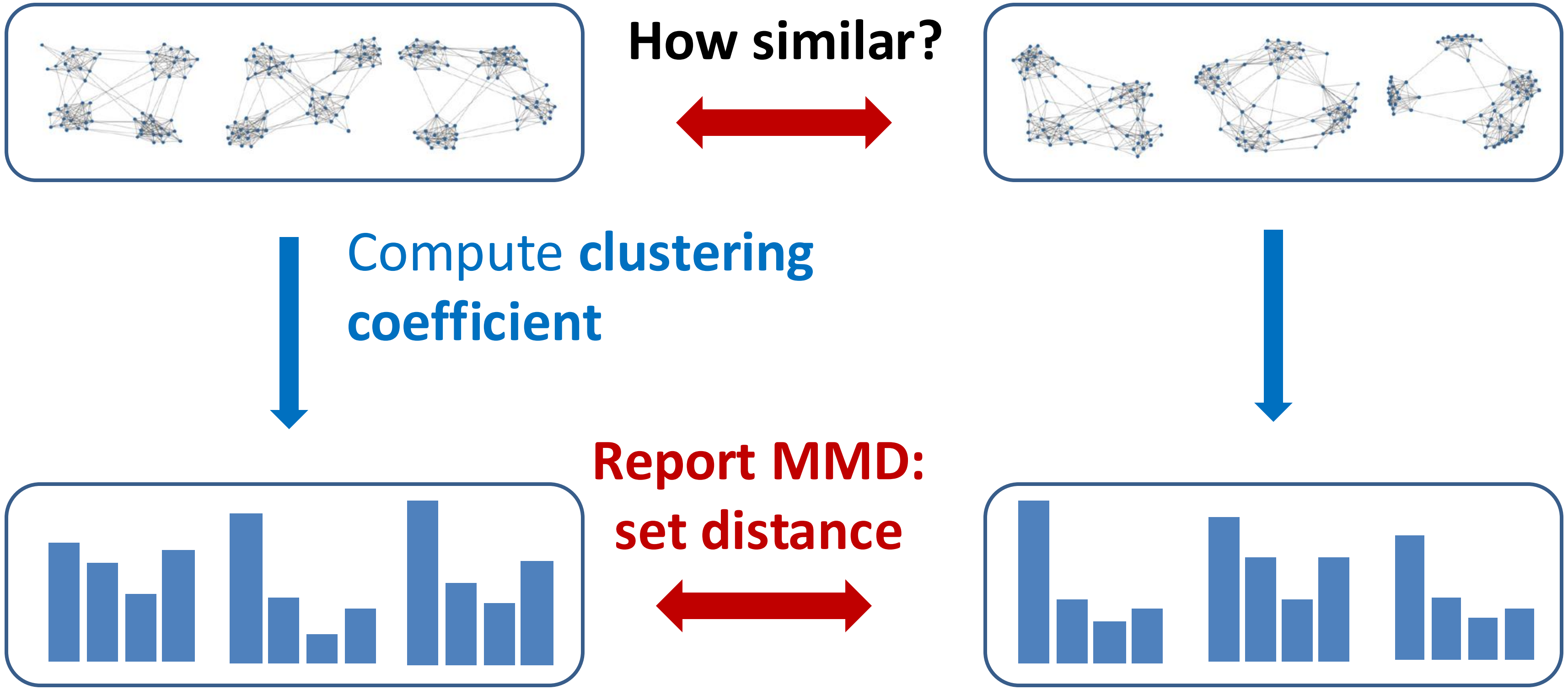
Compute graph statistics

Report MMD: set distance

where similarity between set elements are computed by EMD distribution distance

(2) Graph statistics similarity

- **Example**



How similar?

Compute **clustering coefficient**

Report MMD: set distance

	Erdos-Renyi	Kronecker	GraphRNN
MMD score	1.24	1.67	**0.002**

(2) Graph statistics similarity

- Compared to traditional graph generative models, GraphRNN can generated graphs with statistics **very close to ground-truth graphs**

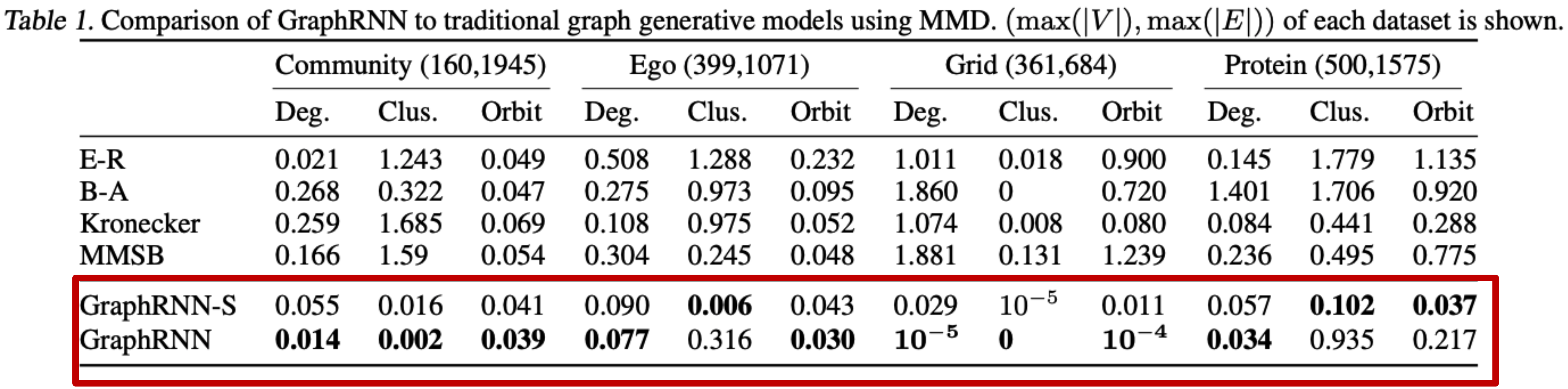


Table 1. Comparison of GraphRNN to traditional graph generative models using MMD. $(\max(|V|), \max(|E|))$ of each dataset is shown.

	Community (160,1945)			Ego (399,1071)			Grid (361,684)			Protein (500,1575)		
	Deg.	Clus.	Orbit	Deg.	Clus.	Orbit	Deg.	Clus.	Orbit	Deg.	Clus.	Orbit
E-R	0.021	1.243	0.049	0.508	1.288	0.232	1.011	0.018	0.900	0.145	1.779	1.135
B-A	0.268	0.322	0.047	0.275	0.973	0.095	1.860	0	0.720	1.401	1.706	0.920
Kronecker	0.259	1.685	0.069	0.108	0.975	0.052	1.074	0.008	0.080	0.084	0.441	0.288
MMSB	0.166	1.59	0.054	0.304	0.245	0.048	1.881	0.131	1.239	0.236	0.495	0.775
GraphRNN-S	0.055	0.016	0.041	0.090	**0.006**	0.043	0.029	10^{-5}	0.011	0.057	**0.102**	**0.037**
GraphRNN	**0.014**	**0.002**	**0.039**	**0.077**	0.316	**0.030**	$\mathbf{10^{-5}}$	**0**	$\mathbf{10^{-4}}$	**0.034**	0.935	0.217

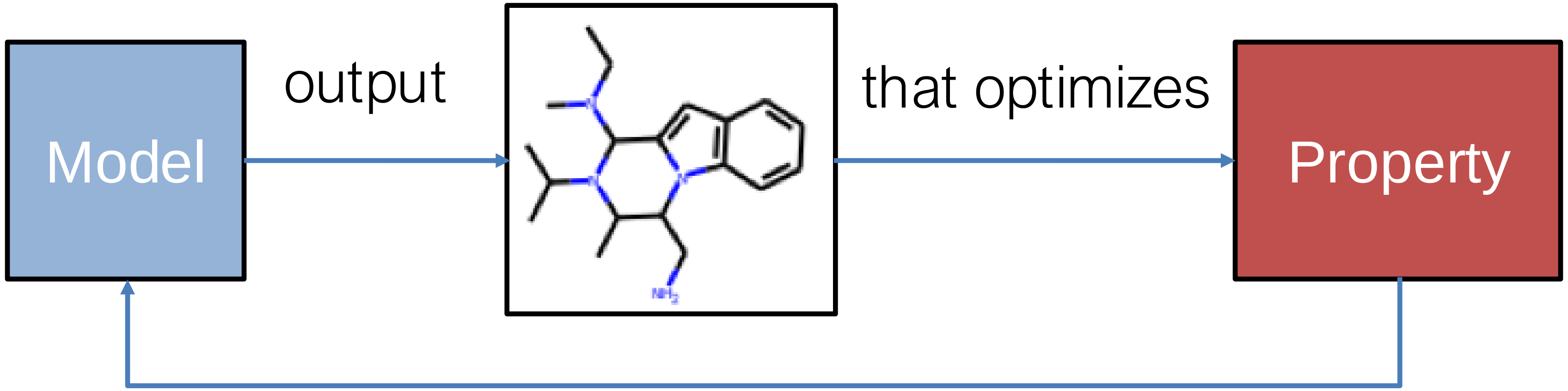
Beyond Prediction: Graph Generative Models

Application of Deep Graph Generative Models to Molecule Generation

Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation. J. You, B. Liu, R. Ying, V. Pande, J. Leskovec. *NeurIPS*, 2018.

Application: Drug Discovery

- **Question:** Can we learn a model that can generate **valid** and **realistic** molecules with **optimized** property scores?



Model

output

that optimizes

Property

e.g., `drug_likeness=0.95`

Goal-Directed Graph Generation

Generating graphs that:

- **Optimize a given objective** (High scores)
  - e.g., drug-likeness
- **Obey underlying rules** (Valid)
  - e.g., chemical validity rules
- **Are learned from examples** (Realistic)
  - Imitating a molecule graph dataset
    - We have just covered this part

Goal-Directed Graph Generation

Generating graphs that:

- **Optimize a given objective** (High scores)
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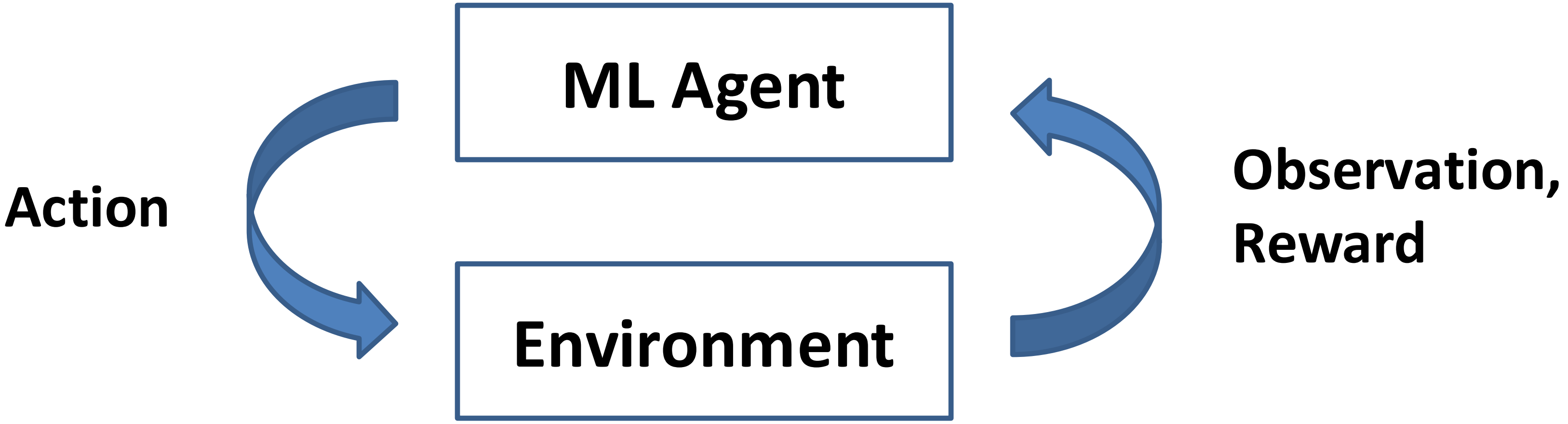
- **Are learned from examples** (Realistic)
  - Imitating a molecule graph dataset
    - We have just covered this part

A "Black-box" to Graph Generation:

Objectives like drug-likeness are governed by physical law

Idea: Reinforcement Learning

- A ML agent **observes** the environment, takes an **action** to interact with the environment, and receives positive or negative **reward**
- The agent then **learns from this loop**
- **Key idea**: Agent can directly learn from environment, which is a **blackbox** to the agent



ML Agent

Action

Observation,
Reward

Environment

Solution: GCPN

Graph Convolutional Policy Network (GCPN) combines graph representation + RL

Key component of GCPN:

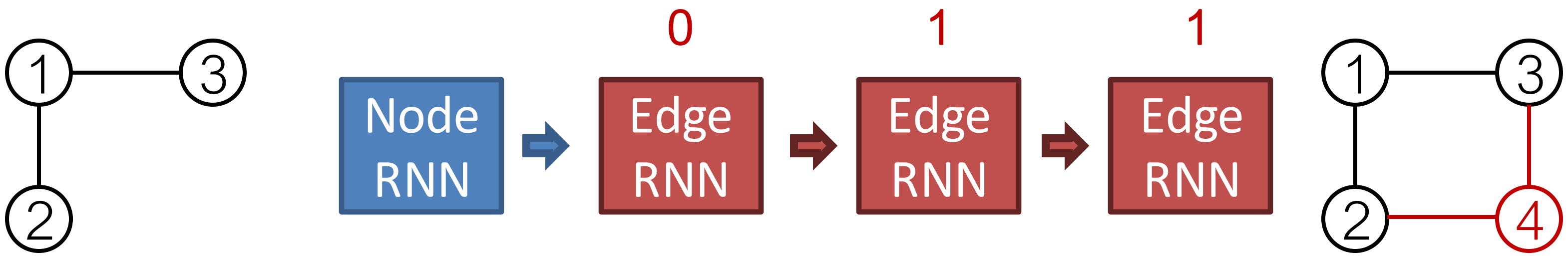
- Graph Neural Network captures graph structural information
- Reinforcement learning guides the generation towards the desired objectives
- Supervised training imitates examples in given datasets

GCPN vs. GraphRNN

- **Commonality of GCPN & GraphRNN:**
  - Generate graphs sequentially
  - Imitate a given graph dataset
- **Main Differences:**
  - GCPN uses **GNN** to predict the generation action
    - **Pros:** GNN is more expressive than RNN
    - **Cons:** GNN takes longer time to compute than RNN
  - GCPN further uses **RL** to direct graph generation to our goals
    - RL enables goal-directed graph generation

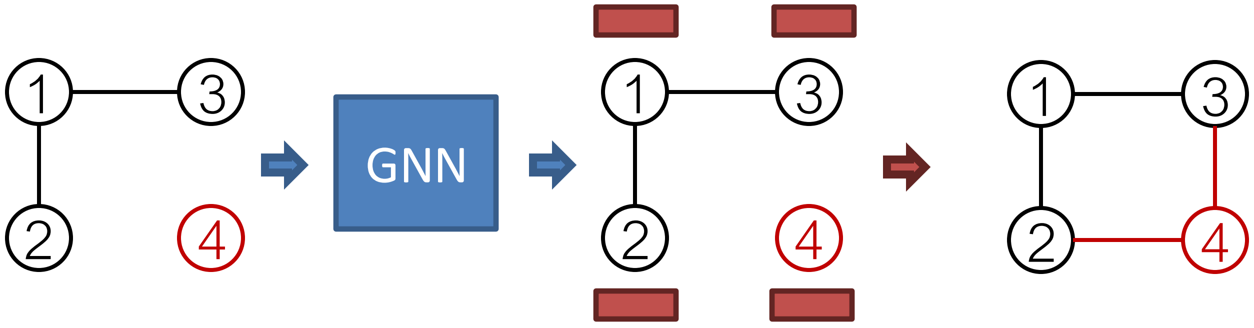
GCPN vs. GraphRNN

- **Sequential graph generation**
- **GraphRNN**: predict action based on **RNN hidden states**



RNN hidden state captures the generated graph so far

- **GCPN:** predict action based on **GNN node embeddings**



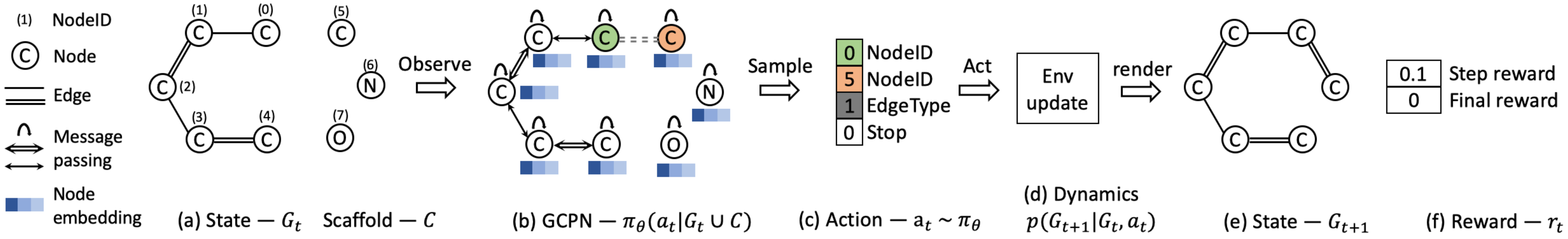
Node embeddings

Predict potential links using node embeddings

Recall the link prediction head:

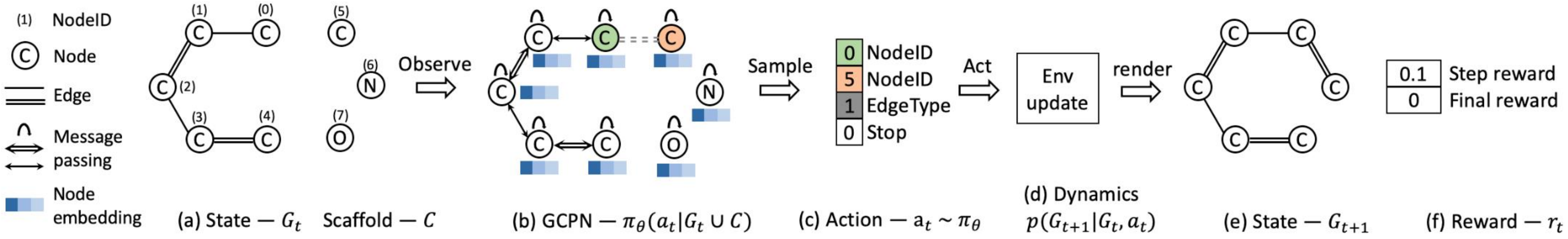
$$\text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}) := \text{Linear}(\text{Concat}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}))$$

Overview of GCPN



- **(a)** Insert nodes
- **(b,c)** Use GNN to predict which nodes to connect
- **(d)** Take an action (check chemical validity)
- **(e, f)** Compute reward

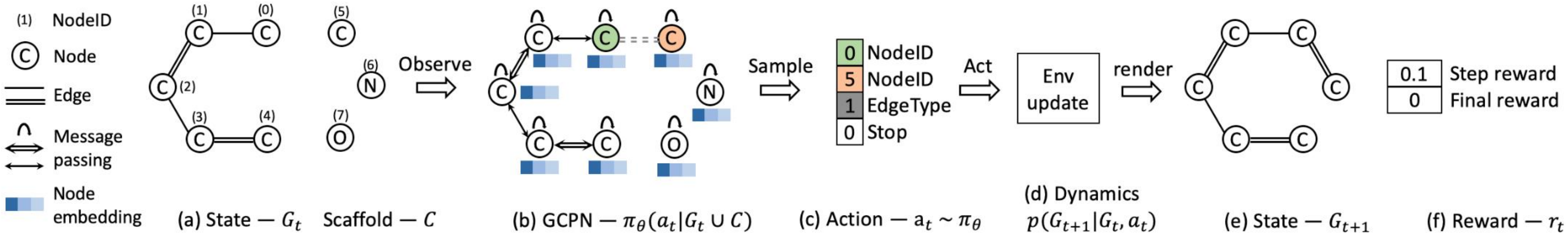
How Do We Set the Reward?



- **Step reward:** Learn to take valid action
  - At each step, assign small positive reward for valid action
- **Final reward:** Optimize desired properties
  - At the end, assign positive reward for high desired property

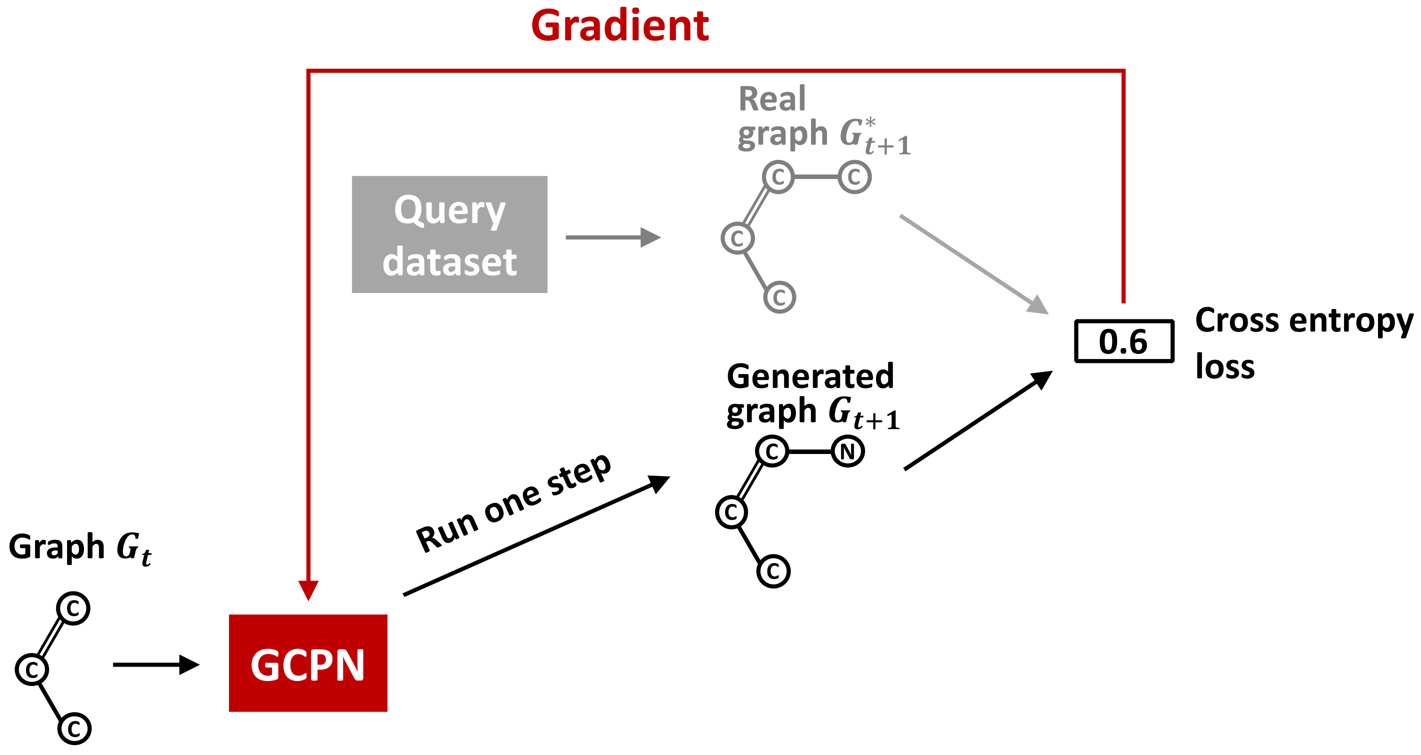
Reward = **Final reward** + **Step reward**

How Do We Train?



- **Two parts:**
- **(1) Supervised training:** Train policy by imitating the action given by real observed graphs. Use gradient.
  - We have covered this idea in GraphRNN
- **(2) RL training:** Train policy to optimize rewards. Use standard policy gradient algorithm.
  - Refer to any RL course, e.g., CS443 or CS542

Training Graph Conv. Policy Network



(1) Self-supervised training: Imitating the action given by real observed graphs with gradient

→ **Goal 1: imitation**

(2) RL training: Train policy to optimize rewards with policy gradient (PPO)

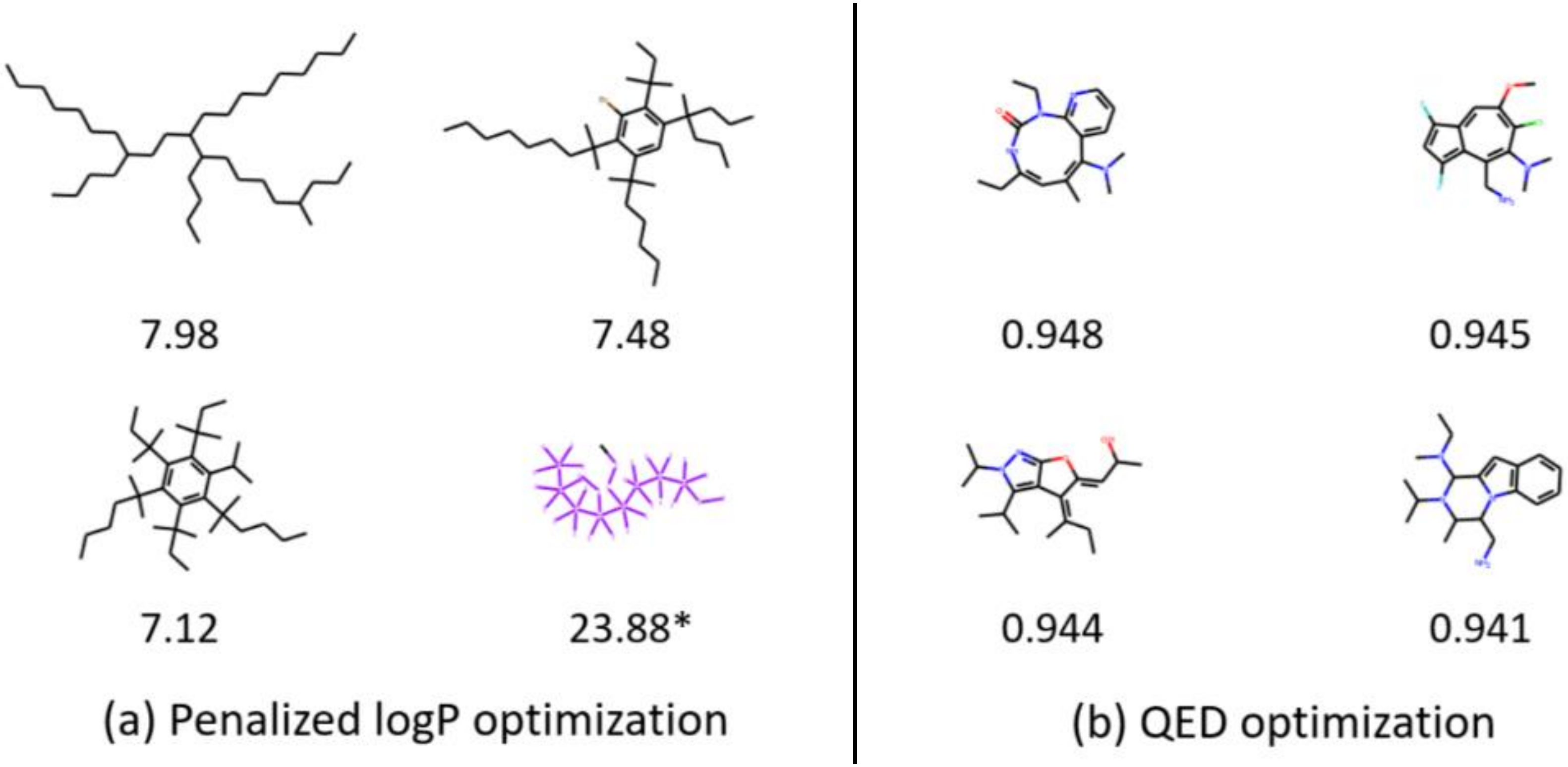
→ **Goal 2: optimization**

ChatGPT [OpenAI, 2022] uses the similar idea: **self-supervised** + **RL training**

Qualitative Results

Visualization of GCPN graphs:

- Property optimization Generate molecules with high specified property score



(a) Penalized logP optimization

(b) QED optimization

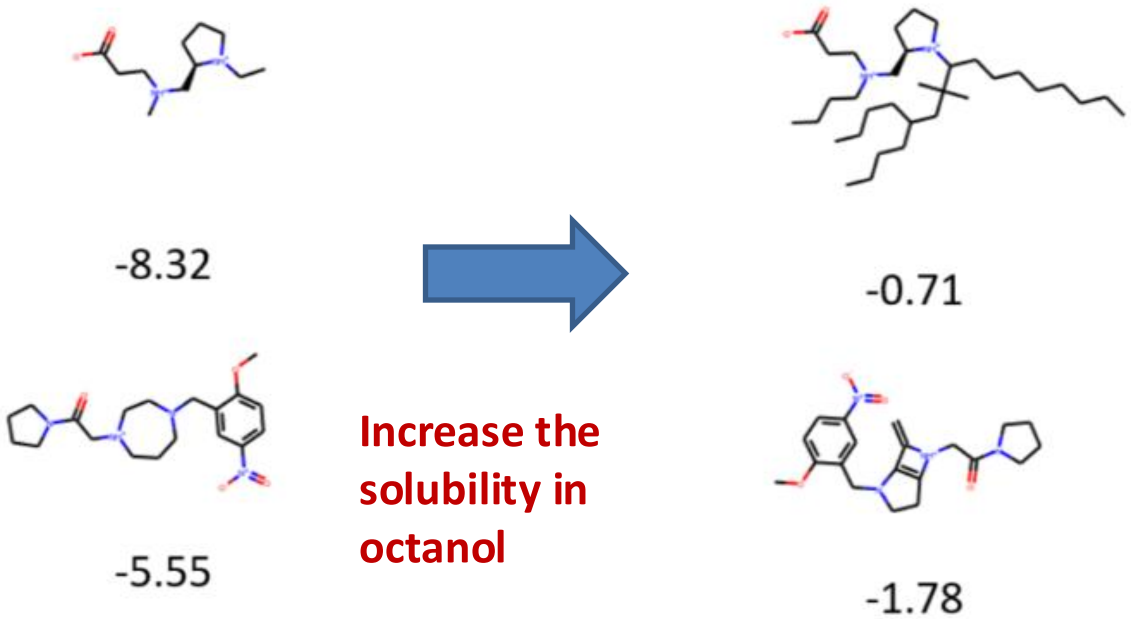
Qualitative Results

Visualization of GCPN graphs:

- Constrained optimization: Edit a given molecule for a few steps to achieve higher property score

Starting structure

Finished structure



Increase the solubility in octanol

(c) Constrained optimization of penalized logP

Summary of Graph Generation

- Complex graphs can be successfully generated via autoregressive sequential generation using deep learning
- Each step a decision is made based on hidden state, which can be
  - Implicit: vector representation, decode with RNN
  - Explicit: intermediate generated graphs, decode with GCN
- Objectives and tasks:
  - Imitating a set of given graphs: ***SFT***
  - Optimizing graphs towards given goals: ***RLHF***
  - 5 years before ChatGPT ☺