Strategies for Pre-training Graph Neural Networks

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ICLR 2020

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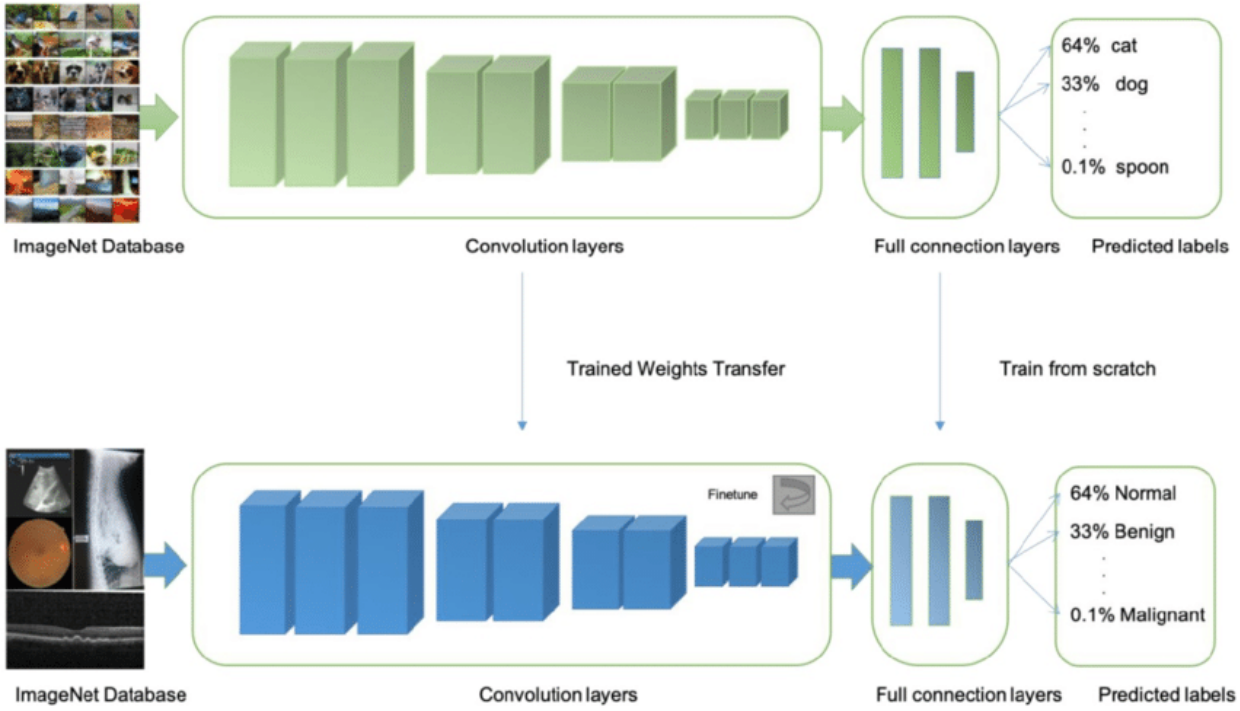
2020. 10. 20.

Transfer Learning (ImageNET, VGG, Resnet, BERT, GPT...)



https://www.researchgate.net/publication/336874848_Current_status_and_future_trends_of_clinical_diagnoses_via_image-based_deep_learning

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Challenges with Learning on Graph Data

1. Scarcity of labeled data

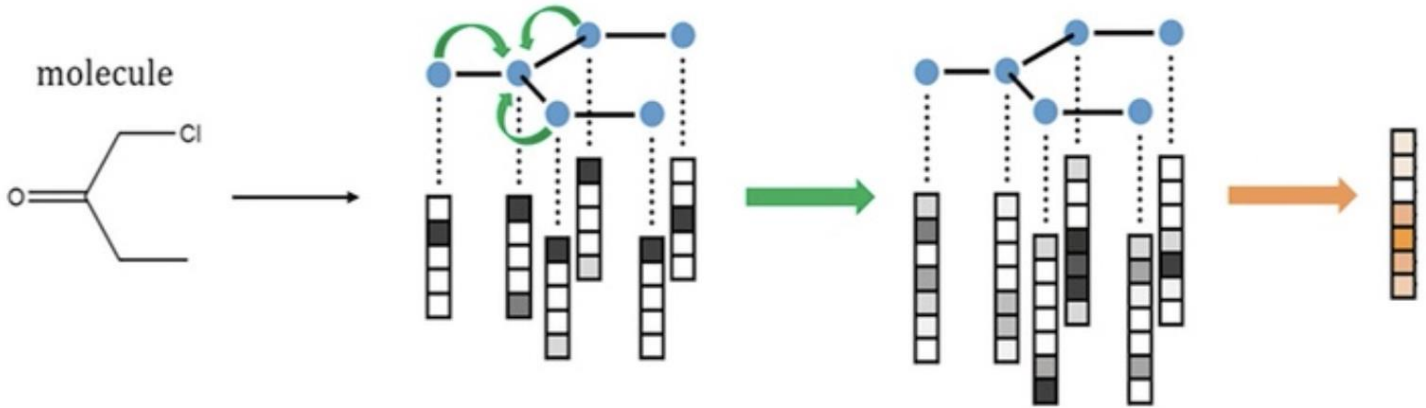
- ✓ Test examples tend to be very different from training examples.
- ✓ GNNs overfit to small training datasets.

2. Out-of-distribution Prediction

- ✓ Obtaining labels requires expensive lab experiments.
- ✓ GNNs extrapolate poorly.

Supervised Learning of Graphs

✓ To learn a representation vector h_G that predicts the label of a graph G.



Graph Neural Networks (GNNs)

- ✓ GNNs use the graph connectivity as well as node and edge features to learn a representation vector h_v for every node.

k-hop neighborhood

feature vector of edge between u and v

$$h_v^{(k)} = \text{COMBINE}^{(k)}\left(h_v^{(k-1)}, \text{AGGREGATE}^{(k)}\left(\left\{\left(h_v^{(k-1)}, h_u^{(k-1)}, e_{uv}\right): u \in \mathcal{N}(v)\right\}\right)\right)$$

representation of node v at the k-th iteration

set of neighbors of v

Graph Representation Learning

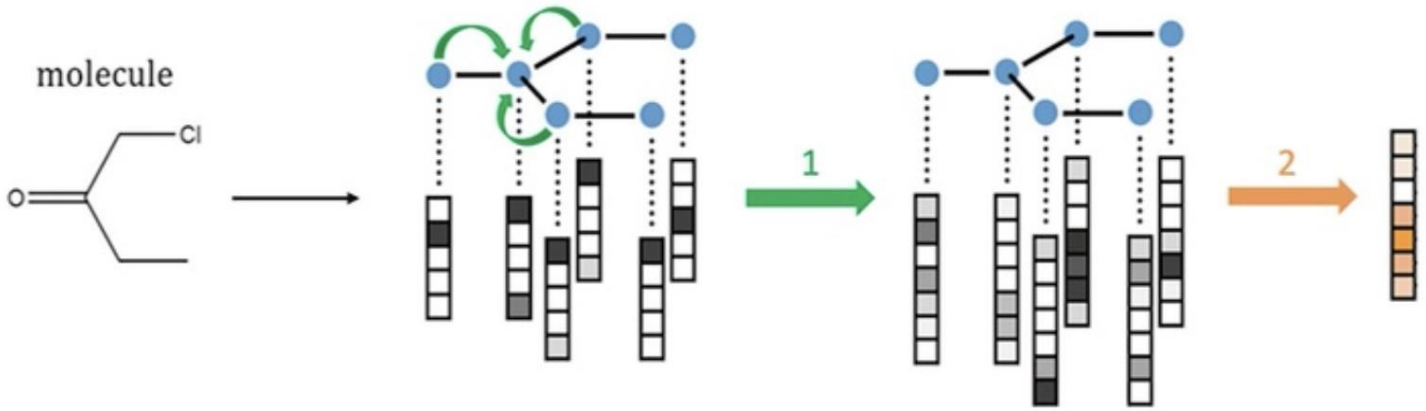
✓ The READOUT function pools node features from the final iteration *K* to obtain the entire graph's representation h_G.

permutation-invariant function

$$h_G = \mathrm{READOUT}\left(\left\{h_v^{(K)} \mid v \in G\right\}\right)$$

graph representation

Graph Representation Learning

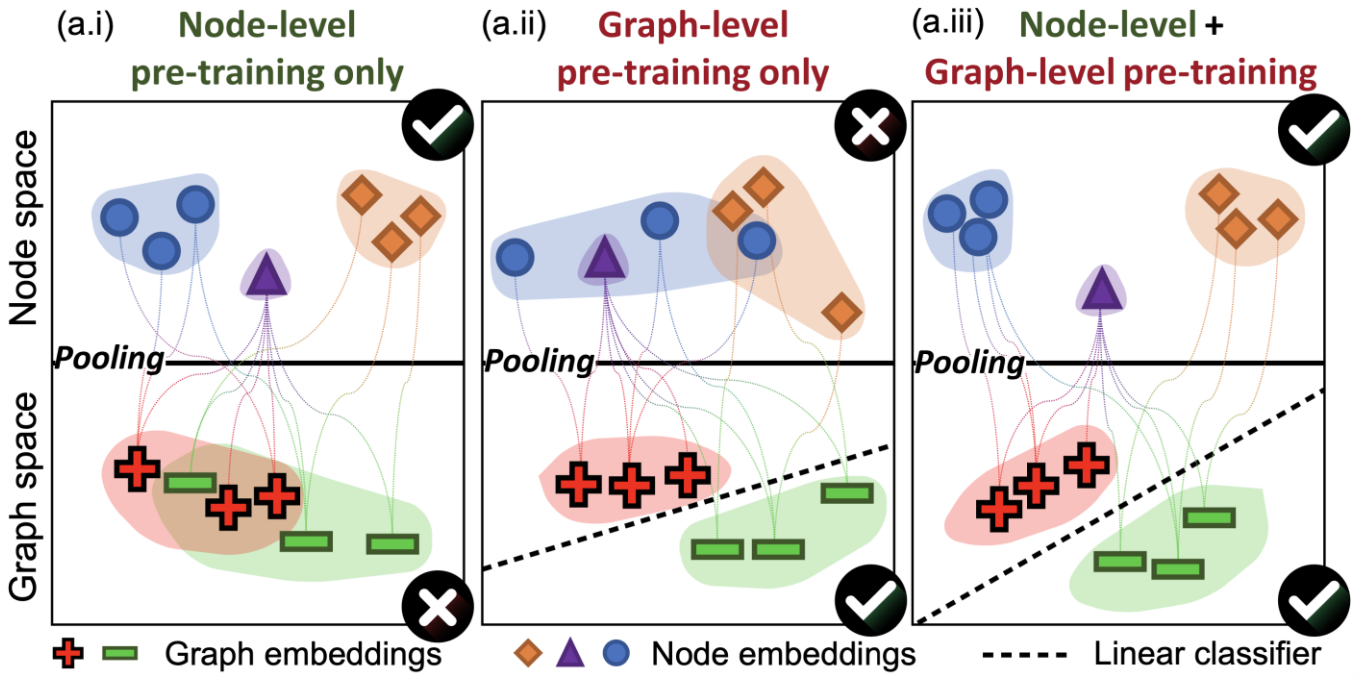


1. Iteratively aggregating neighboring information to obtain node embeddings.

2. Pooling node embeddings to obtain graph embedding.

Strategies for Pre-training GNNs

✓ **Key idea:** Pre-train both **node** and **graph** embeddings.



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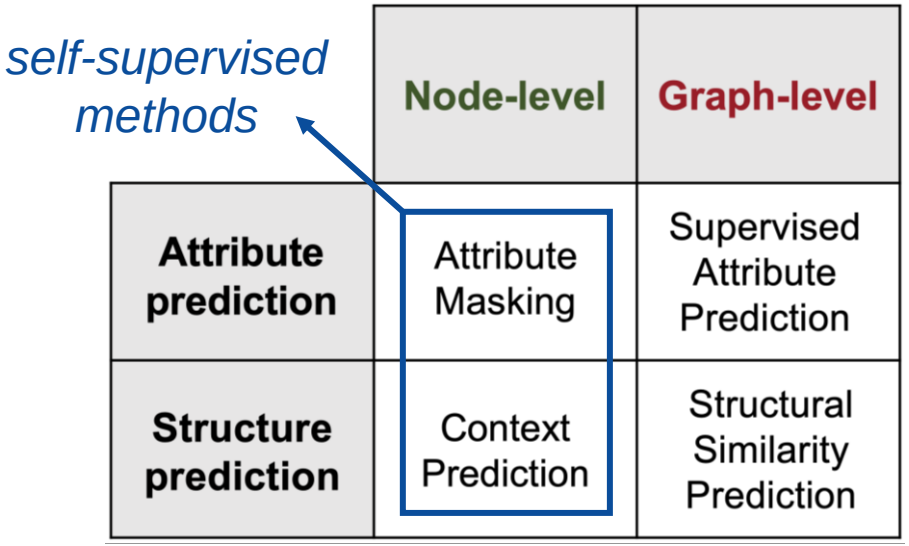


Node-level Pre-training

✓ To use easily-accessible unlabeled data to capture domain-specific knowledge/regularities in the graph.

❑ **Context Prediction**: Exploiting Distribution of Graph Structure

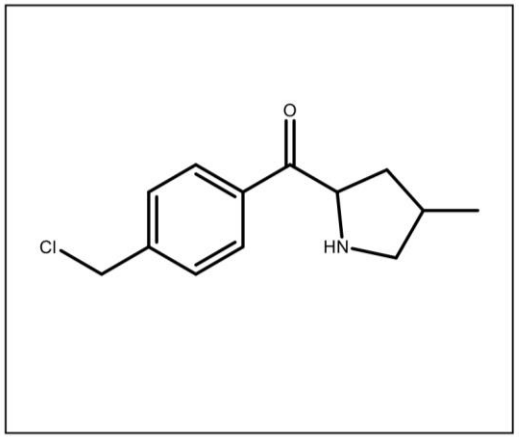
- ✓ To use subgraphs to predict their surrounding graph structures.
- ✓ Mapping nodes appearing in similar structural contexts to nearby embeddings.

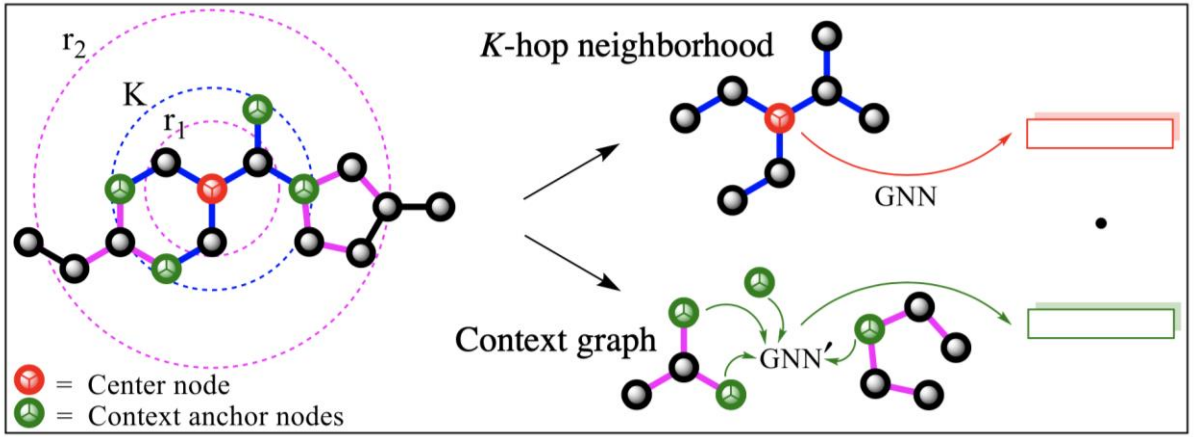
❑ **Attribute Masking**: Exploiting Distribution of Graph Attributes

- ✓ To capture domain knowledge by learning the regularities of the node/edge attributes distributed over graph structure.

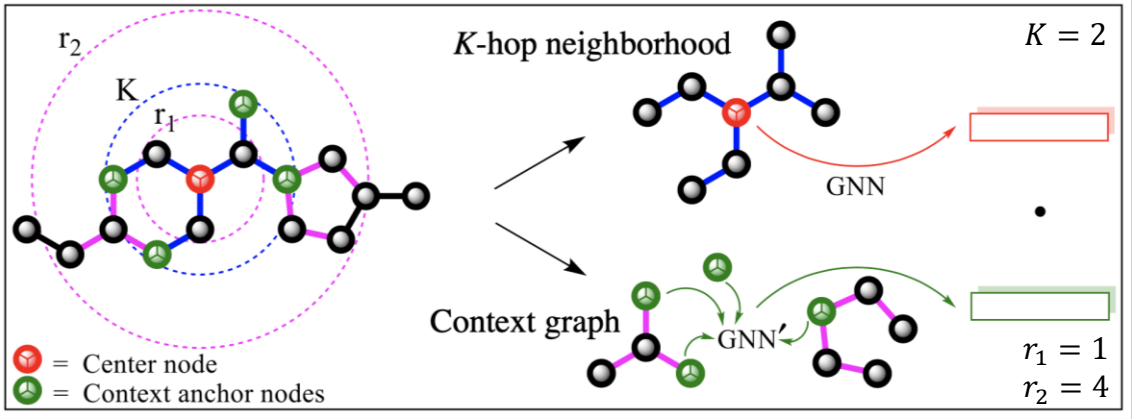
Neighborhood and Context Graphs

- ✓ To pre-train a GNN so that it maps nodes appearing in similar structural contexts to nearby embeddings.





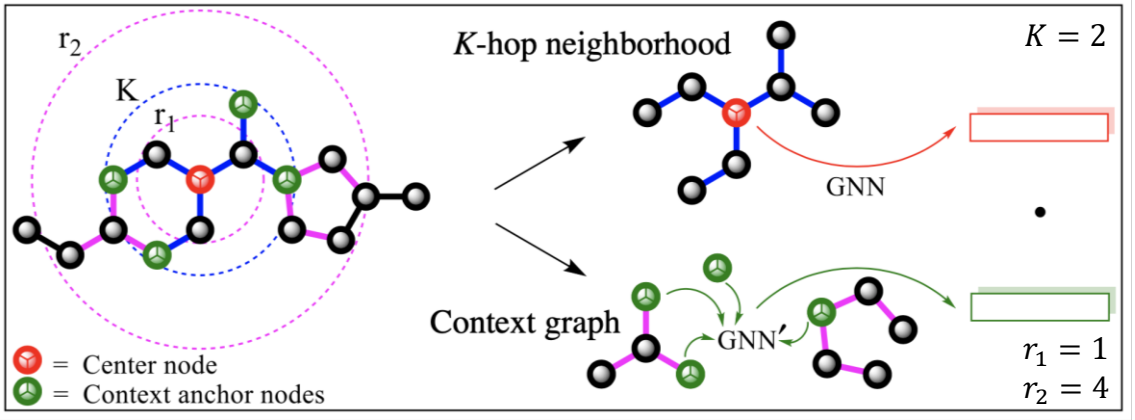
Neighborhood Graphs



✓ Motivated by *K*-layer GNN aggregation.

✓ *K*-hop neighborhood contains all nodes and edges that are at most *K*-hops.

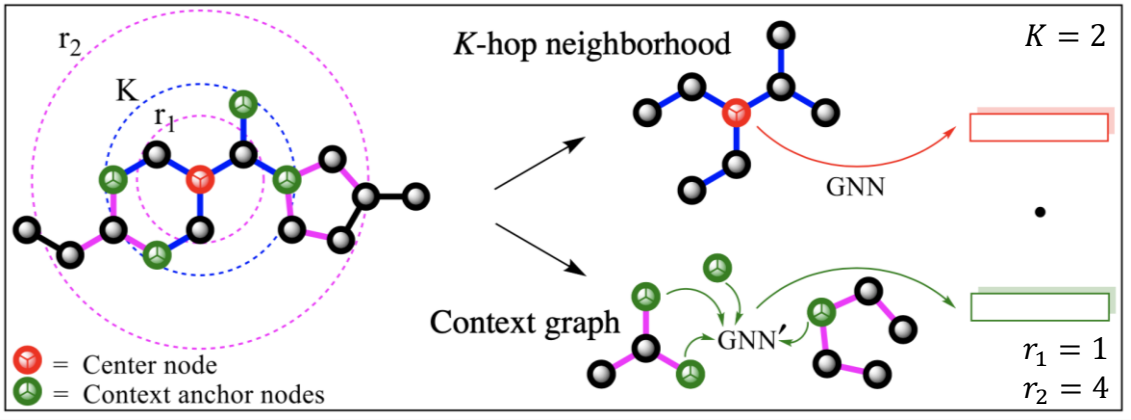
Context Graphs



✓ Context graph of v as graph structure that surrounds v's neighborhood.

✓ Context graph is a subgraph that is between r_1-hops and r_2-hops.

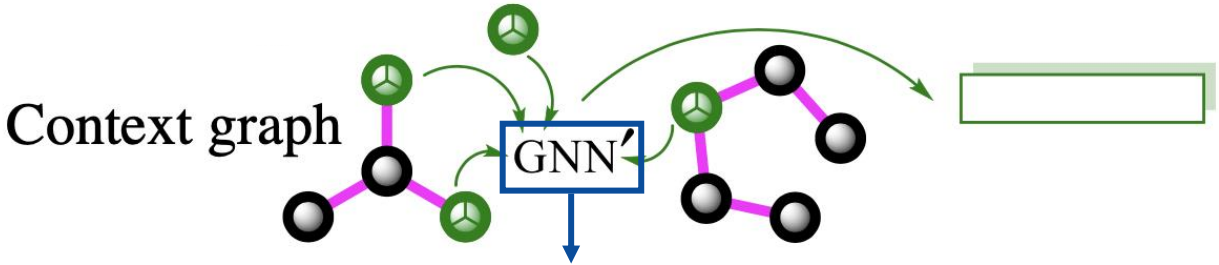
Context Anchor Nodes



- ✓ Context anchor nodes are shared between the neighborhood and the context graph.
- ✓ Context anchor nodes provide information about how the neighborhood and context graphs are connected with each other.

Encoding context into a fixed vector using an auxiliary GNN

- ✓ Directly predicting the context graph is intractable.
- ✓ To encode context graph as *fixed-length vectors* for context prediction.
- ✓ To average embeddings of *context anchor nodes* to obtain a *fixed-length context embedding* c_v^G.



Learning via Negative Sampling

- ✓ The learning objective of Context Prediction is a binary classification of whether a particular neighborhood and a particular context graph belong to the same node.

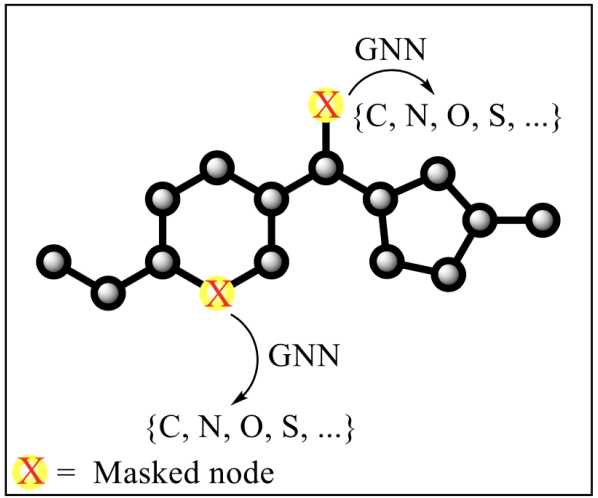
node embedding *indicator function*

$$\sigma\left(h_v^{(K)\top} c_{v'}^{G'}\right) \approx \mathbf{1}\{v \text{ and } v' \text{ are the same nodes}\}$$

sigmoid function *context embedding*

Masking node and Edges Attributes

- ✓ Masking node/edge attributes and let GNNs predict attributes based on neighboring structure.
- ✓ Beneficial for richly-annotated graphs from scientific domains.

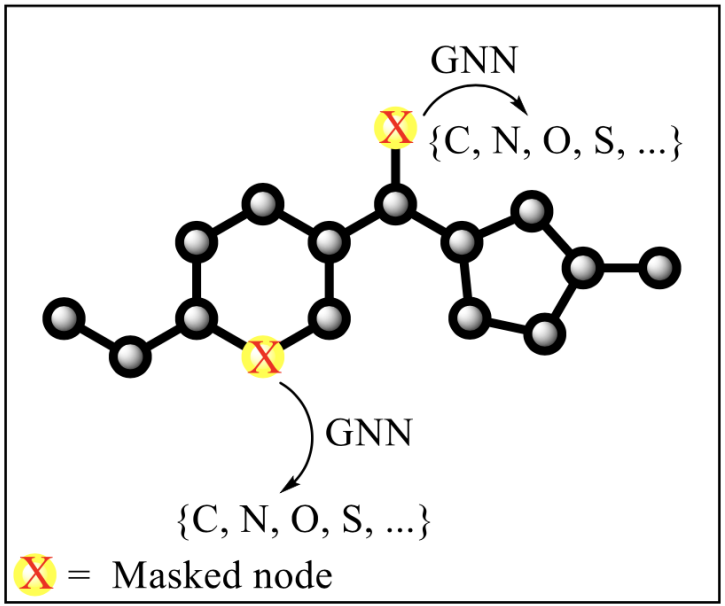


Masking node and Edges Attributes

1. Mask node/edge attributes.

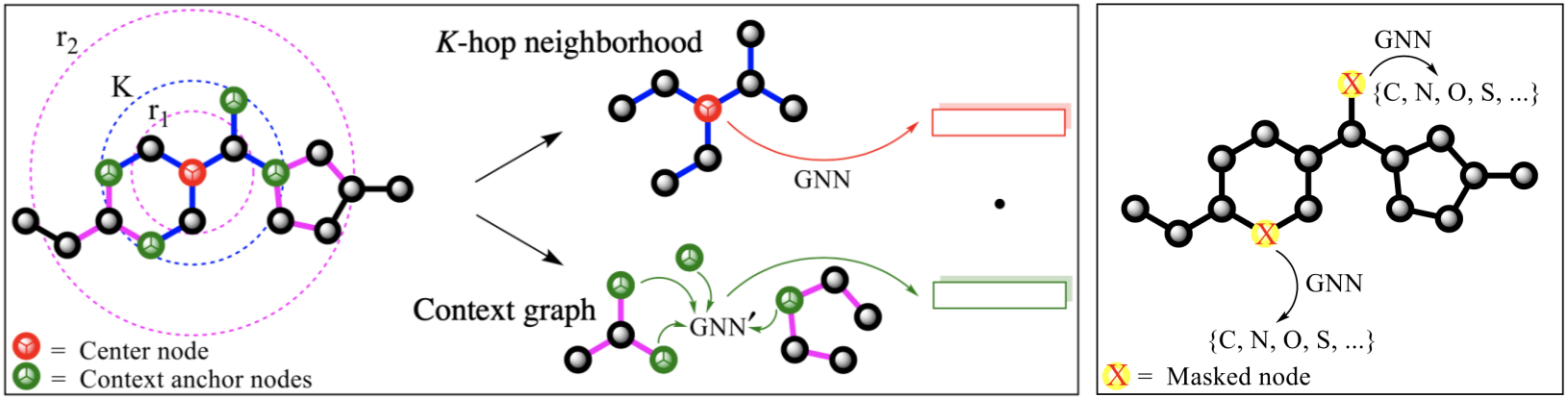
2. Obtain the corresponding node/edge embedding applying GNN.

3. Predict a masked node/edge attribute from a linear model that is applied on top of embeddings.



Node-level Pre-training

- ✓ To use easily-accessible unlabeled data to capture domain-specific knowledge/regularities in the graph.



Graph-level Pre-training

✓ To generate useful graph embeddings composed of the meaningful node embeddings obtained by node-level pre-training.

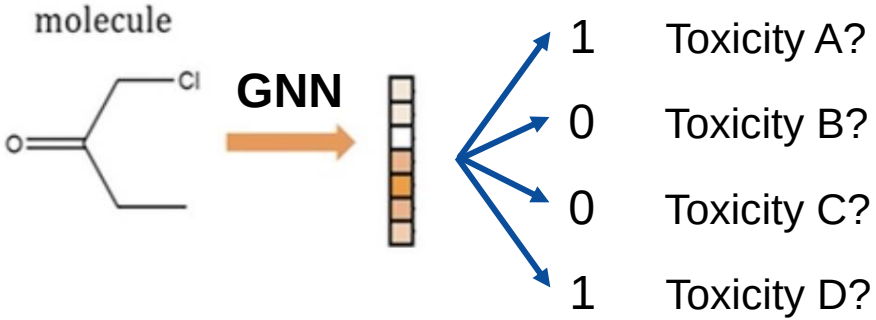
	Node-level	Graph-level
Attribute prediction	Attribute Masking	Supervised Attribute Prediction
Structure prediction	Context Prediction	Structural Similarity Prediction

Making predictions about domain-specific attributes of entire graphs.

Making predictions about graph structure.

Supervised Graph-level Property Prediction

- ✓ Inject graph-level domain-specific knowledge into our pretrained embeddings by defining supervised graph-level prediction tasks.
- ✓ Graph-level multi-task supervised pre-training to jointly predict a diverse set of supervised labels of individual graphs



Negative Transfer

- ✓ Naively performing the extensive multi-task graph-level pre-training alone can fail to give transferable graph-level representations.

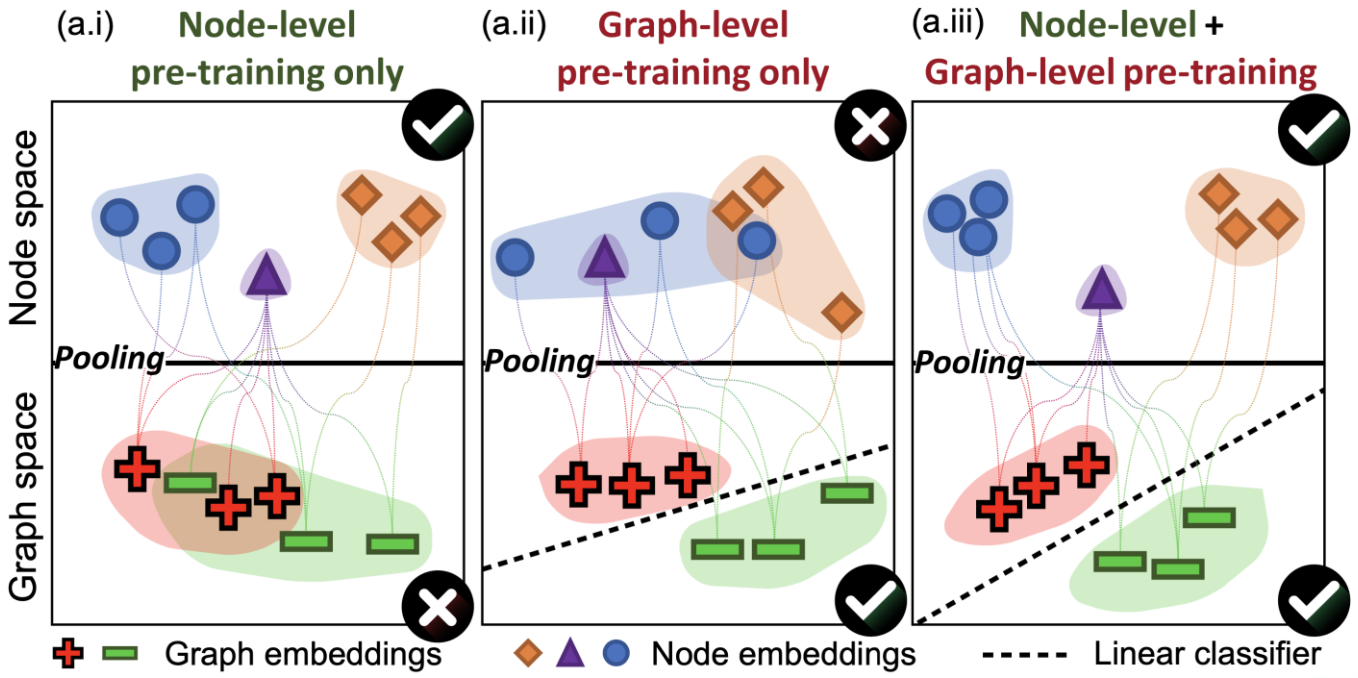
- ✓ To select "truly-relevant" supervised pre-training tasks.

  → selecting the relevant task requires significant domain expertise.

- ✓ To first **regularize** GNNs at the level of individual nodes via node-level pre-training methods before performing graph-level pre-training.

Strategies for Pre-training GNNs

✓ **Key idea:** Pre-train both **node** and **graph** embeddings.



Structural Similarity Prediction

- ✓ To define a graph-level predictive task where the goal would be to model the structural similarity of two graphs.
- ✓ However, finding the ground truth graph distance values is a difficult problem, and in large datasets there is a quadratic number of graph pairs to consider.

future work...

Pre-training GNNs and Fine-tunning for Downstream Tasks

1. **Node-level** self-supervised pre-training on unlabeled data

2. **Graph-level** multi-task supervised pre-training on labeled data

3. **Fine-tune** on downstream data (add linear classifiers)

Experiments

Pre-training Datasets

❑ For the Chemistry Domain

- ✓ 2 million unlabeled molecules sampled from the ZINC15 database.
- ✓ 456K molecules with 1310 kinds of diverse and extensive biochemical assays.

❑ For the Biology Domain

- ✓ 395K unlabeled protein ego-networks derived from PPI networks of 50 species.
- ✓ 88K labeled protein ego-network to jointly predict 5000 coarse-grained biological.

Downstream Classification Datasets

❑ For the Chemistry Domain

- ✓ 8 binary classification tasks
- ✓ scaffold split

❑ For the Biology Domain

- ✓ 40 binary classification tasks
- ✓ species split

Experimental Setup

❑ GNN architectures

- ✓ mainly study Graph Isomorphism Networks(GINs, 2019)
- ✓ GCN(2016), GraphSAGE(2017) and GAT(2019)
- ✓ 5 GNN layers($K = 5$)
- ✓ Average pooling for the READOUT function

❑ Pre-training

- ✓ Molecular networks ($r_1 = 4, r_2 = 7$)
- ✓ PPI networks ($r_1 = 1, r_2 = 4$)
- ✓ 3 GNN layers to encode the context structure
- ✓ Randomly mask 15% of node(molecular) or edge attribute(PPI)

Test ROC-AUC Performance on Molecular Prediction Using Different Pre-training Strategies with GIN

negative transfer

Dataset		BBBP	Tox21	ToxCast	SIDER	ClinTox	MUV	HIV	BACE	**Average**
# Molecules		2039	7831	8575	1427	1478	93087	41127	1513	/
# Binary prediction tasks		1	12	617	27	2	17	1	1	/
Pre-training strategy		Out-of-distribution prediction (scaffold split)								
Graph-level	Node-level									
–	–	65.8 ±4.5	74.0 ±0.8	63.4 ±0.6	57.3 ±1.6	58.0 ±4.4	71.8 ±2.5	75.3 ±1.9	70.1 ±5.4	67.0
–	Infomax	**68.8 ±0.8**	75.3 ±0.5	62.7 ±0.4	58.4 ±0.8	69.9 ±3.0	75.3 ±2.5	76.0 ±0.7	75.9 ±1.6	70.3
–	EdgePred	67.3 ±2.4	76.0 ±0.6	64.1 ±0.6	60.4 ±0.7	64.1 ±3.7	74.1 ±2.1	76.3 ±1.0	79.9 ±0.9	70.3
–	AttrMasking	64.3 ±2.8	76.7 ±0.4	64.2 ±0.5	61.0 ±0.7	71.8 ±4.1	74.7 ±1.4	77.2 ±1.1	79.3 ±1.6	71.1
–	ContextPred	68.0 ±2.0	75.7 ±0.7	63.9 ±0.6	60.9 ±0.6	65.9 ±3.8	75.8 ±1.7	77.3 ±1.0	79.6 ±1.2	70.9
Supervised	–	68.3 ±0.7	77.0 ±0.3	64.4 ±0.4	62.1 ±0.5	57.2 ±2.5	79.4 ±1.3	74.4 ±1.2	76.9 ±1.0	70.0
Supervised	Infomax	68.0 ±1.8	77.8 ±0.3	64.9 ±0.7	60.9 ±0.6	**71.2 ±2.8**	**81.3 ±1.4**	77.8 ±0.9	80.1 ±0.9	72.8
Supervised	EdgePred	66.6 ±2.2	**78.3 ±0.3**	**66.5 ±0.3**	**63.3 ±0.9**	70.9 ±4.6	78.5 ±2.4	77.5 ±0.8	79.1 ±3.7	72.6
Supervised	AttrMasking	66.5 ±2.5	77.9 ±0.4	65.1 ±0.3	**63.9 ±0.9**	**73.7 ±2.8**	**81.2 ±1.9**	77.1 ±1.2	80.3 ±0.9	73.2
Supervised	ContextPred	**68.7 ±1.3**	**78.1 ±0.6**	65.7 ±0.6	62.7 ±0.8	**72.6 ±1.5**	**81.3 ±2.1**	**79.9 ±0.7**	**84.5 ±0.7**	**74.2**

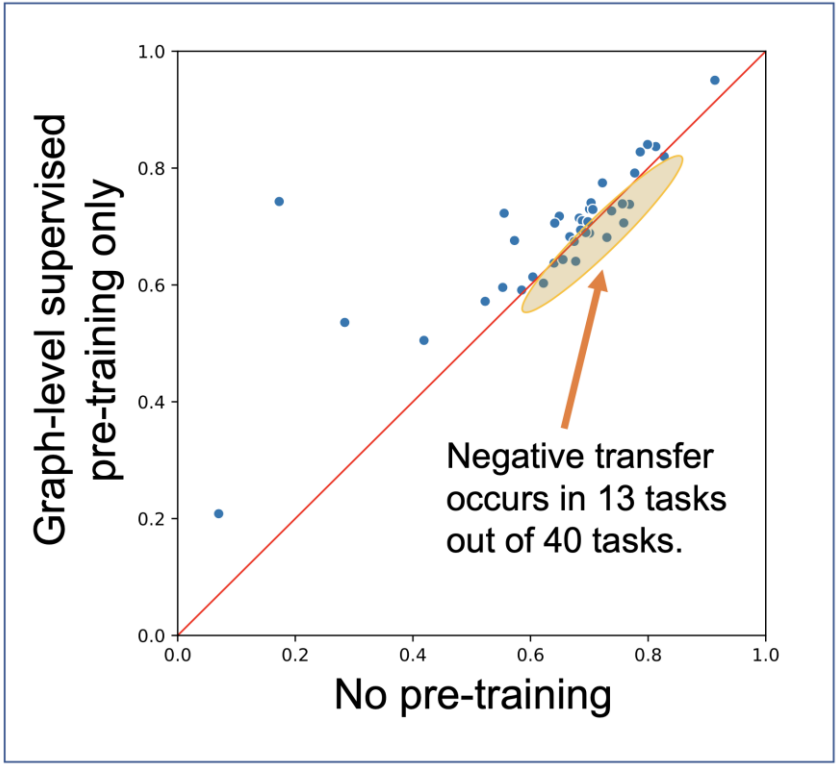
Test ROC-AUC Performance of Different GNN Architectures with and without Pre-training

	Chemistry			Biology		
	Non-pre-trained	Pre-trained	Gain	Non-pre-trained	Pre-trained	Gain
GIN	67.0	**74.2**	**+7.2**	64.8 ± 1.0	**74.2 ± 1.5**	**+9.4**
GCN	**68.9**	72.2	+3.4	63.2 ± 1.0	70.9 ± 1.7	+7.7
GraphSAGE	68.3	70.3	+2.0	65.7 ± 1.2	68.5 ± 1.5	+2.8
GAT	66.8	60.3	-6.5	**68.2 ± 1.1**	67.8 ± 3.6	-0.4

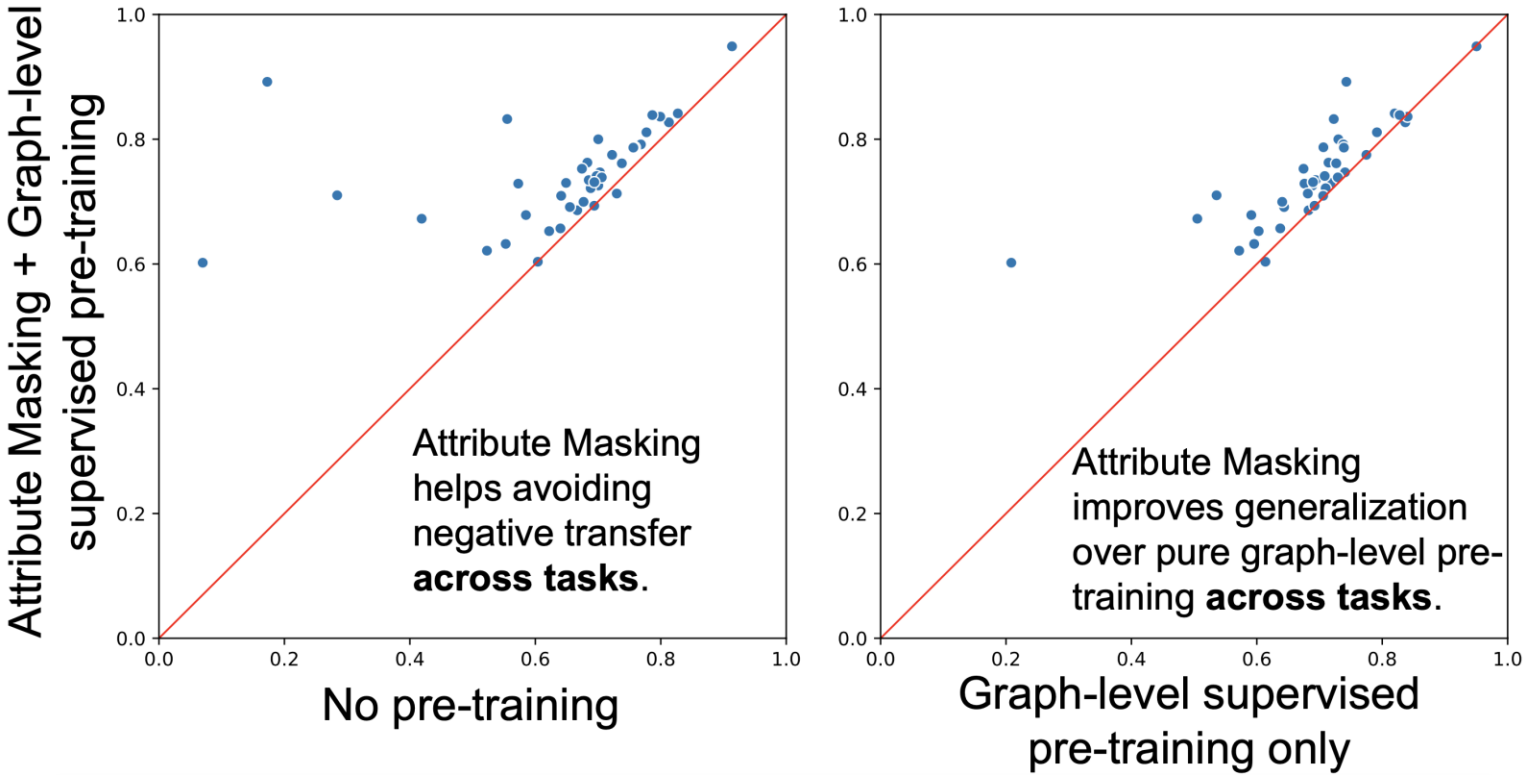
Test ROC-AUC of Protein Function Prediction Using Different Pre-training Strategies with GIN

Pre-training strategy		Out-of-dist. (species split)
Graph-level	Node-level	
–	–	64.8 ±1.0
–	Infomax	64.1 ±1.5
–	EdgePred	65.7 ±1.3
–	ContextPred	65.2 ±1.6
–	AttrMasking	64.4 ±1.3
Supervised	–	69.0 ±2.4
Supervised	Infomax	72.8 ±1.5
Supervised	EdgePred	72.3 ±1.4
Supervised	ContextPred	73.8 ± 1.0
Supervised	AttrMasking	**74.2 ±1.5**

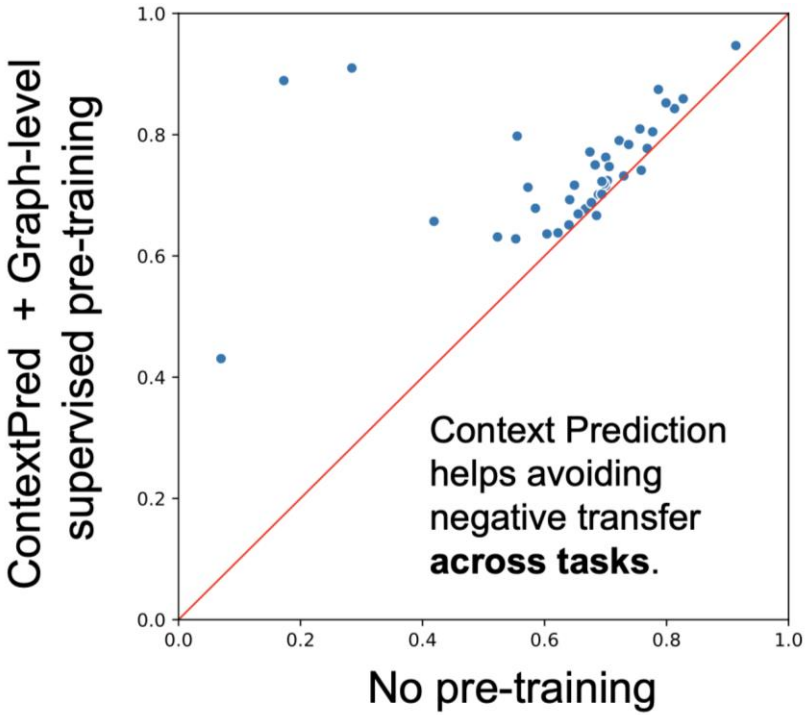
Negative Transfer

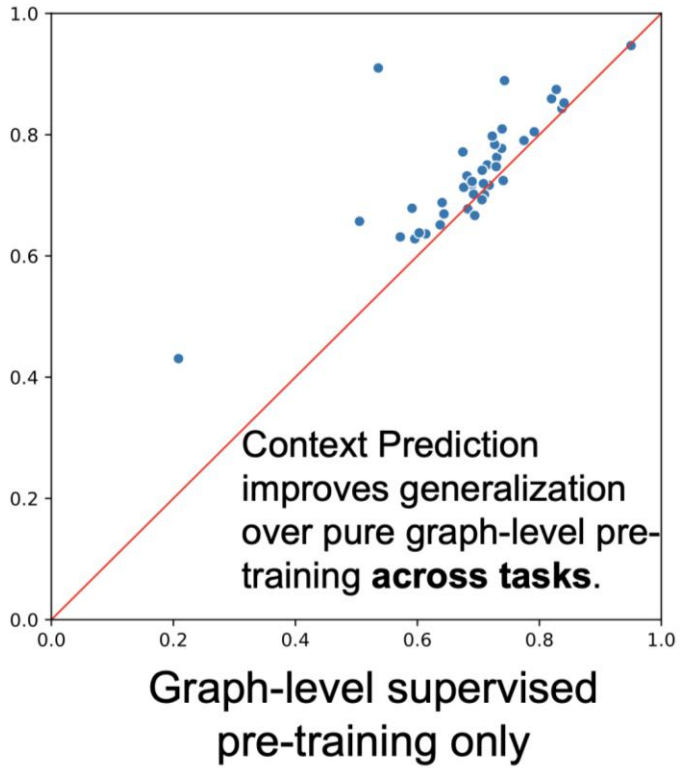


Avoiding Negative Transfer (1)

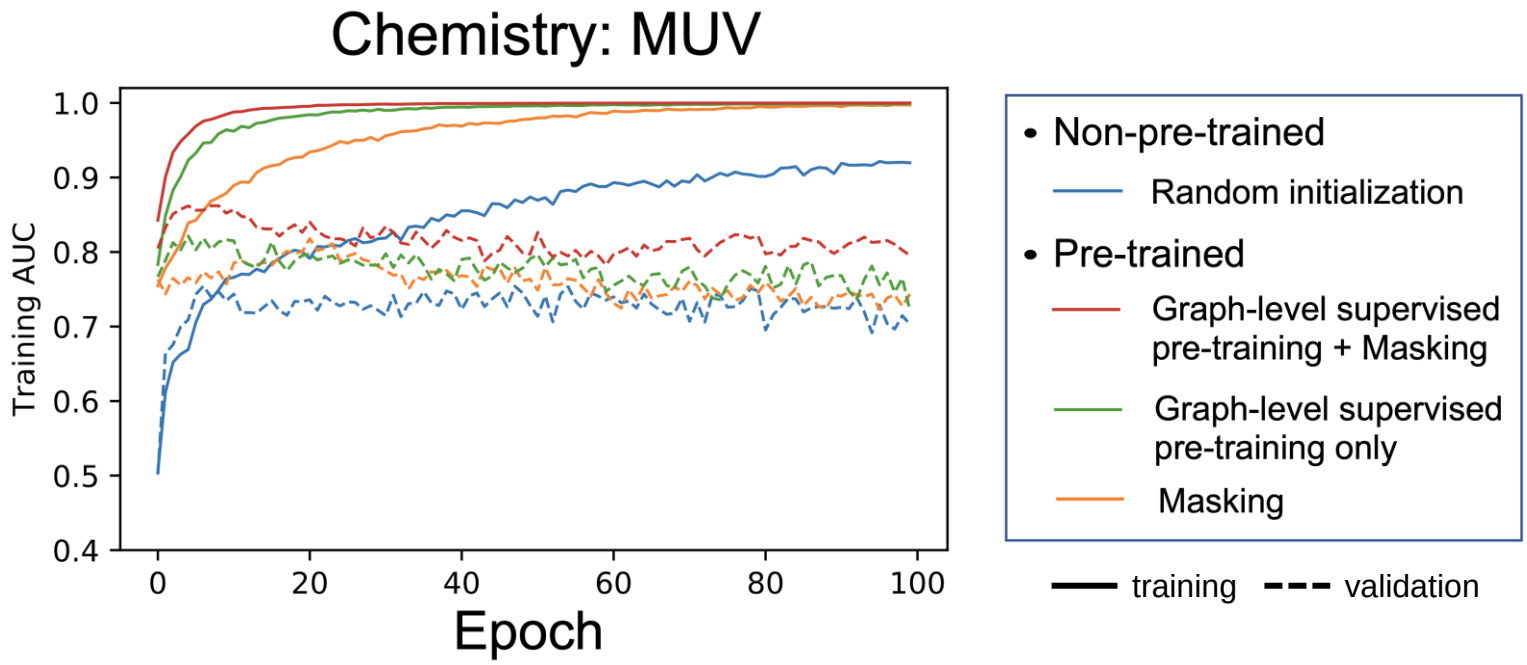


Avoiding Negative Transfer (2)

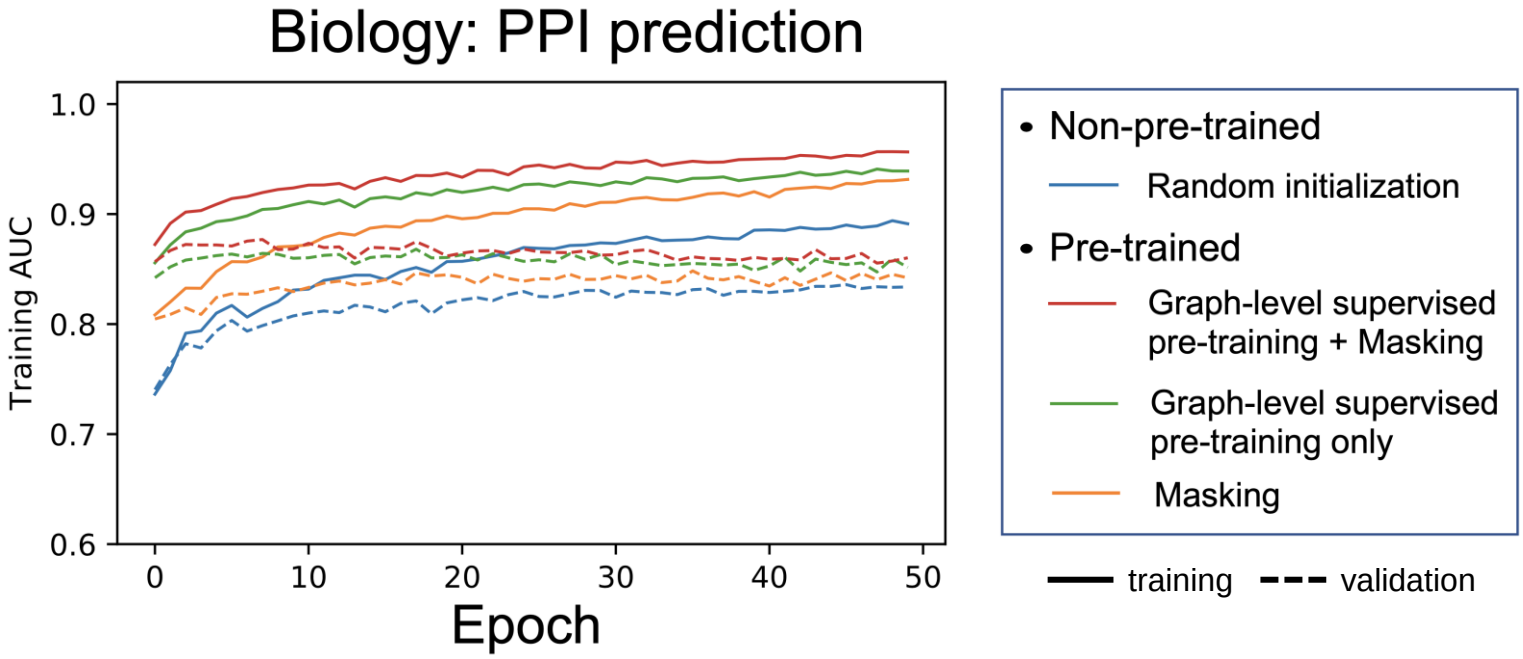




Training and Validation Curves of Different Pre-training strategies on GINs (1)



Training and Validation Curves of Different Pre-training strategies on GINs (2)



Thank you ☺