



中國人民大學
RENMIN UNIVERSITY OF CHINA



高瓴人工智能學院
Gaoling School of Artificial Intelligence

图表示学习

魏哲巍 教授

中国人民大学



报告提纲

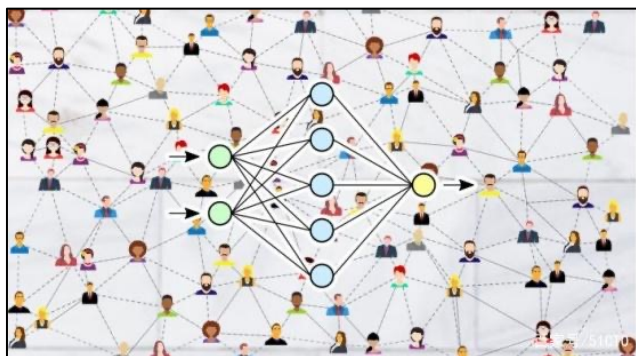
- 图表示学习的简介
- 图表示学习的年度进展
- 总结与展望




图表示学习

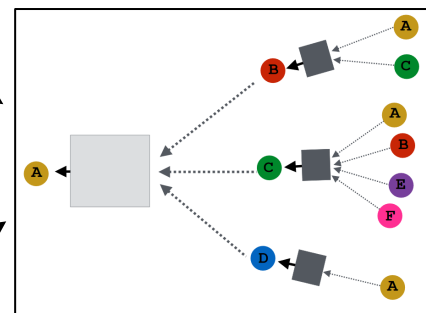
■ 以社交网络为例

连接关系：用户之间的连接关系

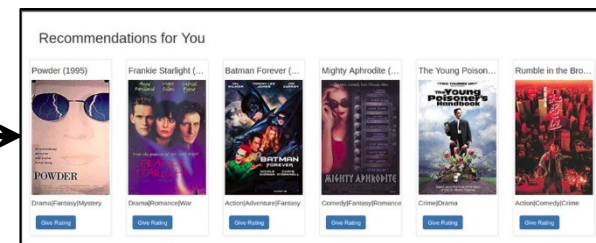


特征信息：用户的兴趣、年龄等特征

	Movies	Reviews Given	Rating
 Nikhil	Mission Impossible	✓	Good
	James Bond	✓	Good
	Toy Story	✓	Bad



图神经网络

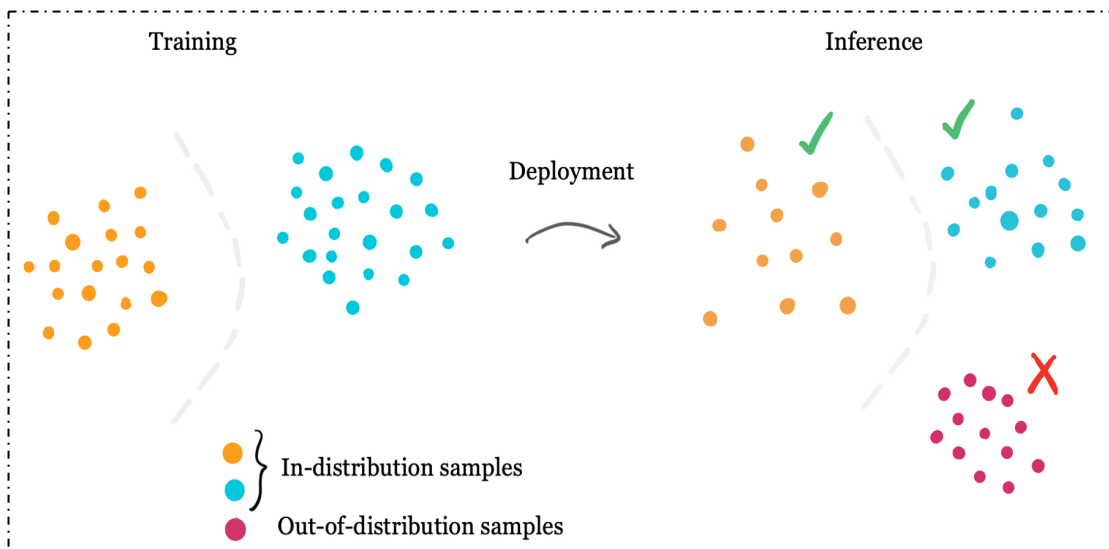


预测、推荐任务

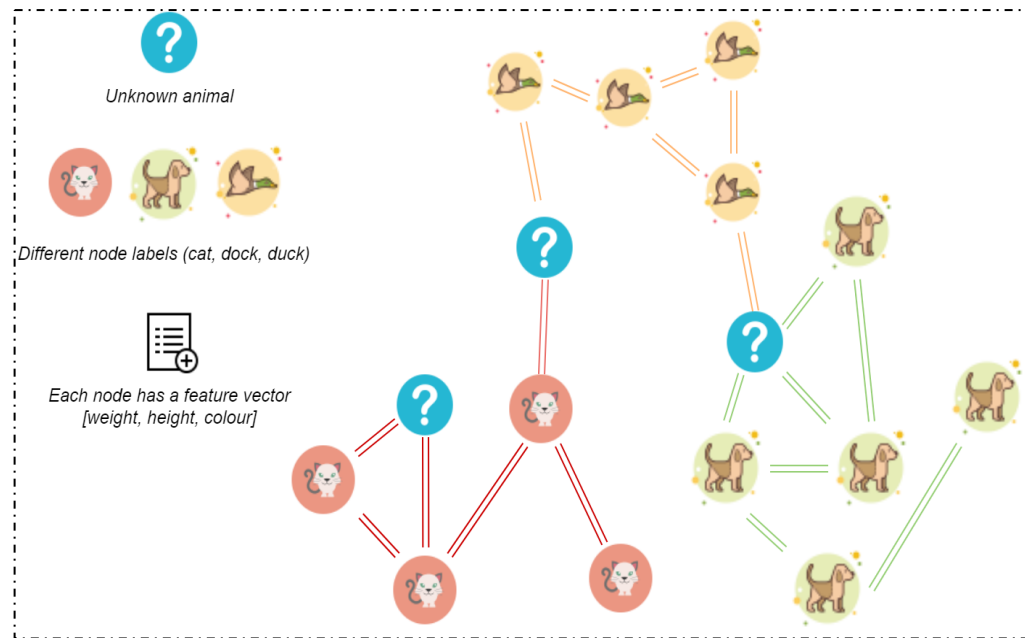


图表示学习

图表示学习与传统机器学习的区别



i.i.d假设



关联假设

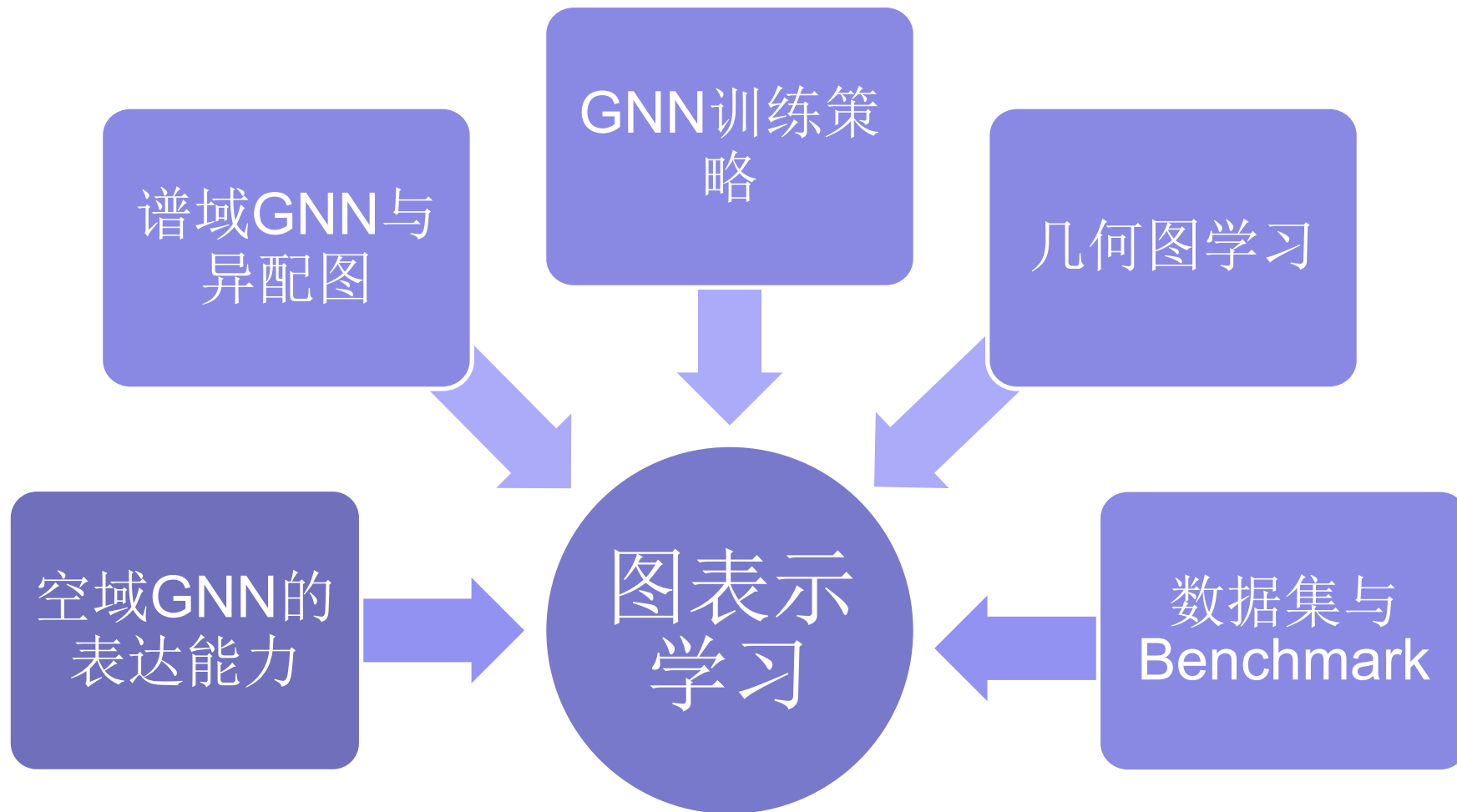


报告提纲

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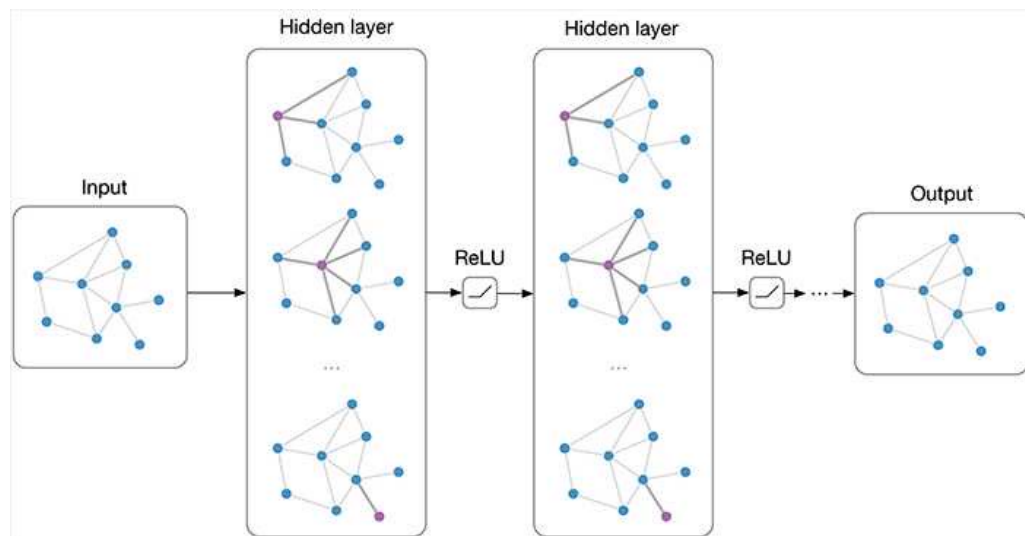


图表示学习





图表示学习



空域GNN的
表达能力

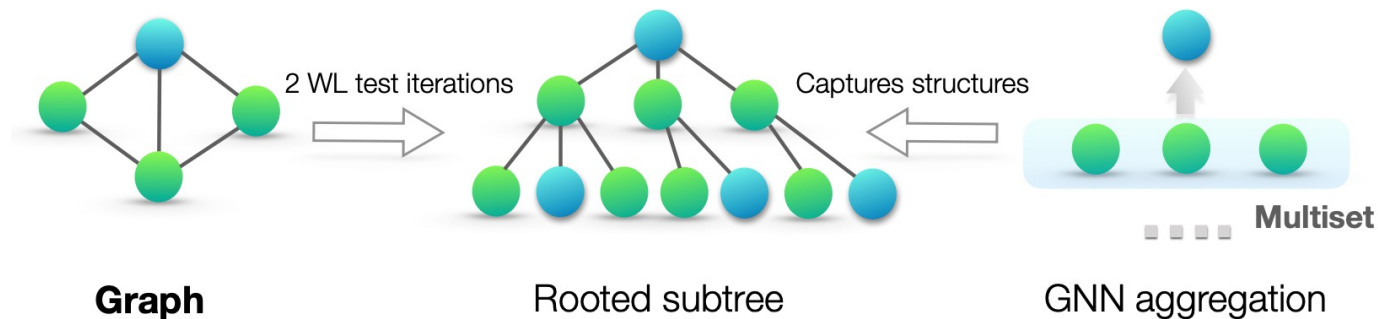


图表示
学习

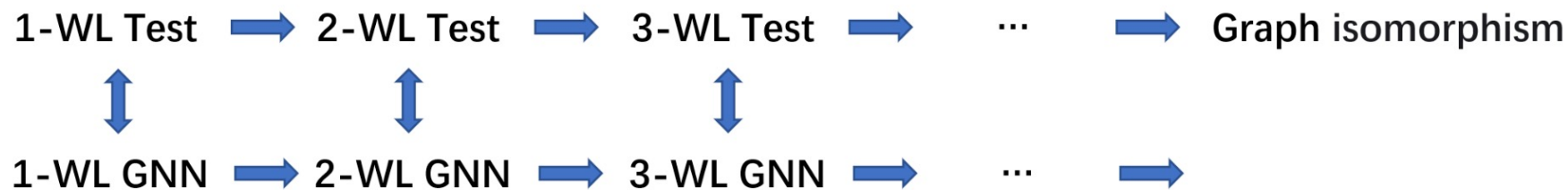


空域GNN的表达能力

- 在空域评估并提高GNN的表达能力一直是研究的热门
 - GIN [Xu et al., ICLR'19]提出，GNN 在区分图结构方面至多与 1-WL test一样强大



- 利用高阶WL变体设计表达能力更强的GNN [Maron et al., ICML'19, Balcilar et al., ICLR'21, Horn et al., ICLR'22]





空域GNN的表达能力

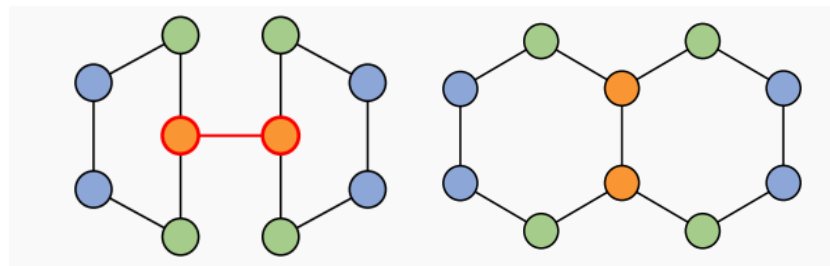
■ 年度研究进展

北大研究发现K-hop消息传递的表达能力被**3-WL bounded**，且利用每一跳中的**外围子图信息**可以改进 K-hop 消息传递 [Feng et al., NeurIPS'22]

CMU提出了比k-WL更细粒度的指标来衡量GNN的表达能力——**SetWL层次结构**，其复杂性低于k-WL [Zhao et al., NeurIPS'22]

ANU的研究也提出了一个新的图同构测试层次结构 **Neighbourhood WL (N-WL)**，并基于此设计了GNN模型G3N [Wang et al., ICLR'23]

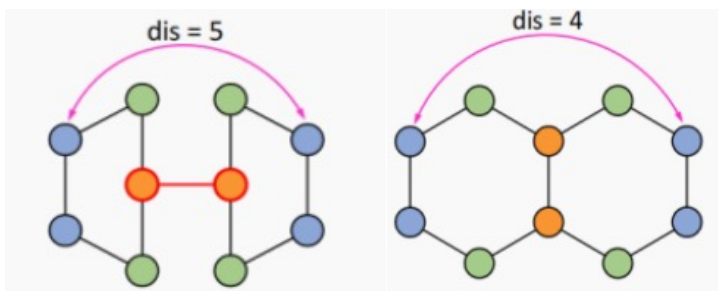
■ 从双连通判别问题出发



□ 左图有割边，右图没有；现有GNN模型都不能区分两图。

■ 提出的广义距离WL (GD-WL) 算法能解决所有双连通性判别问题

□ 通过添加距离信息可以区分两图 □ 基于GD-WL设计的GNN模型

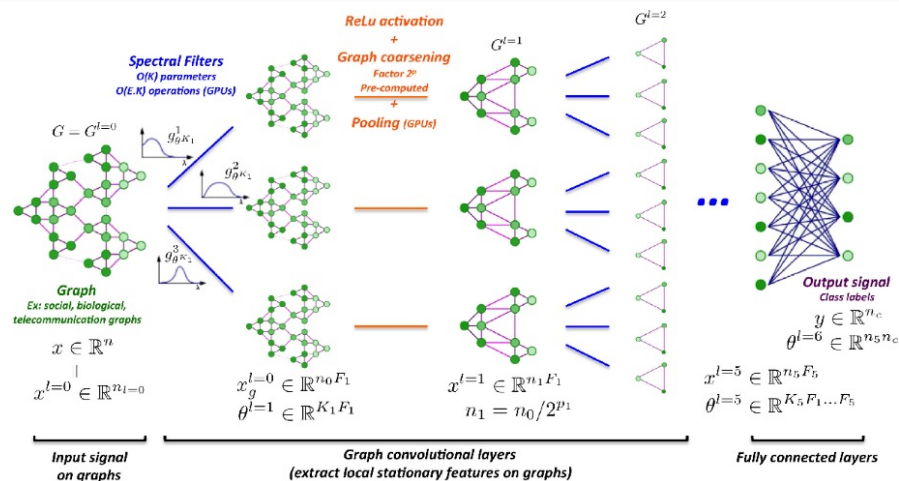


Model	Cut Vertex Detection	Cut Edge Detection
GCN [Kipf and Welling, 2017]	51.5%±1.3%	62.4%±1.8%
GAT [Veličković et al., 2018]	52.0%±1.3%	62.8%±1.9%
GIN [Xu et al., 2019]	53.9%±1.7%	63.1%±2.2%
GSN [Bouritsas et al., 2022]	60.1%±1.9%	70.7%±2.1%
Graphormer [Ying et al., 2021]	76.4%±2.8%	84.5%±3.3%
Graphormer-GD (ours)	100%	100%
- w/o. Resistance Distance	83.3%±2.7%	100%



图表示学习

谱域GNN与
异配图



空域GNN的
表达能力

图表示
学习

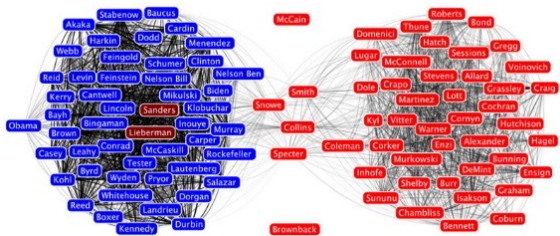
谱域GNN与异配图

- 谱域GNN核心：设计/学习多项式滤波器

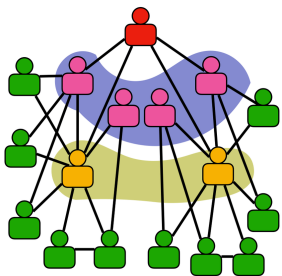
$$y = \sum_{k=0}^K w_k g_k(L)x$$

□ w_k 为多项式系数； $g_k(\cdot)$ 为多项式基，不同的系数可以表达不同的滤波器

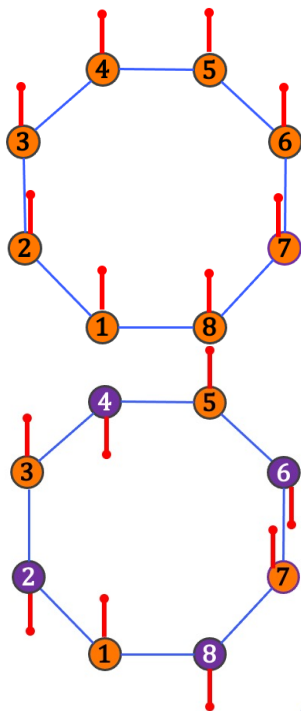
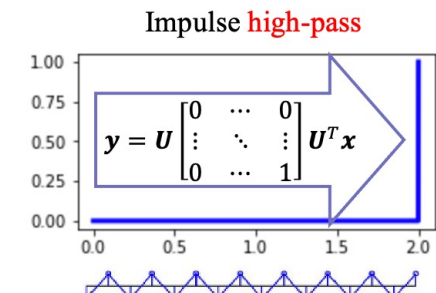
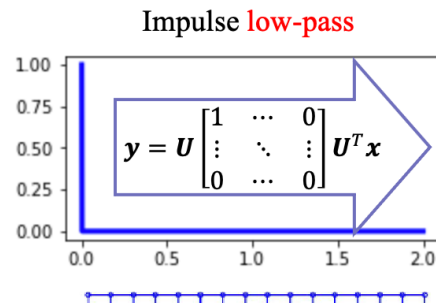
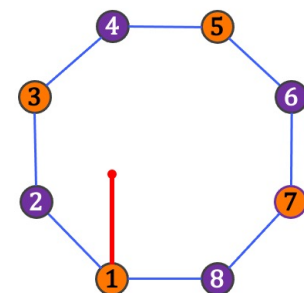
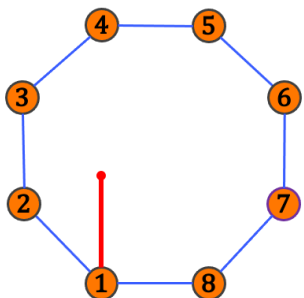
- 同配图对应低通滤波器，异配图对应高通滤波器



同配图：边相连的节点通常属于同一类



异配图：边相连的节点通常属于不同类





谱域GNN与异配图

■ 年度研究进展

北大从理论上研究了谱域GNN的表达能力，证明了使用**正交多项式基**有助于滤波器的学习，并提出了**JacobiConv** [Wang et al., ICML'22]

大连理工从谱域光滑度(Spectral smoothness)入手分析了多项式滤波器近似能力的限制，并提出了**Correlation-free**架构 [Yang et al., ICML'22]

人大重新审视了使用切比雪夫基近似滤波器的方法，并提出了基于切比雪夫插值的GNN模型**ChebNetII** [He et al., NeurIPS'22] (Ours)

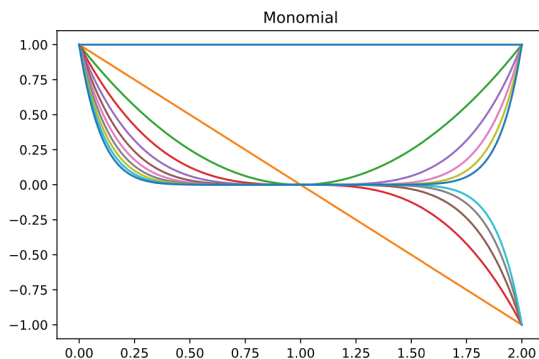
MIT从不变性的角度提出了两个新的谱域GNN架构**SignNet**和**BasisNet**，可以证明该架构比现有谱方法更具表达能力 [Lim et al., ICLR'23]



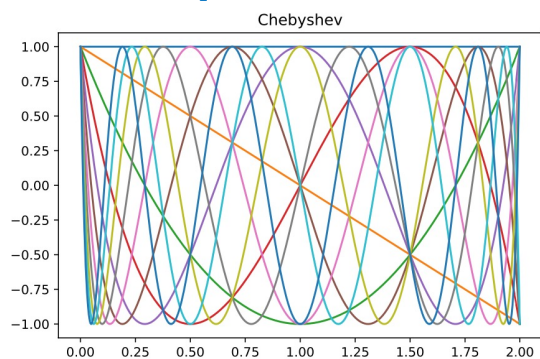
FavardGNN/OptBasisGNN [Guo et al., ICML'23]

- FavardGNN : 利用Favard定理学习任意多项式基
- OptBasisGNN: 计算收敛速度最快的最优多项式基

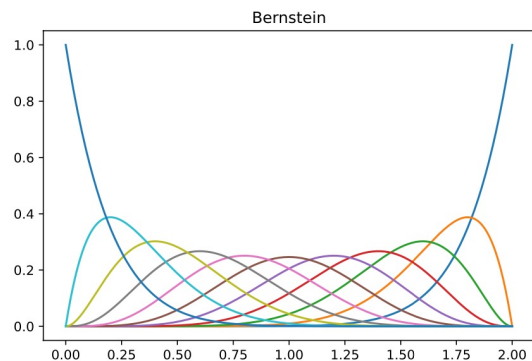
GPR-GNN [Chien et al., 2021]



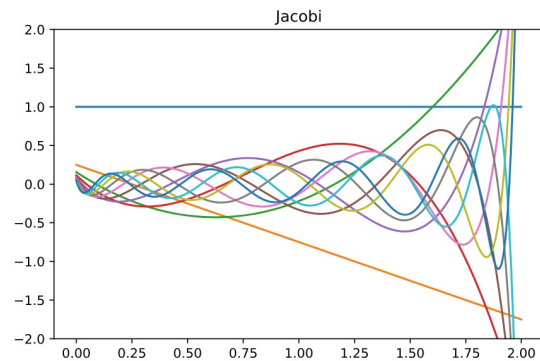
ChebNet [Defferrard et al., 2016]



BernNet [He et al., 2021]



JacobiConv [Wang et al., 2022]

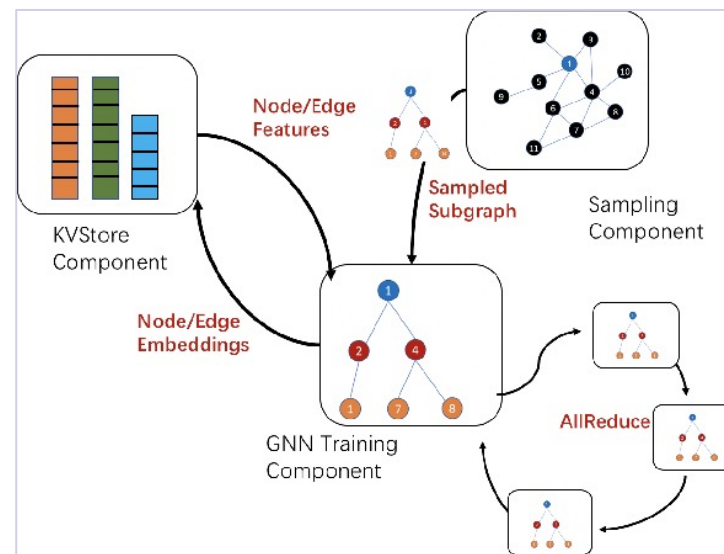
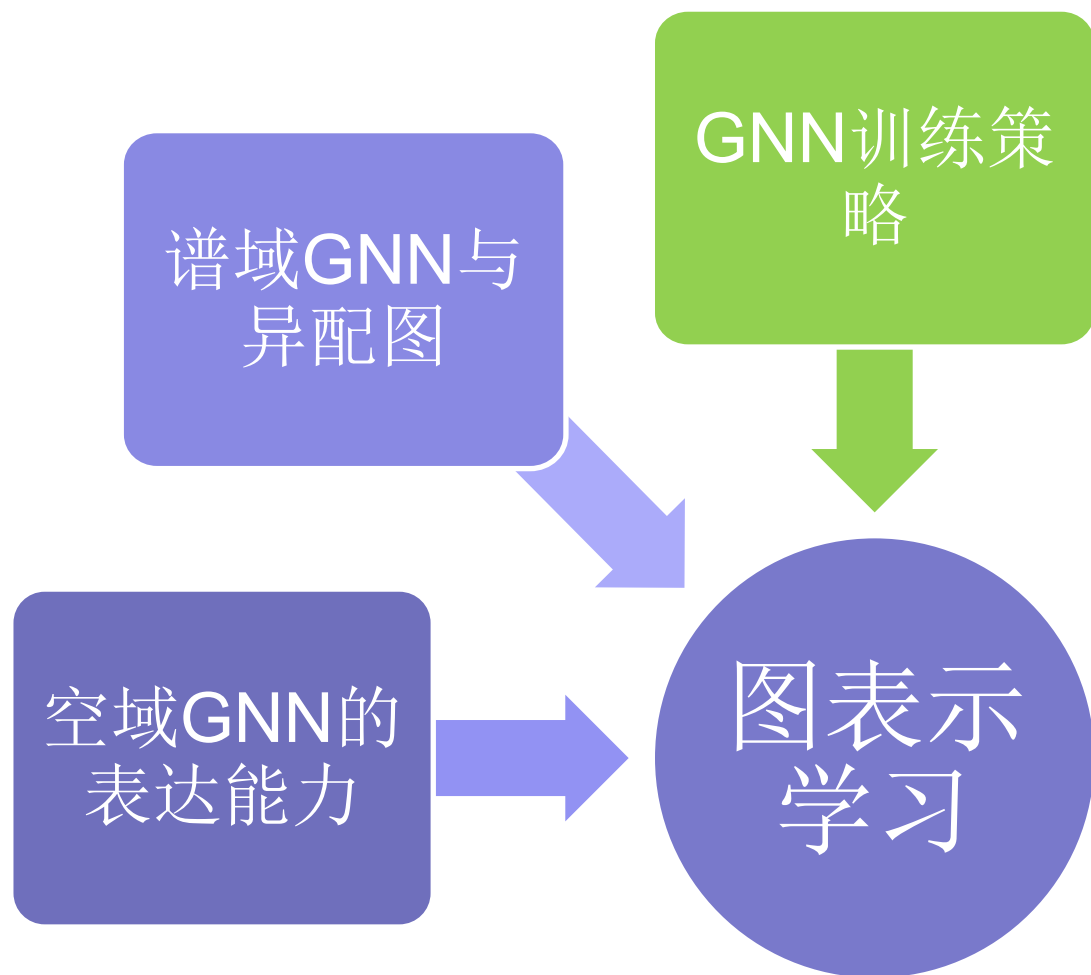


Dataset	Chameleon	Squirrel	Actor	Citeseer	Pubmed
$\ V\ $	2,277	5,201	7,600	3,327	19,717
$\mathcal{H}(G)$.23	.22	.22	.74	.80
MLP	46.59 ± 1.84	31.01 ± 1.18	40.18 ± 0.55	76.52 ± 0.89	86.14 ± 0.25
GCN	60.81 ± 2.95	45.87 ± 0.8	33.26 ± 1.15	79.85 ± 0.78	86.79 ± 0.31
ChebNet	59.51 ± 1.25	40.81 ± 0.42	37.42 ± 0.58	79.33 ± 0.57	87.82 ± 0.24
ARMA	60.21 ± 1.00	36.27 ± 0.62	37.67 ± 0.54	80.04 ± 0.55	86.93 ± 0.24
APPNP	52.15 ± 1.79	35.71 ± 0.78	39.76 ± 0.49	80.47 ± 0.73	88.13 ± 0.33
GPRGNN	67.49 ± 1.38	50.43 ± 1.89	39.91 ± 0.62	80.13 ± 0.84	88.46 ± 0.31
BernNet	68.53 ± 1.68	51.39 ± 0.92	41.71 ± 1.12	80.08 ± 0.75	88.51 ± 0.39
ChebNetll	71.37 ± 1.01	57.72 ± 0.59	41.75 ± 1.07	80.53 ± 0.79	88.93 ± 0.29
JacobiConv	74.20 ± 1.03	57.38 ± 1.25	41.17 ± 0.64	80.78 ± 0.79	89.62 ± 0.41
FavardGNN	72.32 ± 1.90	63.49 ± 1.47	43.05 ± 0.53	81.89 ± 0.63	90.90 ± 0.27
OptBasisGNN	74.26 ± 0.74	63.62 ± 0.76	42.39 ± 0.52	80.58 ± 0.82	90.30 ± 0.19

Dataset	Penn94	Genius	Twitch-Gamers	Pokec	Wiki
$\ V\ $	41,554	421,961	168,114	1,632,803	1,925,342
$\ E\ $	1,362,229	984,979	6,797,557	30,622,564	303,434,860
$\mathcal{H}(G)$.470	.618	.545	.445	.389
MLP	73.61 ± 0.40	86.68 ± 0.09	60.92 ± 0.07	62.37 ± 0.02	37.38 ± 0.21
GCN	82.47 ± 0.27	87.42 ± 0.31	62.18 ± 0.26	75.45 ± 0.17	OOM
GCNII	82.92 ± 0.59	90.24 ± 0.09	63.39 ± 0.61	78.94 ± 0.11	OOM
MixHop	83.47 ± 0.71	90.58 ± 0.16	65.64 ± 0.27	81.07 ± 0.16	49.15 ± 0.26
LINK	80.79 ± 0.49	73.56 ± 0.14	64.85 ± 0.21	80.54 ± 0.03	57.11 ± 0.26
LINKX	84.71 ± 0.52	90.77 ± 0.27	66.06 ± 0.19	82.04 ± 0.07	59.80 ± 0.41
GPRGNN	83.54 ± 0.32	90.15 ± 0.30	62.59 ± 0.38	80.74 ± 0.22	58.73 ± 0.34
BernNet	83.26 ± 0.29	90.47 ± 0.33	64.27 ± 0.31	81.67 ± 0.17	59.02 ± 0.29
ChebNetll	84.86 ± 0.33	90.85 ± 0.32	65.03 ± 0.27	82.33 ± 0.28	60.95 ± 0.39
FavardGNN	84.92 ± 0.41	90.29 ± 0.14	64.26 ± 0.12	-	-
OptBasisGNN	84.85 ± 0.39	90.83 ± 0.11	65.17 ± 0.16	82.83 ± 0.04	61.85 ± 0.03



图表示学习

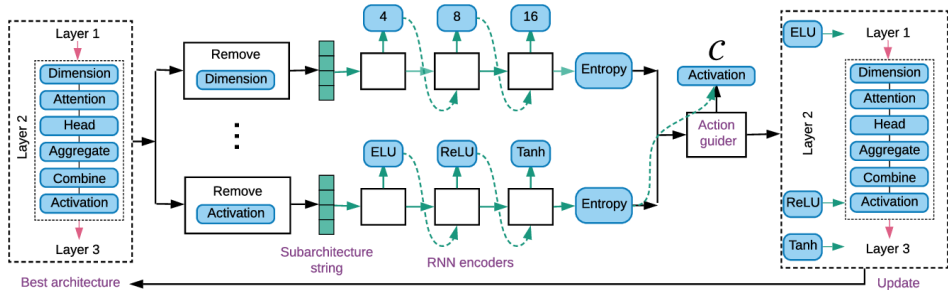




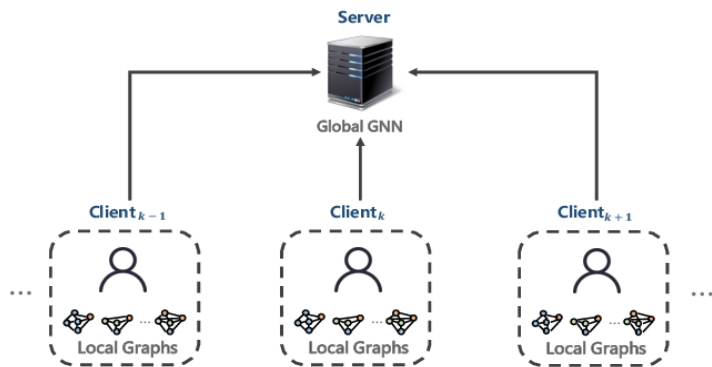
GNN训练策略

■ GNN的训练策略包括了多个方面

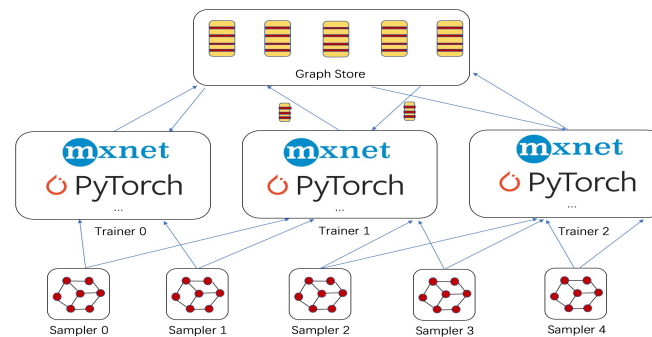
□ 自动化神经结构搜索



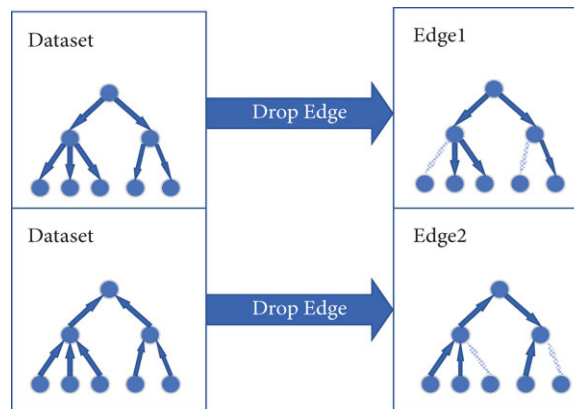
□ GNN与联邦学习



□ 分布式训练GNN模型



□ 解决GNN的过平滑问题



- PaSca是一种基于新型结构范式的可扩展的图神经结构搜索系统
 - 自动搜索性能良好且可扩展的 GNN 架构，并通过多目标优化来平衡多个标准（准确性、效率等）之间的权衡

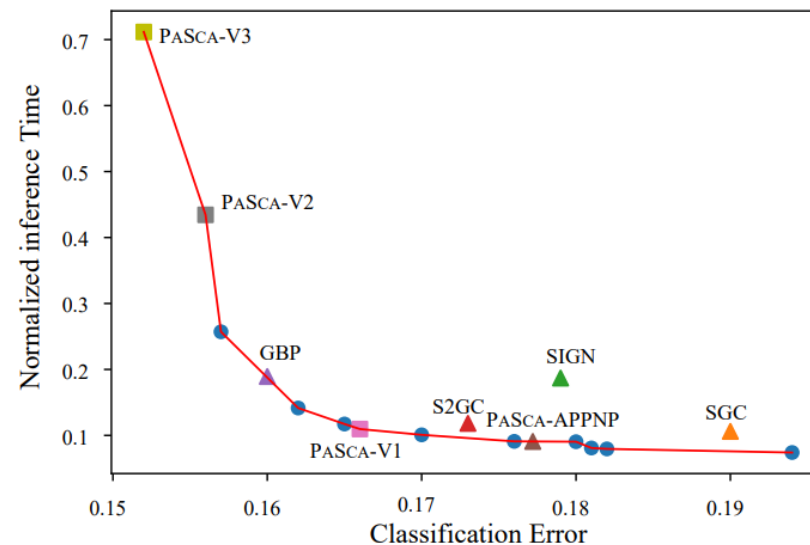
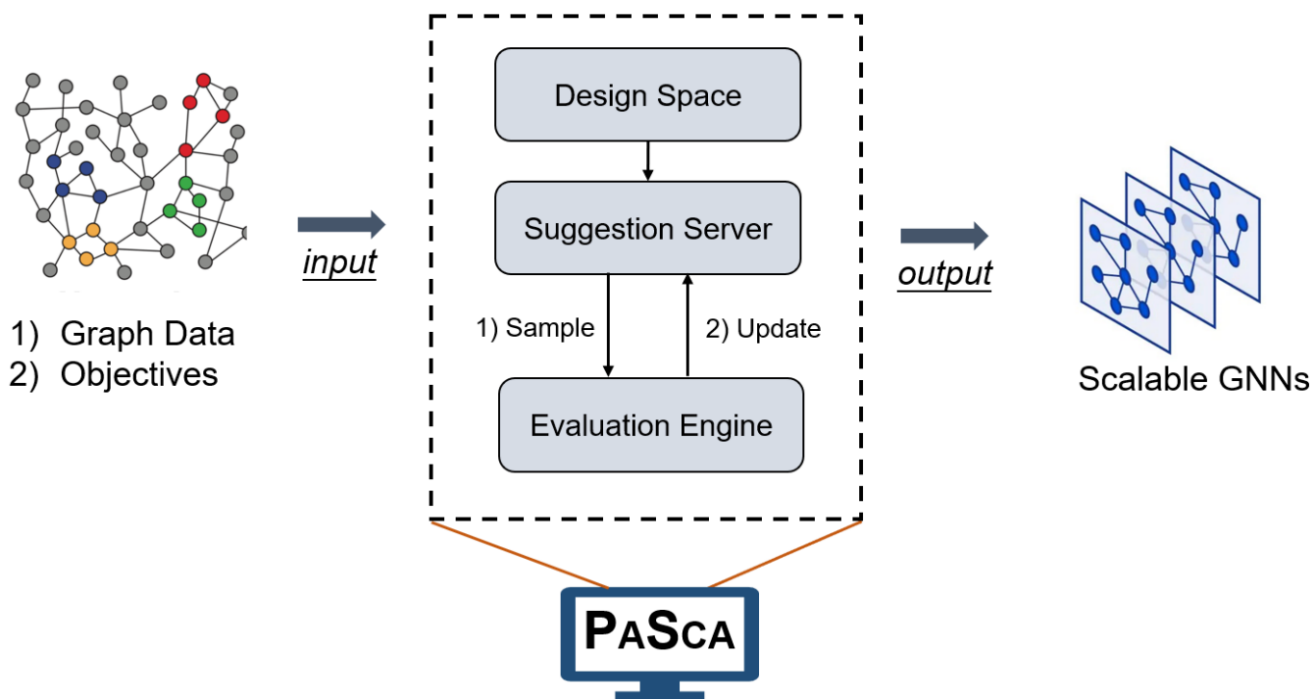
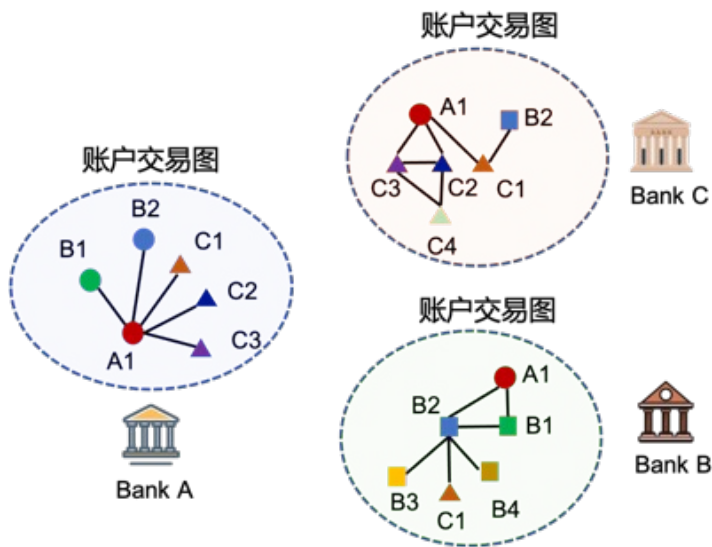


Figure 6: Pareto Front found on Cora.

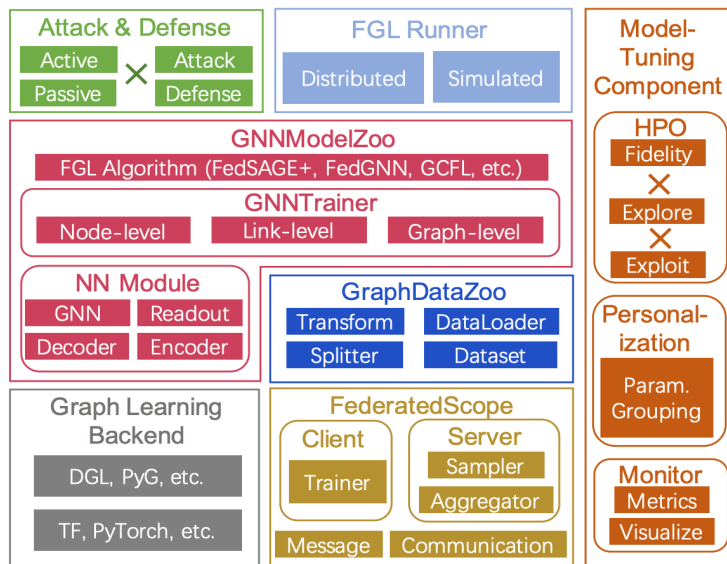


FS-GNN——KDD 2022 Best Paper

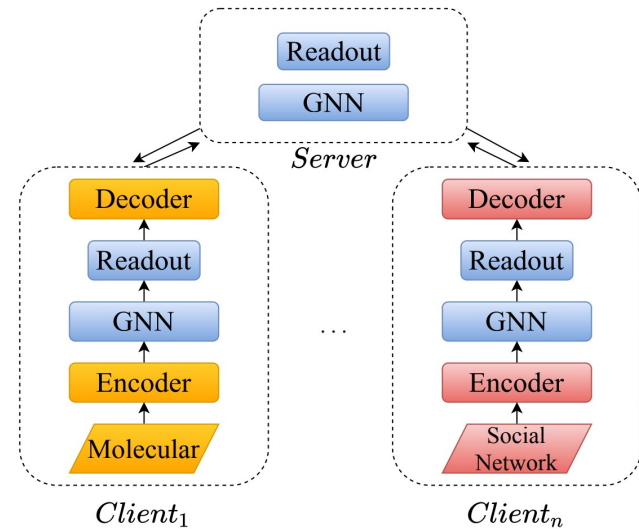
- 在银行反洗钱任务中，预测银行账户是否是风险账户
 - 当前联邦学习的框架普遍缺乏对图学习的灵活支持
 - FederatedScope-GNN建立了一个当前最标准最完善的联邦图学习基准



银行反洗钱场景



FS-GNN 联邦图学习框架

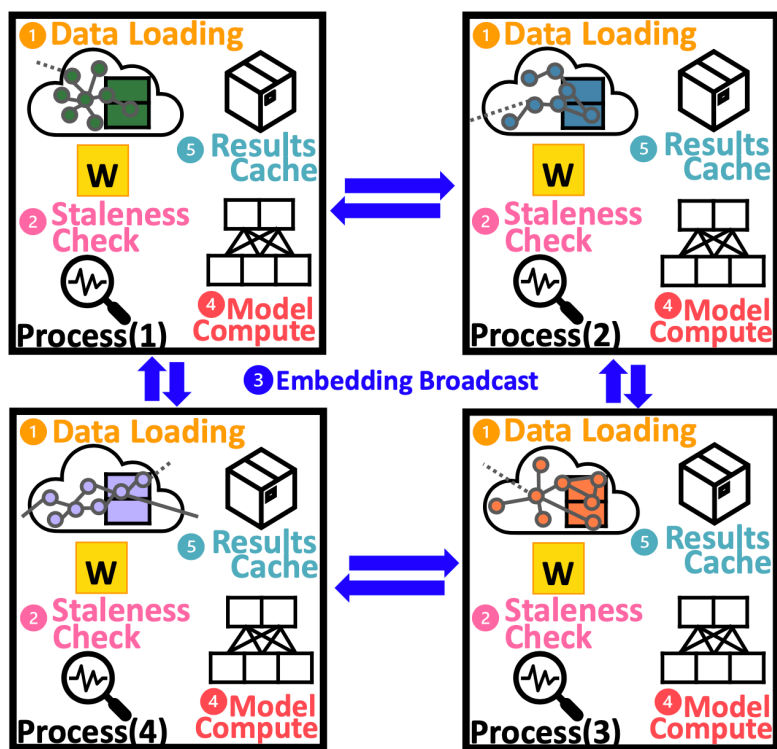


基于FS-GNN的个性化GNN

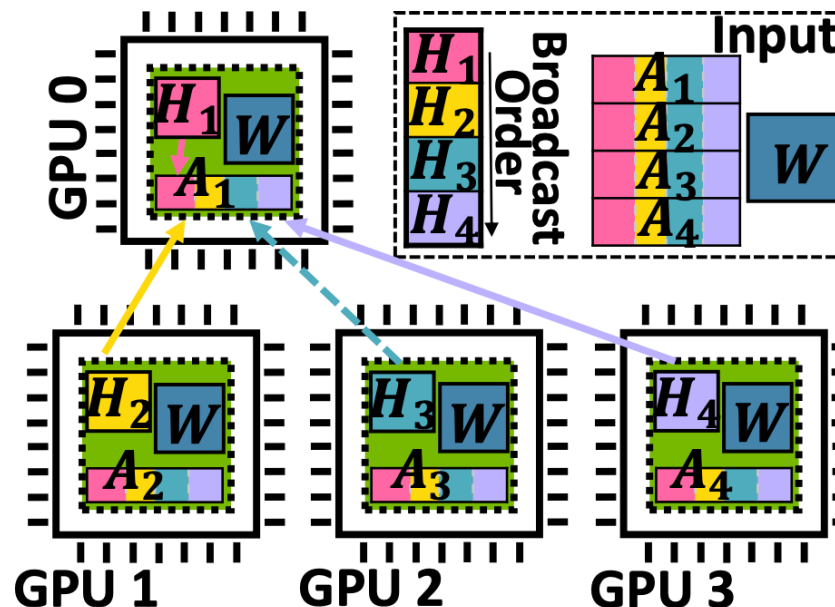


SANCUS——VLDB 2022 Best Paper

- SANCUS框架提出了用于维护历史嵌入的陈旧性指标，既能保证收敛性，又可以去中心化而避免大量通信，高效地实现了GNN分布式训练



SANCUS框架概述



基于SANCUS的两层GNN示例

- DropMessage 对传播的消息进行删除操作
 - 允许一个节点将不同的消息传递给不同的邻居，可以证明现有的随机删除方法均可统一到 DropMessage 框架中；
 - 从理论上证明了随机删除消息的有效性。

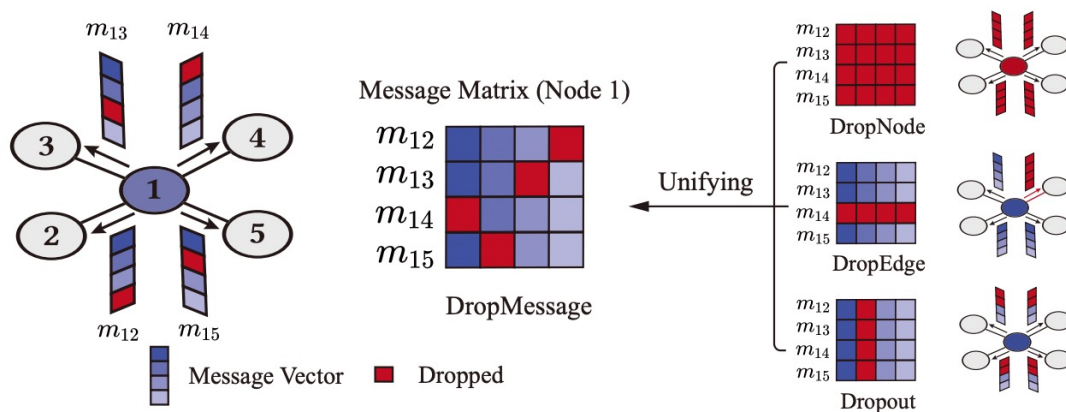


Figure 1: Illustrations of DropMessage and other existing random dropping methods. Considering the messages propagated by the center node (*i.e.*, Node 1), DropMessage allows to propagate distinct messages to different neighbor nodes, and its induced message matrix can be arbitrary. The induced message matrices of other methods obey some explicit constraints and can be regarded as special forms of DropMessage.

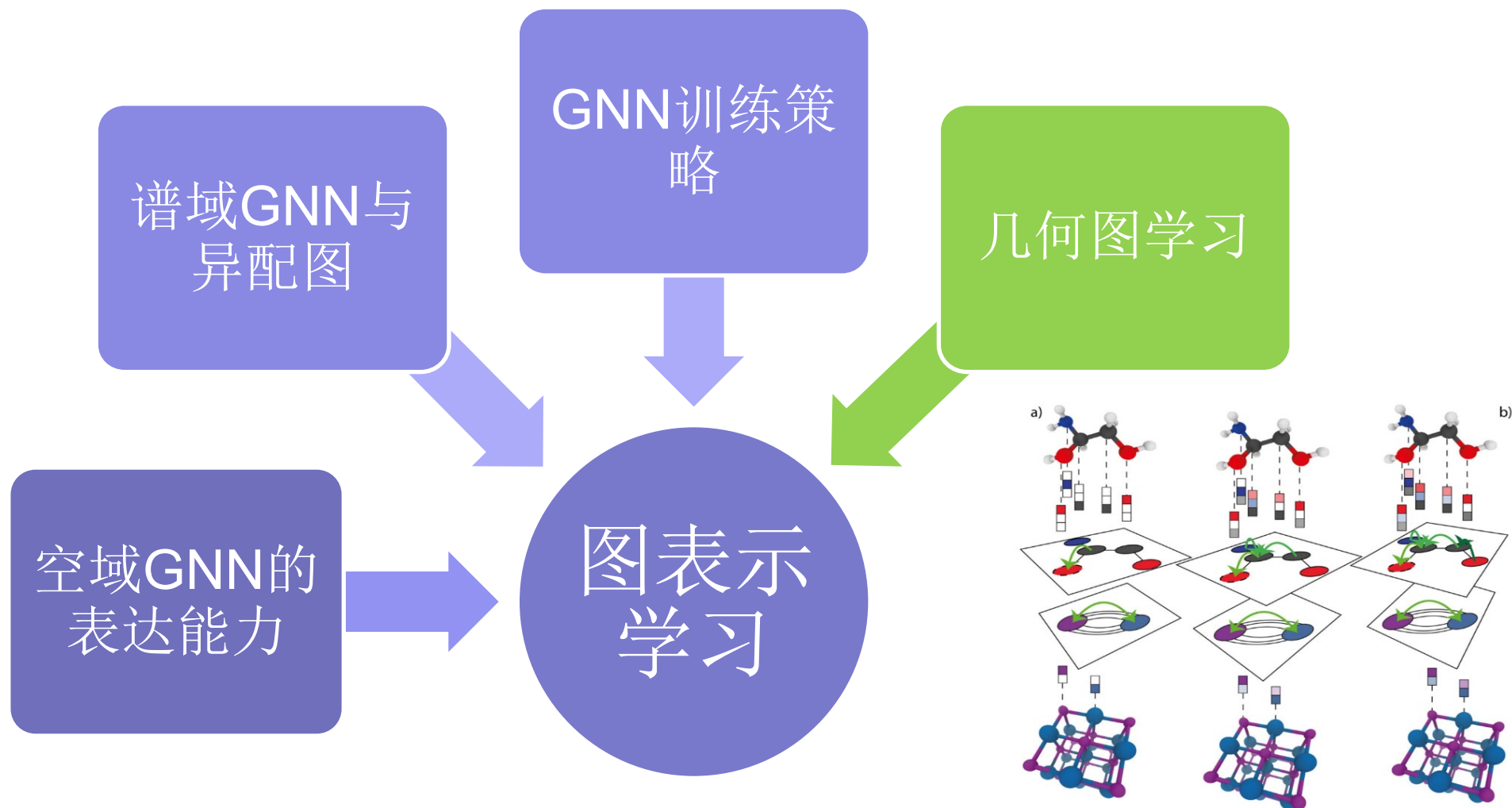
Table 1: Overview of different random dropping methods in a view of Bernoulli sampling process.

Method	Formula
Dropout	$\tilde{\mathbf{X}}_{i,j} = \epsilon \mathbf{X}_{i,j}$
DropEdge	$\tilde{\mathbf{A}}_{i,j} = \epsilon \mathbf{A}_{i,j}$
DropNode	$\tilde{\mathbf{X}}_i = \epsilon \mathbf{X}_i$
DropMessage	$\tilde{\mathbf{M}}_{i,j} = \epsilon \mathbf{M}_{i,j}$

s.t. $\epsilon \sim \text{Bernoulli}(1 - \delta)$



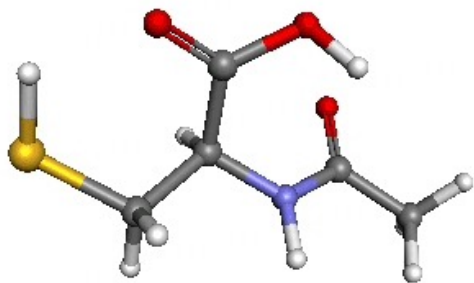
图表示学习



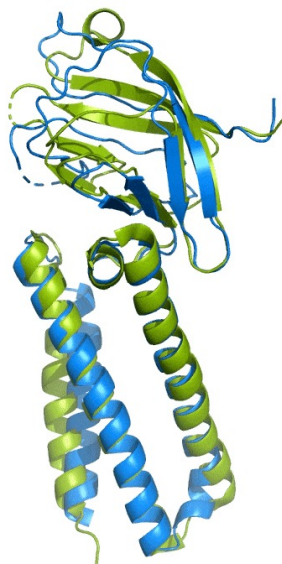


几何图学习

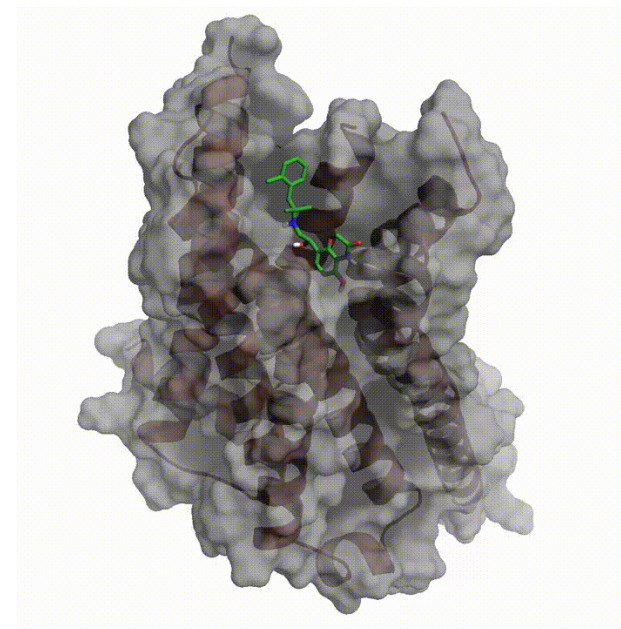
- 许多科学问题，特别是物理和化学问题，需要以**几何图** (geometric) 的形式处理。结合GNN，可用于药物研发、分子生成.....
- 核心科学问题：节点具备**坐标**特征，如何保持图的**3D不变性**？



小分子



蛋白质



蛋白质配体结合



几何图学习

■ 年度研究进展

Google研究发现，在许多情况下，**小分子数据**的**自监督图预训练**带来的好处可以忽略不计 [Sun et al., NeurIPS'22]

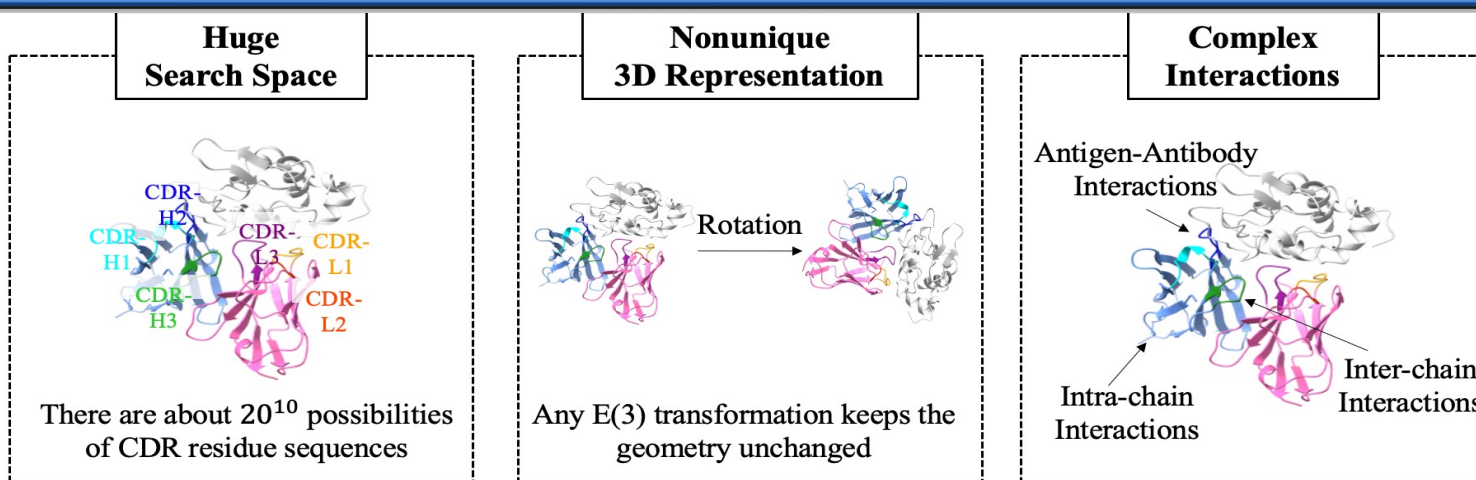
MIT研究证明了**Transformer**可以很好地泛化到**3D原子图**，提出了结合Transformer的GNN模型Equiformer [Liao et al., ICLR'23]

人大与深势科技提出了一种泛用的**3D分子表示学习**框架**Uni-Mol**，扩展了分子表示学习方法的表示能力和应用范围 [Zhou et al., ICLR'23](Ours)

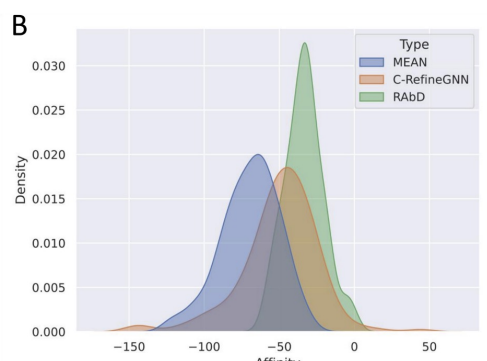
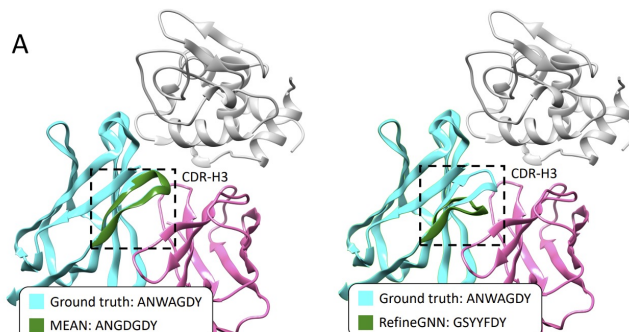


MEAN—ICLR 2023 Outstanding Paper Honorable Mention

■ 抗体设计的挑战性

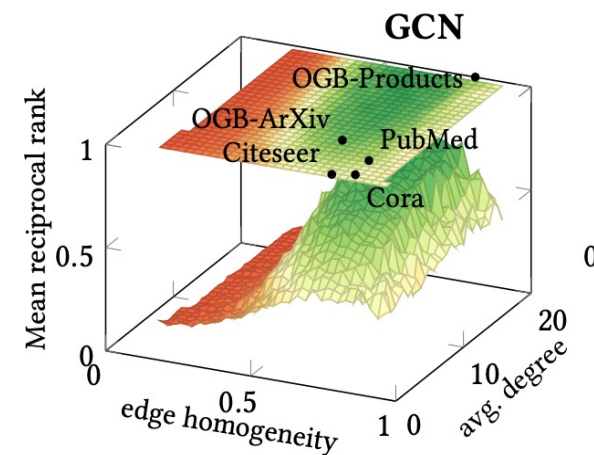
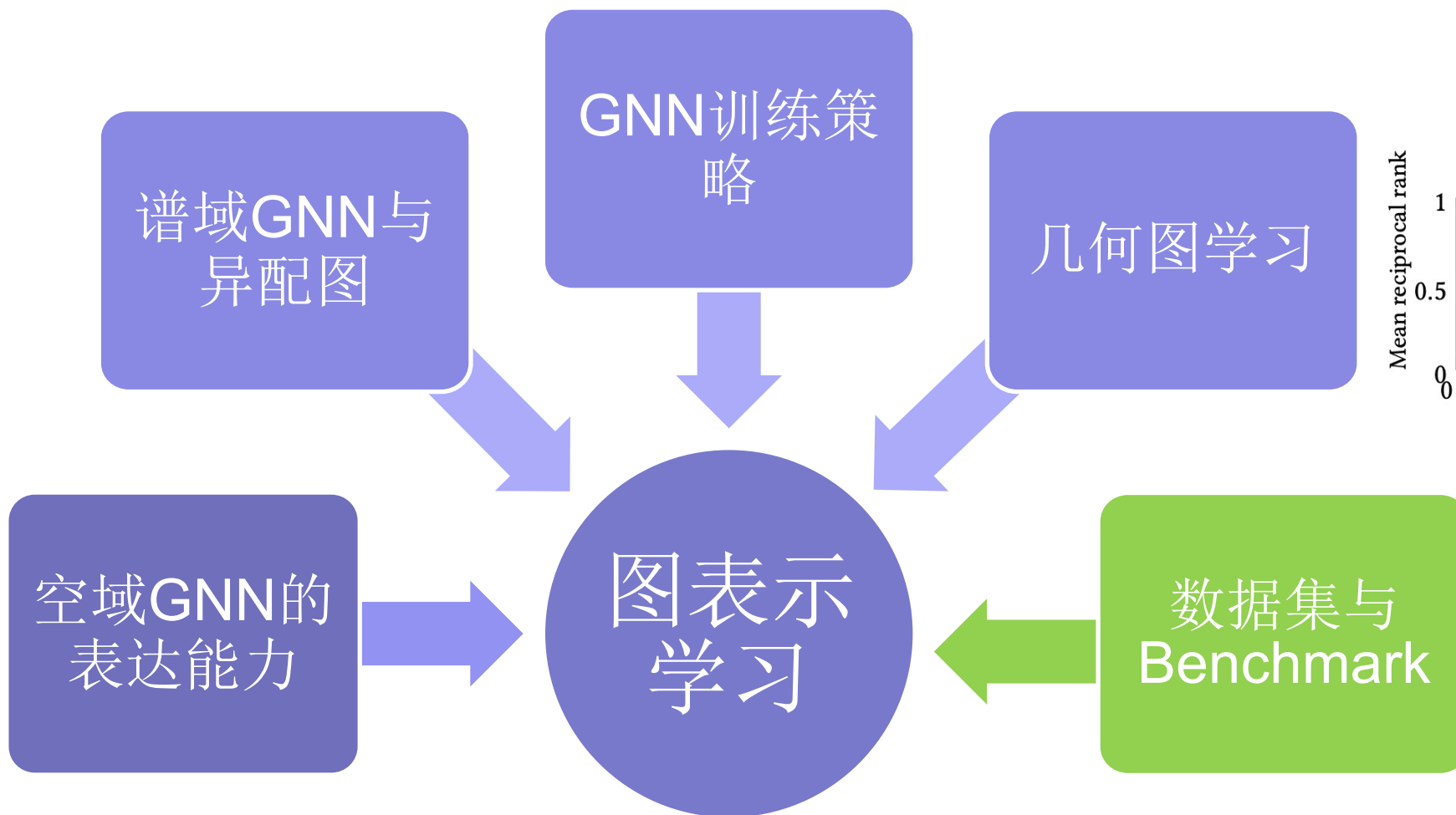


- 多通道等变注意力网络MEAN，一种基于E(n)-equivariant GNNs的抗体设计方法
 - 将抗体生成视为**三维等变图翻译问题**：给定抗体-抗原三维复合体，输出抗体CDR区域一维氨基酸序列和对接后的三维结构
 - 在靶向抗原的抗体设计任务上，MEAN的CDR重构精度比国际主流方法RefineGNN提高了**23%**





图表示学习





数据集和Benchmark

- 数据集和Benchmark对图表示学习的研究起到了很大的促进作用
 - 本年度提出了一些新的数据集和Benchmark:

GraphWorld: Google开发的用于图学习研究人员在合成图数据集上系统地测试新模型的方法和工具箱 [Palowitch et al., KDD'22]

Long Range Graph Benchmark (LRGB): 南洋理工大学提出的用于评估和发展具有长程依赖关系的GNN模型 [Dwivedi et al., NeurIPS'22]

Table 2: Statistics of the five proposed LRGB datasets.

Dataset	Total Graphs	Total Nodes	Avg Nodes	Mean Deg.	Total Edges	Avg Edges	Avg Short.Path.	Avg Diameter
PascalVOC-SP	11,355	5,443,545	479.40	5.65	30,777,444	2,710.48	10.74±0.51	27.62±2.13
COCO-SP	123,286	58,793,216	476.88	5.65	332,091,902	2,693.67	10.66±0.55	27.39±2.14
PCQM-Contact	529,434	15,955,687	30.14	2.03	32,341,644	61.09	4.63±0.63	9.86±1.79
Peptides-func	15,535	2,344,859	150.94	2.04	4,773,974	307.30	20.89±9.79	56.99±28.72
Peptides-struct	15,535	2,344,859	150.94	2.04	4,773,974	307.30	20.89±9.79	56.99±28.72



数据集和Benchmark

- 本年度提出了一些新的数据集和Benchmark:

CGLB: 悉尼大学提出的用于评估连续图学习(Continual Graph Learning)的数据集和Benchmark [Zhang et al., NeurIPS'22]

Yandex Research提出现存的一些**异配图数据集**的构造存在问题, 他们构造了新的真实数据集 [Platonov et al., ICLR'23]

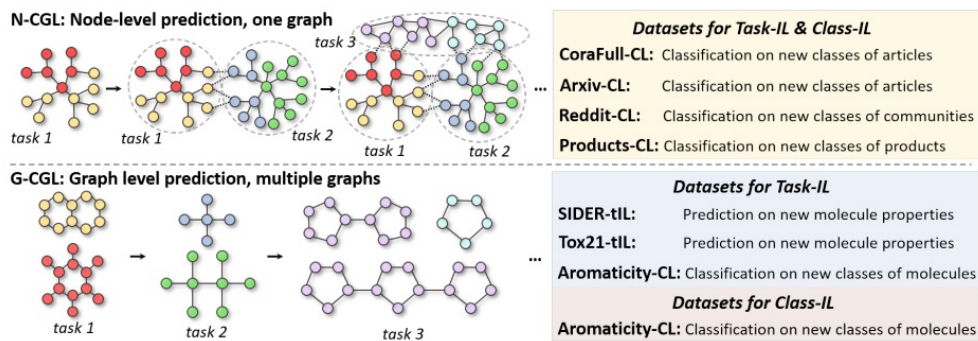


Figure 1: Overview of 4 different benchmark tasks with N-CGL or G-CGL setting under task-IL or class-IL scenario (applied to different datasets).

Table 3: Statistics of the new heterophilous datasets

	roman-empire	amazon-ratings	minesweeper	tolokers	questions
nodes	22662	24492	10000	11758	48921
edges	32927	93050	39402	519000	153540
avg degree	2.91	7.60	7.88	88.28	6.28
global clustering	0.29	0.32	0.43	0.23	0.02
avg local clustering	0.39	0.58	0.44	0.53	0.03
diameter	6824	46	99	11	16
node features	300	300	7	10	301
classes	18	5	2	2	2
edge homophily	0.05	0.38	0.68	0.59	0.84
adjusted homophily	-0.05	0.14	0.01	0.09	0.02
LI	0.11	0.04	0.00	0.01	0.00



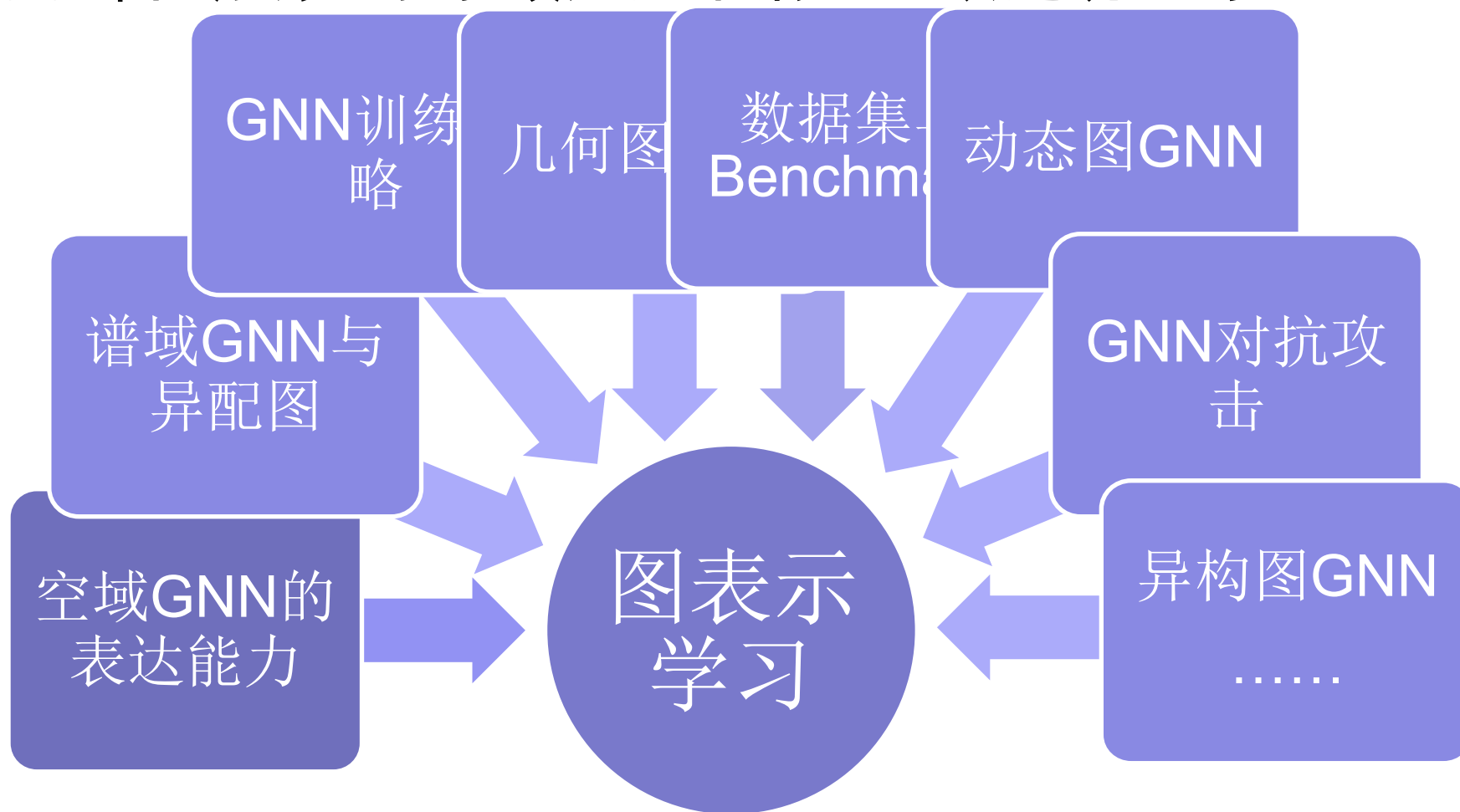
报告提纲

- 图表示学习的简介
- 图表示学习的年度进展
- 总结与展望



总结与展望

- 图表示学习领域方兴未艾：研究方向众多，最佳论文数目显著增加
- 理论基础不明确、杀手级应用不清楚、缺乏统一的Benchmark





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论文列表

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- Platonov, et al. A critical look at the evaluation of gnn under heterophily: are we really making progress? ICLR 2023.

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谢谢!
Q&A



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