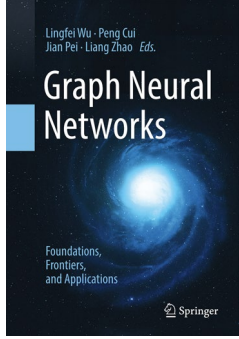


Graph Neural Networks: Foundations, Frontiers, Applications

Lingfei Wu, Liang Zhao, Xiaojie Guo,

Peng Cui and Jian Pei

IJCAI 2022 Tutorial

2022-07-24

Outline

GNNs Foundations

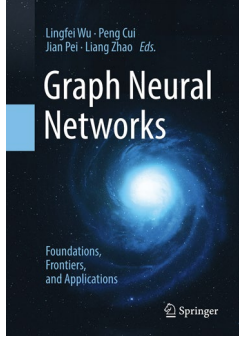
- Time History of GNNs
- GNNs: Foundations and Models
- GNNs: Theory, Scalability, Interpretability

GNNs Frontiers

- Graph Generation and Transformation
- Dynamic Graph Neural Networks
- Graph Matching
- Graph Structure Learning

GNNs Applications

- GNNs in Natural Language Processing
- GNNs in Program Analysis
- GNNs in Predicting Protein Function & Interaction

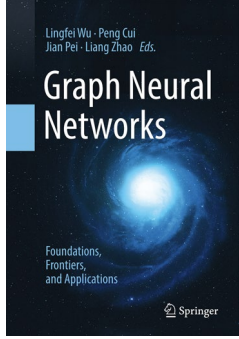


GNN book website：
https://graph-neural-networks.github.io/index.html

GNN Springer：
https://link.springer.com/book/10.1007/978-981-16-6054-2

Amazon：
https://www.amazon.com/Graph-Neural-Networks-Foundations-Applications/dp/9811660530

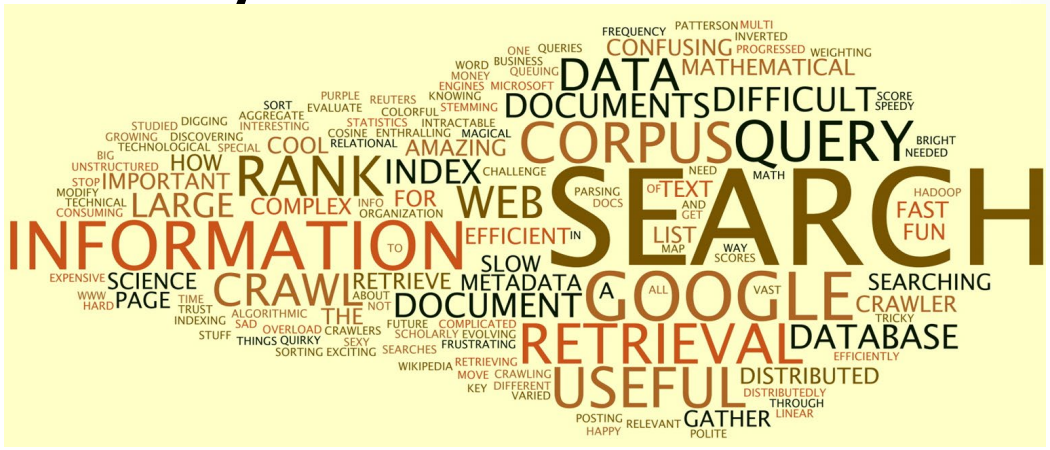
JD.com (京东商城)：
https://item.jd.com/10043589466641.html



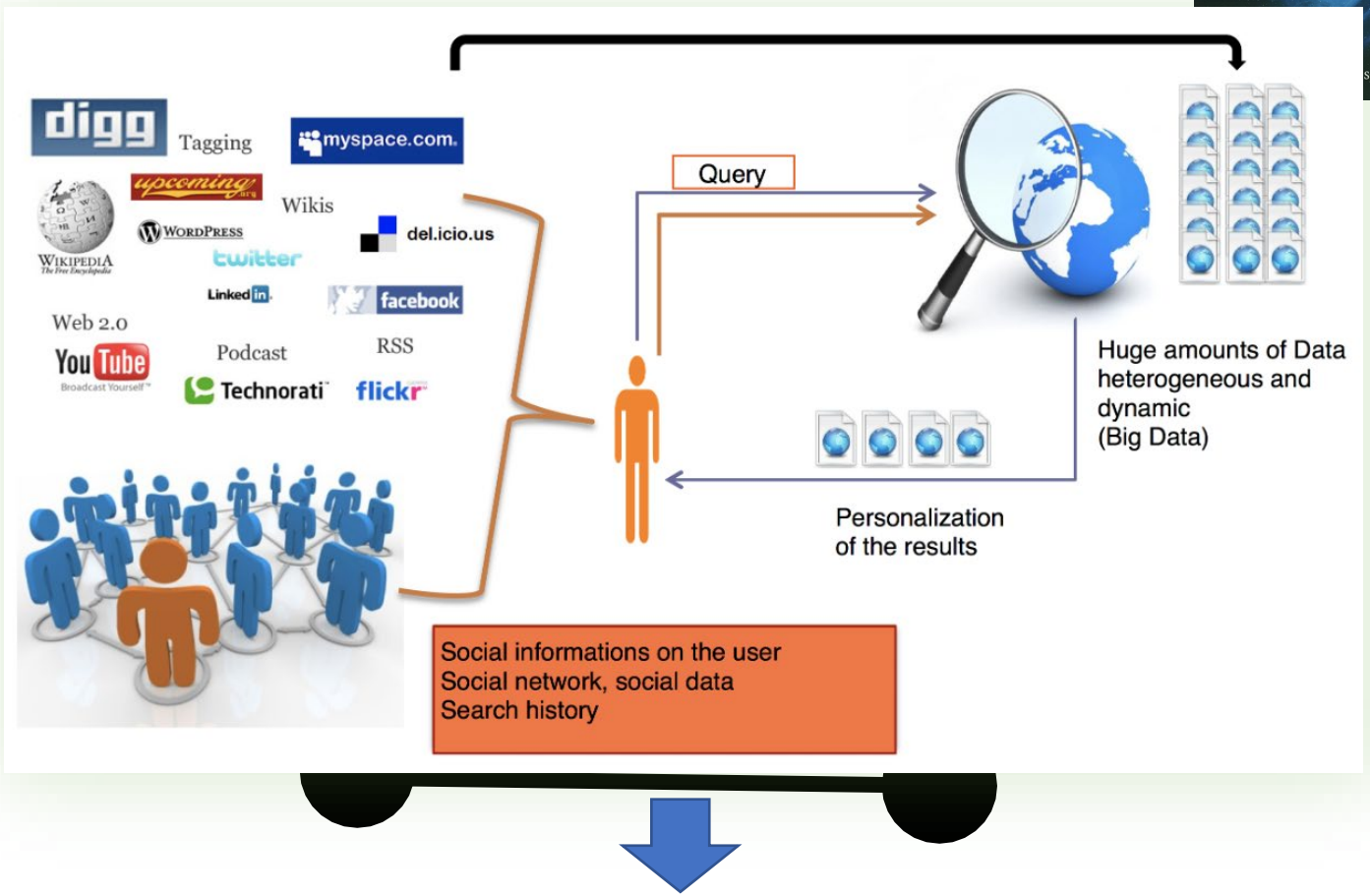
GNNs
Introduction

Why graphs?

- Graphs are a general language for describing and modeling complex systems

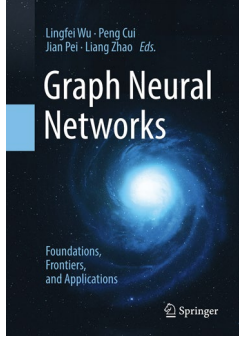


Source from Laboratoire Hubert Curien - Université Jean Monnet

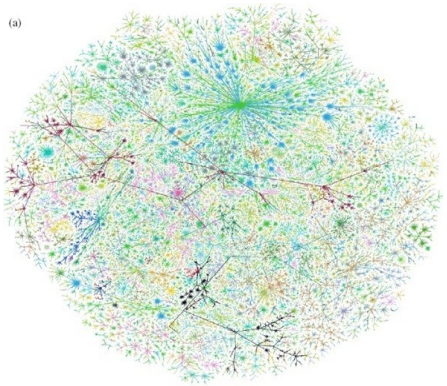


Graph Topology + Node Attributes + Node Types

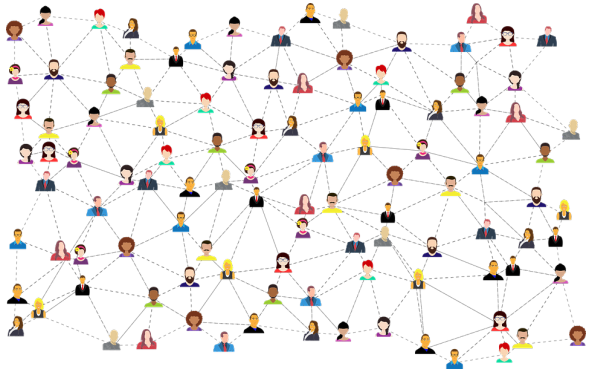
Graph!



Graph-structured data are ubiquitous

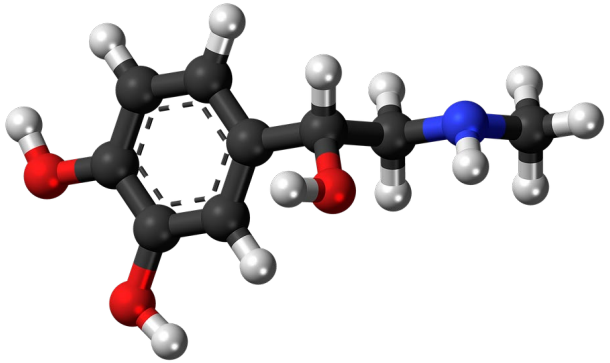


Internet

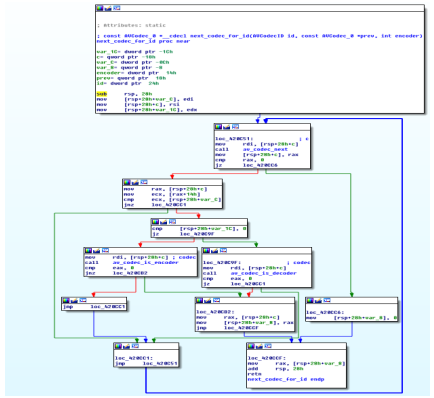


Social networks

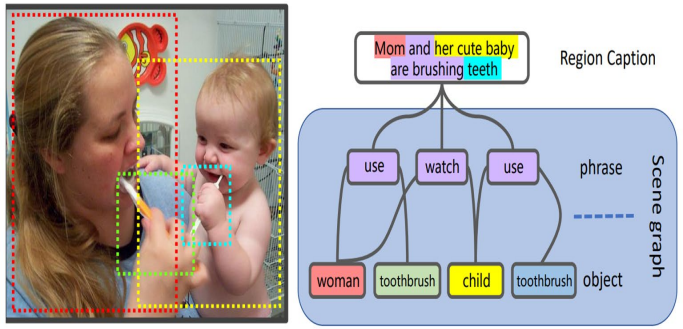
Information retrieval



Biomedical graphs

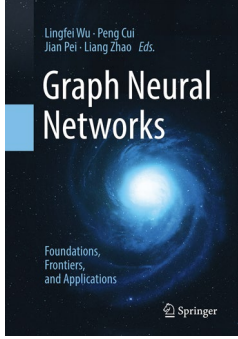


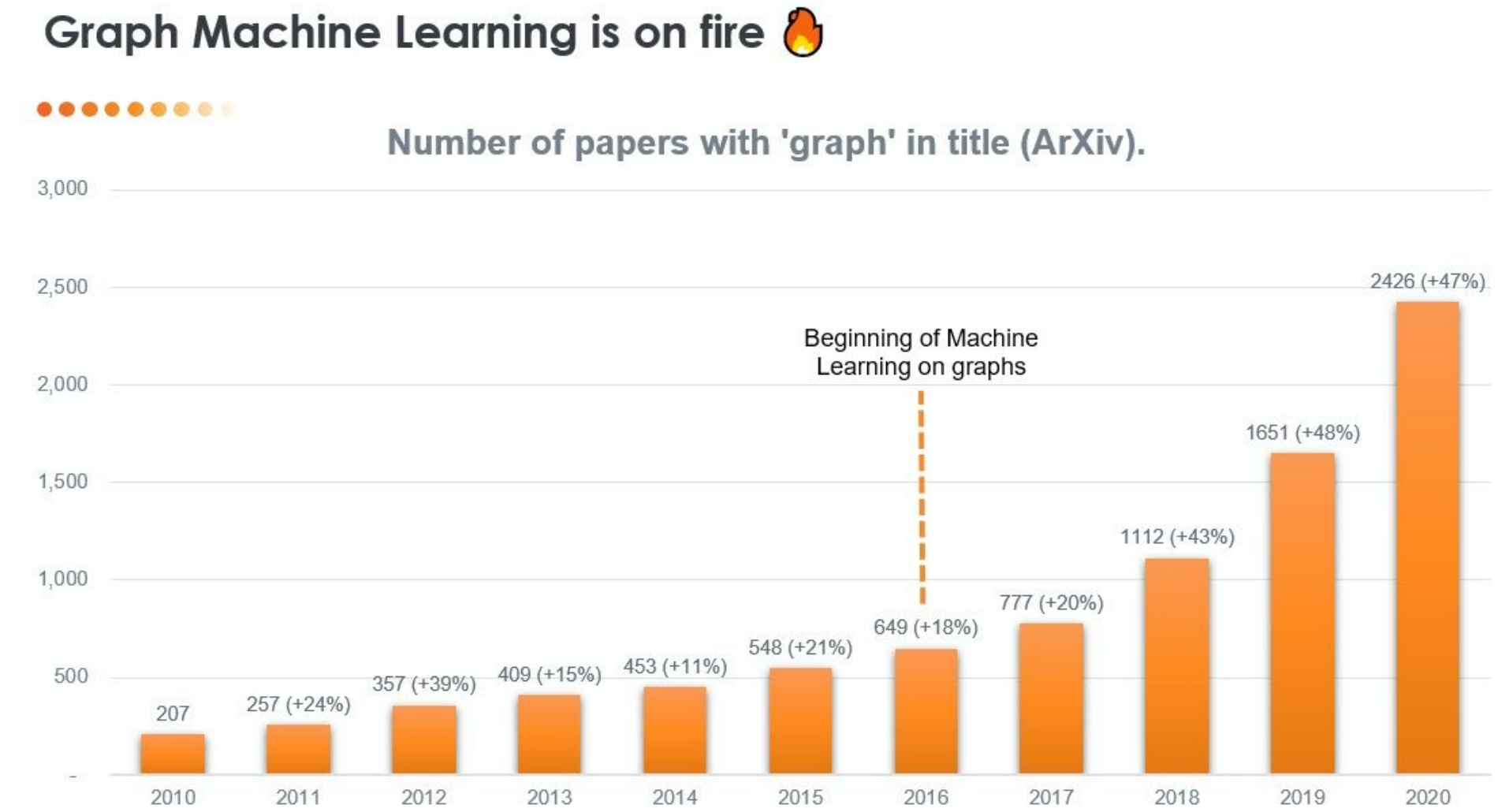
Program graphs



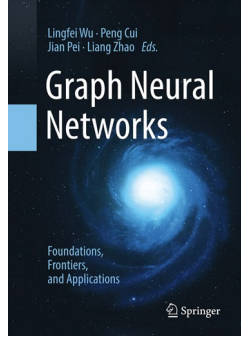
Scene graphs

Graph Machine Learning: Recent Trending





GNNs: A Brief History



Year 2009

First GNNs Paper (Scarselli et al., 2009)

Year 2016, 2017

First GRU-based Modern GNNs paper: GGNN

First graph convolution-based paper GCN, Start a new era of GNNs history

Year 2017-2021

A series of Graph Convolution (GCN), Message Passage (MPNN, GraphSage, GIN), Attention-based (GAT)

Year 2019-2021

GNNs–based applications, such as search, Recommendation, drug discovery, NLP, intelligent Transport…

Many open-source Githubs like DGL, Pytorch Geometric, Graph4NLP, TorchDrug…

Year 2021

3 GNN books released simultaneously:

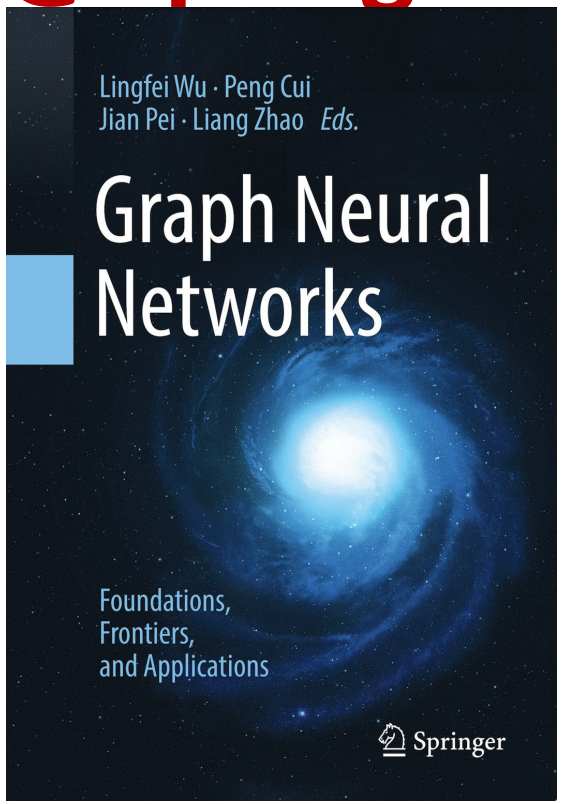
1）Prof. Liu (Tsinghua) et al.: "Introduction to Graph Neural Networks"

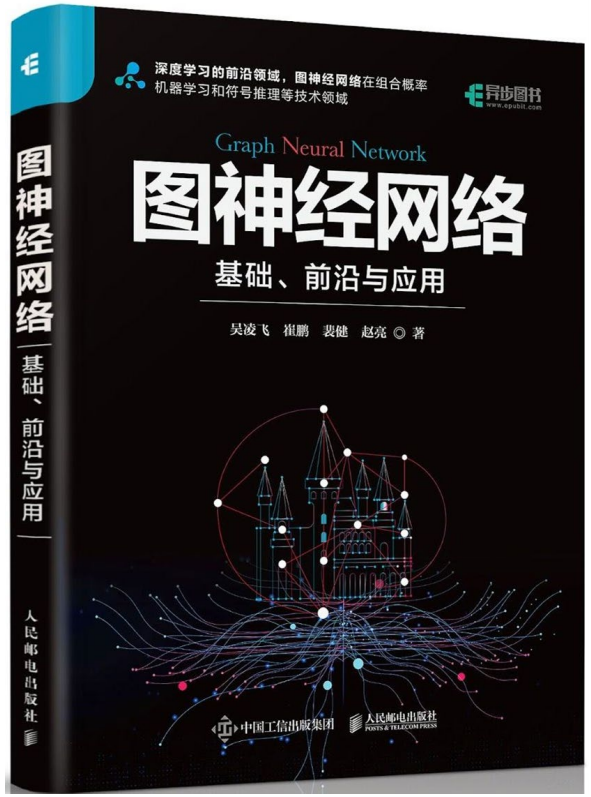
2）Prof. Tang (MSU) et al.: "Deep learning on

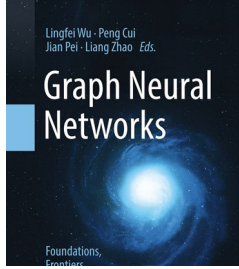
Year 2022

Most comprehensive GNN book: "Graph Neural Networks: Foundations, Frontiers, Applications" by Springer

Graph Neural Networks Book @Springer2022







Free download: https://graph-neural-networks.github.io/index.html

The English version of the book is available for pre-order on Springer, Amazon and JD.COM !

The Chinese version (人民邮电出版社) will be officially published in August 2022!!

PART I: Introduction

1. Representative Learning
2. Graph Representative Learning
3. Graph Neural Networks

PART II: Foundations

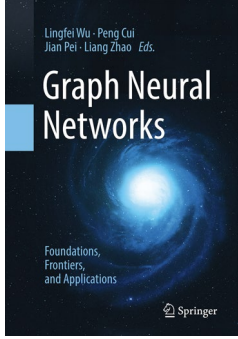
4. Graph Neural Networks for Node Classification
5. The Express Power of Graph Neural Networks
6. Graph Neural Networks: Scalability
7. Interpretability in Graph Neural Networks
8. Graph Neural Networks: Adversarial Robustness

PART III: Frontiers

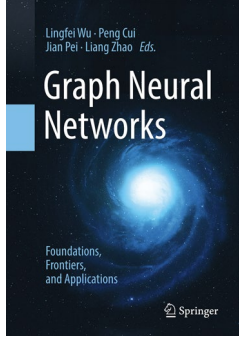
9. Graph Classification
10. Link Prediction
11. Graph Generation
12. Graph Transformation
13. Graph Matching
14. Graph Structure Learning
15. Dynamic Graph Neural Networks
16. Heterogenous Graph Neural Networks
17. Auto ML
18. Self-supervised Learning

PART IV: Broad and Emerging Applications

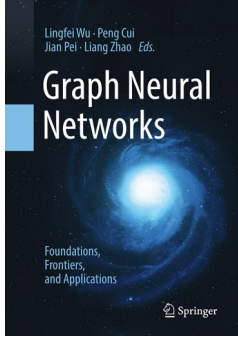
19. Graph Neural Networks in Modern Recommender System
20. Graph Neural Networks in Computer Vision
21. Graph Neural Networks in Natural Language Processing
22. Graph Neural Networks in Program Analysis
23. Graph Neural Networks in Software Mining
24. Graph Neural Networks in Drug Development
25. Graph Neural Networks in Predicting Protein functions and Interactions
26. Graph Neural Networks in Anomaly Detection
27. Graph Neural Networks in Urban Intelligence



GNNs
Foundations

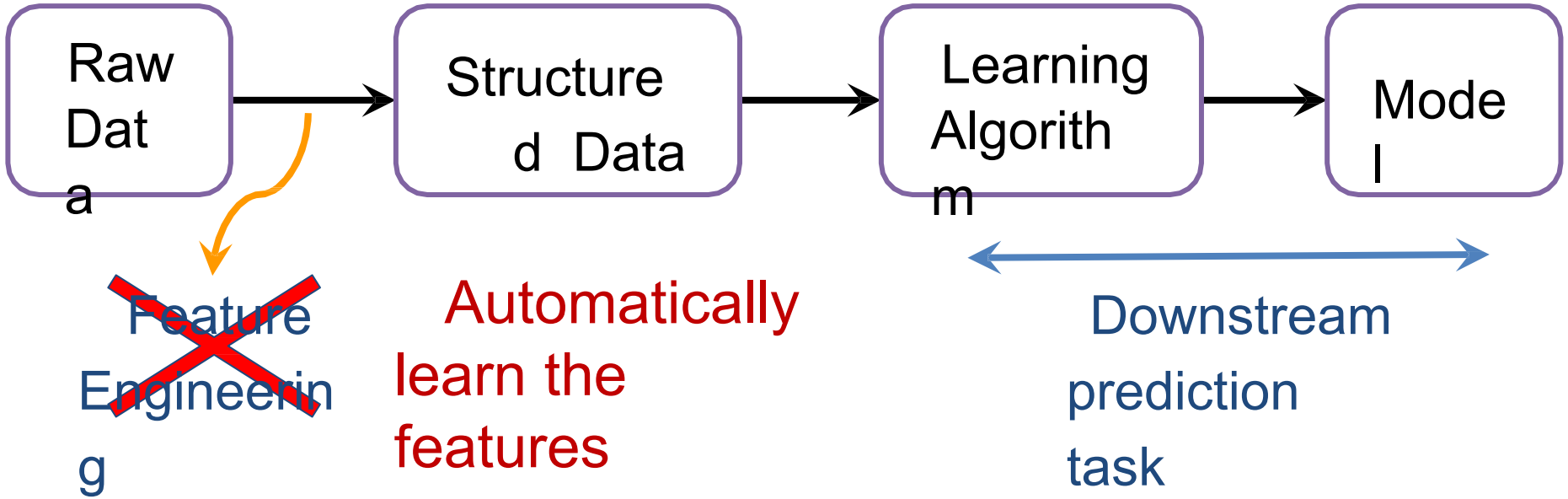


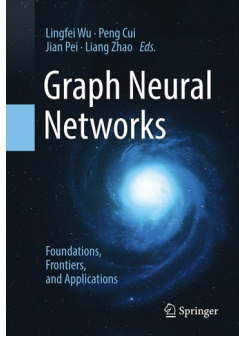
GNNs for Node Classification (Chapter 4)



Machine Learning Lifecycle

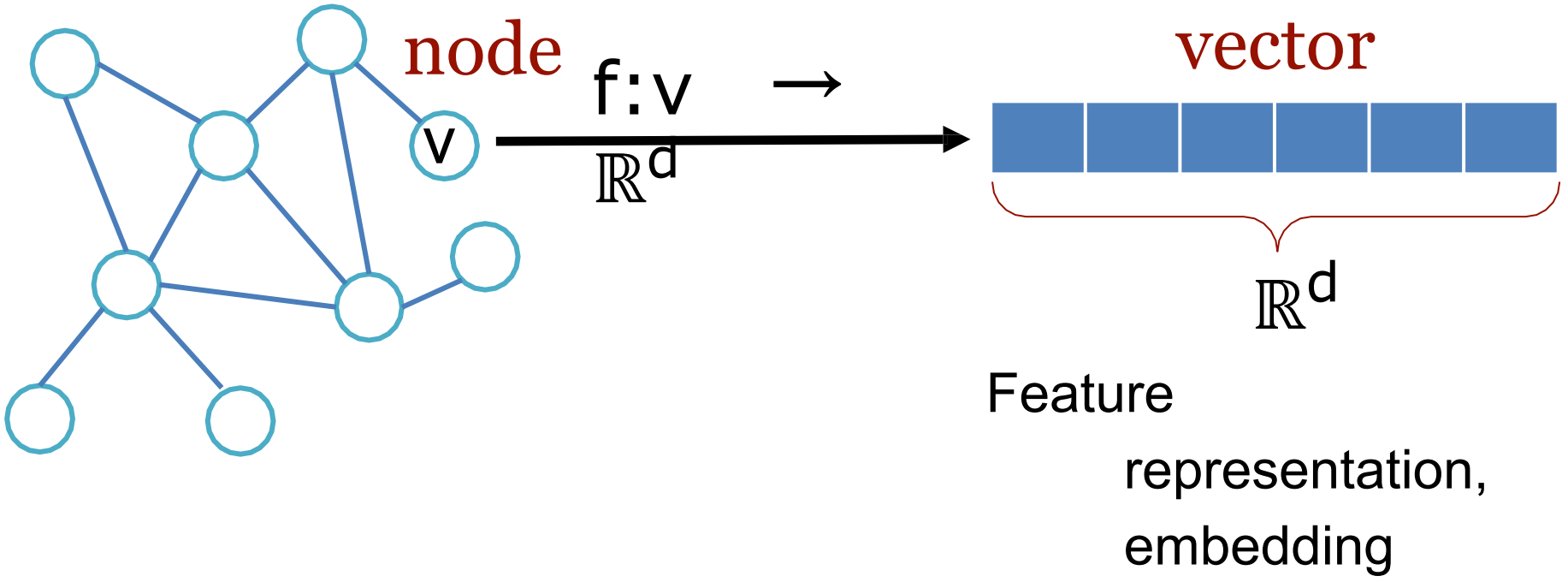
- (Supervised) Machine Learning Lifecycle: feature learning is the key

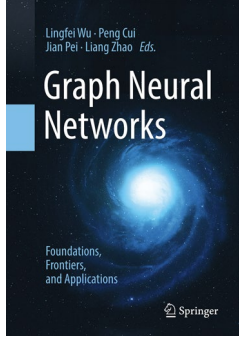




Feature Learning in Graphs

- Our Goal: Design efficient task-independent/ task-dependent feature learning for machine learning in graphs!





Graph Neural Networks: Foundations

- Learning node embeddings:

A graph filter adjacency matrix

$$\mathbf{h}_i^{(l)} = f_{\text{filter}}(A, \mathbf{H}^{(l-1)})$$

Updated node embeddings Input node embeddings

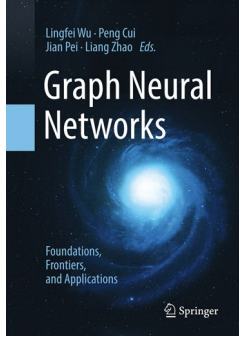
$f_{\text{filter}}(\cdot,\cdot)$
- Spectral-based
- Spatial-based
- Attention-based
- Recurrent-based

- Learning graph-level embeddings:

$$A', \mathbf{H}' = f_{\text{pool}}(A, \mathbf{H})$$

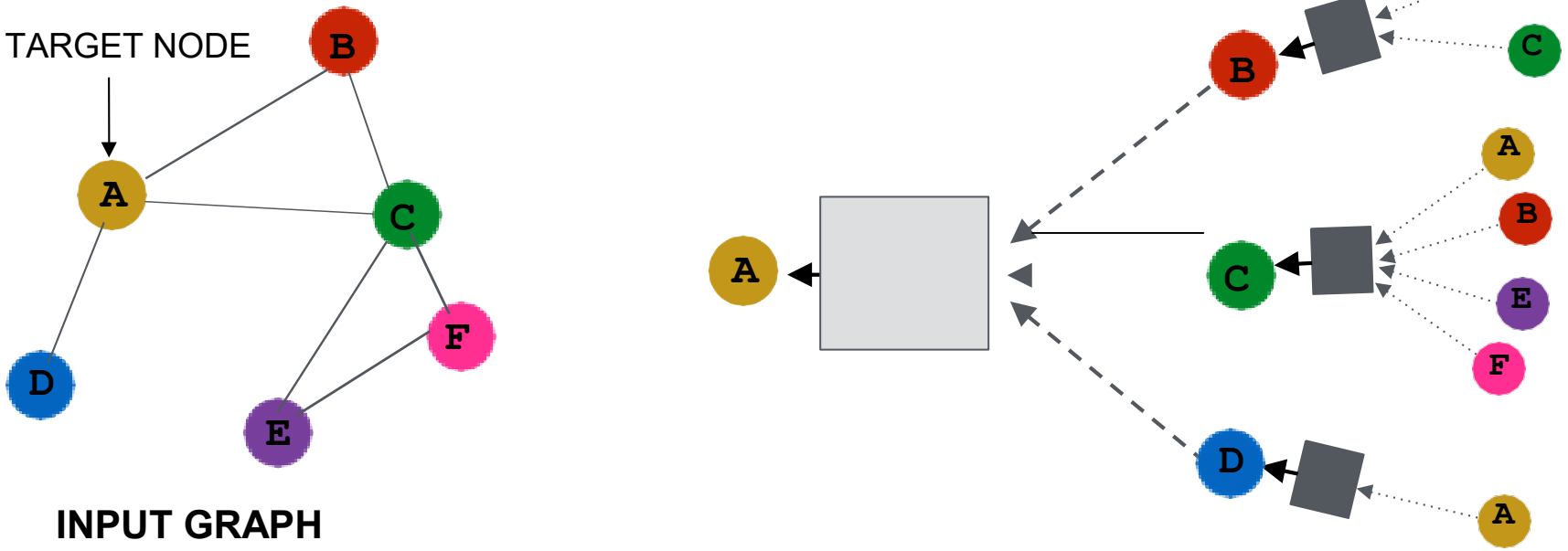
A small graph w/ fewer nodes New node embeddings Input graph Input node embeddings

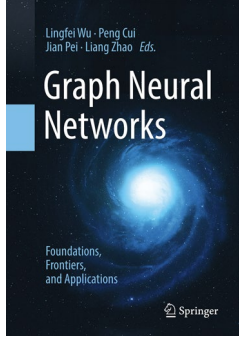
$f_{\text{pool}}(\cdot,\cdot)$
- Flat Graph Pooling (i.e. Max, Ave, Min)
- Hierarchical Graph Pooling (i.e. Diffpool)



Graph Neural Networks: Basic Model

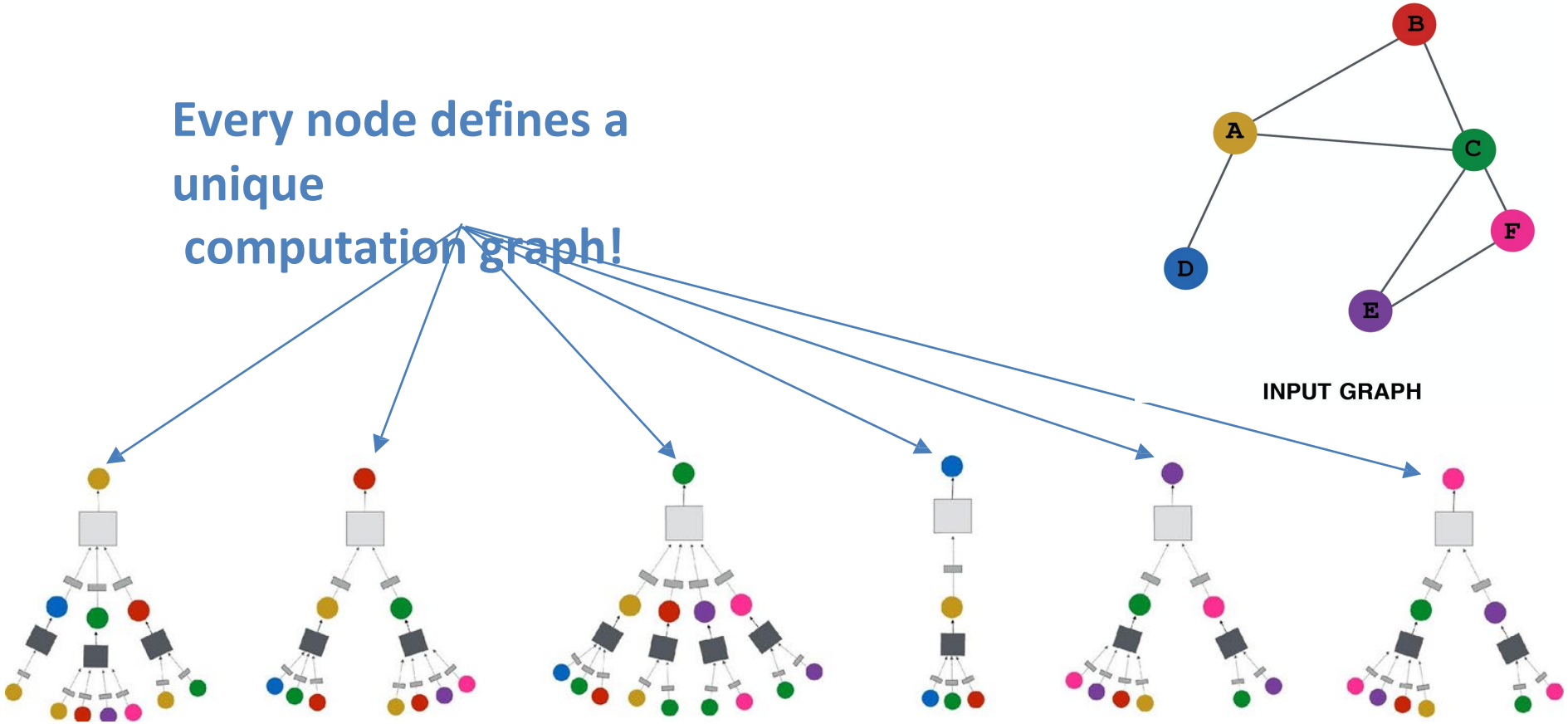
- Key idea: Generate node embeddings based on local neighborhoods.

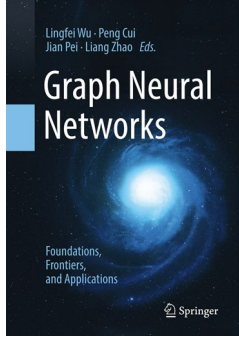




Neighborhood Aggregation

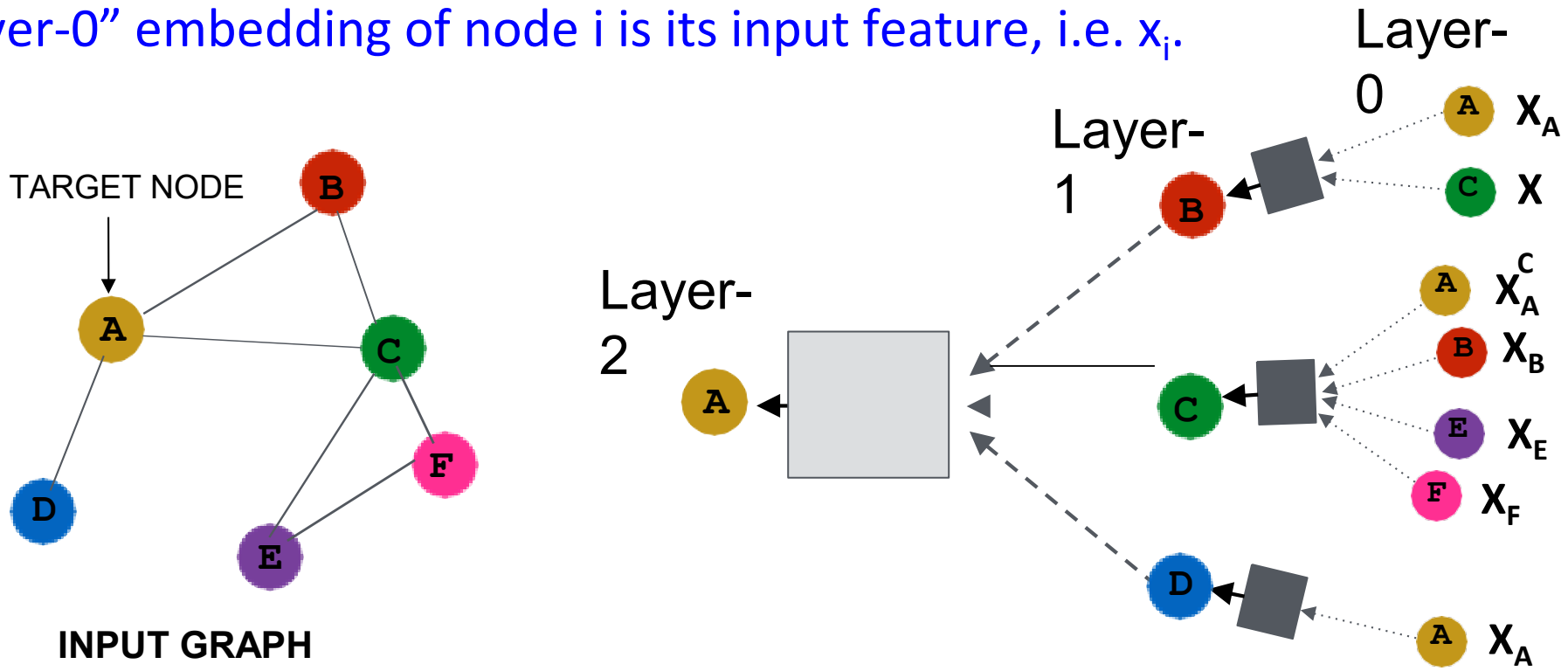
- Intuition: Network neighborhood defines a computation graph

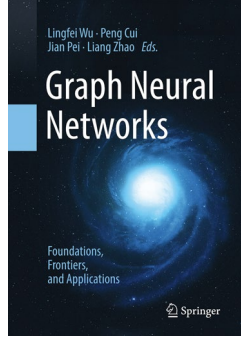




Neighborhood Aggregation

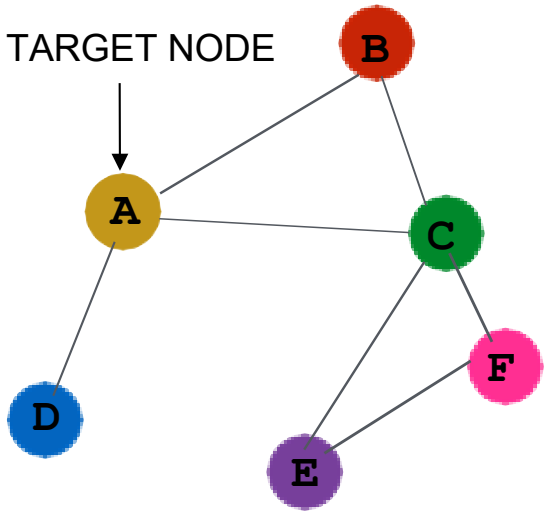
- Nodes have embeddings at each layer.
- Model can be arbitrary depth.
- "layer-0" embedding of node i is its input feature, i.e. x_i.

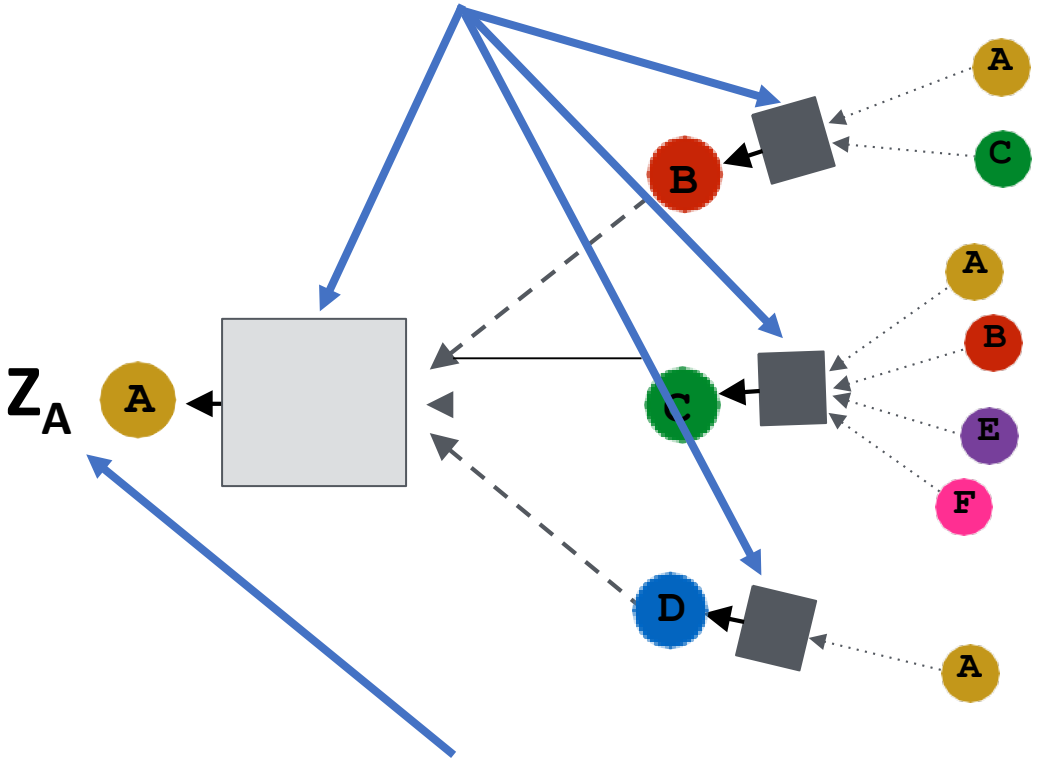




Overview of GNN Model

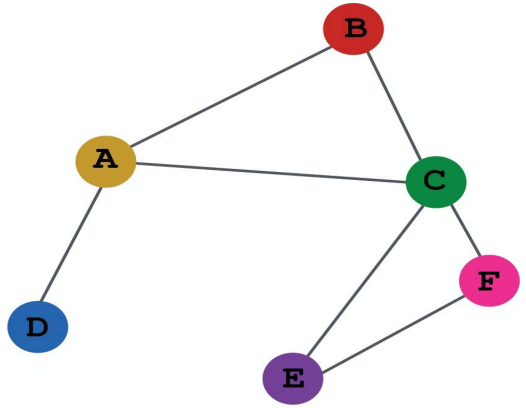
1) Define a neighborhood aggregation function





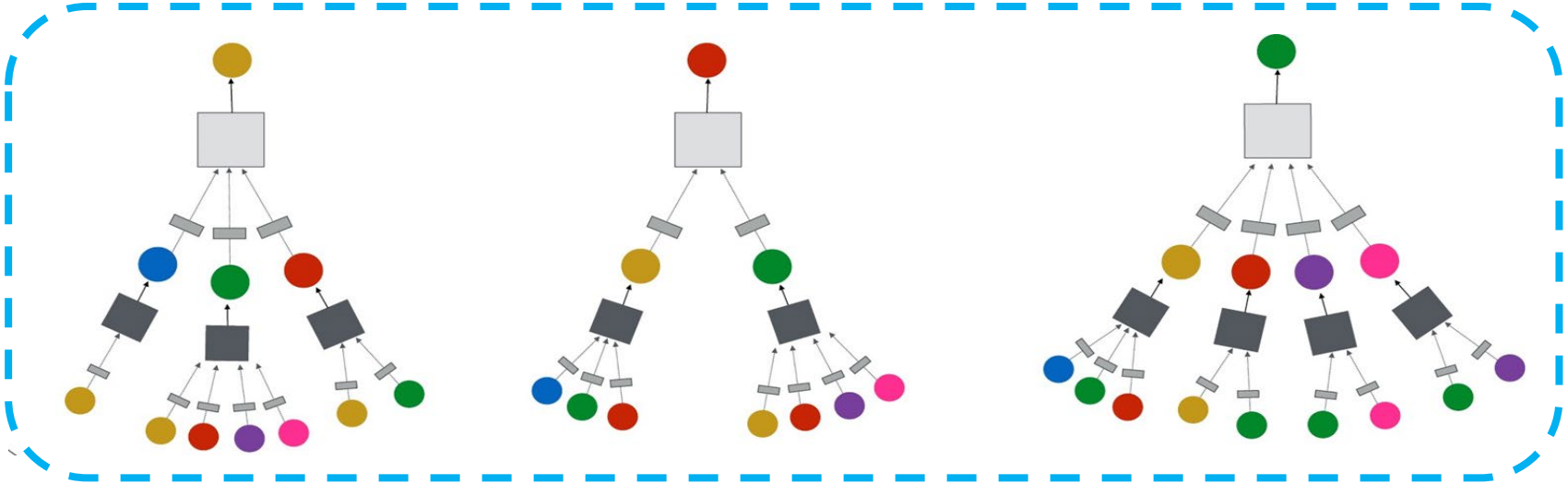
2) Define a loss function on the embeddings, $\mathbf{L(z_v)}$

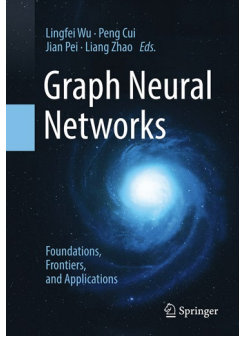
Overview of GNN Model

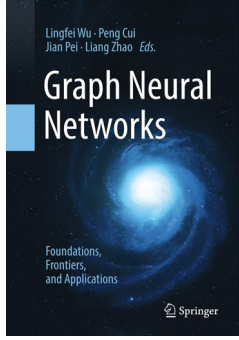


INPUT GRAPH

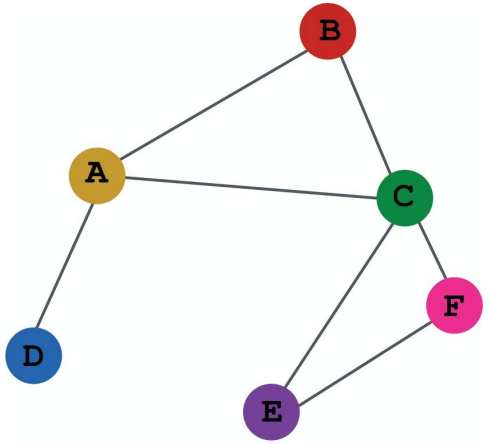
3) Train on a set of nodes, i.e., a batch of computation graphs







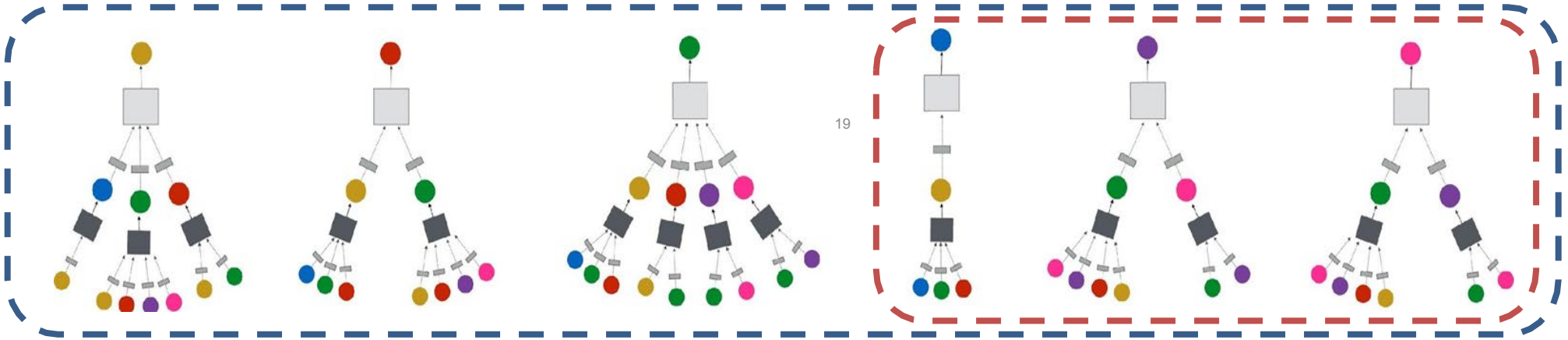
Overview of GNN Model

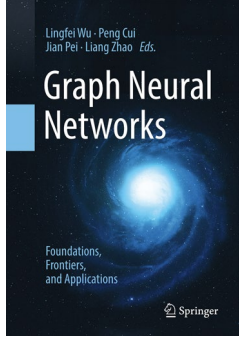


INPUT GRAPH

4) Generate embeddings for nodes as needed

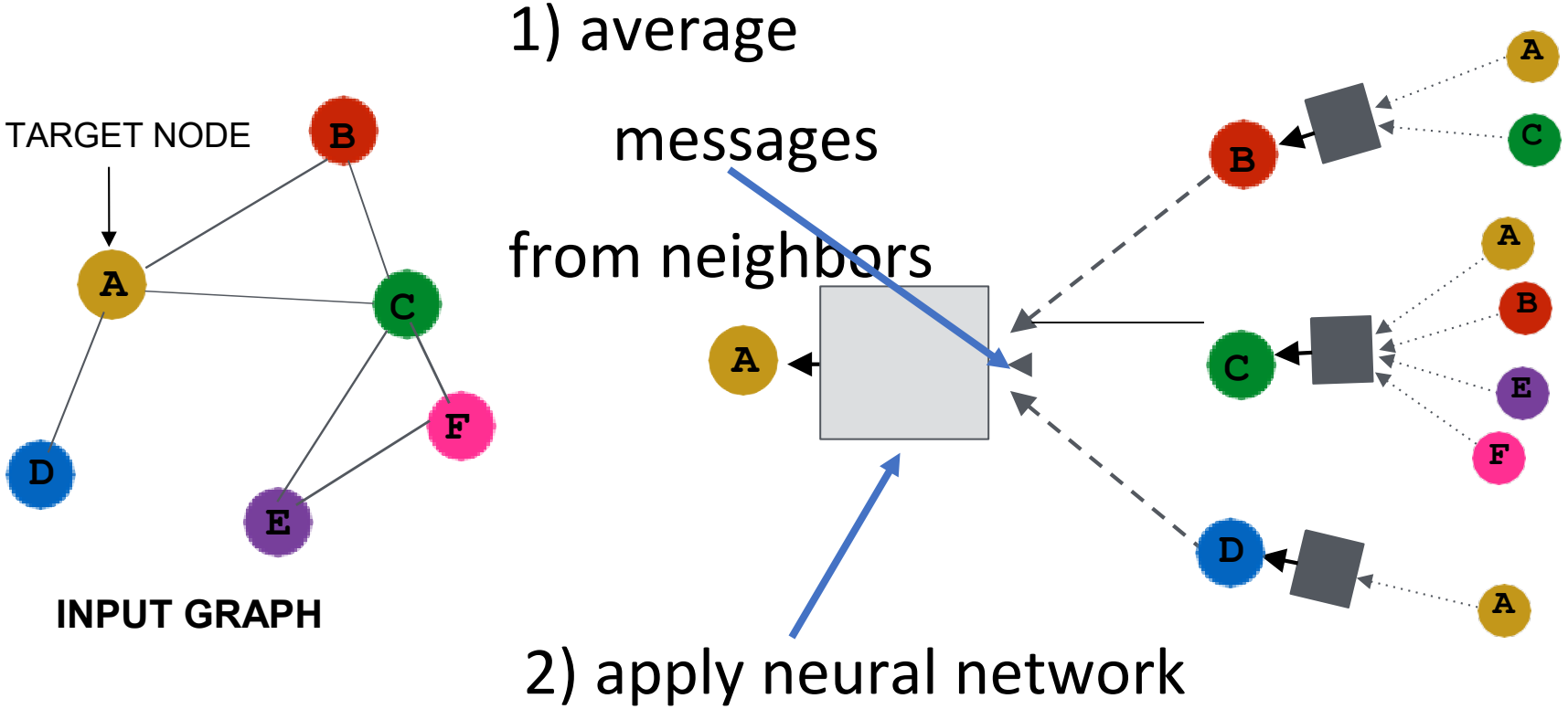
Even for nodes we never trained on!

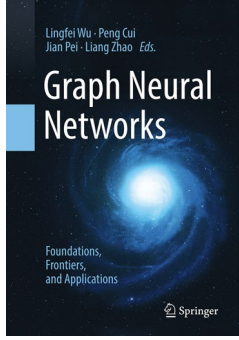




GNN Model: A Case Study

- Basic approach: Average neighbor information and apply a neural network





GNN Model: A Case Study

- Basic approach: Average neighbor information and apply a neural network.

Initial "layer 0" embeddings are equal to node features

previous layer embedding of v

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

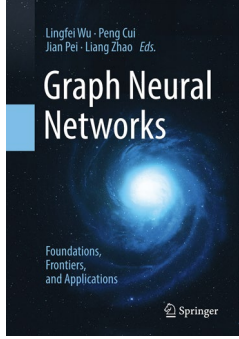
$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \quad \forall k > 0$$

kth layer embedding of v

non-linearity (e.g., ReLU or tanh)

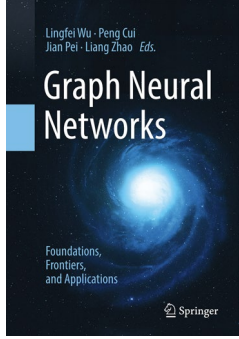
average of neighbor's previous layer embeddings

GNN Model: Quick Summary

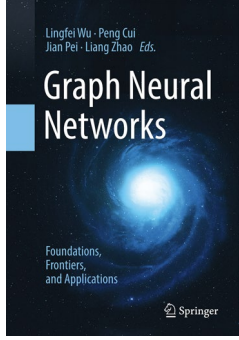


- Key idea: generate node embeddings by aggregating neighborhood information.
  - Allows for parameter sharing in the encoder
  - Allows for inductive learning

Graph Neural Networks: Popular Models



- Spectral-based Graph Filters
  - GCN (Kipf & Welling, ICLR 2017), Chebyshev-GNN (Defferrard et al. NIPS 2016)
- Spatial-based Graph Filters
  - MPNN (Gilmer et al. ICML 2017), GraphSage (Hamilton et al. NIPS 2017)
  - GIN (Xu et al. ICLR 2019)
- Attention-based Graph Filters
  - GAT (Velickovic et al. ICLR 2018)
- Recurrent-based Graph Filters
  - GGNN (Li et al. ICLR 2016)



Graph Convolution Networks (GCN)

Key idea: spectral convolution on graphs

Eigen-decomposition is expensive

$$f_{\text{filter}} * \mathbf{x}_i = \mathbf{U} f(\Lambda) \mathbf{U}^T \mathbf{x}_i$$

Chebyshev polynomials accelerates but still not powerful

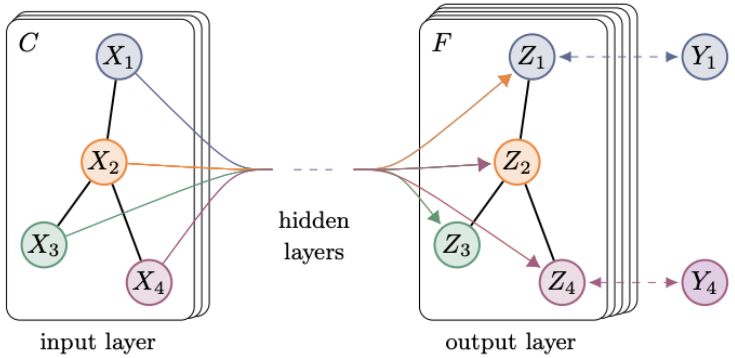
$$f'_{\text{filter}} * \mathbf{x}_i \approx \sum_{p=0}^{P} \theta'_p \mathbf{T}_p(\tilde{\mathbf{L}}) \mathbf{x}_i$$

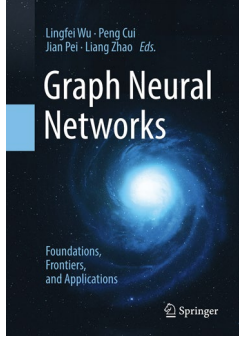
First-order approximation fast and powerful

$$f_{\text{filter}} * \mathbf{h}_i^{(l)} \approx \theta(I_n + D^{-\frac{1}{2}} A D^{-\frac{1}{2}}) \mathbf{h}_i^{(l)}$$

Renormalization trick stabilizes the numerical computation

$$\mathbf{H}^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} \mathbf{H}^{(l)} \mathbf{W}^{(l)})$$

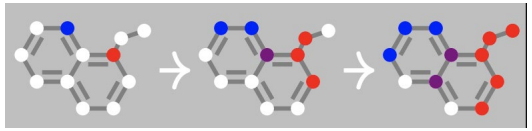




Message Passing Neural Network (MPNN)

Key idea: graph convolutions as a message passing process

MPNN: $$\mathbf{h}_i^{(l)} = f_{\text{filter}}(A, \mathbf{H}^{(l-1)}) = f_U(\mathbf{h}_i^{(l-1)}, \sum_{v_j \in N(v_i)} f_M(\mathbf{h}_i^{(l-1)}, \mathbf{h}_j^{(l-1)}, \mathbf{e}_{i,j}))$$

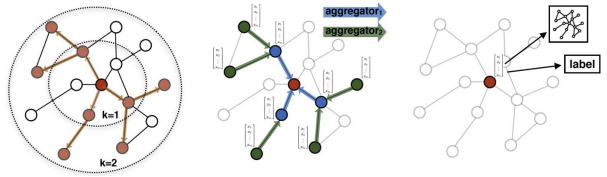


expensive if the number of nodes are large

Update and aggregation functions

Node and edge embeddings

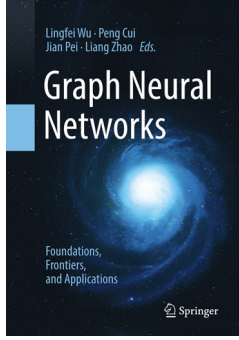
GraphSage: $$f_{\text{filter}}(A, \mathbf{H}^{(l-1)}) = \sigma(\mathbf{W}^{(l)} \cdot f_M(\mathbf{h}_i^{(l-1)}, \{\mathbf{h}_j^{(l-1)}, \forall v_j \in N(v_i)\}))$$



sampling to obtain a fixed number of neighbors

Aggregation functions

Node embeddings



Graph Attention Network (GAT)

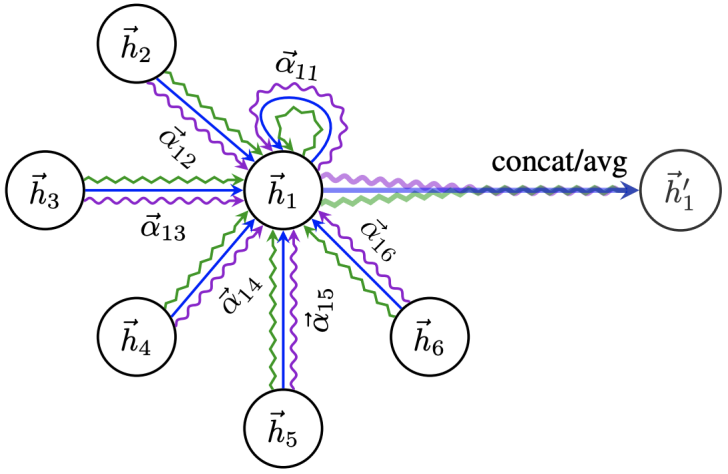
Key idea: dynamically learn the weights (attention scores) on the edges when performing message passing

Weighted sum of node embeddings

$$\mathbf{h}_i^{(l)} = f_{\text{filter}}(A, \mathbf{H}^{(l-1)}) = \sigma\Big(\sum_{v_j \in N(v_i)} \alpha_{ij} \mathbf{W}^{(l)} \mathbf{h}_j^{(l-1)}\Big)$$

Learned local weights with self-attention

$$\alpha_{ij} = \frac{\exp(\text{LeakyReLU}(\mathbf{u}^{(l)T}[\mathbf{W}^{(l)}\mathbf{h}_i^{(l-1)} || \mathbf{W}^{(l)}\mathbf{h}_j^{(l-1)}]))}{\sum_{v_k \in N(v_i)} \exp(\text{LeakyReLU}(\mathbf{u}^{(l)T}[\mathbf{W}^{(l)}\mathbf{h}_i^{(l-1)} || \mathbf{W}^{(l)}\mathbf{h}_k^{(l-1)}]))}$$

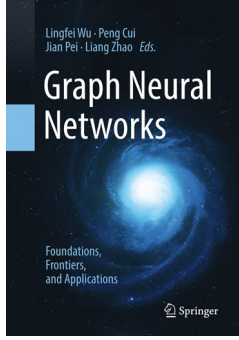


Intermediate node embeddings

$$f_{\text{filter}}(A, \mathbf{H}^{(l-1)}) = ||_{k=1}^{K} \sigma\Big(\sum_{v_j \in N(v_i)} \alpha_{ij}^k \mathbf{W}_k^{(l)} \mathbf{h}_j^{(l-1)}\Big)$$

Final node embeddings

$$f_{\text{filter}}(A, \mathbf{H}^{(L-1)}) = \sigma\Big(\frac{1}{K}\sum_{k=1}^{K}\sum_{v_j \in N(v_i)} \alpha_{ij}^k \mathbf{W}_k^{(L)} \mathbf{h}_j^{(L-1)}\Big)$$



Gated Graph Neural Networks (GGNN)

Key idea: the use of Gated Recurrent Units while taking into account edge type and directions

Zero-padding input node embeddings

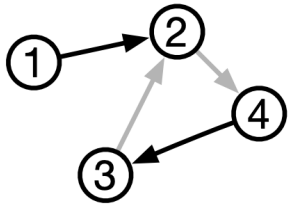
Incoming & outcoming edges for node v_i

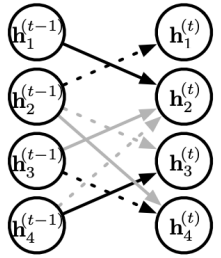
$$\mathbf{h}_i^{(0)} = [\mathbf{x}_i^T, \mathbf{0}]^T$$

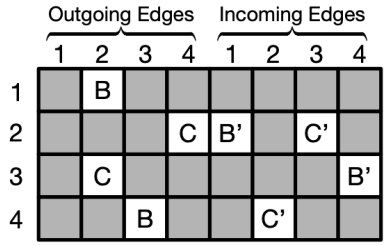
$$\mathbf{a}_i^{(l)} = A_{i:}^T [\mathbf{h}_1^{(l-1)} \ldots \mathbf{h}_n^{(l-1)}]^T$$

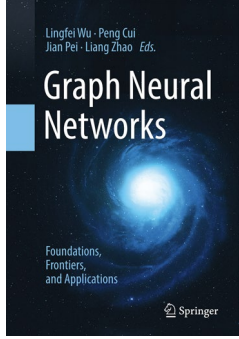
$$\mathbf{h}_i^{(l)} = \mathrm{GRU}(\mathbf{a}_i^{(l)}, \mathbf{h}_i^{(l-1)})$$

GRU for fusing node embeddings



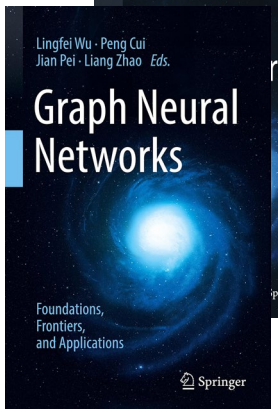






GNNs: Expressive Power (Chapter 5)

Graph Representation Learning and Problem Formulation

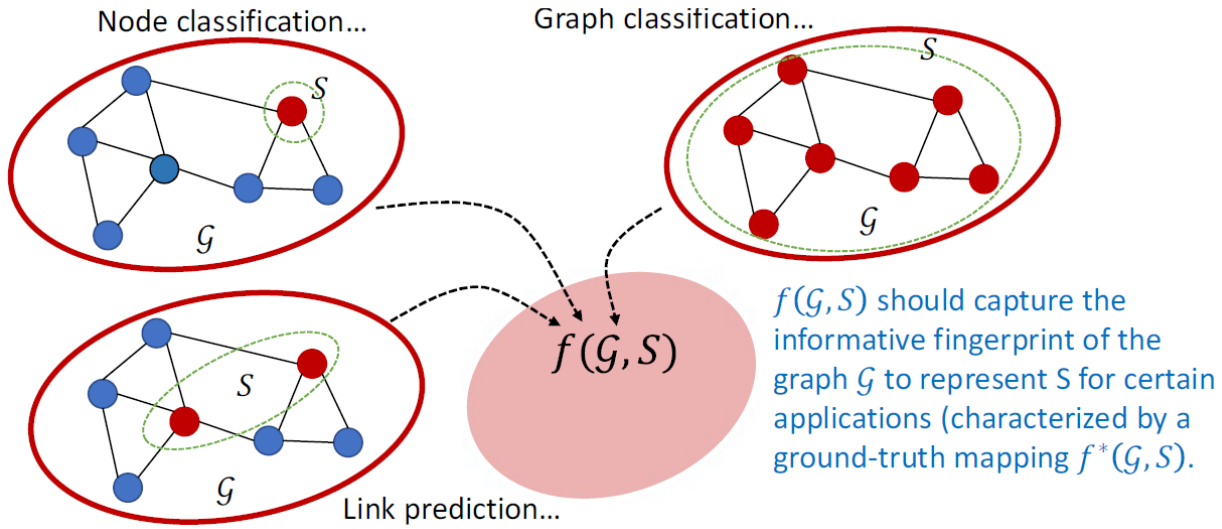


Feature Space $\mathscr{X} := \Gamma \times \mathscr{S}$.

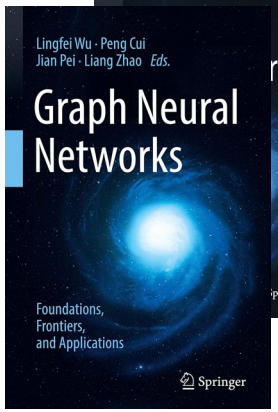
Space of graph-structured data

All node set of interest

Point in Feature Space $f^*(\mathscr{G}, S) = y$



Graph Representation Learning and Problem Formulation



Isomorphism:

$$(\mathcal{G}^{(1)}, S^{(1)}), (\mathcal{G}^{(2)}, S^{(2)})$$

$$\mathcal{G}^{(1)} = (A^{(1)}, X^{(1)})$$

$$\mathcal{G}^{(2)} = (A^{(2)}, X^{(2)})$$

$$\pi : \mathcal{V}[\mathcal{G}^{(1)}] \to \mathcal{V}[\mathcal{G}^{(2)}]$$

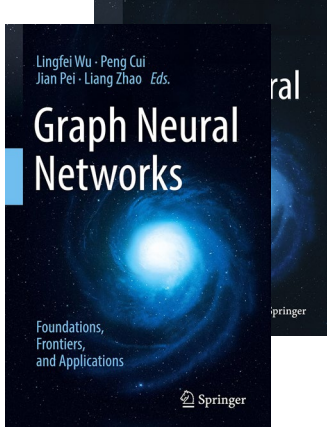
$$A^{(1)}_{uv} = A^{(2)}_{\pi(u)\pi(v)}, X^{(1)}_{u} = X^{(2)}_{\pi(u)}$$

condition

$$(\mathcal{G}^{(1)}, S^{(1)}) \cong (\mathcal{G}^{(2)}, S^{(2)})$$

Permutation invariance: $(\mathcal{G}^{(1)}, S^{(1)}) \cong (\mathcal{G}^{(2)}, S^{(2)}), f(\mathcal{G}^{(1)}, S^{(1)}) = f(\mathcal{G}^{(2)}, S^{(2)})$

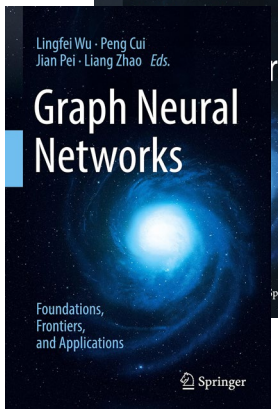
Graph Representation Learning and Problem Formulation



Expressive Power: how a model can distinguish non-isomorphic GRL examples

Definition 5.5. (Expressive power) Consider a feature space $\mathscr{X}$ of a graph representation learning problem and a model f defined on $\mathscr{X}$. Define another space $\mathscr{X}(f)$ as a subspace of the quotient space $\mathscr{X}/\cong$ such that for two GRL examples $(\mathscr{G}^{(1)}, S^{(1)})$, $(\mathscr{G}^{(2)}, S^{(2)}) \in \mathscr{X}(f)$, $f(\mathscr{G}^{(1)}, S^{(1)}) \neq f(\mathscr{G}^{(2)}, S^{(2)})$. Then, the size of $\mathscr{X}(f)$ characterizes the expressive power of f. For two models, $f^{(1)}$ and $f^{(2)}$, if $\mathscr{X}(f^{(1)}) \supset \mathscr{X}(f^{(2)})$, we say that $f^{(1)}$ is more expressive than $f^{(2)}$.

How to build the most expressive permutation invariant GNNs for graph representation learning problems?



The Expressive Power of GNNs

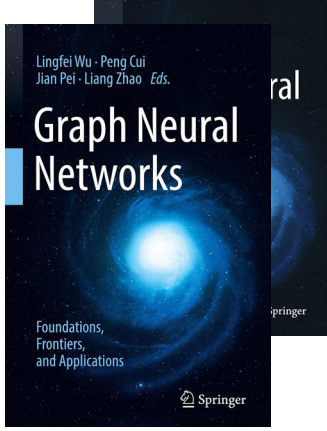
Question 1: **Function approximation**

What class of functions can GNNs approximate?

Question 2: Distinguishing graph structures

Whether can GNNs distinguish two different graph structures or not ?

Message Passing Graph Neural Networks

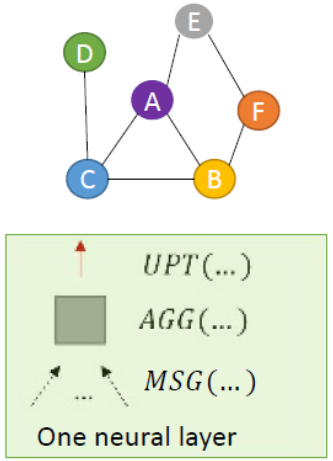


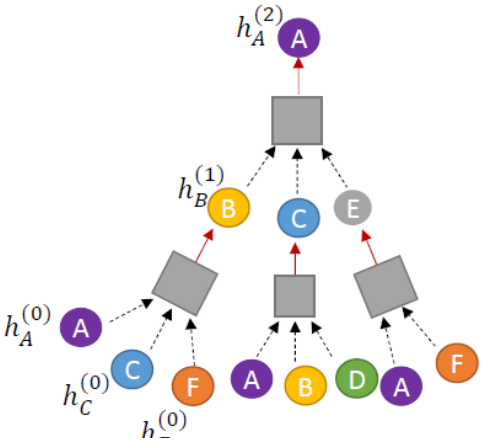
1. Initialize node vector representations as node attributes: $\mathbf{h}_v^{(0)} \leftarrow X_v, \forall v \in \mathcal{V}$.
2. Update each node representation based on message passing over the graph structure. In l-th layer, $l = 1, 2, ..., L$, perform the following steps:

$$\text{Message:} \quad \mathbf{m}_{vu}^{(l)} \leftarrow \text{MSG}(\mathbf{h}_v^{(l-1)}, \mathbf{h}_u^{(l-1)}), \forall (u,v) \in \mathcal{E},$$

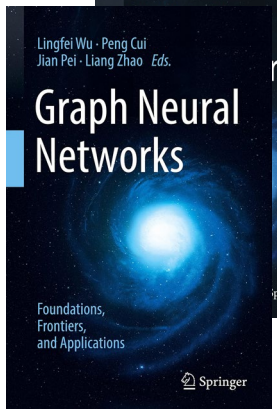
$$\text{Aggregation:} \quad \mathbf{a}_v^{(l)} \leftarrow \text{AGG}(\{\mathbf{m}_{vu}^{(l)} | u \in \mathcal{N}_v\}), \forall v \in \mathcal{V},$$

$$\text{Update:} \quad \mathbf{h}_v^{(l)} \leftarrow \text{UPT}(\mathbf{h}_v^{(l-1)}, \mathbf{a}_v^{(l)}), \forall v \in \mathcal{V}.$$





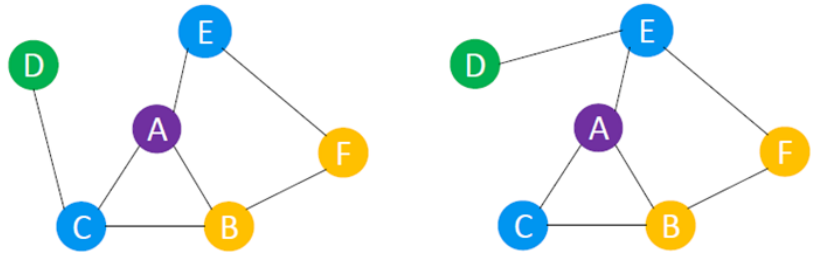
Theorem 5.1. *(Invariance of MP-GNN) $f_{MP-GNN}(\cdot,\cdot)$ satisfies permutation invariance (Def. 5.4) as long as the AGG and READOUT operations are invariant pooling operations (Def. 5.7).*



The Expressive Power of MP-GNN

MP-GNN is at most as powerful as the 1-WL test in distinguishing different graph-structured features (upper bounds).

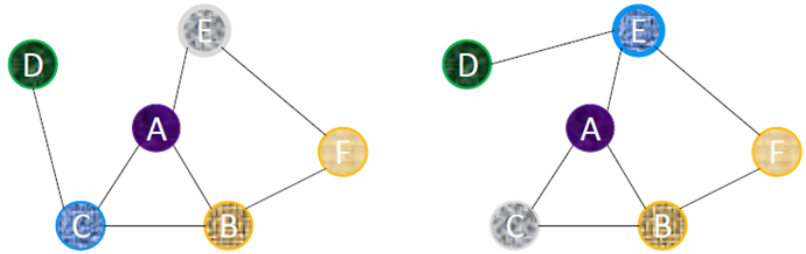
Step 1: Each node is initialized with some color according to its attribute (if no attributes, use the same color).



The mapping "attributes → colors" is injective.

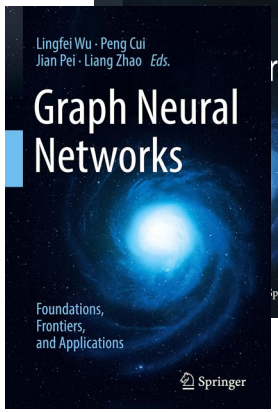
Step 2: Each node will collect the colors from their neighbors:

Node A: (p,{bby})
Left node E: (b,{py});
Right node E: (b,{pyg}) ...



The mapping "(self-color, set of colors from neighbors) → a new color" is injective

The Expressive Power of MP-GNN



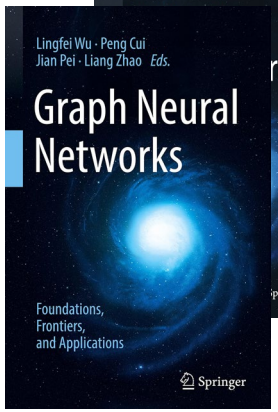
What kinds of GNNs that are, in principle, as powerful as the 1-WL test?

Theorem 5.3. *(Theorem 3 in (Xu et al, 2019d)) After sufficient iterations, MP-GNN may map any GRL examples* $(\mathcal{G}^{(1)}, S^{(1)})$ *and* $(\mathcal{G}^{(2)}, S^{(2)})$*, that the 1-WL test decides as non-isomorphic, to different representations if the following two conditions hold:*

a) The composition of MSE, AGG and UPT (Eqs.equation 11.45-equation 5.3) constructs an injective mapping from $(\mathbf{h}_v^{(k-1)}, \{\mathbf{h}_u^{(k-1)} | u \in \mathcal{N}_v\})$ *to* $\mathbf{h}_v^{(k)}$.

b) The READOUT (Eq.equation 5.4) is injective.

MP-GNN with the Power of the 1-WL Test



a) The composition of MSE, AGG and UPT (Eqs.equation 11.45-equation 5.3) constructs an injective mapping from $(\mathbf{h}_v^{(k-1)}, \{\mathbf{h}_u^{(k-1)} | u \in \mathcal{N}_v\})$ *to* $\mathbf{h}_v^{(k)}$.

AGG operation is suggested to adopt the sum pooling operation

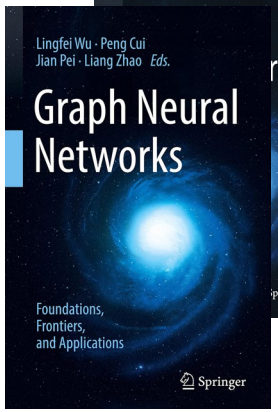
(Injective multiset functions: record the number of repetitive elements)

$$\text{Expressive Message:} \quad \mathbf{m}_{vu}^{(k)} \leftarrow MLP_1^{(k-1)}(\mathbf{h}_v^{(k-1)} \oplus \mathbf{h}_u^{(k-1)}), \ \forall (u,v) \in \mathcal{E},$$

$$\text{Expressive Aggregation:} \quad \mathbf{a}_v^{(k)} \leftarrow \sum_{u \in \mathcal{N}_v} \mathbf{m}_{vu}^{(k)}, \ \forall v \in \mathcal{V},$$

$$\text{Expressive Update:} \quad \mathbf{h}_v^{(k)} \leftarrow MLP_2^{(k-1)}(\mathbf{h}_v^{(k-1)} \oplus \mathbf{a}_v^{(k)}), \ \forall v \in \mathcal{V}.$$

MP-GNN with the Power of the 1-WL Test

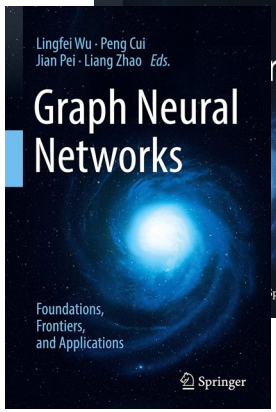


b) The READOUT (Eq.equation 5.4) is injective.

Expressive Inference: $\hat{y}_S = MLP(\sum_{v \in S} \mathbf{h}_v^{(L)})$.

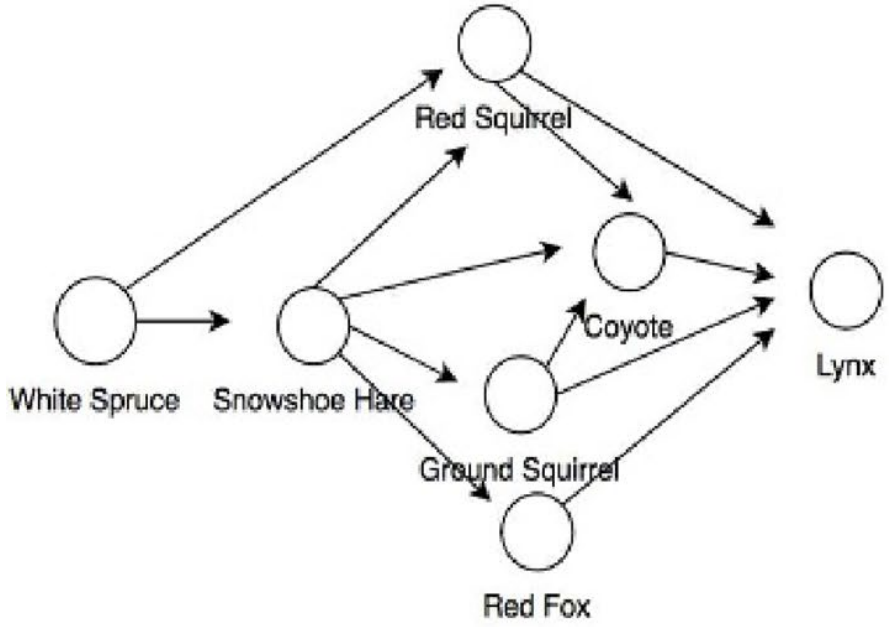
- Combine the proof for injectiveness of the sum aggregation with the universal approximation property of MLP.

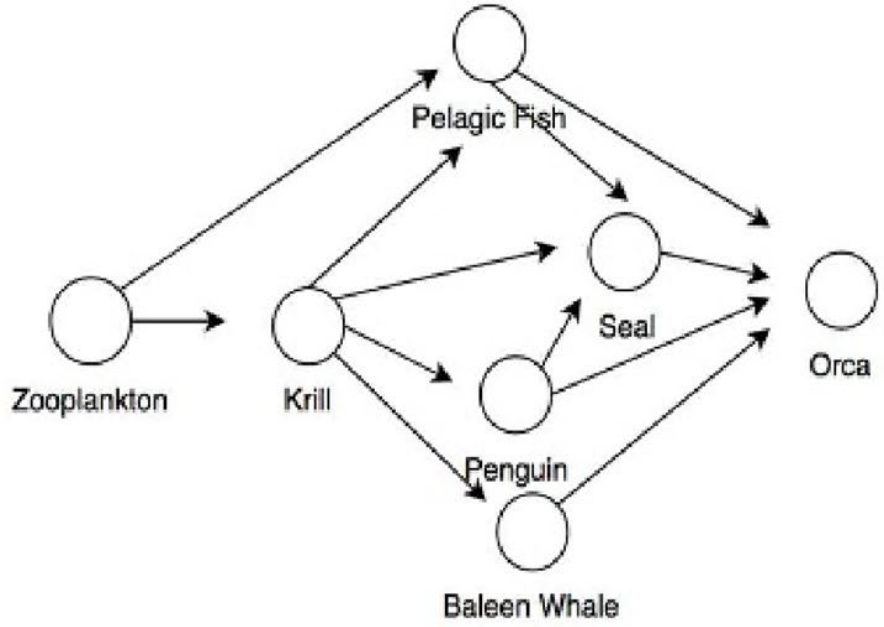
GNNs that are more Powerful than 1-WL Test



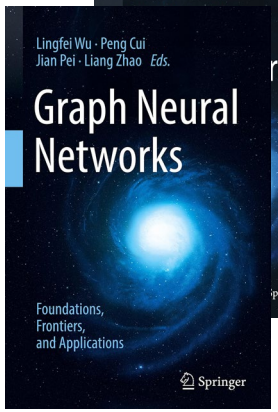
Information lost when using MP-GNN

- The information about the distance between multiple nodes is lost.



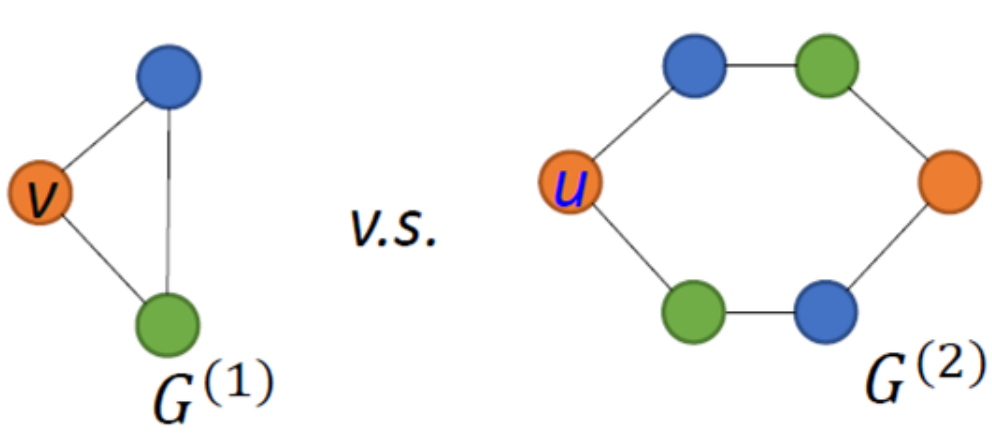


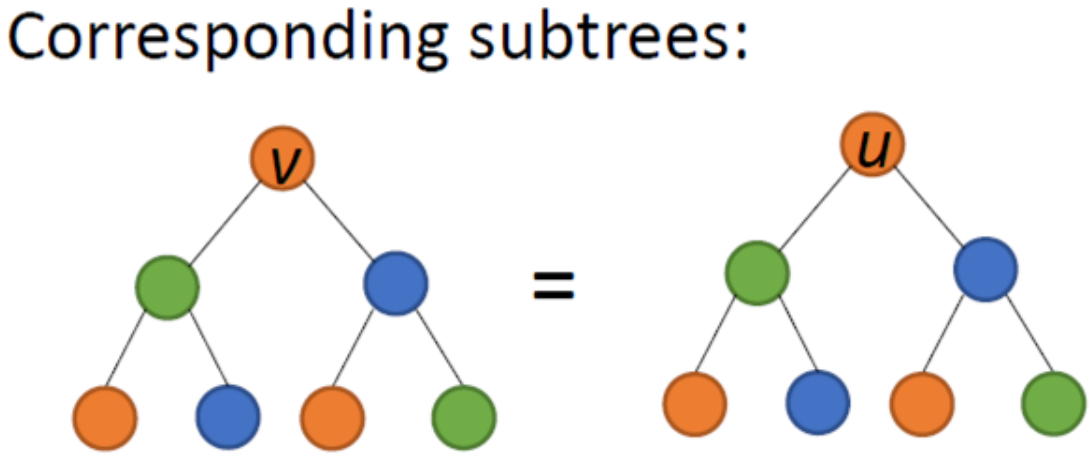
GNNs that are more Powerful than 1-WL Test



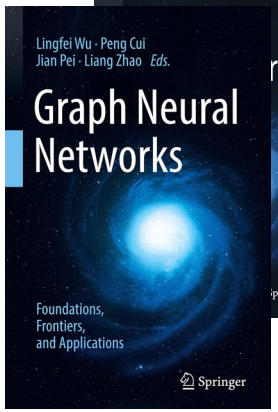
Information lost when using MP-GNN

- The information about cycles is lost.





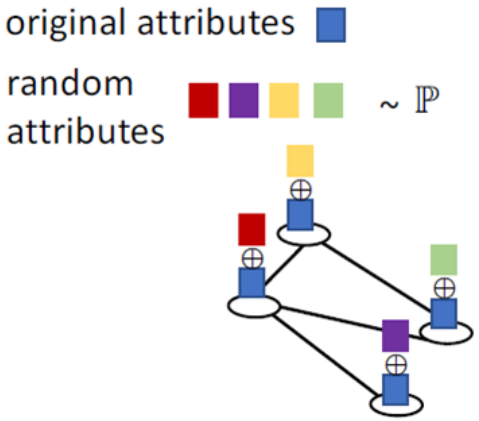
GNNs that are more Powerful than 1-WL Test



$$g_I(\mathcal{G}, S) = (\mathcal{G}_I, S), \quad \text{where } \mathcal{G}_I = (A, X \oplus \mathbf{I}),$$

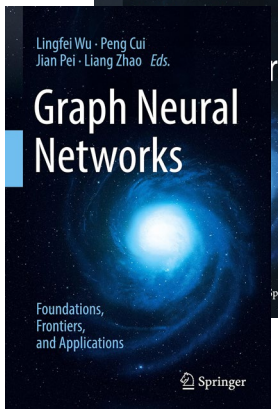
Problem: it is not permutation invariant

Injecting Random Attributes



Types of random attributes	Positional information	Model & reference
Random permutations	No	RP-GNN (Murphy et al, 2019)
(Almost uniform) Discrete r.v.	No	rGIN (Sato et al, 2020)
Distances to random anchor sets	Yes	PGNN (You et al, 2019)
Graph-convoluted Gaussian r.v.	Yes	CGNN (Srinivasan & Ribeiro, 2020)
Random signed Laplacian eigenmap	Yes	LE-GNN (Dwivedi et al, 2020)

GNNs that are more Powerful than 1-WL Test

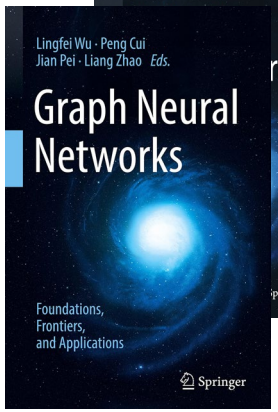


Injecting Deterministic Distance Attributes.

Two important pieces of intuition:

- Effective distance information is typically correlated with the task
- Distance from S to other nodes in G may be also useful side information.

GNNs that are more Powerful than 1-WL Test

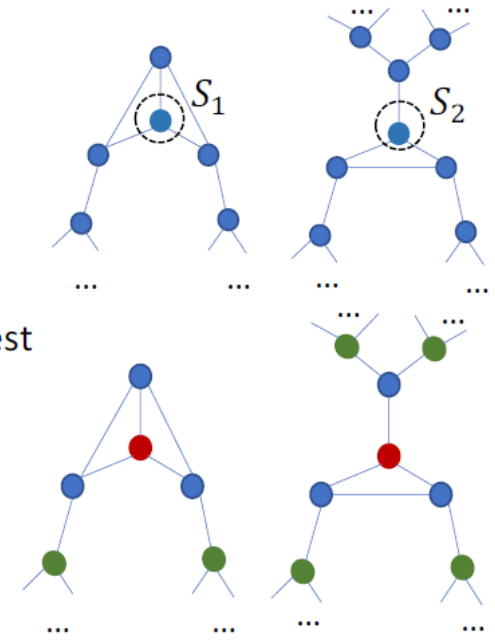


Distance Encoding (Li et al (2020e) DE-GNN)

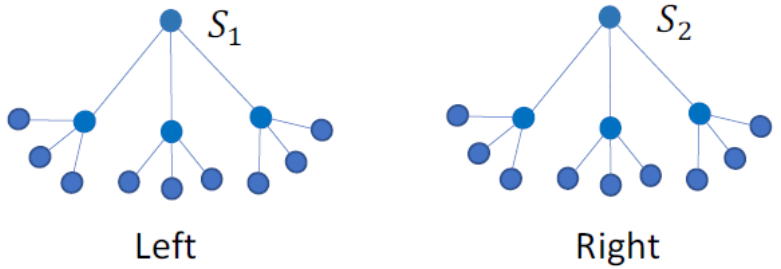
Node classification
for structural-role prediction

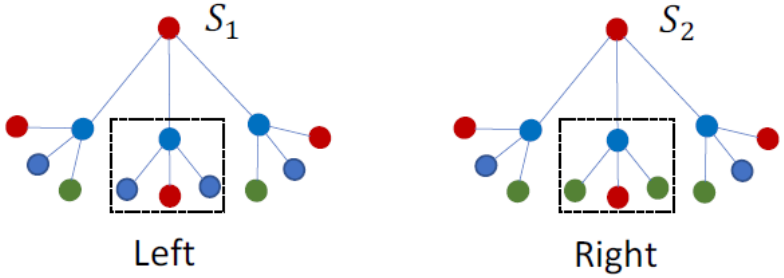
+ distance encoding (use shortest path distance as an example)

- DE = 0
- DE = 1
- DE = 2

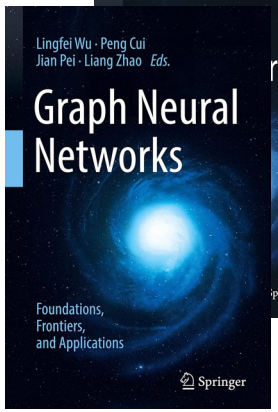


Subtrees rooted at the nodes of interest

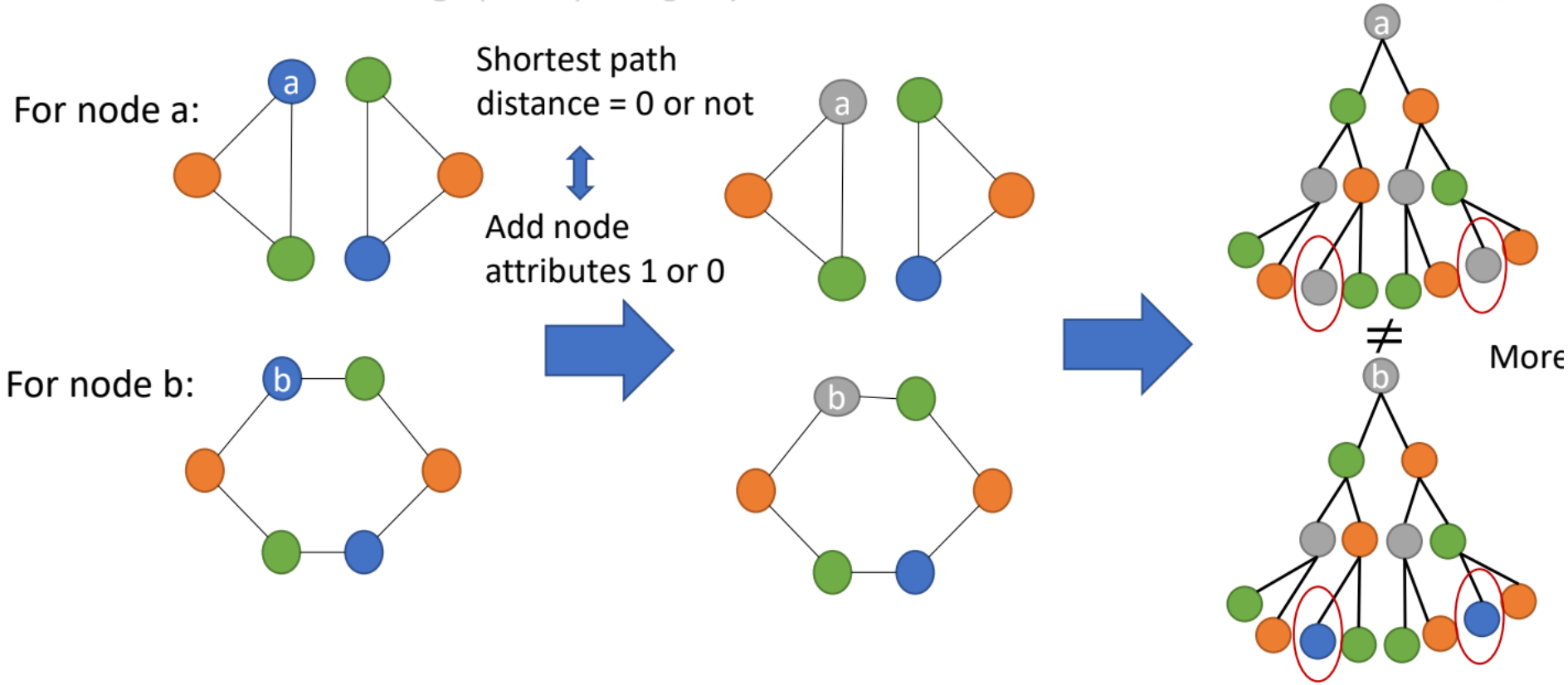




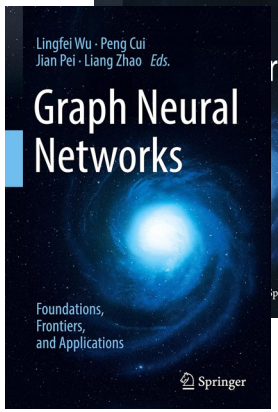
GNNs that are more Powerful than 1-WL Test



Distance Encoding (Identity-aware GNN (You at al, 2(

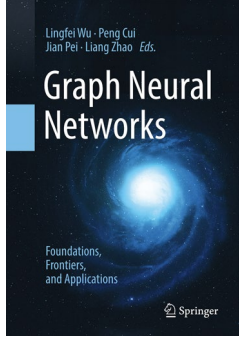


GNNs that are more Powerful than 1-WL Test

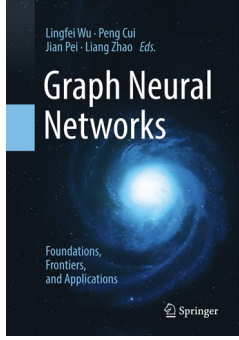


Higher-order Graph Neural Networks.

- k-WL-induced GNNs (Morris et al, 2019)
- Invariant and equivariant GNNs (Maron et al, 2018, 2019b)
- k-FWL-induced GNNs (Maron et al, 2019a; Chen et al, 2019f)



GNNs: Interpretability (Chapter 7)

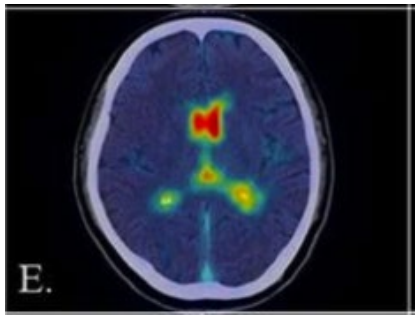


Interpretability of AI models

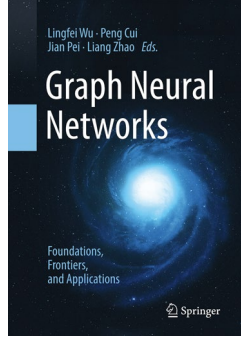
Interpretability is the degree to which an observer can understand the cause of a decision.

An **interpretation** is the mapping of an abstract concept into a domain that the human can understand.

- **Model-Oriented Reasons**
  - Credibility
  - Fairness
  - Adversarial-Attack Robustness
  - Backdoor-Attack Robustness

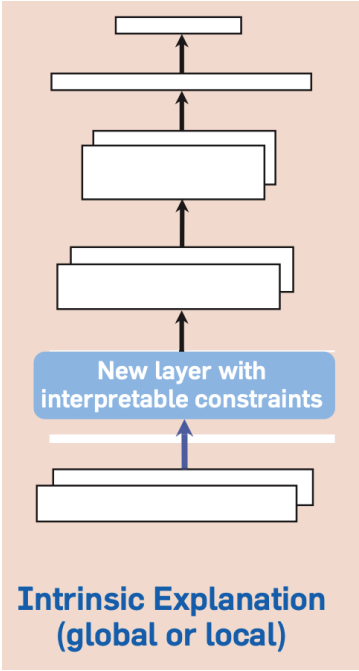


- **User-Oriented Reasons**
  - Improving User Experiences (e.g., cancer diagnosis, recommender system, etc.)
  - Facilitating Decision Making (e.g., outlier detection)

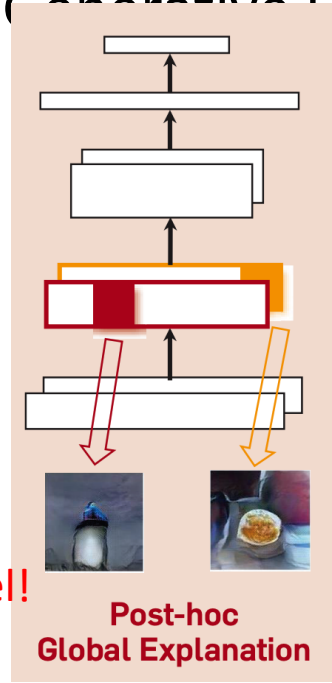


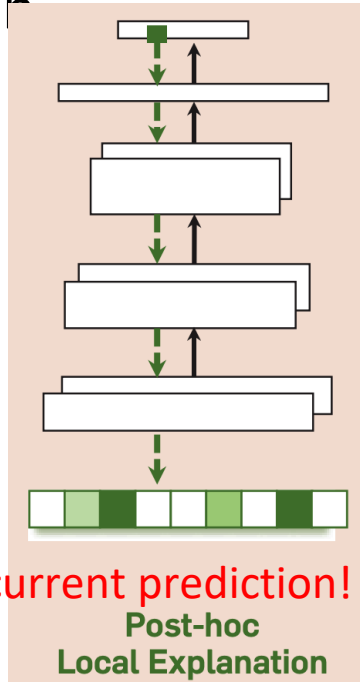
Types of Interpretations

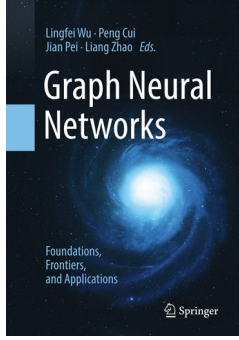
- Intrinsic Explanation
  - Distillation.
  - Attention models.
  - Disentangled representation learning.



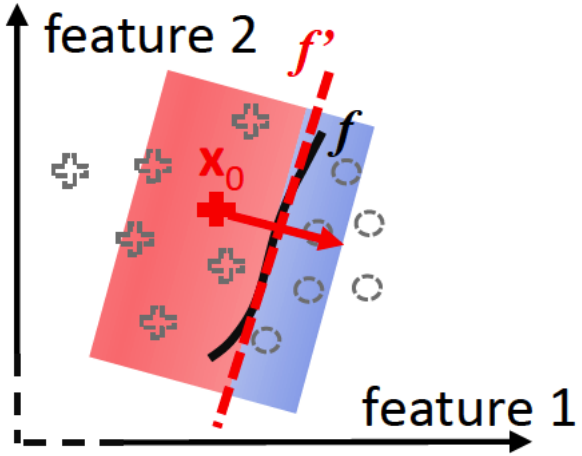
- Post-Hoc Interpretation
  - Approximation-Based Explanation
  - Relevance-Propagation Based Explanation
  - Perturbation-Based Approaches
  - Generative Explanation



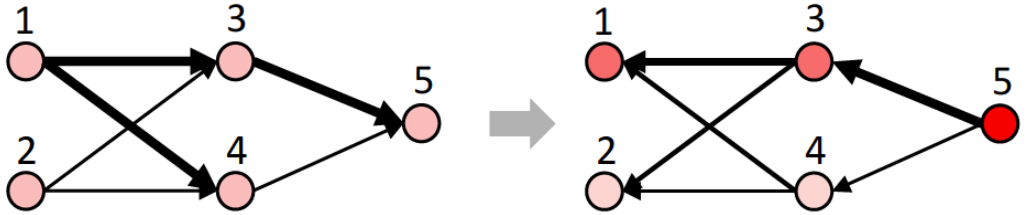




Types of post-hoc interpretations

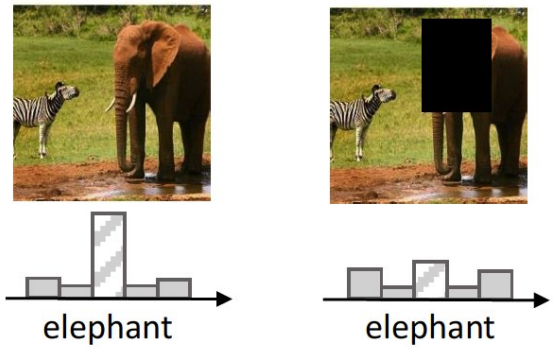


Approximation-Based Explanation

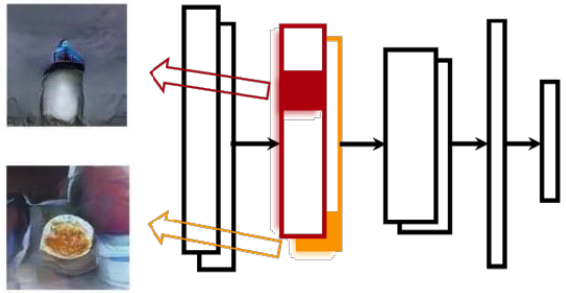


feed-forward connection weights relevance propagation

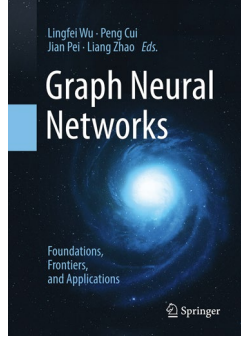
Relevance-Propagation Based Explanation



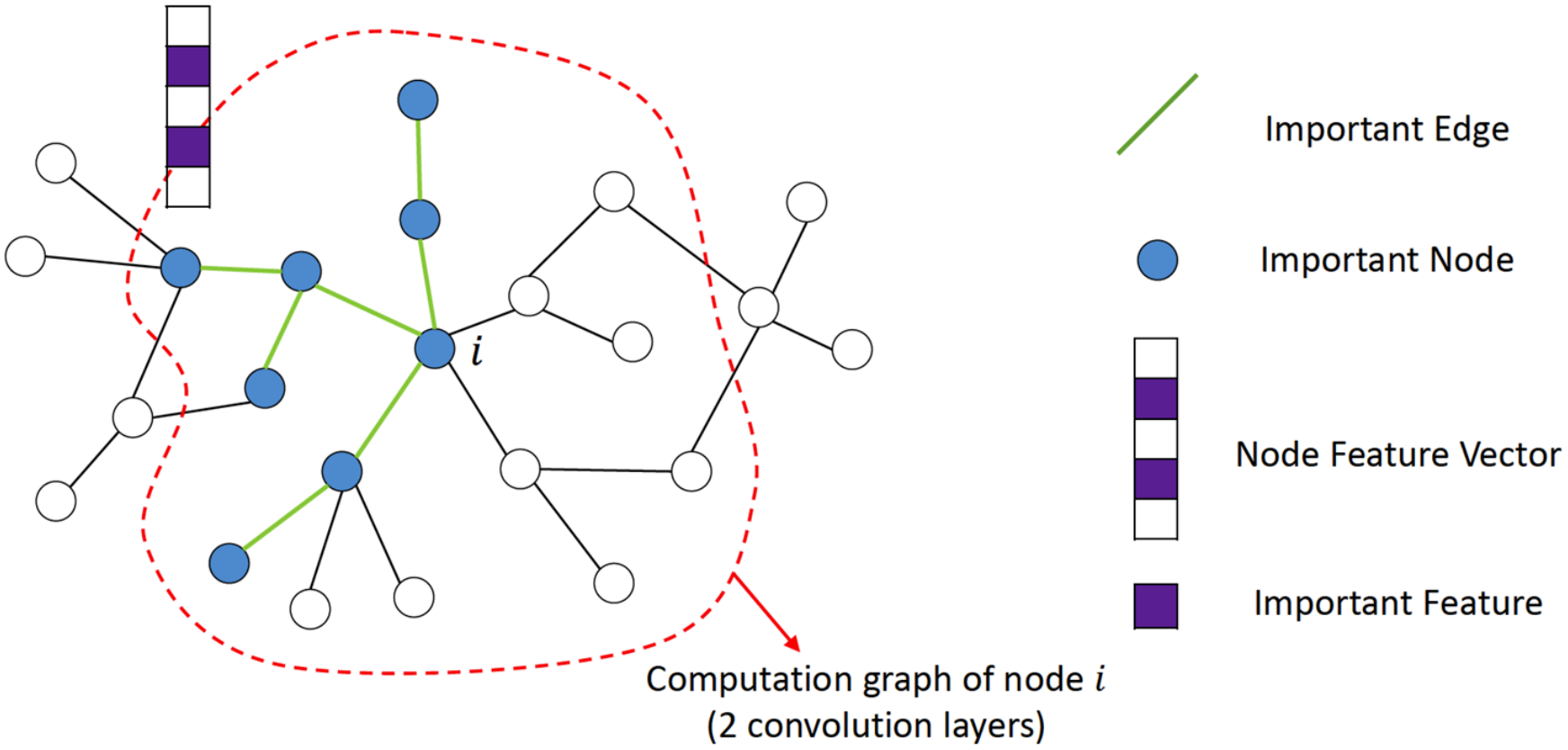
Perturbation-Based Approaches

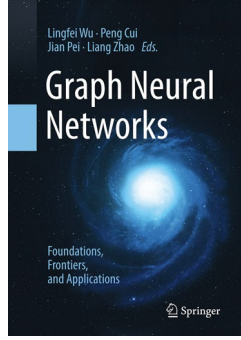


Generative Explanation

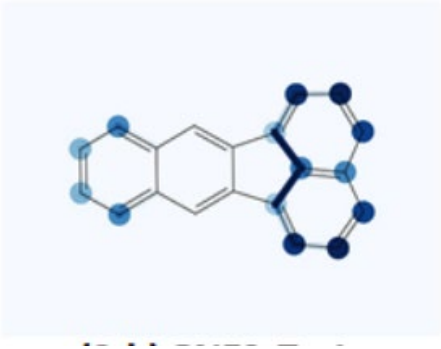


Formats of Explanation on Graphs

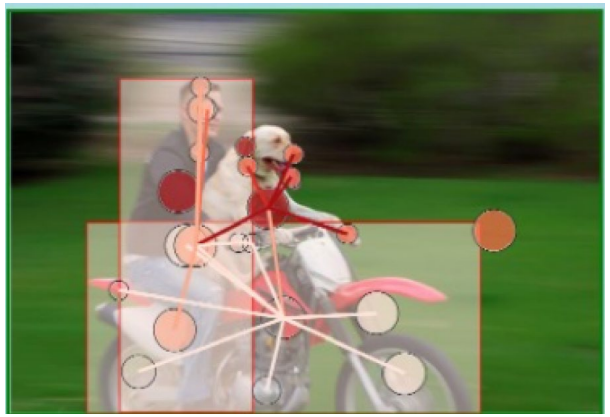




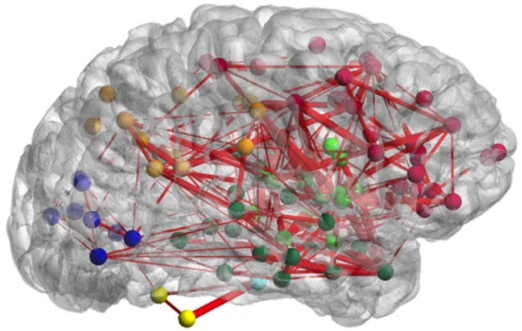
Intepretable GNN on graphs



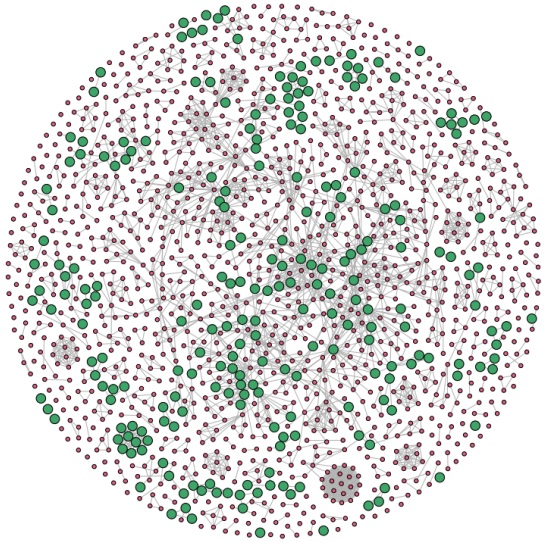
Which part determines the toxicity?



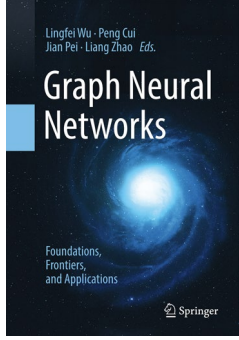
Why this image is about driving?



The rationale of mental disease prediction?



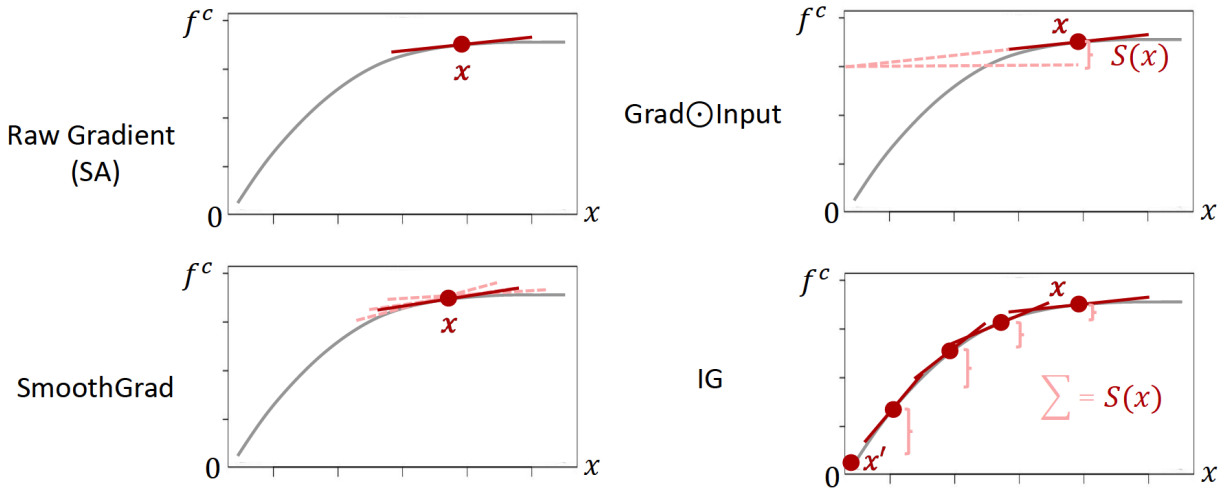
Source of infection in disease contact network?



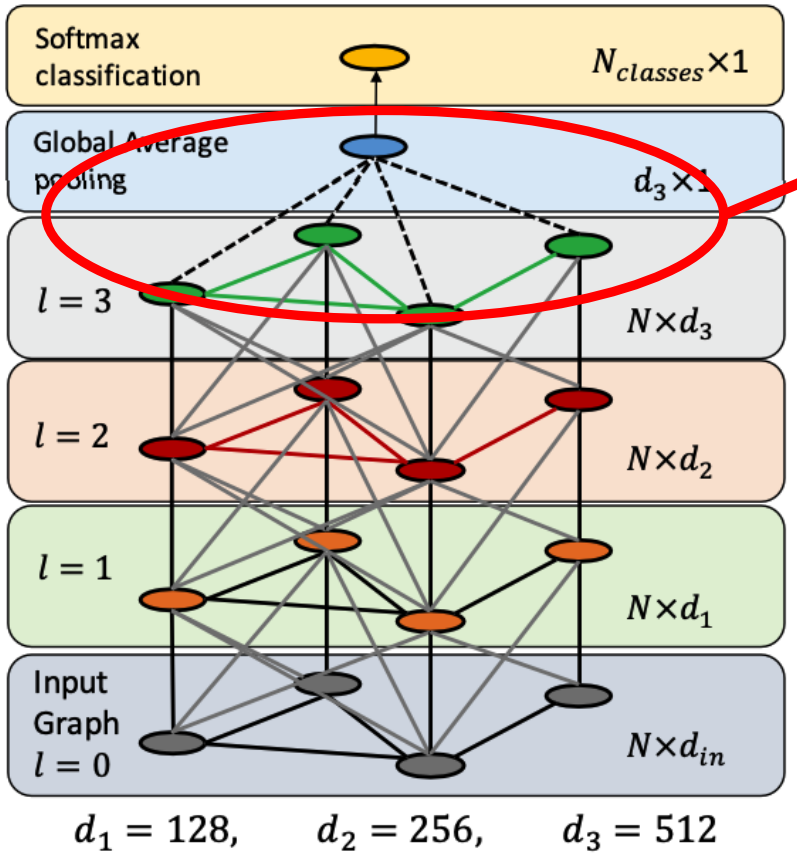
Approximation-Based Explanation

- White-Box Approximation
  - Input Gradient [Baldassarre et al. 2019]
  - Grad*Input [Sanchez-Lengeling et al. 2020]
  - Integrated Gradients (IG)
  - SmoothGrad [Sanchez-Lengeling et al. 2020]
  - Class Activation Mapping (CAM) [Pope et al. 2019]
  - Grad-CAM
  - [Pope et al. 2019]
- Black-Box Approximation Methods
  - GraphLime [Huang et al. 2022]
  - RelEx [Zhang et al. 2020]
  - PGM-Explainer [Vu et al. 2020]

f^c: function for class c.



CAM and GradCAM for GNNs



[Pope et al. 2019]

CAM

$$\mathbf{h} = \frac{1}{n}\sum_{i=1}^{n} H_{i,:}^{L}$$

$$f^c(\mathscr{G}) = \sum_k w_k^c \mathbf{h}_k$$

Extension 1: Generalization to any form of f^c

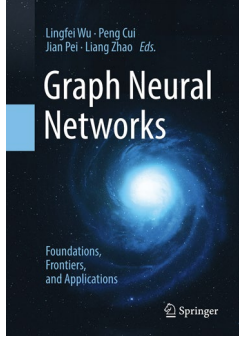
GradCAM

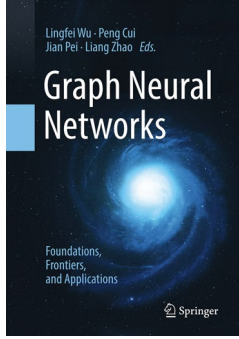
$$w_k^c = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial f^c(\mathscr{G})}{\partial H_{i,k}^{L}}$$

$$\mathscr{S}(i) = \frac{1}{n}\sum_k w_k^c H_{i,k}^{L}.$$

$$\mathscr{S}(i) = ReLU\left(\sum_k w_k^c H_{i,k}^{L}\right)$$

Extension 2: Add ReLU to get rid of negative features.

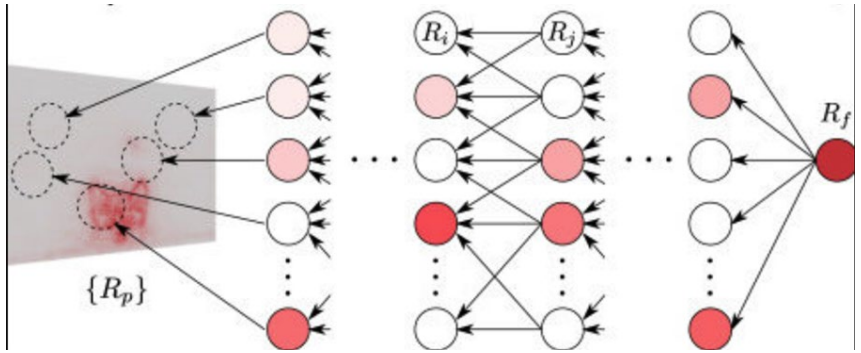




Relevance-Propagation Based Explanation

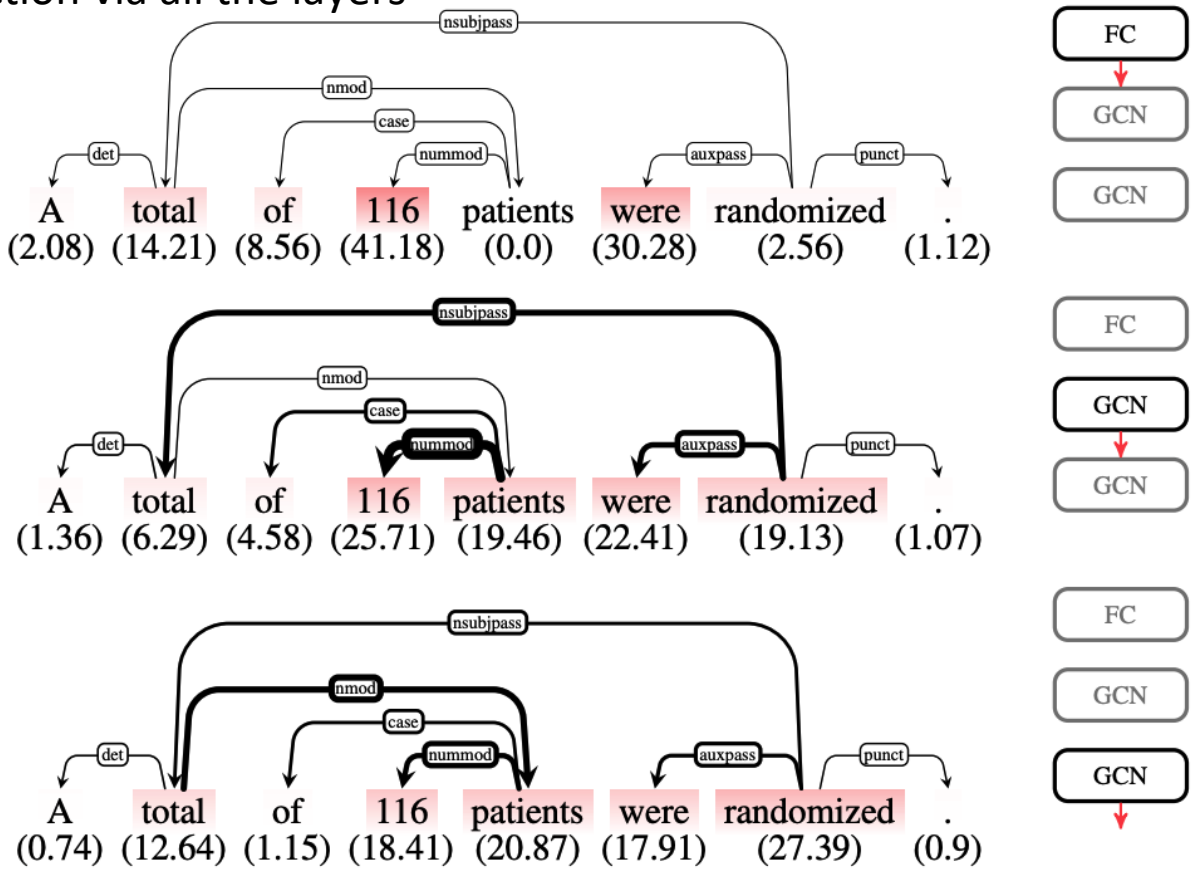
- Layer-wise Relevance Propagation (LRP) [Bach et al. 2015, Baldassarre and Azizpour. 2019; Schwarzenberg et al. 2019]

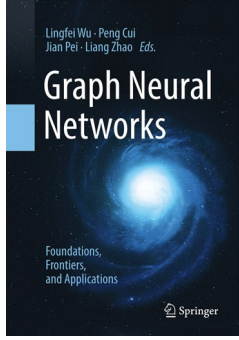
Quantify the Contribution of each input neuron to the prediction via all the layers



$$R_i^l = \sum_j \frac{z_{i,j}^+}{\sum_k z_{k,j}^+ + b_j^+ + \varepsilon} R_j^{l+1}$$

$$z_{i,j} = x_i^l w_{i,j}$$



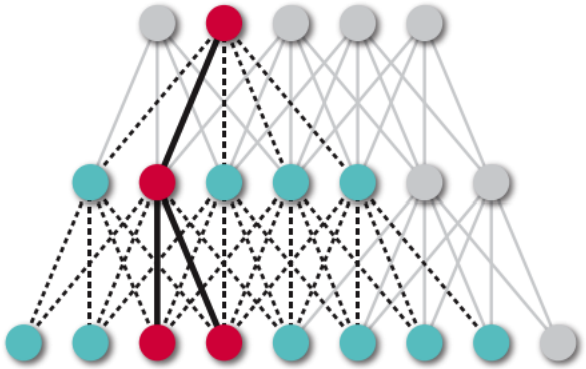


Relevance-Propagation Based Explanation

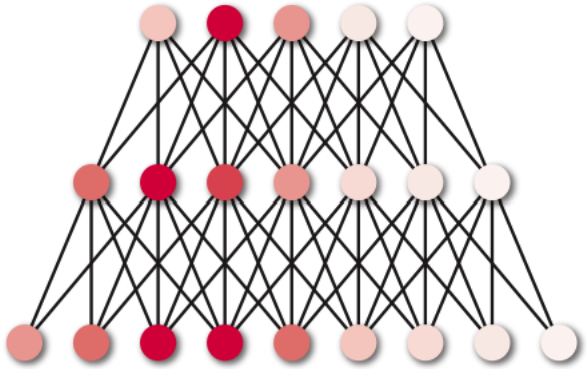
- Excitation BackPropagation (EBP) [Zhang et al, 2018]

$$P(a_i) = \sum_{a_j \in \mathcal{P}_i} P(a_i|a_j)P(a_j),$$

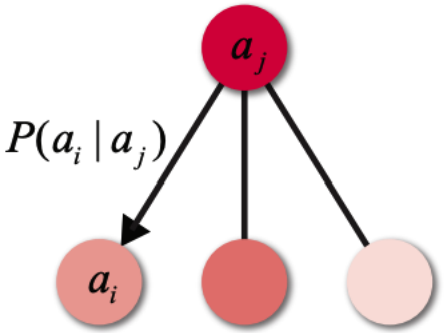
- Only non-negative weights are considered and negative weights are set to zero.



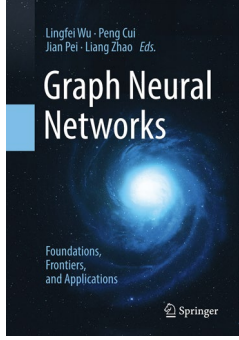
(a) Deterministic WTA



(b) Probabilistic WTA



(c) Winner Sampling



Approximation-Based Explanation

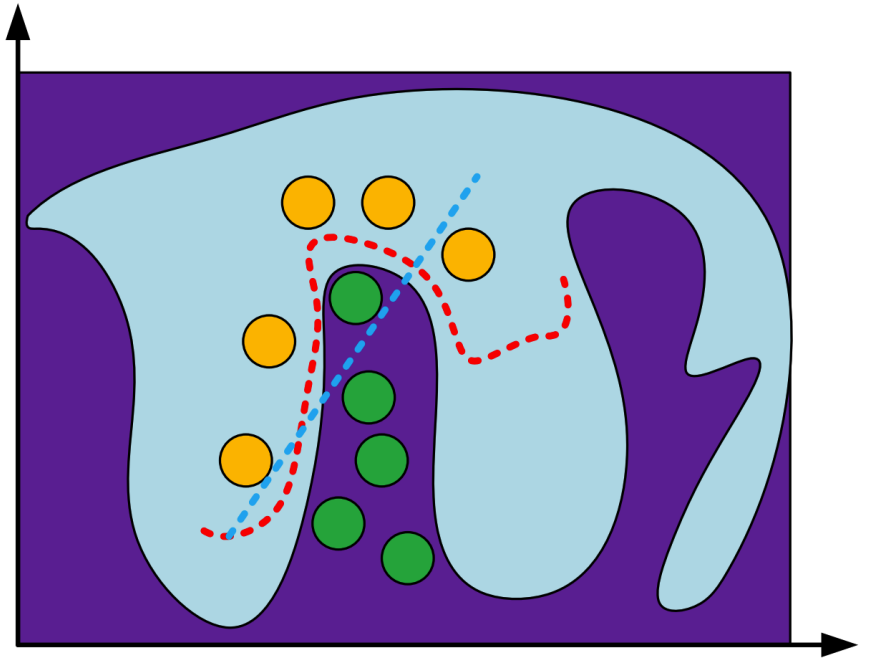
- GraphLime: Extend LIME to GNN [Huang et al. 2022]
  - Consider the N-hop neighbors

$$\boldsymbol{X}_n = [\boldsymbol{x}_1, \boldsymbol{x}_2, ...\boldsymbol{x}_m]$$

  - Use non-linear kernel-based model parameterized by β to approximate the original model

$$\min_{\boldsymbol{\beta}\in\mathbb{R}^d} \frac{1}{2}\|\bar{\boldsymbol{L}} - \sum_{k=1}^{d} \beta_k \bar{\boldsymbol{K}}^{(k)}\|_F^2 + \rho\|\boldsymbol{\beta}\|_1$$

$$\text{s.t.} \quad \beta_1, \ldots, \beta_d \geq 0,$$



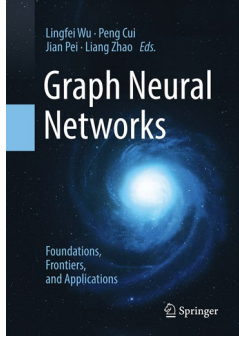
top K non-zero β_k are indicating representative K features

$$\bar{\boldsymbol{L}} = \boldsymbol{HLH}/\|\boldsymbol{HLH}\|_F$$

$$\bar{\boldsymbol{K}}^{(k)} = \boldsymbol{HK}^{(k)}\boldsymbol{H}/\|\boldsymbol{HK}^{(k)}\boldsymbol{H}\|_F$$

$$K(\boldsymbol{x}_i^{(k)}, \boldsymbol{x}_j^{(k)}) = \exp\left(-\frac{(\boldsymbol{x}_i^{(k)} - \boldsymbol{x}_j^{(k)})^2}{2\sigma_x^2}\right),$$

$$L(y_i, y_j) = \exp\left(-\frac{\|y_i - y_j\|_2^2}{2\sigma_y^2}\right),$$



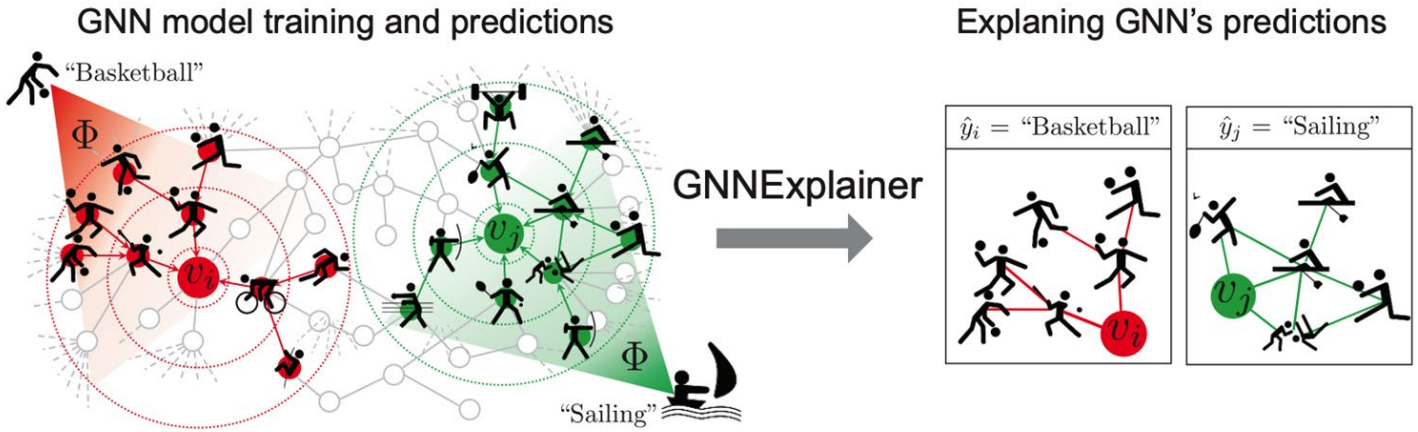
Perturbation-Based Approaches

- GNNExplainer [Ying et al. 2019]: Find the portion of graphs that has largest mutual information with the prediction

$$\max_{G_S} MI\left(Y, (G_S, X_S)\right) = H(Y) - H(Y|G = G_S, X = X_S).$$

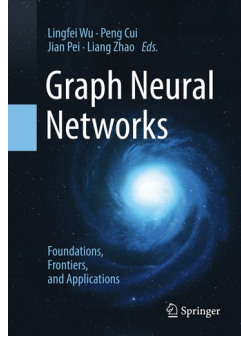
$$H(Y|G{=}G_S, X{=}X_S) = -\mathbb{E}_{Y|G_S,X_S}\left[\log P_\Phi(Y|G{=}G_S, X{=}X_S)\right].$$

$$\min_M -\sum_{c=1}^{C} \mathbb{1}[y=c] \log P_\Phi(Y=y|G=A_c \odot \sigma(M), X=X_c),$$

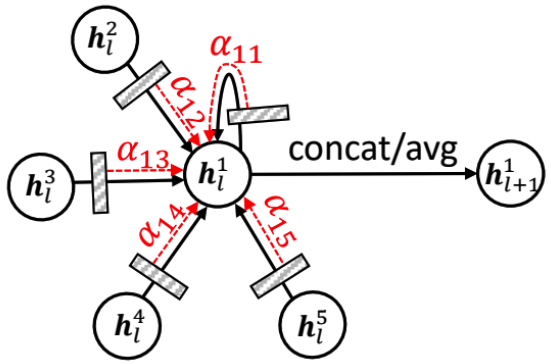


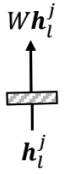
- PGExplainer $M_{i,j} = \mathrm{MLP}_\Psi\left([\mathbf{z}_i; \mathbf{z}_j]\right),$

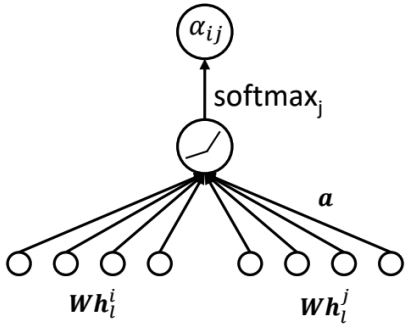
Interpretable Modeling on Graph Neural Networks



- GNN-Based Attention Models [Velčković et al. 2018]







multi-head extension

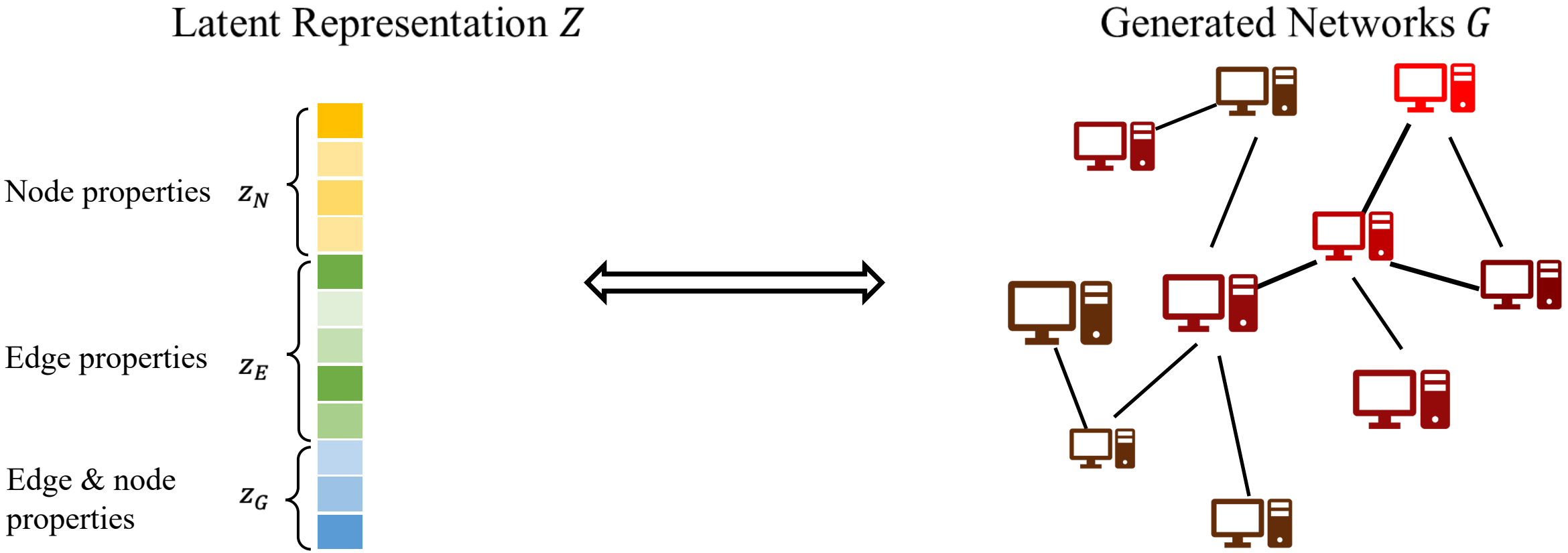
$$\mathbf{h}_{l+1}^i = \sigma\Big(\sum_{j\in\mathcal{V}_i\cup\{i\}} \alpha_{i,j} W\mathbf{h}_l^j\Big), \quad \Rightarrow \quad \mathbf{h}_{l+1}^i = \Big\|_{k=1}^{K} \sigma\Big(\sum_{j\in\mathcal{V}_i\cup\{i\}} \alpha_{i,j}^k W^k\mathbf{h}_l^j\Big),$$

$$\alpha_{i,j} = \mathrm{softmax}(e_{i,j}) = \frac{\exp(e_{i,j})}{\sum_{k\in\mathcal{V}_i\cup\{i\}}\exp(e_{i,k})},$$

$$e_{i,j} = \mathrm{LeakyReLU}(\mathbf{a}^\top[W\mathbf{h}_l^i \| W\mathbf{h}_l^j]),$$

Disentangled Representation Learning on Graphs

[Guo et al. 2020]



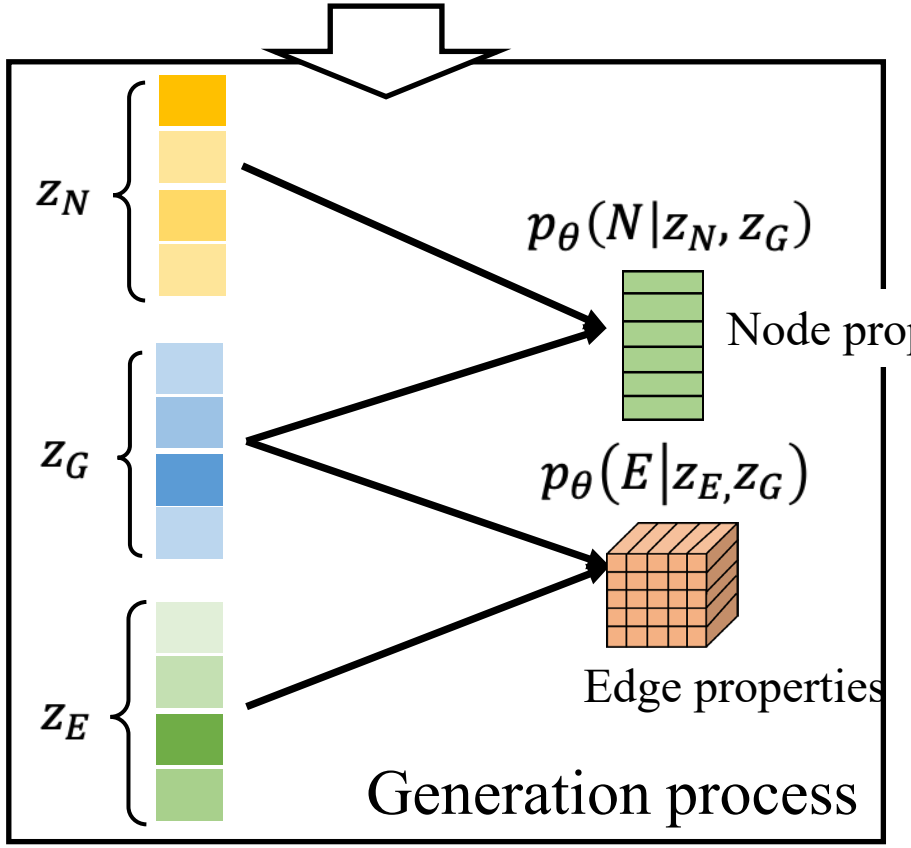
- **Goal:** Learning a graph generative model where each property of the generated graphs can be controlled by each latent variable.

Node-edge Disentangled Variational Autoencoder

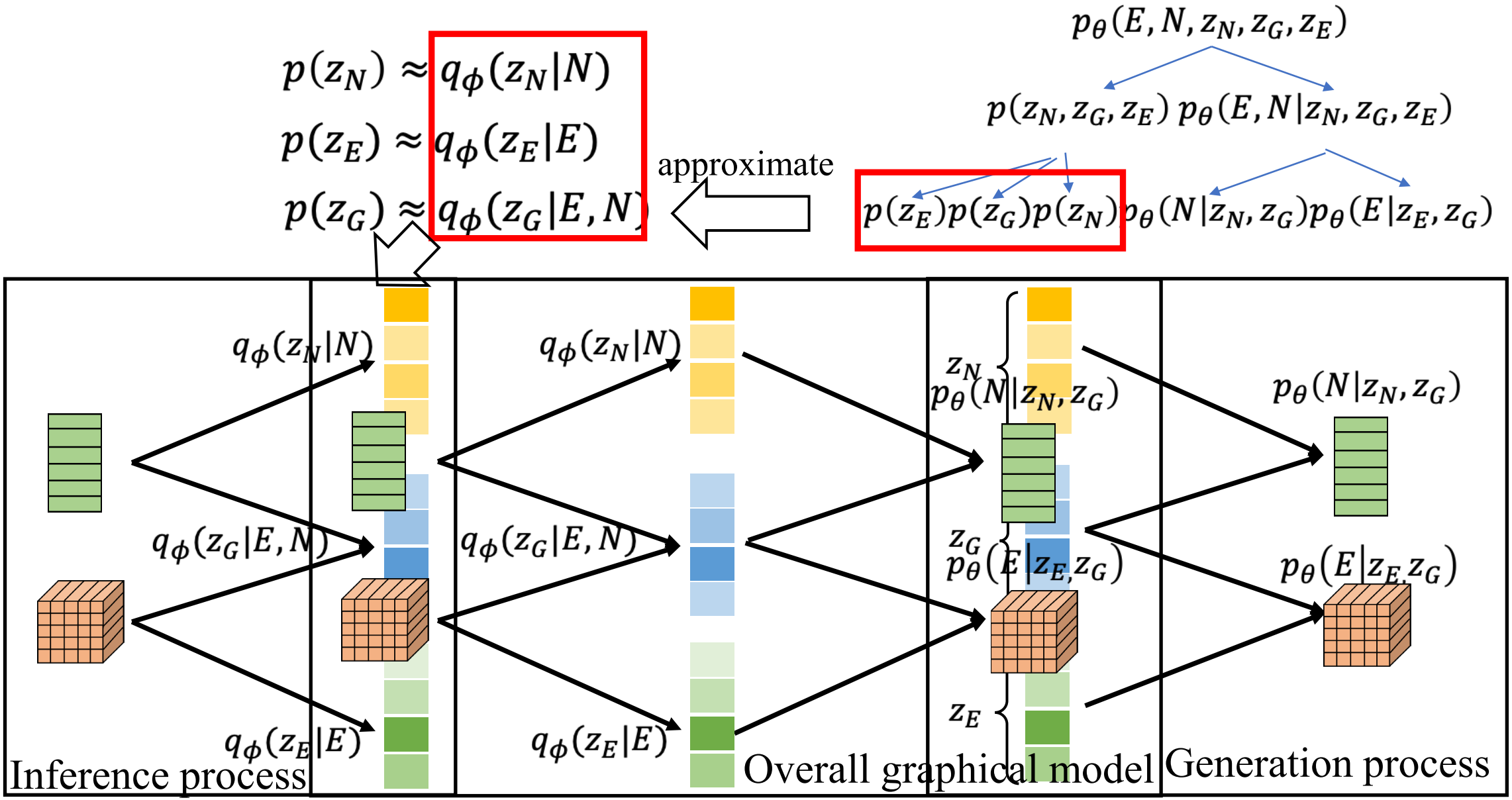
$$p_\theta(E, N, z_N, z_G, z_E)$$

$$p(z_N, z_G, z_E)\; p_\theta(E, N | z_N, z_G, z_E)$$

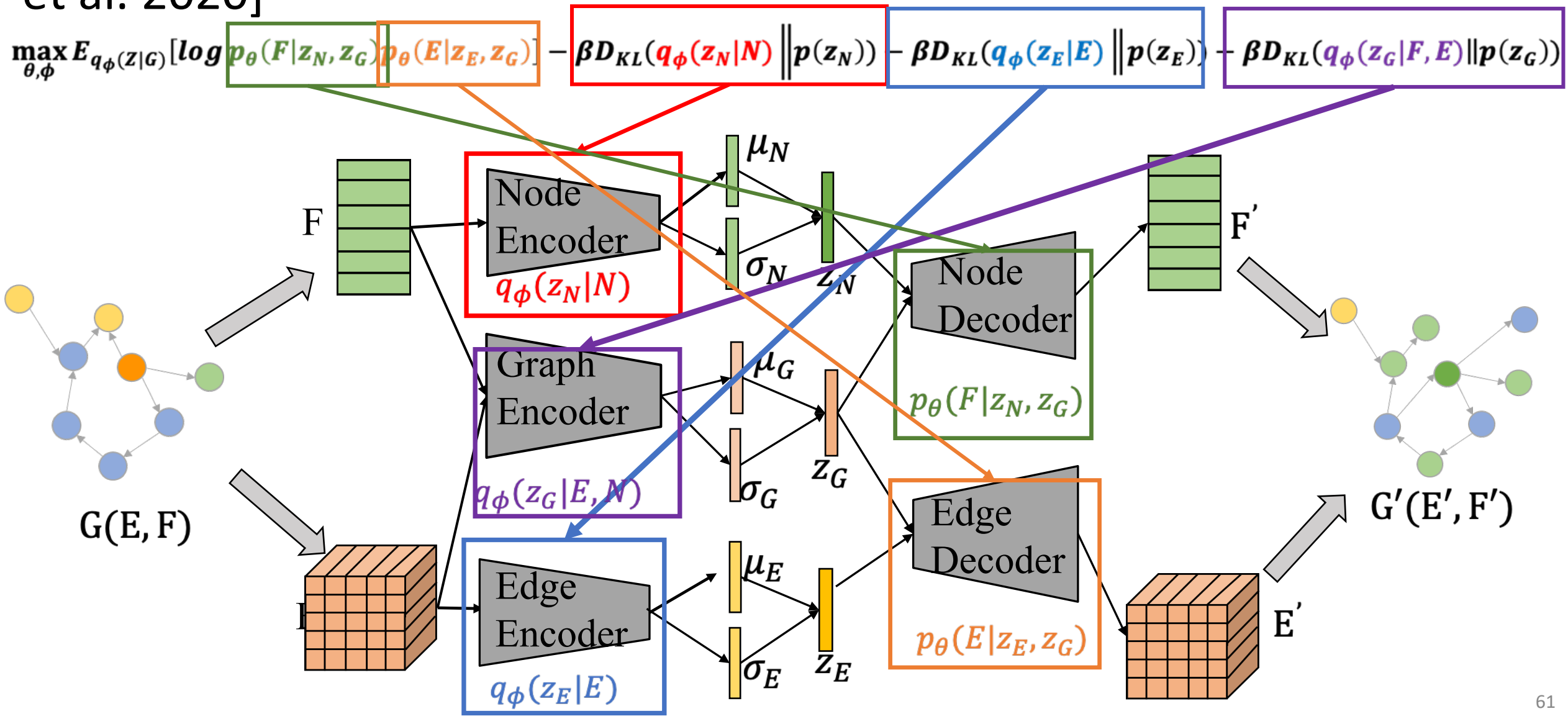
$$p(z_E)p(z_G)p(z_N)p_\theta(N|z_N, z_G)p_\theta(E|z_E, z_G)$$



Node-edge Disentangled Variational Autoencoder



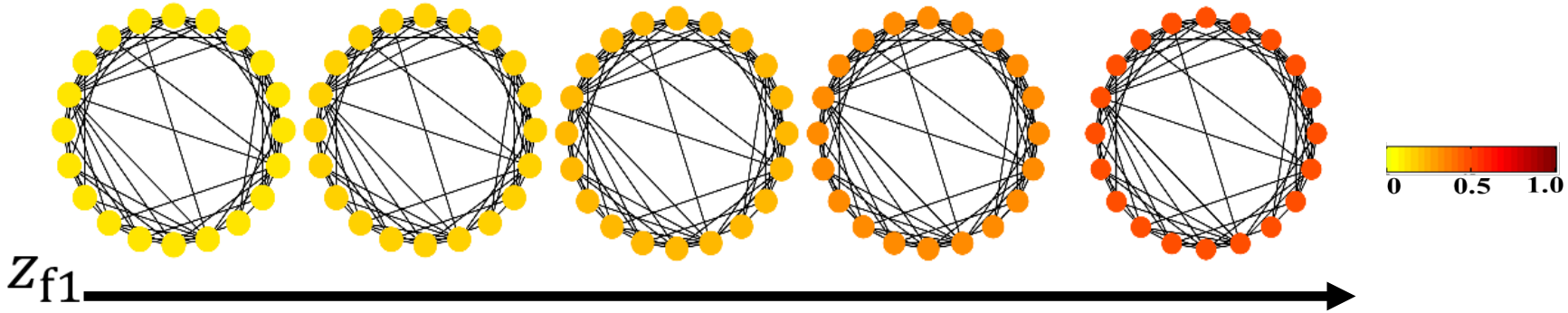
Node-edge Disentanglement VAE (NED-VAE) [Guo et al. 2020]



Experiment: Qualitative evaluation (WS graphs)

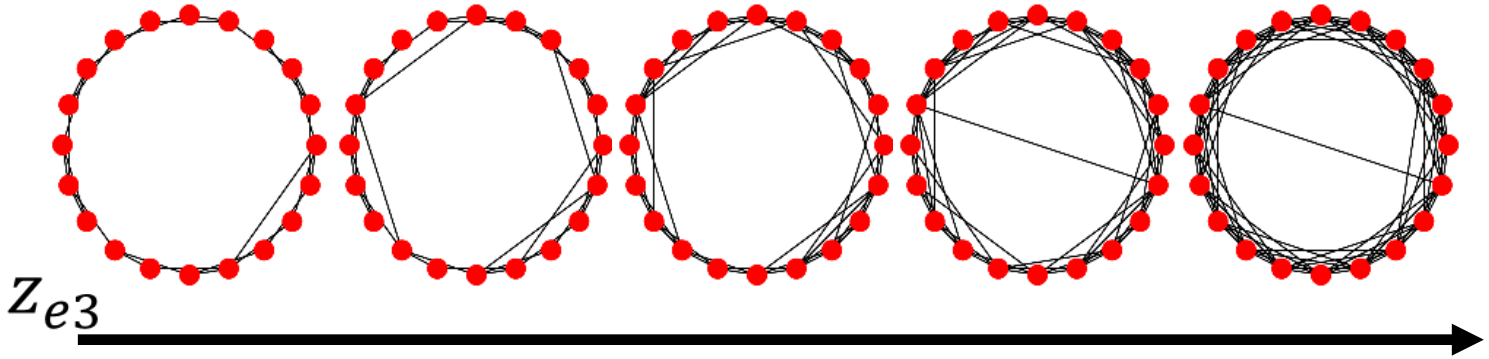
Node related factor

(**node value**)



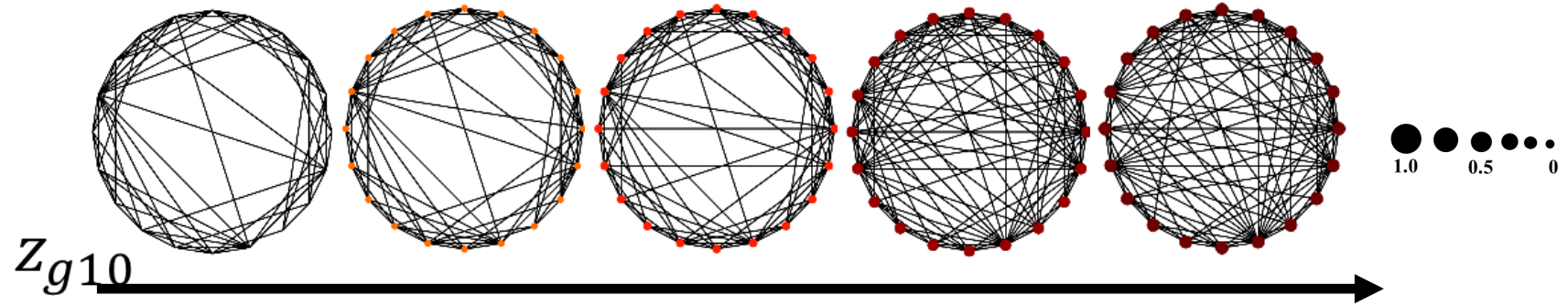
Edge related factor

(**number of rings**)

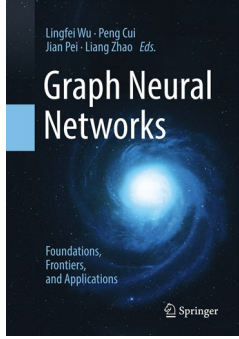


Node-edge-joint related factor

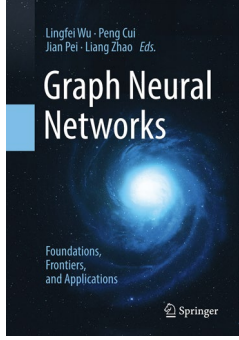
(**density** and **node value**)



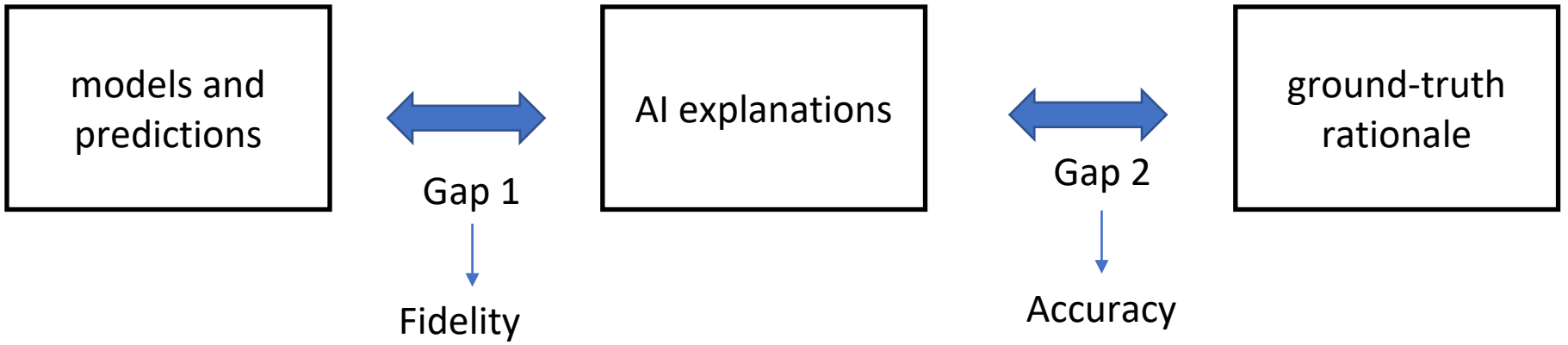
Evaluation of Graph Neural Networks Explanations: Benchmark Datasets



- Synthetic Datasets
  - BA-Shapes (Ying et al, 2019)
  - BA-Community (Ying et al, 2019)
  - Tree-Cycle (Ying et al, 2019)
  - Tree-Grid (Ying et al, 2019)
  - Noisy BA-Community, Noisy Tree-Cycle, Noisy Tree-Grid (Lin et al, 2020a)
  - BA-2Motifs (Luo et al, 2020)
- Real-World Datasets
  - MUTAG (Debnath et al, 1991)
  - REDDIT-BINARY (Yanardag and Vishwanathan, 2015)
  - Delaney Solubility (Delaney, 2004)
  - Bitcoin-Alpha, Bitcoin-OTC (Kumar et al, 2016)
  - MNIST SuperPixel-Graph (Dwivedi et al, 2020)



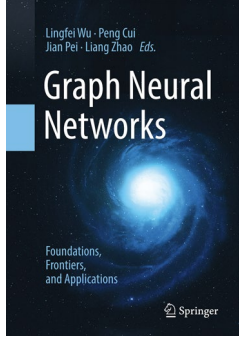
Evaluation Metrics



$$fidelity = \frac{1}{N}\sum_{i=1}^{N}\left(f^{y_i}\left(\mathcal{G}_i\right) - f^{y_i}\left(\mathcal{G}_i \setminus \mathcal{G}_i'\right)\right)$$

(Acc, AUC, F1, etc.)

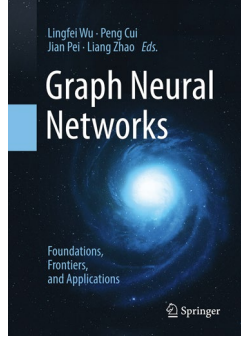
- Fidelity
- Accuracy
- Contrastivity: uses distance measure to quantify the differences between two explanations for different classes
- Sparsity: the ratio of explanation graph size to input graph size
- Stability: how stable the explanations are before and after adding noise to the input

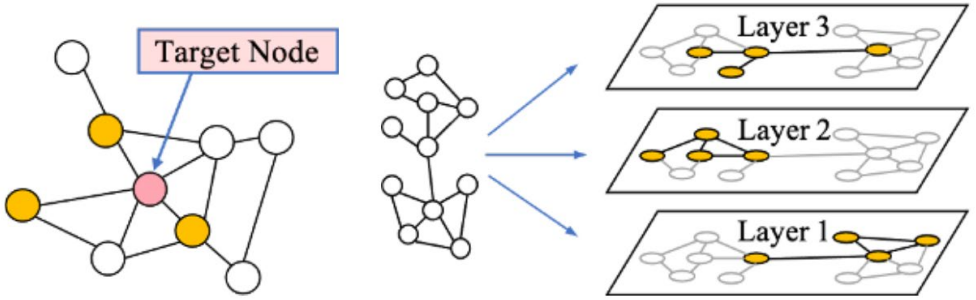


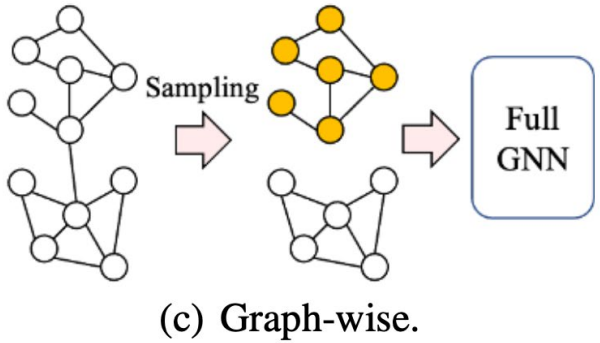
Future directions

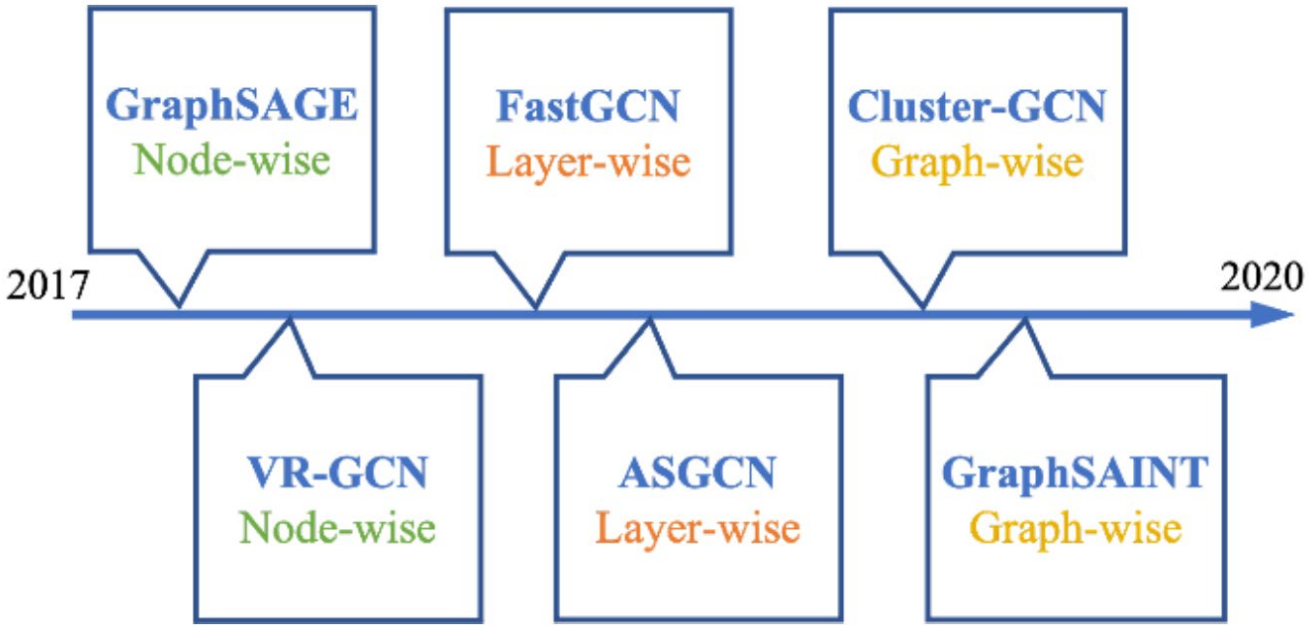
- more efficient explanation algorithms
- utilize interpretation towards identifying GNN model defects and improving model properties
- how to improve the explanation performance
- how to bring causality into GNN learning
- how to incorporate human-computer interaction (HCI) to show explanation in a more user-friendly format

GNNs: Scalability (Chapter 6)

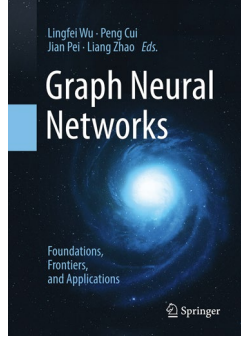


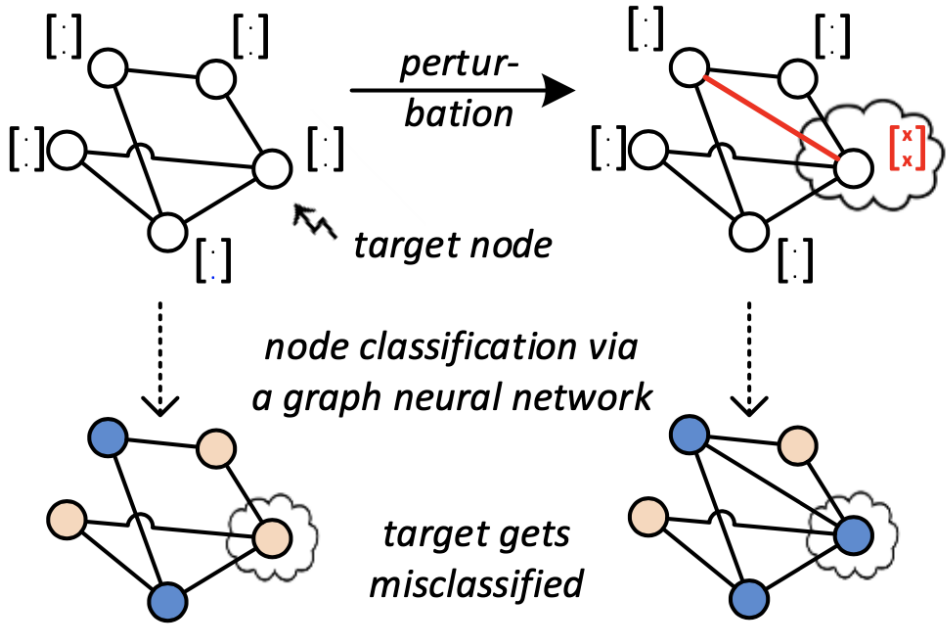


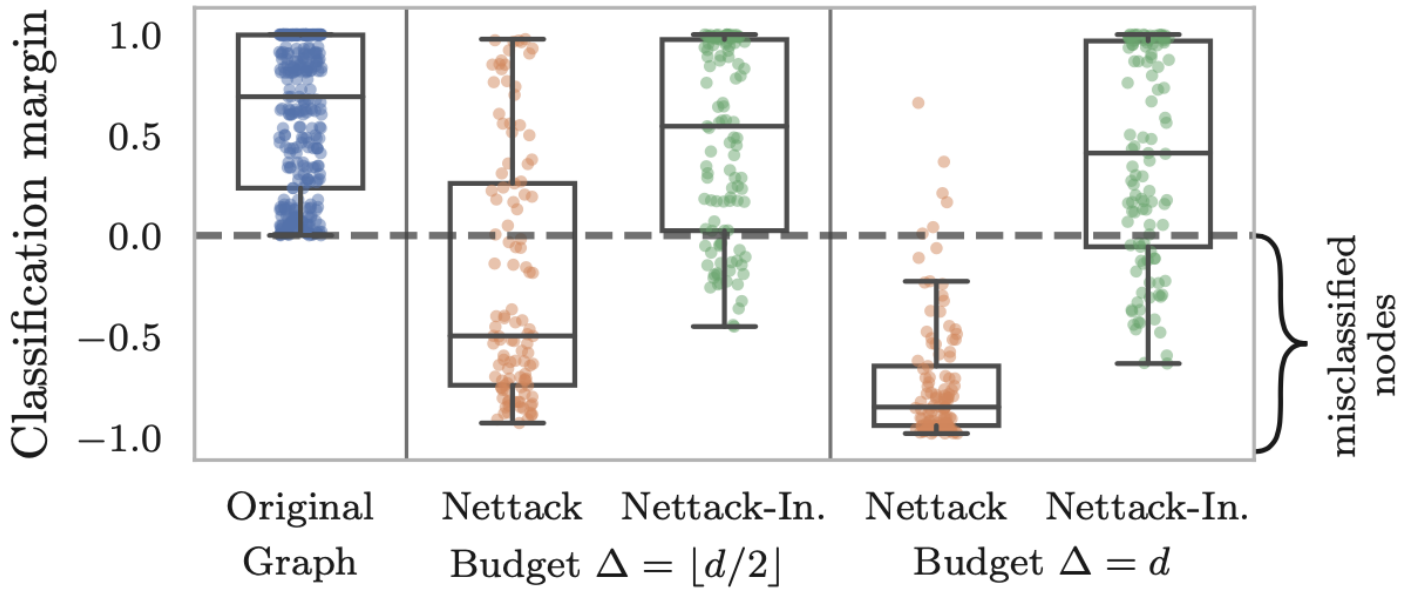




GNNs: Adversarial Robustness (Chapter 8)







Outline

GNNs Foundations

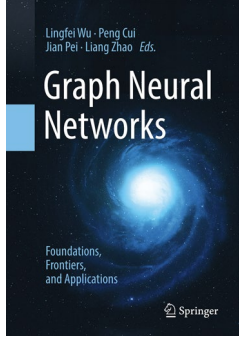
- Time History of GNNs
- GNNs: Foundations and Models
- GNNs: Theory, Scalability, Interpretability

GNNs Frontiers

- Graph Generation and Transformation
- Dynamic Graph Neural Networks
- Graph Matching
- Graph Structure Learning

GNNs Applications

- GNNs in Natural Language Processing
- GNNs in Program Analysis
- GNNs in Predicting Protein Function & Interaction

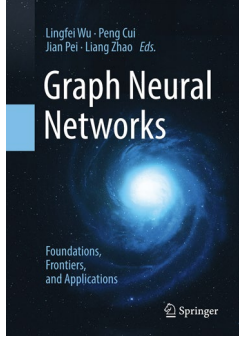


GNN book website：
https://graph-neural-networks.github.io/index.html

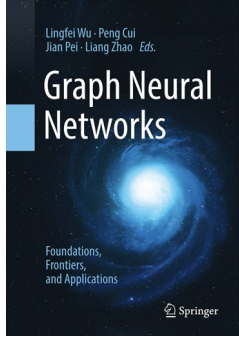
GNN Springer：
https://link.springer.com/book/10.1007/978-981-16-6054-2

Amazon：
https://www.amazon.com/Graph-Neural-Networks-Foundations-Applications/dp/9811660530

JD.com (京东商城)：
https://item.jd.com/10043589466641.html

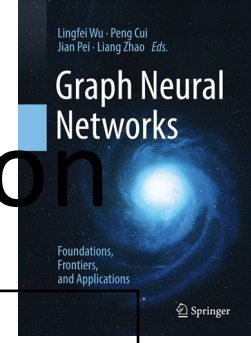


GNNs
Frontiers

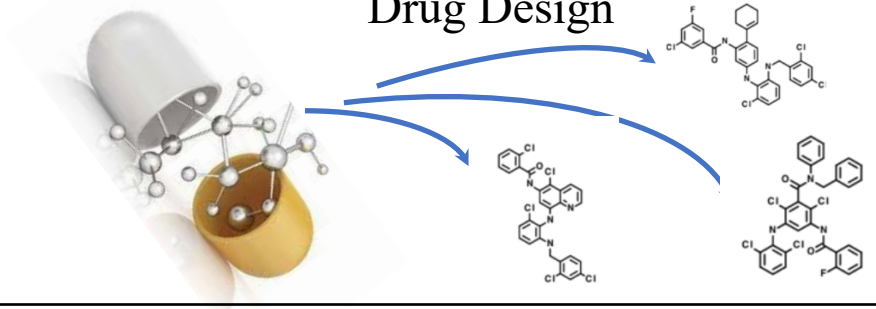


GNNs: Graph Generation and Transformation (Chapter 11 &12)

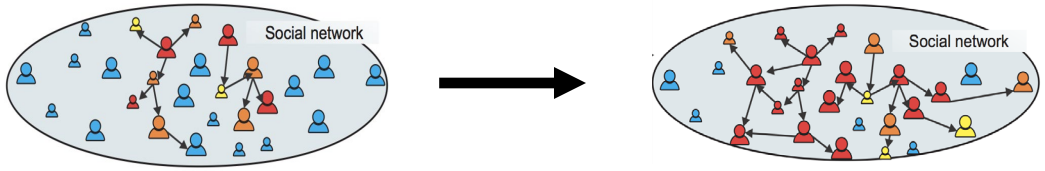
GNN for Graph Generation and Transformation



Drug Design



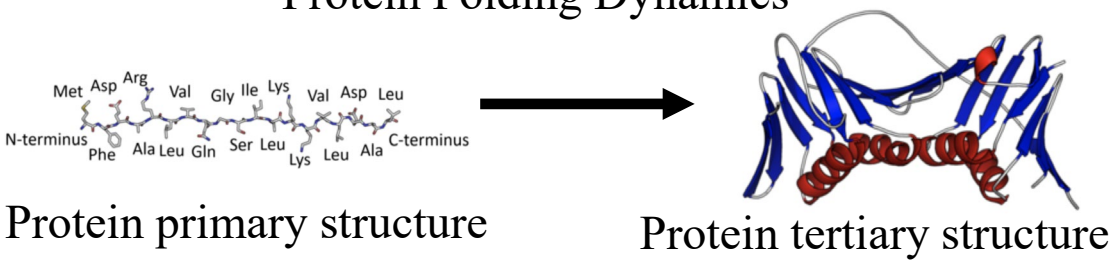
Social Network Synthesis



Without Social Event

With Social Event

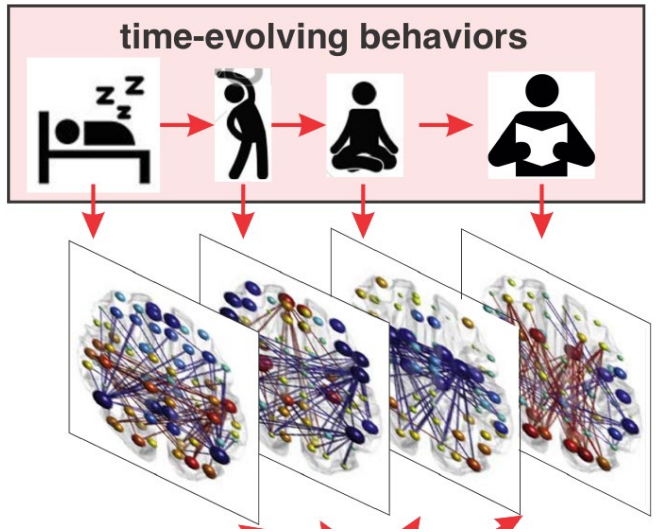
Protein Folding Dynamics



Protein primary structure

Protein tertiary structure

Brain Network Dynamics

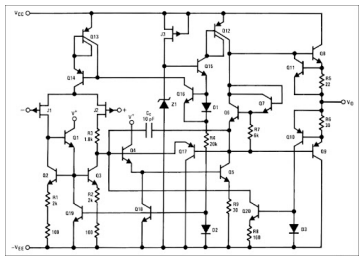


Integrated Circuit Design

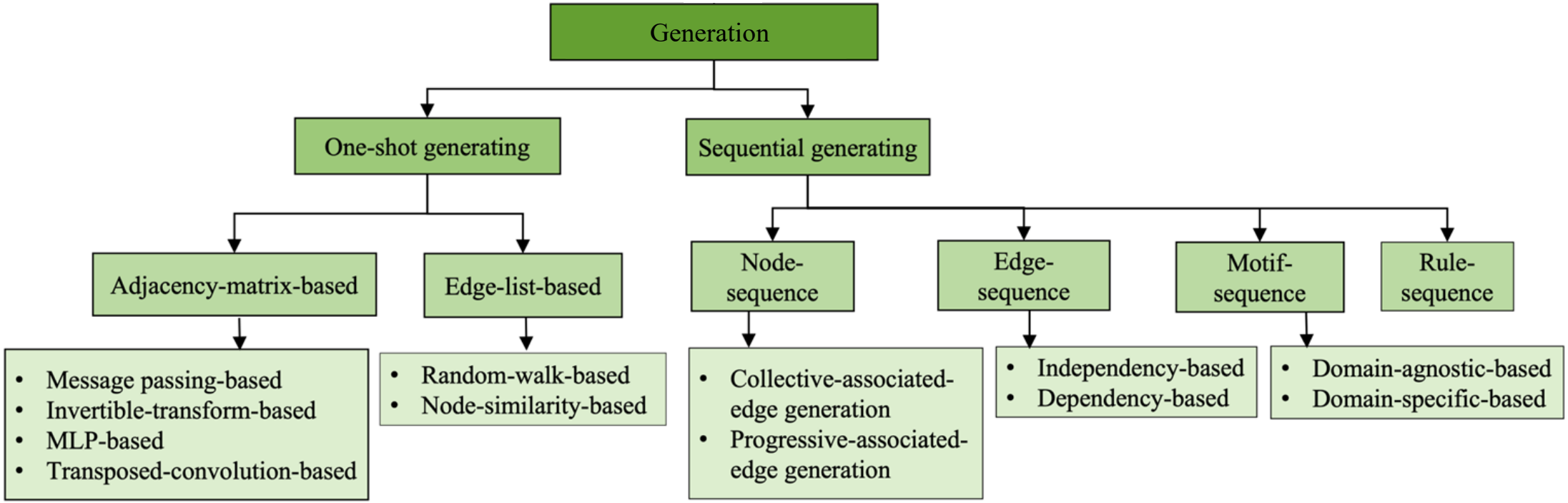
A target function

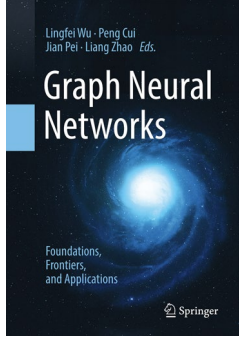
Low energy consumption

Small area

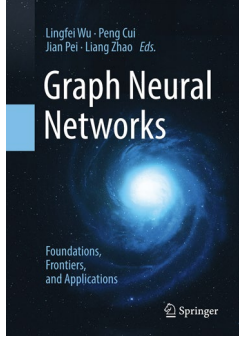


Taxonomy [Guo and Zhao 2022]

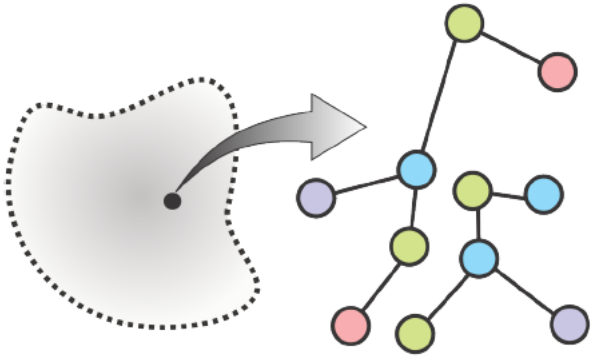




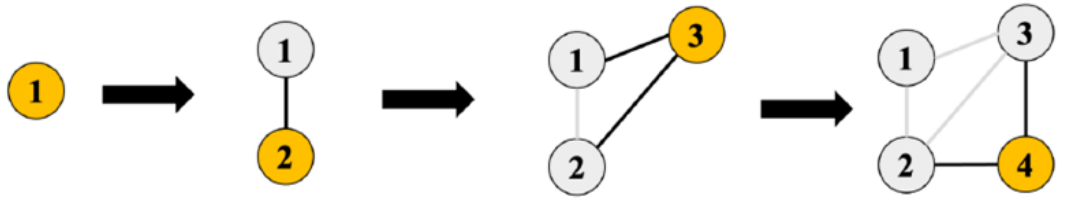
One-shot Generating vs Sequential Generating



One-shot Generation



Sequential Generating



- Advantage and disadvantage

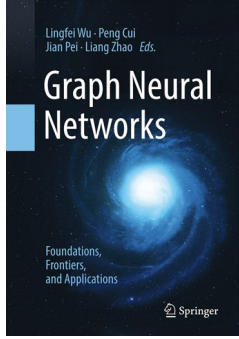
Pros:
capture global patterns
no need to order nodes

Cons:
time consuming

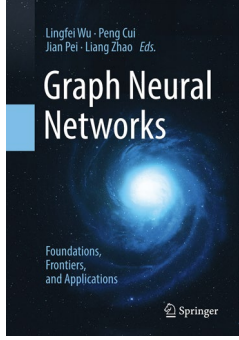
Pros:
efficient for each step
local patterns captured

Cons:
hard to capture global patterns
predefined ordering of nodes

One-shot Generating

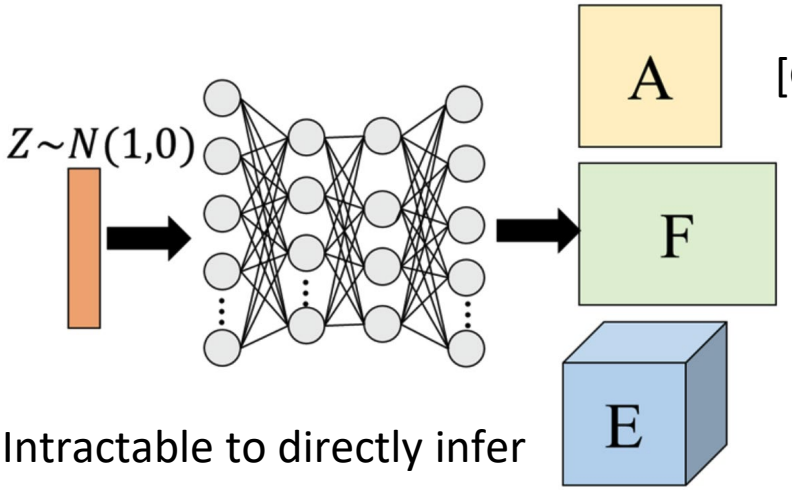


- Adjacency matrix-based
  - MLP-based decoder
  - Message-passing-based decoder
  - Invertible-transform-based decoder
- Edge list based
  - Random-walk-based
  - Node-similarity-based



Adjacency matrix-based: MLP as decoder

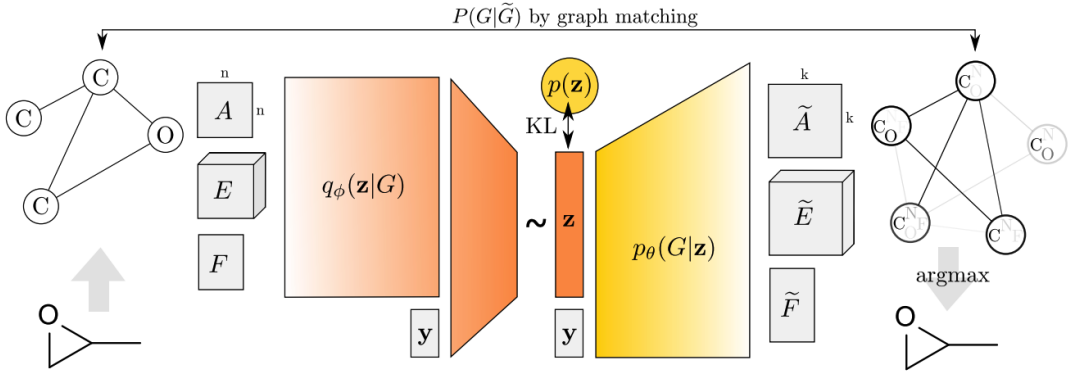
Goal: To learn the graph decoder as generator; typically use GNN as the encoder.



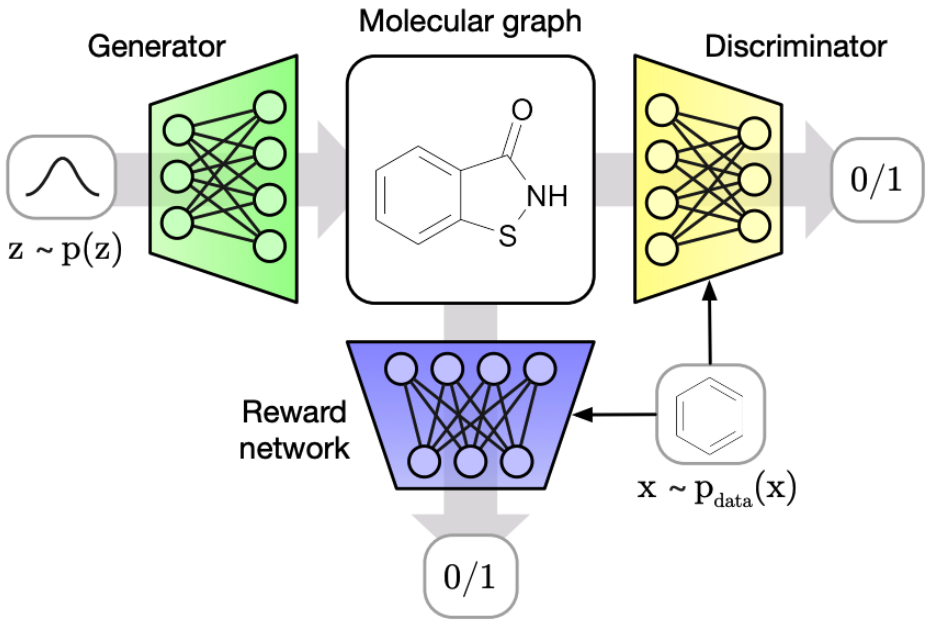
[Guo and Zhao 2022]

Intractable to directly infer

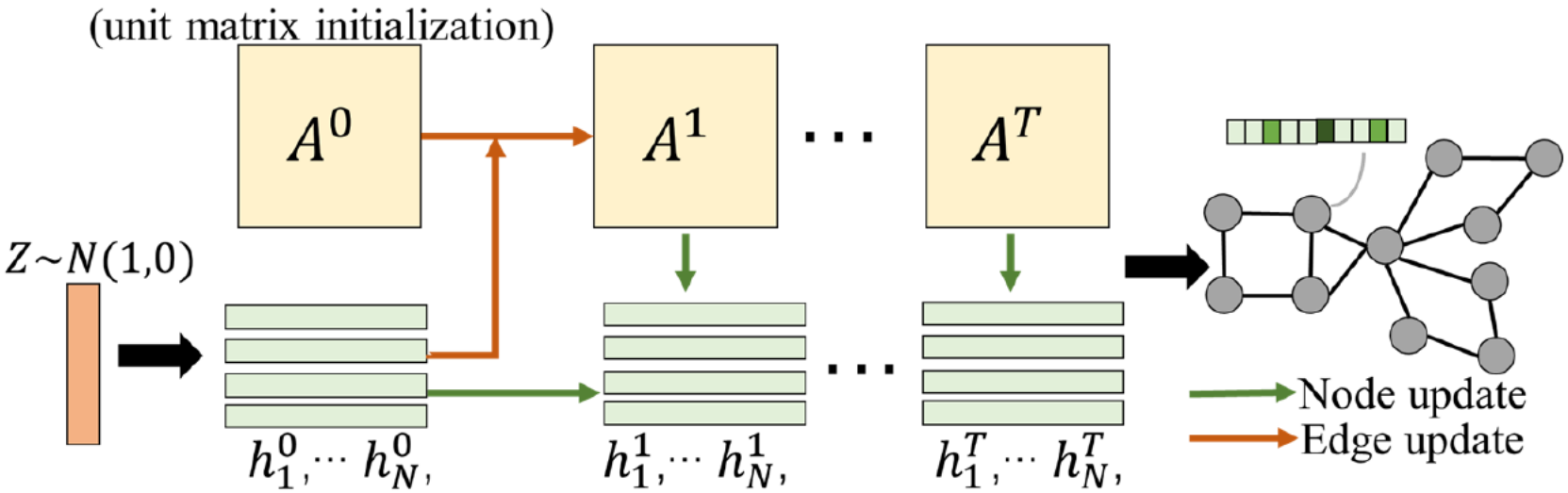
Variational inference
(e.g., GraphVAE [Simonovsky et al. 2018])



Adversarial training
(e.g., MolGAN [DeCao and Kipf 2018])

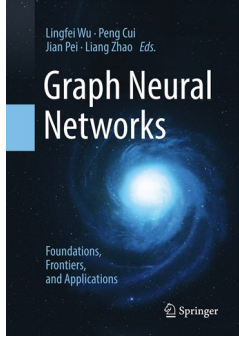


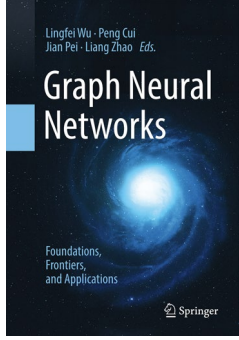
Adjacency matrix-based: Message-passing-based methods



[Guo and Zhao 2022]

$$A_{i,j}^{l+1} = A_{i,j}^{l} + ReLu(\nu_1 A_{i,j}^{l} + \nu_2 h_i^l + \nu_3 h_j^l);$$
$$h_i^{l+1} = h_i^l + ReLu(w_1 h_i^l + \sum_j^N \eta_{i,j} w_2 h_j^l),$$

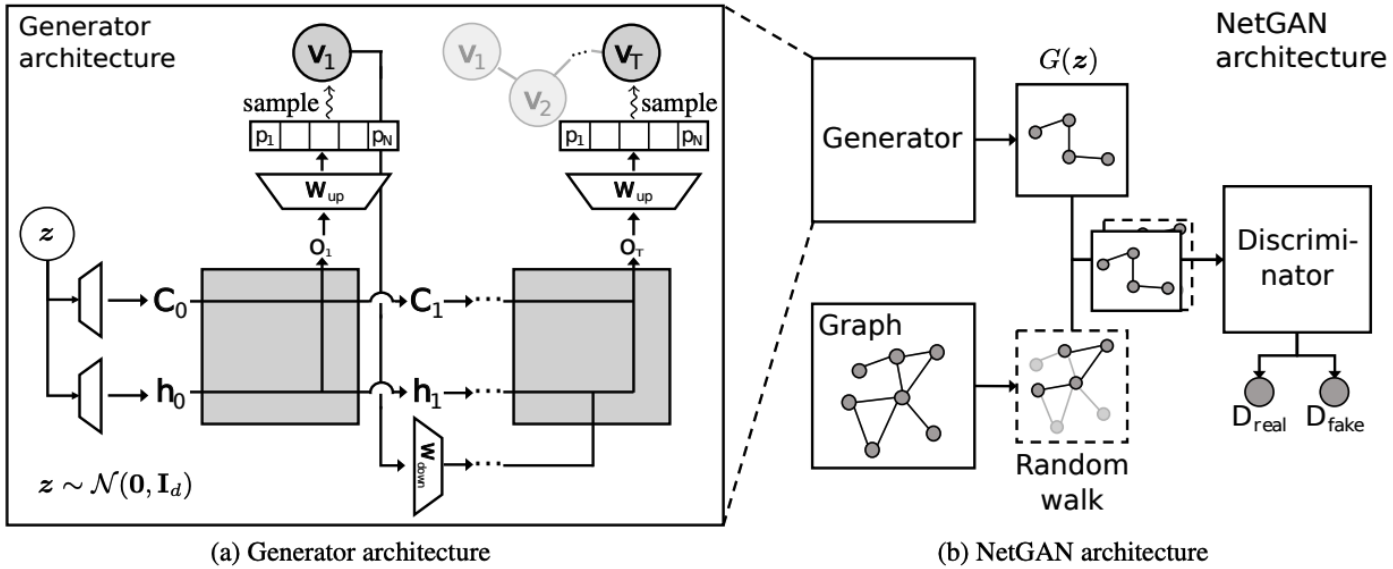




Edge-list based: Random-walk based

- NetGAN [Bojchevski 2018]

Phase 1: Generating random walks.



(a) Generator architecture

(b) NetGAN architecture

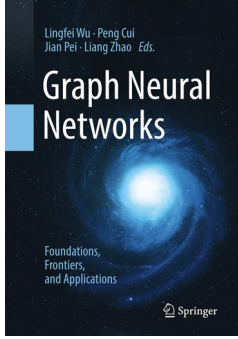
Phase 2: Assembling the Adjacency Matrix.

- Generate many random-walks
- Accumulate all into adjacency matrix
- To ensure no singletons:
  - Step 1: for each node, sample an edge

$$p_{ij} = \frac{s_{ij}}{\sum_v s_{iv}}$$

  - Step 2: sampling edges

$$p_{ij} = \frac{s_{ij}}{\sum_{u,v} s_{uv}}$$



Edge-list based: Node-similarity-based

- Phase 1: Use GNN to learn the node embeddings.
- Phase 2: Generate each edge's probability $\widetilde{\mathrm{A}}_{i,j}$ based on pairs of nodes' embeddings

$$\widetilde{\mathrm{A}}_{i,j} = Sigmoid(Z_i Z_j^T) \quad \text{[Kipf et al. 2018]}$$

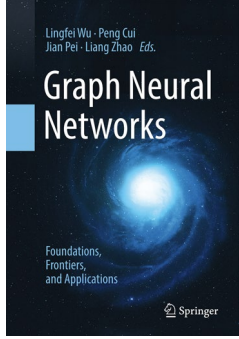
$$\tilde{A}_{i,j} = 1/(1 + exp(C(\| Z_i - Z_j \|_2^2 - 1))) \quad \text{[Liu et al. 2018]}$$

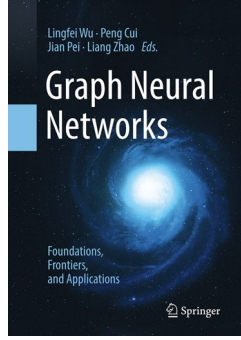
$$\tilde{A}_{i,j} = \mathrm{Sigmoid}(m_j - log \| Z_i - Z_j \|_2^2) \quad \text{[Salha et al. 2019]}$$

- Phase 3: sample each edge using $\widetilde{\mathrm{A}}_{i,j}$

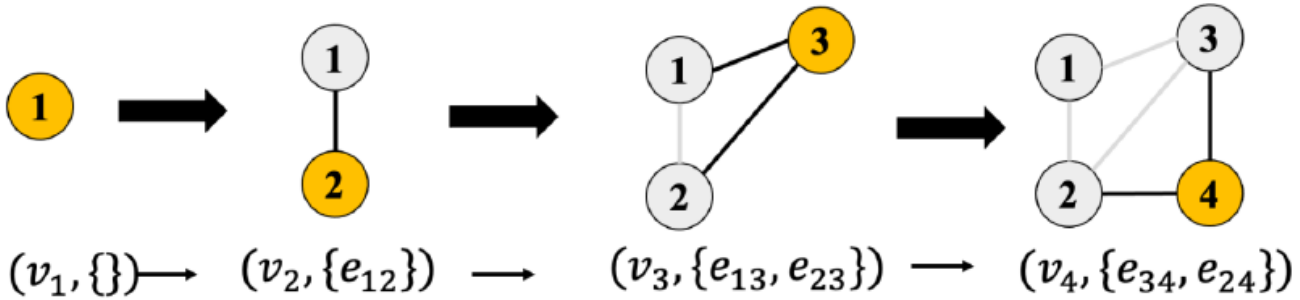
Sequential generating

- node sequence based
- edge sequence based
- graph motif sequence based
- rule-based (e.g., Junction Tree [Jin et al. 2018])





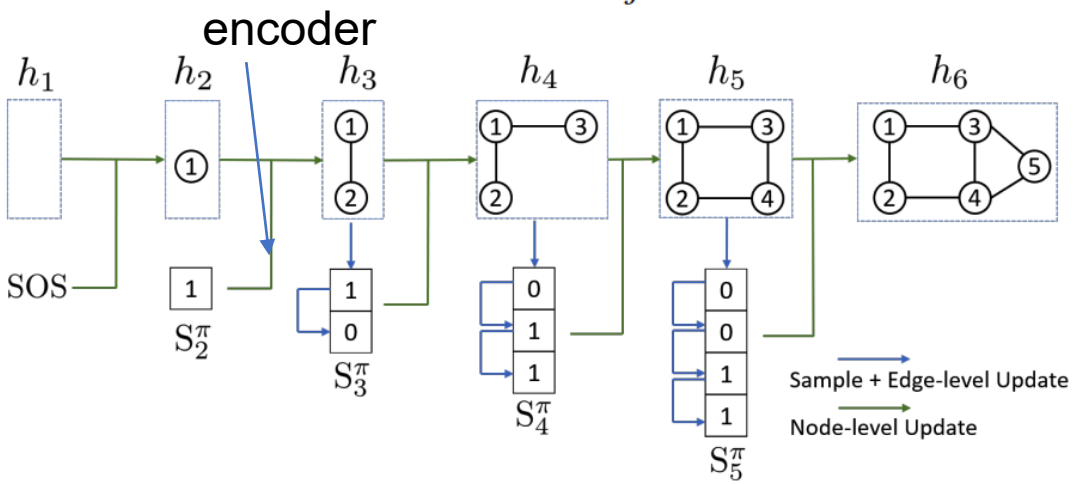
Node sequence based [You et al. 2018]



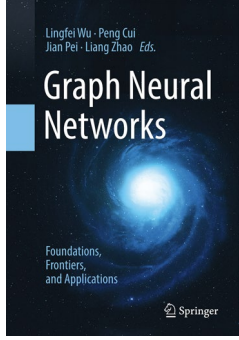
$$p(\mathcal{V}^\pi, A^\pi) = \prod_{i=1}^{N} p(v_i^\pi | v_{<i}^\pi, A_{<i,\cdot}^\pi) p(A_{i,\cdot}^\pi | v_{\leq i}^\pi, A_{<i,\cdot}^\pi),$$

$$p(A_{i,\cdot}^\pi | A_{<i,\cdot}^\pi) = \prod_{j=1}^{i-1} p(A_{i,j}^\pi | A_{i,<j}^\pi, A_{<i,\cdot}^\pi),$$

can be time-consuming for large graphs

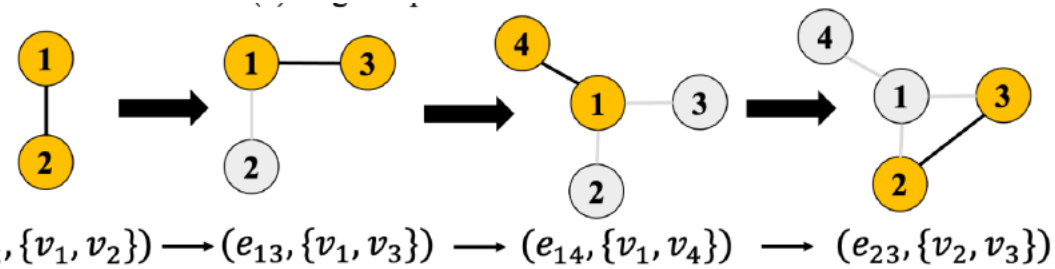


Ways to improve [Liu et al. 2018]
1) an addEdge function to determine the size of the edge set
2) a selectNode function to select the nodes to be connected from the existing graph



Edge Sequence based

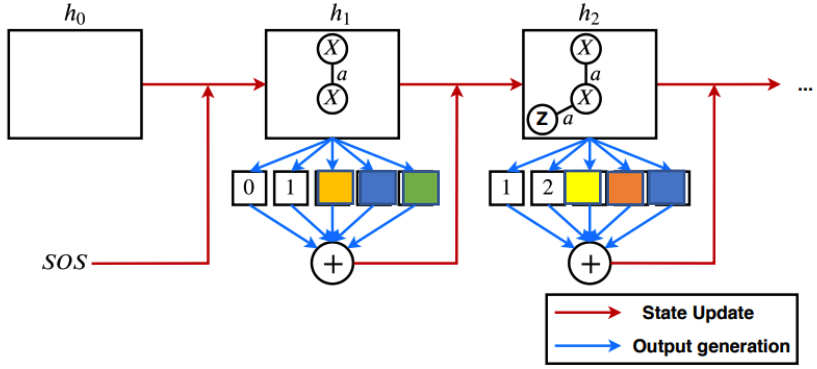
Sometimes edges contain rich information, and sometimes the graph is sparse.



$$(e_{12}, \{v_1, v_2\}) \longrightarrow (e_{13}, \{v_1, v_3\}) \longrightarrow (e_{14}, \{v_1, v_4\}) \longrightarrow (e_{23}, \{v_2, v_3\})$$

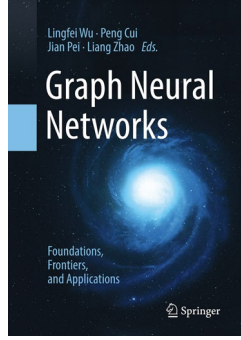
Consider graph as a sequence of tuples where each tuple is denoted as $s_i = (\alpha(u), \alpha(v), F_u, F_v, E^i_{u,v})$ [Goyal et al. 2020]

$$p(s_i|s_{<i}) = p((\alpha(u), \alpha(v), F_u, F_v, E^i_{u,v})|s_{<i})$$
$$= p(\alpha(u)|s_{<i})p(\alpha(v)|s_{<i})p(F_u|s_{<i})p(F_v|s_{<i})p(E^i_{u,v}|s_{<i}),$$

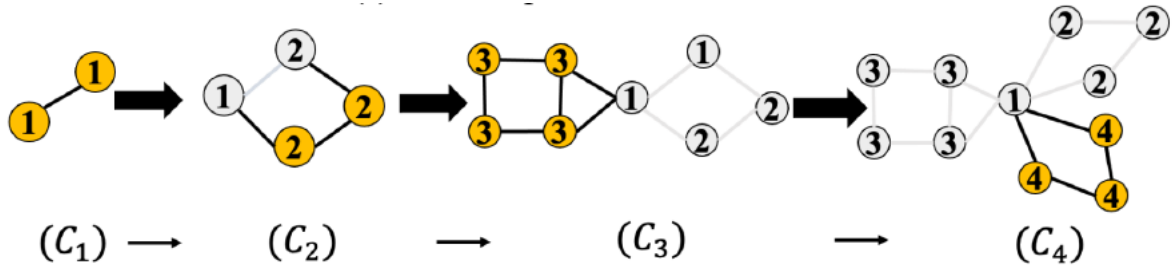


$$p(\alpha(u)|s_{<i})p(\alpha(v)|\alpha(u), s_{<i})$$

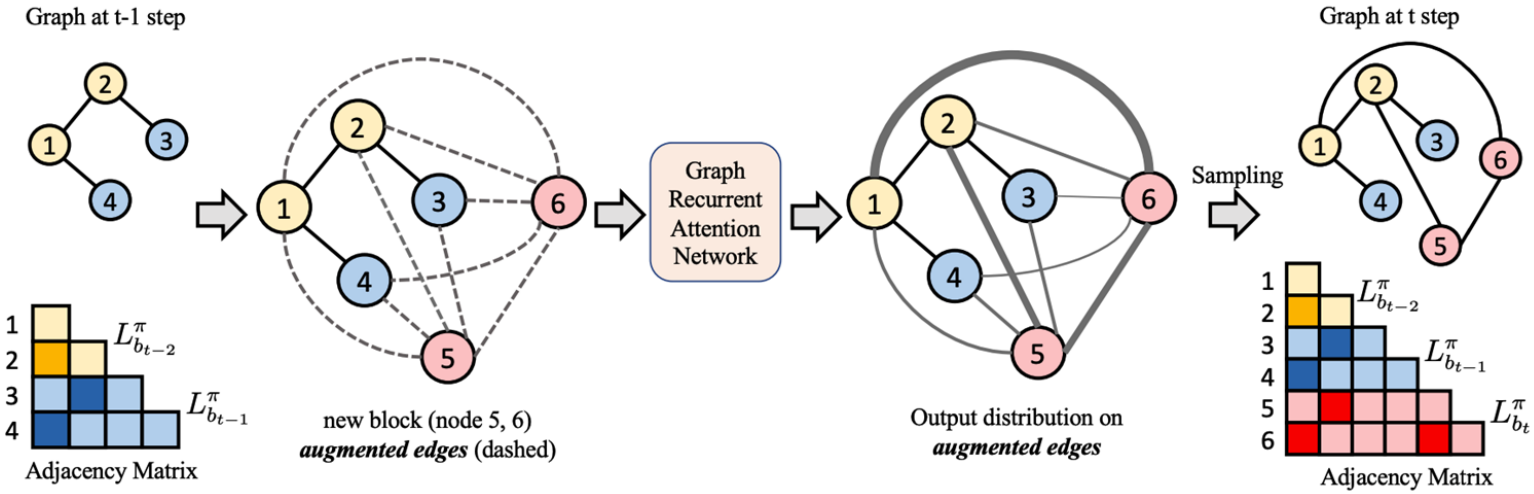
Consider the dependency between u and v. [Bacciu et al. 2020]

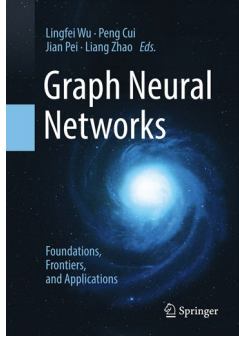


Graph Motif Based [Liao et al. 2019]



$$p(C_t|C_{<t}) = \prod_{B(t-1)<i\leq B} \prod_{1\leq j\leq i} p(A^{\pi}_{i,j}|C_{<t})$$

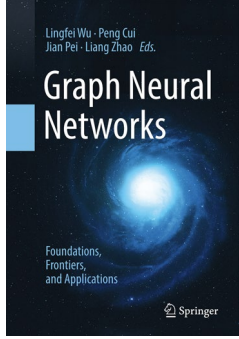




Graph Transformation

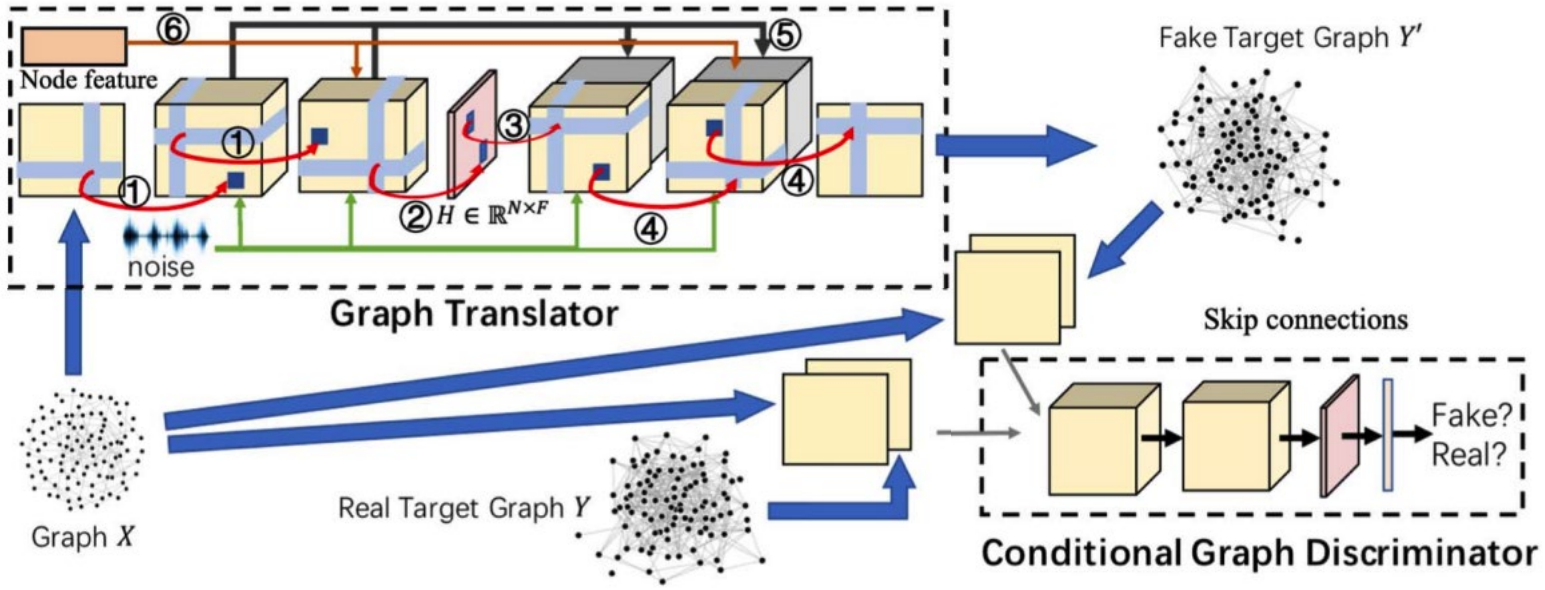
- Edge transformation
  - Applications: protein folding, structure-to-functional connectivity
  - Techniques:
    - GT-GAN [Guo et al. 2022b]
    - DAG2DAG [xx, xx]

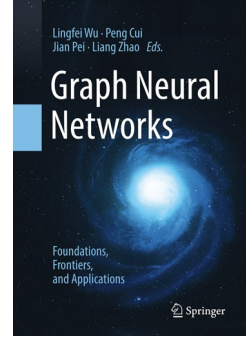
- Node-edge joint translation
  - Techniques:
    - GCPN [You et al.]
    - NEC-DGT [Guo et al. 2019]



Graph Transformation

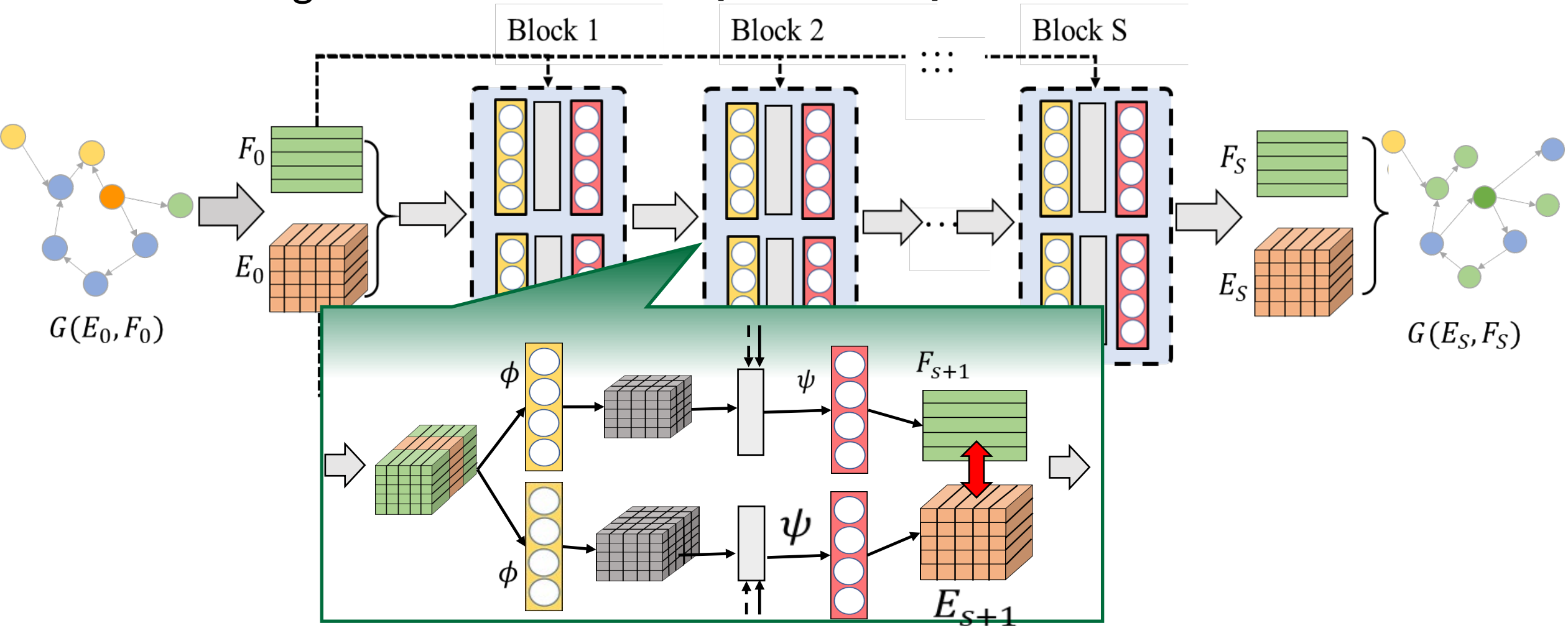
- Edge Transformation
  - GT-GAN [Guo et al. 2022]

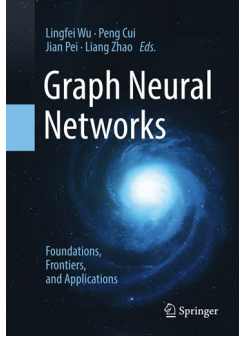




Graph Transformation

- Node-Edge-Co Transformation [Guo et al. 2019]



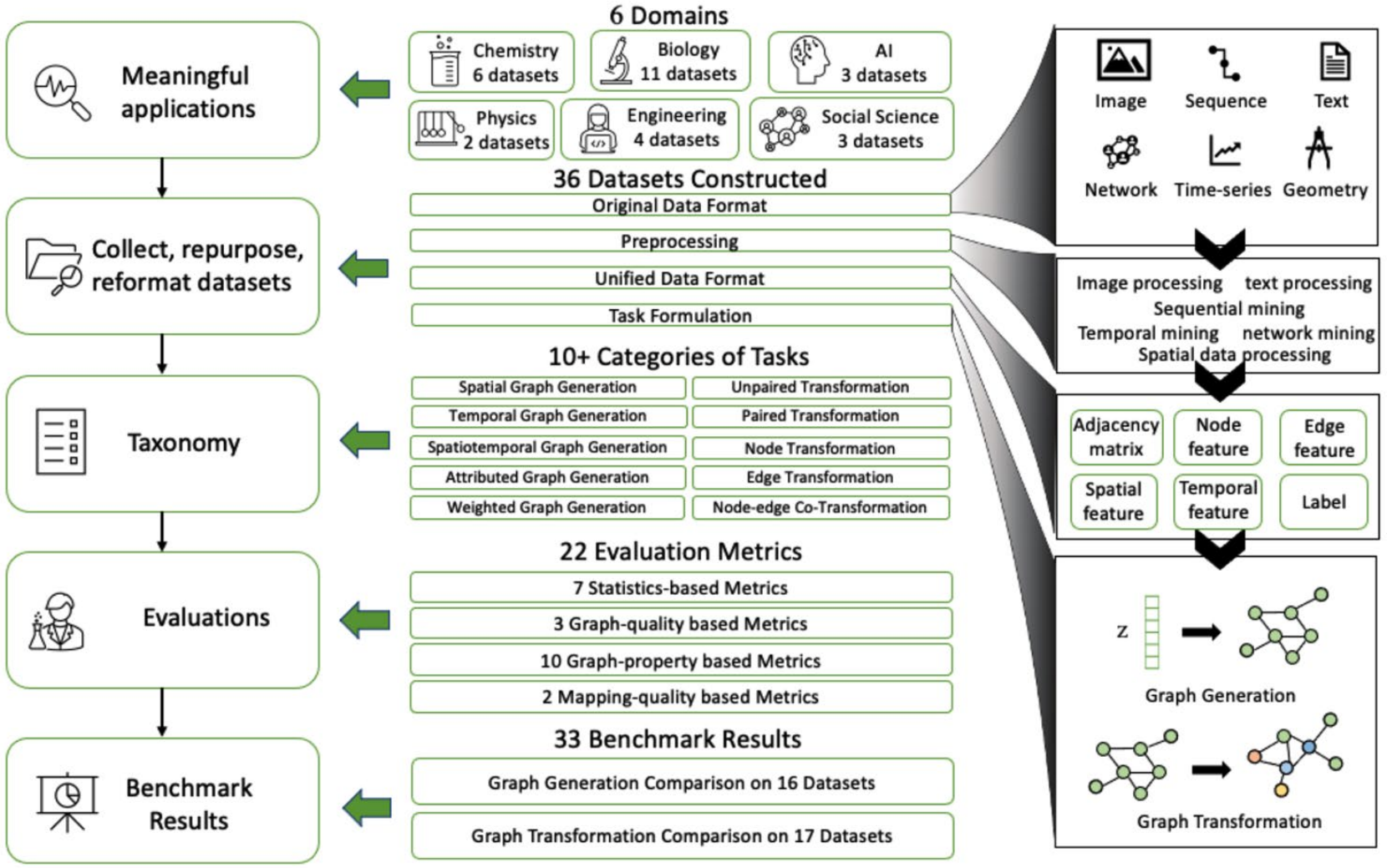


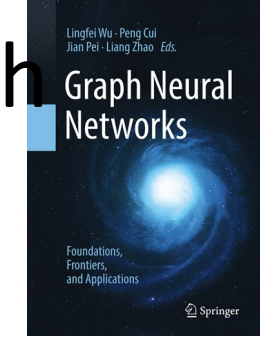
Evaluation metrics [Guo and Zhao 2022]

- Statistics-based
  - Difference between the distributions of generated graphs and real graphs
  - In the graph aspects
    - node degree, cluster coefficient, orbit count, triangle count, Characteristic path length, assortativity, largest component size, etc.
  - With difference measure:
    - Maximum Mean Discrepancy
    - Average KL Divergence
- Classification-based
  - A classifier is trained on a class of real graphs, then it is used to classify the generated graphs under the corresponding class.
  - Metrics: Accuracy and Fréchet Inception Distance
- Intrinsic-quality-based
  - Validity: the percentage of generated graphs that satisify required properties (e.g., cyclic, molecular validity, etc.)
  - Uniqueness: diversity of generated graphs
  - Novelty: percentage of the generated graphs unseen in training set

GraphGT: Benchmark Datasets Repository for Graph Generation

[Du et al. 2021]

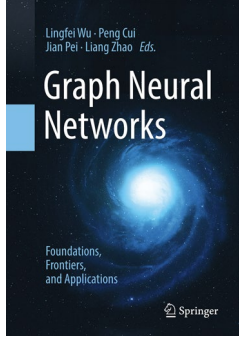


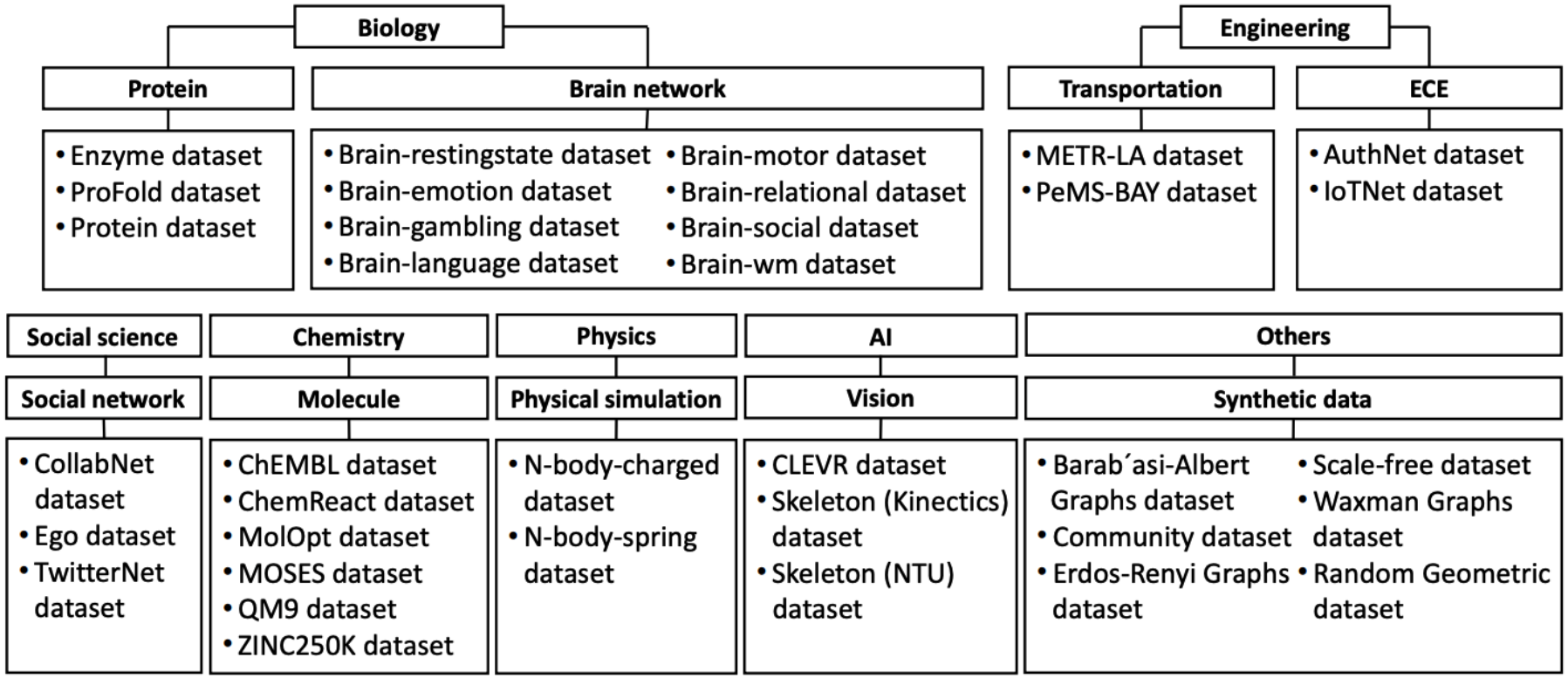


Du, et al. GraphGT: Machine Learning Datasets for Deep Graph Generation and Transformation. NeurIPS 2021.

Visit our website for datasets: https://graphgt.github.io/index.html
Or scan QR code:

GraphGT Benchmark datasets by domains



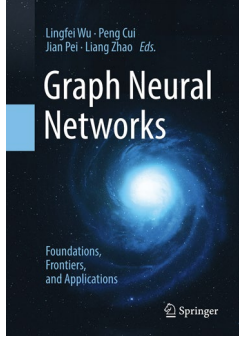


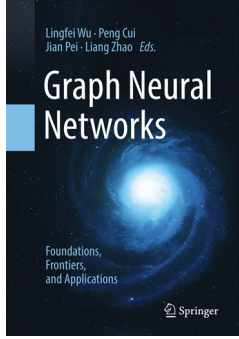
Du, et al. GraphGT: Machine Learning Datasets for Deep Graph Generation and Transformation. NeurIPS 2021.

Visit our website for datasets: https://graphgt.github.io/index.html
Or scan QR code:

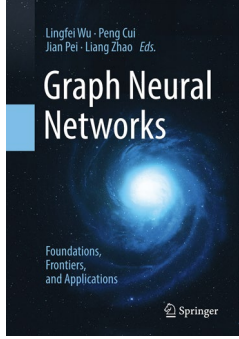
Future Opportunities

- Scalability.
- Validity constraint.
- Interpretability and Controllability.



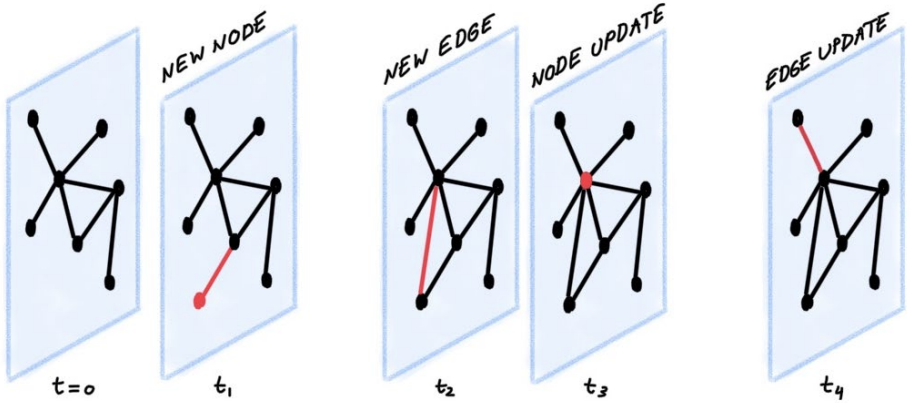


GNNs: Dynamic Graph (Chapter 15)



GNN for Dynamic graph: dynamic graph types

- Discrete-time dynamic graph (DTDG)

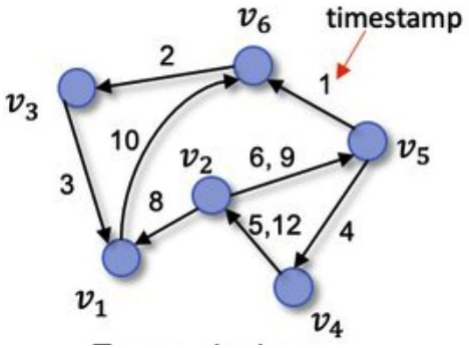


[Rossi 2020]

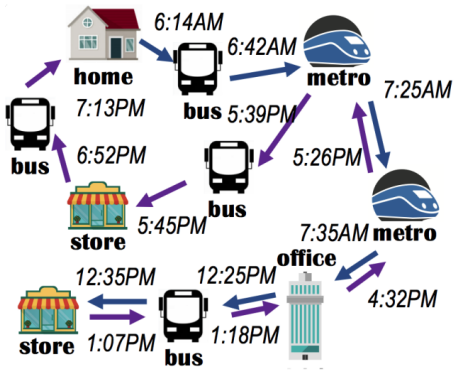
$$[G^{(1)}, G^{(2)}, \ldots, G^{(\tau)}]$$

$$G^{(t)} = (V^{(t)}, A^{(t)}, X^{(t)})$$

- Continuous-time dynamic graph (CTDG)



[Xu

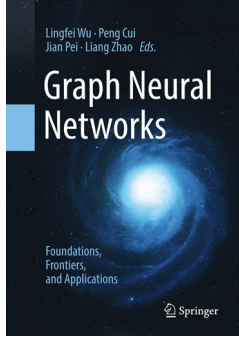


[Zhang et al.

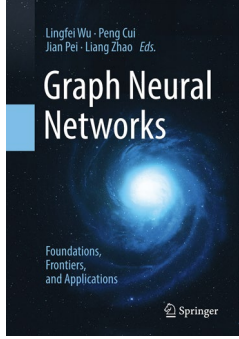
$$(G^{(t_0)}, O)$$

$$O = [(add\ node, v_4, 20\text{-}05\text{-}2020), (add\ edge, (v_2, v_4), 21\text{-}05\text{-}2020),$$
$$(Feature\ update, (v_1, [0.1, 2]), 28\text{-}05\text{-}2020), (add\ edge, (v_3, v_4), 04\text{-}06\text{-}2020)]$$

GNN for Dynamic graph: types of dynamics



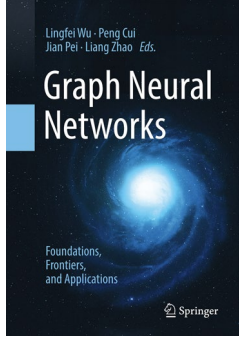
- Operations:
  - Node addition/deletion
  - Feature update
  - edge addition/deletion
  - edge weight updates
- Another categorization:
  - communication: dynamics on graphs. usually fast
  - association: dynamics of graphs. usually slower.



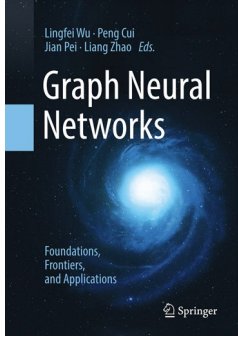
Types of tasks

- Dynamic Node classification/regression
  - interpolation
  - extrapolation
- Dynamic graph classification
- Dynamic link prediction
  - interpolation
  - extrapolation
- Time prediction
  - interpolation
  - extrapolation

Modeling Dynamic Graphs with GNN



- Conversion to Static Graph [Yao et al. 2016]
- GNNs for DTDGs [Seo et al, 2018; Manessi et al, 2020; Xu et al, 2019a]
- GNNs for CTDGs [Kumar et al. 2019b]



Conversion to Static Graph

- Temporal aggregation [Yao et al. 2016]

Involving topology

weighted aggregation of the adjacency matrices

exponentially decaying $\boldsymbol{A}^{(agg)} = \sum_{t=1}^{\tau} \phi(t,\tau)\boldsymbol{A}^{(t)}$

$$\boldsymbol{X}^{(agg)} = \sum_{t=1}^{\tau} \phi(t,\tau)\boldsymbol{X}^{(t)}$$

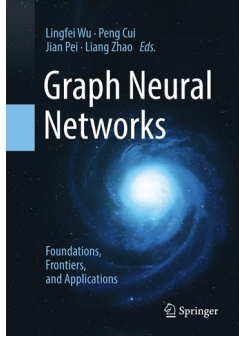
For extrapolation problems

$$\phi(t,\tau) = \exp(-\theta(\tau - t))$$

For interpolation problems

$$\phi(t,t') = \exp(-\theta|t' - t|)$$

θ is a hyperparameter controlling how fast the importance decays

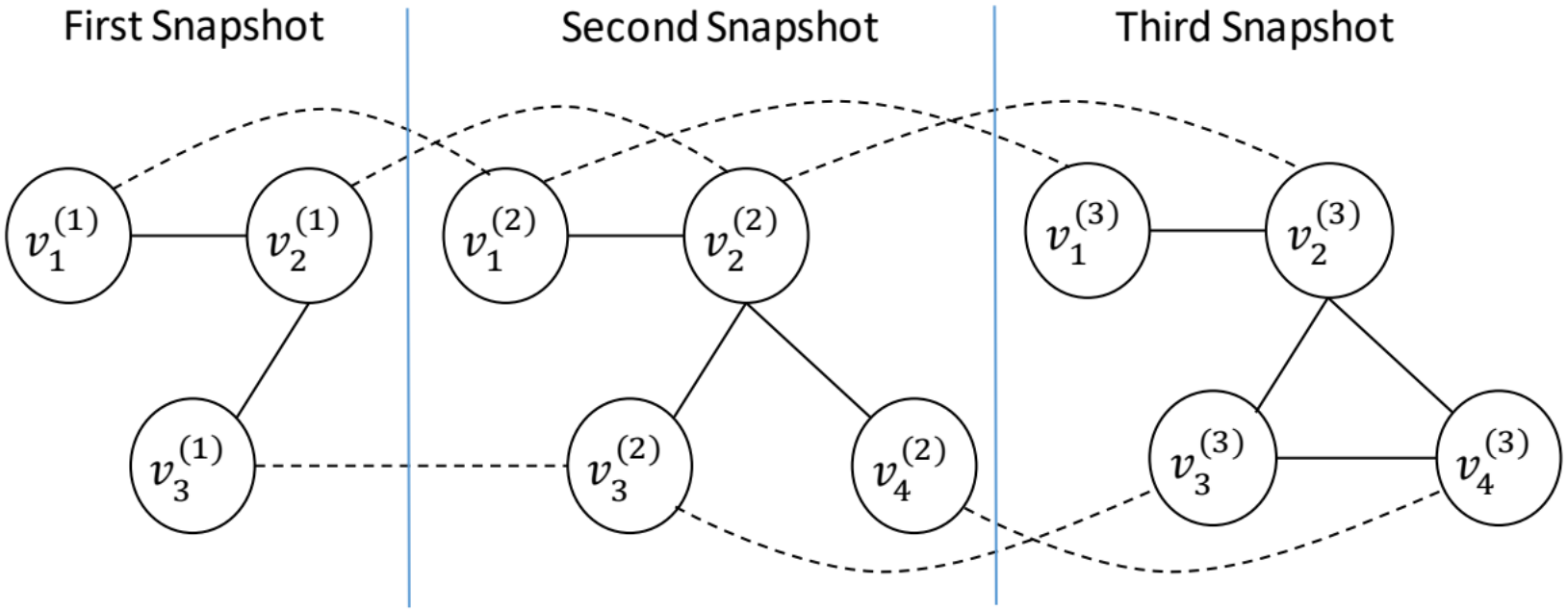


Conversion to Static Graph

- Temporal unrolling

  Connecting the nodes corresponding to the same object across time

GNN(



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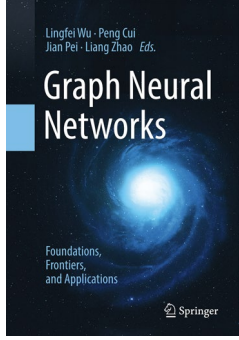
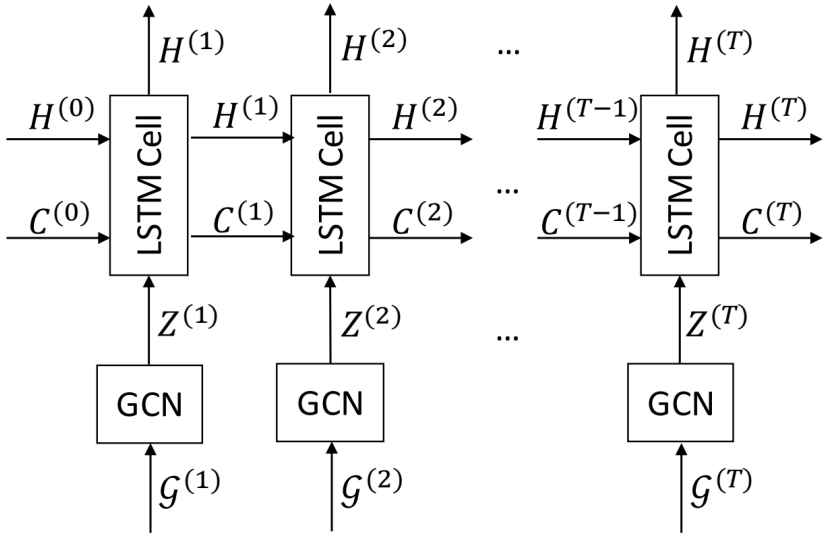


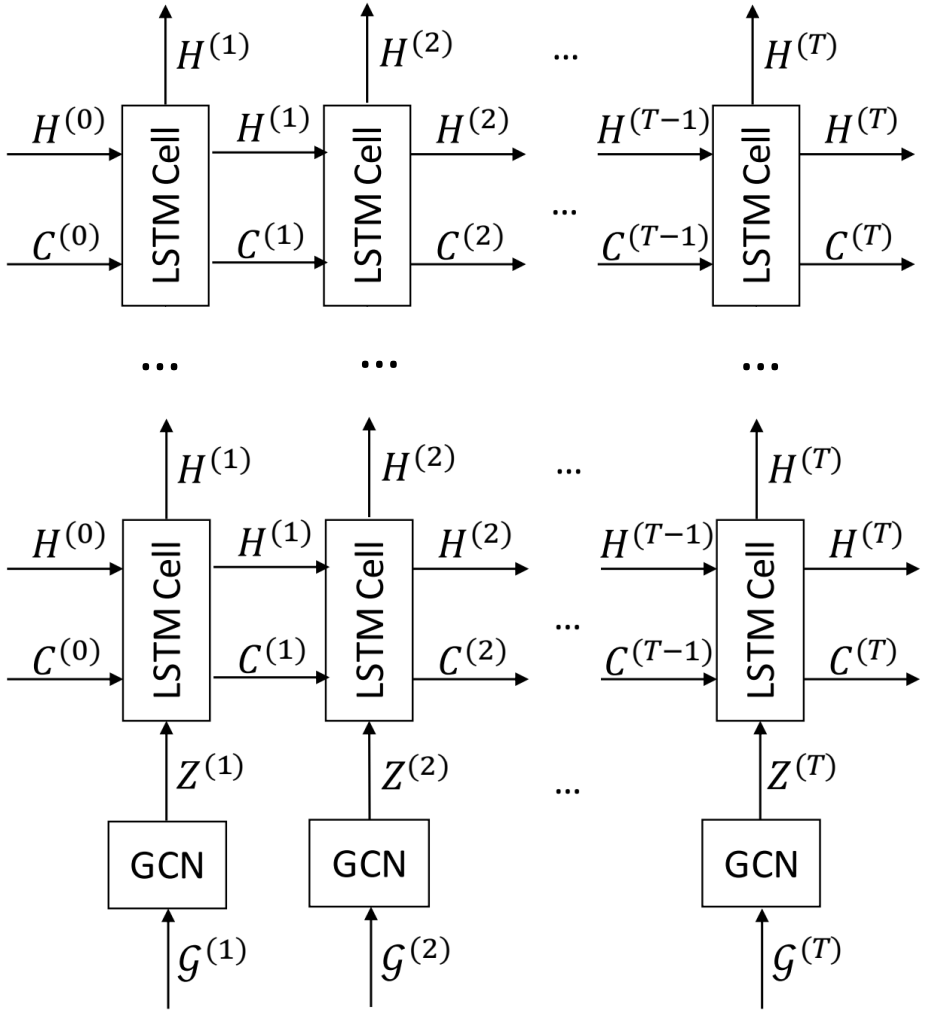
DTDG techniques: GNN-RNN

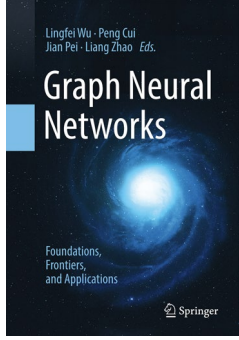
GNN-RNN: sequence of graphs
RNN can be vanilla, LSTM, biRNN, Transformer, etc.

$$\boldsymbol{Z}^{(t)} = GCN(\boldsymbol{X}^{(t)}, \boldsymbol{A}^{(t)})$$

$$\boldsymbol{H}^{(t)}, \boldsymbol{C}^{(t)} = LSTM(\boldsymbol{Z}^{(t)}, \boldsymbol{H}^{(t-1)}, \boldsymbol{C}^{(t-1)})$$





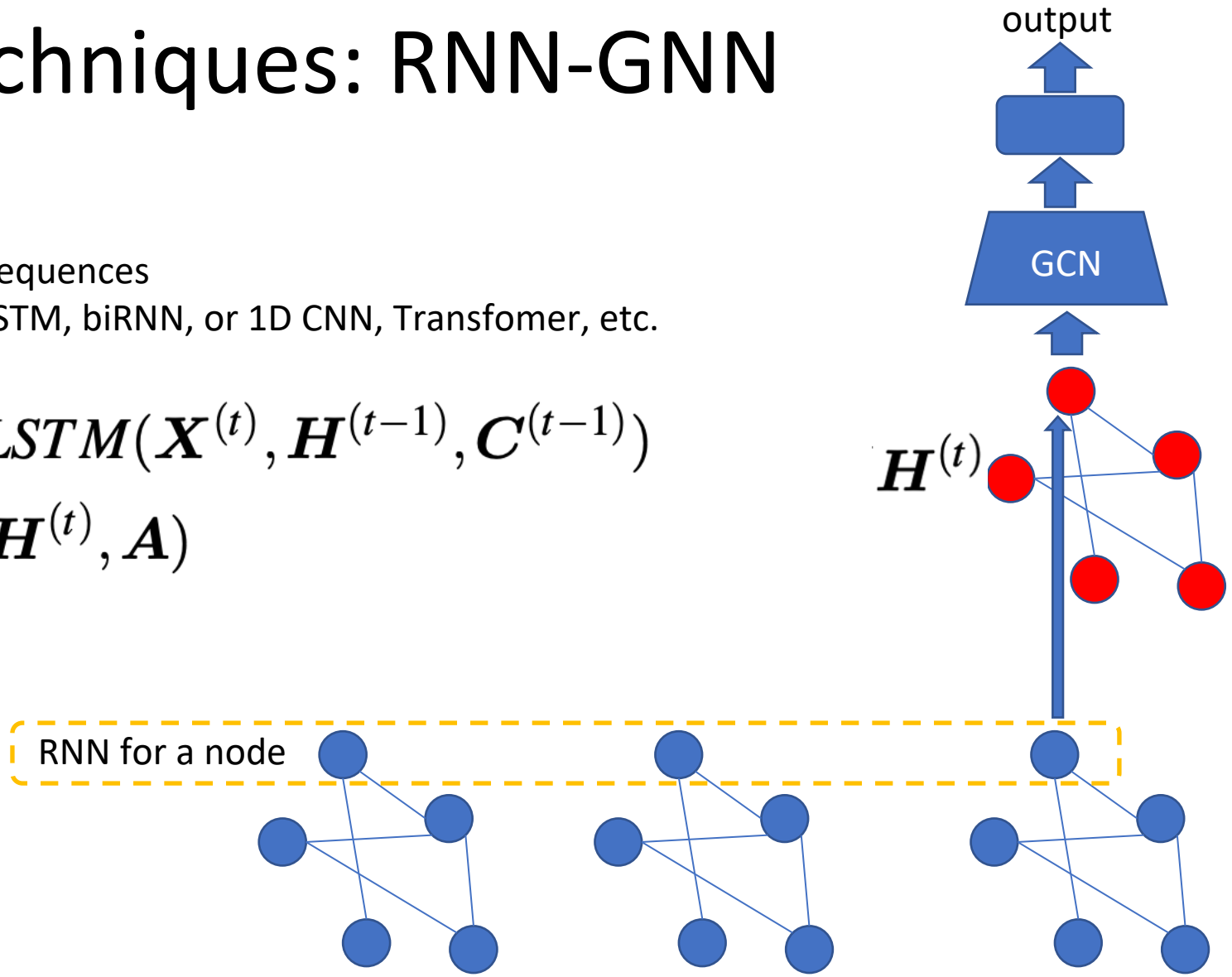


DTDG techniques: RNN-GNN

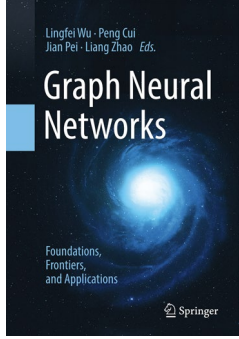
RNN-GNN: graph of sequences
RNN can be vanilla, LSTM, biRNN, or 1D CNN, Transfomer, etc.

$$\boldsymbol{H}^{(t)}, \boldsymbol{C}^{(t)} = LSTM(\boldsymbol{X}^{(t)}, \boldsymbol{H}^{(t-1)}, \boldsymbol{C}^{(t-1)})$$

$$\boldsymbol{Z}^{(t)} = GCN(\boldsymbol{H}^{(t)}, \boldsymbol{A})$$



GNN for CTDG techniques [Kumar et al. 2019b]



Given an observation $(AddEdge, (v_i, v_j), t)$, the embedding of v_i and v_j can be updated as follows.

$$\boldsymbol{Z}_i^{(t)} = RNN_{source}((\boldsymbol{Z}_j^{(t-)} \,||\, \Delta t_i \,||\, \boldsymbol{f}),\ \boldsymbol{Z}_i^{(t-)})$$

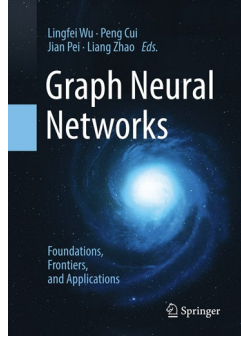
$$\boldsymbol{Z}_j^{(t)} = RNN_{target}((\boldsymbol{Z}_i^{(t-)} \,||\, \Delta t_j \,||\, \boldsymbol{f}),\ \boldsymbol{Z}_j^{(t-)})$$

Then $Z_i^{(t)}$ and $Z_j^{(t)}$ are concatenated to generate the final edge prediction and supervised by $(AddEdge, (v_i, v_j), t)$

1-hop neighbor is considered in [Trivedi et al. (2019],
multi-hop neighbor is considered in TGAT [Xu et al. 2020a].

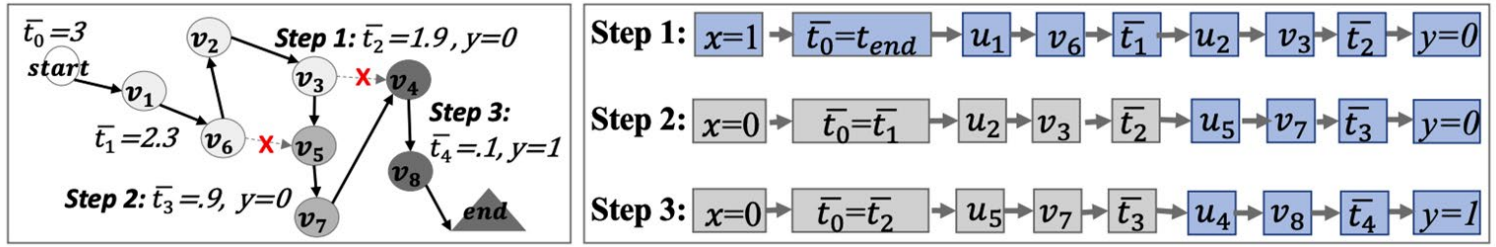
$$\boldsymbol{Z}_i^{(t)} = RNN((\boldsymbol{z}_{\mathcal{N}}(v_j)\Delta t_i),\ \boldsymbol{Z}_i^{(t-)})$$

$\boldsymbol{z}_{\mathcal{N}(v_j)}$ is the neighborhood of v_j

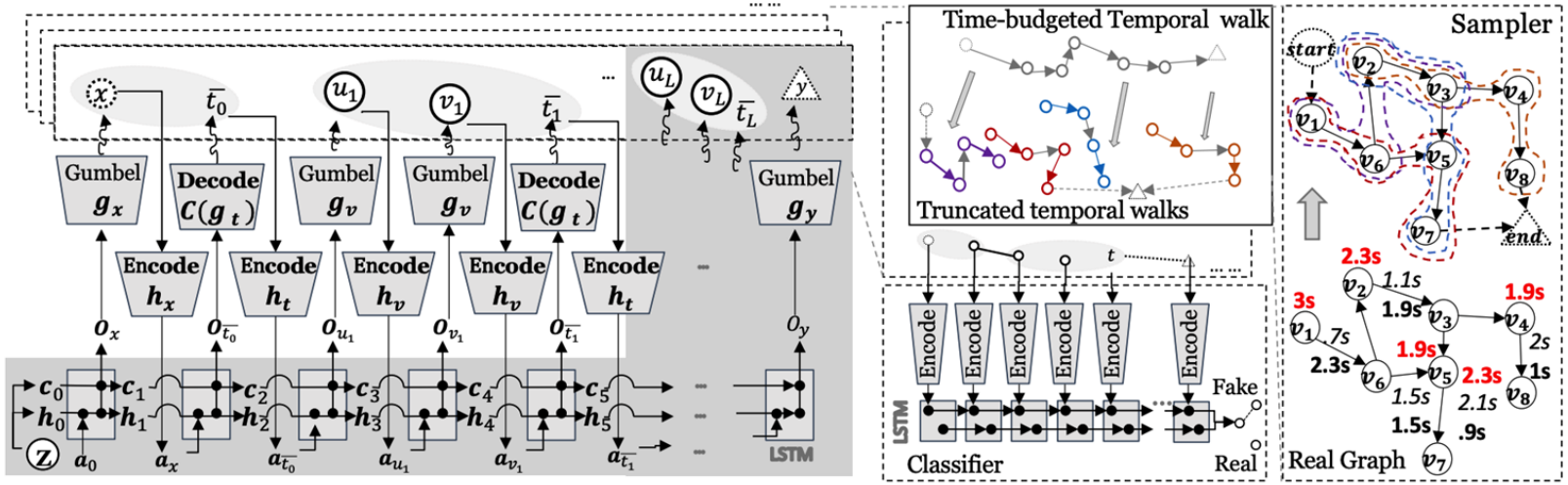


Dynamic Graph Generation for CTDG [Zhang et al. 2021]

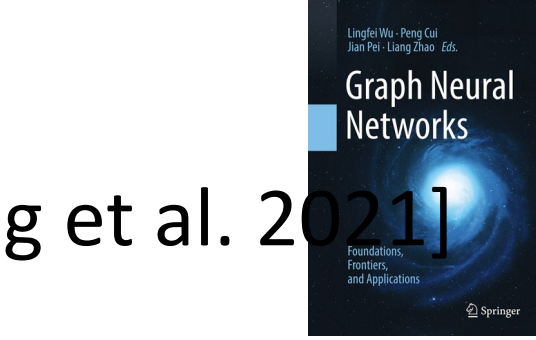
- Continuous-time dynamic graph generation
  - Temporal random walk generation and assembly
    - Challenge: large variance in random walk length: truncated temporal random walk is used



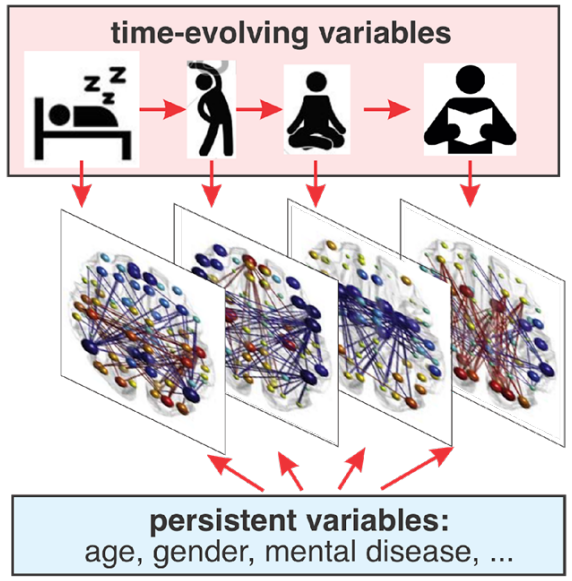
  - Truncated termpoal random walk generator



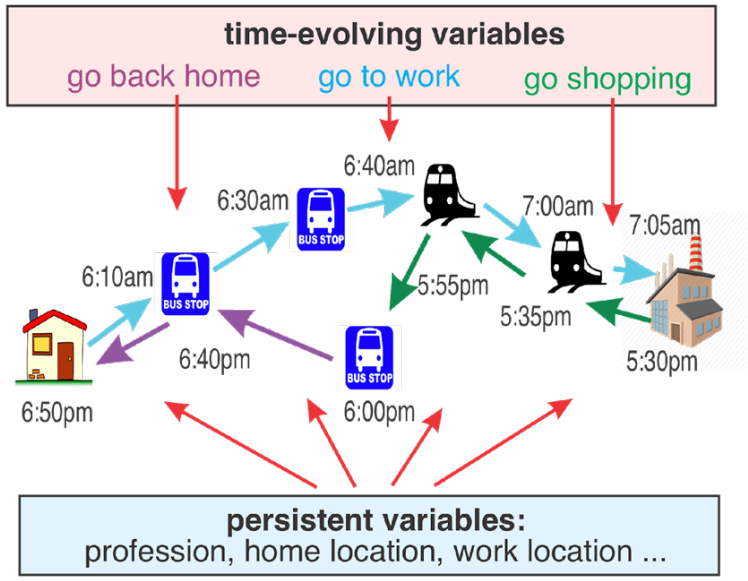
Dynamic Graph Generation for DTDG [Zhang et al. 2021]



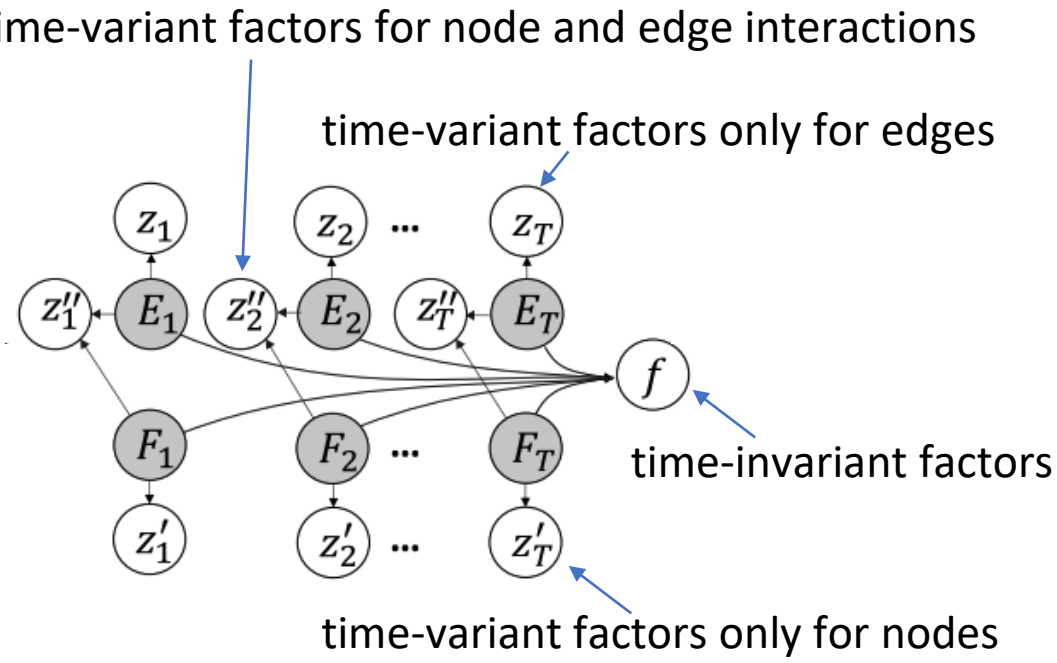
- Discrete-time dynamic graph generation



(d) Dynamic functional connectivity

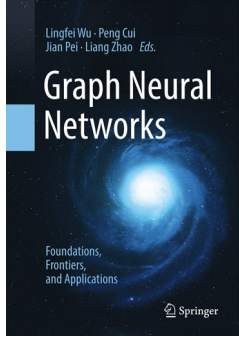


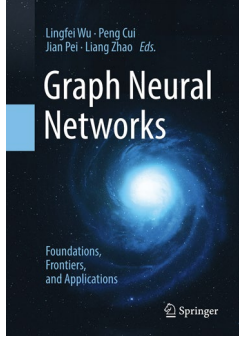
(e) Human mobility network



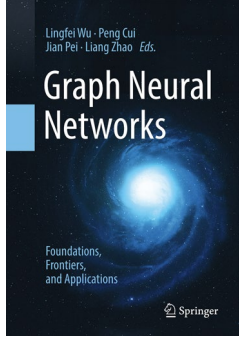
Future directions

- Node addition and removal are still challenges.
- Inverse problem of graph dynamics
- Spatiotemporal



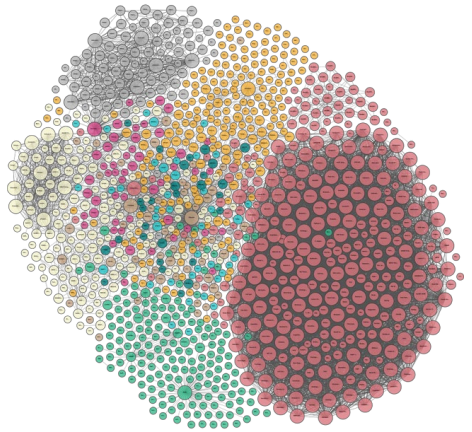


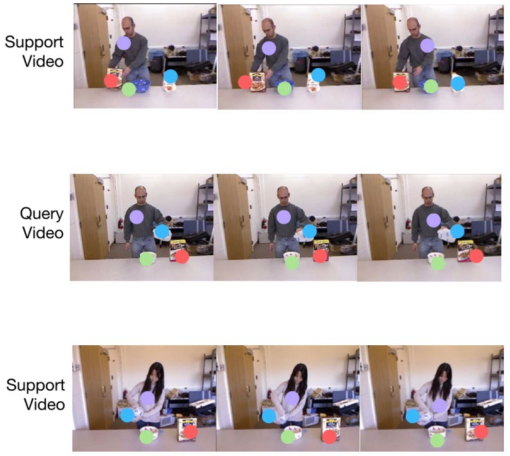
GNNs: Graph Matching (Chapter 13)

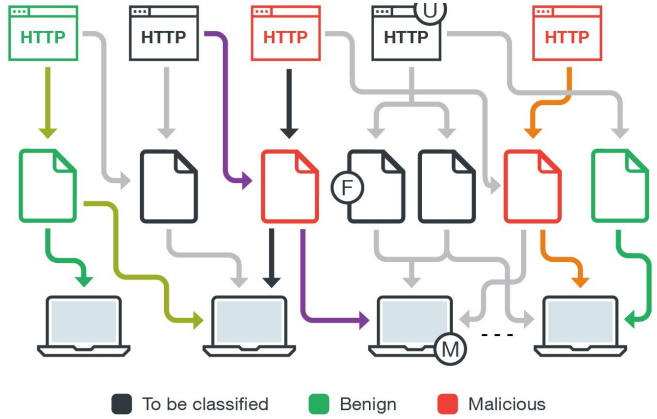


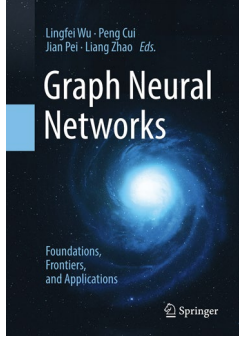
Graph Matching: Applications

- Graph similar searching in graph-based database
- 3D Action Recognition
- Unknown malware detection
- Promising selection in automatic theory proving



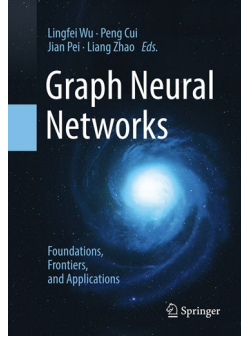






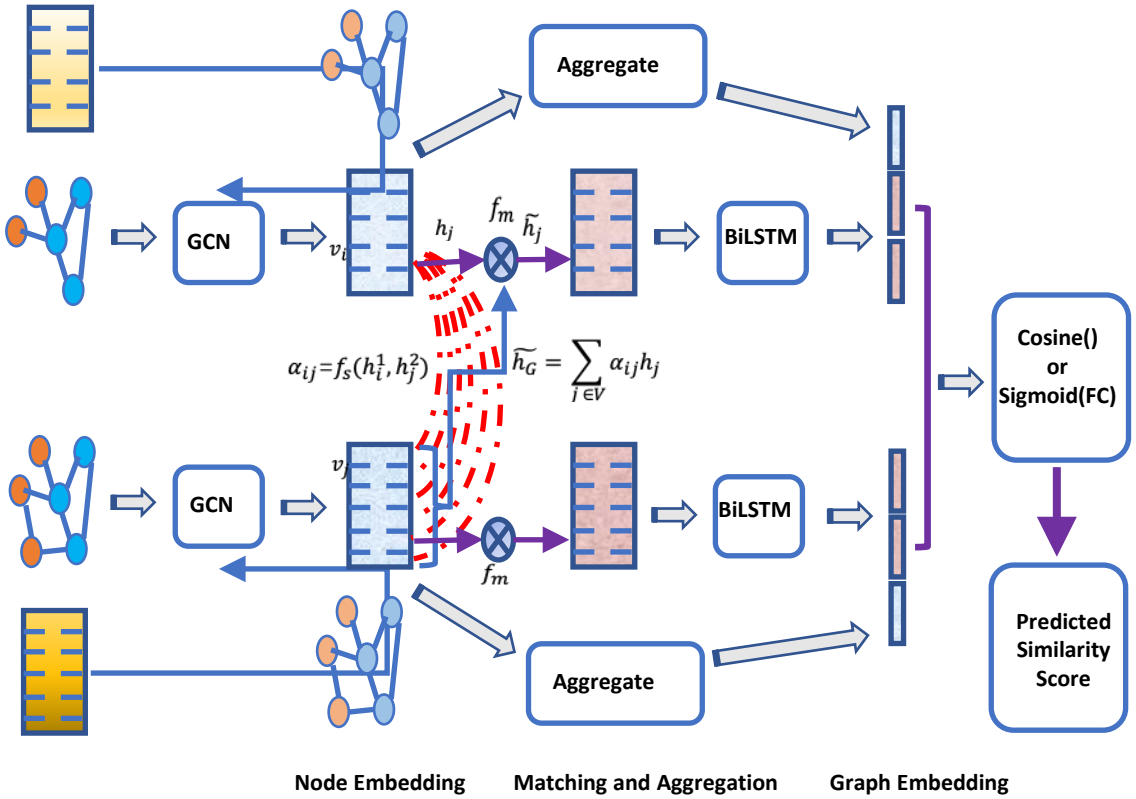
Graph Similarity Learning: Formulation

- Graph Similarity Learning
  - **Input:** a pair of graph inputs $(\mathrm{G}^1, \mathrm{G}^2) \in \boldsymbol{G}\times\boldsymbol{G}$
    - $\mathrm{G}^1 = (\mathrm{V}^1, \mathrm{E}^1)$ with $(\mathrm{X}^1, \mathrm{A}^1)$, where $\mathrm{X}^1 \in \mathrm{R}^{\mathrm{N}\times\mathrm{d}}$, $\mathrm{X}^1 \in \mathrm{R}^{\mathrm{N}\times\mathrm{N}}$
    - $\mathrm{G}^2 = (\mathrm{V}^2, \mathrm{E}^2)$ with $(\mathrm{X}^2, \mathrm{A}^2)$, where $\mathrm{X}^2 \in \mathrm{R}^{\mathrm{M}\times\mathrm{d}}, \mathrm{X}^2 \in \mathrm{R}^{\mathrm{M}\times M}$
  - **Output:** a similarity score $\mathrm{y} \in \boldsymbol{Y}$
    - $\mathbf{Y} = \{-1, 1\}$: graph-graph classification task
    - $\mathbf{Y} = [0, 1]$: graph-graph regression task



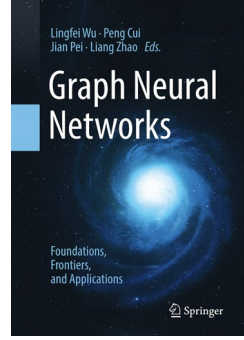
Multi-level Graph Matching Networks

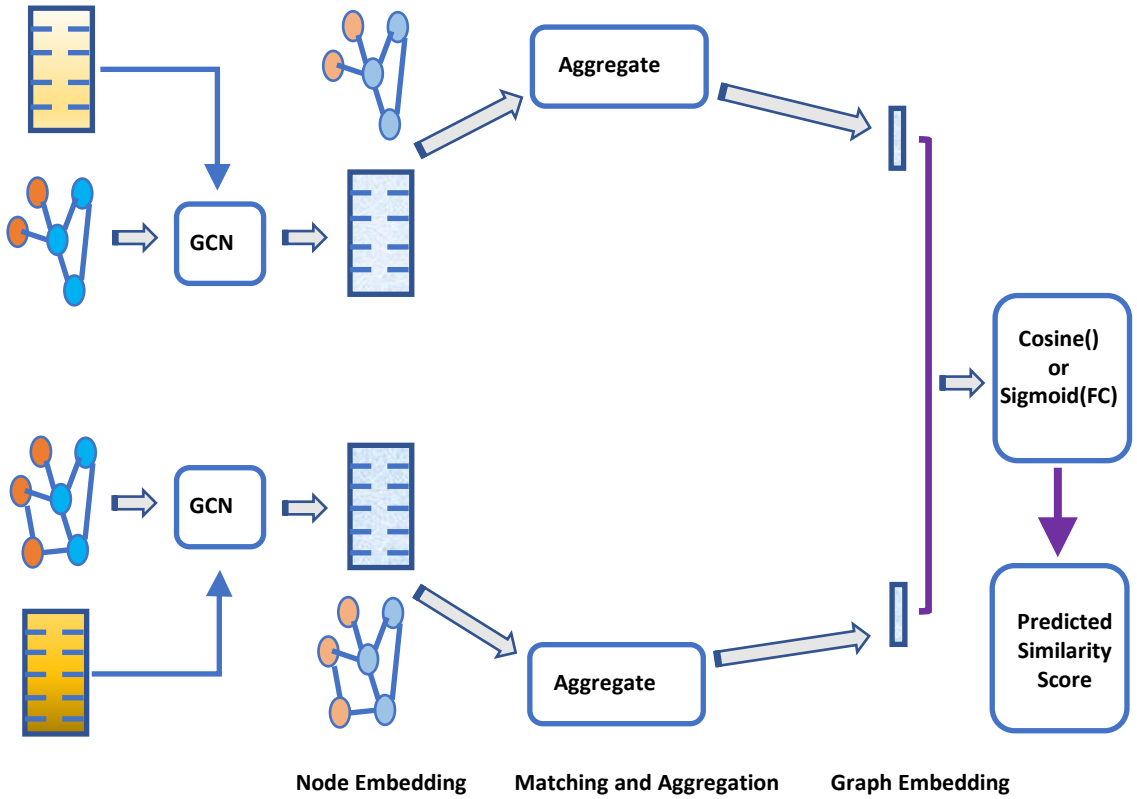
We propose a HGMN to capture different-levels interactions:



- Siamese Graph Neural Networks (SGNN): learning the global-level interactions
- Multi-perspective Node-Graph Matching Network (MPNGMN): learning the cross-level node-graph interactions

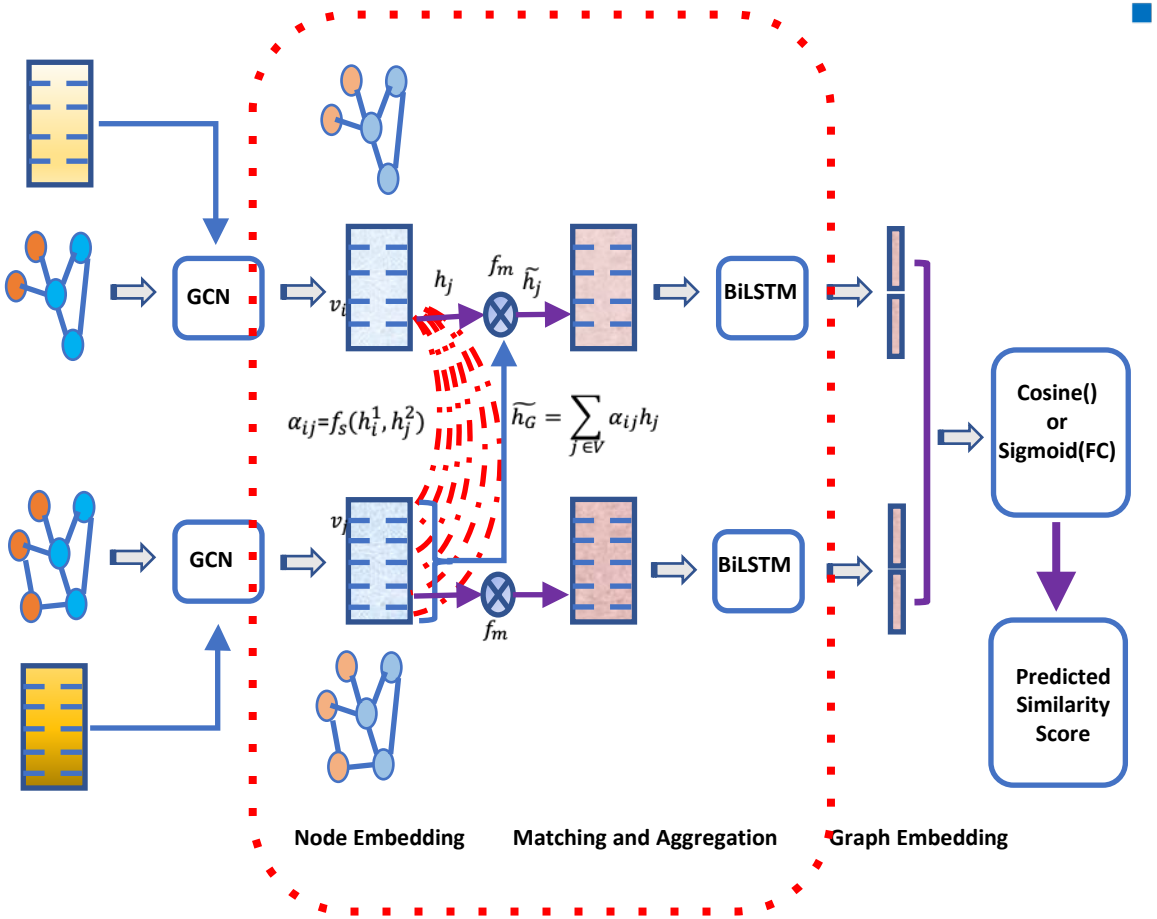
Siamese Graph Neural Networks





- Node Embedding Layer:
  - ✓ Graph siamese network with 3-layer GCNs
  - ✓ Generate node embeddings for G^1 and G^2
  - ✓ $H^l = \{\vec{h}_i^l\}_{i=1}^{\{N,M\}} \in \mathcal{R}^{\{N,M\}\times d'}, l = \{1,2\}$
- Graph-level Embedding Aggregation Layer:
  - ✓ Max / FCMax / Avg / FCAvg / BiLSTM
  - ✓ [redacted]
- Graph-Graph Matching and Prediction Layers:
  - ✓ Classification: $\widetilde{y} = cosine(\vec{h_G^1}, \vec{h_G^2})$
  - ✓ Regression: $\widetilde{y} = \mathrm{sigmoid}\left(\mathrm{MLP}\left([\vec{h_G^1}, \vec{h_G^2}]\right)\right)$

Multi-perspective Node-Graph Matching Networks



- **Node-Graph Matching Layers:**

① For each node $v_i \in V^1$ and V^2 compute node embeddings ($\overrightarrow{h_i^1}$) in G^1 or G^2

② Compute attention weights

$$\alpha_{i,j} = f_s(\mathbf{h}_i^1, \mathbf{h}_j^2), \; j \in \mathcal{V}^2$$

③ Attentive graph-level embeddings of G^2

$$\tilde{\vec{h}}_G^2 = \sum_{j \in \mathcal{V}^2} \alpha_{i,j} \vec{h}_j^2$$

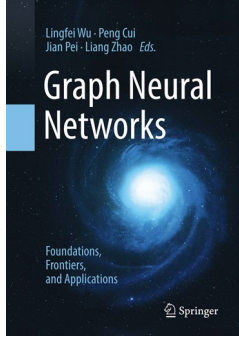
④ Multi-perspective matching function f_m

[redacted]

Trainable weights: $W_m = \{\vec{w}_i\}_{i=1}^{\tilde{d}} \in \mathcal{R}^{d' \times \tilde{d}}$

⑤ update the node features for node v_i

$$\tilde{\vec{h}}_i^1 = f_m(\vec{h}_i^1, \tilde{\vec{h}}_G^2, W_m)$$



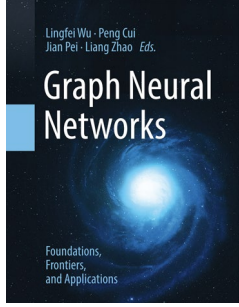
Experimental Setup

We evaluate our model on **four datasets** for both **classification** and **regression** tasks.

Table 1: Summary statistics of datasets for both classification & regression tasks.

Tasks	Datasets	Sub-datasets	# of Graphs	# of Functions	Min # Nodes	Max # Nodes	AVG # Nodes	Init Feature Dimensions
classif-ication	**FFmpeg**	[3, 200]	83008	10376	3	200	18.83	6
		[20, 200]	31696	7668	20	200	51.02	
		[50, 200]	10824	3178	50	200	90.93	
	OpenSSL	[3, 200]	73953	4249	3	200	15.73	6
		[20, 200]	15800	1073	20	200	44.89	
		[50, 200]	4308	338	50	200	83.68	
regre-ssion	**AIDS700**	-	700	-	2	10	8.90	29
	LINUX1000	-	1000	-	4	10	7.58	1

Experiments: Classification Tasks



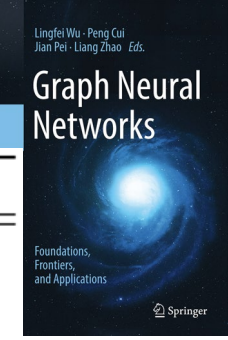
Model	FFmpeg			OpenSSL		
	[3, 200]	[20, 200]	[50, 200]	[3, 200]	[20, 200]	[50, 200]
SimGNN	95.38±0.76	94.31±1.01	93.45±0.54	95.96±0.31	93.58±0.82	94.25±0.85
GMN	94.15±0.62	95.92±1.38	94.76±0.45	96.43±0.61	93.03±3.81	93.91±1.65
GraphSim	97.46±0.30	96.49±0.28	94.48±0.73	96.84±0.54	94.97±0.98	93.66±1.84
SGNN (Max)	93.92±0.07	93.82±0.28	85.15±1.39	91.07±0.10	88.94±0.47	82.10±0.51
SGNN (FCMax)	95.37±0.04	96.29±0.14	95.98±0.32	92.64±0.15	93.79±0.17	93.21±0.82
SGNN (BiLSTM)	96.92±0.13	97.62±0.13	96.35±0.33	95.24±0.06	96.30±0.27	93.99±0.62
NGMN (Max)	73.74±8.30	73.85±1.76	77.72±2.07	67.14±2.70	63.31±3.29	63.02±2.77
NGMN (FCMax)	97.28±0.08	96.61±0.17	96.65±0.30	95.37±0.19	96.08±0.48	**95.90±0.73**
NGMN (BiLSTM)	97.73±0.11	98.29±0.21	96.81±0.96	96.56±0.12	**97.60±0.29**	92.89±1.31
MGMN (Max + BiLSTM)	97.44±0.32	97.84±0.40	97.22±0.36	94.77±1.80	97.44±0.26	94.06±1.60
MGMN (FCMax + BiLSTM)	**98.07±0.06**	**98.29±0.10**	**97.83±0.11**	96.87±0.24	97.59±0.24	95.58±1.13
MGMN (BiLSTM + BiLSTM)	97.56±0.38	98.12±0.04	97.16±0.53	**96.90±0.10**	97.31±1.07	95.87±0.88

Classification Tasks:

- ✓ detecting whether two binaries are compiled from the same one source code function
- ✓ learning a similarity score $y \in \mathbf{Y} = \{-1, 1\}$ between two control flow graphs G^1 and G^2

Evaluation metric: *Area Under the ROC Curve* (**AUC**)

Experiments: Regression Tasks

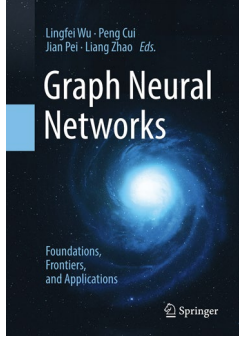


Datasets	Model	mse (10^{-3})	ρ	τ	$p@10$	$p@20$
AIDS700	SimGNN	1.376±0.066	0.824±0.009	0.665±0.011	0.400±0.023	0.489±0.024
	GMN	4.610±0.365	0.672±0.036	0.497±0.032	0.200±0.018	0.263±0.018
	GraphSim	1.919±0.060	0.849±0.008	0.693±0.010	0.446±0.027	0.525±0.021
	SGNN (Max)	2.822±0.149	0.765±0.005	0.588±0.004	0.289±0.016	0.373±0.012
	SGNN (FCMax)	3.114±0.114	0.735±0.009	0.554±0.008	0.278±0.021	0.364±0.017
	SGNN (BiLSTM)	1.422±0.044	0.881±0.005	0.718±0.006	0.376±0.020	0.472±0.014
	NGMN (Max)	2.378±0.244	0.813±0.015	0.642±0.013	**0.578±0.199**	**0.583±0.169**
	NGMN (FCMax)	2.220±1.547	0.808±0.145	0.656±0.122	0.425±0.078	0.504±0.064
	NGMN (BiLSTM)	1.191±0.048	0.904±0.003	0.749±0.005	0.465±0.011	0.538±0.007
	MGMN (Max + BiLSTM)	1.210±0.020	0.900±0.002	0.743±0.003	0.461±0.012	0.534±0.009
	MGMN (FCMax + BiLSTM)	1.205±0.039	0.904±0.002	0.749±0.003	0.457±0.014	0.532±0.016
	MGMN (BiLSTM + BiLSTM)	**1.169±0.036**	**0.905±0.002**	**0.751±0.003**	0.456±0.019	0.539±0.018
LINUX1000	SimGNN	2.479±1.038	0.912±0.031	0.791±0.046	0.635±0.328	0.650±0.283
	GMN	2.571±0.519	0.906±0.023	0.763±0.035	0.888±0.036	0.856±0.040
	GraphSim	0.471±0.043	0.976±0.001	**0.931±0.003**	**0.956±0.006**	0.942±0.007
	SGNN (Max)	11.832±0.698	0.566±0.022	0.404±0.017	0.226±0.106	0.492±0.190
	SGNN (FCMax)	17.795±0.406	0.362±0.021	0.252±0.015	0.239±0.000	0.241±0.000
	SGNN (BiLSTM)	2.140±1.668	0.935±0.050	0.825±0.100	0.878±0.012	0.865±0.007
	NGMN (Max)*	16.921±0.000	-	-	-	-
	NGMN (FCMax)	4.793±0.262	0.829±0.006	0.665±0.011	0.764±0.170	0.767±0.166
	NGMN (BiLSTM)	1.561±0.020	0.945±0.002	0.814±0.003	0.743±0.085	0.741±0.086
	MGMN (Max + BiLSTM)	1.054±0.086	0.962±0.003	0.850±0.008	0.877±0.054	0.883±0.047
	MGMN (FCMax + BiLSTM)	1.575±0.627	0.946±0.019	0.817±0.034	0.807±0.117	0.784±0.108
	MGMN (BiLSTM + BiLSTM)	**0.439±0.143**	**0.985±0.005**	0.919±0.016	0.955±0.011	**0.943±0.014**

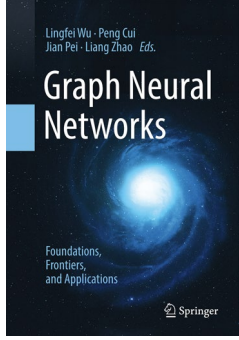
* As all duplicated experiments running on this setting do not converge in their training processes, their corresponding results cannot be calculated.

Regression Tasks: learning the graph edit distance $y \in \mathbf{Y} = [0,1]$ between two graphs G^1 and G^2

Evaluation metrics: mean square error (**mse**), spearman's rank correlation coefficient (**ρ**), kendall's rank correlation coefficient (**τ**), and precision at k (**p@k**, $k = 10/20$)

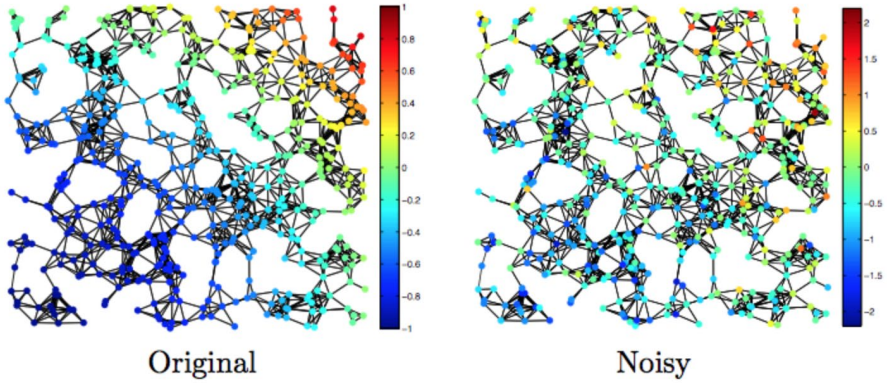


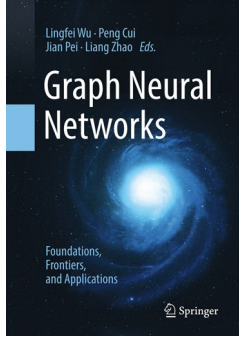
GNNs: Graph Structure Learning (Chapter 14)



Graph Learning: Motivations

- GNNs are powerful, unfortunately, it requires graph-structured data available.
- Questionable if the given intrinsic graph-structures are optimal (i.e., noisy, incomplete, etc.) for the downstream tasks.
- Many applications (e.g., NLP tasks) may only have non-graph structured data or even just the original feature matrix, requiring additional graph construction.

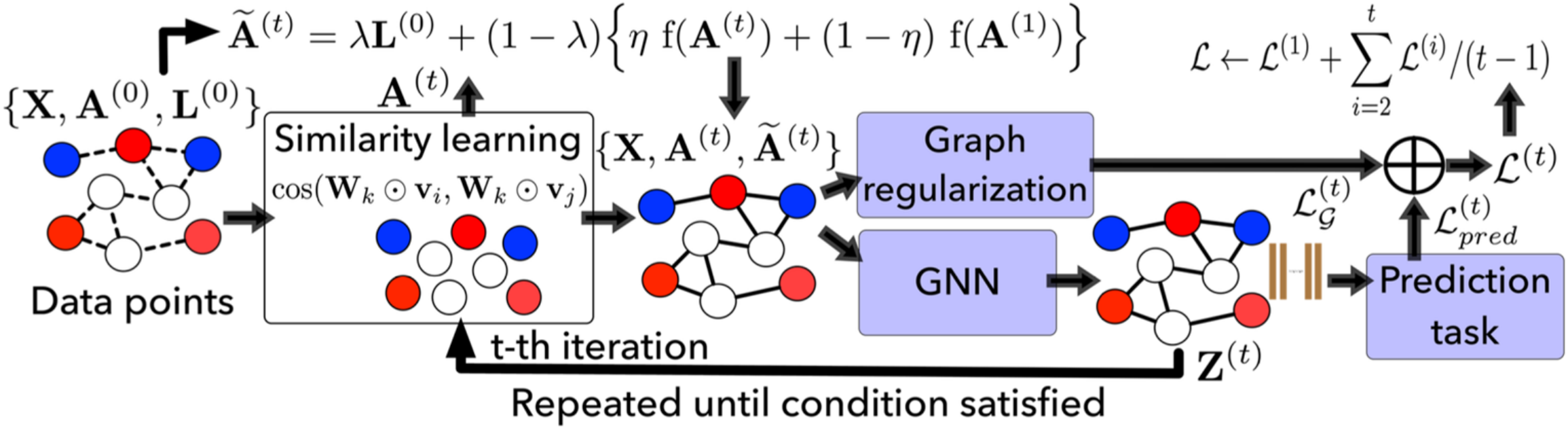




Graph Learning: Formulation

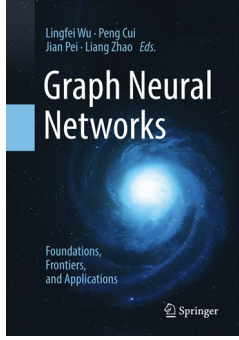
- Deep graph Learning
  - **Input:** A raw graph input $G \in \boldsymbol{G}$
    - Given a noisy $G = (V, E)$ with (X, A^0), where $X \in R^{N \times d}$, $A^0 \in R^{N \times N}$
    - Given initial feature matrix X, where $X \in R^{N \times d}$
  - **Output:** An optimal graph adjacency $A \in R^{N \times N}$ and node embeddings $Z \in R^{N \times d'}$

Iterative Deep Graph Learning : System Overview



- Graph learning as similarity metric learning
- Graph regularization to control smoothness, sparsity, and connectivity
- Iterative method to refine the graph structures and graph embeddings

IDGL: Graph Learning as Similarity Metric Learning



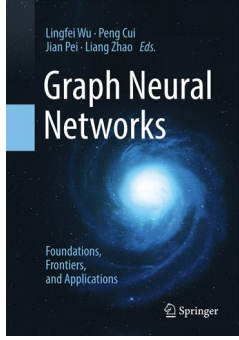
- We design a multi-head weighted cosine similarity metric function to learn a similarity matrix S for all pairs of nodes.

$$s_{ij}^k = \cos(\mathbf{W}_k \odot \mathbf{x}_i, \mathbf{W}_k \odot \mathbf{x}_j) \quad s_{ij} = \frac{1}{m}\sum_{k=1}^{m} s_{ij}^k$$

- We proceed to extract a symmetric sparse adjacency matrix from the similarity matrix S by considering only the ε-neighborhood for each node.

$$\mathbf{A}_{ij} = \begin{cases} \mathbf{S}_{ij} & \mathbf{S}_{ij} > \varepsilon \\ 0 & \text{otherwise} \end{cases} \qquad \tilde{\mathbf{A}} = \lambda \mathbf{L}_0 + (1-\lambda)\frac{\mathbf{A}_{ij}}{\sum_j \mathbf{A}_{ij}}$$

where $\mathbf{L}_0$ is the normalized adjacency matrix of the initial graph (or kNN-graph).



IDGL: Graph Regularization

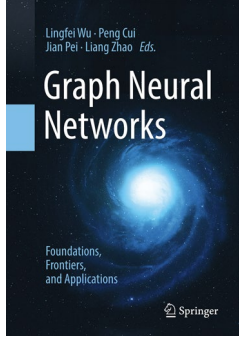
- We adapt the techniques designed for learning graphs from smooth and apply them as regularization for controlling smoothness, connectivity and sparsity

$$\Omega(\mathbf{A}, \mathbf{X}) = \frac{1}{2}\sum_{i,j}\mathbf{A}_{ij}||\mathbf{x}_i - \mathbf{x}_j||^2 = \mathrm{tr}(\mathbf{X}^T\mathbf{L}\mathbf{X})$$ Smoothness

$$f(\mathbf{A}) = -\beta\mathbf{1}^T\log(\mathbf{A}\mathbf{1}) + \gamma||\mathbf{A}||_F^2$$ Connectivity & sparsity

$$\mathcal{L}_{\mathcal{G}} = \alpha\Omega(\mathbf{A}, \mathbf{X}) + f(\mathbf{A})$$ Graph regularization loss

IDGL: Iterative Method for Joint Graph Structure and Representation Learning



- Iterative method repeatedly
  - refines the adjacency matrix with the updated node embeddings
  - refines the node embeddings with the updated adjacency matrix
- Iterative procedure dynamically stops
  - the learned adjacency matrix converges with certain threshold
  - the maximal number of iterations is reached

while $(t == 0 \quad or \quad ||\mathbf{A}^{(t)} - \mathbf{A}^{(t-1)}||_F^2 > \delta||\mathbf{A}^{(0)}||_F^2)$ c

$t \leftarrow t + 1$

$\mathbf{A}^{(t)}, \tilde{\mathbf{A}}^{(t)} \leftarrow \{\mathbf{Z}^{(t-1)}, \mathbf{A}_0\}$ using Eqs. (2), (3) and (10)

$\tilde{\mathbf{A}}^{(t)} \leftarrow \eta\tilde{\mathbf{A}}^{(t)} + (1-\eta)\tilde{\mathbf{A}}^{(0)}$

$\mathbf{Z}^{(t)} \leftarrow \{\tilde{\mathbf{A}}^{(t)}, \mathbf{X}\}$ using Eq. (7)

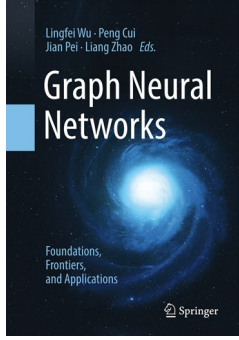
$\hat{\mathbf{y}} \leftarrow \{\tilde{\mathbf{A}}^{(t)}, \mathbf{Z}^{(t)}\}$ using Eq. (8)

$\mathcal{L}_{\text{pred}}^{(t)} \leftarrow \{\hat{\mathbf{y}}, \mathbf{y}\}$ using Eq. (9)

$\mathcal{L}_{\mathcal{G}}^{(t)} \leftarrow \{\mathbf{A}^{(t)}, \mathbf{X}\}$ using Eqs. (4)–(6)

$\mathcal{L}^{(t)} \leftarrow \mathcal{L}_{\text{pred}}^{(t)} + \mathcal{L}_{\mathcal{G}}^{(t)}$

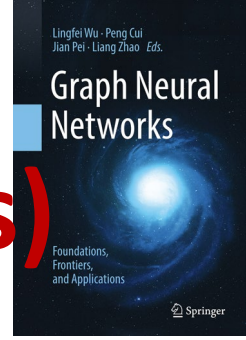
end

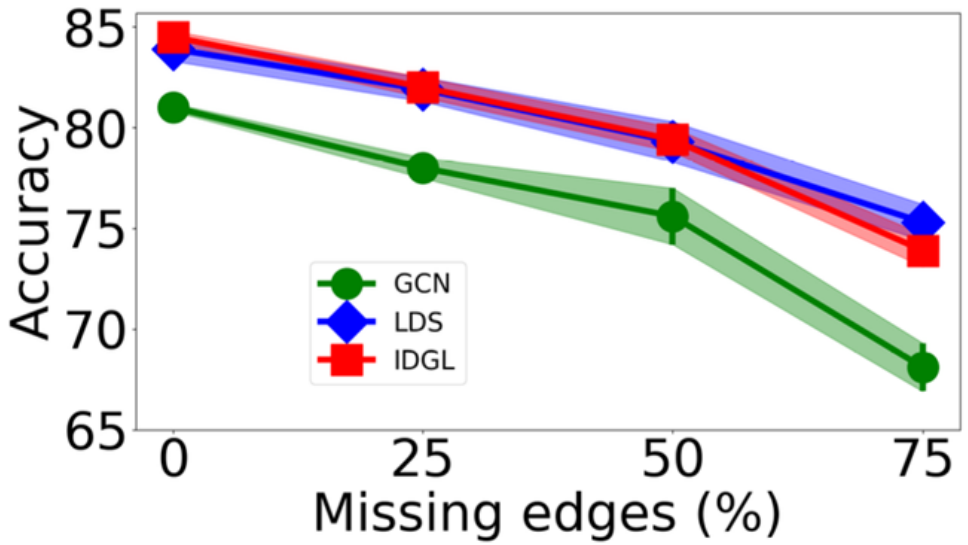


Results (Transudative Setting)

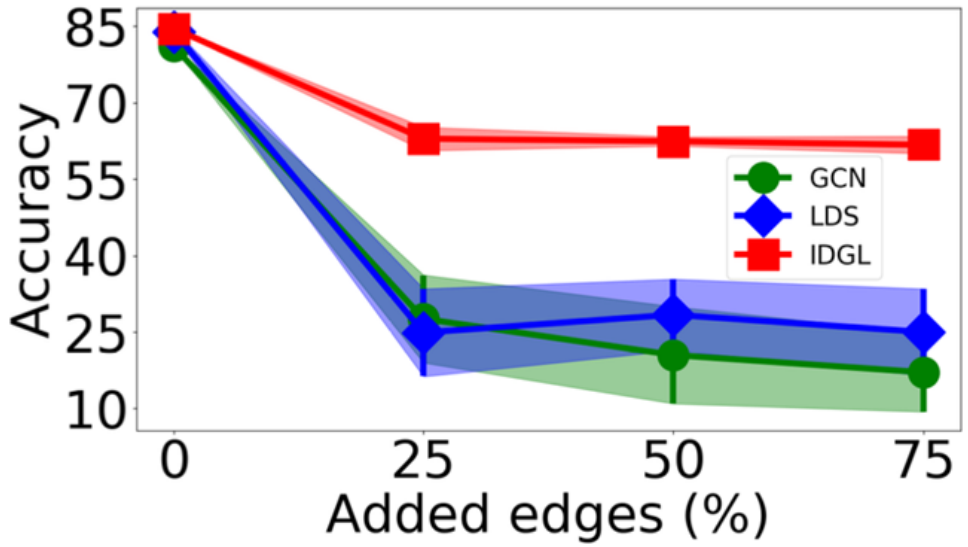
Model	Cora	Citeseer	Pubmed	ogbn-arxiv	Wine	Cancer	Digits
GCN	81.5	70.3	79.0	71.7 (0.3)	—	—	—
GAT	83.0 (0.7)	72.5 (0.7)	79.0 (0.3)	—	—	—	—
GraphSage	77.4 (1.0)	67.0 (1.0)	76.6 (0.8)	71.5 (0.3)	—	—	—
APPNP	—	**75.7 (0.3)**	79.7 (0.3)	—	—	—	—
H-GCN	**84.5 (0.5)**	72.8 (0.5)	79.8 (0.4)	—	—	—	—
GCN+GDC	83.6 (0.2)	73.4 (0.3)	78.7 (0.4)	—	—	—	—
LDS	84.1 (0.4)	75.0 (0.4)	—	—	97.3 (0.4)	94.4 (1.9)	92.5 (0.7)
GCN_{kNN}*	—	—	—	—	95.9 (0.9)	94.7 (1.2)	89.5 (1.3)
LDS*	83.9 (0.6)	74.8 (0.3)	—	—	96.9 (1.4)	93.4 (2.4)	90.8 (2.5)
IDGL	**84.5 (0.3)**	74.1 (0.2)	—	—	97.8 (0.6)	**95.1 (1.0)**	93.1 (0.5)
IDGL-ANCH	84.4 (0.2)	72.0 (1.0)	**82.7 (0.4)**	**72.0 (0.3)**	**98.1 (1.1)**	94.8 (1.4)	**93.2 (0.9)**

Results (Robustness to Missing/Adding Edges)





(a) Edge deletion



(b) Edge addition

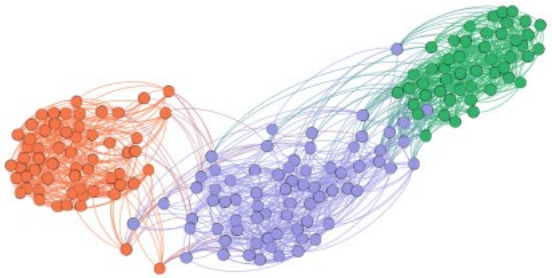
Visualization of the Initial and Learned Graphs

(a) Initial graph ($\mathbf{A}^{(0)}$)

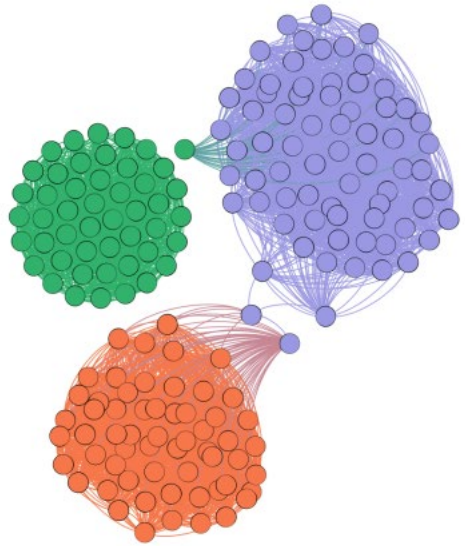
(b) Learned graph ($\mathbf{A}^{(t)}$)

Dataset: Cora (having initial graph data)

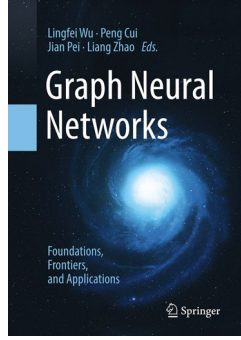
Dataset: Wine (having no initial graph data)



(a) kNN graph ($\mathbf{A}^{(0)}$)



(b) Learned graph ($\mathbf{A}^{(t)}$)



GNNs: Graph Classification (Chapter 9)

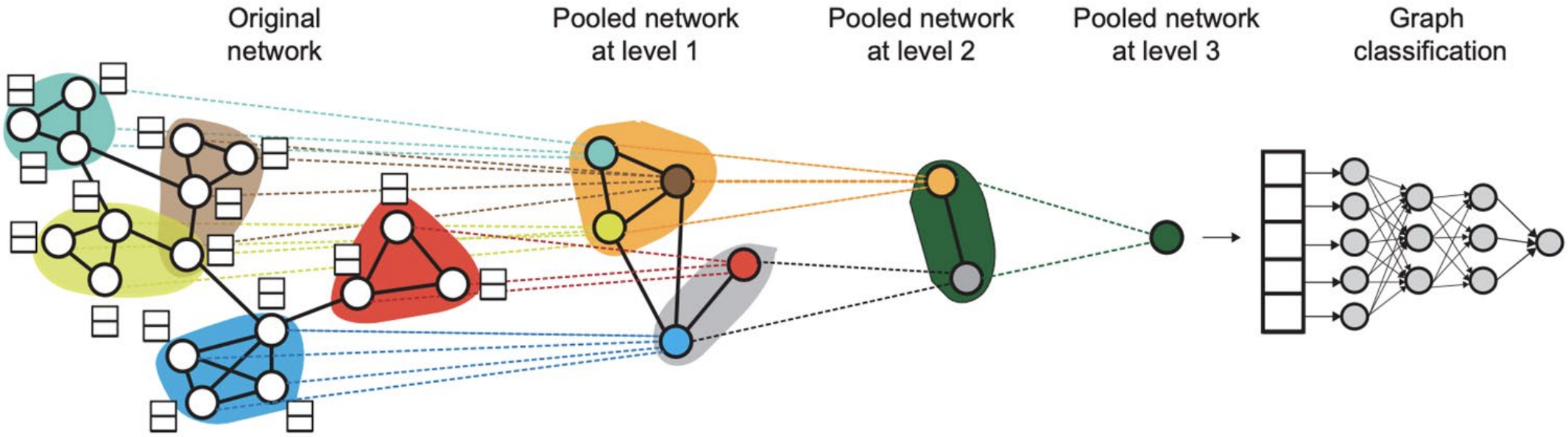
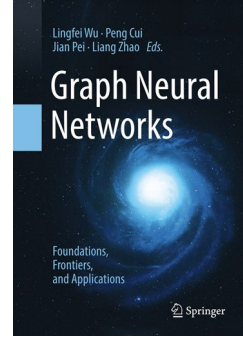
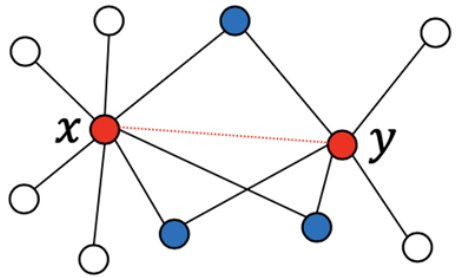


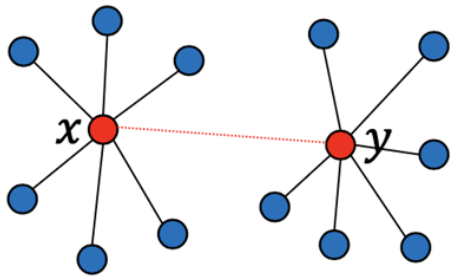
Image credit: Rex Ying et al., “Hierarchical Graph Representation Learning with Differentiable Pooling”, NeurIPS 2018.



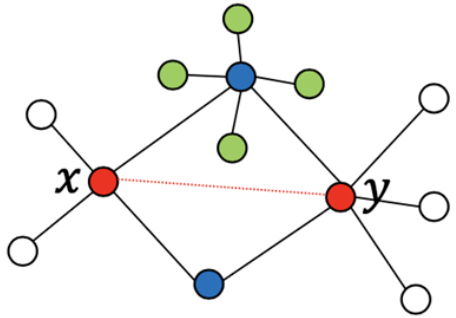
GNNs: Link Prediction (Chapter 10)



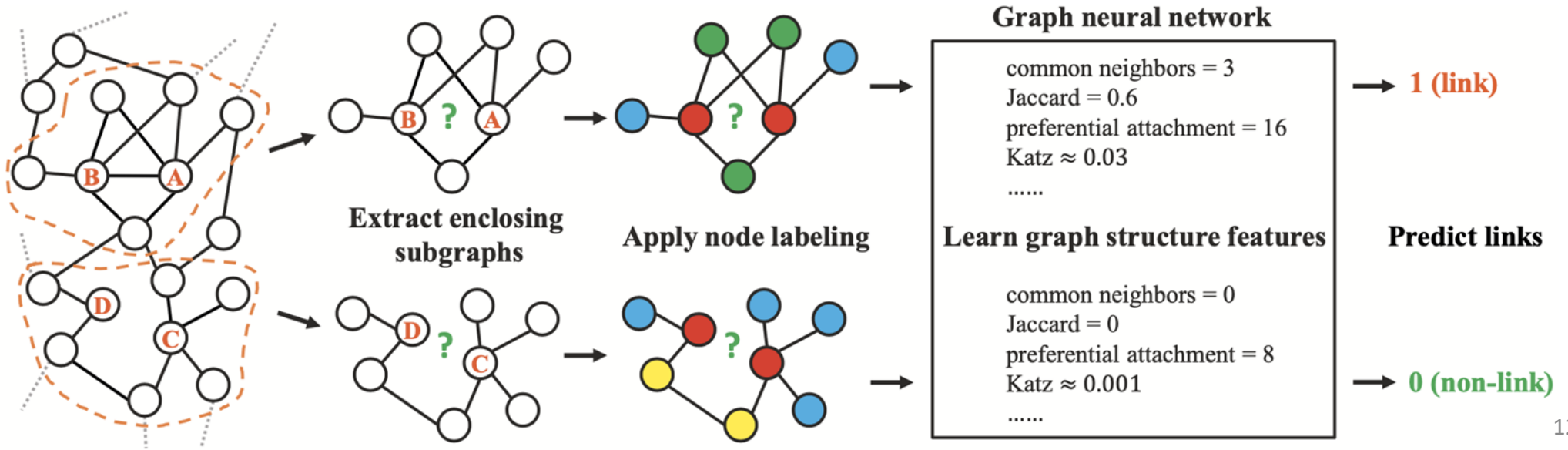
common neighbors (CN):
$|\Gamma(x) \cap \Gamma(y)|$



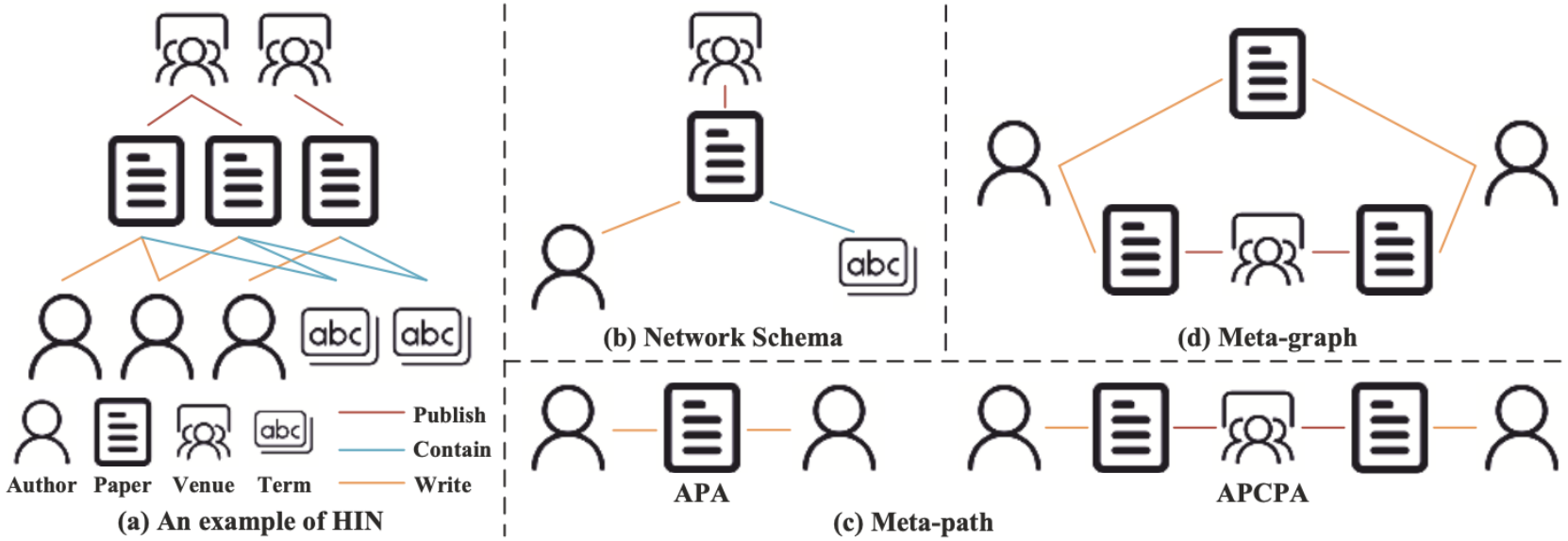
preferential attachment (PA):
$|\Gamma(x)| \cdot |\Gamma(y)|$

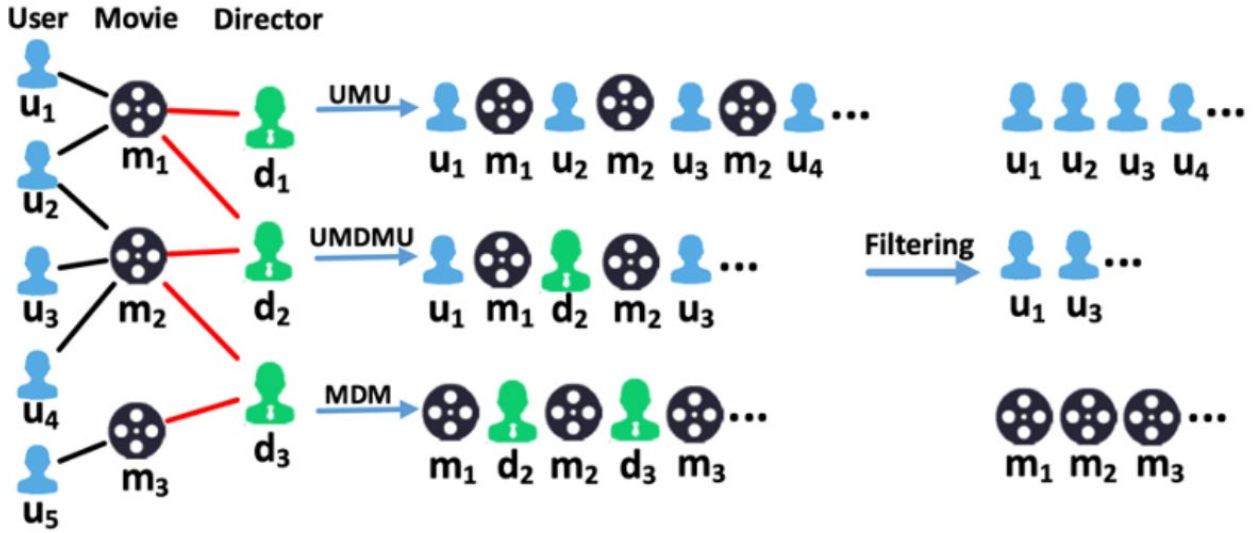


Adamic-Adar (AA):
$\sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{1}{\log |\Gamma(z)|}$

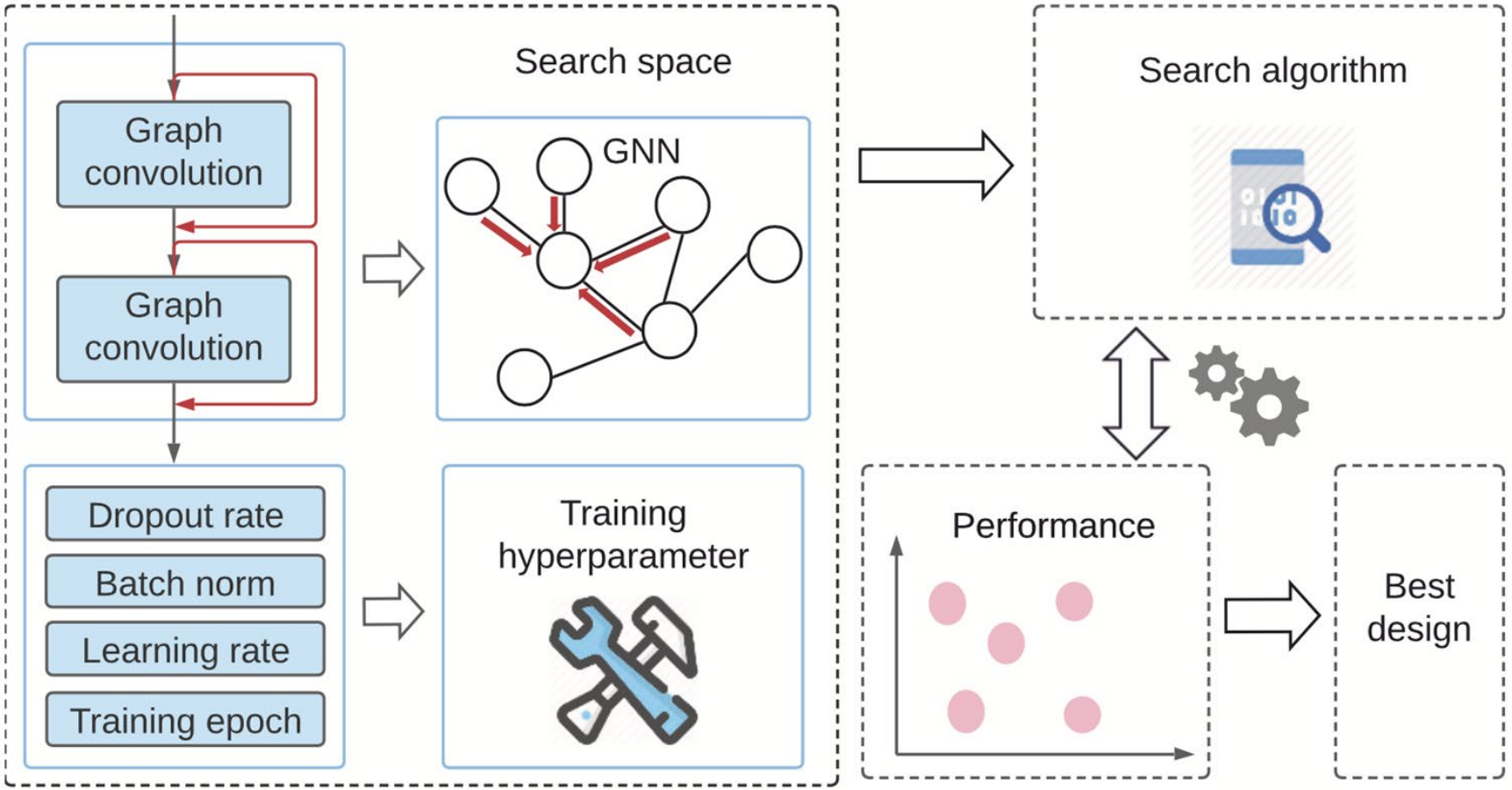


Heterogeneous GNNs (Chapter 16)

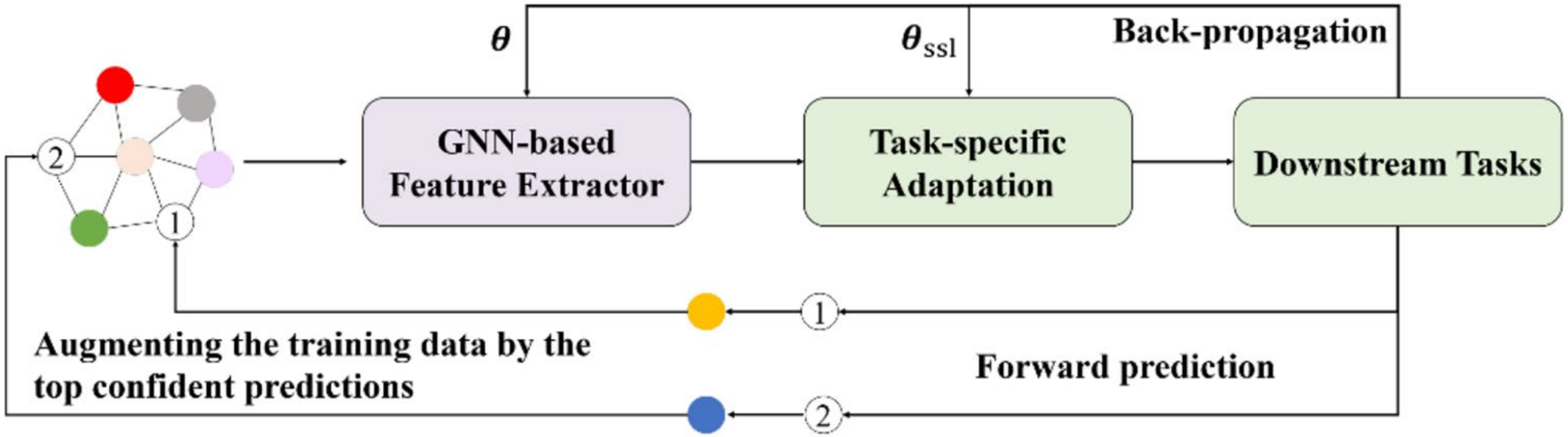




GNNs: AutoML (Chapter 17)



GNNs: Self-supervised Learning (Chapter 18)



Outline

GNNs Foundations

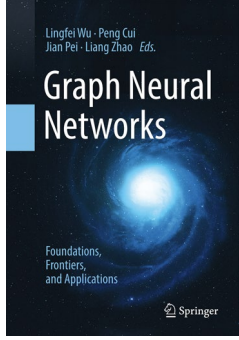
- Time History of GNNs
- GNNs: Foundations and Models
- GNNs: Theory, Scalability, Interpretability

GNNs Frontiers

- Graph Generation and Transformation
- Dynamic Graph Neural Networks
- Graph Matching
- Graph Structure Learning

GNNs Applications

- GNNs in Natural Language Processing
- GNNs in Program Analysis
- GNNs in Predicting Protein Function & Interaction

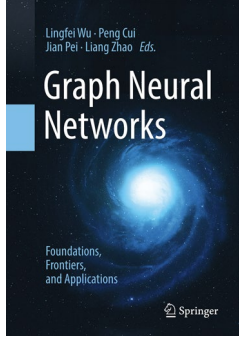


GNN book website：
https://graph-neural-networks.github.io/index.html

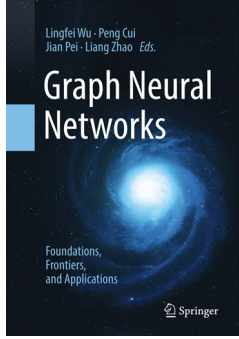
GNN Springer：
https://link.springer.com/book/10.1007/978-981-16-6054-2

Amazon：
https://www.amazon.com/Graph-Neural-Networks-Foundations-Applications/dp/9811660530

JD.com (京东商城)：
https://item.jd.com/10043589466641.html

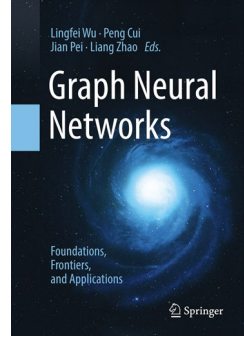


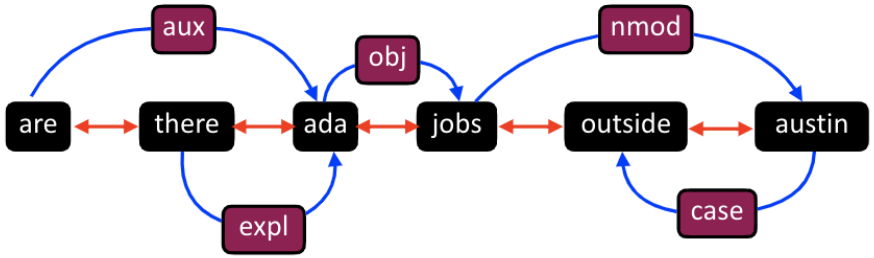
GNNs
Applications



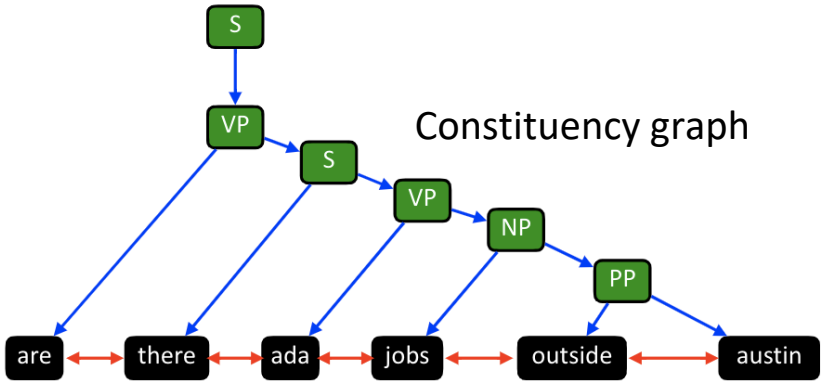
GNNs in Natural Language Processing (Chapter 21)

Graphs are ubiquitous in NLP As Well

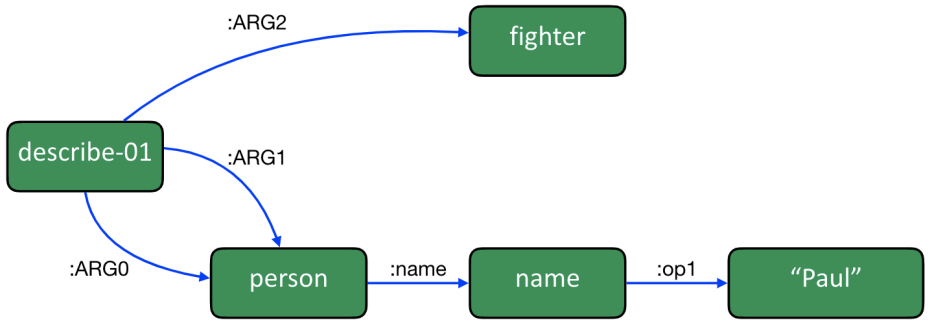




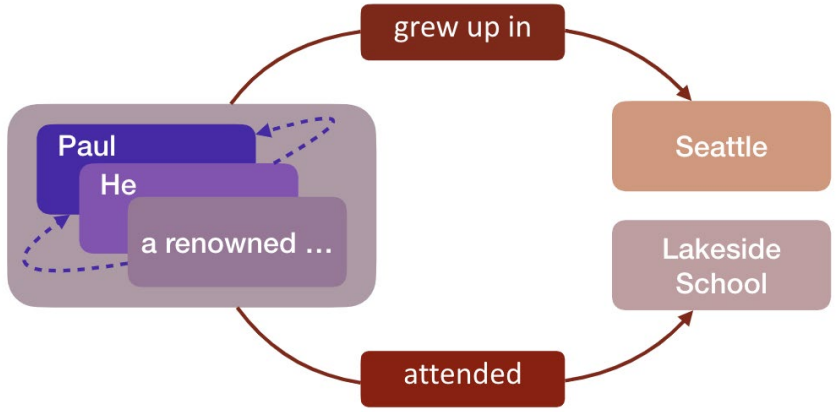
Dependency graph



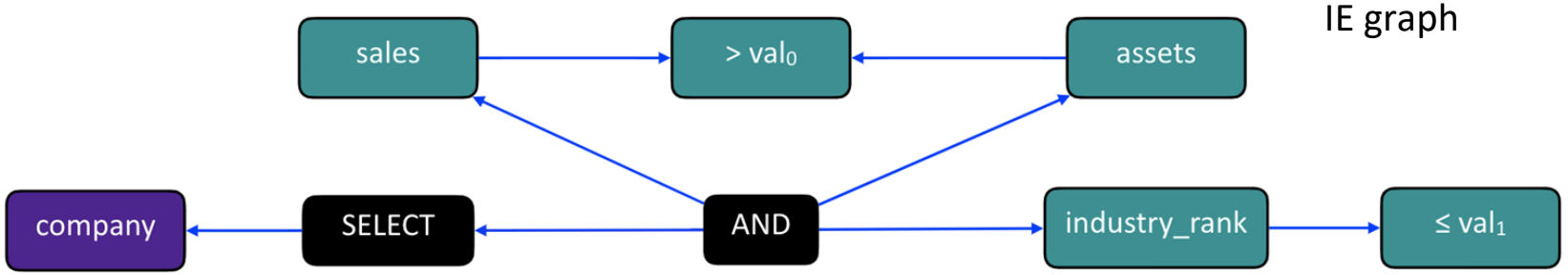
Constituency graph



AMR graph

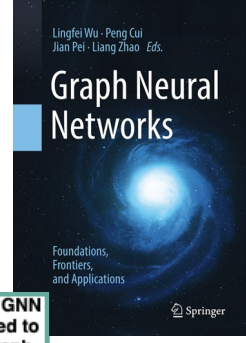


IE graph



SQL graph

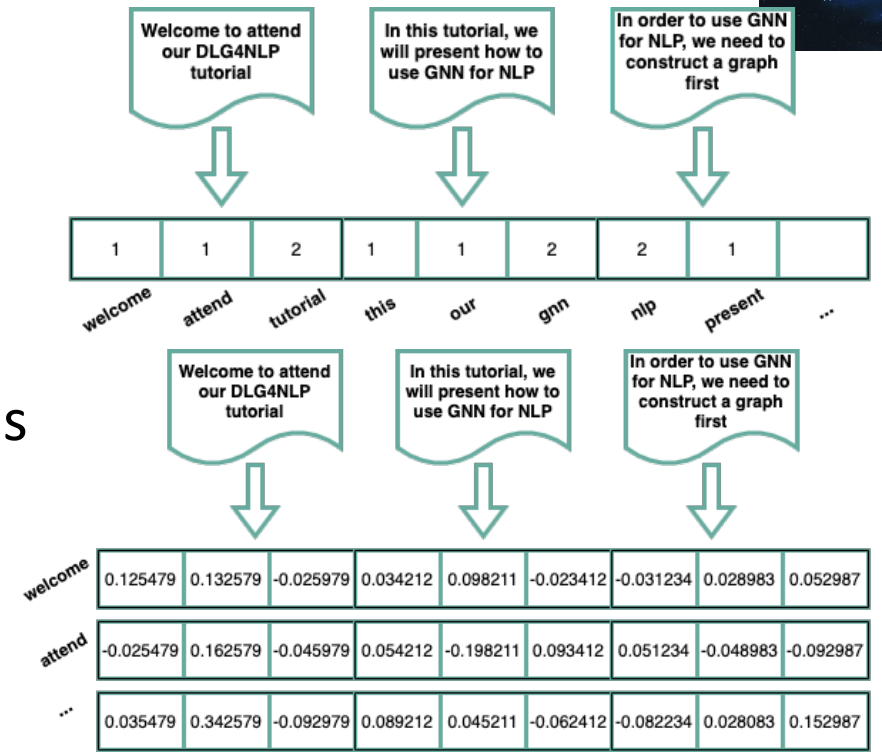
Natural Language Processing: A Graph Perspective

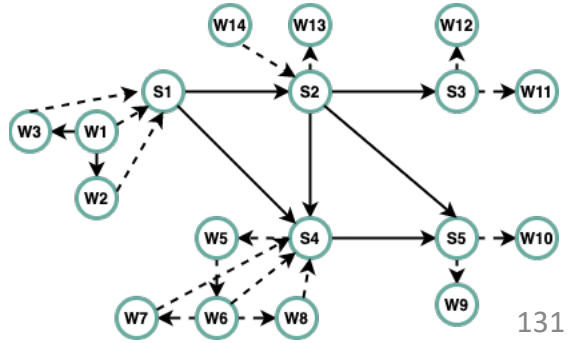


- Represent natural language as a bag of tokens
  - BOW, TF-IDF
  - Topic Modeling: text as a mixture of topics

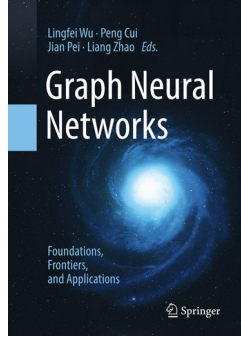
- Represent natural language as a sequence of tokens
  - Linear-chain CRF
  - Word2vec, Glove

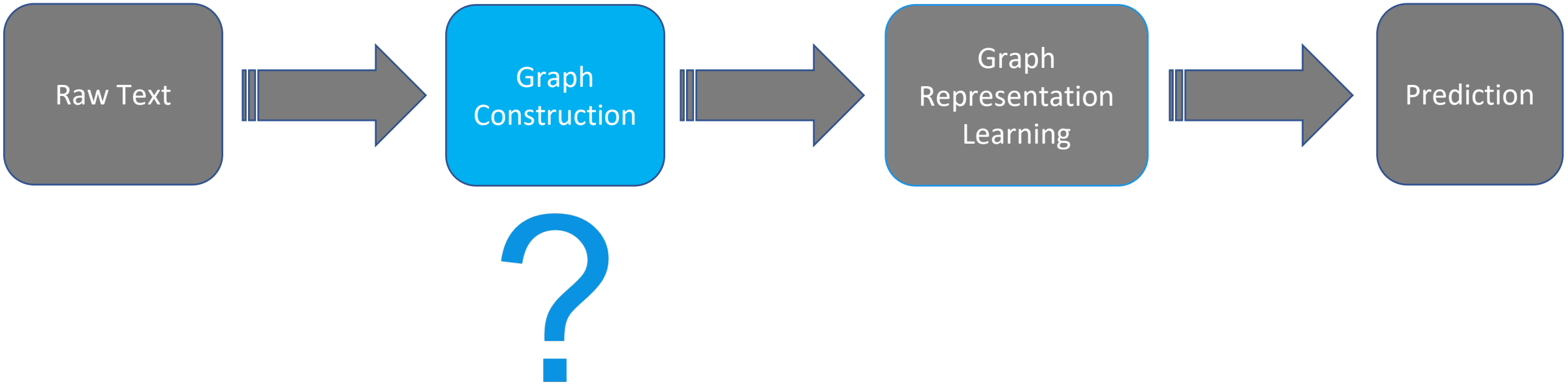
- Represent natural language as a graph
  - Dependency graphs, constituency graphs, AMR graphs, IE graphs, and knowledge graphs
  - Text graph containing multiple hierarchies of elements, i.e. document, sentence and word

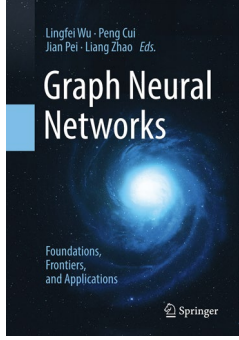




GNNs for Natural Language Processing

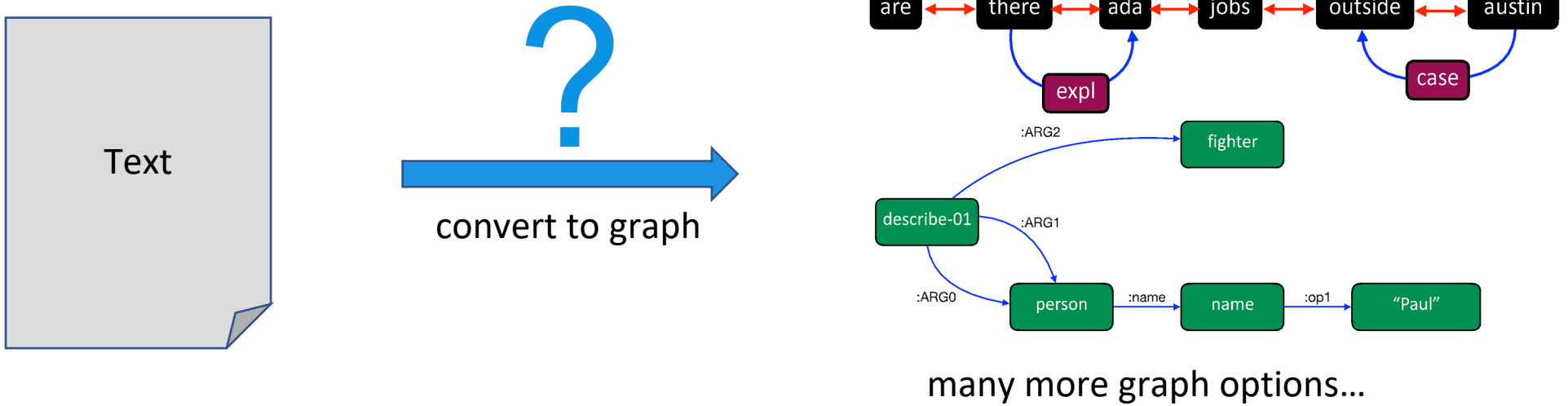




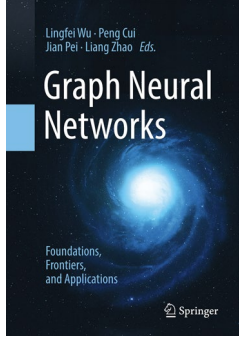


Why Graph Construction for NLP?

- Representation power: graph > sequence > bag
- Different NLP tasks require different aspects of text , e.g., syntax, semantics.
- Different graphs capture different aspects of the text
- Two categories: static vs dynamic graph construction
- Goal: good downstream task performa

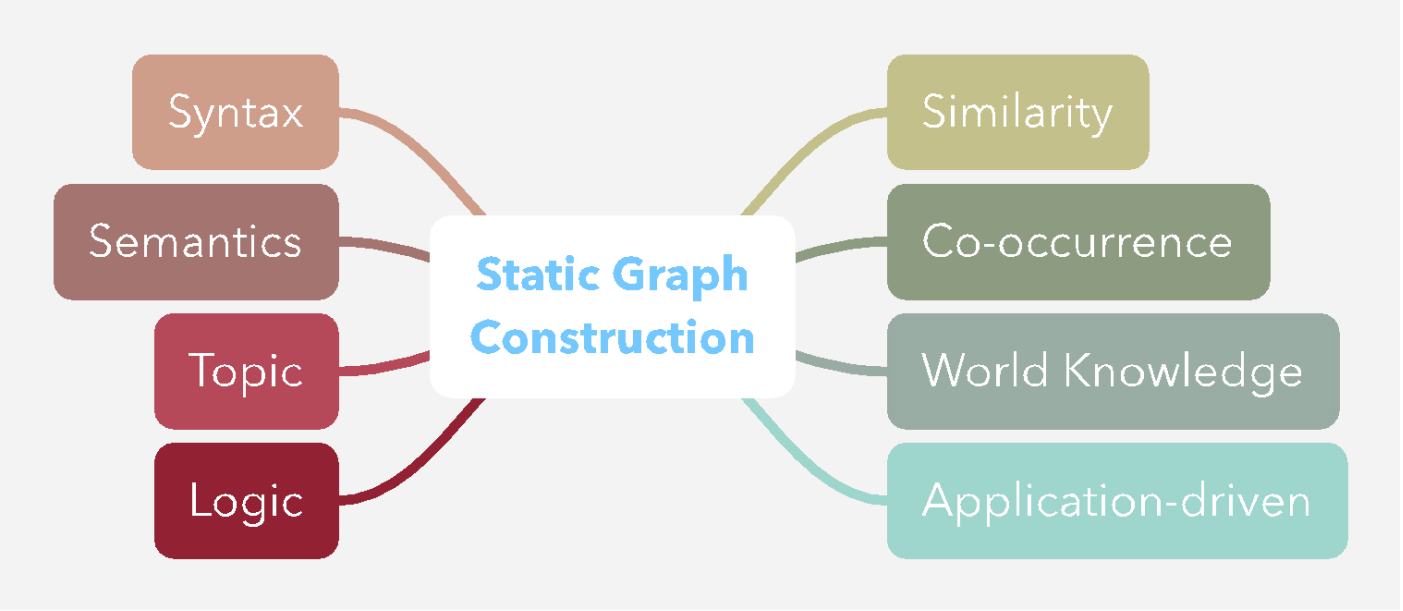


many more graph options…

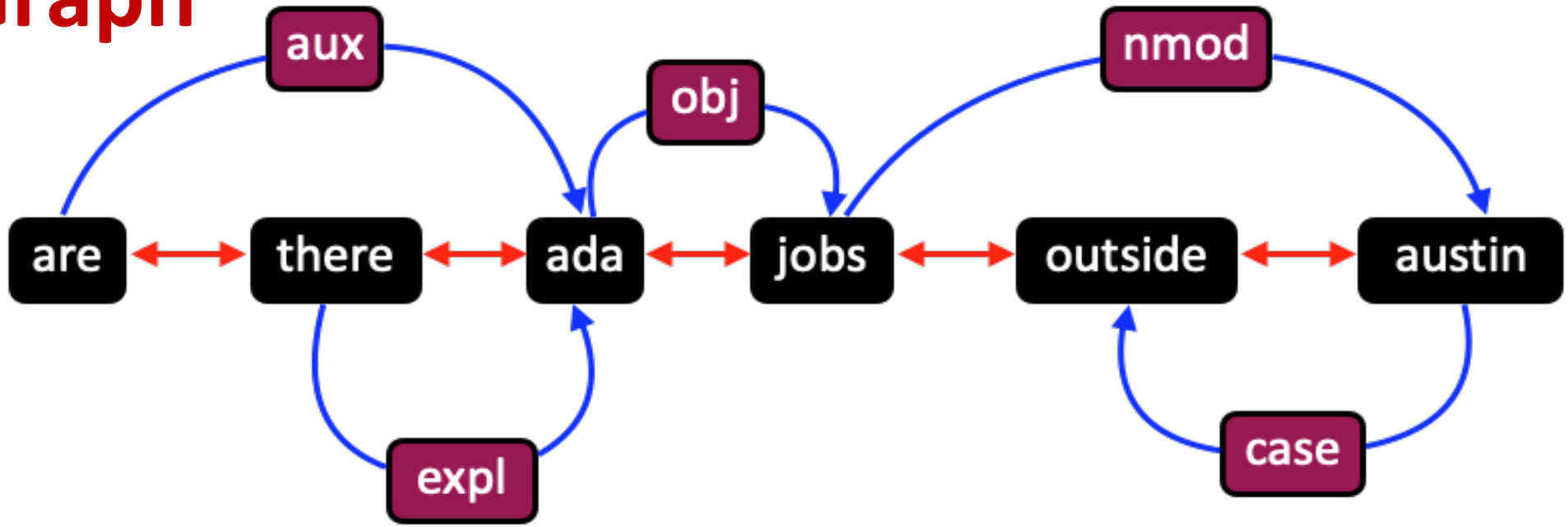


Static Graph Construction

- Problem setting:
  - Input: raw text (e.g., sentence, paragraph, document, corpus)
  - Output: graph
- Conducted during preprocessing by augmenting text with domain knowledge



Static Graph Construction: Dependency Graph

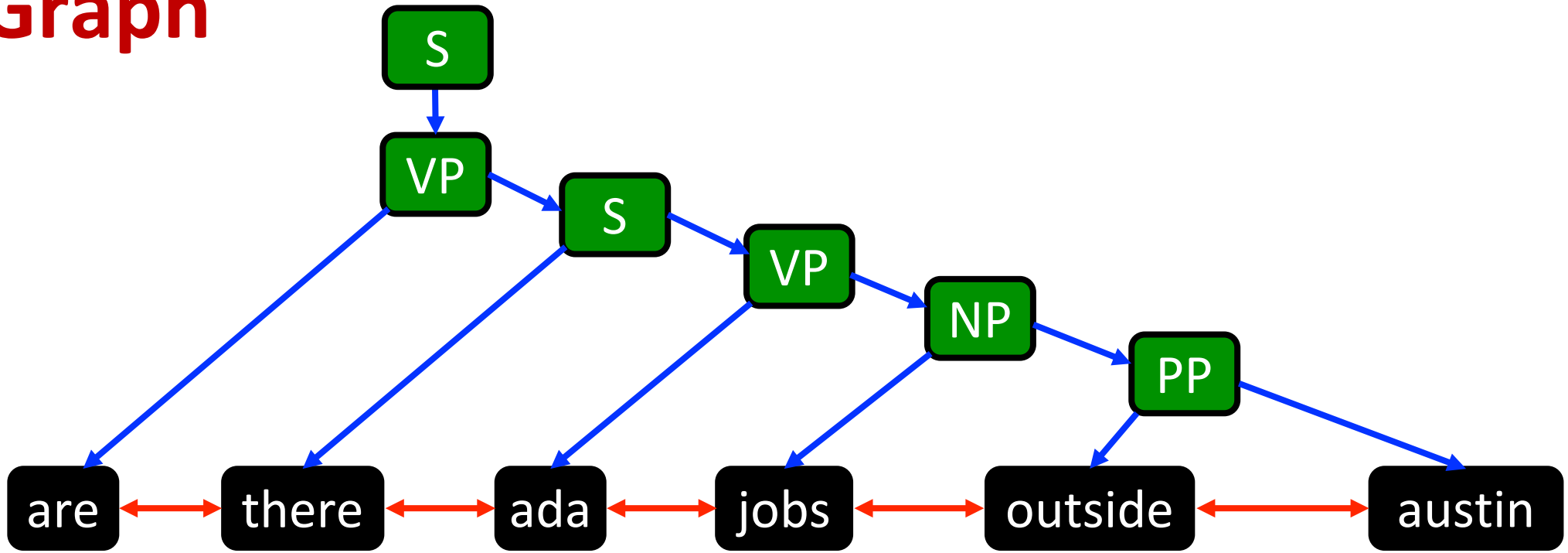


Dependency parsing

Add additional sequential edges to
1) reserve sequential information in raw text
2) connect multiple dependency graphs in a paragraph

Text input: are there ada jobs outside austin

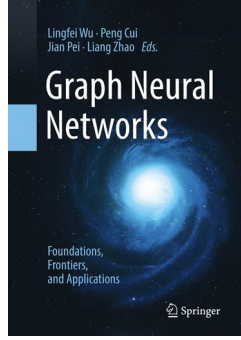
Static Graph Construction: Constituency Graph



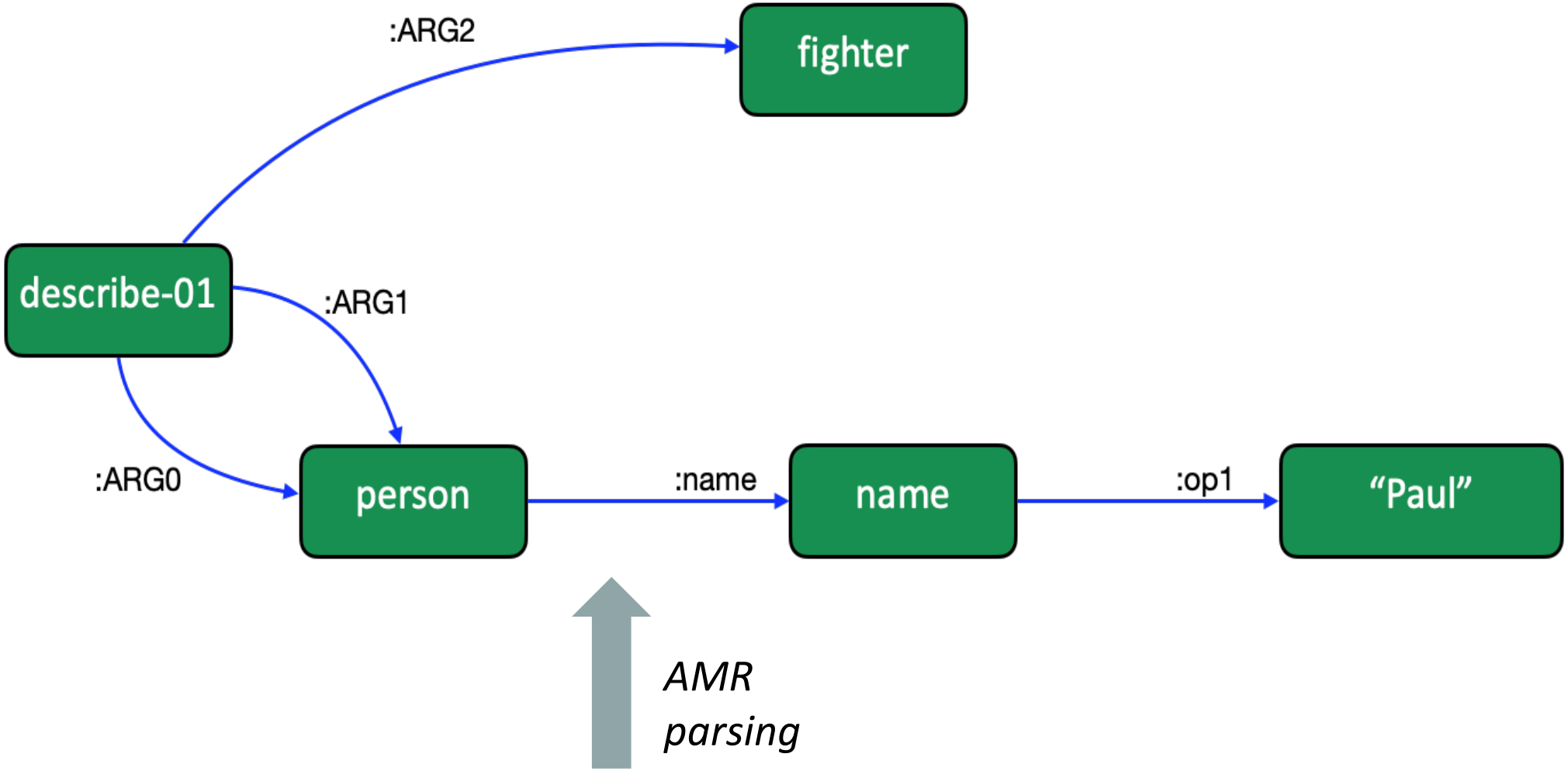
Constituency parsing

Again, add additional sequential edges

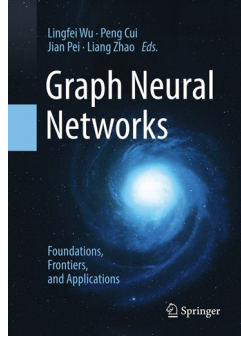
Text input: are there ada jobs outside austin



Static Graph Construction: AMR Graph



Text input: Paul's description of himself: a fighter

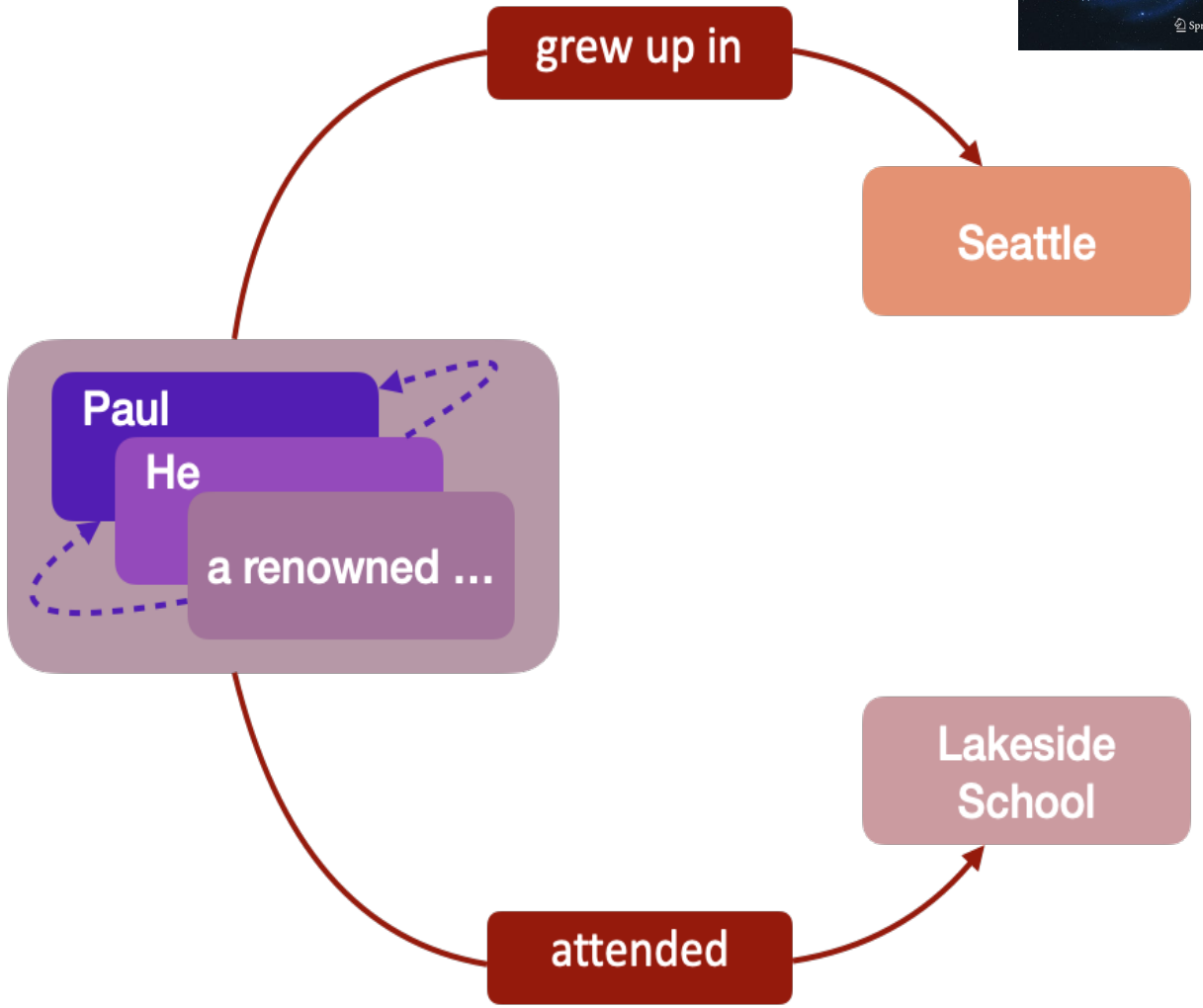


Static Graph Construction: IE Graph

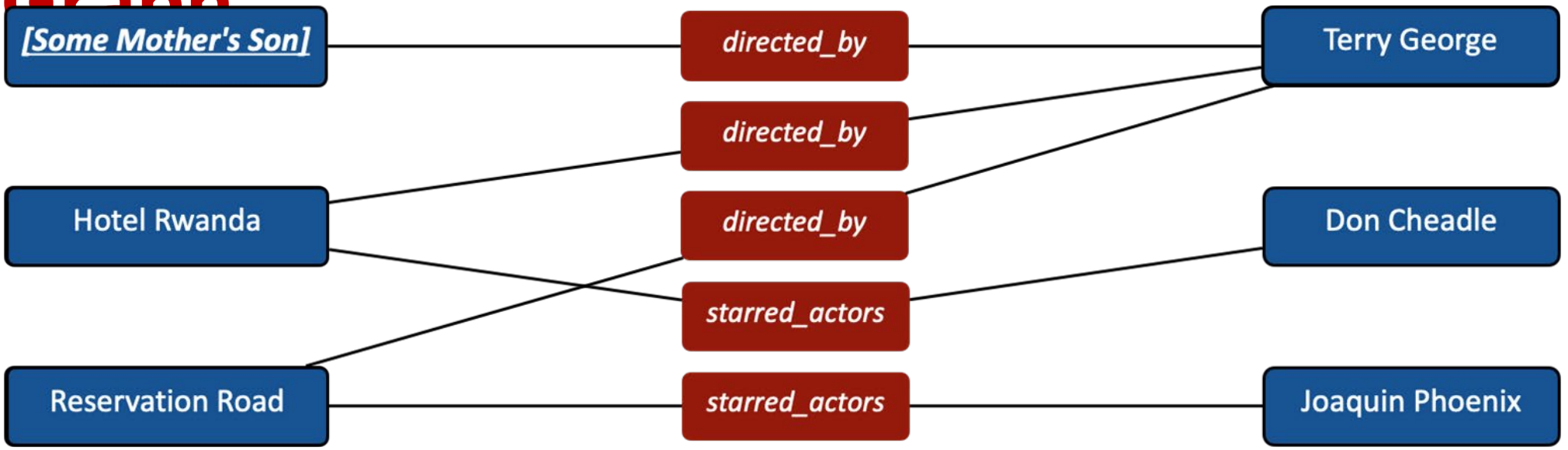
Text input: *Paul, a renowned computer scientist, grew up in Seattle. He attended Lakeside School.*

OpenIE

Coreference

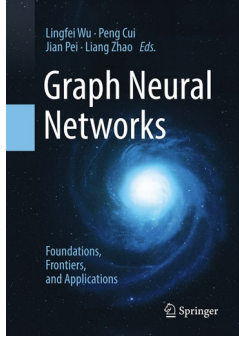


Static Graph Construction: Knowledge Graph

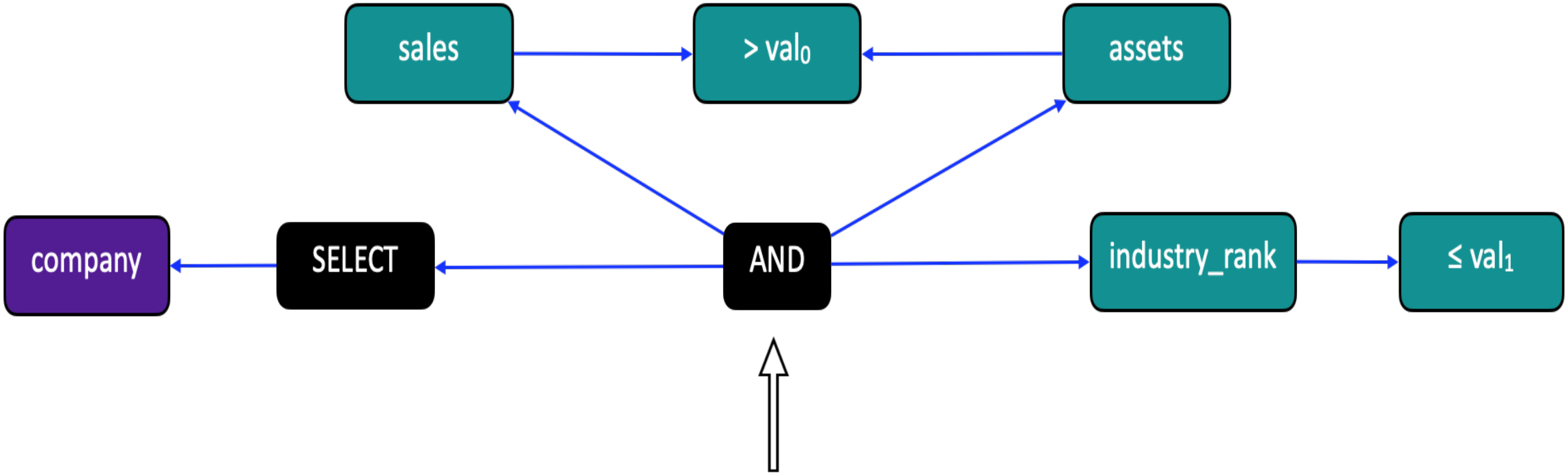


Get the concept sub-graph from KB

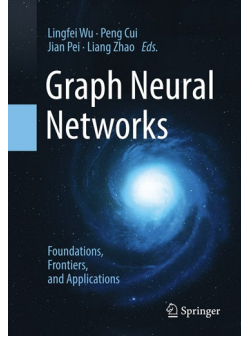
Question: *who acted in the movies directed by the director of* ***[Some Mother's Son]***
Answer: *Don Cheadle, Joaquin Phoenix*



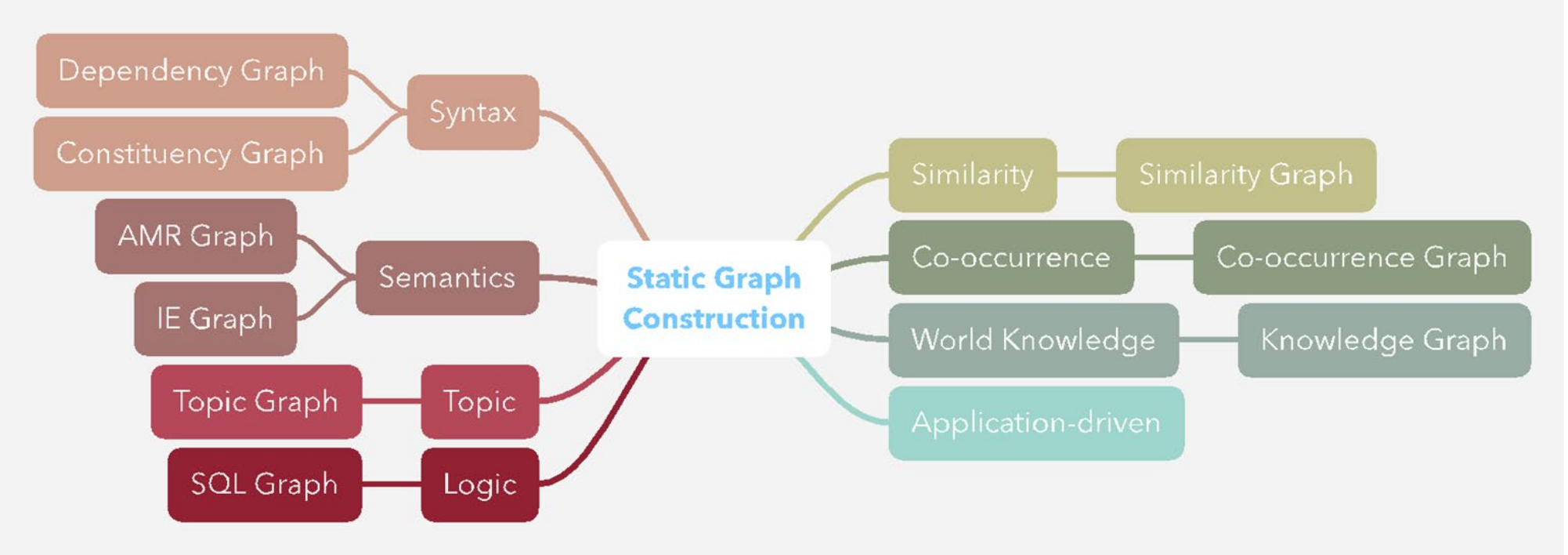
Static Graph Construction: SQL Graph



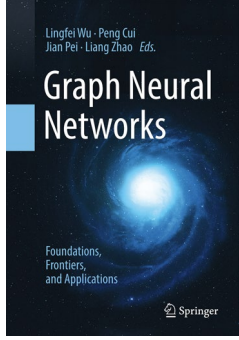
SQL query input: SELECT *company* ***WHERE*** *assets* $>$ *val*$_0$ ***AND*** *sales* $>$ *val*$_0$ ***AND*** *industry_rank* $\leq$ *val*$_1$



Static Graph Construction: Summary

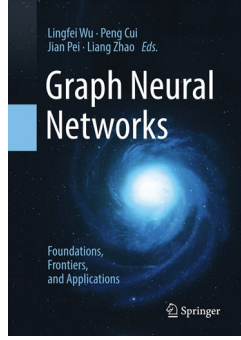


Widely used in various NLP applications such as NLG, MRC, semantic parsing, etc.

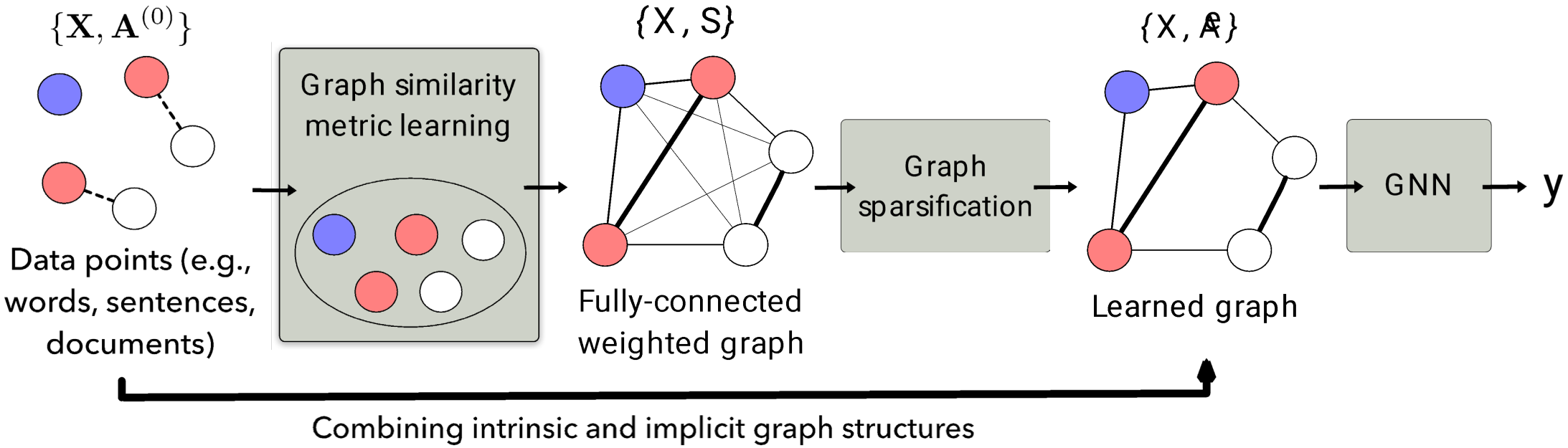


Dynamic Graph Construction

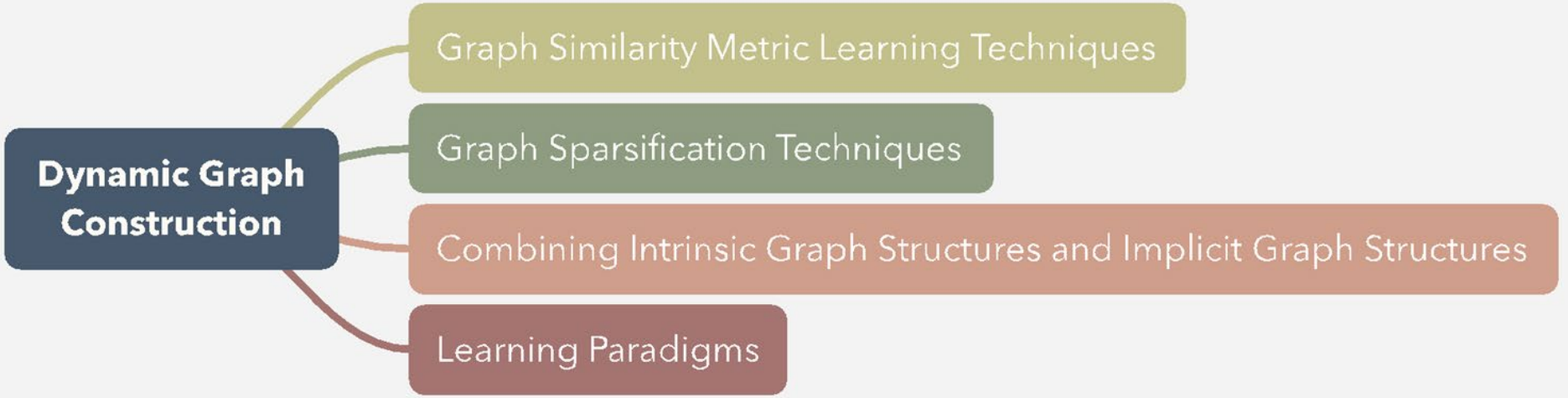
- Problem setting:
  - Input: raw text (e.g., sentence, paragraph, document, corpus)
  - Output: graph
- Graph structure (adjacency matrix) learning on the fly, joint with graph representation learning

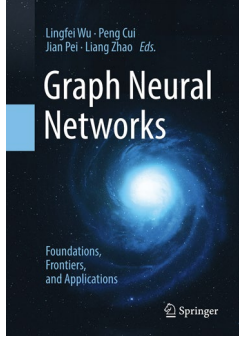


Dynamic Graph Construction: Overview

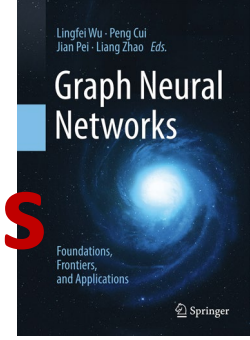


Dynamic Graph Construction Outline



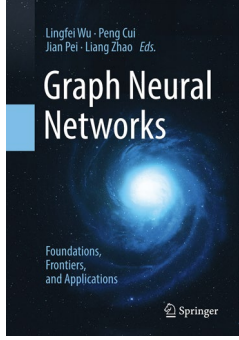


Graph Similarity Metric Learning Techniques

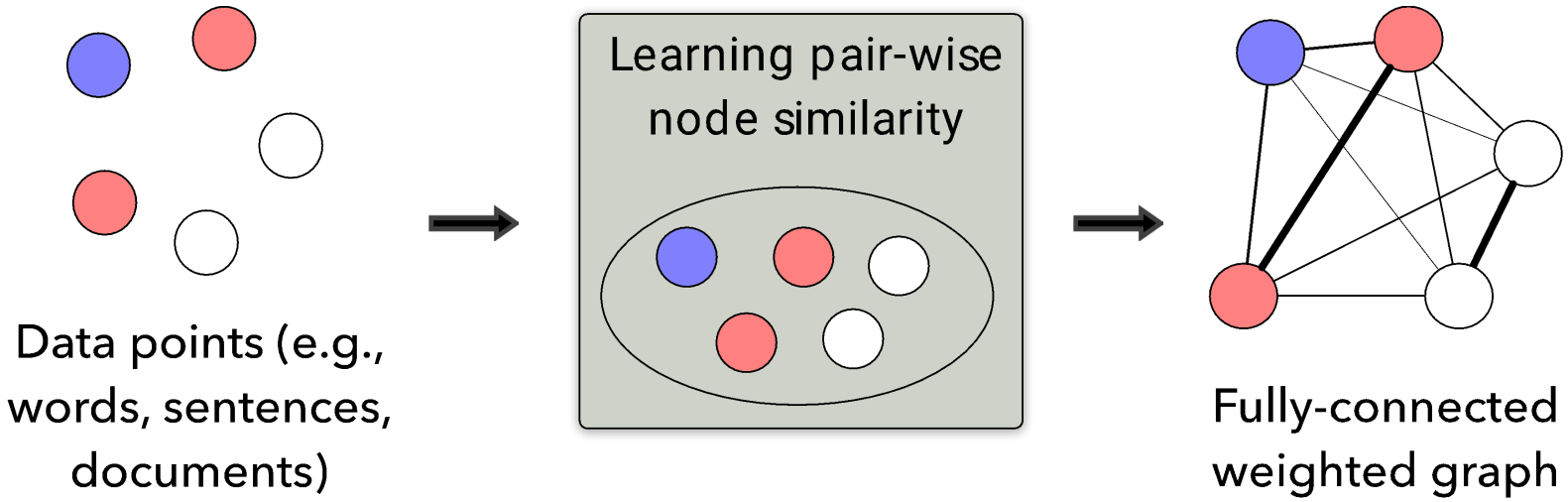


- Graph structure learning as similarity metric learning (in the node embedding space)
- Enabling inductive learning
- Various metric functions

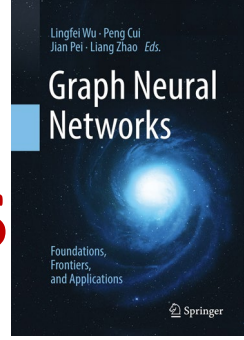
Node Embedding Based Similarity Metric Learning



- Learning a weighted adjacency matrix by computing the pair-wise node similarity in the embedding space
- Common metrics functions
  - Attention-based similarity metric functions
  - Cosine-based similarity metric functions



Attention-based Similarity Metric Functions

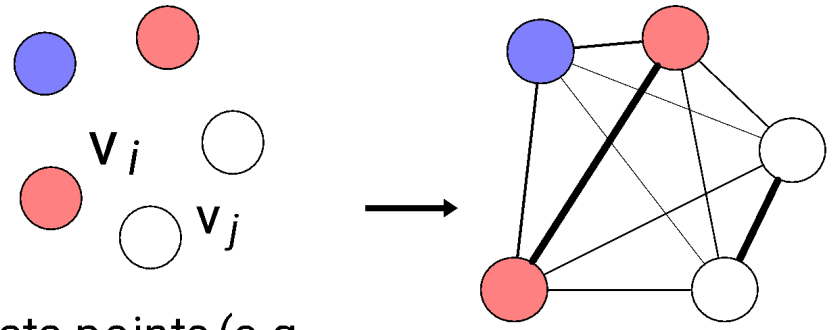


Variant 1)

$$S_{i,j} = (\mathbf{v}_i \odot \mathbf{u})^T \mathbf{v}_j$$

Node feature vector

Non-negative learnable weight vector



Data points (e.g., words, sentences, documents)

Fully-connected weighted graph

Variant 2)

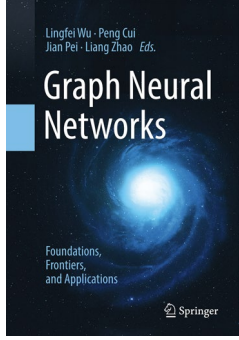
$$S_{i,j} = \mathrm{ReLU}(\mathbf{W}\mathbf{v}_i)^T \mathrm{ReLU}(\mathbf{W}\mathbf{v}_j)$$

Learnable weight matrix

Chen at al. "GraphFlow: Exploiting Conversation Flow with Graph Neural Networks for Conversational Machine Comprehension". IJCAI 2020.

Chen et al. "Reinforcement Learning Based Graph-to-Sequence Model for Natural Question Generation". ICLR 2020.

Cosine-based Similarity Metric Functions

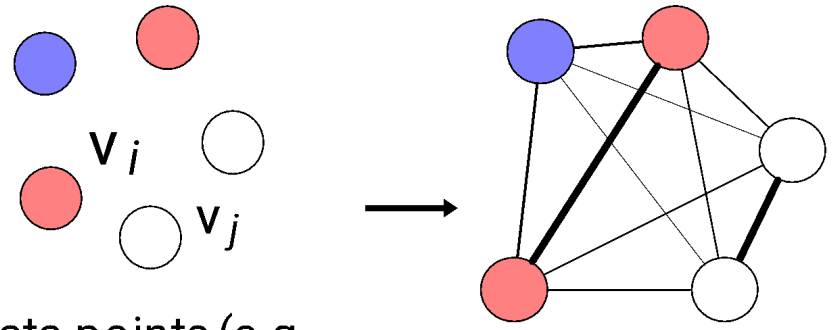


$$S_{i,j}^p = \cos\left(\mathbf{w}_p \odot \mathbf{v}_i, \mathbf{w}_p \odot \mathbf{v}_j\right)$$

Learnable weight vector

$$S_{i,j} = \frac{1}{m}\sum_{p=1}^{m} S_{ij}^p$$

Multi-head similarity scores

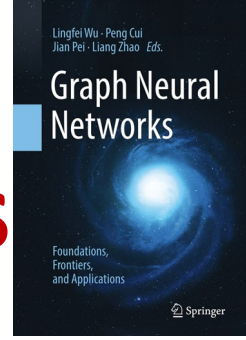


Data points (e.g., words, sentences, documents)

Fully-connected weighted graph

Chen et al. “Iterative Deep Graph Learning for Graph Neural Networks: Better and Robust Node Embeddings”. NeurIPS 2021.

Attention-based Similarity Metric Functions



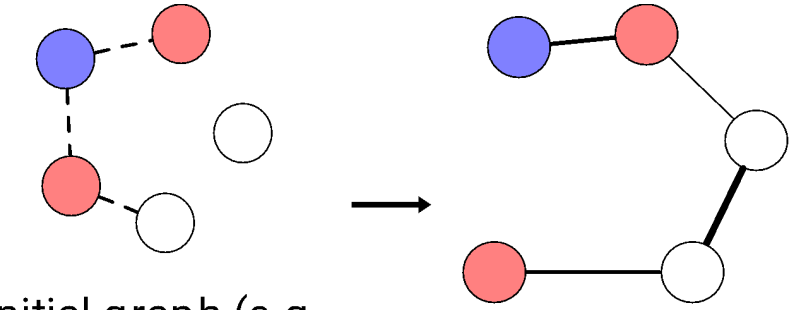
Variant 1)

$$S^l_{i,j} = \text{softmax}(\mathbf{u}^T \tanh(\mathbf{W}[\mathbf{h}^l_i, \mathbf{h}^l_j, \mathbf{v}_i, \mathbf{v}_j, \mathbf{e}_{i,j}]))$$

Edge embeddings

Variant 2)

$$S_{i,j} = \frac{\text{ReLU}(\mathbf{W}^Q \mathbf{v}_i)^T (\text{ReLU}(\mathbf{W}^K \mathbf{v}_i) + \text{ReLU}(\mathbf{W}^R \mathbf{e}_{i,j}))}{\sqrt{d}}$$

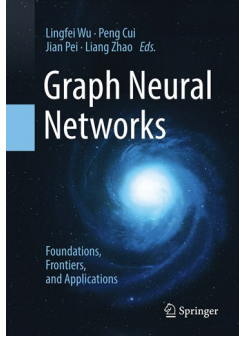


Initial graph (e.g., words, sentences, documents)

Fully-connected weighted graph

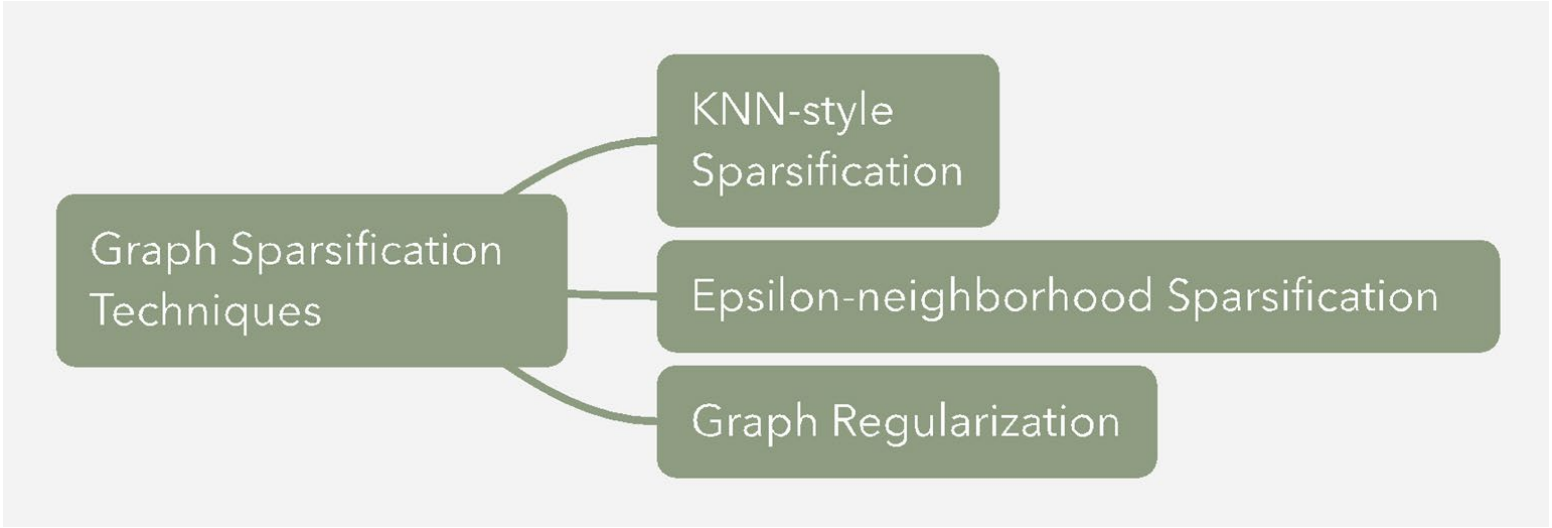
Liu et al. "Contextualized Non-local Neural Networks for Sequence Learning". AAAI 2019.

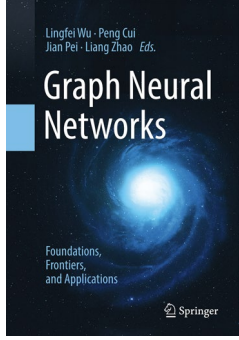
Liu et al. "Retrieval-Augmented Generation for Code Summarization via Hybrid GNN". ICLR 2021.



Graph Sparsification Techniques

- Similarity metric functions learn a fully-connected graph
- Fully-connected graph is computationally expensive and might introduce noise
- Enforcing sparsity to the learned graph structure
- Various techniques





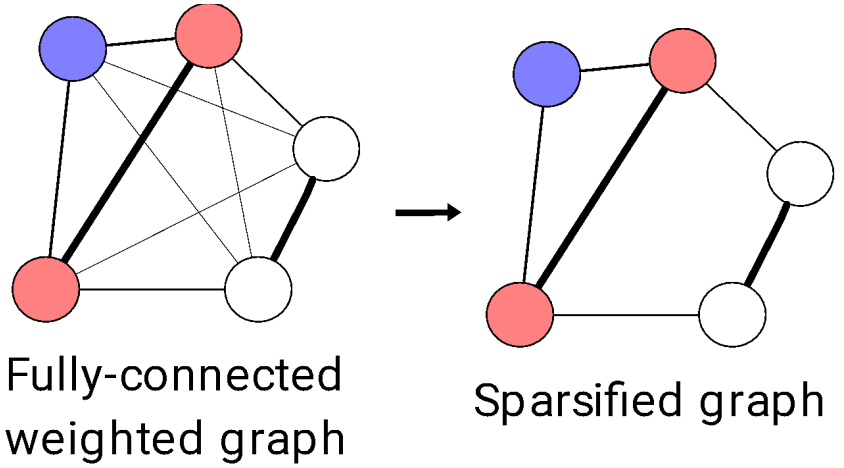
Common Graph Sparsification Options

Option 1) KNN-style Sparsification

$$\mathbf{A}_{i,:} = \text{topk}(\mathbf{S}_{i,:})$$

Option 2) epsilon-neighborhood Sparsification

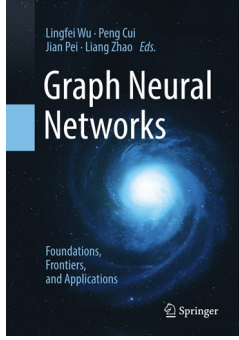
$$A_{i,j} = \begin{cases} S_{i,j} & S_{i,j} > \varepsilon \\ 0 & \text{otherwise} \end{cases}$$



Option 3) graph Regularization

$$\frac{1}{n^2}||A||_F^2$$

Combining Intrinsic and Implicit Graph Structures



- Intrinsic graph typically still carries rich and useful information
- Learned implicit graph is potentially a "shift" (e.g., substructures) from the intrinsic graph structure

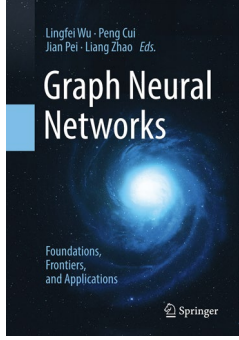
$$\widetilde{A} = \lambda L^{(0)} + (1 - \lambda)\mathrm{f}(A)$$

Normalized graph Laplacian

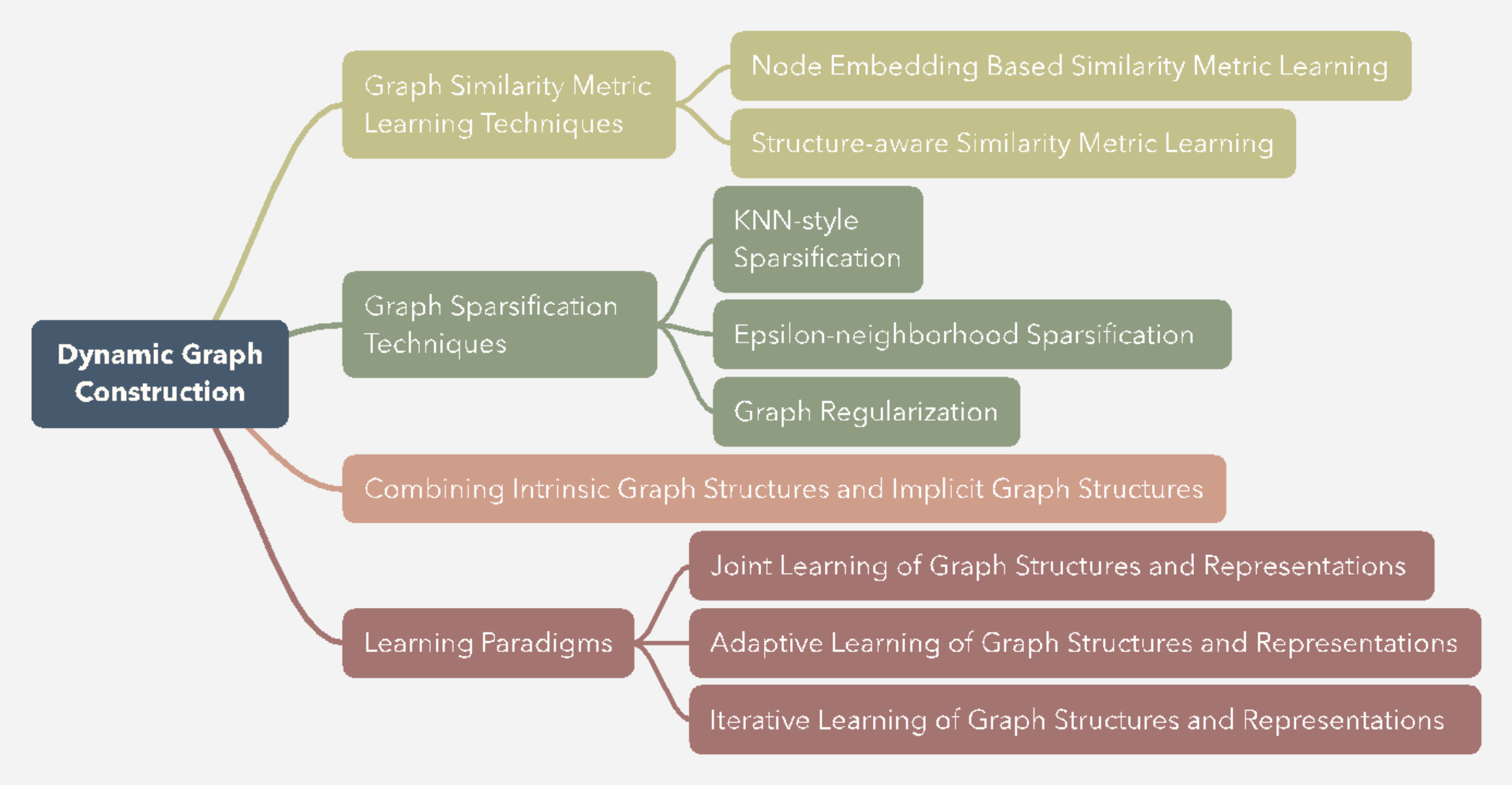
f(A) can be arbitrary operation, e.g., graph Laplacian, row-normalization

Li et al. "Adaptive Graph Convolutional Neural Networks". AAAI 2018.

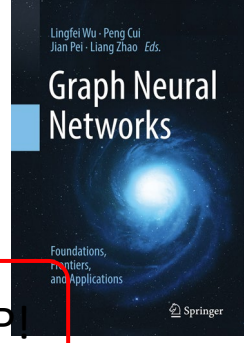
Chen et al. "Iterative Deep Graph Learning for Graph Neural Networks: Better and Robust Node Embeddings". NeurIPS 2021.



Dynamic Graph Construction Summary



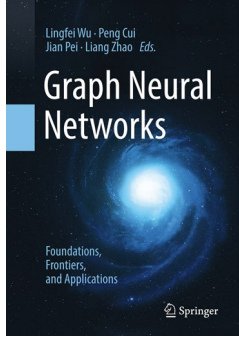
Static vs. Dynamic Graph Construction

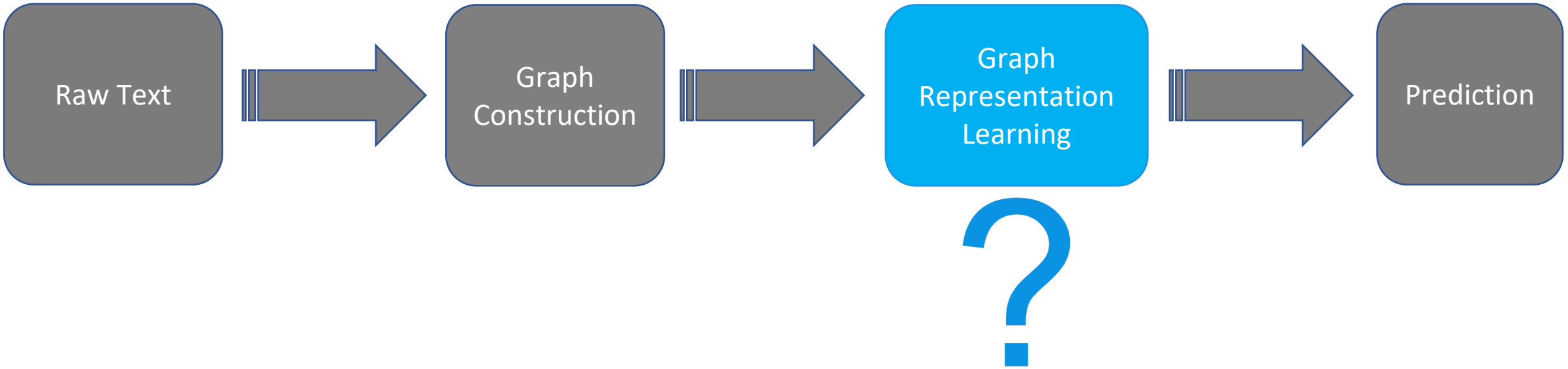


New topic in DLG4NLP!

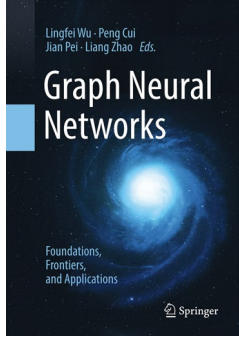
Static graph construction	Dynamic graph construction
Pros	Pros
prior knowledge	no domain expertise
	joint graph structure & representation learning
Cons	Cons
extensive domain expertise	scalability
• error-prone (e.g., noisy, incomplete) • sub-optimal	explainability
• disjoint graph structure & representation learning • error accumulation	

GNNs for Natural Language Processing



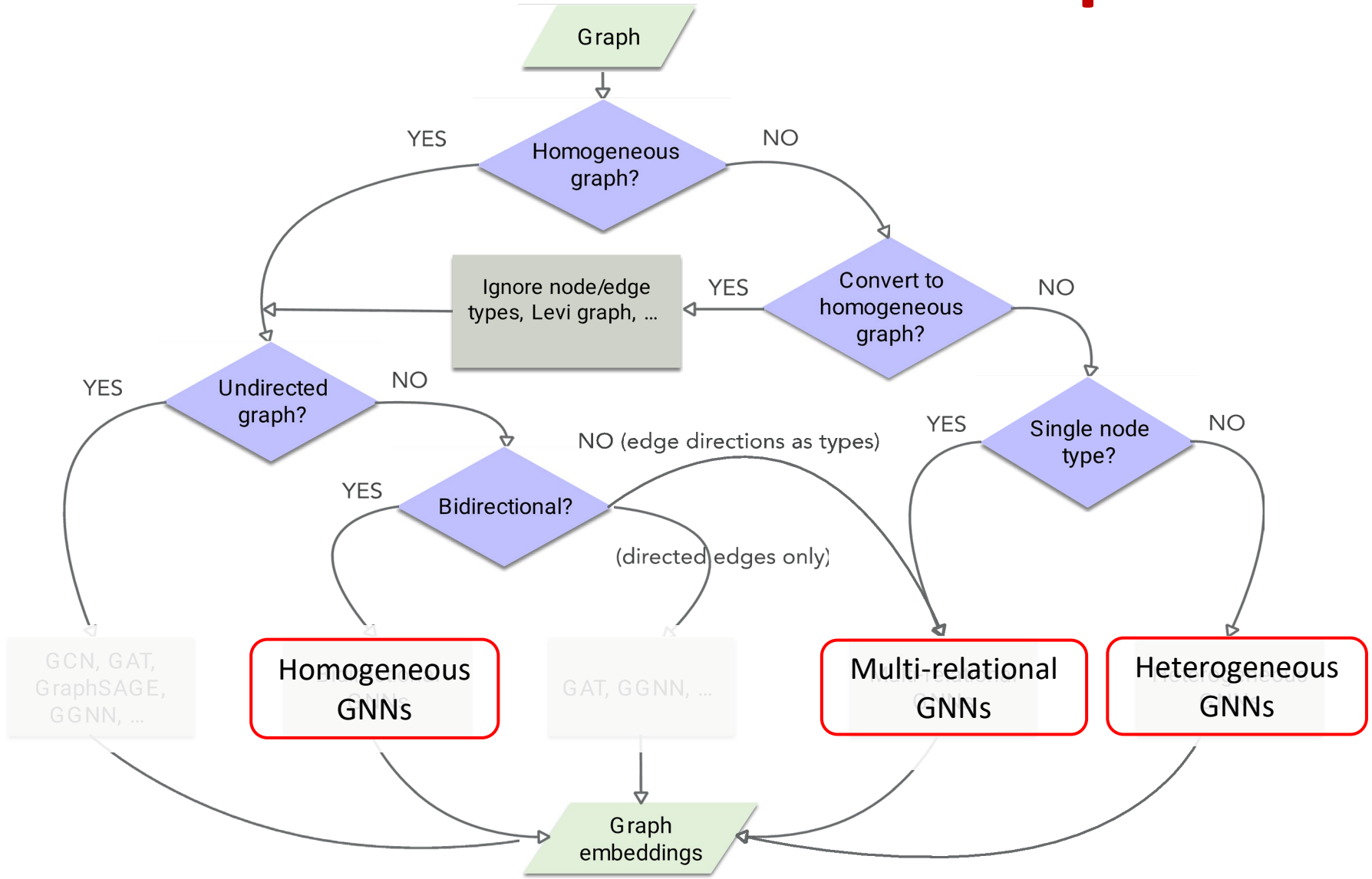


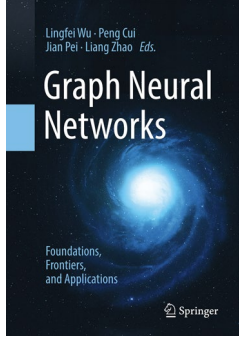
Homogeneous vs Multi-relational vs Heterogeneous Graphs



Graph types	Homogeneous	Multi-relational	Heterogeneous
# of node types	1	1	> 1
# of edge types	1	> 1	>= 1

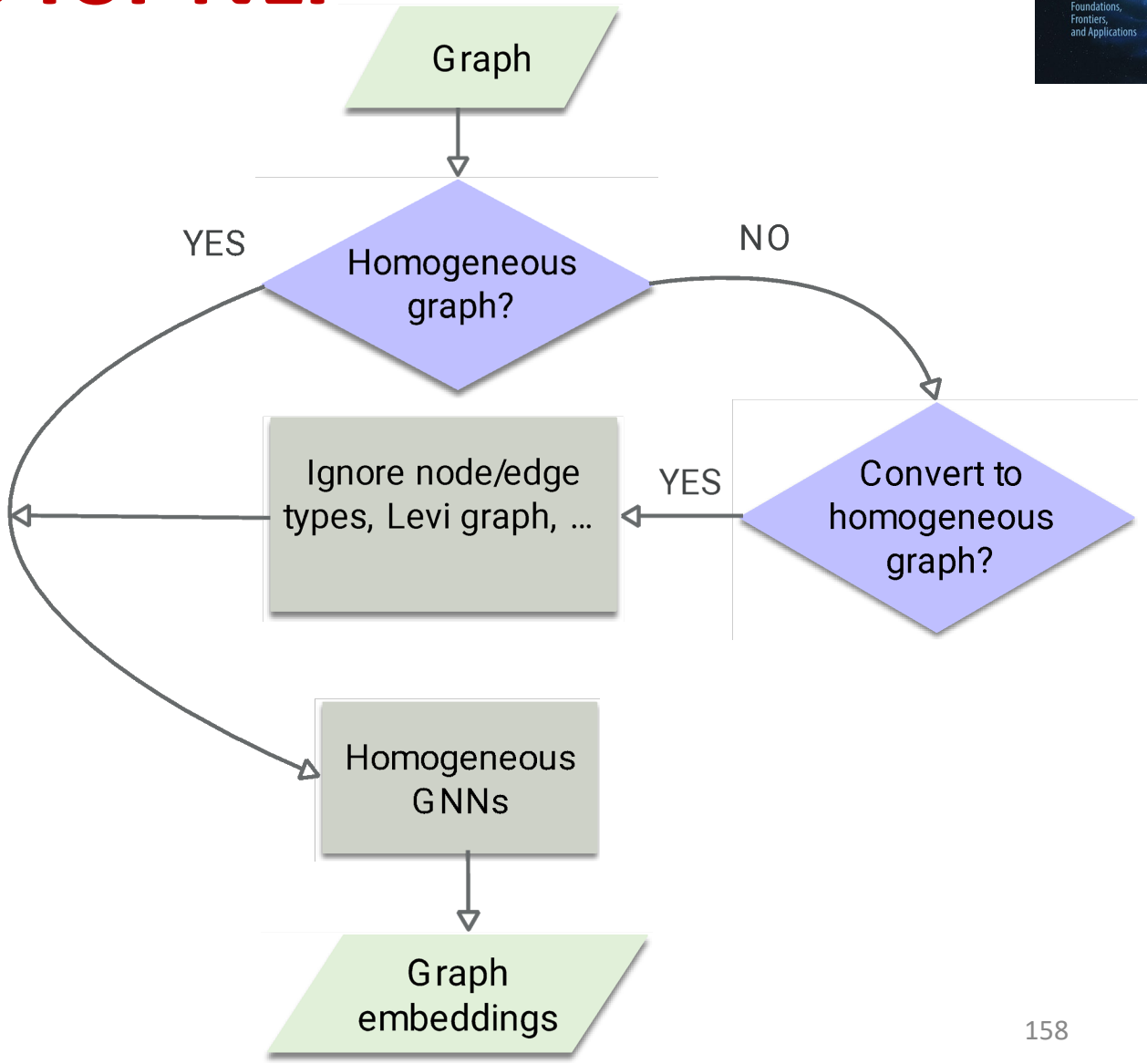
Which GNNs to Use Given a Graph?



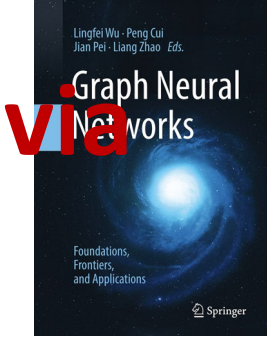


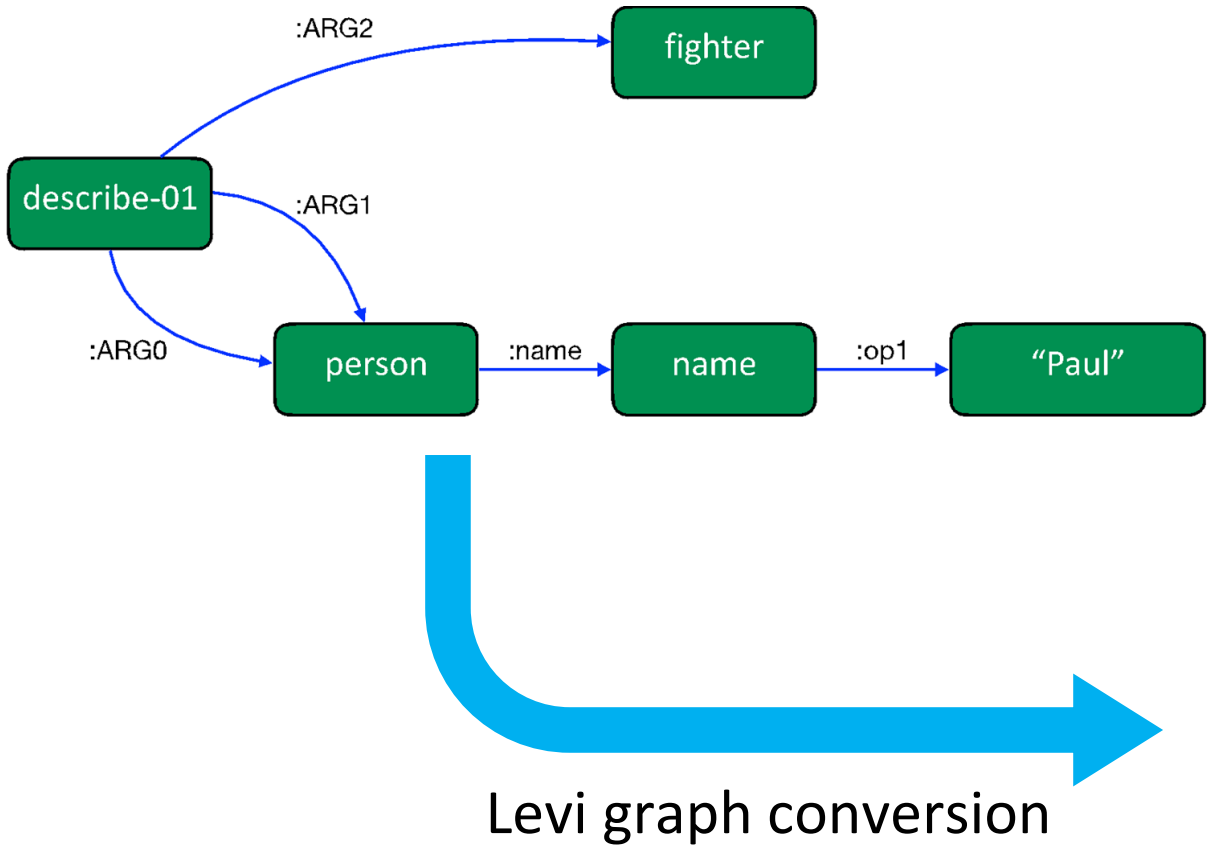
Homogeneous GNNs for NLP

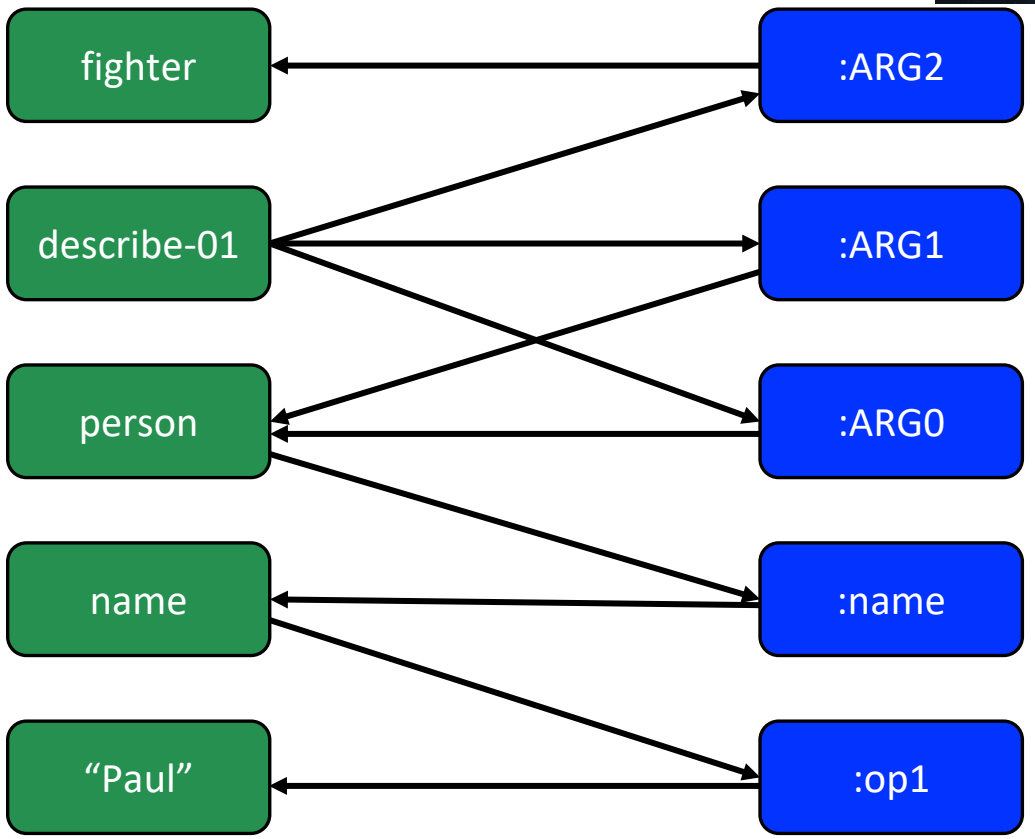
- When to use homogeneous GNNs?
- Homogeneous GNNs
  - GCN
  - GAT
  - GraphSAGE
  - GGNN
  - …



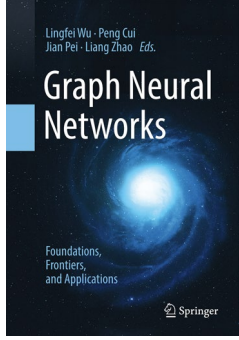
Non-homogeneous to Homogeneous Conversion via Levi Graph





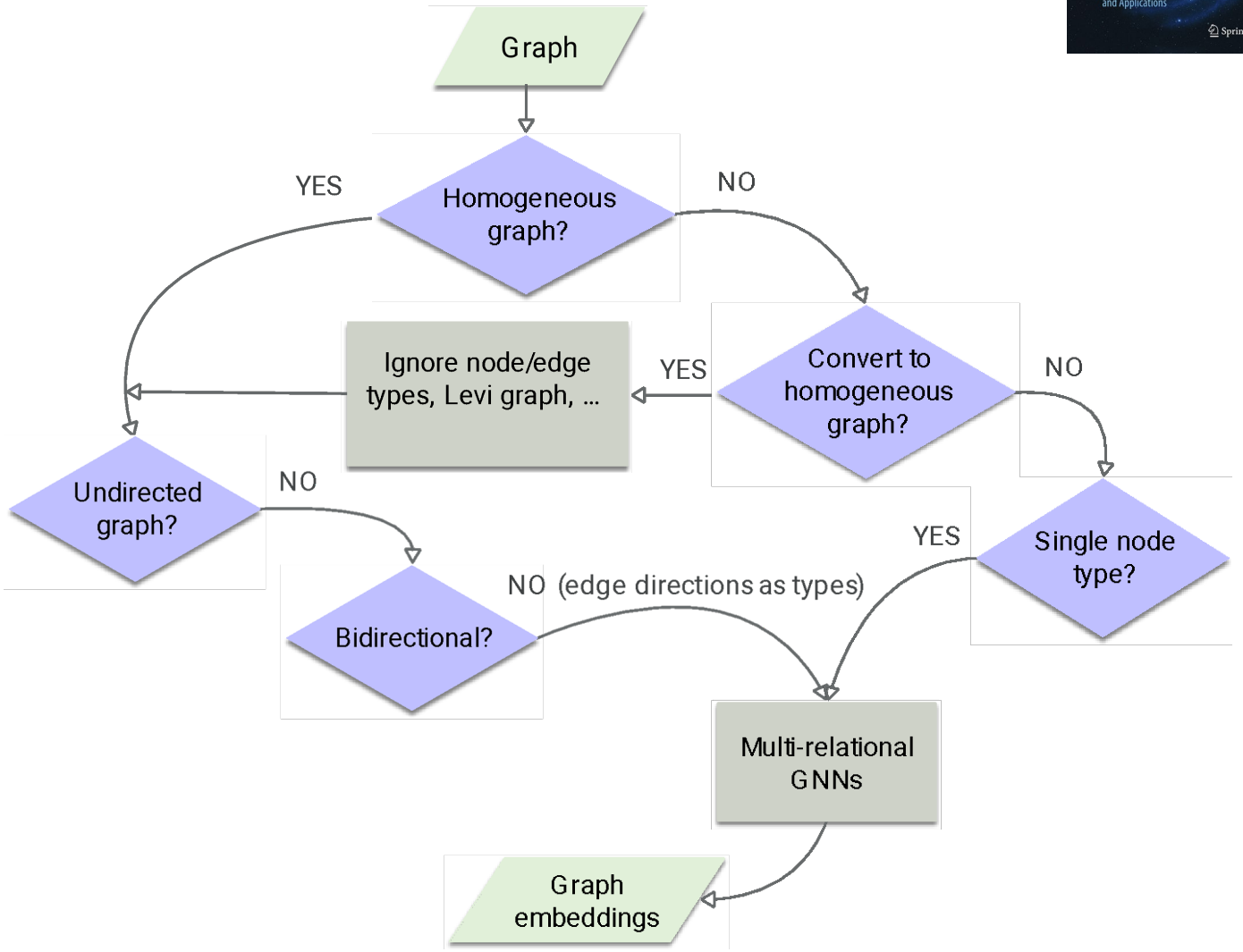


Levi graph: edges as new nodes



Multi-relational GNNs for NLP

- When to use multi-relational GNNs?
- Multi-relational GNNs
  a) Including relation-specific transformation parameters in GNN
  b) Including edge embeddings in GNN
  c) Multi-relational Graph Transformers



R-GNN: Overview

$$\mathbf{h}_i^k = \sigma(\mathbf{h}_i^{k-1}, \sum_{v_j \in \mathcal{N}(v_i)} AGG(\mathbf{h}_j^{k-1}, \theta^k))$$

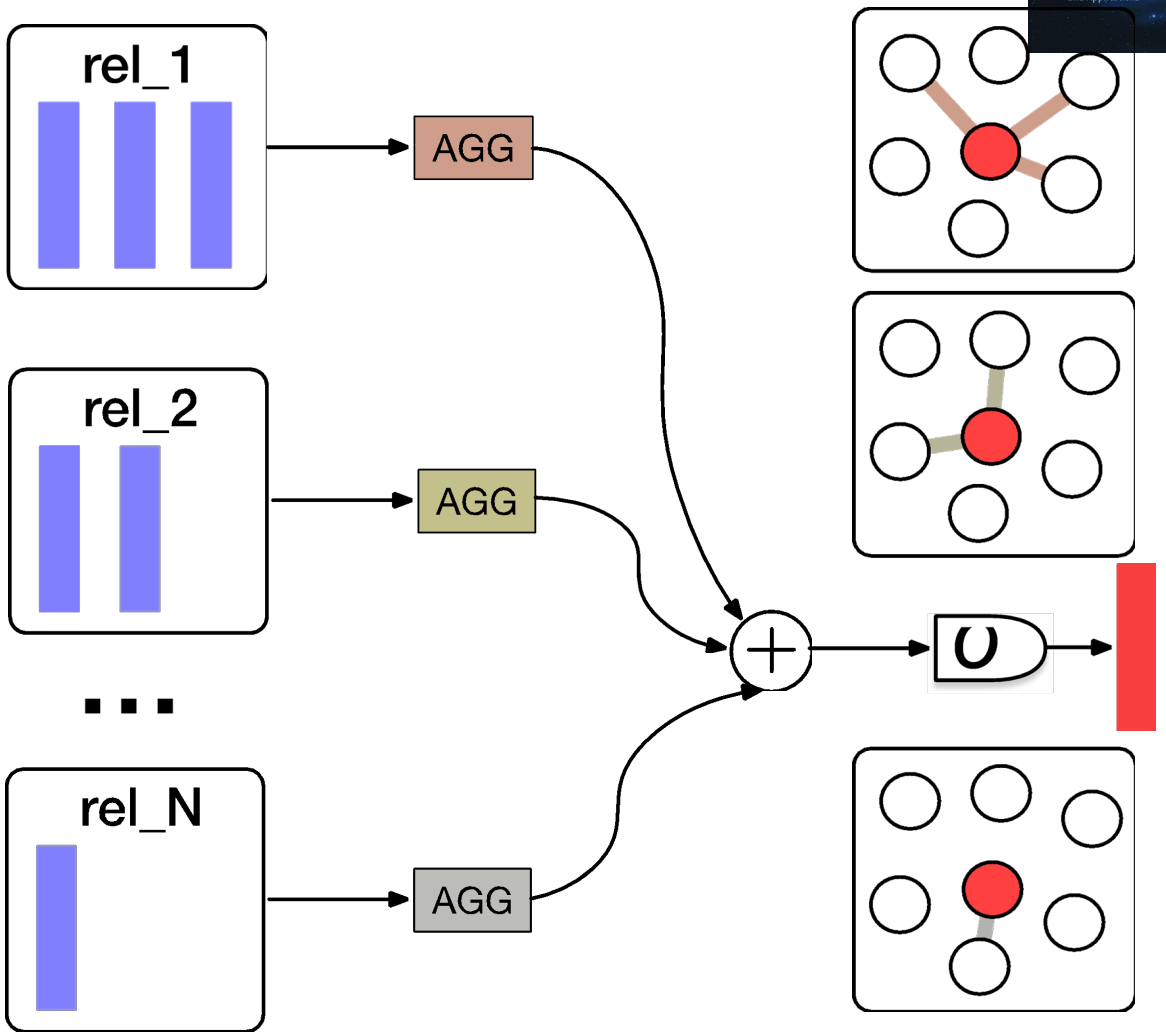
GNN

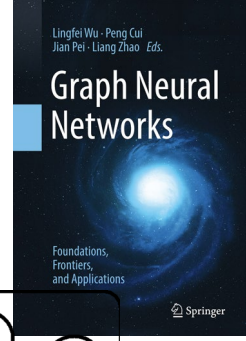
R-GNN

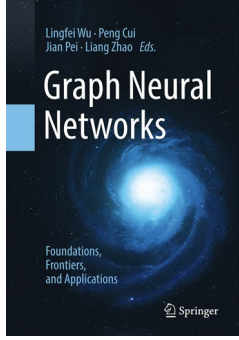
1) relation-specific transformation, e.g., node feature transformation, attention weight …

$$\mathbf{h}_i^k = \sigma(\mathbf{h}_i^{k-1}, \sum_{r \in \mathcal{E}} \sum_{v_j \in \mathcal{N}_r(v_i)} AGG(\mathbf{h}_j^{k-1}, \theta_r^k))$$

2) aggregation per relation-specific subgraph







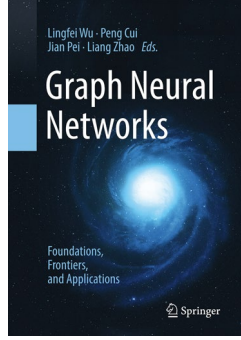
R-GNN Variant: R-GCN

- Relation-specific node feature transformation during neighborhood aggregation

$$\mathbf{h}_i^k = \sigma\Big(\sum_{r\in\mathcal{E}}\sum_{v_j\in\mathcal{N}_r(v_i)}\frac{1}{c_{i,r}}\mathbf{W}_r^k\mathbf{h}_j^{k-1} + \mathbf{W}_0^k\mathbf{h}_i^{k-1}\Big), \quad c_{i,r} = |\mathcal{N}_r(v_i)$$

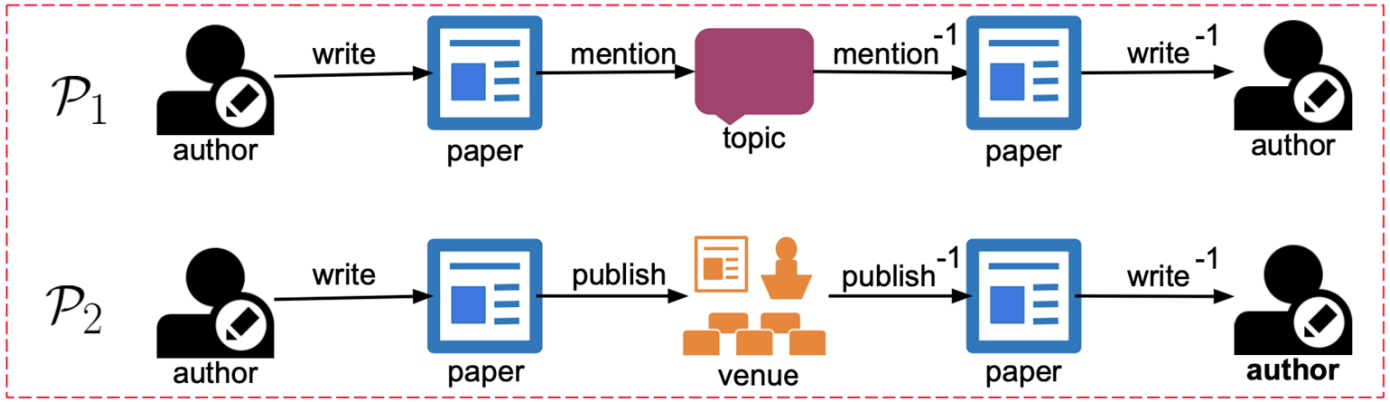
Relation-specific d x d learnable weight matrix

Schlichtkrull et al. "Modeling Relational Data with Graph Convolutional Networks". 2017.

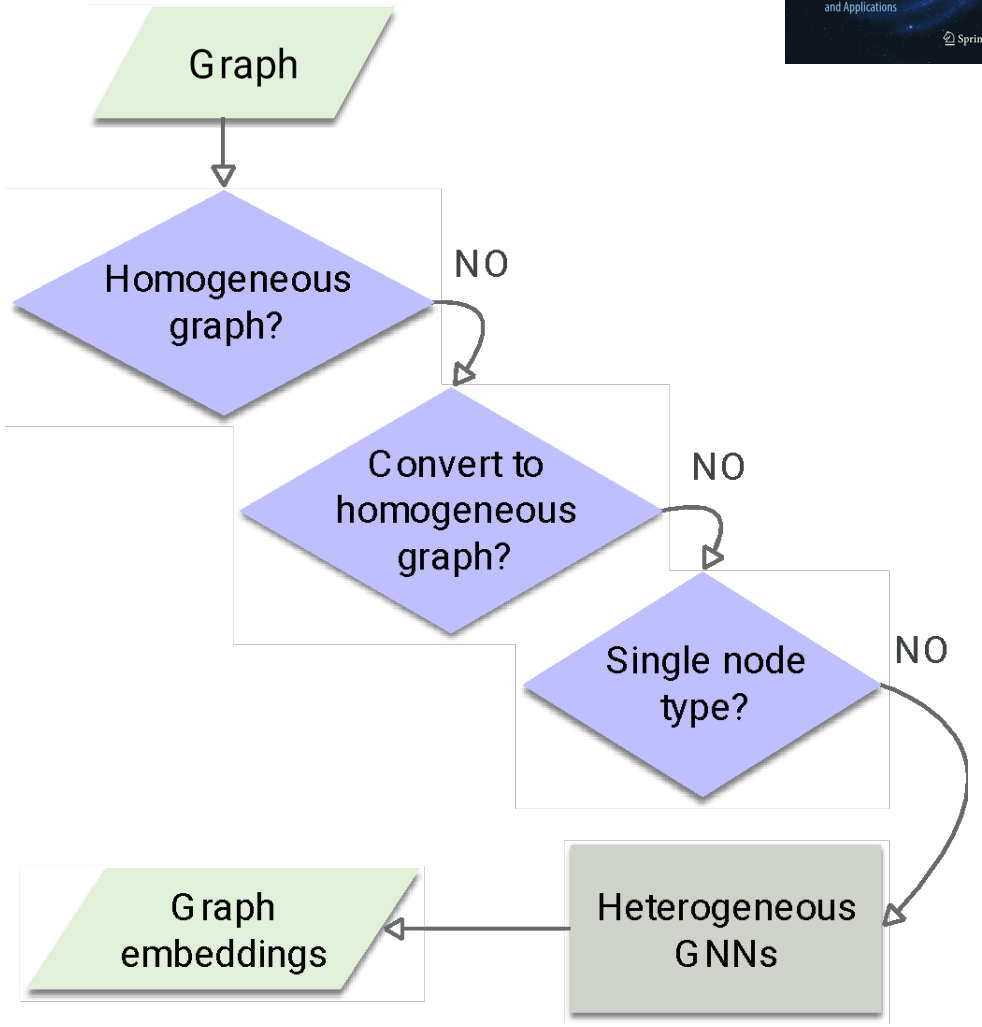


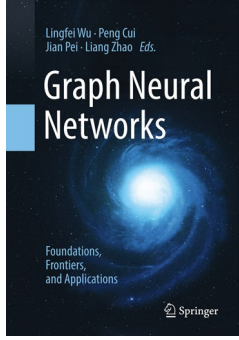
Heterogeneous GNNs

- When to use Heterogeneous GNNs?
- Heterogeneous GNNs
  a) Meta-path based Heterogeneous GNNs



Meta paths among author nodes





Meta-path based Heterogeneous GNN example: HAN

Step 1) type-specific node feature transformation

$$\mathbf{h}_i = \mathbf{W}_{\tau(v_i)}\mathbf{v}_i$$

Node-type specific learnable weight matrix

Step 2) node-level aggregation along each meta path

$$\mathbf{z}_{i,\Phi_k} = \sigma\Big(\sum_{v_j \in \mathcal{N}_{\Phi_k}(v_i)} \alpha_{i,j}^{\Phi_k}\mathbf{h}_j\Big)$$

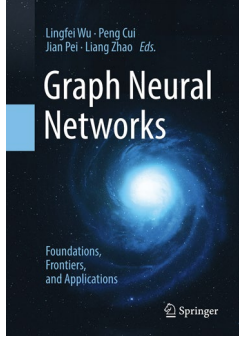
Aggregate over neighboring nodes in k-length meta path

Step 3) meta-path level aggregation

$$\mathbf{z}_i = \sum_{k=1}^{p} \beta_{\Phi_k}\mathbf{z}_{i,\Phi_k}$$

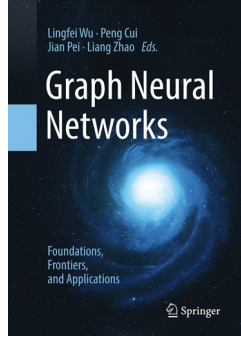
Attention weights over meta paths

Wang et al. "Heterogeneous Graph Neural Networks for Extractive Document Summarization". ACL 2020.



Graph4NLP: A Library for Deep Learning on Graphs for NLP

Graph4NLP: A Brief History and Future



Year June/2021

Graph4NLP v0.4.1 Released, first library for promoting easy use of GNN for NLP

Year September/2021

Our **DLG4NLP website** launched: survey, library, tutorial, workshop and many more.

Year September/2021

Graph4NLP v0.5.1 released, Lint the codes, support testing with users' own data, and fix many reported bugs.

Year 01/20/2022

Graph4NLP v0.5.5 released, Support model.predict API by introducing wrapper functions, separate graph Topology and graph Embedding and many more…

Year 07/31/2022 (planning)

- Graph4NLP v0.6.1 will be released, new configuration system, relational GNN support.

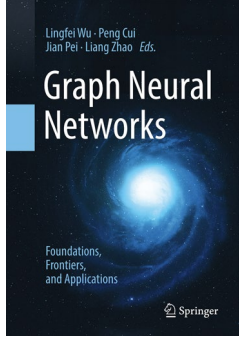
- DLG4NLP@NAACL2022 workshop is coming!

Year 2022

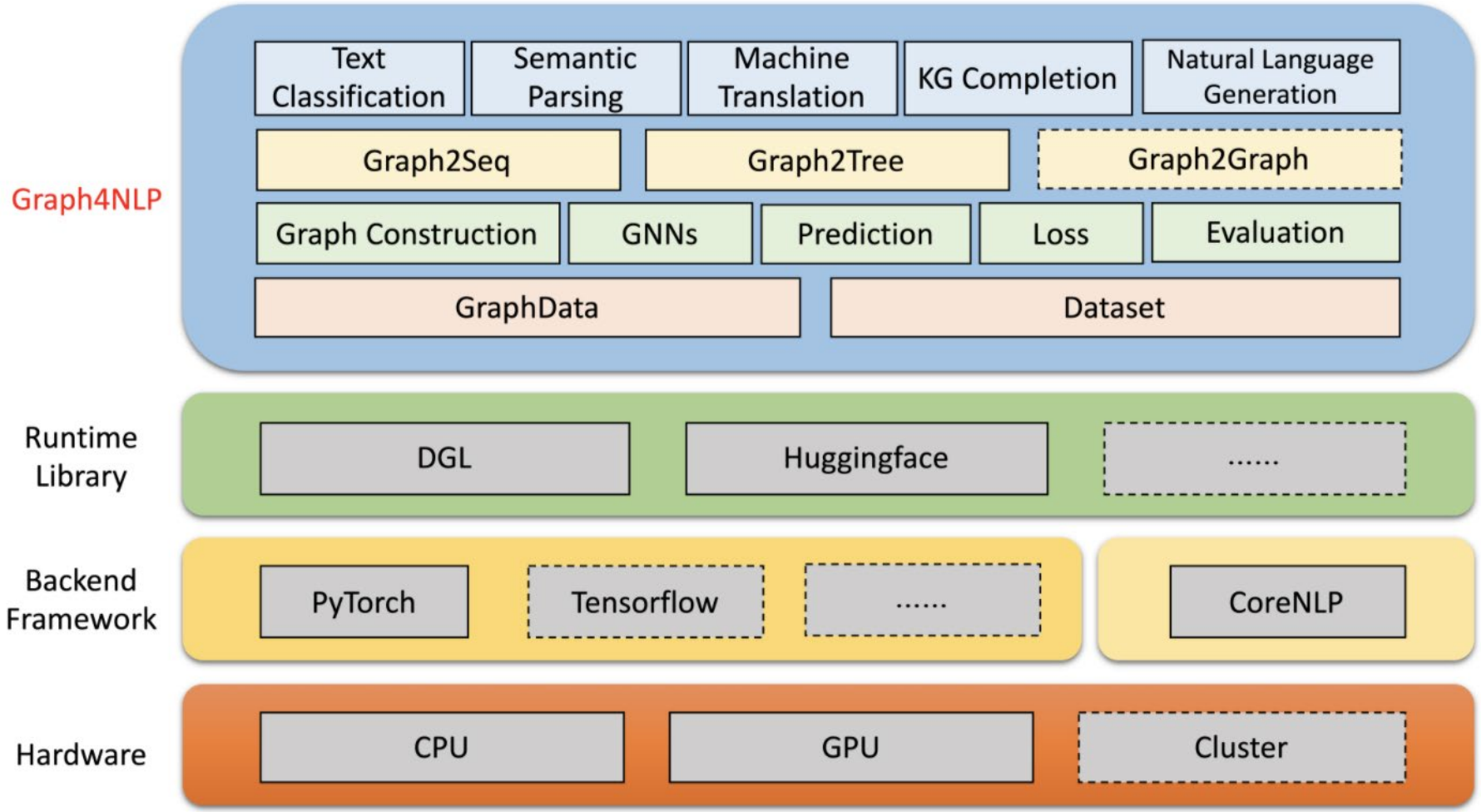
- Graph4NLP v0.6.1 will be released,

- More tutorials, and workshops

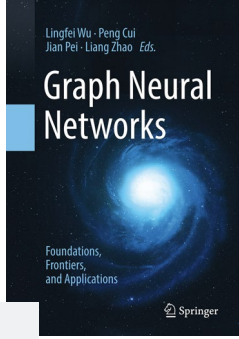
- Release a New Graph4NLP book by Cambridge Press



Overall Architecture of Graph4NLP Library



DGL: https://github.com/dmlc/dgl, DIG: https://github.com/divelab/DIG, Huggingface: https://github.com/huggingface/transformers



Key Features and Future Releases

Easy-to-use and Flexible

Provides both full implementations of state-of-the-art models and also flexible interfaces to build customized models with whole-pipeline support

Rich Set of Learning Resources

Provide a variety of learning materials including code demos, code documentations, research tutorials and videos, and paper survey

High Running Efficiency and Extensibility

Build upon highly-optimized runtime libraries including DGL and provide highly modulization blocks

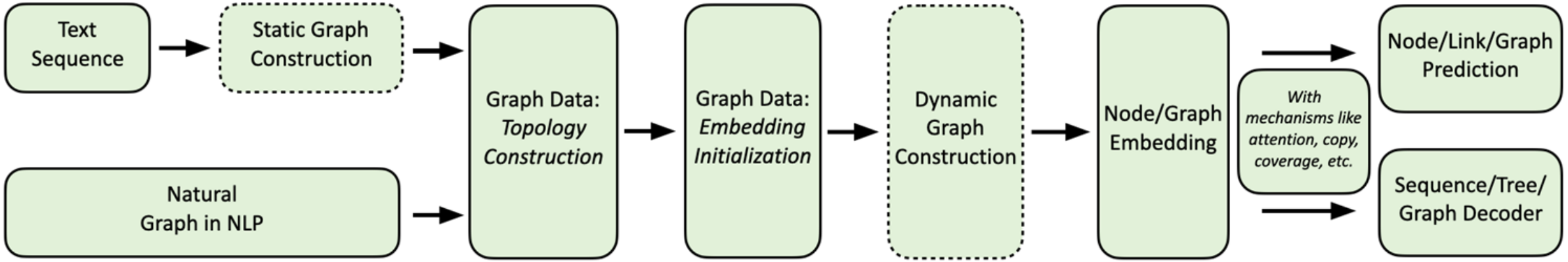
Comprehensive Code Examples

Provide a comprehensive collection of NLP applications and the corresponding code examples for quick-start

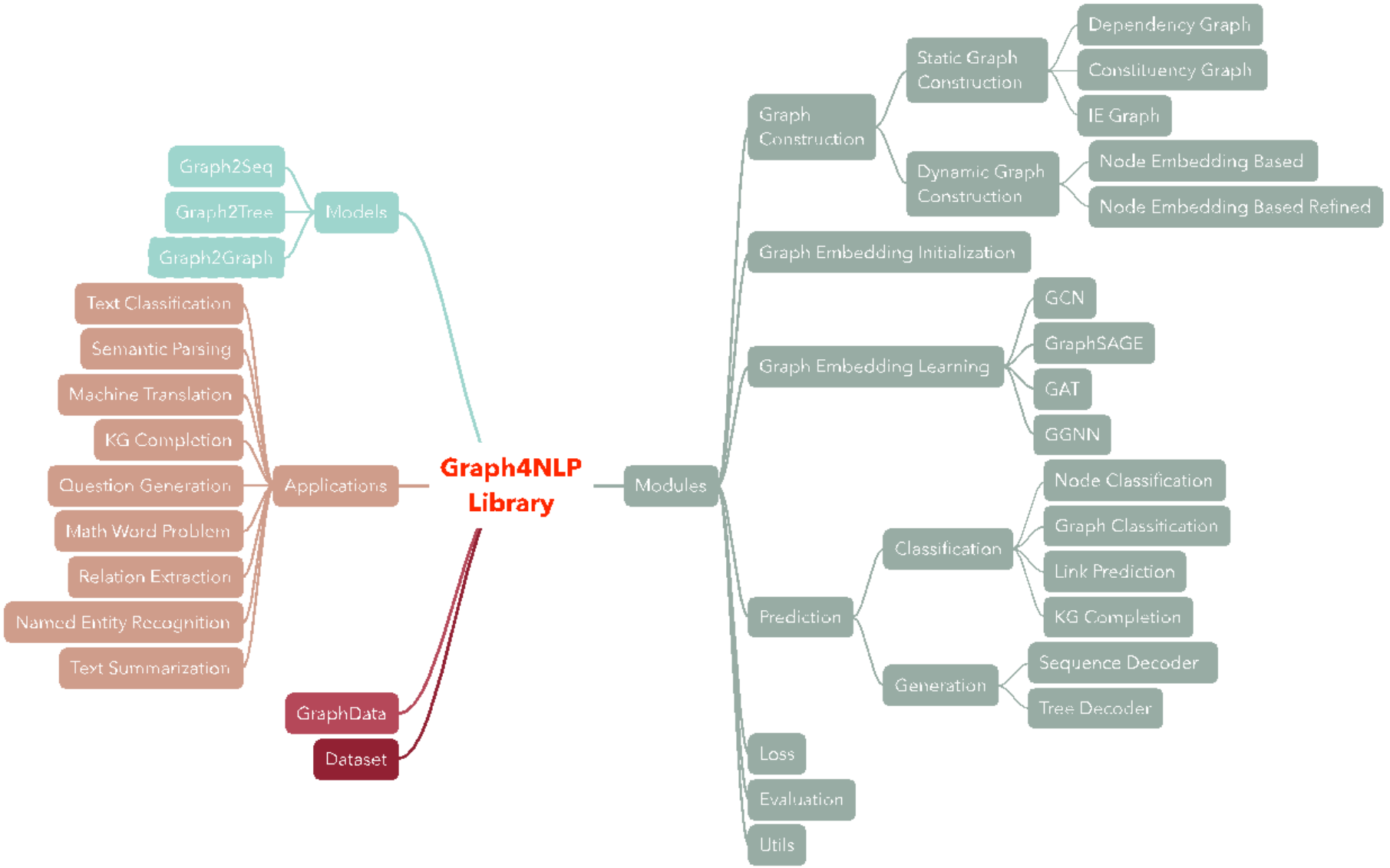
Future Releases

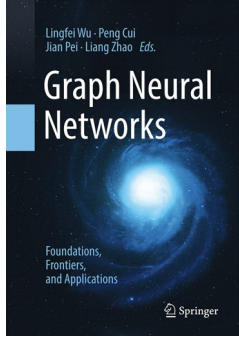
- **V0.6 new features: new configuration system, relational GNN support, etc.**
- **Future todo: Native multi-GPU support, better support for customized graph construction, etc.**

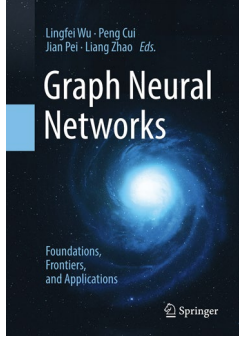
Computing Flow of Graph4NLP



Dive Into Graph4NLP Library

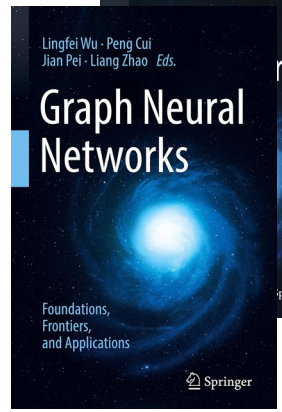


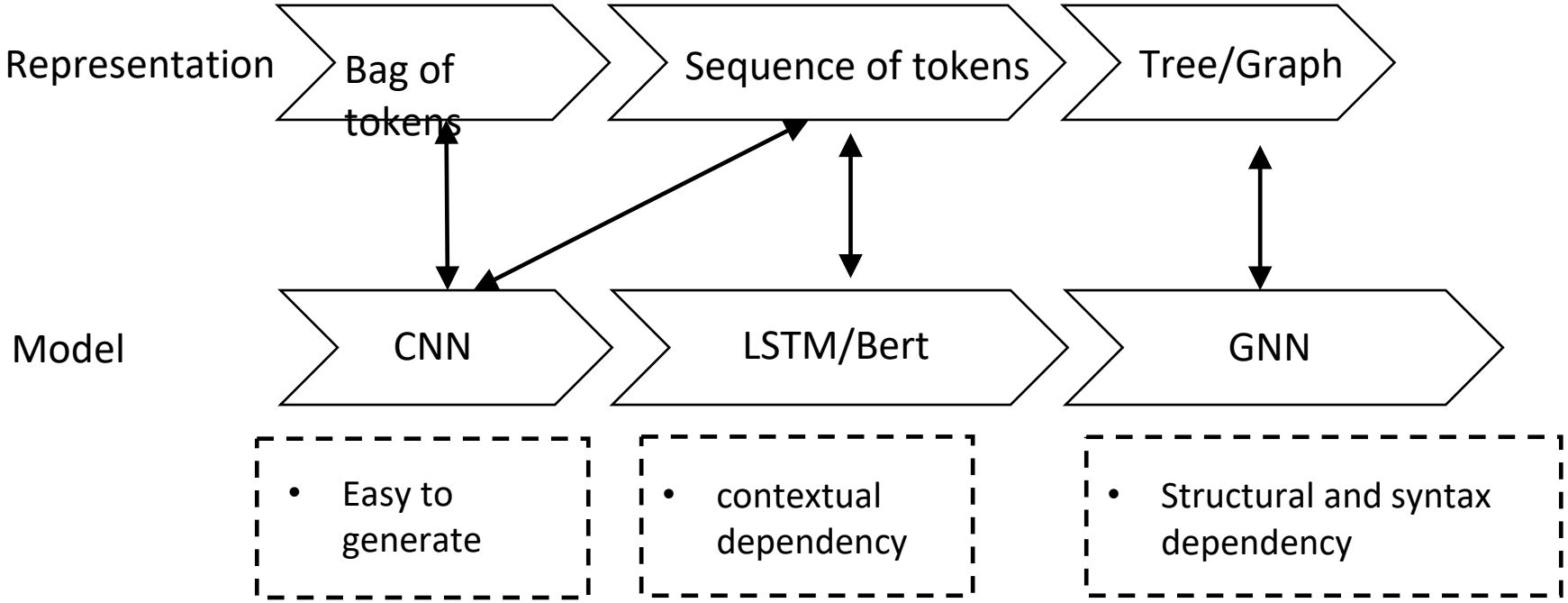




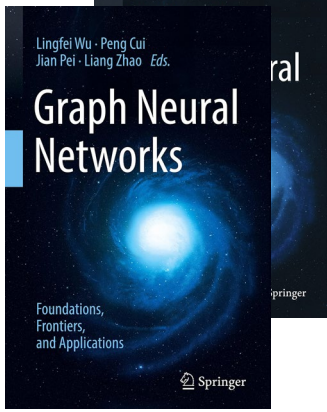
GNNs in Program Analysis (Chapter 22)

Representation of Programs in DL

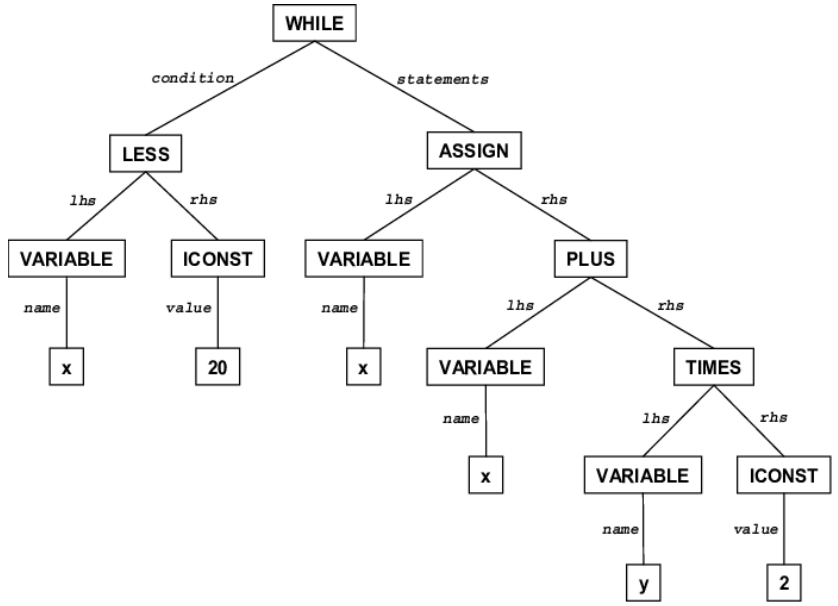




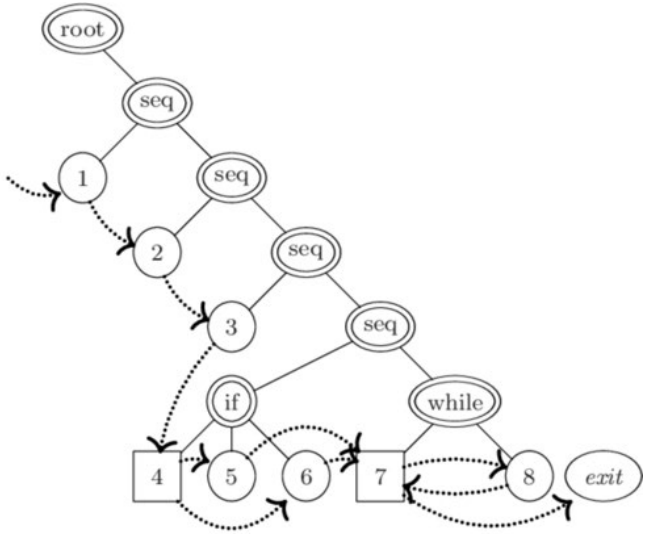
A Graph Representation of Programs



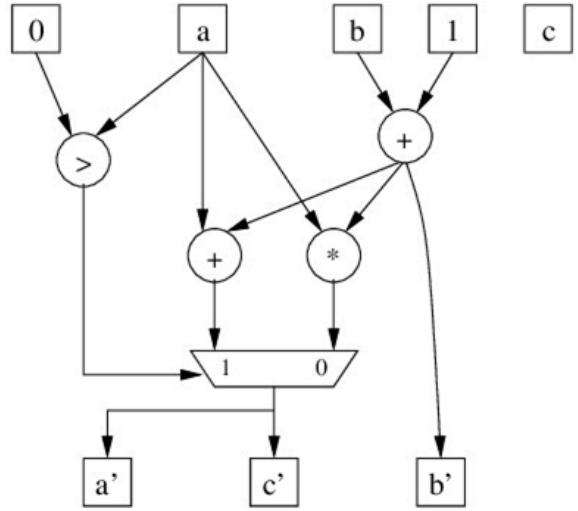
Trade-offs between expressing various program properties, the size of the graph representation, and the effort required to generate them.



Syntax Tree
(Fritzson P, et al 2009)

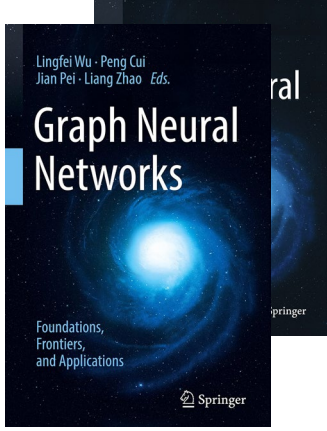


Control Flow Graph
(Va E , et al 2007)
n

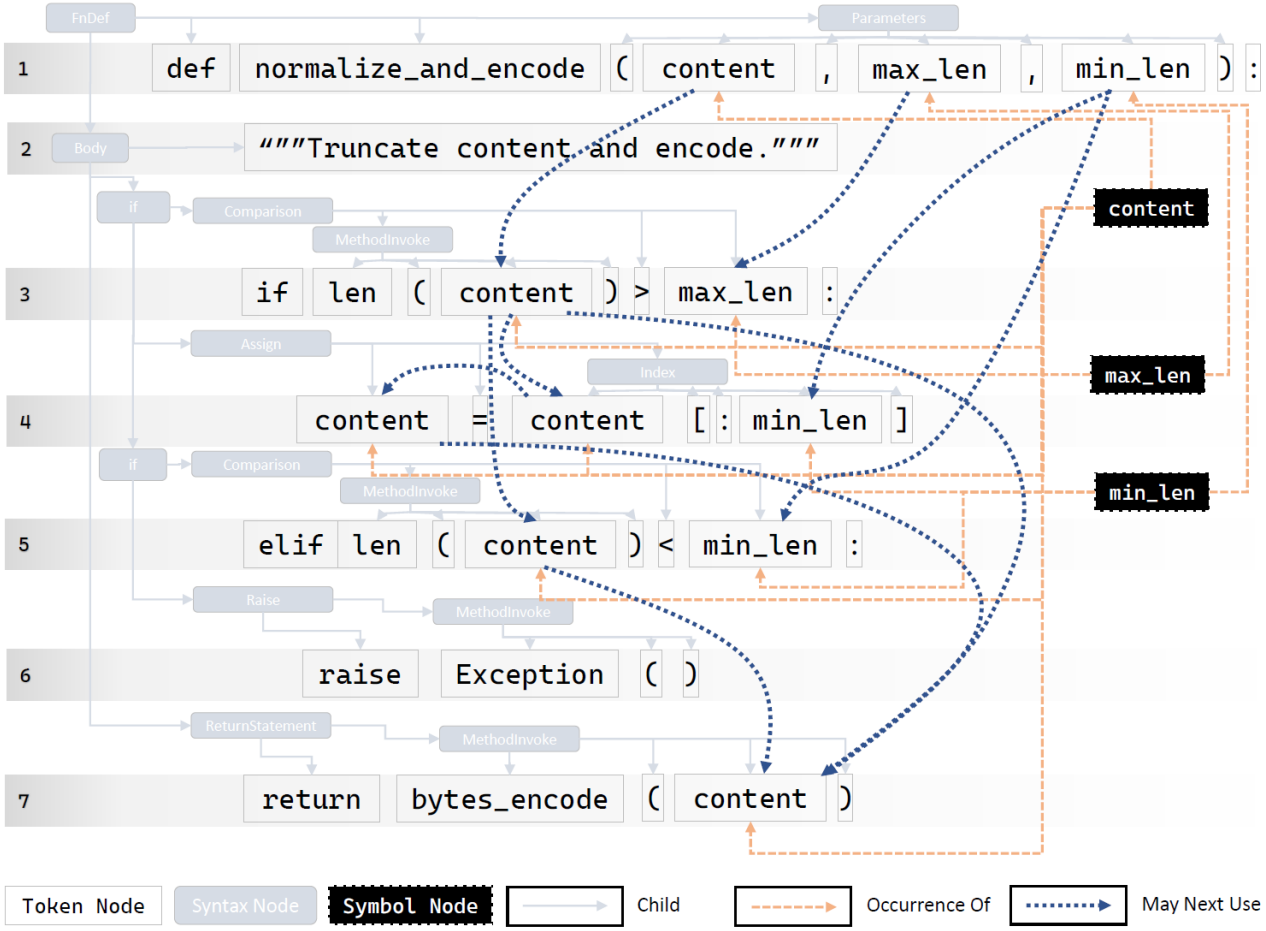


Data Flow Graph
(A. Koelbl, et al 2009)

A Graph Representation of Programs



Model each source code file as a single graph (Allamanis et al, 2018b)

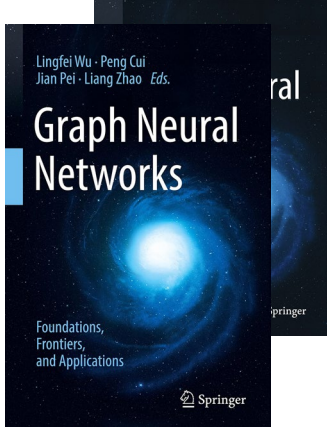


Token node: Program language can be tokenized into a sequence of tokens. (NextToken edge)

Syntax node: The sequence of tokens is parsed into a syntax tree. **(**Child edge**)**

Symbol node: variables, functions, packages (Occurrence edge)

A Graph Representation of Programs



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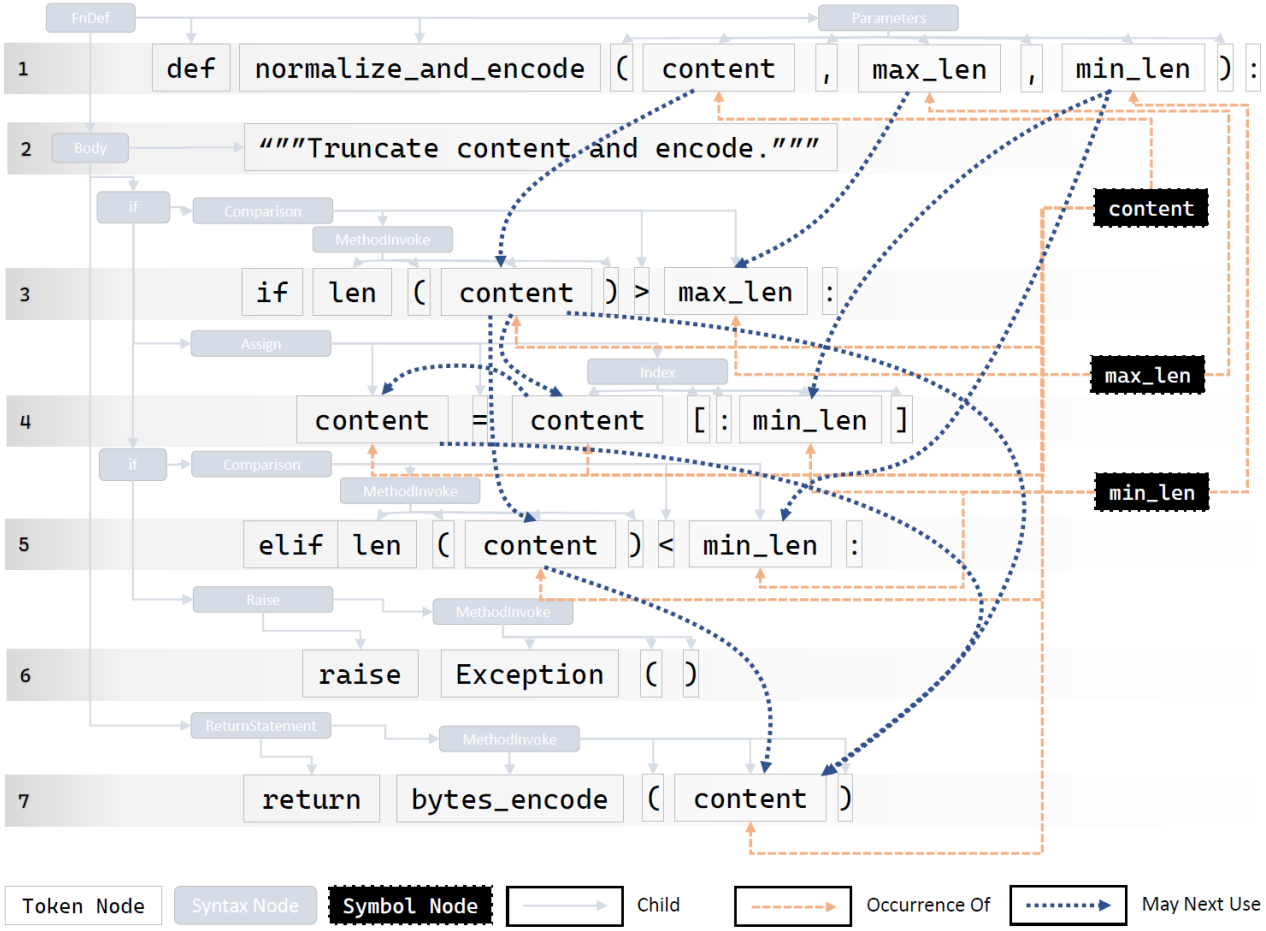


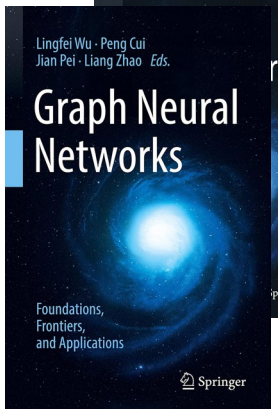
Data Flow: all the valid paths that data may flow through the program.

(MayNextUse)

Program Dependence Graph

- Less model capacity for learning deterministic facts.
- Inductive biases help on program analysis tasks.

Case Study 1: Detecting Variable Misuse Bugs



Variable misuse: the incorrect use of one variable instead of another already in the scope

Significance: 12% of the bugs in a large set of Java codebases are variable misuses, 6% of Java build errors in the Google engineering systems are variable misuses.

Goal: (1) localize the bug (2) suggest a repair.

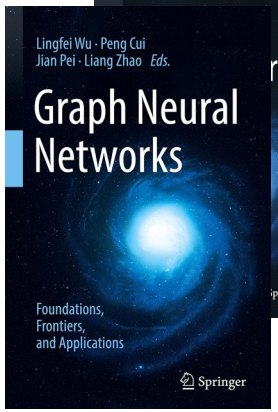
$$\{\mathbf{h}_{v_i}\} = \text{GNN}\left(\mathscr{G}', \{\mathbf{n}_{v_i}\}\right)$$

GNN for directed heterogeneous graphs.

$$p_{loc}(v_i) = \underset{v_j \in \mathscr{V}_{vu} \cup \{\emptyset\}}{\text{softmax}}\left(\mathbf{u}^\top \mathbf{h}_{v_i}\right)$$

Pointer network (Vinyalset al, 2015)

Case Study 1: Detecting Variable Misuse Bugs



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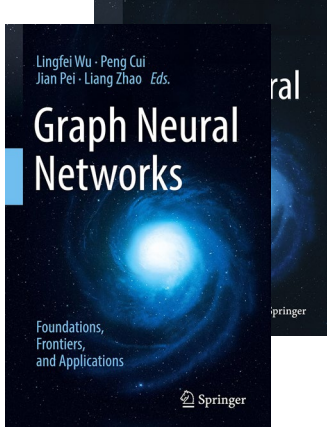
GNN for directed heterogeneous graphs.

$$p_{rep}(s_i) = \underset{s_j \in \mathscr{V}_{s@v_{bug}}}{\text{softmax}}\left(\mathbf{w}^\top [\mathbf{h}_{v_{bug}}, \mathbf{h}_{s_j}]\right),$$

Embedding of correct candidates

Embedding of misuse nodes

Case Study 1: Detecting Variable Misuse Bugs



Variable misuse: the incorrect use of one variable instead of another already in the scope

Significance: 12% of the bugs in a large set of Java codebases are variable misuses, 6% of Java build errors in the Google engineering systems are variable misuses.

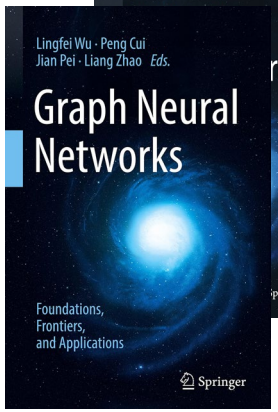
Goal: (1) localize the bug (2) suggest a repair.

```
def describe_identity_pool(self, identity_pool_id):
  identity_pool = self.identity_pools.get(identity_pool_id, None)

  if not identity_pool:
-     raise ResourceNotFoundError(identity_pool)
+     raise ResourceNotFoundError(identity_pool_id)
...
```

A diff snippet of code with a real-life variable misuse error caught by a GNN-based model.

Case Study 2: Predicting Types in Dynamically Typed Languages



Type check: Guarantee that the values of variables will only take the values of the annotated type (e.g., int, float, str)

Issues: many programming languages either forgo the guarantees provided by types or require their users to explicitly provide type annotations.

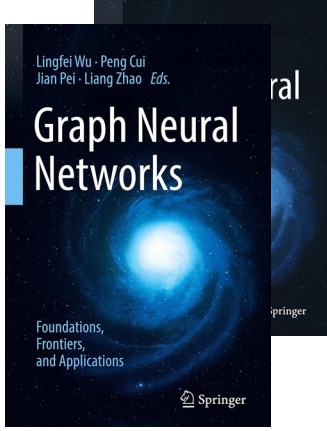
Probabilistic type inference: Node classification tasks

$$p(s_j : \tau) = \underset{\tau' \in Z}{\text{softmax}} \left(E_\tau{}^\top \mathbf{h}_{v_{s_j}} + b_\tau \right),$$

fixed vocabulary of type annotations

Open-source project and datasets: https://github.com/microsoft/dpu-utils

Case Study 2: Predicting Types in Dynamically Typed Languages



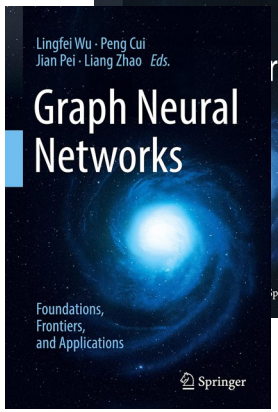
Current Limitations:

- Type annotations are highly structured and sparse.
  e.g., *Dict[Tuple[int, str], List[bool]]* appear infrequently
- Dynamic/open set recognition environment
  e.g., new user-defined types (classes) will also appear at test time.

```
def __init__(
  self,
- embedding_dim: float = 768,
- ffn_embedding_dim: float = 3072,
- num_attention_heads: float = 8,
+ embedding_dim: int = 768,
+ ffn_embedding_dim: int = 3072,
+ num_attention_heads: int = 8,
  dropout: float = 0.1,
  attention_dropout: float = 0.1,
```

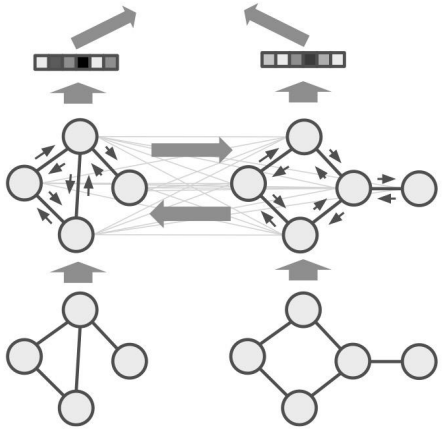
Typilus (Allamanis et al, 2020).

The variables cannot contain floats but instead should contain integers.

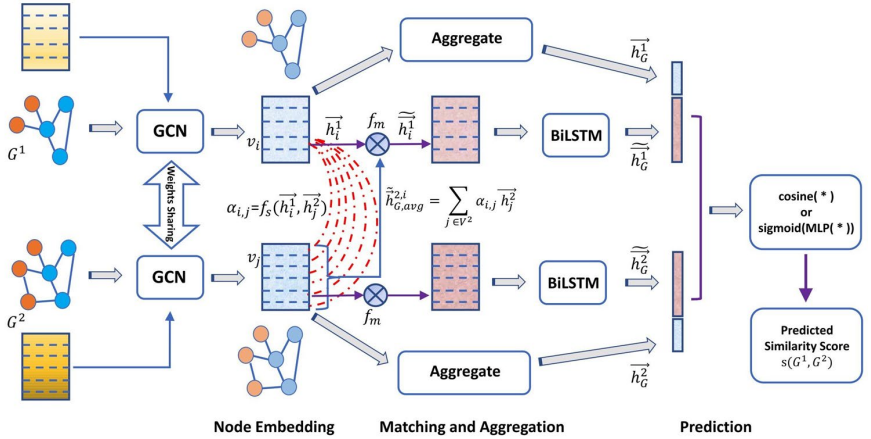


Case Study 3: code similarity analysis

Goal: Compare and predict whether two codes are solving the same problem.
Graph Matching problem: finding a similarity between graphs



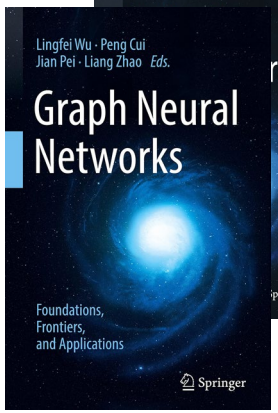
Graph Matching Networks w/ SPT [1]



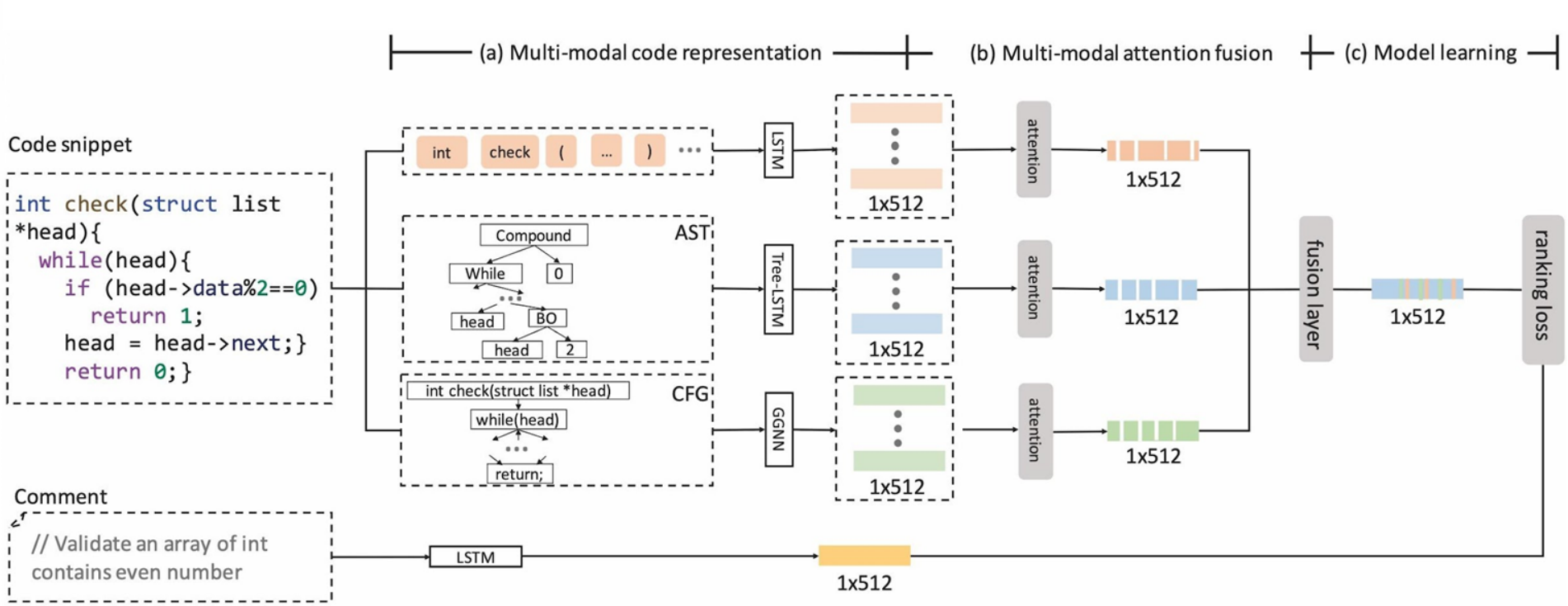
Multilevel Graph Matching Networks [2]

1. Abstract syntax tree (AST): more semantic information and capture the “problem” semantics
2. Both **Node-graph-interaction**, node-node-interaction and graph-graph interaction interaction

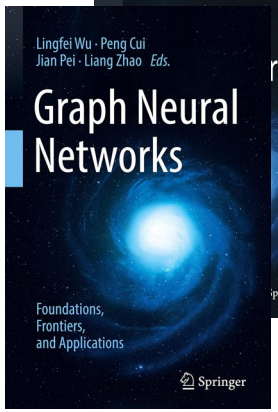
[1] Li Y, et al. Graph matching networks for learning the similarity of graph structured objects. InInternational conference on machine learning 2019 May 24 (pp. 3835-3845). PMLR
[2] Ling X, et al. Multilevel Graph Matching Networks for Deep Graph Similarity Learning. IEEE Transactions on Neural Networks and Learning Systems. 2021 Aug 18



Case Study 3: code similarity analysis

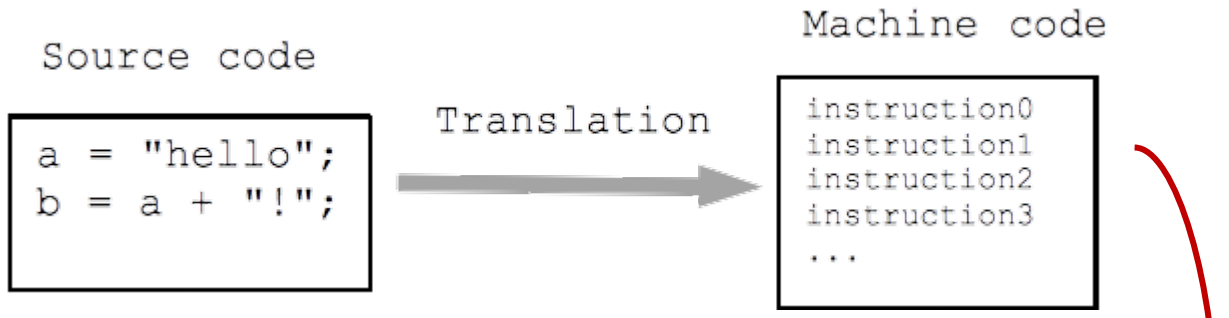


Wan Y, Shu J, Sui Y, Xu G, Zhao Z, Wu J, Yu P. Multi-modal attention network learning for semantic source code retrieval. In2019 34th IEEE/ACM International Conference on Automated Software Engineering (ASE) 2019 Nov 11 (pp. 13-25). IEEE.

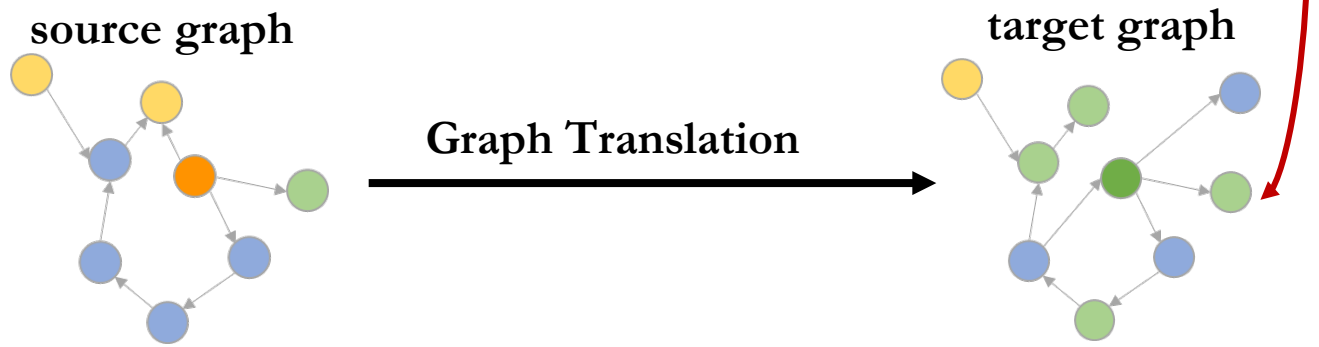


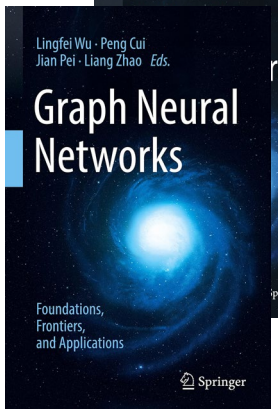
Case Study 4: Code Translation

Code Translation: Translating source code from one language to another language.
e.g., program modernization



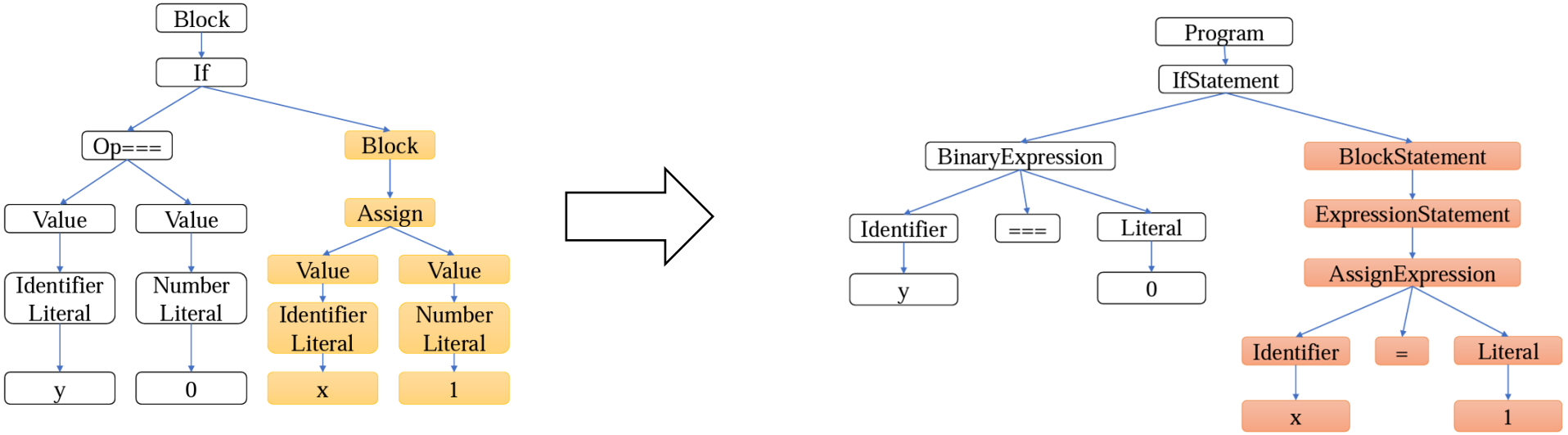
Graph-to-graph translation: Learning the mapping from graph in the source domain to the graph in the target domain.



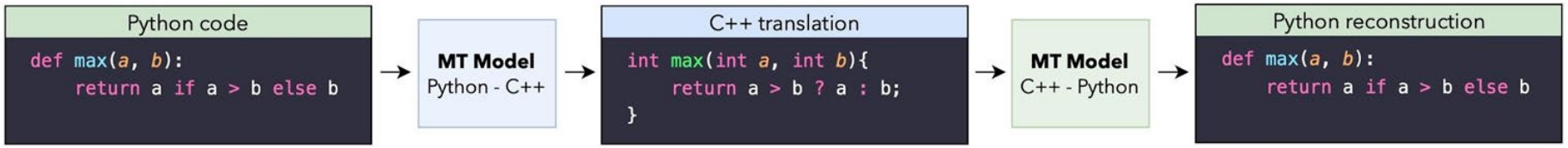


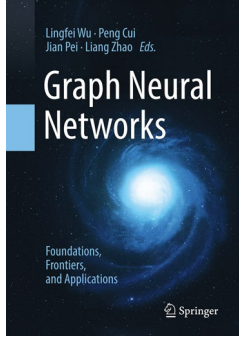
Case Study 4: Code Translation

Supervised setting: Tree-to-tree neural networks for program translation (Chen X et al,. 2018)

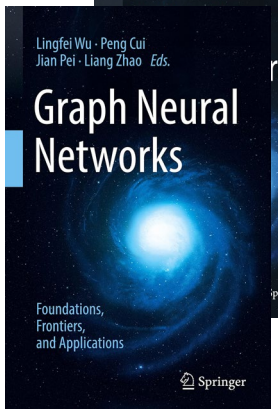


Unsupervised setting: Unsupervised Circle Translation (Roziere B et al,. 2020)





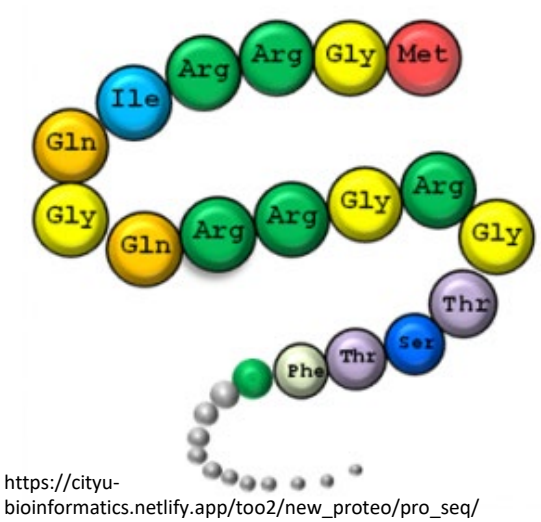
GNNs in Protein Modeling (Chapter 25)



From Protein Interactions to Function

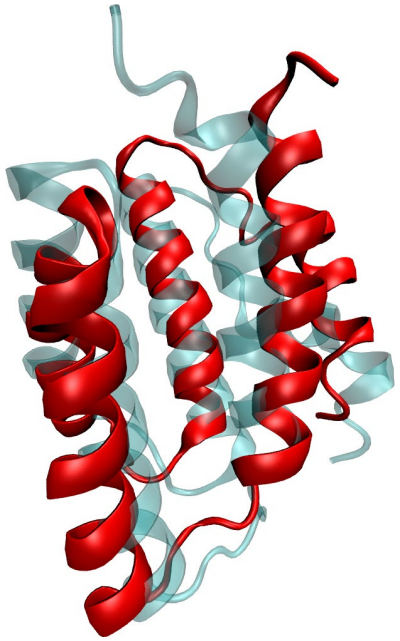
- Millions of protein products in database to be explored

  -----What function a protein molecule performs.

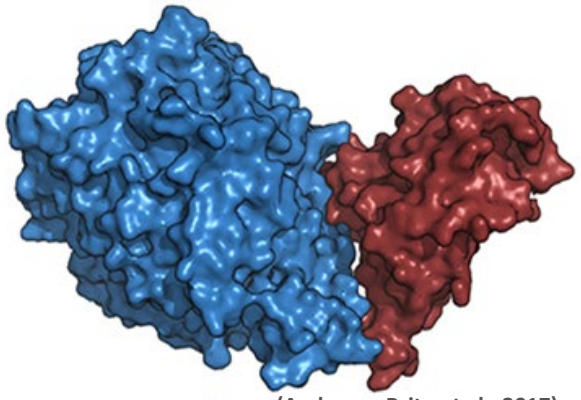


https://cityu-bioinformatics.netlify.app/too2/new_proteo/pro_seq/

Biological sequence



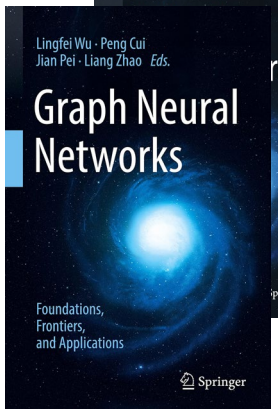
Protein structure



(Anderson Brito et al,. 2017)

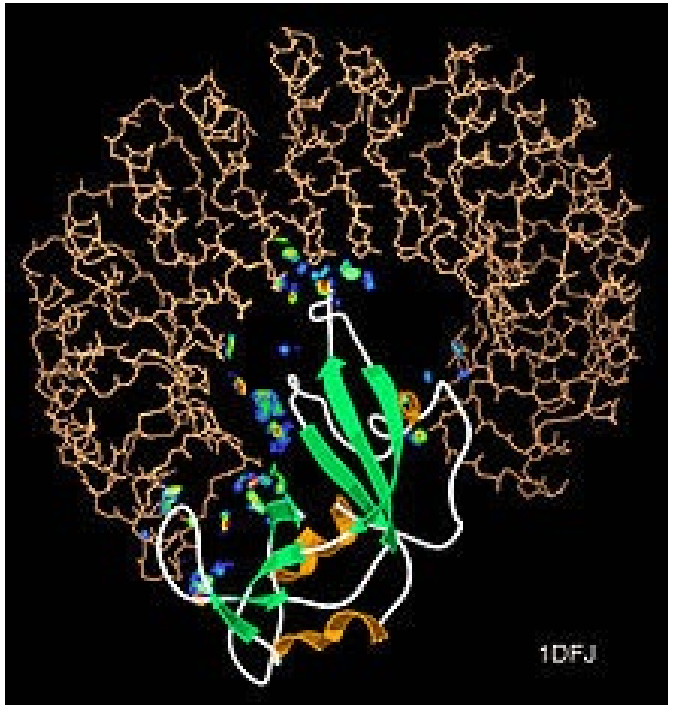
Protein Interaction

Protein-Protein Interaction Networks



PPI networks: edges denoting interacting protein nodes, of many species, such as human, yeast, mouse, and others, suddenly became available to researchers.

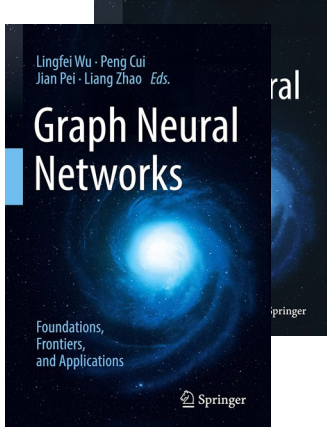
- few nodes to ten thousands of nodes



https://en.wikipedia.org/wiki/Protein%E2%80%93protein_interaction

Shehu A, Barbará D, Molloy K. A survey of computational methods for protein function prediction. InBig data analytics in genomics 2016 (pp. 225-298). Springer, Cham.

Problem Formulation(s), Assumptions, and Noise



What to predict with regards to protein function?

- PPI networks are incomplete: high type-I error, type-II error, and low inclusion

Problem formulation: predicting whether there exists a connection between two nodes in a PPI network (**link prediction**)

Protein function annotation schemes:

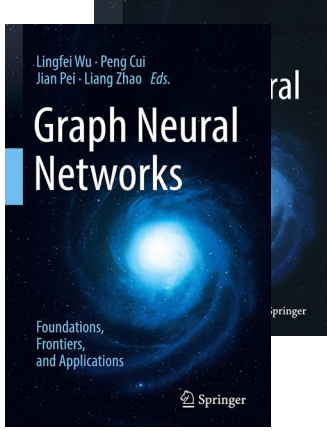
Gene Ontology (Lovell et al, 2003)

- Cellular Component (CC): describes the component or anatomical structure in a cell where a gene product operates.
- Biological Process (BP): captures the physiological description of protein function and allows specifying the processes in which a gene product participates in the cell.
- Molecular Function (MF): action of a single macromolecular machine, e.g., direct physical interactions with other molecular entities

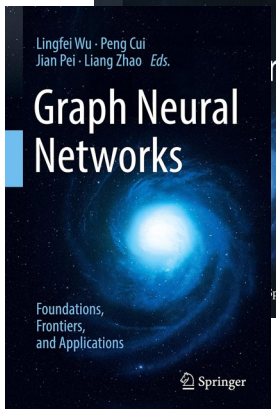
Shallow Machine Learning Models over the Years

Summary of performance of shallow models

Literature	Model	Dataset	Sensitivity (%)	Specificity (%)	Accuracy (%)
Chen and Liu (2005)	RF	*Saccharomyces cerevisiae*	79.78	64.38	NA*
Guo et al (2010)	SVM	Human	89.17	92.17	90.67
		Yeast	88.17	89.81	88.99
		Drosophila	99.53	80.65	90.09
		Escherichia coli	95.11	90.35	92.73
		Caenorhabditis elegans	96.46	98.55	97.51
Lin and Chen (2012)	Tree-Augmented Naïve Bayes (TAN)	Human	88	70	NA*
You et al (2015a)	RF	*Saccharomyces cerevisiae*	94.34	NA*	94.72
You et al (2015b)	SVM	*Saccharomyces cerevisiae*	85.74	94.37	90.06



GNN for Protein Interaction



Molecular-interaction graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, $A \in \mathbb{R}^{n \times n}$ connectivity of the proteins;

Proteins

Interactions among Proteins

Message passing for protein embedding :

$$H^{t+1} = F(H^t, P||A||L||X)$$

$$O = G(H, P||A||L||X)$$

Link prediction task:

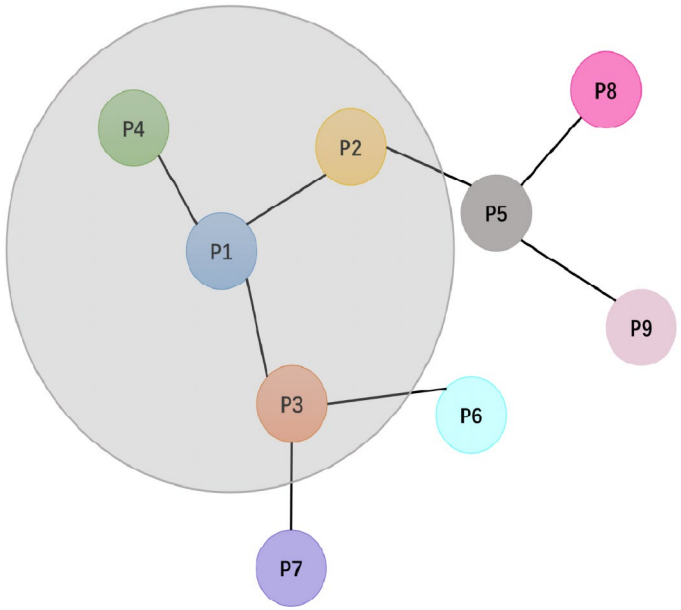
$p(A_{i,j}) \approx 1$ indicates there exists an interaction with high confidence;

$p(A_{i,j}) \approx 0$ indicates a low interaction confidence.

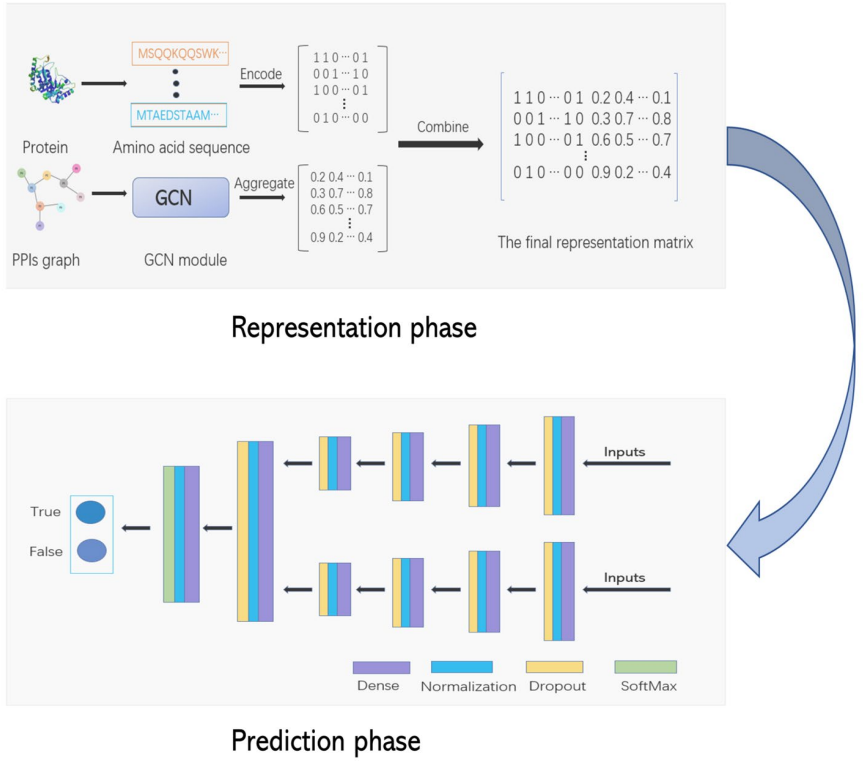
$$A' = DECODER(Z|P, A; \theta_{decoder})$$

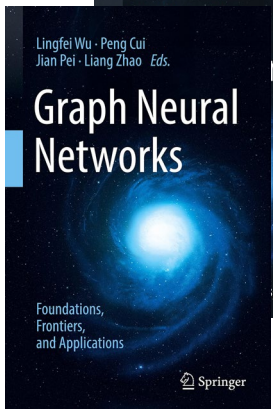
Automated Function Prediction (binary multi-label classification): interactions among m proteins

Case Study 1: Prediction of Protein-Protein and Protein-Drug Interactions: The Link Prediction Problem



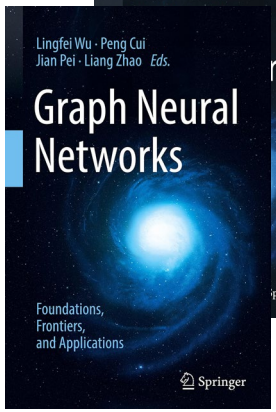
The PPIs networks: The vertex in the graph represents protein, and the edge between two vertexes represents the protein-protein interaction



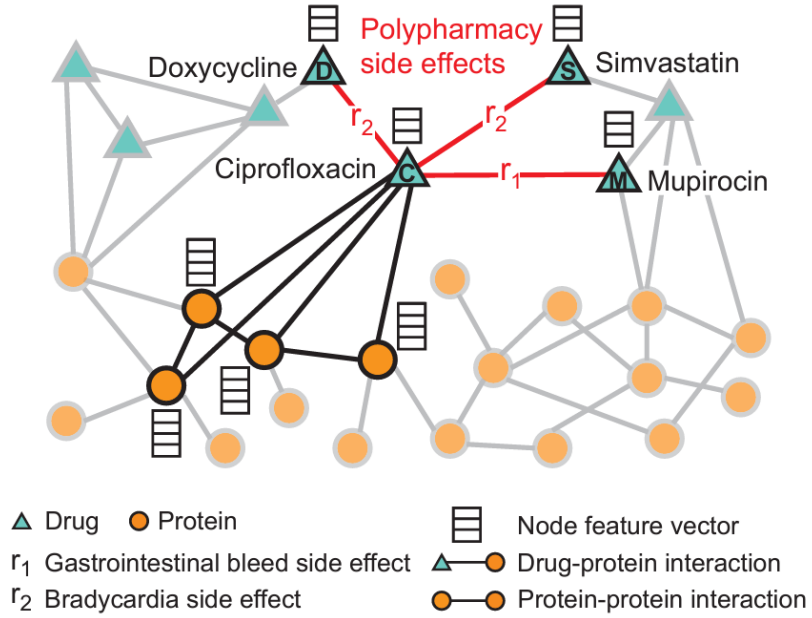


Liu L, Ma Y, Zhu X, et al (2019) Integrating sequence and network information to enhance protein-protein interaction prediction using graph convolutional networks. In: 2019 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), pp 1762–1768, DOI 10.1109/BIBM47256.2019.8983330

Case Study 1: Prediction of Protein-Protein and Protein-Drug Interactions: The Link Prediction Problem

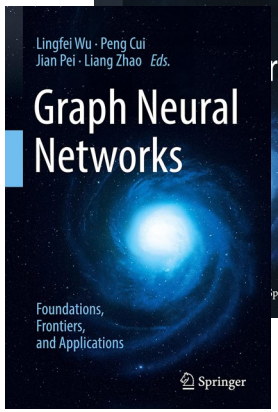


Modeling polypharmacy side effects with graph convolutional networks



Zitnik M, Agrawal M, Leskovec J (2018) Modeling polypharmacy side effects with graph convolutional networks. Bioinformatics 34(13):i457–i466

Case Study 1: Prediction of Protein-Protein and Protein-Drug Interactions: The Link Prediction Problem



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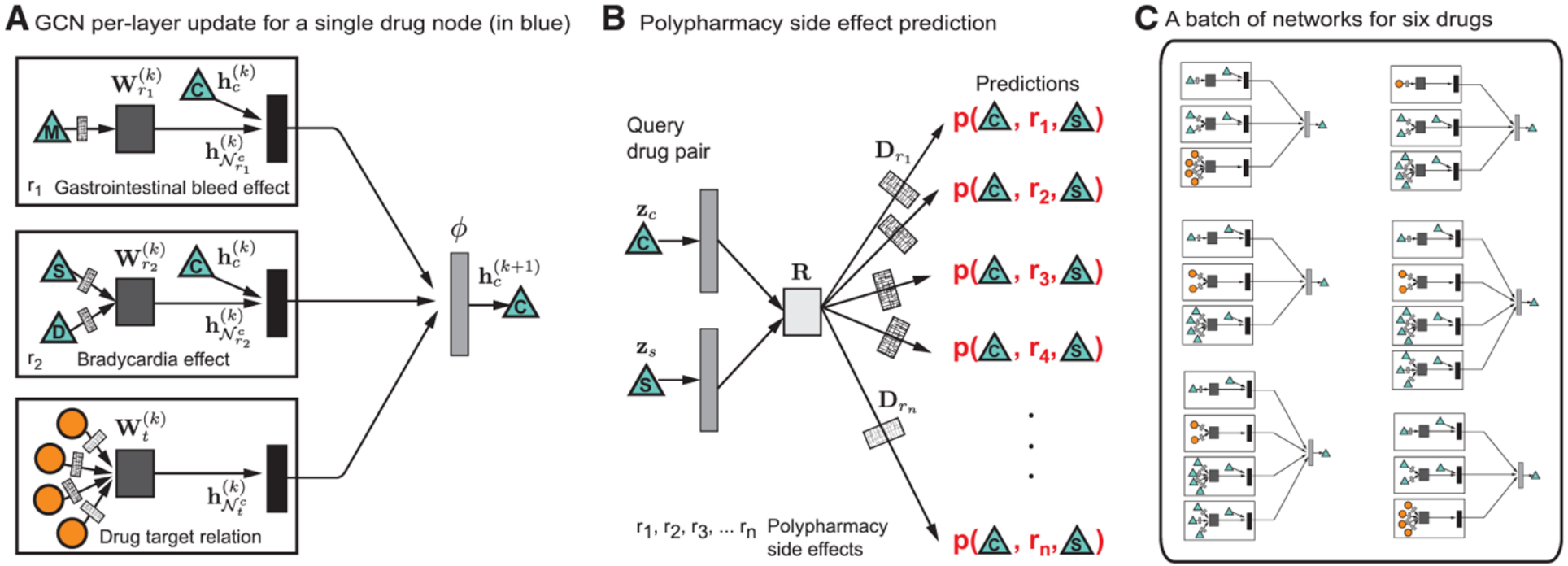
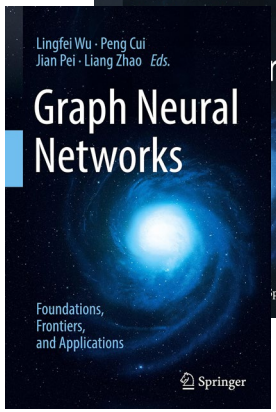
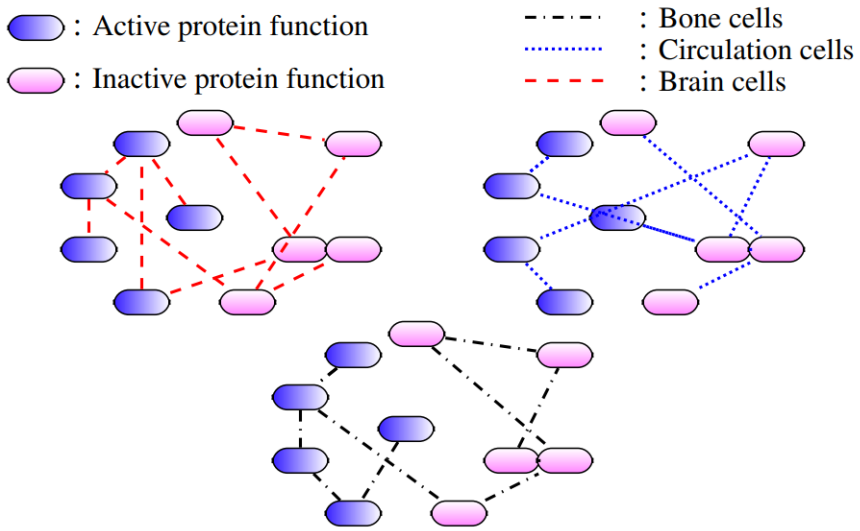


Zitnik M, Agrawal M, Leskovec J (2018) Modeling polypharmacy side effects with graph convolutional networks. Bioinformatics 34(13):i457–i466

Case Study 2: Prediction of Protein Function and Functionally-important Residues



Automated Function Prediction (AFP) : multilabel classification among several components



A multi-relational network of proteins.

neighborhood aggregation $H_{n,i}^{(l)} = \sum_{n' \in \mathcal{N}_n^{(i)}} S_{n,n',i} \check{Z}_{n',i}^{(l-1)}$

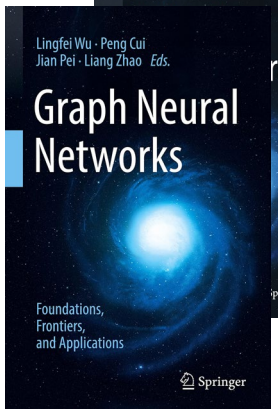
relation aggregation:

$$\mathbf{g}_{ni}^{(l)} := \sum_{i'=1}^{I} R_{ii'n}^{(l)} \mathbf{h}_{ni'}^{(l)} \quad \text{for all } n,$$

$$\underline{Z}_{inp}^{(l)} := \mathbf{g}_{ni}^{\top} \mathbf{w}_{nip}^{(l)}, \quad \text{for all } i, n, p,$$

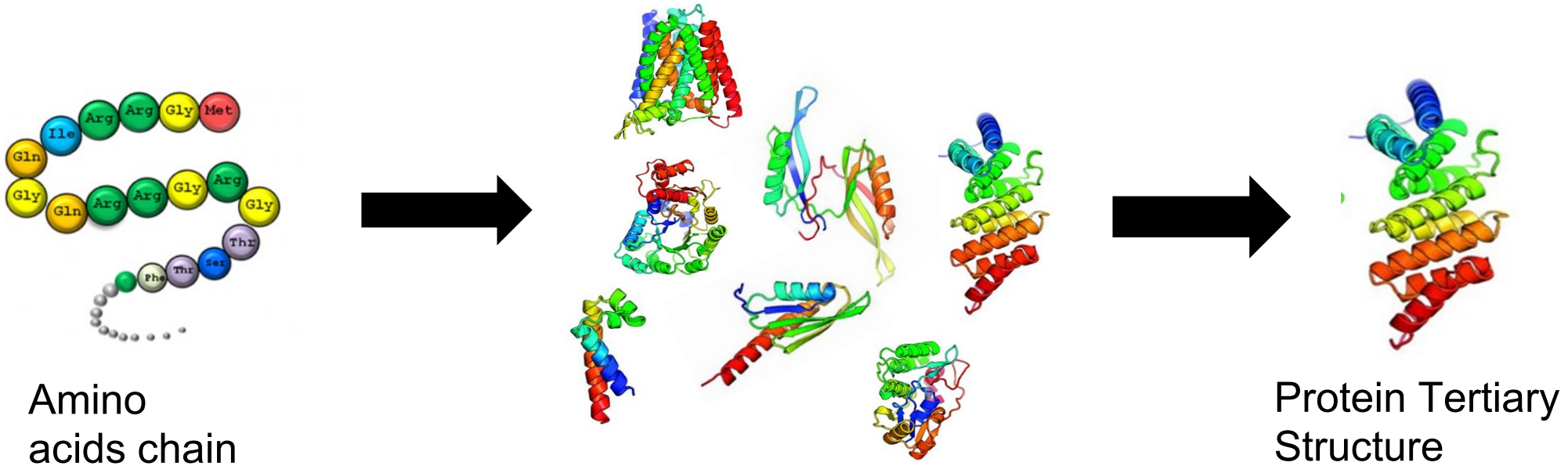
residual updating: $Z^{(l)} = f(Z^{(l-1)}; \theta_z^{(l)}) + f(X; \theta_x^{(l)})$

Ioannidis VN, Marques AG, Giannakis GB (2019) Graph neural networks for predicting protein functions. In: 2019 IEEE 8th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP), pp 221–225, DOI 10.1109/CAMSAP45676.2019.9022646



Case Study 3: De-novo protein generation

- **Protein structure prediction (PSP)** seeks to determine one or more biologically-active/native forms/structures of a protein molecule from the sequence of amino acids chain.

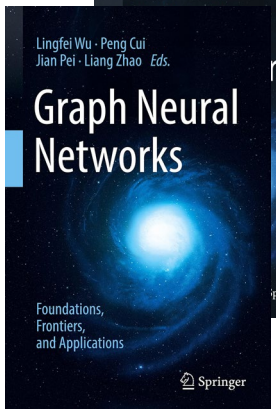


Amino acids chain

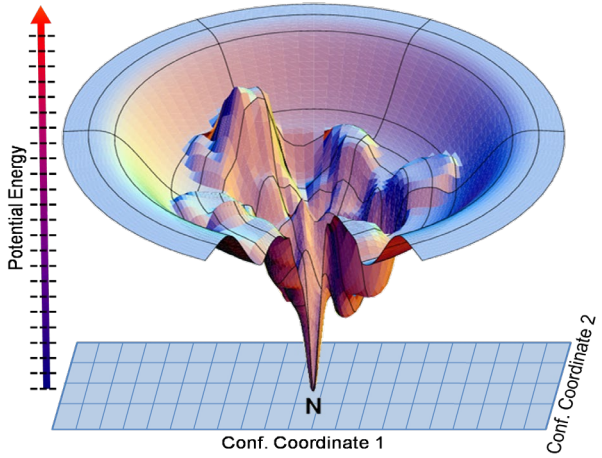
Protein Tertiary Structure

2^N complexity

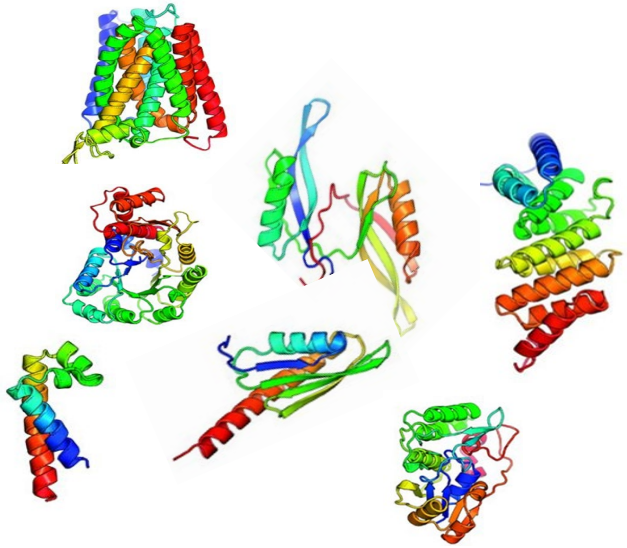
Case Study 3: De-novo protein generation



Given tertiary structures, can the model generate protein-like (physically realistic) tertiary structures without any particular amino acid sequence in mind?

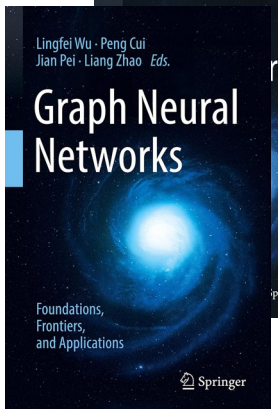


Protein structure space

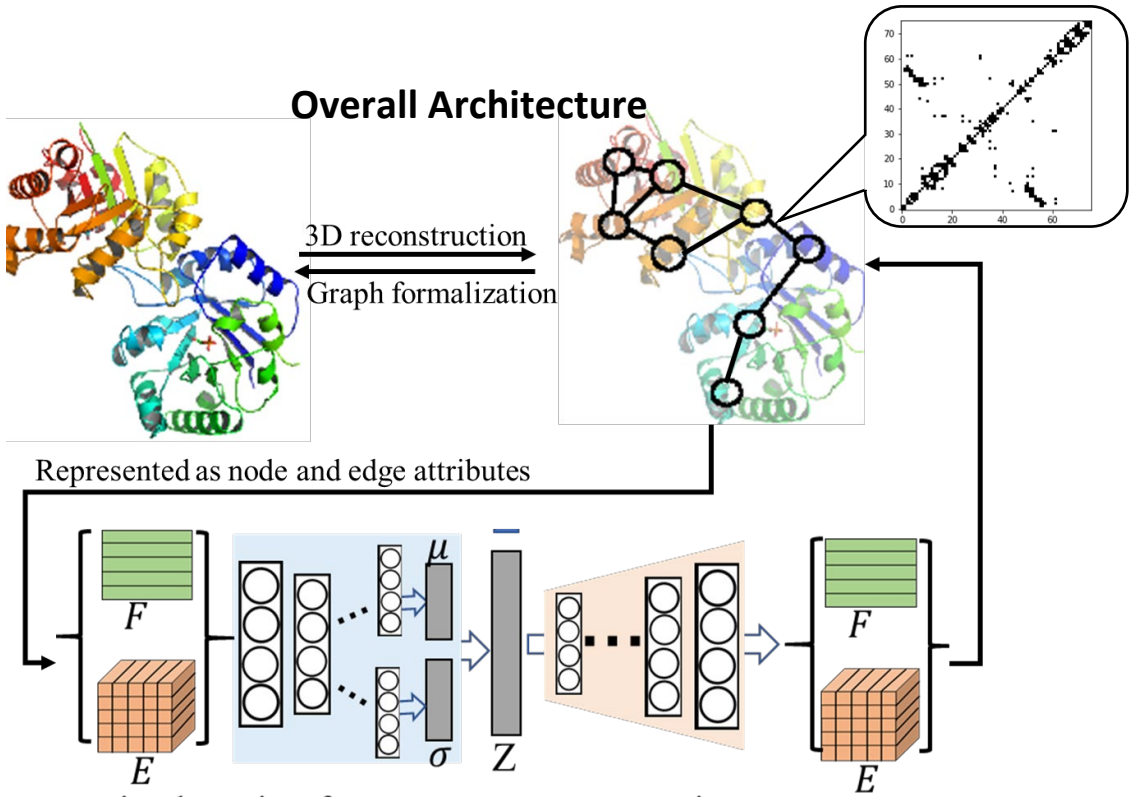


More various structures

Case Study 3: De-novo protein generation



Learning the protein structure distribution via Variational autoencoder



Protein contact graph: $G = (E, F)$

Objective function:

$$\ell = \mathbb{E}_{q(Z|F,E)}[\log p(E, F|Z)] - KL[q(Z|F, E)||p(Z)]$$

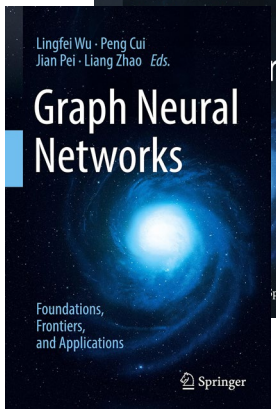
encoder

decoder

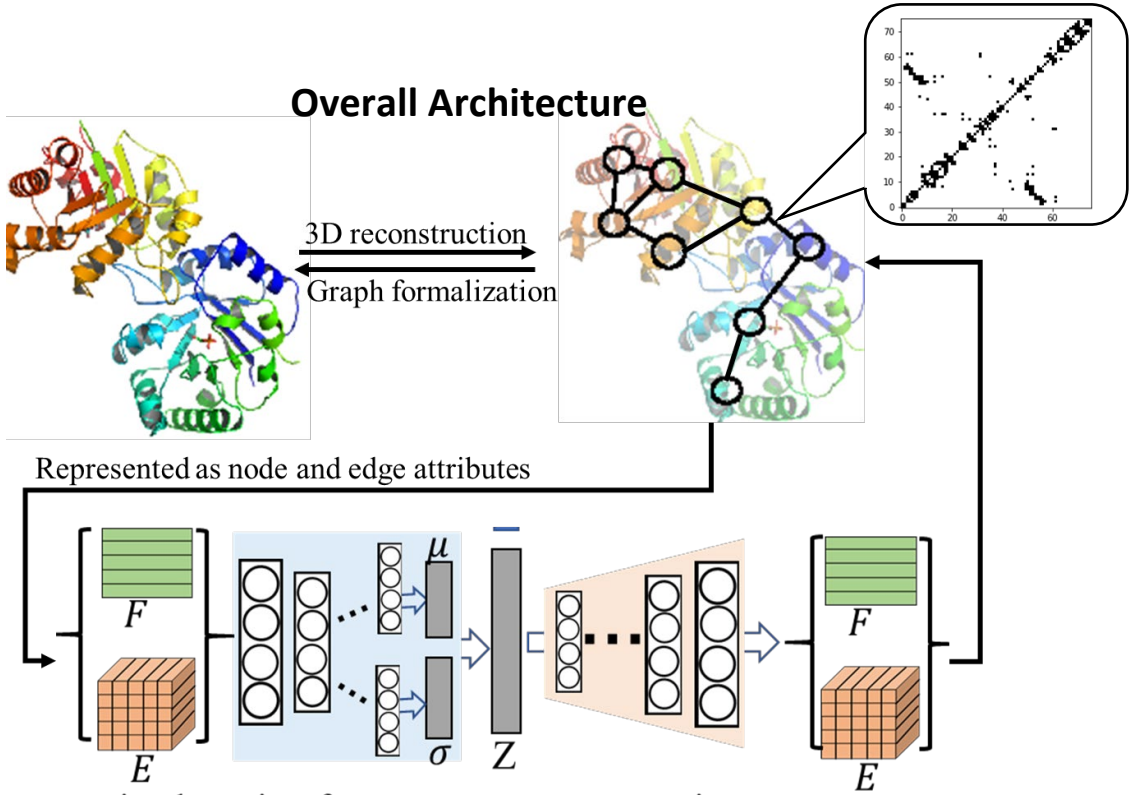
$$q(Z|F, E) = \prod_{i=1}^{N} q(z_i|F, E), \text{ where } q(z_i|F, E) = \mathcal{N}(z_i|\mu_i, \sigma_i^2),$$

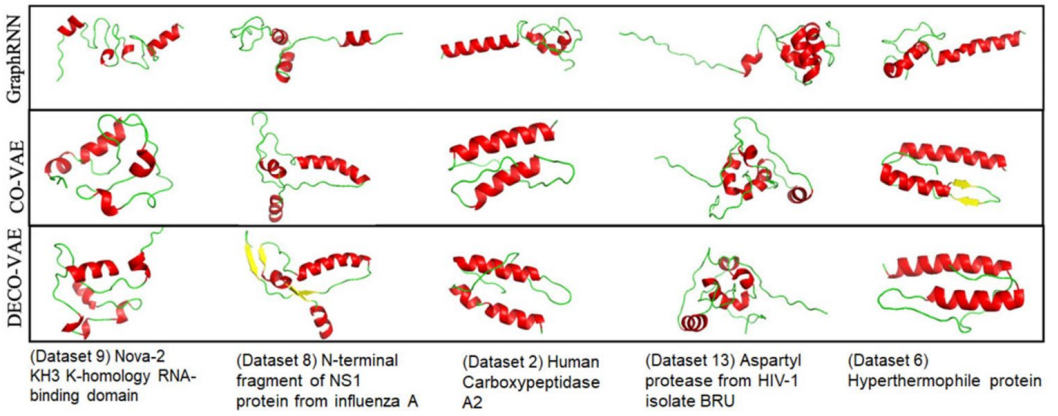
Guo X, Du Y, Tadepalli S, Zhao L, Shehu A. Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances. 2021;1(1):vbab036.

Case Study 3: De-novo protein generation



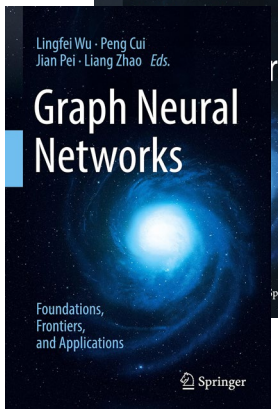
Learning the protein structure distribution via Variational autoencoder



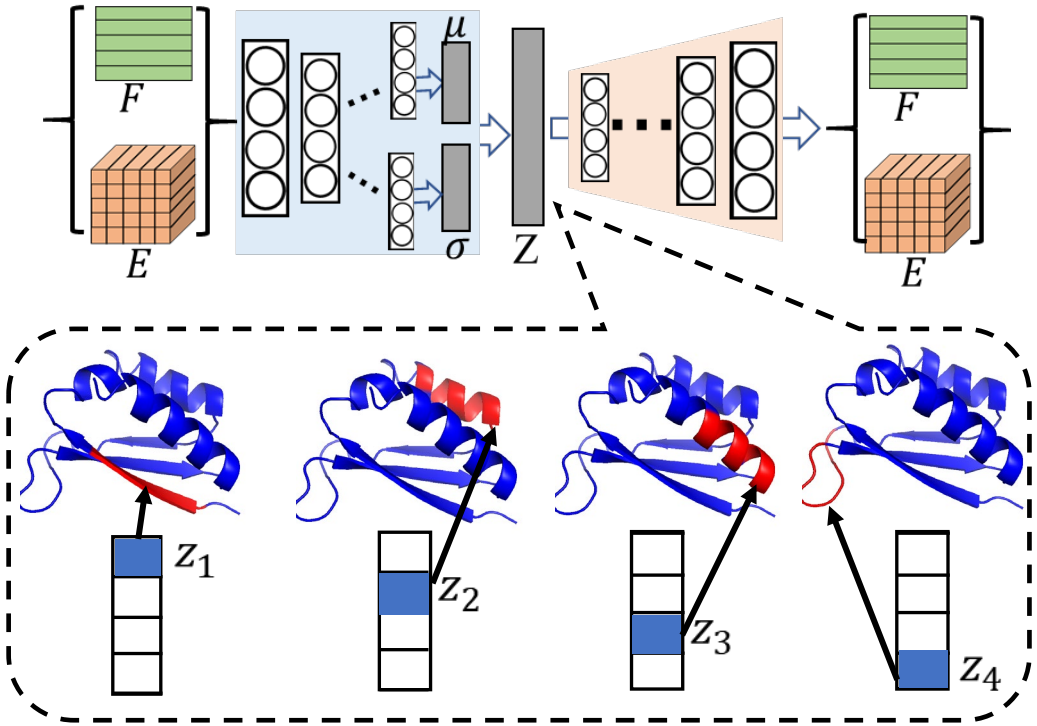


Guo X, Du Y, Tadepalli S, Zhao L, Shehu A. Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances. 2021;1(1):vbab036.

Case Study 3: De-novo protein generation



Interpretability Enhancement



Protein contact graph: $G = (E, F)$

Objective function:

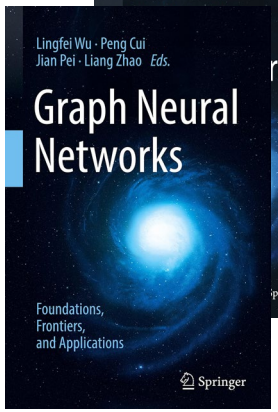
$$\ell = \mathbb{E}_{q(Z|F,E)}[\log p(E, F|Z)] - KL[q(Z|F, E)||p(Z)]$$

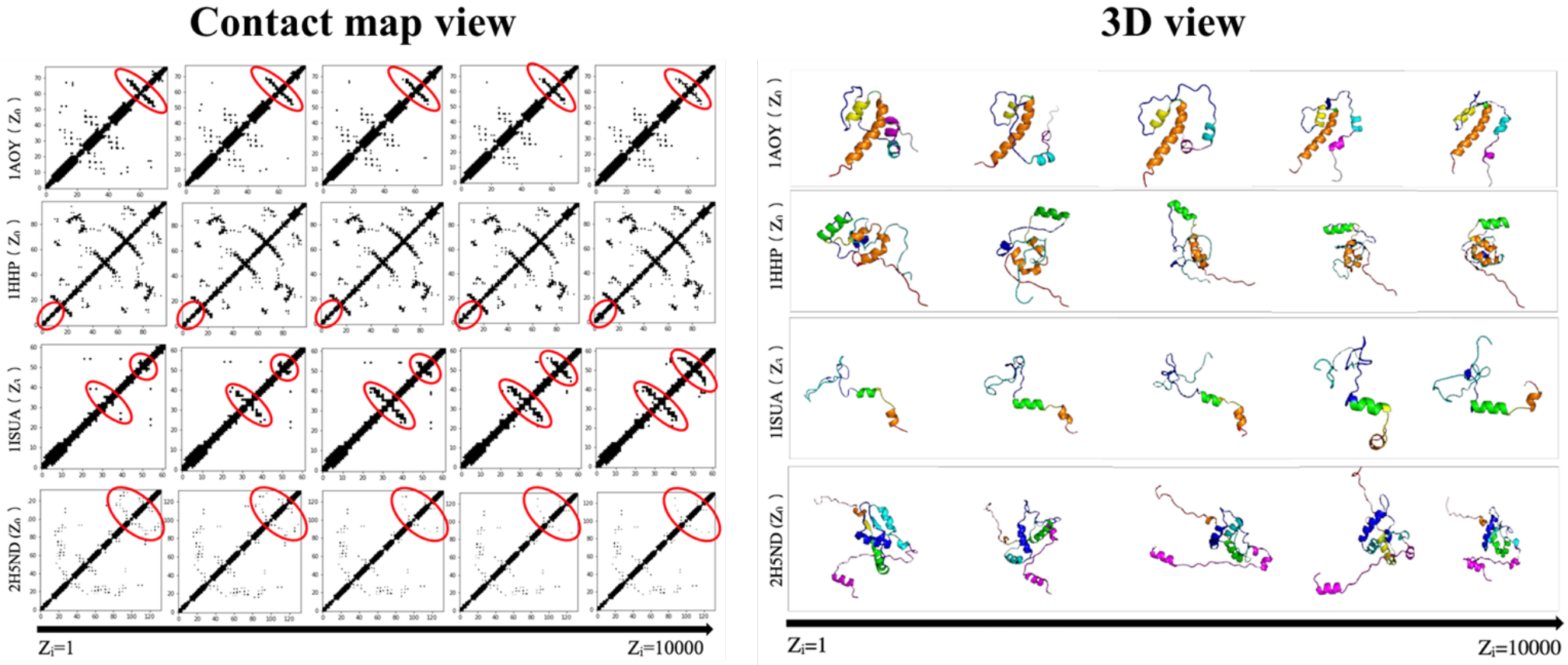
$$\Downarrow$$

$$\ell = \mathbb{E}_{q(Z|F,E)}[\log p(E, F|Z)] - \beta KL[q(Z|F, E)||p(Z)].$$

Guo X, Du Y, Tadepalli S, Zhao L, Shehu A. Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances. 2021;1(1):vbab036.

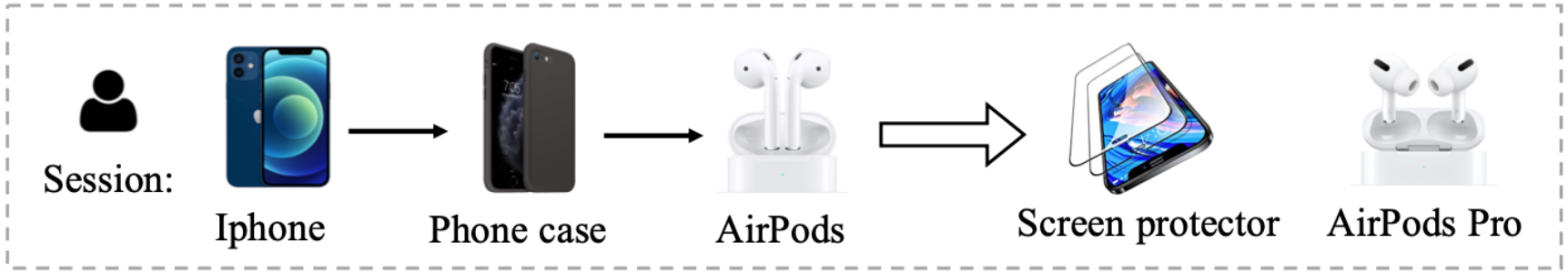
Case Study 3: De-novo protein generation

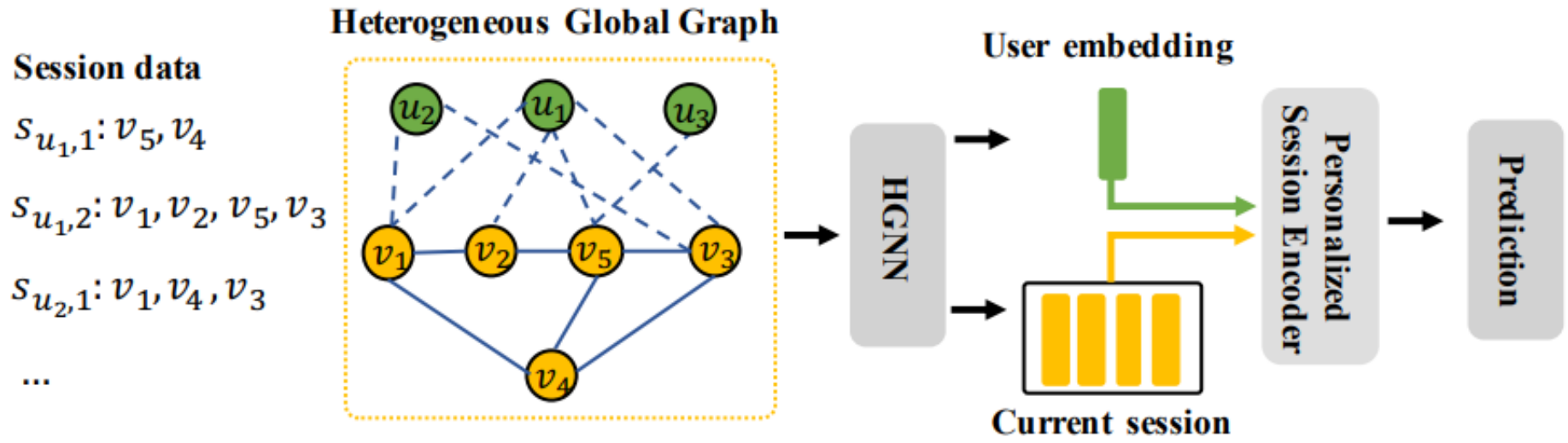


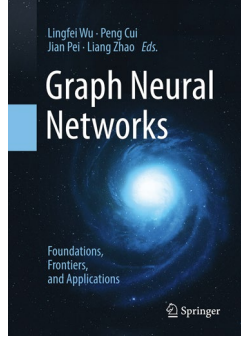


Guo X, Du Y, Tadepalli S, Zhao L, Shehu A. Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances. 2021;1(1):vbab036.

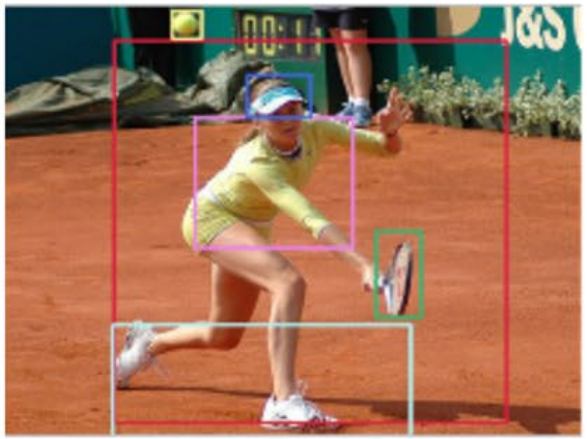
GNNs in Recommendation (Chapter 19)



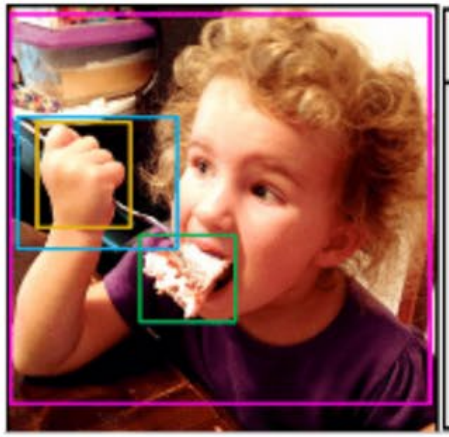


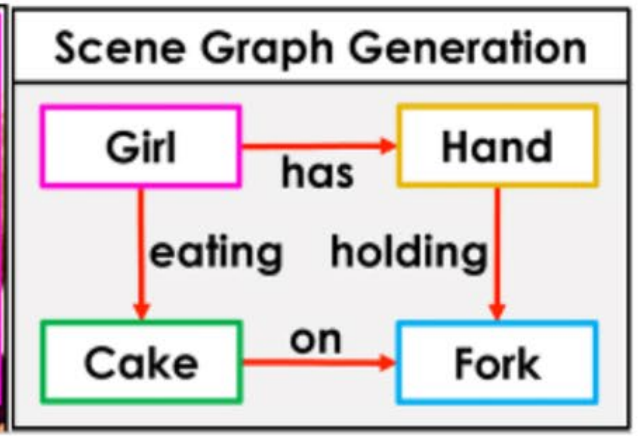


GNNs in Computer Vision (Chapter 20)

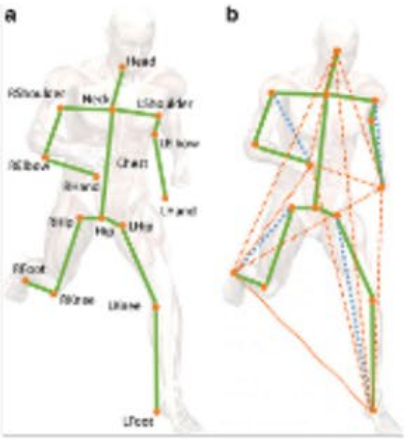


object detection

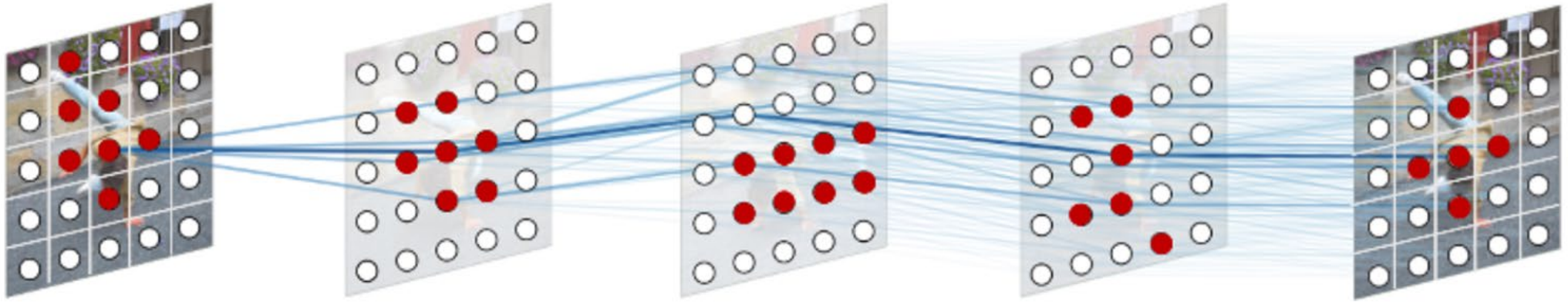




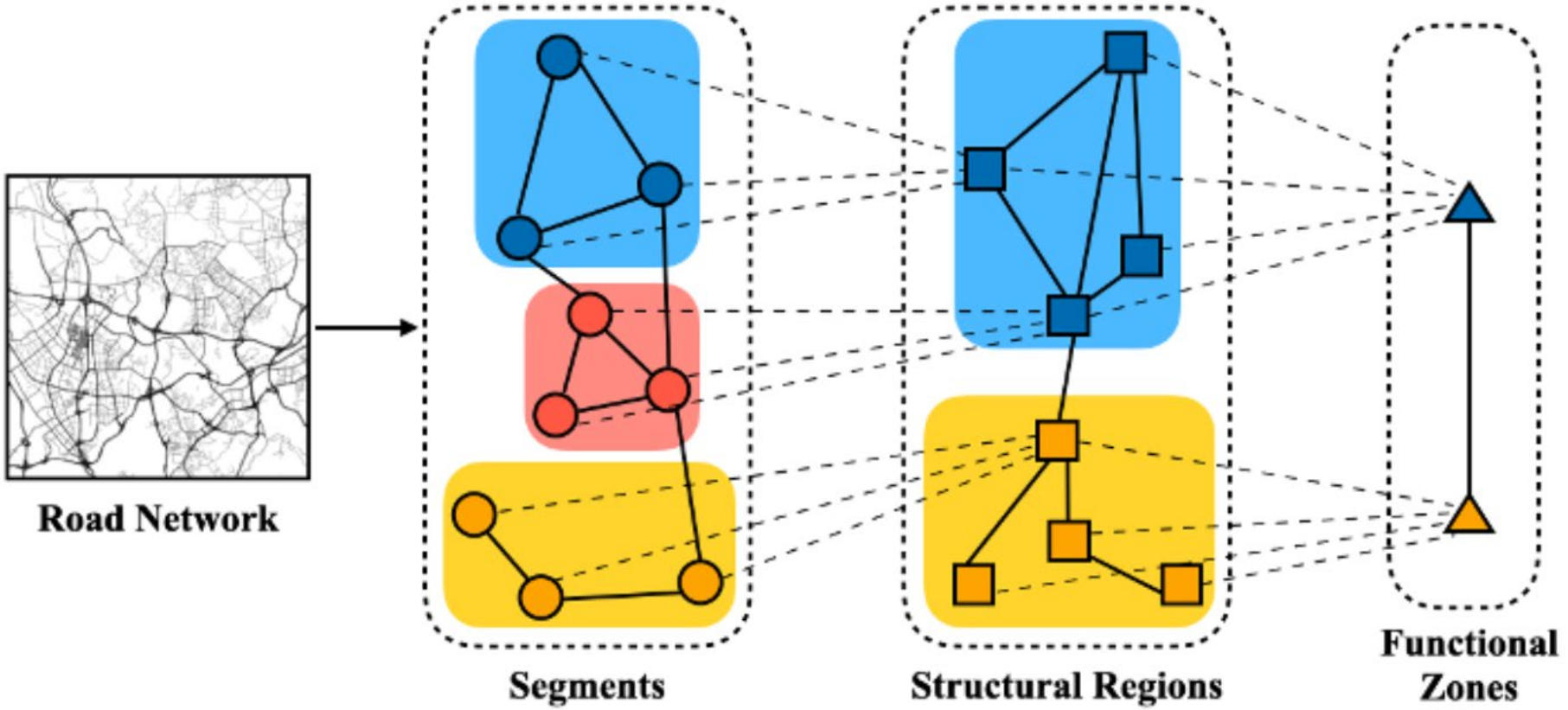
scene graph generation



skeleton



GNNs in Urban Intelligence (Chapter 27)



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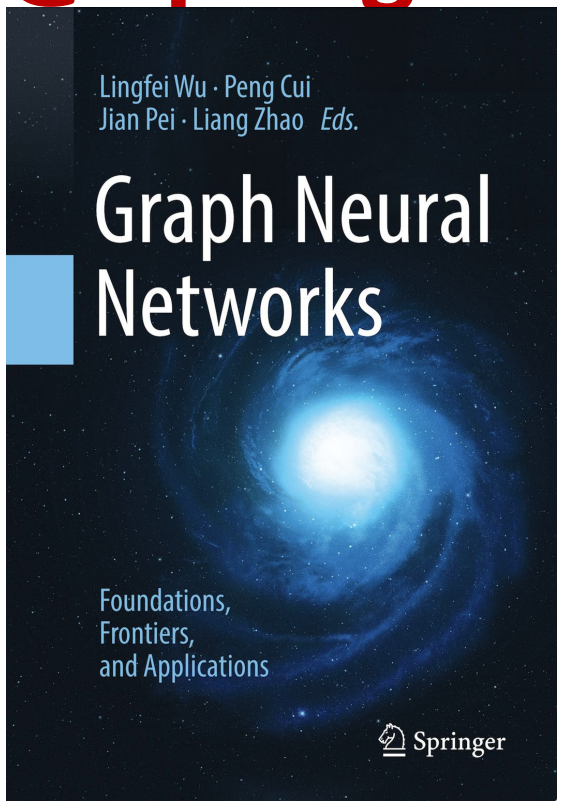

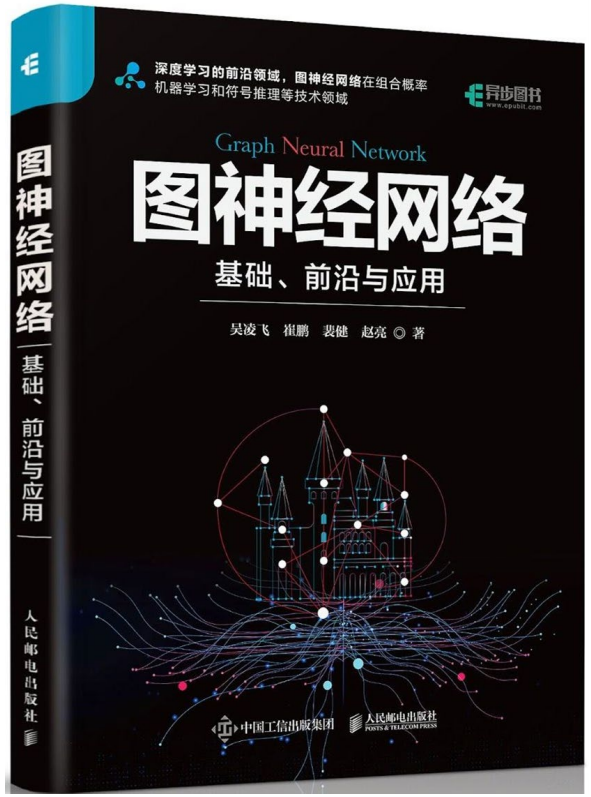

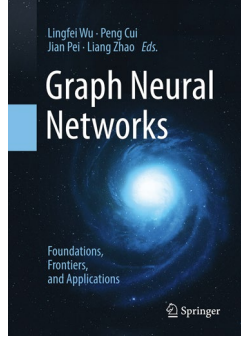

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The English version of the book is available for pre-order on Springer, Amazon and JD.COM !
The Chinese version (人民邮电出版社) will be officially published in August 2022!!

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2. Graph Representative Learning
3. Graph Neural Networks

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4. Graph Neural Networks for Node Classification
5. The Express Power of Graph Neural Networks
6. Graph Neural Networks: Scalability
7. Interpretability in Graph Neural Networks
8. Graph Neural Networks: Adversarial Robustness

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25. Graph Neural Networks in Predicting Protein functions and Interactions
26. Graph Neural Networks in Anomaly Detection
27. Graph Neural Networks in Urban Intelligence