

Propagation on Residuals and Rethinking

马佳明

2023.09.20

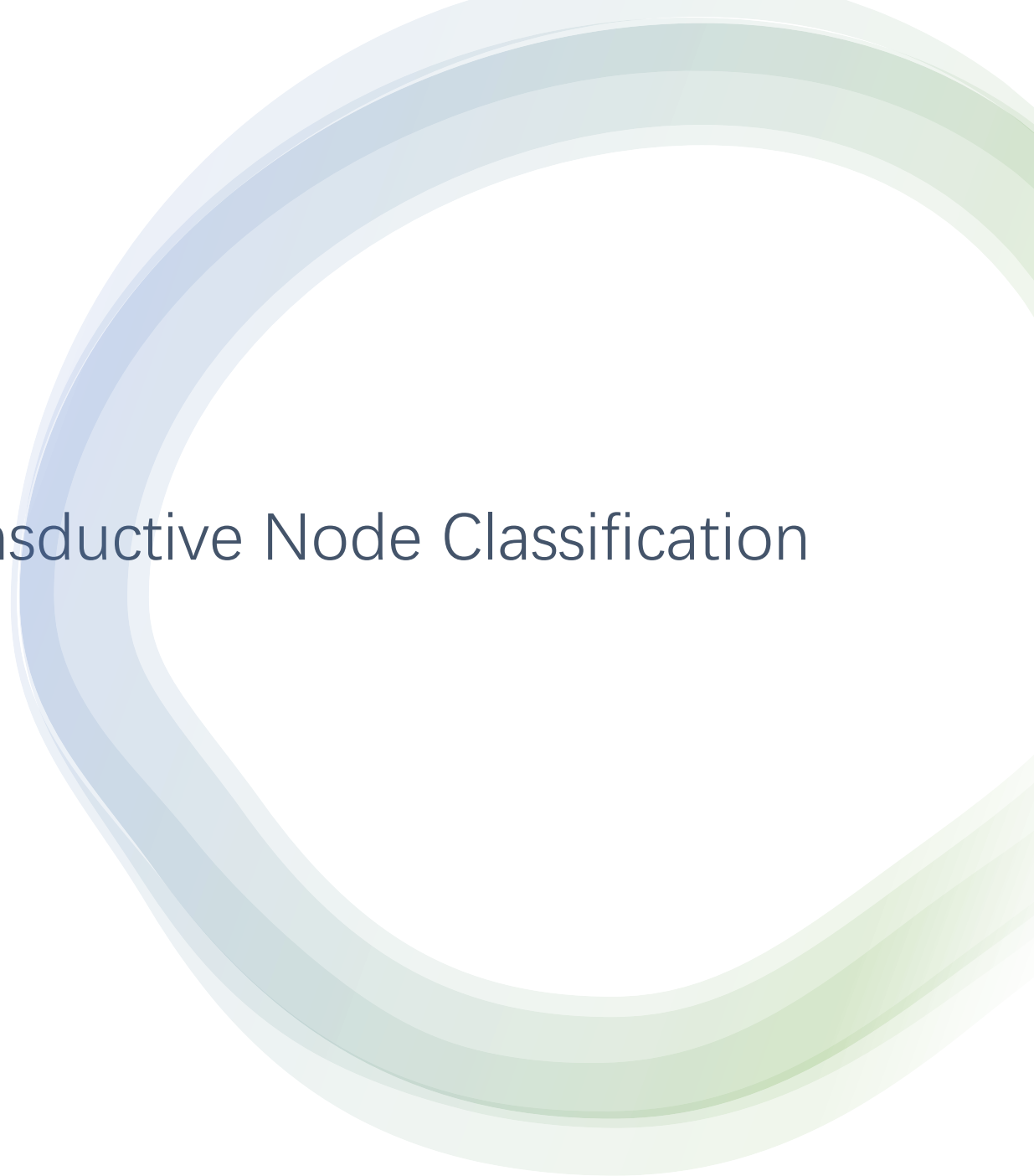
中国科学技术大学 大数据学院 数据智能实验室



中国科学技术大学
University of Science and Technology of China

Content

- Few-Shot on Graph
- Scenarios and Definition of Transductive Node Classification
- Traditional Method for TNC
- **Propagation on Residuals**
- Rethinking about Future



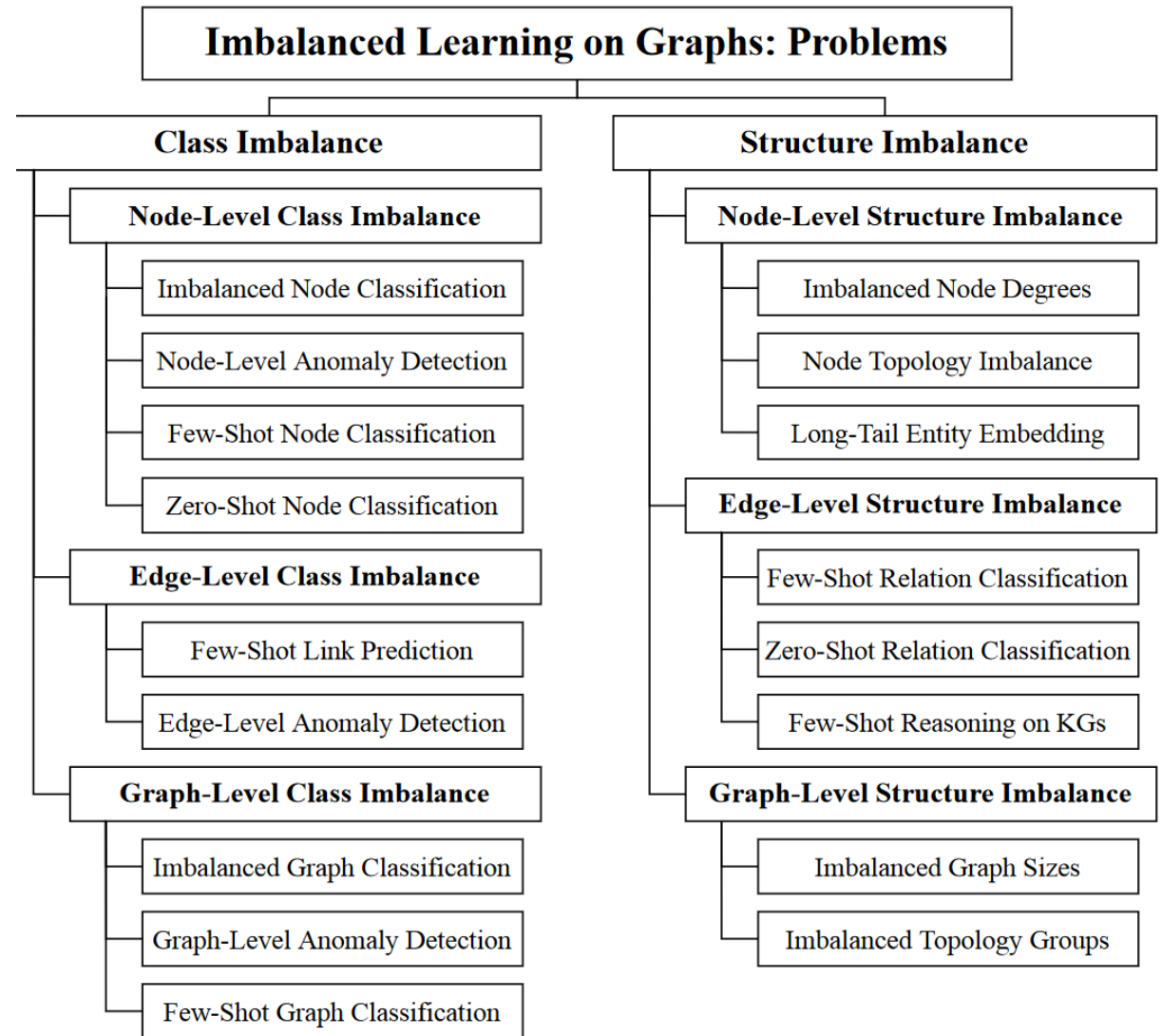
A decorative graphic consisting of several overlapping, semi-transparent rings in shades of blue and green, arranged in a circular pattern around the central text.

1. Few-show on Graph

Few-shot on Graph?

- Node Classification (Transductive)
- Link Prediction
- Graph Classification

- Relation Classification
- Reasoning on Knowledge-Graph



— *Deep Long-Tailed Learning: A Survey, Zhang & etc., PAMI 2023.*

— *A Survey of Imbalanced Learning on Graphs: Problems, Techniques, and Future Directions, Liu & etc., arXiv 2023.*

— *A Survey on Graph Neural Networks for Time Series: Forecasting, Classification, Imputation, and Anomaly Detection, Jin & etc., arXiv 2023.*

- **CV: 1st Transductive Inference Explicitly in Few-Shot Learning.**

—— Learning to Propagate Labels: Transductive Propagation Network for Few-shot Learning. Liu & etc., ICLR 2019.

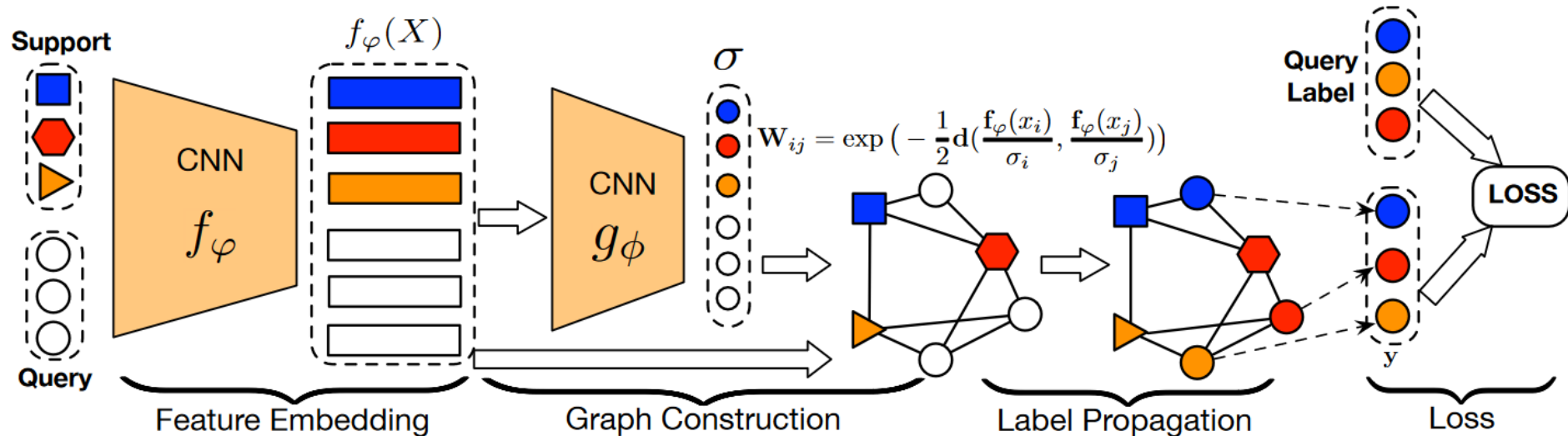


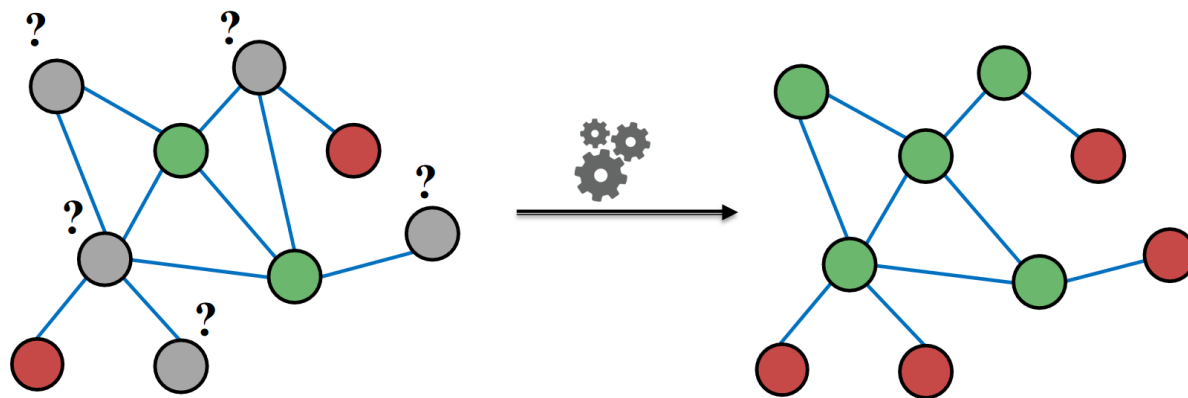
Figure 2: The overall framework of our algorithm in which the manifold structure of the entire query set helps to learn better decision boundary. The proposed algorithm is composed of four components: feature embedding, graph construction, label propagation, and loss generation.



2. Scenarios and Definition on Transductive Node Classification

Scenarios: Transductive Node Classification

- 通过使用图上已知标记(Label)的节点, 来预测图上未知标记的节点的标记。
- 仅关注于当前图中的节点, 而不考虑将来可能出现的新节点。
- Always Few-shot!



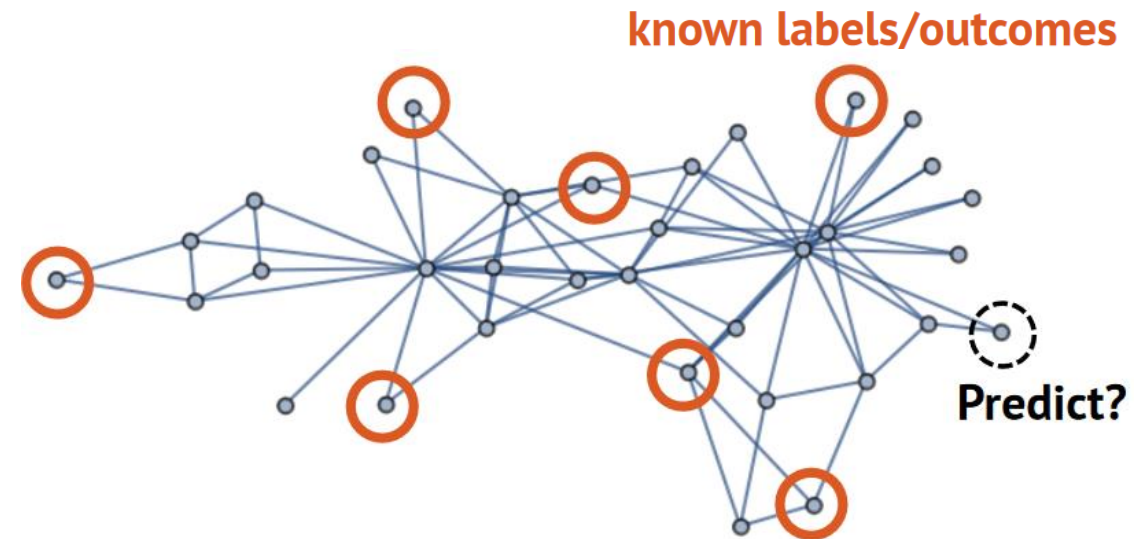
// **Semi-supervised:** 训练数据集中只有部分数据标记有标签, 而大部分数据没有标签。目标是通过利用有标签数据 and 无标签数据的信息 (feature), 来进行模型训练和预测。

// **Inductive:** 通过使用已知标记的节点来构建一个模型, 然后将该模型应用于未来出现的新节点。它更加关注于构建通用的模型, 可以应用于未来的节点分类任务。(GraphSAGE)

—— *Inductive Representation Learning on Large Graphs. Hamilton & etc., NIPS 2017.*

Naïve Definition

- Input:
 - Graph $G = (V, E, X, Y)$.
 - Node Feature $X \in \mathbb{R}^{|V| \times d}$.
 - Known Node Label $y_L \in \{0, 1\}^{|V_L|}$.
($V_L \in V$ The labeled node set.)
- Output:
 - Unknown Node Label $y_u \in \{0, 1\}^{|V_U|}$.
($V_U = V \setminus V_L \in V$ the unlabeled node set.)





3. Traditional Method for TNC

- **1. Simplicial Label Propagation or GNNs.**

—— Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions. Zhu & etc., ICML 2003.

1. Simplicial Label Propagation or GNNs

- **LP assumptions:**

1. Homophily

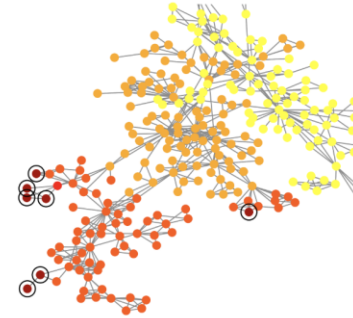
- **GNNs assumptions:**

1. Labels only depend on neighbor features.

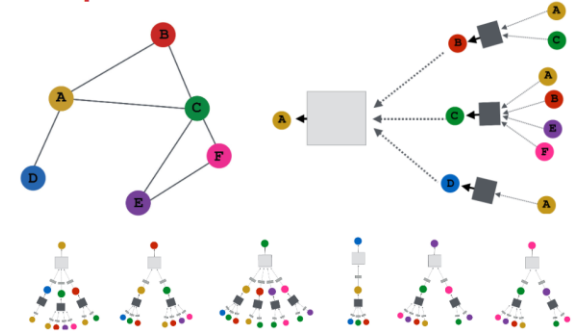
2. Features are informative.

- **Propagation \approx Smoothness**

Label Propagation [early 2000s]



Graph Neural Networks [late 2010s]



Model	Training		Inference	
	Feature	Label	Feature	Label
LPA		✓		✓
GCN	✓		✓	

- **1. Simplicial Label Propagation or GNNs.**

—— Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions. Zhu & etc., ICML 2003.

- **2. GNNs + Propagation.**

—— Predict then Propagate: Graph Neural Networks meet Personalized PageRank. Gasteiger & etc., ICLR 2019.

—— Unifying Graph Convolutional Neural Networks and Label Propagation. Wang & Leskovec., arXiv 2020.

2. GNNs + Propagation

PPNP & APPNP:

- GCN + PageRank :

1. Personalization

2. Approximation

3. **Embedding** Propagation

(\approx Feature Propagation)

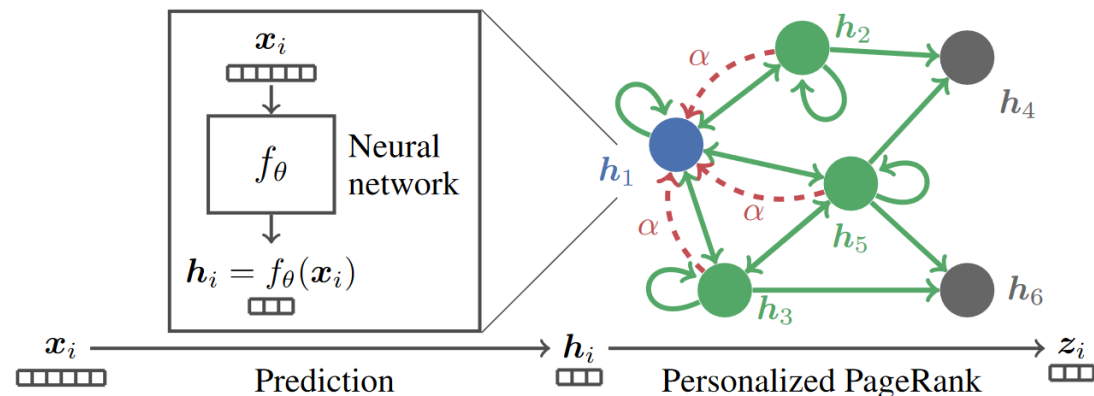


Figure 1: Illustration of (approximate) personalized propagation of neural predictions (PPNP, APPNP). Predictions are first generated from each node’s own features by a neural network and then propagated using an adaptation of personalized PageRank. The model is trained end-to-end.

Table 2: Average accuracy with uncertainties showing the 95 % confidence level calculated by bootstrapping. Previously reported improvements vanish on our rigorous experimental setup, while PPNP and APPNP significantly outperform the compared models on all datasets.

Model	CITeseer	CORA-ML	PUBMED	MS ACADEMIC
V. GCN	73.51 \pm 0.48	82.30 \pm 0.34	77.65 \pm 0.40	91.65 \pm 0.09
GCN	75.40 \pm 0.30	83.41 \pm 0.39	78.68 \pm 0.38	92.10 \pm 0.08
N-GCN	74.25 \pm 0.40	82.25 \pm 0.30	77.43 \pm 0.42	92.86 \pm 0.11
GAT	75.39 \pm 0.27	84.37 \pm 0.24	77.76 \pm 0.44	91.22 \pm 0.07
JK	73.03 \pm 0.47	82.69 \pm 0.35	77.88 \pm 0.38	91.71 \pm 0.10
Bt. FP	73.55 \pm 0.57	80.84 \pm 0.97	72.94 \pm 1.00	91.61 \pm 0.24
PPNP*	75.83 \pm 0.27	85.29 \pm 0.25	-	-
APPNP	75.73 \pm 0.30	85.09 \pm 0.25	79.73 \pm 0.31	93.27 \pm 0.08

*out of memory on PUBMED, MS ACADEMIC (see efficiency analysis in Section 3)

— *Predict then Propagate: Graph Neural Networks meet Personalized PageRank. Gasteiger & etc., ICLR 2019.*

— *The Anatomy of a Large-Scale Hypertextual Web Search Engine. Brin & Page, Computer networks and ISDN systems, 1998.*

2. GNNs + Propagation

PPNP & APPNP:

- GCN + PageRank :

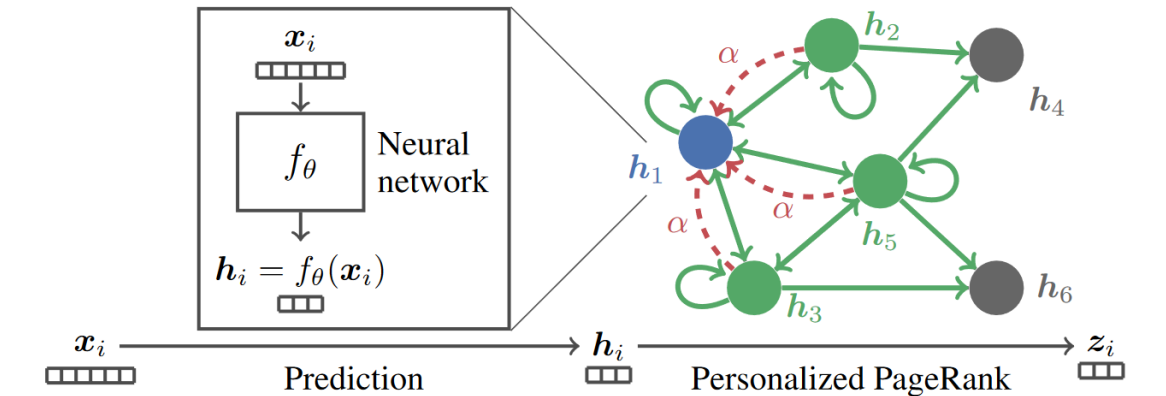
1. Personalization

2. Approximation

3. **Embedding** Propagation (\approx Feature Propagation)

4. No labels utilized during training and inference.

5. Marginal improvement.



Model	Training		Inference	
	Feature	Label	Feature	Label
LPA		✓		✓
GCN	✓		✓	
APPNP	✓		✓	

—— *Predict then Propagate: Graph Neural Networks meet Personalized PageRank. Gasteiger & etc., ICLR 2019.*

—— *The Anatomy of a Large-Scale Hypertextual Web Search Engine. Brin & Page, Computer networks and ISDN systems, 1998.*

2. GNNs + Propagation

GCN-LPA:

- GCN + LPA :

1. LPA during training weight.

2. Overemphasis to Label.

3. Depending on GNNs with **trainable weight edge** like GAT.

Method	Cora	Citeseer	Pubmed	Coauthor-CS	Coauthor-Phy
MLP	64.6 ± 1.7	62.0 ± 1.8	85.9 ± 0.3	91.7 ± 1.4	94.1 ± 1.2
LR	77.3 ± 1.8	71.2 ± 1.8	86.0 ± 0.6	91.1 ± 0.6	93.8 ± 1.1
LPA	85.3 ± 0.9	70.0 ± 1.7	82.6 ± 0.6	91.3 ± 0.2	94.9 ± 0.4
GCN	88.2 ± 0.8	77.3 ± 1.5	87.2 ± 0.4	93.6 ± 1.5	96.2 ± 0.2
GAT	87.7 ± 0.3	76.2 ± 0.9	86.9 ± 0.5	93.8 ± 0.4	96.3 ± 0.7
JK-Net	89.1 ± 1.2	78.3 ± 0.9	85.8 ± 1.1	92.4 ± 0.4	94.8 ± 0.4
GraphSAGE	86.8 ± 1.9	75.2 ± 1.1	84.7 ± 1.6	92.6 ± 1.6	94.5 ± 1.1
GCN-LPA	88.5 ± 1.5	78.7 ± 0.6	87.8 ± 0.6	94.8 ± 0.4	96.9 ± 0.2

Table 2: Mean and the 95% confidence intervals of test set accuracy for all methods and datasets.

Model	Training		Inference	
	Feature	Label	Feature	Label
LPA		✓		✓
GCN	✓		✓	
APPNP	✓		✓	
GCN-LPA	✓	✓	✓	

—— *Unifying Graph Convolutional Neural Networks and Label Propagation. Wang & Leskovec., arXiv 2020.*

—— *Graph Attention Networks. Velickovic & etc., ICLR 2018.*

- **1. Simplicial Label Propagation or GNNs.**

—— Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions. Zhu & etc., ICML 2003.

- **2. GNNs + Propagation.**

—— Predict then Propagate: Graph Neural Networks meet Personalized PageRank. Gasteiger & etc., ICLR 2019.

—— Unifying Graph Convolutional Neural Networks and Label Propagation. Wang & Leskovec., arXiv 2020.

- **3. Not only Propagation on Feature but also done so on Label.**

—— Masked Label Prediction: Unified Message Passing Model for Semi-Supervised Classification. Shi & etc., IJCAI 2021.

3. GNNs + L&F Propagation

UniMP:

- GAT+ All Propagation:
 1. L&F Propagation;
 2. Masked Known Label.

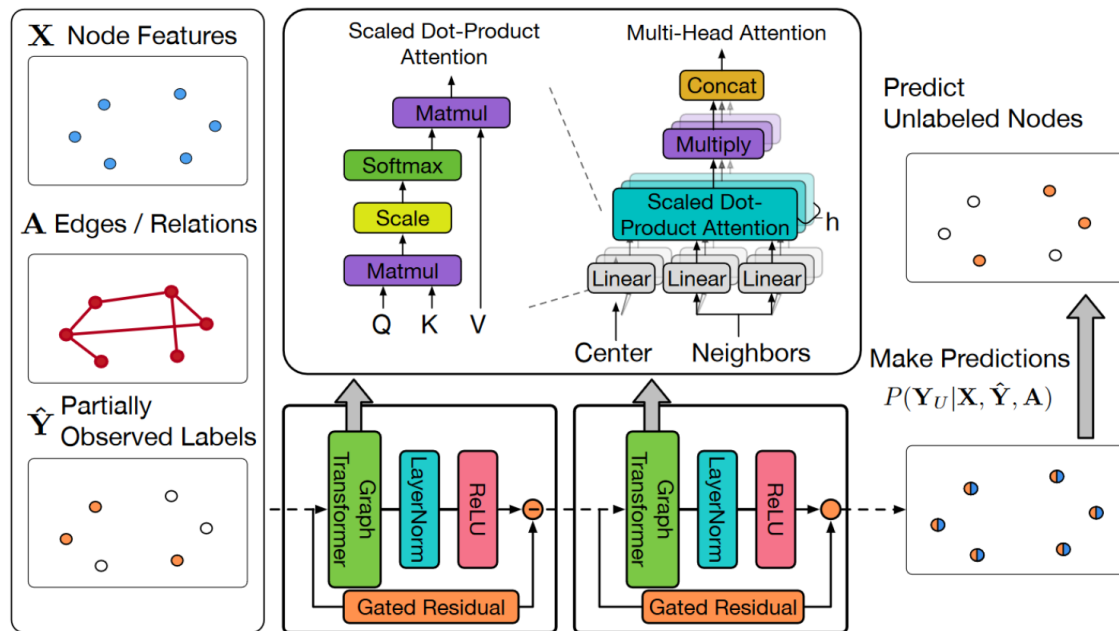


Figure 1: The architecture of UniMP.

Model	Training		Inference	
	Feature	Label	Feature	Label
LPA		✓		✓
GCN	✓		✓	
APPNP	✓		✓	
GCN-LPA	✓	✓	✓	✓
UniMP (Ours)	✓	✓	✓	✓

Table 1: Comparison the input information that message passing models use in training and inference.

3. GNNs + L&F Propagation

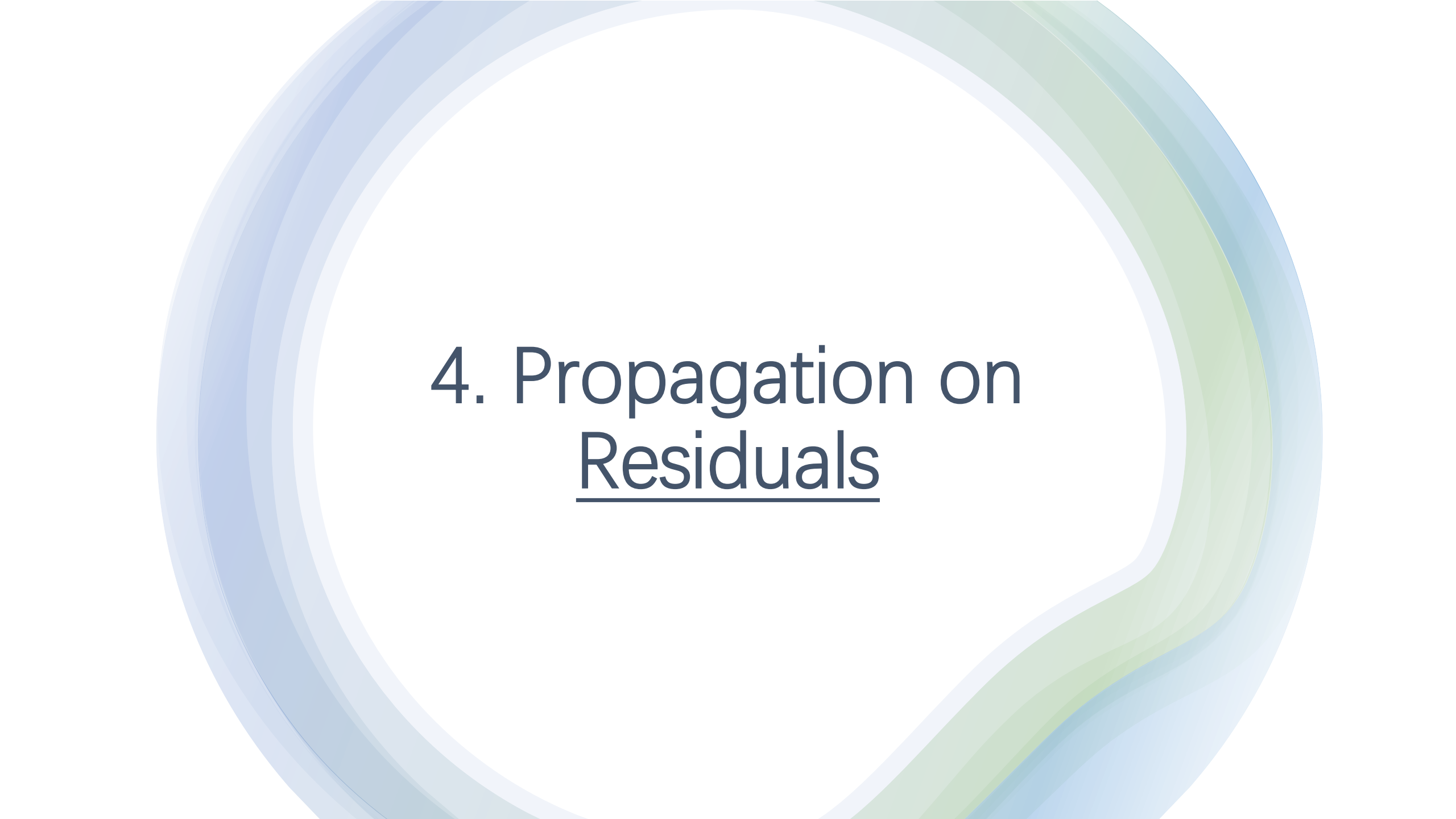
UniMP:

- GAT+ All Propagation:
 1. L&F Propagation;
 2. Masked Known Label.
- SOTA ! (2022.09)

Model	Test Accuracy	Validation Accuracy	Params
GCN-Cluster [Chiang <i>et al.</i> , 2019]	0.7897 ± 0.0036	0.9212 ± 0.0009	206,895
GAT-Cluster	0.7923 ± 0.0078	0.8985 ± 0.0022	1,540,848
GAT-NeighborSampling	0.7945 ± 0.0059	-	1,751,574
GraphSAINT [Zeng <i>et al.</i> , 2019]	0.8027 ± 0.0026	-	331,661
DeeperGCN [Li <i>et al.</i> , 2020]	0.8090 ± 0.0020	0.9238 ± 0.0009	253,743
UniMP	0.8256 ± 0.0031	0.9308 ± 0.0017	1,475,605

Table 4: Results for ogbn-products

Inputs	Model	Datasets
		ogbn-products Test ACC
X	Multilayer Perceptron	0.6106 ± 0.0008
X, A	GCN	0.7851 ± 0.0011
	GAT	0.8002 ± 0.0063
	Graph Transformer	0.8137 ± 0.0047
A, \hat{Y}	GCN	0.7832 ± 0.0013
	GAT	0.7751 ± 0.0054
	Graph Transformer	0.7987 ± 0.0104
X, A, \hat{Y}	GCN	0.7987 ± 0.0104
	GAT	0.8193 ± 0.0017
	Graph Transformer	0.8256 ± 0.0031
	⊥ w/ Edge Feature	*



4. Propagation on Residuals

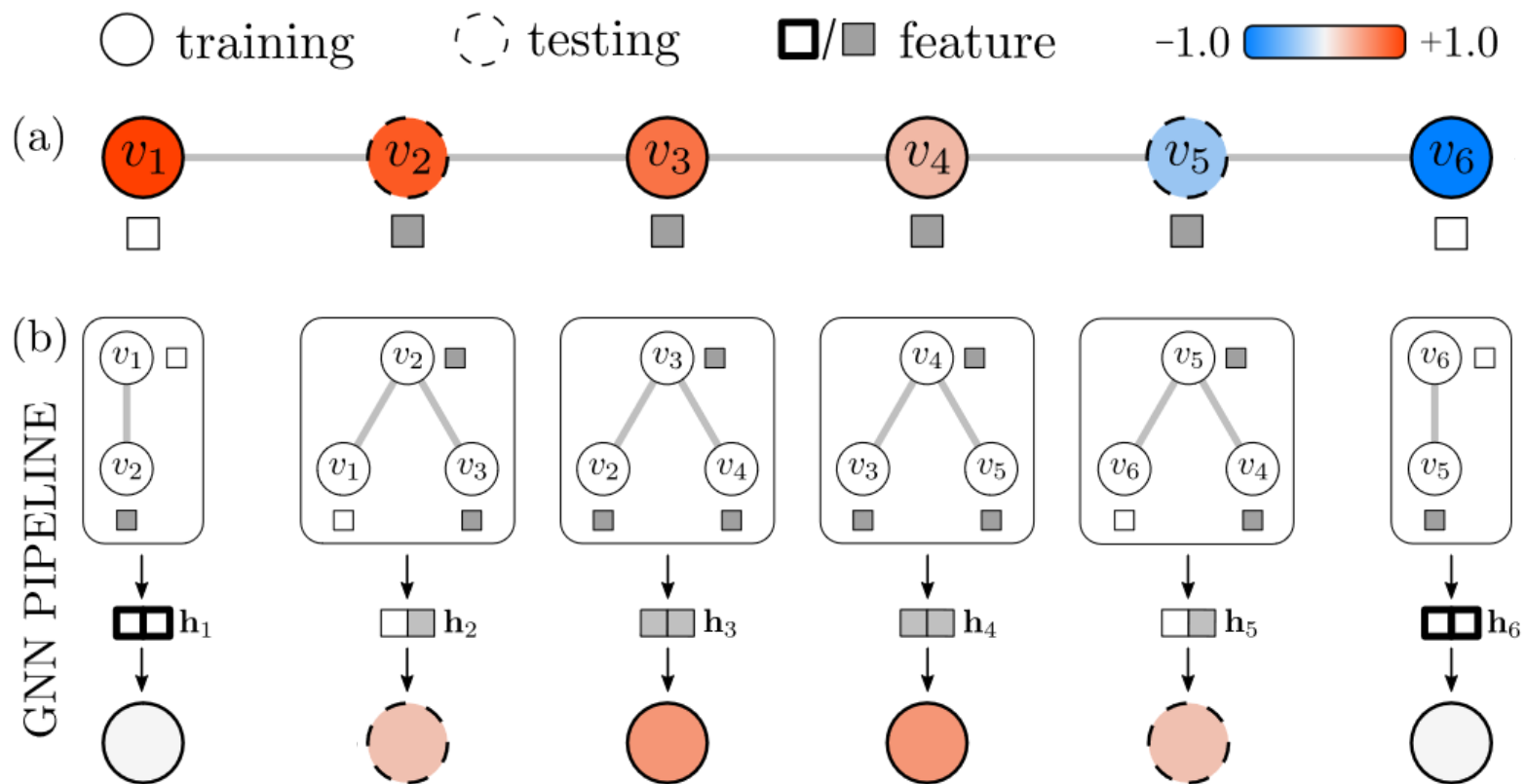
- **1. LP on residuals.**

—— Residual Correlation in Graph Neural Network Regression. Jia & Benson, KDD 2020.

1. LP on residuals for improving GNN regression algorithms.

Claim: GNNs tend to generate biased predictions, resulting in residuals.

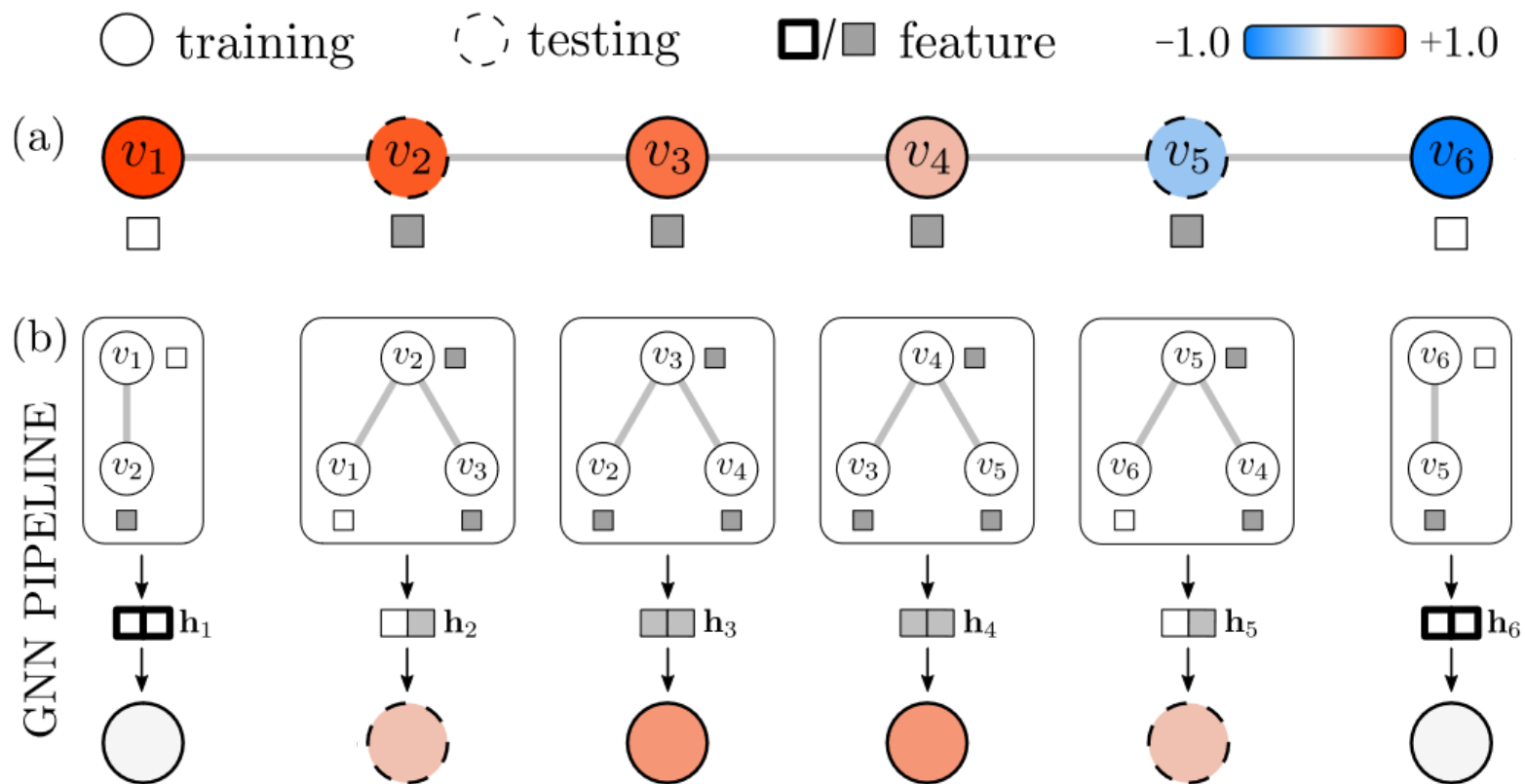
Reason: Labels and features are not necessarily strongly correlated.



1. LP on residuals for improving GNN regression algorithms.

Problem: LPA appended can not figure out this situation.

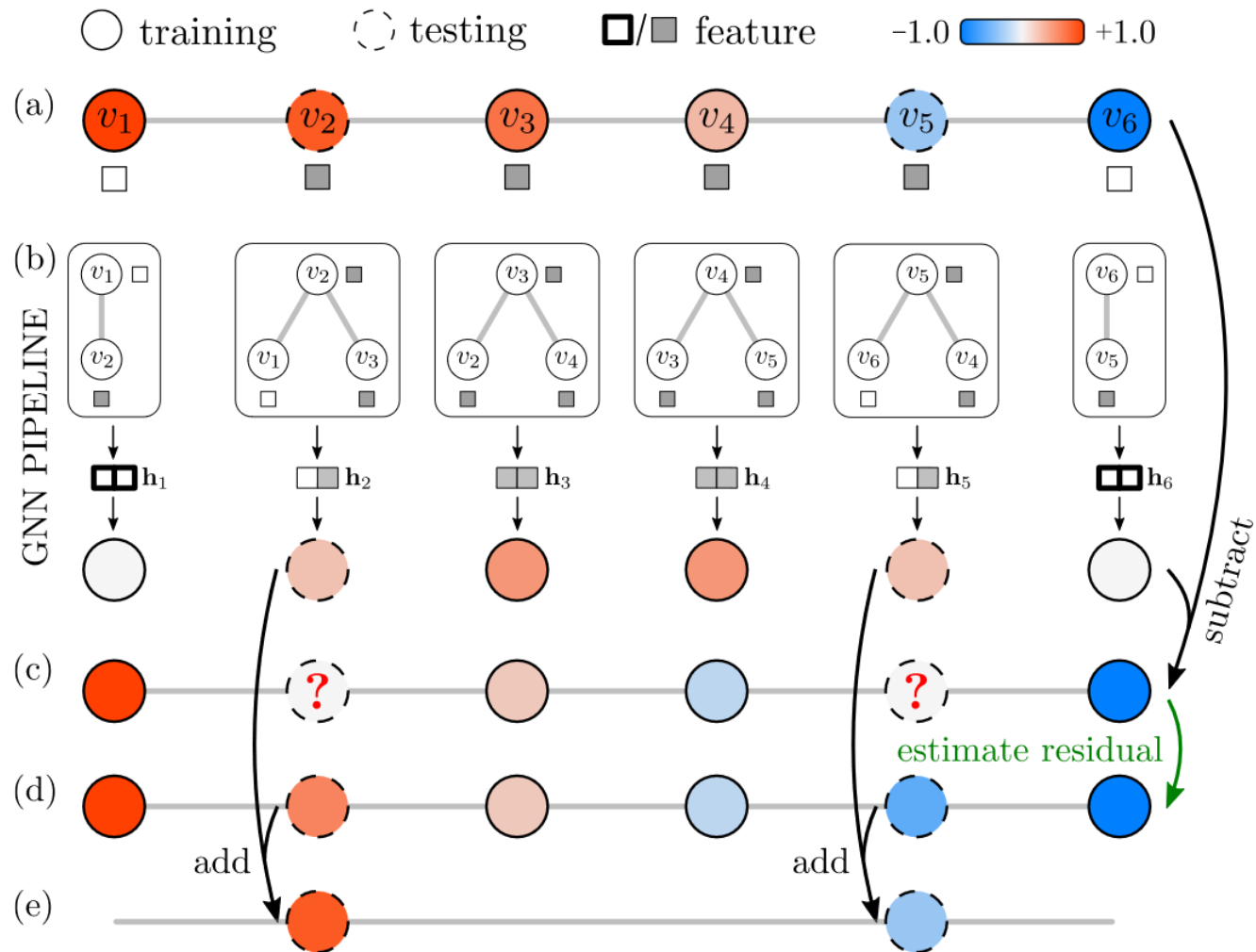
Reason: The pseudo-label distribution has changed.



1. LP on residuals for improving GNN regression algorithms.

Solution: Residual Propagation

1. Base prediction.
2. Residual Cal. on labeled nodes.
3. Residual propagation.
4. Final prediction
= smoothed residual + base prediction
(= true value on labeled nodes)



1. LP on residuals for improving GNN regression algorithms.

Table 1: Transductive learning accuracy of our C-GNN and LP-GNN models compared to competing baselines. The best accuracy is in green. Our C-GNN outperforms GNN on all datasets, often by a substantial margin. Even C-MLP, which does not use neighbor features, outperforms GNN in many cases, highlighting the importance of label correlation. LP, LP-MLP and LP-GNN assume positive label correlation among neighboring vertices and perform poorly for datasets where most edges encode negative interactions, as highlighted in orange. We also report the learned $\{\alpha_i\}$ values from C-GNN.

Dataset	n	m	LP	MLP	LP-MLP	C-MLP	GNN	LP-GNN	C-GNN	$\{\alpha_i\}$
Ising(+)	1.2K	2.4K	0.76 \pm 0.02	0.68 \pm 0.03	0.76 \pm 0.02	0.76 \pm 0.02	0.67 \pm 0.04	0.76 \pm 0.02	0.76 \pm 0.02	+0.89
Ising(-)	1.2K	2.4K	0.30 \pm 0.03	0.47 \pm 0.02	0.30 \pm 0.03	0.77 \pm 0.03	0.47 \pm 0.03	0.30 \pm 0.03	0.77 \pm 0.03	-0.93
income	3.2K	12.7K	0.54 \pm 0.04	0.64 \pm 0.03	0.73 \pm 0.03	0.74 \pm 0.03	0.75 \pm 0.03	0.81 \pm 0.03	0.81 \pm 0.02	+0.92
education	3.2K	12.7K	0.36 \pm 0.05	0.67 \pm 0.03	0.71 \pm 0.02	0.72 \pm 0.02	0.70 \pm 0.02	0.72 \pm 0.03	0.72 \pm 0.03	+0.78
unemployment	3.2K	12.7K	0.70 \pm 0.03	0.43 \pm 0.05	0.69 \pm 0.04	0.77 \pm 0.03	0.55 \pm 0.04	0.75 \pm 0.05	0.78 \pm 0.03	+0.99
election	3.2K	12.7K	0.58 \pm 0.02	0.37 \pm 0.02	0.61 \pm 0.03	0.63 \pm 0.03	0.51 \pm 0.04	0.69 \pm 0.03	0.69 \pm 0.03	+0.95
Anaheim	914	3.8K	0.49 \pm 0.08	0.75 \pm 0.02	0.81 \pm 0.04	0.82 \pm 0.03	0.76 \pm 0.03	0.81 \pm 0.04	0.82 \pm 0.03	+0.95, +0.17
Chicago	2.2K	15.1K	0.59 \pm 0.05	0.60 \pm 0.05	0.65 \pm 0.06	0.65 \pm 0.05	0.68 \pm 0.04	0.72 \pm 0.04	0.71 \pm 0.04	+0.85, +0.68
sexual	1.9K	2.1K	0.37 \pm 0.06	0.68 \pm 0.02	0.64 \pm 0.03	0.83 \pm 0.03	0.88 \pm 0.02	0.86 \pm 0.02	0.93 \pm 0.01	-0.98
Twitch-PT	1.9K	31.3K	0.00 \pm 0.04	0.61 \pm 0.03	0.60 \pm 0.04	0.66 \pm 0.03	0.69 \pm 0.03	0.69 \pm 0.03	0.74 \pm 0.03	+0.99

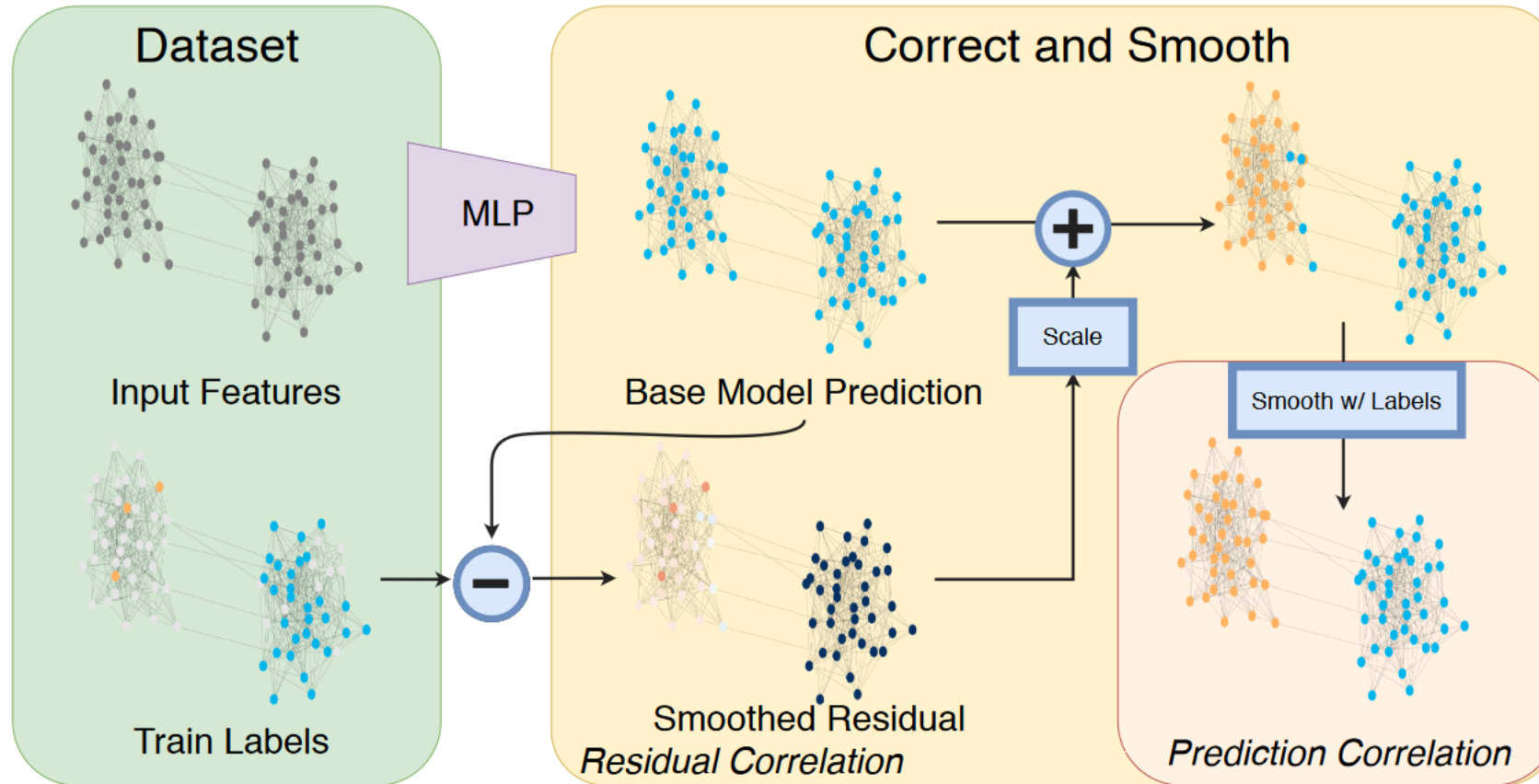
- **1. LP on residuals.**

—— Residual Correlation in Graph Neural Network Regression. Jia & Benson, KDD 2020.

- **2. Using LP on residuals but removing GNNs altogether.**

—— Combining Label Propagation and Simple Models Out-performs Graph Neural Networks. Huang et al., ICLR 2021.

2. Using LP but removing GNNs altogether for good classification performance.



• Leaderboard for **ogbn-products**.

— https://ogb.stanford.edu/docs/leader_nodeprop/

• Amazon product co-purchasing network:

- Undirected and unweighted;
- Node: products sold in Amazon (# 2,449,029);
- Edge: indicates the products are purchased together (# 61,859,140);
- Node features: the product descriptions (PCA).

• Prediction task:

- Category of a product (# 47).

• Methods related to C&S (up to now):

- Top 5: 4/5 90%
- Top 20: 9/20 45%

Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	GLEM+GIANT+SAGN+SCR	Yes	0.8737 ± 0.0006	0.9400 ± 0.0003	Jianan Zhao (Mila & MSRA Team)	Paper, Code	139,792,525	Tesla V100 (32GB)	Oct 27, 2022
2	**GradBERT+GIANT & SAGN+SLE-CnS**	Yes	0.8692 ± 0.0007	0.9371 ± 0.0003	Costas Mavromatis (UMN & AWS)	Paper, Code	1,154,654	GeForce RTX 3090 (24GB GPU)	Apr 20, 2023
3	GIANT-XRT+R-SAGN+SCR-C&S	Yes	0.8684 ± 0.0005	0.9365 ± 0.0003	LeeXue (HIT Team)	Paper, Code	1,154,142	TITAN RTX (24GB GPU)	Sep 30, 2022
4	GIANT-XRT+SAGN+SCR-C&S	Yes	0.8680 ± 0.0007	0.9357 ± 0.0004	Yufei He (CogDL Team)	Paper, Code	1,154,654	GeForce RTX 3090 24GB (GPU)	Jun 13, 2022
5	GIANT-XRT+SAGN+MCR-C&S	Yes	0.8673 ± 0.0008	0.9387 ± 0.0002	Yufei He (CogDL Team)	Paper, Code	1,154,654	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
6	GIANT-XRT+SAGN+SCR	Yes	0.8667 ± 0.0009	0.9364 ± 0.0005	Yufei He (CogDL Team)	Paper, Code	1,154,654	GeForce RTX™ 3090 24GB (GPU)	Jun 13, 2022
7	GIANT-XRT+SAGN+MCR	Yes	0.8651 ± 0.0009	0.9389 ± 0.0002	Yufei He (CogDL Team)	Paper, Code	1,154,654	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
8	GIANT-XRT+SAGN+SLE-C&S (use raw text)	Yes	0.8643 ± 0.0020	0.9352 ± 0.0005	Eli Chien (UIUC)	Paper, Code	1,548,382	Tesla T4 (16GB GPU)	Nov 8, 2021
9	GIANT-XRT+SAGN+SLE (use raw text)	Yes	0.8622 ± 0.0022	0.9363 ± 0.0005	Eli Chien (UIUC)	Paper, Code	1,548,382	Tesla T4 (16GB GPU)	Nov 8, 2021
10	GIANT-XRT+GAMLP+MCR	Yes	0.8591 ± 0.0008	0.9402 ± 0.0004	Yufei He (CogDL Team)	Paper, Code	2,144,151	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
11	GAMLP+RLU+SCR-C&S	No	0.8520 ± 0.0008	0.9304 ± 0.0005	Yufei He (CogDL Team)	Paper, Code	3,335,831	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
12	GAMLP+RLU+SCR	No	0.8505 ± 0.0009	0.9292 ± 0.0005	Yufei He (CogDL Team)	Paper, Code	3,335,831	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
13	SAGN+SLE (4 stages)-C&S	No	0.8485 ± 0.0010	0.9302 ± 0.0003	Chuxiong Sun (CTRI)	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Sep 21, 2021
14	SAGN+SLE (4 stages)	No	0.8468 ± 0.0012	0.9309 ± 0.0007	Chuxiong Sun (CTRI)	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Sep 21, 2021
15	GAMLP+MCR	No	0.8462 ± 0.0003	0.9319 ± 0.0003	Yufei He (CogDL Team)	Paper, Code	3,335,831	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
16	GAMLP+RLU	No	0.8459 ± 0.0010	0.9324 ± 0.0005	Wentao Zhang (PKU Tencent Joint Lab)	Paper, Code	3,335,831	Tesla V100 (32GB)	Aug 19, 2021
17	Spec-MLP-Wide + C&S	No	0.8451 ± 0.0006	0.9132 ± 0.0010	Huixuan Chi (AML@ByteDance)	Paper, Code	406,063	Tesla V100 (32GB)	Jul 27, 2021
18	SAGN+MCR	No	0.8441 ± 0.0005	0.9325 ± 0.0004	Yufei He (CogDL Team)	Paper, Code	2,179,678	GeForce RTX™ 3090 24GB (GPU)	Dec 8, 2021
19	SAGN+SLE	No	0.8428 ± 0.0014	0.9287 ± 0.0003	Chuxiong Sun	Paper, Code	2,179,678	Tesla V100 (16GB GPU)	Apr 19, 2021
20	MLP + C&S	No	0.8418 ± 0.0007	0.9147 ± 0.0009	Horace He (Cornell)	Paper, Code	96,247	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020

20	MLP + C&S	No	0.8418 ± 0.0007	0.9147 ± 0.0009	Horace He (Cornell)	Paper , Code	96,247	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020
----	----------------------	----	--------------------	--------------------	-------------------------------------	---	--------	--------------------------------	-----------------

...

25	Linear + C&S	No	0.8301 ± 0.0001	0.9134 ± 0.0001	Horace He (Cornell)	Paper , Code	10,763	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020
----	-------------------------	----	--------------------	--------------------	-------------------------------------	---	--------	--------------------------------	-----------------

26	UniMP	No	0.8256 ± 0.0031	0.9308 ± 0.0017	Yunsheng Shi (PGL team)	Paper , Code	1,475,605	Tesla V100 (32GB)	Sep 8, 2020
----	--------------	----	--------------------	--------------------	---	---	-----------	----------------------	----------------

...

GAT (Neighbor sampling or Cluster) (+ C&S)

...

GraphSAGE (+ C&S)

...

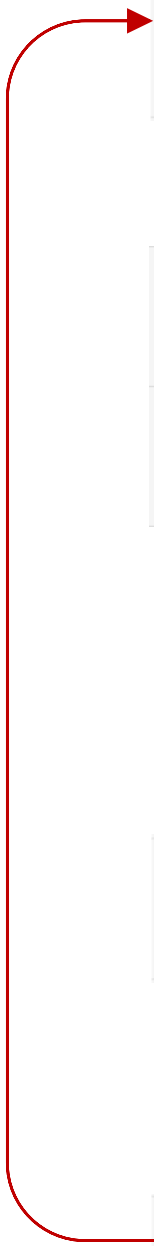
49	Label Propagation	No	0.7434 ± 0.0000	0.9091 ± 0.0000	Horace He (Cornell)	Paper , Code	0	GeForce RTX 2080 (11GB GPU)	Oct 3, 2020
----	-------------------	----	--------------------	--------------------	-------------------------------------	---	---	--------------------------------	----------------

...

Node2vec

...

54	MLP	No	0.6106 ± 0.0008	0.7554 ± 0.0014	Matthias Fey – OGB team	Paper , Code	103,727	GeForce RTX 2080 (11GB GPU)	Jun 10, 2020
----	-----	----	--------------------	--------------------	---	---	---------	--------------------------------	-----------------



- **1. LP on residuals.**

—— Residual Correlation in Graph Neural Network Regression. Jia & Benson, KDD 2020.

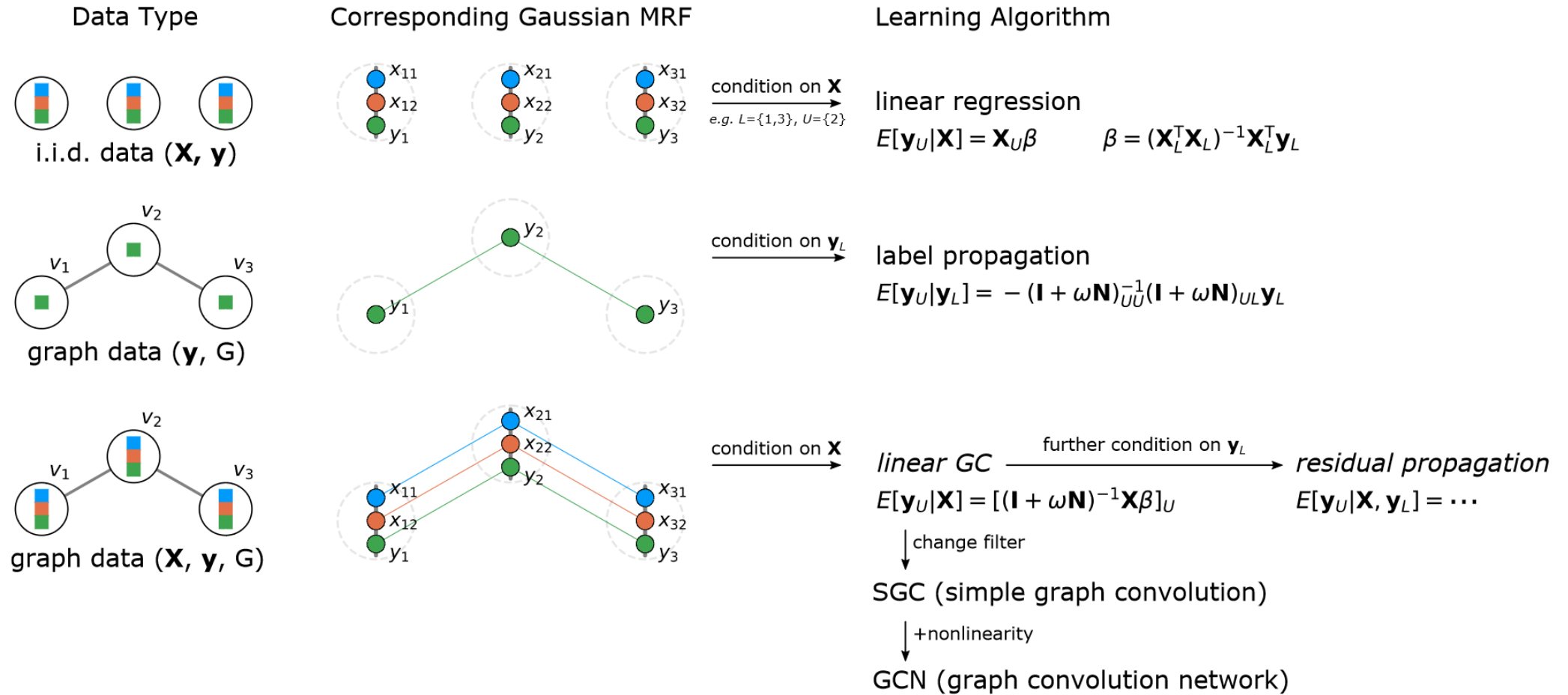
- **2. Using LP on residuals but removing GNNs altogether.**

—— Combining Label Propagation and Simple Models Out-performs Graph Neural Networks. Huang et al., ICLR 2021.

- **3. Statistical framework that unifies LP and GNN ideas.**

—— A Unifying Generative Model for Graph Learning Algorithms: Label Propagation, Graph Convolutions, and Combinations. Jia & Benson, SIAM Journal on Mathematics of Data Science 2022.

3. Statistical framework that unifies LP and GNN ideas.



— A Unifying Generative Model for Graph Learning Algorithms: Label Propagation, Graph Convolutions, and Combinations. Jia & Benson, SIAM Journal on Mathematics of Data Science 2022.

3. Statistical framework that unifies LP and GNN ideas.

- Input:

- Graph $G = (V, E, X, Y)$.
- Node Feature $X \in \mathbb{R}^{|V| \times d}$.
- Known Node Label $y_L \in \{0, 1\}^{|V_L|}$, ($V_L \in V$ The labeled node set.)

- Output:

- Unknown Node Label $y_U \in \{0, 1\}^{|V_U|}$, ($V_U = V \setminus V_L \in V$ the unlabeled node set.)

- **Solution:**

- $y_U = \mathbb{E}[y_U | G, X, y_L]$

3. Statistical framework that unifies LP and GNN ideas.

Linear Graph Conv. (LGC)	Simplified Graph Conv. (SGC)	Graph Conv. Network (GCN)
$(1 - \alpha)(I + \alpha S + \alpha^2 S^2 + \dots)X\beta$	$\tilde{S}^k X\beta$	$\sigma(\tilde{S} \dots \sigma(\tilde{S}XW^1) \dots W^k)\beta$
$S = D^{-1/2}AD^{-1/2}$	$\tilde{S} = (D + I)^{-1/2}(A + I)(D + I)^{-1/2}$	$\tilde{S} = (D + I)^{-1/2}(A + I)(D + I)^{-1/2}$

Dataset	Outcome	LP	LR	LGC (α)	SGC (K)	GCN (K)	LGC/RP	SGC/RP	GCN/RP	h_0	LP (α)	LR	LGC (α)	SGC (K)	GCN (K)	LGC/RP (α)	SGC/RP (K, α)	GCN/RP (K, α)
U.S.	income	0.40	0.63	0.66 (0.46)	0.51 (1.0)	0.53 (1.3)	0.69	0.55	0.55	1	0.19 (0.79)	0.68	0.70 (0.28)	0.37 (1.8)	0.34 (1.7)	0.73 (0.29)	0.40 (1.8, 0.21)	0.37 (1.7, 0.21)
	education	0.31	0.71	0.71 (0.00)	0.43 (1.0)	0.47 (1.0)	0.71	0.46	0.48	10	0.43 (0.95)	0.48	0.58 (0.57)	0.45 (2.1)	0.45 (2.0)	0.68 (0.56)	0.56 (2.1, 0.46)	0.54 (2.0, 0.43)
	unemployment	0.47	0.34	0.39 (0.59)	0.32 (1.3)	0.45 (2.5)	0.54	0.52	0.53	100	0.59 (0.99)	0.24	0.42 (0.85)	0.38 (2.3)	0.45 (2.5)	0.64 (0.85)	0.63 (2.3, 0.81)	0.62 (2.5, 0.79)
	election	0.52	0.42	0.49 (0.68)	0.43 (1.1)	0.52 (2.1)	0.64	0.61	0.61									
CDC	airT	0.95	0.85	0.86 (0.78)	0.86 (2.6)	0.95 (3.0)	0.96	0.97	0.97									
	landT	0.89	0.81	0.81 (0.09)	0.79 (1.0)	0.91 (2.4)	0.90	0.93	0.93									
	precipitation	0.89	0.59	0.61 (0.93)	0.61 (2.3)	0.79 (3.0)	0.89	0.90	0.90									
	sunlight	0.96	0.75	0.81 (0.97)	0.80 (3.0)	0.90 (3.0)	0.96	0.97	0.97									
	pm2.5	0.96	0.21	0.27 (0.99)	0.23 (2.7)	0.78 (3.0)	0.96	0.96	0.97									
London	income	0.46	0.85	0.85 (0.00)	0.64 (1.0)	0.63 (1.0)	0.85	0.65	0.64									
	education	0.65	0.81	0.83 (0.40)	0.74 (1.6)	0.79 (1.4)	0.86	0.77	0.79									
	age	0.65	0.73	0.73 (0.17)	0.66 (1.2)	0.70 (1.7)	0.75	0.72	0.72									
	election	0.67	0.73	0.81 (0.74)	0.74 (2.0)	0.76 (2.1)	0.85	0.78	0.78									
Twitch	days	0.08	0.58	0.59 (0.67)	0.22 (1.4)	0.26 (1.7)	0.60	0.23	0.26									

- GCN more expressive but prone to overfitting.
- More homophily \rightarrow larger K, α
- Adding residual prop never hurts!
- GCN better with more homophily?
“memorizing” neighborhood features (zero training error)
+ smoothness in data \rightarrow better out-of-sample prediction

— *A Unifying Generative Model for Graph Learning Algorithms: Label Propagation, Graph Convolutions, and Combinations.* Jia & Benson, *SIAM Journal on Mathematics of Data Science* 2022.

— *Graph Signal Processing: Overview, Challenges and Applications.* Ortega & etc., *Proceedings of the IEEE* 2018.

A decorative graphic consisting of several overlapping, semi-transparent rings in shades of blue and green, arranged in a circular pattern around the central text.

5. Rethinking about Future



LP is a powerful tool:

- Applied to residuals (correlated errors), features (smoothing / de-noising), final predictions (more smoothness)
- Linear models are often superior to nonlinear ones (GNNs) in TNC.

Few-shot on Graph:

- Even nothing holds meaning.
- Even a lack can suffice.

Feature? Label?

- Feature: attribute we use.
- Label: attribute we predict.



Residual?

- Explicitness: What we need to correct.
- Implicitness: **Influence** we have modeled.



Transductive? Inductive?

- Learning the influence of the lack component in the Few-shot Problem.
- Latent law.

Reference

- [1] Deep Long-Tailed Learning: A Survey, Zhang & etc., PAMI 2023.
- [2] A Survey of Imbalanced Learning on Graphs: Problems, Techniques, and Future Directions, Liu & etc., arXiv 2023.
- [3] A Survey on Graph Neural Networks for Time Series: Forecasting, Classification, Imputation, and Anomaly Detection, Jin & etc., arXiv 2023.
- [4] Learning to Propagate Labels: Transductive Propagation Network for Few-shot Learning. Liu & etc., ICLR 2019.
- [5] Inductive Representation Learning on Large Graphs. Hamilton & etc., NIPS 2017.
- [6] Semi-Supervised Learning Using Gaussian Fields and Harmonic Functions. Zhu & etc., ICML 2003.
- [7] Predict then Propagate: Graph Neural Networks meet Personalized PageRank. Gasteiger & etc., ICLR 2019.
- [8] The Anatomy of a Large-Scale Hypertextual Web Search Engine. Brin & Page, Computer networks and ISDN systems, 1998.
- [9] Unifying Graph Convolutional Neural Networks and Label Propagation. Wang & Leskovec., arXiv 2020.
- [10] Graph Attention Networks. Velickovic & etc., ICLR 2018.
- [11] Masked Label Prediction: Unified Message Passing Model for Semi-Supervised Classification. Shi & etc., IJCAI 2021.
- [12] Training Sparse Neural Networks. Srinivas& etc., CVPR Workshops, 2017.
- [13] Residual Correlation in Graph Neural Network Regression. Jia & Benson, KDD 2020.
- [14] Combining Label Propagation and Simple Models Out-performs Graph Neural Networks. Huang et al., ICLR 2021.
- [15] A Unifying Generative Model for Graph Learning Algorithms: Label Propagation, Graph Convolutions, and Combinations. Jia & Benson, SIAM Journal on Mathematics of Data Science 2022.
- [16] Graph Signal Processing: Overview, Challenges and Applications. Ortega & etc., Proceedings of the IEEE 2018.
- [17] Stanford CS224W: Label propagation on graph, Leskovec, <http://web.stanford.edu/class/cs224w/slides/08-message.pdf>.
- [18] Label Propagation and Graph Neural Networks, Benson & etc., <https://www.cs.cornell.edu/~arb/slides/2021-03-12-northeastern.pdf>.

Thx for Q&A :)

