



PASCA:可扩展的图神经网络搜索系统

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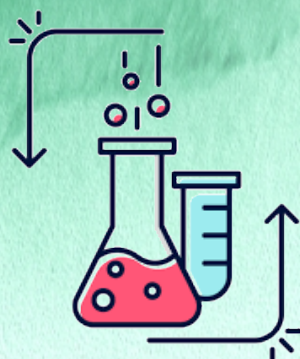
大纲



1. □□



2. 方法



3. □□



4. □□



1.问题





图数据

许多数据都是以图的形式存在:



社交网络



知识图谱



药物和新材料

图神经网络被广泛应用于多个场景:

- 推荐系统
- 异常检测
- 药物发现
- 蛋白质结构预测



图卷积神经网络(GCN)的表达形式:

第 $l+1$ 层的节点表示

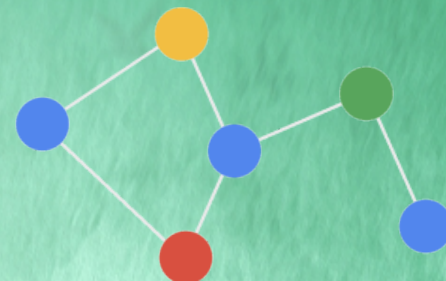
度矩阵

第 l 层的节点表示

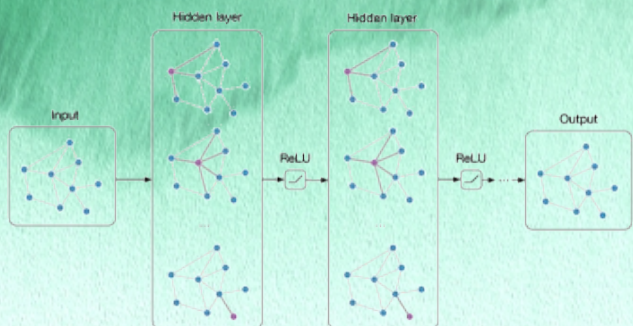
$$\mathbf{X}^{(l+1)} = \delta \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \mathbf{X}^{(l)} \mathbf{W}^{(l)} \right)$$

含自环的邻接矩阵

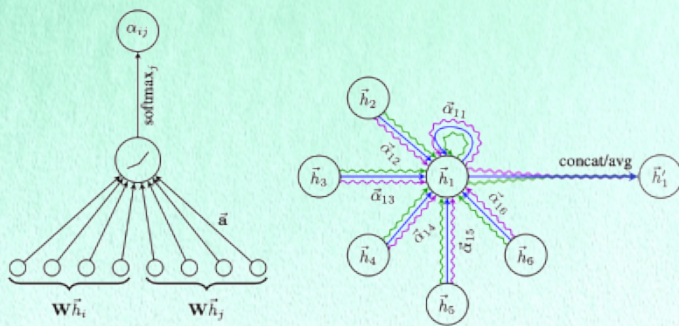
第 l 层的模型参数



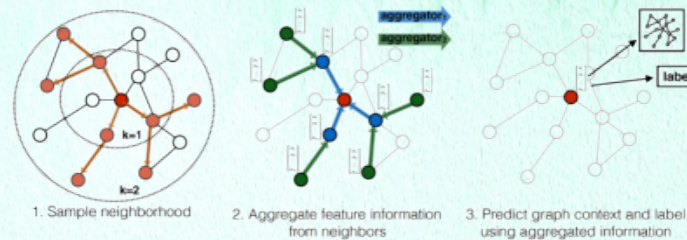
- 通过消息传播机制聚合高阶邻居的信息
- 提升自身的表达能力



GCN



GAT



GraphSAGE



- [1] Kipf T N, Welling M. Semi-supervised classification with graph convolutional networks. ICLR, 2017.
- [2] Veličković P, Cucurull G, Casanova A, et al. Graph Attention Networks. ICLR. 2018.
- [3] Hamilton W, Ying Z, Leskovec J. Inductive representation learning on large graphs. NeurIPS, 2017.



Neural Message Passing (消息传递机制)

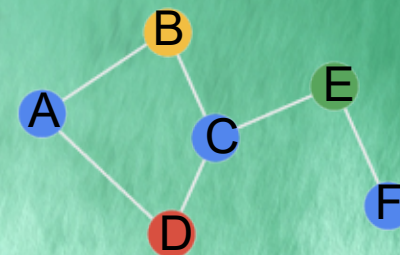
- 传统的GNN (如GCN[1], GAT[2]) 都遵循 neural message passing (NMP, 消息传递机制) paradigm:

- Aggregate the neighborhood information (通信)

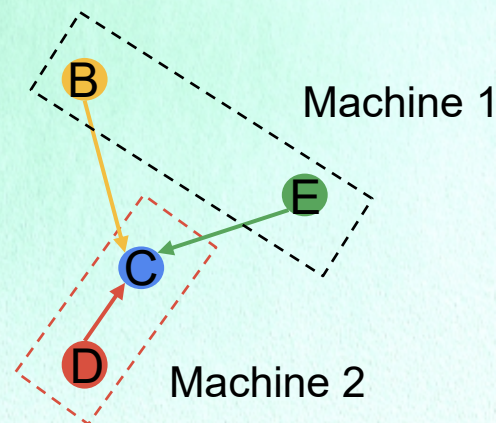
- Update the message via neural networks (计算)
$$\mathbf{m}_v^t \leftarrow \text{aggregate}(\{\mathbf{h}_u^{t-1} | u \in \mathcal{N}_v\})$$

$$\mathbf{h}_v^t \leftarrow \text{update}(\mathbf{m}_v^t)$$

- 缺点: **频繁地** 从其他机器上拉取信息 \rightarrow 大规模图数据上每个epoch都有的高通信开销



输入图



[1] Thomas N Kipf and Max Welling. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In ICLR.

[2] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. 2018. Graph Attention Networks. In ICLR.





GNN 系统

大多数GNN系统使用消息传播机制

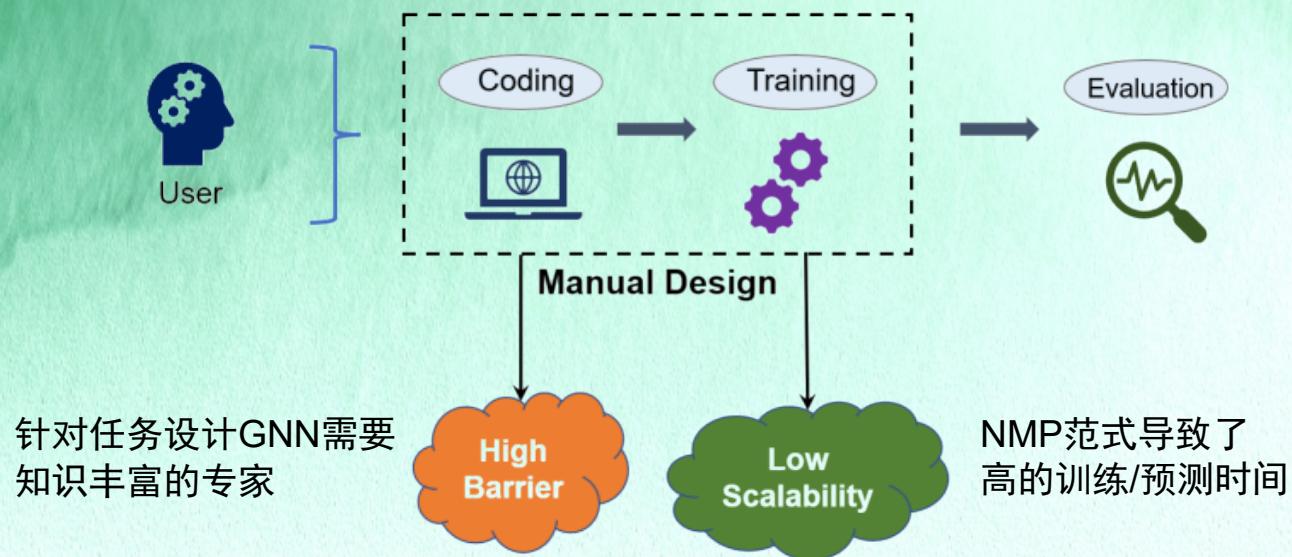


DGL[1]



PyG[2]

大□模□数据□来的挑□



[1] <https://github.com/dmlc/dgl>

[2] https://github.com/pyg-team/pytorch_geometric





瓶颈

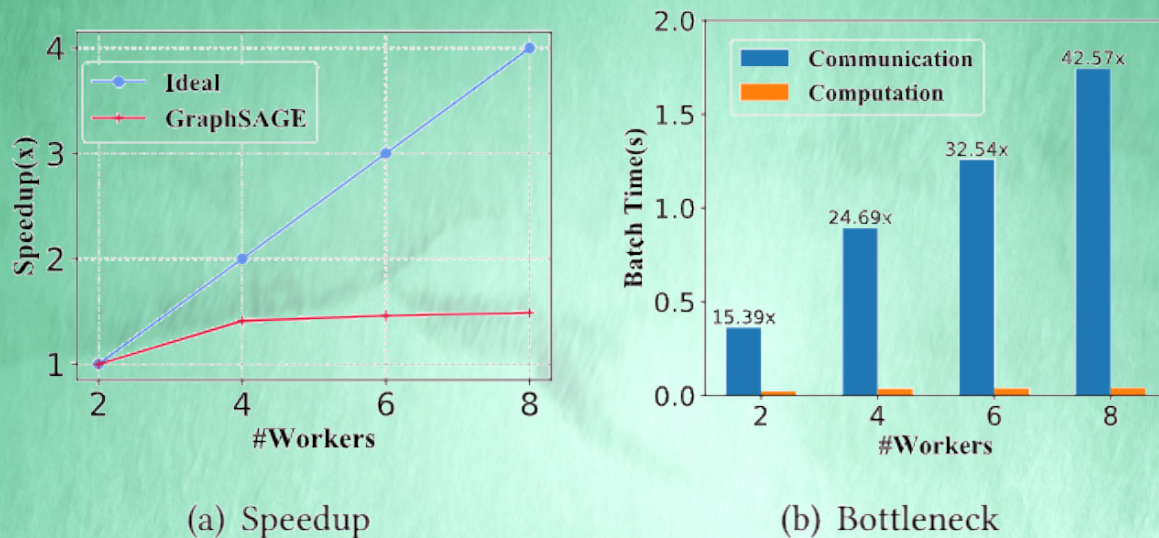


Figure 2: The speedup and bottleneck of a two-layer GraphSAGE along with the increased workers on Reddit dataset.

可扩展性：受制于单机的存储开销和分布式通讯开销，现有的消息传递机制不能很好地扩展到大图上。

- 增加更多机器时候，加速比增长不明显
- 通信开销占比过大

目标：如何兼顾GNN的可扩展性，设计使用门槛低的图神经网络系统？





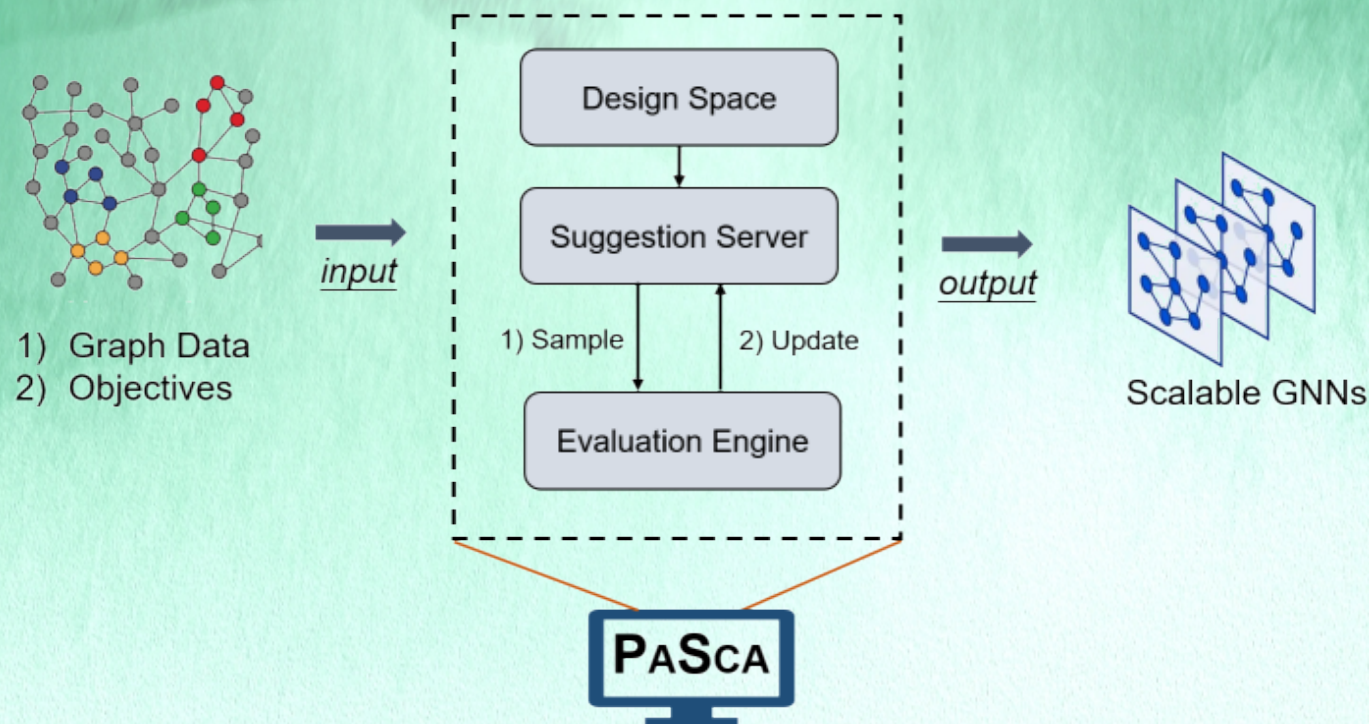
2.方法





系统目标

- 输入: 图数据 + 优化目标
- 输出: 能兼顾多个优化目标的**Scalable GNN**



端到端系统，无需人为定义网络结构和训练流程

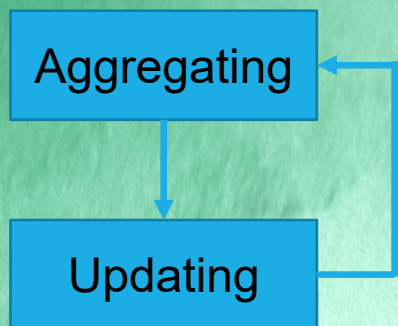




方法概览

- Scalable Graph Neural Architecture Paradigm (SGAP建模范式)
 - 定义可扩展训练流程的抽象
- 自动搜索系统 (PaSca)

不可扩展的设计



Fetch information **during** training

The number of training epochs

可扩展的设计



Fetch information **before and after** training

Twice

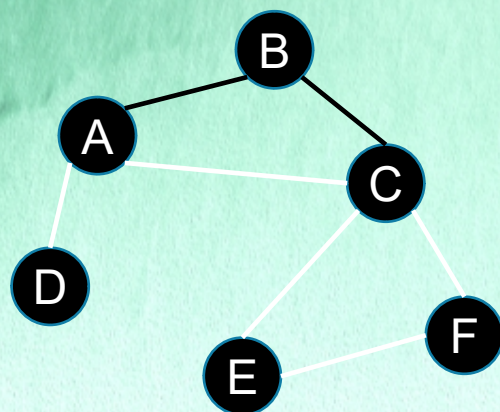
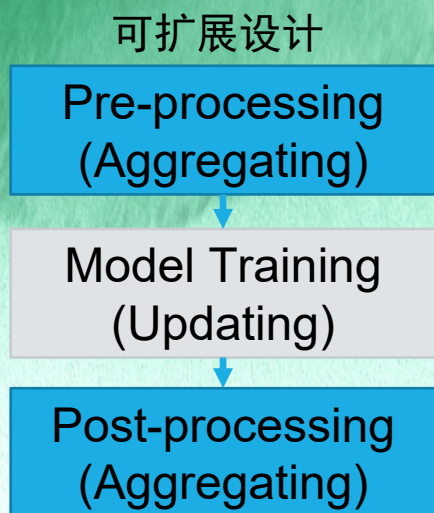




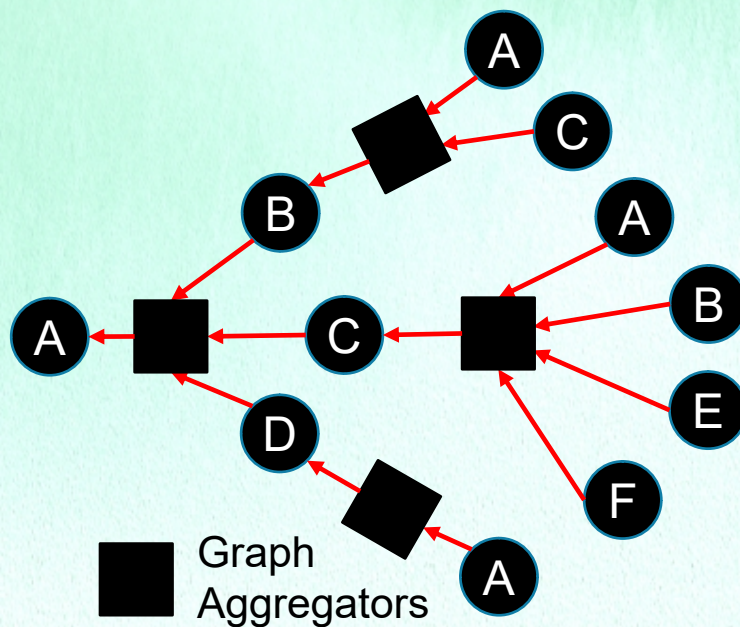
SGAP 抽象

- 预处理
 - 从邻居节点聚合消息 (特征)
- 后处理
 - 从邻居节点聚合消息 (软标签)

$$\mathbf{m}_v^t \leftarrow \text{graph_aggregator} \left(\{ \mathbf{m}_u^{t-1} | u \in \mathcal{N}_v \} \right)$$



Input Graph





Graph Aggregator (图聚合器)

- 抽象 $\mathbf{m}_v^t \leftarrow \text{graph_aggregator} \left(\{ \mathbf{m}_u^{t-1} | u \in \mathcal{N}_v \} \right)$
- Augmented normalized adjacency (used in GCN[1])

$$\mathbf{m}_v^t = \sum_{u \in \mathcal{N}_v} \frac{1}{\tilde{d}_u} \mathbf{m}_u^{t-1}$$

- Personalized PageRank (used in APPNP[2])

$$\mathbf{m}_v^t = \alpha \mathbf{m}_v^0 + (1 - \alpha) \sum_{u \in \mathcal{N}_v} \frac{1}{\sqrt{\tilde{d}_v \tilde{d}_u}} \mathbf{m}_u^{t-1}$$

- Triangle-induced adjacency (used MotifNet[3])

$$\mathbf{m}_v^t = \sum_{u \in \mathcal{N}_v} \frac{1}{d_v^{tri}} \mathbf{m}_u^{t-1}$$

[1] Thomas N Kipf and Max Welling. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In ICLR.

[2] Johannes Klicpera, Aleksandar Bojchevski, and Stephan Günnemann. 2019. Predict then Propagate: Graph Neural Networks meet Personalized PageRank. In ICLR.

[3] Federico Monti, Karl Otness, and Michael M Bronstein. 2018. Motifnet: a motif-based graph convolutional network for directed graphs. In 2018 IEEE Data Science Workshop (DSW). IEEE, 225–228.





SGAP 抽象

• 训练

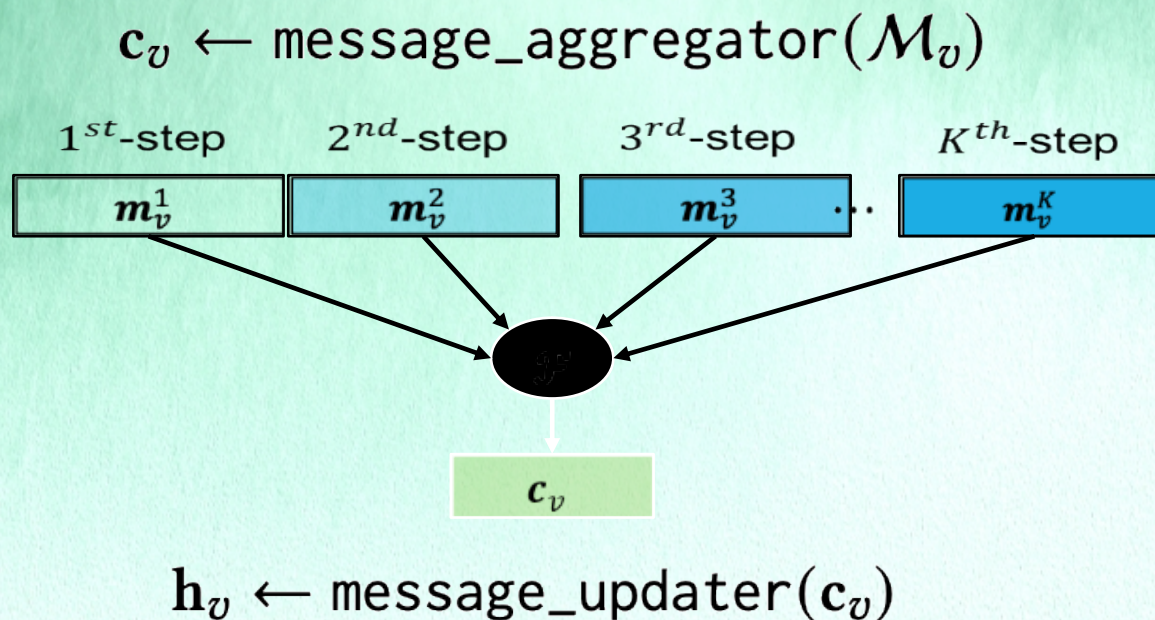
- 聚合来自预处理阶段的消息
- 更新聚合后的消息

可扩展设计

Pre-processing
(Aggregating)

Model Training
(Updating)

Post-processing
(Aggregating)





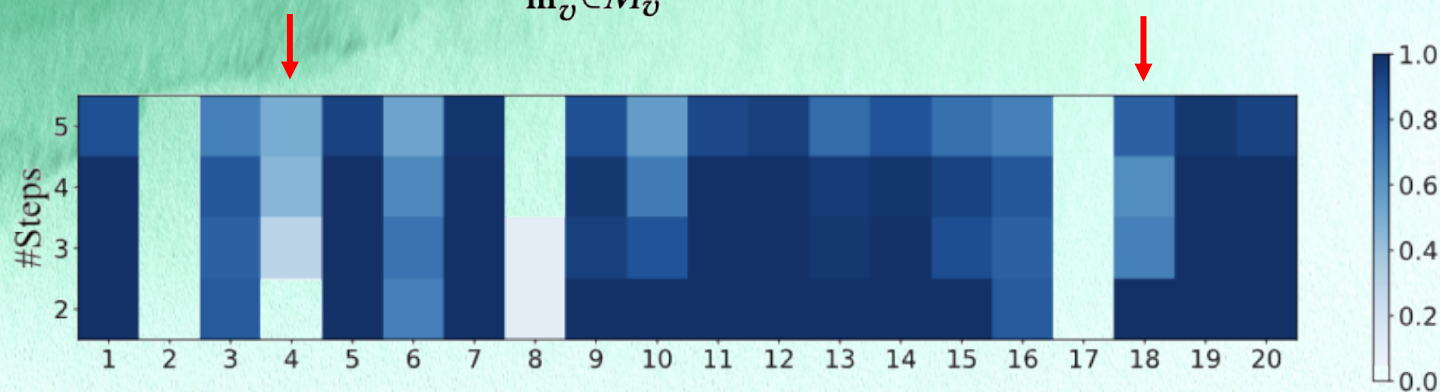
Message Aggregator (消息聚合器)

- 抽象 $c_v \leftarrow \text{message_aggregator}(\mathcal{M}_v)$
- 非自适应聚合器 (mean, max)

$$c_{msg} \leftarrow \oplus_{\mathbf{m}_v^i \in \mathcal{M}_v} w_i f(\mathbf{m}_v^i)$$

- 自适应聚合器 (gate with trainable parameters)

$$c_{msg} \leftarrow \sum_{\mathbf{m}_v^i \in \mathcal{M}_v} w_i \mathbf{m}_v^i, \quad w_i = \sigma(\mathbf{s} \mathbf{m}_v^i)$$



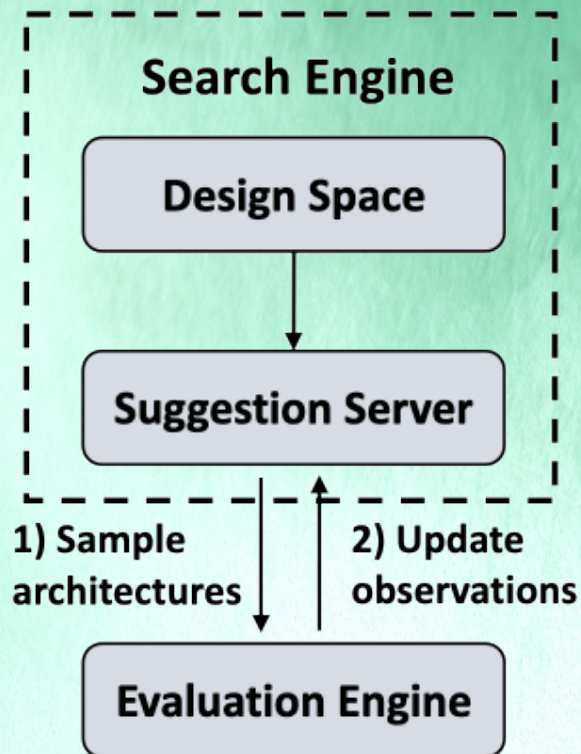
应该给不同节点的不同层表示消息不同的权重!





方法概览

- 可扩展范式 (SGAP)
- 自动化搜索系统 (PaSca)
 - 两个模块
 - (自动化) 搜索引擎
 - (分布式) 评估引擎
 - 搜索引擎推荐一个 configuration instance.
 - 评估引擎 **评估 被推荐的** configuration instance.



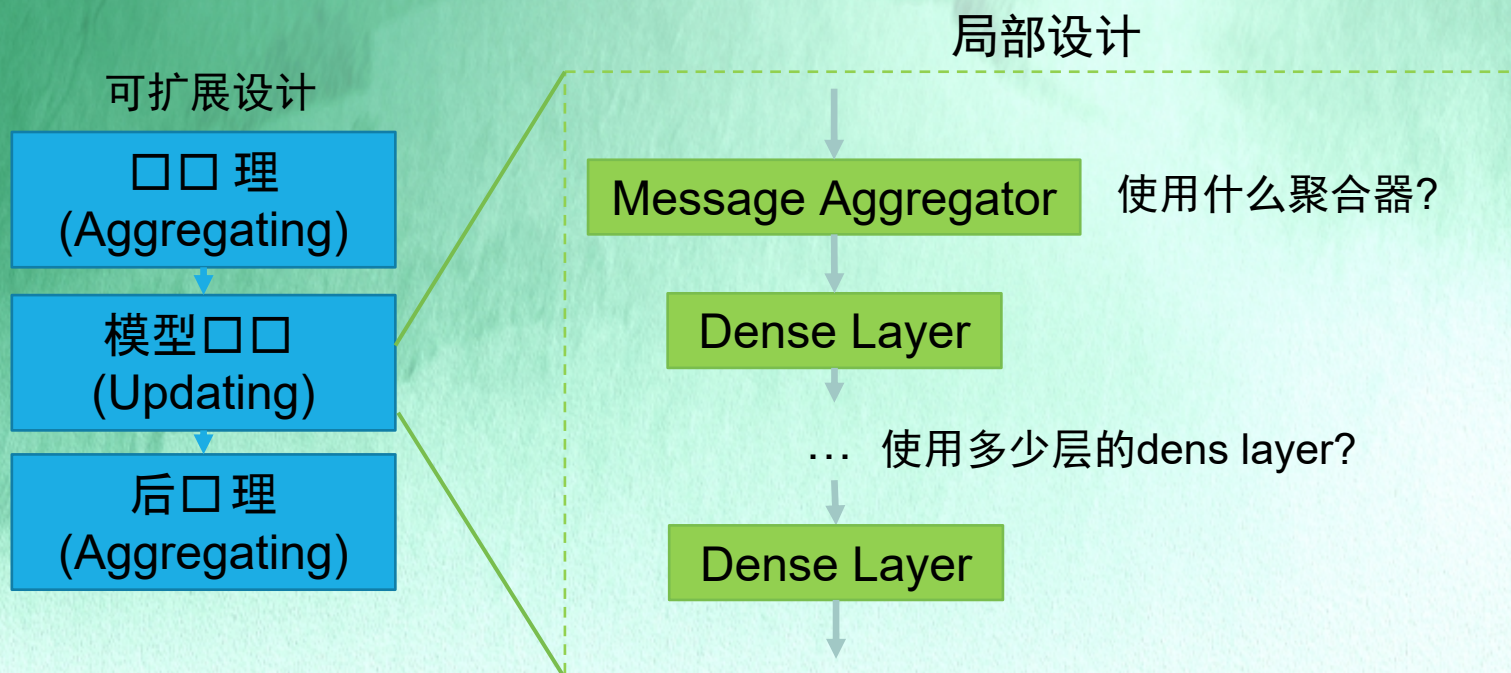
Searching





Search Engine (搜索引擎)

- 处理不同优化目标之间的 tradeoff
- 设计空间: 在SGAP 3 个阶段的局部设计 (参数)





Design Space (设计空间)

- 6 个参数可供选择 + 每个阶段2个参数
- 超过 150k 种可能的 configuration instances

Stages	Name	Range/Choices	Type
Pre-processing	Aggregation steps (K_{pre})	[0, 10]	Integer
	Graph aggregators (GA_{pre})	{Aug.NA, PPR($\alpha = 0.1$), PPR($\alpha = 0.2$), PPR($\alpha = 0.3$), Triangle. IA}	Categorical
Model training	Message aggregators (MA)	{None, Mean, Max, Concatenate, Weighted, Adaptive}	Categorical
	Transformation steps (K_{trans})	[1, 10]	Integer
Post-processing	Aggregation steps (K_{post})	[0, 10]	Integer
	Graph aggregators (GA_{post})	{Aug.NA, PPR($\alpha = 0.1$), PPR($\alpha = 0.2$), PPR($\alpha = 0.3$), Triangle. IA}	Categorical

- 现有的Scalable GNN都存在于我们设定的空间中

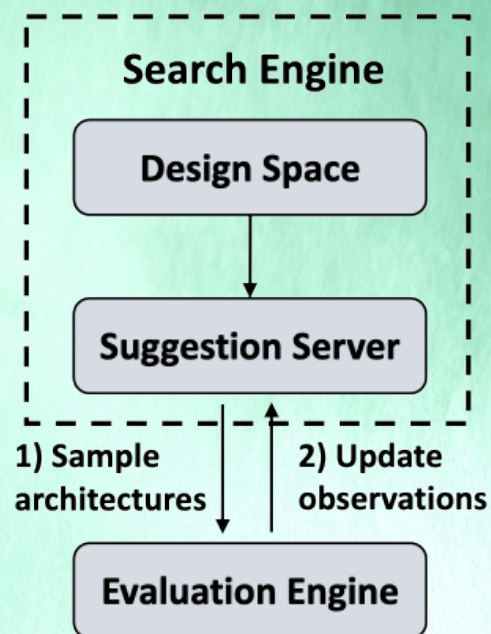
Models	Pre-processing	Model training		Post-processing
	GA_{pre}	MA	K_{trans}	GA_{post}
SGC	Aug.NA	None	1	/
SIGN	Optional	Concatenate	1	/
S ² GC	PPR	Mean	1	/
GBP	Aug.NA	Weighted	≥ 2	/
PASCA-APPNP	/	/	≥ 2	PPR





Suggestion Server (推荐服务器)

- 建模 配置 和 优化目标之间的关系
- 推荐 能兼容多个优化目标的配置
- 更新 历史得到的历史数据

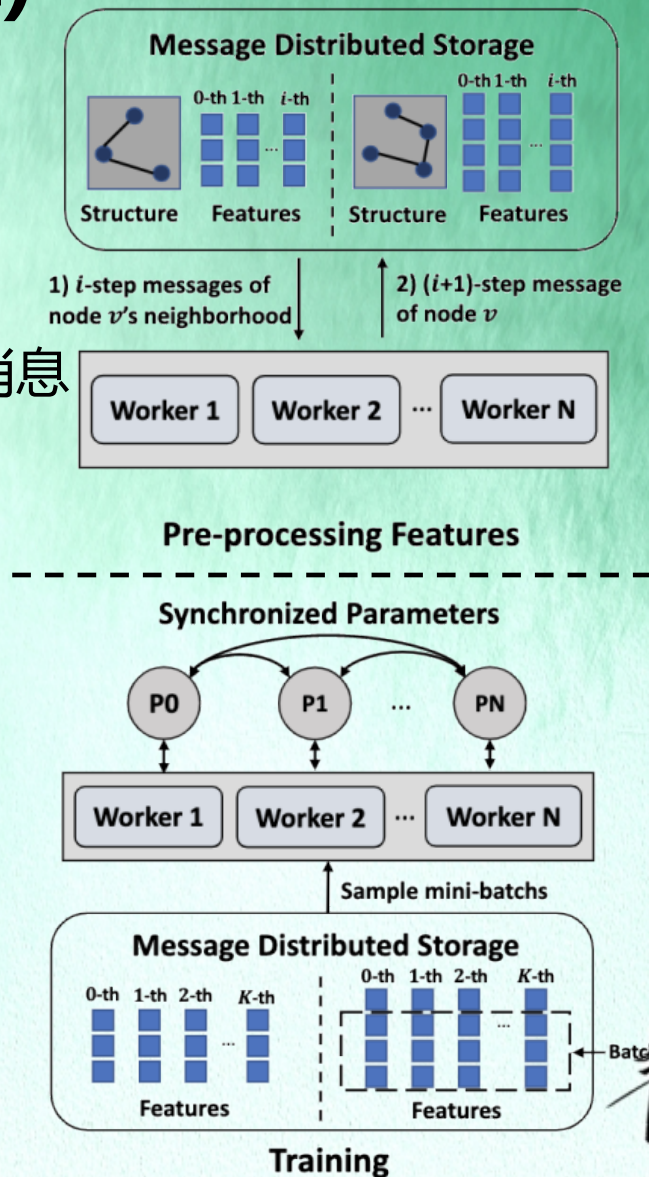


Searching



Evaluation Engine (评估引擎)

- Graph data aggregator (图数据聚合器)
 - 切分大图
 - 基于已经计算好的第 (i) 步消息来 计算第(i+1) 步消息
- Neural architecture trainer (网络结构训练器)
 - Mini-batch 训练
 - 基于parameter server的异步网络更新





3.实验





实验设置

数据集

Dataset	#Nodes	#Features	#Edges	#Classes	#Train/Val/Test	Task type	Description
Cora	2,708	1,433	5,429	7	140/500/1000	Transductive	citation network
Citeseer	3,327	3,703	4,732	6	120/500/1000	Transductive	citation network
Pubmed	19,717	500	44,338	3	60/500/1000	Transductive	citation network
Amazon Computer	13,381	767	245,778	10	200/300/12881	Transductive	co-purchase graph
Amazon Photo	7,487	745	119,043	8	160/240/7,087	Transductive	co-purchase graph
ogbn-products	2,449,029	100	61,859,140	47	195922/489811/204126	Transductive	co-purchase network
Coauthor CS	18,333	6,805	81,894	15	300/450/17,583	Transductive	co-authorship graph
Coauthor Physics	34,493	8,415	247,962	5	100/150/34,243	Transductive	co-authorship graph
Flickr	89,250	500	899,756	7	44,625/22,312/22,312	Inductive	image network
Reddit	232,965	602	11,606,919	41	155,310/23,297/54,358	Inductive	social network
Industry	1,000,000	64	1,434,382	253	5,000/10,000/30,000	Transductive	user-video graph

验证目标

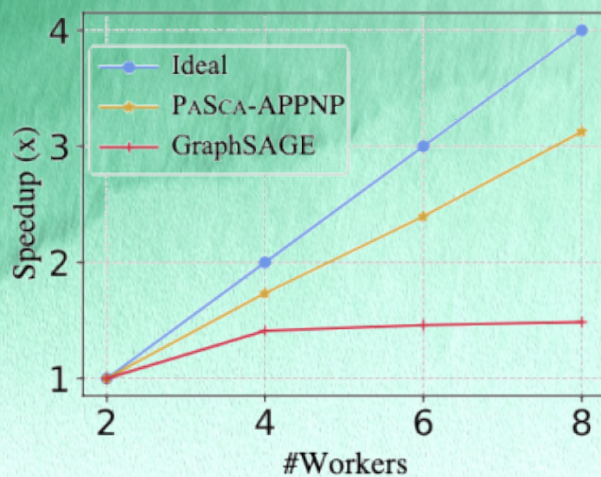
- SGAP 比基于NMP的消息传递机制 **更 *scalable***。
- PaSca搜索出来的结果能够很好地处理 **不同搜索目标之间的tradeoff**。
- 搜索结构能够取得 **更高的预测性能**。



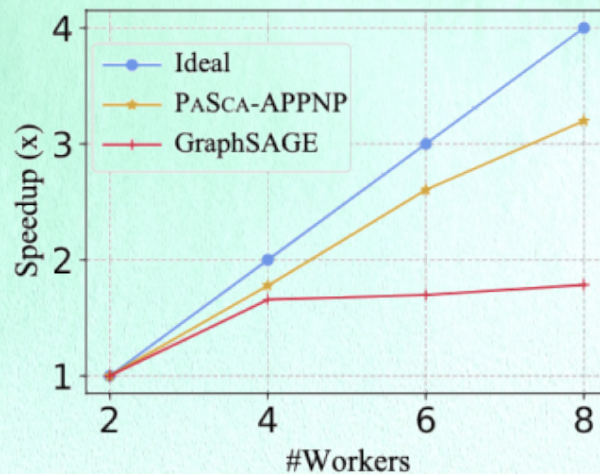


Scalability Analysis (可扩展性分析)

- 对比方法
 - SGAP: 基于 SGAP 和 PaSca评估引擎的APPNP
 - NMP: 基于DistDGL的GraphSAGE
- 基于 SGAP 可以取得接近线性的加速比并且更加接近理想的加速比。



Reddit (>230K
nodes)



ogbn-product (>2.4M
nodes)





Search Representatives (代表性方法)

- 代表性方法 (在帕累托平面上的)
 - 从SGAP设计空间搜索出来的方法能兼顾多个搜索目标之间的tradeoff。
 - PaSca-V3 取得了最低的预测误差但带来了比PaSca-V2更长的预测时间。
- 我们搜索出来的结果GBP[1], 一个 SOTA 的可扩展网络结构

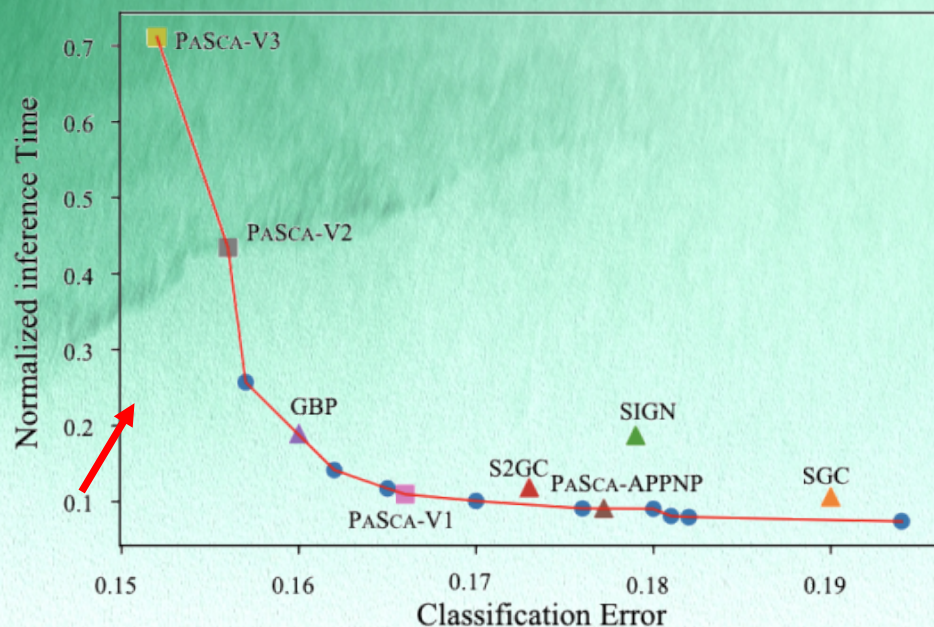


Table 3: Scalable GNNs found by PaSca.

Models	Pre-processing			Model training K_{trans}	Post-processing	
	GA_{pre}	MA	K_{pre}		GA_{post}	K_{post}
PaSca-V1	PPR($\alpha = 0.1$)	Weighted	3	2	/	/
PaSca-V2	Aug.NA	Adaptive	6	2	/	/
PaSca-V3	Aug.NA	Adaptive	6	3	PPR ($\alpha = 0.3$)	4

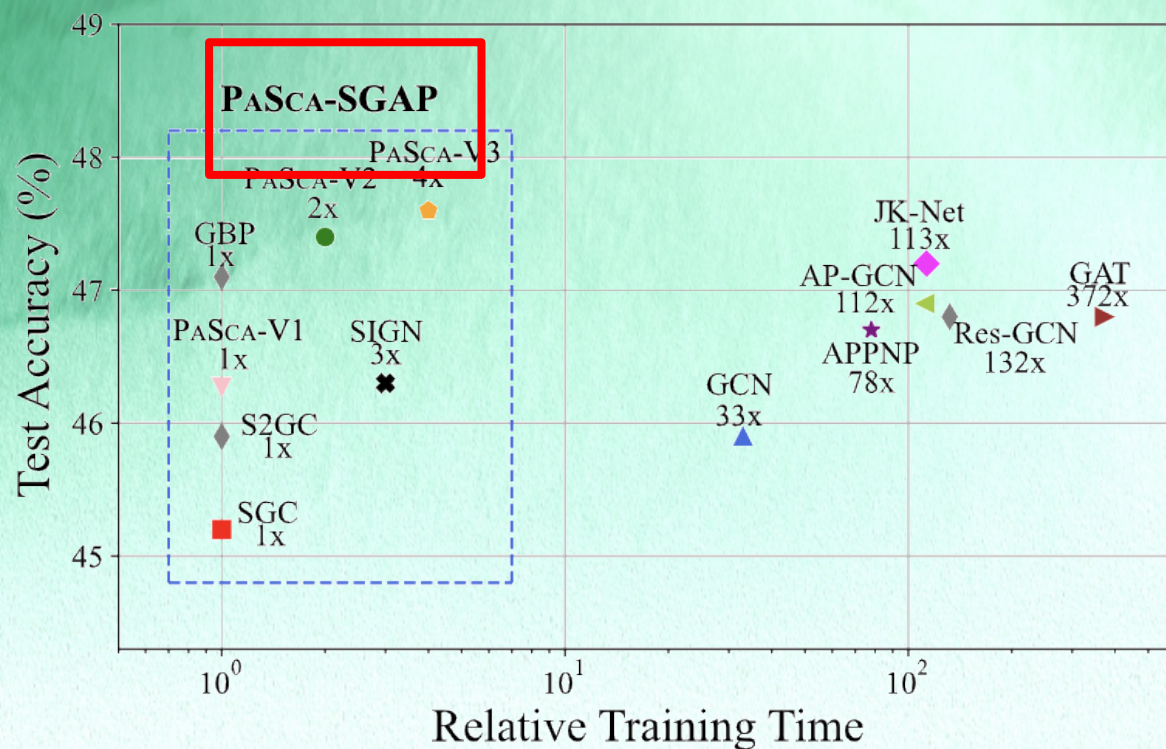
[1] Chen M, Wei Z, Ding B, et al. 2020. Scalable graph neural networks via bidirectional propagation[J]. In NeurIPS.





Search Representatives (代表性方法)

- 搜索出来的模型能很好兼顾训练时间与测试准确率。
- PaSca V2 和 V3 都获得了比 JK-Net 更好的准确率，但是只需要明显更少的训练时间。





预测性能

- 和其他不scalable的建模范式相比，基于SGAP的网络结构 能取得有竞争力的模型性能。
- PaSca-V3 在不同数据集上都取得了最好的性能。

Type	Models	Cora	Citeseer	PubMed	Amazon Computer	Amazon Photo	Coauthor CS	Coauthor Physics	Industry
NMP	GCN	81.8±0.5	70.8±0.5	79.3±0.7	82.4±0.4	91.2±0.6	90.7±0.2	92.7±1.1	45.9±0.4
	GAT	83.0±0.7	72.5±0.7	79.0±0.3	80.1±0.6	90.8±1.0	87.4±0.2	90.2±1.4	46.8±0.7
	JK-Net	81.8±0.5	70.7±0.7	78.8±0.7	82.0±0.6	91.9±0.7	89.5±0.6	92.5±0.4	47.2±0.3
	ResGCN	82.2±0.6	70.8±0.7	78.3±0.6	81.1±0.7	91.3±0.9	87.9±0.6	92.2±1.5	46.8±0.5
DNMP	APNP	83.3±0.5	71.8±0.5	80.1±0.2	81.7±0.3	91.4±0.3	92.1±0.4	92.8±0.9	46.7±0.6
	AP-GCN	83.4±0.3	71.3±0.5	79.7±0.3	83.7±0.6	92.1±0.3	91.6±0.7	93.1±0.9	46.9±0.7
SGAP	SGC	81.0±0.2	71.3±0.5	78.9±0.5	82.2±0.9	91.6±0.7	90.3±0.5	91.7±1.1	45.2±0.3
	SIGN	82.1±0.3	72.4±0.8	79.5±0.5	83.1±0.8	91.7±0.7	91.9±0.3	92.8±0.8	46.3±0.5
	S ² GC	82.7±0.3	73.0±0.2	79.9±0.3	83.1±0.7	91.6±0.6	91.6±0.6	93.1±0.8	45.9±0.4
	GBP	83.9±0.7	72.9±0.5	80.6±0.4	83.5±0.8	92.1±0.8	92.3±0.4	93.3±0.7	47.1±0.6
	PaSca-V1	83.4±0.5	72.2±0.5	80.5±0.4	83.7±0.7	92.1±0.7	91.9±0.3	93.2±0.6	46.3±0.4
	PaSca-V2	84.4±0.3	73.1±0.3	80.7±0.7	84.1±0.7	92.4±0.7	92.6±0.4	93.6±0.8	47.4±0.6
	PaSca-V3	84.6±0.6	73.4±0.5	80.8±0.6	84.8±0.7	92.7±0.8	92.8±0.5	93.8±0.9	47.6±0.3





4.总结





总结

- **系统实现**：我们设计了PaSca, 一个新颖的构建和探索可扩展 GNNs的网络结构搜索系统，而不是仅研究单个的网络结构设计。
- **多目标自动化搜索**：PaSca搜索出来的代表性模型能够在预测性能、效率以及可扩展性等多个方面超越现有的SOTA GNN 模型。
- **SGAP建模范式**：PaSca能够帮助研究者来探索不同的Scalable GNN结构设计，并且理解不同设计的特点和功能。





工作应用与影响力

- 与腾讯TEG机器学习平台部合作，实现了能自动化建模10亿节点的**超大规模图神经网络系统**，部署于腾讯太极机器学习平台，并广泛应用于**视频推荐**和**内容风控**等场景
- 系统部分功能已在Github开源：<https://github.com/PKU-DAIR/SGL>
- 系统论文获得**CCF A类数据挖掘旗舰会议WWW 2022** 唯一**“最佳学生论文奖”**（中国第2个）
- 系统相关工作刷新了国际图学习榜单**OGB的3项第一**，获腾讯**年度开源协同创新奖**和**世博会领先科技成果奖**

Best Student Paper Award

PaSca: a Graph Neural Architecture Search System under the Scalable Paradigm
Systems and Infrastructure Track



<https://www2022.thewebconf.org/awards/>

Leaderboard for ogbn-mag

The classification accuracy on the test and validation sets. The higher, the better.

Package: $\geq 1.2.1$

Rank	Method	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	NARS-GAMILP+RLU	0.5590 ± 0.0027	0.5702 ± 0.0041	Wentao Zhang (PKU Tencent Joint Lab)	Paper, Code	6,734,882	Tesla V100 (32GB)	Aug 19, 2021

腾讯Angel Graph团队刷新GNN最强榜单OGB世界纪录!



腾讯大数据 2021-09-01 17:39

刷新国际图学习榜单

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





第一作者论文总结

- 共发表论文29篇，含CCF推荐**A类论文24篇**，**第一作者**论文覆盖**机器学习三大会**(ICML*2, NeurIPS*2和ICLR*1)、**数据库三大会**(SIGMOD*2, VLDB*1和ICDE*1) 和**数据挖掘顶会**(KDD*3和WWW*1)
 - 以**第一作者**发表在CCF A类**数据挖掘旗舰会议WWW 2022** (国际万维网大会) 的论文获得1822篇投稿中**唯一“最佳学生论文奖”**
 - 以**第一作者**在CCF A类**机器学习旗舰会议NeurIPS 2021**发表**2篇“Spotlight 焦点论文”** (录取率 < 3%)
1. [WWW 2022] PASCA : a New Paradigm and System to Build Scalable Graph Neural Network (CCF A, 第一作者, **最佳学生论文奖**)
 2. [KDD 2022] Graph Attention Multi-Layer Perceptron (CCF A, 第一作者)
 3. [KDD 2022] An Empirical Study of Deep Graph Neural Networks (CCF A, 第一作者)
 4. [KDD 2021] ROD : Reception-aware Online Distillation for Sparse Graphs (CCF A, 第一作者)
 5. [SIGMOD 2021] ALG : Fast and Accurate Active Learning Framework for Graph Convolutional Networks (CCF A, 第一作者)
 6. [SIGMOD 2020] Reliable Data Distillation on Graph Convolutional Network (CCF A, 第一作者)
 7. [VLDB 2021] Grain : Improving Data Efficiency of Graph Neural Networks via Diversified Influence Maximization (CCF A, 第一作者)
 8. [ICDE 2020] Efficient Diversity-Driven Ensemble for Deep Neural Networks (CCF A, 第一作者)
 9. [ICLR 2022] Information Gain Propagation : a New Way to Graph Active Learning with Soft Labels (ML三大会之一, 第一作者)
 - 10.[ICML 2022] NAFS: A Simple yet Tough-to-beat Baseline for Graph Representation Learning. (CCF A, 第一作者)
 - 11.[ICML 2022] Deep and Flexible Graph Neural Architecture Search. (CCF A, 第一作者)
 - 12.[NeurIPS 2021] Node Dependent Local Smoothing for Scalable Graph Learning (CCF A, 第一作者, **Spotlight论文**)
 - 13.[NeurIPS 2021] RIM : Reliable Influence-based Active Learning on Graphs (CCF A, 第一作者, **Spotlight论文**)
 - 14.[SCIS 2020] Snapshot Boosting : A Fast Ensemble Framework for Deep Neural Networks (CCF B, 第一作者)
 - 15.[软件学报] 图嵌入算法的分布式优化与实现 (中文CCF A, 第一作者)





其他论文（共同一作*，通讯作者+）

1. [CSUR 2022] Shiwen Wu, Fei Sun, **Wentao Zhang**⁺, Xu Xie, Bin Cui⁺. Graph Neural Networks in Recommender Systems: A Survey. ACM Computing Survey 2022. (CCF A).
2. [TKDE 2021] Xupeng Miao*, **Wentao Zhang**^{*}, Yingxia Shao et al. Lasagne : A Multi-Layer Graph Convolutional Network Framework via Node-aware Deep Architecture. (CCF A).
3. [KDD 2021] Xupeng Miao*, Nezihe Merve Gürel*, **Wentao Zhang**^{*}, ..., Shuai Zhang, Yujie Wang, Bin Cui, Ce Zhang. DeGNN: Characterizing and Improving Graph Neural Networks with Graph Decomposition. (CCF A).
4. [ICDE 2021] Xupeng Miao*, **Wentao Zhang**^{*}, Yingxia Shao et al. Lasagne : A Multi-Layer Graph Convolutional Network Framework via Node-aware Deep Architecture (Extended Abstract). (CCF A).
5. [KDD 2022] Yang Li, Yu Shen, Huaijun Jiang, Tianyi Bai, **Wentao Zhang**, Ce Zhang, Bin Cui. Transfer Learning based Search Space Design for Hyperparameter Tuning. (CCF A).
6. [KDD 2022] Yang Li, Yu Shen, Huaijun Jiang, **Wentao Zhang**, Zhi Yang, Ce Zhang, Bin Cui. TransBO: Hyperparameter Optimization via Two-Phase Transfer Learning. (CCF A).
7. [ICDE 2022] Yuezihan Jiang, Yu Cheng, Hanyu Zhao, Wentao Zhang, Xupeng Miao, Liang Wang, Yu He, Zhi Yang, Bin Cui. Zoomer : Improving and Accelerating Recommendation on Web-Scale Graphs via Regions of Interests. (CCF A).
8. [VLDB 2022] Yang Li, Yu Shen, Huaijun Jiang, Wentao Zhang, Jixiang Li, Ji Liu, Ce Zhang, Bin Cui. Hyper-Tune : Towards Efficient Hyper-parameter Tuning at Scale. (CCF A).
9. [VLDB 2021] Yang Li, Yu Shen, **Wentao Zhang**, ..., Wentao Wu, Ce Zhang, Bin Cui. VolcanoML : Speeding up End-to-End AutoML via Scalable Search Space. International Conference on Very Large Data Bases. (CCF A).
10. [KDD 2021] Yang Li, Yu Shen, **Wentao Zhang**, ..., Ce Zhang, Bin Cui. OpenBox : A Generalized Black-box Optimization Service. SIGKDD Conference on Knowledge Discovery and Data Mining. (CCF A).
11. [KBS 2021] Shiwen Wu, Yuanxing Zhang, **Wentao Zhang**, Kaigui Bian, Bin Cui. Enhanced review-based rating prediction by exploiting aside information and user influence. Knowledge Based System (JCR Q1, IF=8.038).
12. [VLDBJ] Yang Li, Yu Shen, Wentao Zhang, Ce Zhang, Bin Cui. VolcanoML : Speeding up End-to-End AutoML via Scalable Search Space. International Conference on Very Large Data Bases. (CCF A).
13. [ACM SAC 2022] Shicheng Gao, Jie Xu, Xiaosen Li, Fangcheng Fu, **Wentao Zhang**, Wen Ouyang, Yangyu Tao and Bin Cui. K-Core Decomposition on Super Large Graphs with Limited Resources.
14. [Bioinformatics 2022] Yang Bai, Yang Li, Yu Shen, Mingyu Yang, **Wentao Zhang**, Bin Cui. AutoDC: an Automatic Machine Learning Framework for Disease Classification. (CCF B).





在学期间所获荣誉奖励

荣誉

1. WWW最佳学生论文奖, 2022 (中国第2个)
2. Apple PhD Fellowship, 2021 (亚太地区1人, 全球15人)
3. 北京大学优秀博士论文奖, 2022 (计算机软件与理论方向1人)
4. 北京大学学生五·四奖章候选人, 2022 (学院1人, 北大27人)
5. 北京大学年度人物候选人, 2021 (学院1人, 北大42人)
6. 北京市三好学生, 2021 (学院2人, 北大58人)
7. 百度奖学金提名奖, 2021 (全球20人)
8. 腾讯年度开源协同创新奖 (Angel Graph团队), 2021
9. 数博会领先科技成果奖 (Angel Graph团队), 2022
10. 国家奖学金, 2021
11. 北京大学三好学生标兵, 2021
1. 北京大学学术创新奖, 2021
2. 北京市普通高等学校优秀毕业生, 2022 (学院6人)
3. 北京大学优秀毕业生, 2022 (学院17人)
4. 北京大学明略奖学金, 2021
5. 北京大学廖凯原奖学金, 2020
6. 北京大学学术创新奖, 2020
7. 北京大学三好学生标兵, 2020
8. 国家奖学金, 2019
9. 北京大学三好学生, 2019
10. 北京大学学习优秀奖, 2018

竞赛获奖

1. 中国软件开源创新大赛决赛特等奖, 2021 (1/3814)
2. 刷新图机器学习榜单记录, OGB评测第1名, 2021
3. 全国高校大数据应用创新大赛特等奖, 2018 (1/575)





谢谢观看！

