





Automated Graph Neural Network for Recommendation System

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Outline

- Introduction
 - Graph Neural Network (GNN)
 - GNN for recommendation
 - Automated machine learning (AutoML) for GNN

- Neural Architecture Search (NAS) for GNN
 - Reinforcement learning
 - Differentiable architecture search

Automated GNN for recommendation

Graph Neural Network

- GNN is a very hot topic in recent years
 - Representation learning in graphs
 - Define "convolution" on non-grid data

- Applications
 - Recommendation [Ying et al. KDD 2018]
 - Fraud Detection [Liu et al. AAAI 2019]
 - Spam detection [Li et al. CIKM 2019]
 - Bioinformatics [Zitnik et al. Bioinformatics 2017]

Graph Neural Network

- Message passing framework
 - Node embedding updated by neighbors
 - K-layer GNN access K-hop neighbors
 - "Neighborhood aggregation"

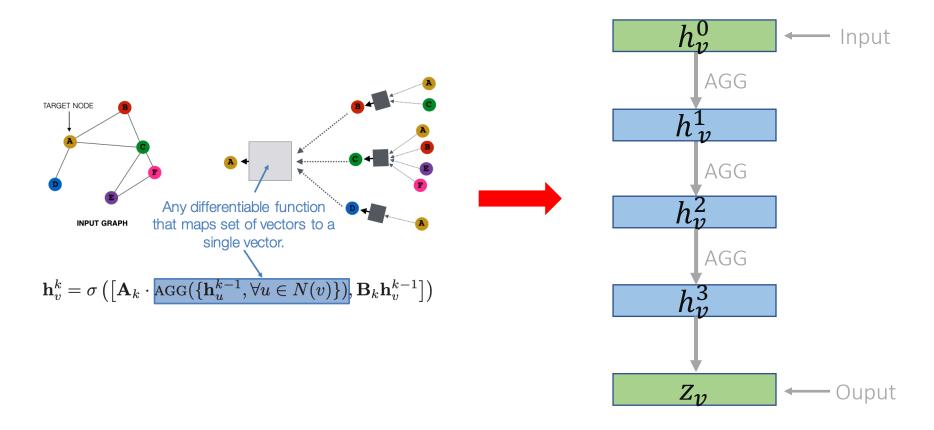
Self contained Neighborhood

$$\mathbf{h}_{v}^{l} = \sigma \left(\mathbf{W}^{(l)} \cdot \mathbf{AGG}_{\text{node}} \left(\left\{ \mathbf{h}_{u}^{(l-1)}, \forall u \in \widetilde{N}(v) \right\} \right) \right)$$

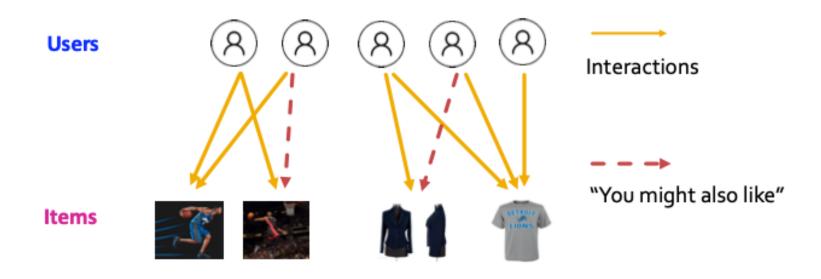
- Variants of GNN
 - GCN: normalized sum aggregator
 - GraphSAGE: MEAN, MAX, SUM, LSTM
 - GAT: Attention aggregator
 - GIN: Multi-Layer Perceptrons (MLP)

Graph Neural Network

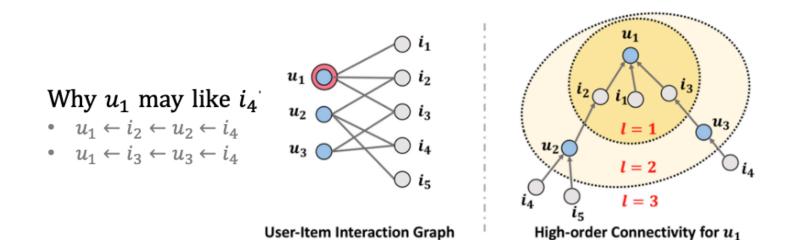
An example GNN architecture.



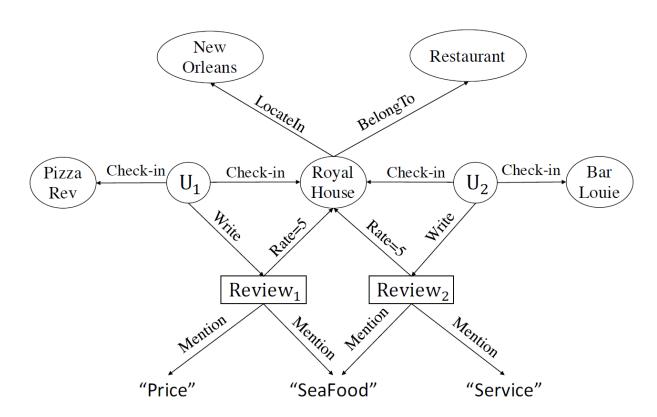
- Recommendation can be naturally modeled by graph.
 - Bipartite graph for collaborative filtering.



- Recommendation can be naturally modeled by graph.
 - Neural Graph collaborative filtering (NGCF)



- Recommendation can be naturally modeled by graph.
 - Heterogeneous graph for rich side information

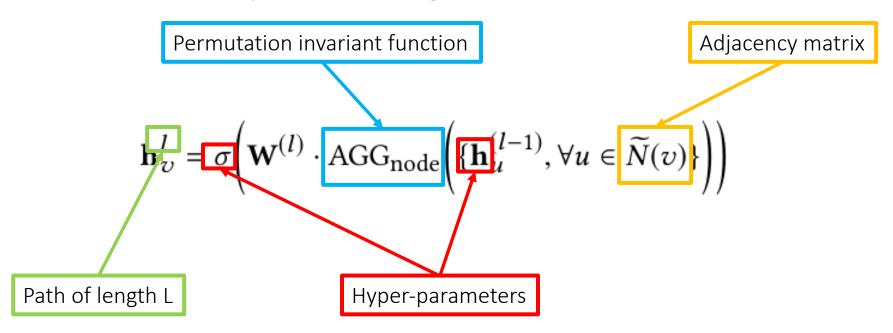


- Recommendation can be naturally modeled by graph.
 - Similarity computation between user and item
 - User and item representation by GNN.
 - Scenario-specific GNNs are needed.
 - AutoML can help.

Neural Architecture Search (NAS) can be exploited.

AutoML for GNN

- What can be searched?
 - Revisiting message passing framework
 - the l-th layer embedding of node v:



Neural Architecture Search (NAS) can be exploited.

NAS for GNN

- Background
 - Graph Neural Network (GNN)
 - Neural Architecture Search (NAS)

- Two methods
 - Reinforcement Learning
 - Differentiable architecture search

Discussion

NAS for GNN

- Background
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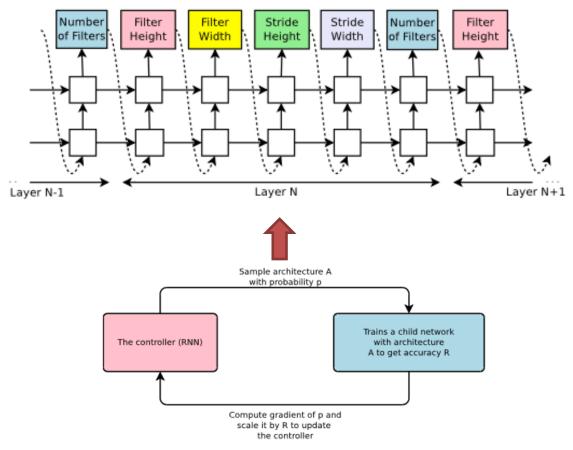
Discussion

Neural Architecture Search

- Neural Architecture Search (NAS)
 - Exploring the possibility of automatically searching for unexplored architectures beyond human-designed ones.
 - Can obtain data-specific models.

NAS

- Trial and Error
 - Iteratively train and evaluate the candidate architectures, keeping tracking of the best ones



NAS for GNN

- Motivation
 - Existing challenges of GNN
 - Architecture challenge
 - Efficiency challenge

- How can NAS help?
 - Automatically search for unexplored and optimal GNN architectures.
 - Transfer searched architecture from smaller graphs to larger graphs.

NAS for GNN

- Background
 - Graph Neural Network (GNN)
 - Neural Architecture Search (NAS)

- Two methods
 - Reinforcement Learning (RL)
 - Differentiable architecture search

Discussion

RL-based NAS

- RL framework
 - Sample an child model and train from scratch.
 - Update based on the validation accuracy (reward)

- Existing works
 - GraphNAS [Gao et al. 2020]
 - Auto-GNN[Zhou et al. 2019]
 - Policy-GNN[Zhou et al. 2020]

- Ongoing work
 - Differentiable architecture search for GNN

Search Space

Macro

Actions	Contents
SAM	Sample neighbors
ATT	Const, gcn, gat, sym-gat, cos
AGG	Sum, mean, max, mlp
Heads K	1, 2, 4, 8, 16
DIM	16, 32, 64, 128
ACT	Relu, elu, tanh, linear, sigmoid

- Combine with Message Passing

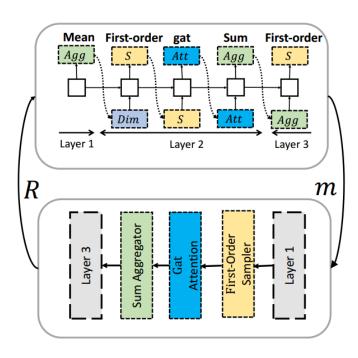
$$\mathbf{m}_{\mathbf{v}}^{t+1} = \sum_{\omega \in N(v)} M_t(h_v^t, h_\omega^t, e_{v\omega}) \qquad h_v^{t+1} = U_t(h_v^t, \mathbf{m}_{\mathbf{v}}^{t+1})$$
 [AGG , SAM] DIM [ATT , Heads K] ACT

Search Space

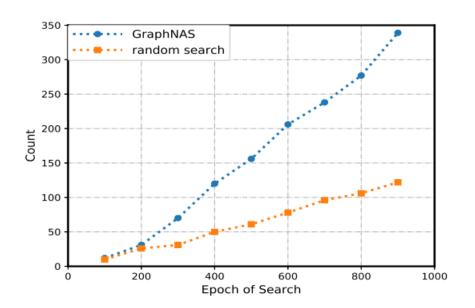
- Micro
 - Each layer contains several cells(2 cells in this paper).
 - Generate hyper params for sub-models.
 - For each cell, select input, GNN method and activation function.
 - Select concatenation type for each layer.

Actions	Contents
Hyper	Ir, dropout, weight_deacy, hidden_unit
His_index	$L_{current-1}, L_{current-2}, C_{< current}$
GNN	Sage, gcn, gat_x, linear, zero
ACT	Relu, elu, tanh, linear, sigmoid
concat_type	concat, add, product

- Search algorithm
 - RNN generates child architectures
 - Train child models and get valid acc
 - Update RNN parameters.



Experiment results



Model	Cora	Citeseer	Pubmed
GCN	81.5+/-0.4	70.9+/-0.5	79.0+/-0.4
SGC	81.0+/-0.0	71.9+/-0.1	78.9+/-0.0
GAT	83.0+/-0.7	72.5+/-0.7	79.0+/-0.3
LGCN	83.3+/-0.5	73.0+/-0.6	79.5+/-0.2
DGCN	82.0+/-0.2	72.2+/-0.3	78.6+/-0.1
ARMA	82.8+/-0.6	72.3+/-1.1	78.8+/-0.3
APPNP	83.3+/-0.6	71.8+/-0.4	80.2+/-0.2
simple-NAS	81.4+/-0.6	71.7+/-0.6	79.5+/-0.5
GraphNAS	84.3+/-0.4	73.7+/-0.2	80.6+/-0.2

Left: Count models whose acc over 0.81 on Cora datasets Right: Semi-supervised node classification w.r.t. accuracy

Auto-GNN [Zhou et al. 2019]

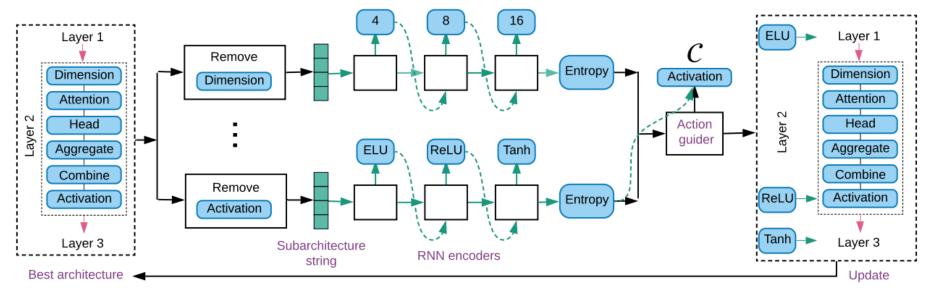
Search space

Macro

Actions	Contents
ATT	Const, gcn, gat, cos, linear
AGG	Sum, mean, max
Heads K	1,2,4,6,8,16
DIM	4,8,16,32,64,128,256
ACT	Relu, elu, tanh, linear, sigmoid

Auto-GNN [Zhou et al. 2019]

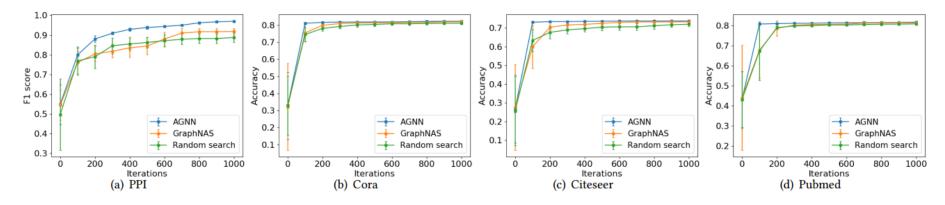
- Search algorithm
 - Modification based on a well-performed architecture.
 - Modify architecture
 - Individual RNN controller for each class
 - Action guider selects a class with decision entropy
 - Use policy gradient to update parameters.



Auto-GNN [Zhou et al. 2019]

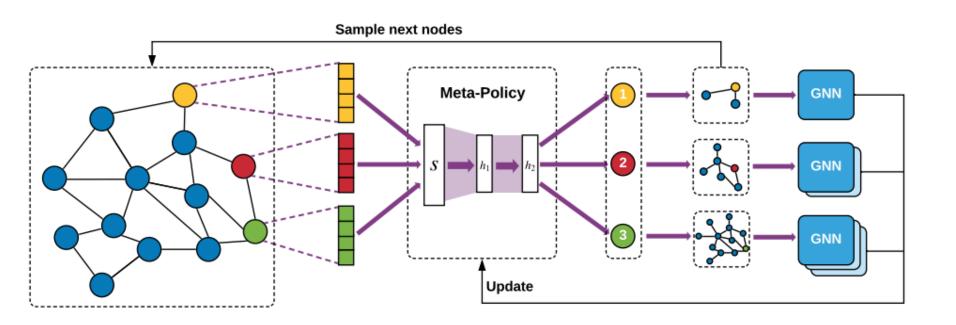
Experiment results

Baseline Class	Model	#Layers	Cora		Citeseer		Pubmed	
Daseille Class	Model	#Layers	#Params	Accuracy	#Params	Accuracy	#Params	Accuracy
	Chebyshev	2	0.09M	81.2%	0.09M	69.8%	0.09M	74.4%
Handcrafted	GCN	2	0.02M	81.5%	0.05M	70.3%	0.02M	79.0.5%
Architectures	GAT	2	0.09M	$83.0\pm0.7\%$	0.23M	$72.5\pm0.7\%$	0.03M	$79.0\pm0.3\%$
	LGCN	3 ~ 4	0.06M	$83.3\pm0.5\%$	0.05M	$73.0\pm0.6\%$	0.05M	$79.5 \pm 0.2\%$
	GraphNAS-w/o share	2	0.09M	$82.7 \pm 0.4\%$	0.23M	$73.5 \pm 1.0\%$	0.03M	$78.8 \pm 0.5\%$
NAS Baselines	GraphNAS-with share	2	0.07M	$83.3 \pm 0.6\%$	1.91M	$72.4 \pm 1.3\%$	0.07M	$78.1 \pm 0.8\%$
NAS daselines	Random-w/o share	2	0.37M	$81.4\pm1.1\%$	0.95M	$72.9 \pm 0.2\%$	0.13M	$77.9 \pm 0.5\%$
	Random-with share	2	2.95M	$82.3 \pm 0.5\%$	0.95M	$69.9 \pm 1.7\%$	0.13M	$77.9 \pm 0.4\%$
AGNN	AGNN-w/o share	2	0.05M	83.6 ± 0.3%	0.71M	$73.8 \pm 0.7\%$	0.07M	79.7 ± 0.4%
AGININ	AGNN-with share	2	0.37M	$82.7 \pm 0.6\%$	1.90M	$72.7 \pm 0.4\%$	0.03M	$79.0 \pm 0.5\%$



Policy-GNN [Lai et al. 2020]

- Search for the number of hops per node based on node attributes.
 - Plugged into existing GNN architectures.



Policy-GNN [Lai et al. 2020]

- Search for the number of hops per node based on node attributes.
 - Performance gain is significant.

Baseline Class	Model	#T arrana	Cora		Citese	er	Pubme	ed
baseline Class	Model	#Layers	Accuracy	1	Accuracy	1	Accuracy	1
Network	DeepWalk [32]	-	0.672	+36.8%	0.432	+107.6%	0.653	+41.0%
Embedding	Node2vec [10]	-	0.749	+22.7%	0.547	+64.0%	0.753	+22.3%
	Chebyshev [5]	2	0.812	+13.2%	0.698	+28.5%	0.744	+23.8%
	GCN [20]	2	0.815	+12.8%	0.703	+27.6%	0.790	+16.6%
	GraphSAGE [14]	2	0.822	+11.8%	0.714	+25.6%	0.871	+5.7%
Static-GNNs	FastGCN [4]	2	0.850	+8.1%	0.776	+15.6%	0.880	+4.7%
	GAT [37]	2	0.830 ± 0.006	+10.7%	0.725 ± 0.005	23.7%	0.790 ± 0.002	+16.6%
	LGCN [8]	2	0.833 ± 0.004	+10.3%	0.730 ± 0.004	+22.9%	0.795± 0.002	+15.8%
	g-U-Nets [7]	4	0.844 ± 0.005	+8.9%	0.732±0.003	+22.5%	0.796± 0.002	+15.7%
	Adapt [17]	2	0.874 ± 0.003	+5.1%	0.796 ± 0.002	+12.7%	0.906± 0.002	+1.7%
NAC ONN	GraphNAS [9]	2	0.833 ± 0.002	+10.3%	0.735± 0.007	+22.0%	0.781± 0.003	+17.9%
NAS-GNNs	AGNN [45]	2	0.836 ± 0.003	+9.9%	0.738 ± 0.005	+21.5%	0.797± 0.003	+15.6%
Dalian CNN	Random Policy	2 ~ 5	0.770 ± 0.021	+19.4%	0.656± 0.024	+36.7%	0.788 ± 0.011	+16.9%
Policy-GNN	Policy-GNN	2 ~ 5	0.919 ± 0.014	-	0.897 ± 0.021	-	0.921± 0.022	-

Policy-GNN [Lai et al. 2020]

- Search for the number of hops per node based on node attributes.
 - Distribution of number of GNN layers

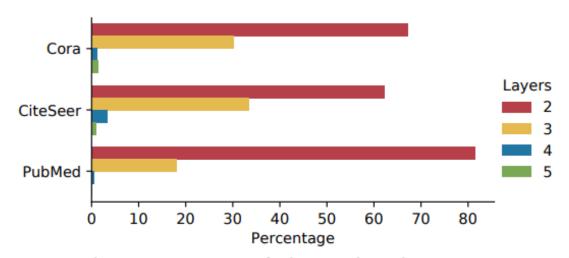


Figure 4: The percentage of the nodes that are assigned to different layers of GCN by *Policy-GNN*.

NAS for GNN

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 - Neural Architecture Search (NAS)

- Two methods
 - Reinforcement Learning (RL)
 - Differentiable architecture search

Discussion

Differentiable architecture search

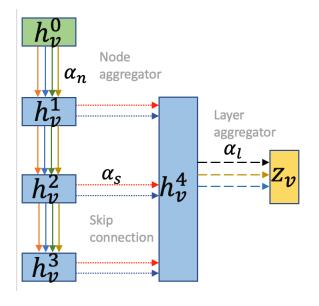
- Search to Aggregate Neighborhood (SANE) for GNN.
 - Ongoing work.

- Contributions
 - Novel and effective search space
 - Differentiable search algorithm
 - Transfer learning in large graphs

Search Space

- Message passing framework
 - Node aggregator
 - Layer aggregator

	Operations
O_n	SAGE-SUM, SAGE-MEAN, SAGE-MAX, SAGE-LSTM, GCN, GAT,GAT-SYM, GAT-COS, GAT-LINEAR, GAT-GEN-LINEAR, CNN, MLP, GeniePath
O_l	CONCAT, MAX, SUM, MIN, LSTM
O_s	IDENTITY, ZERO



Comparing to existing GNNs

	model	node aggregator	layer aggregator	scale to large graph	emulate by SANE
	GCN [17]	GCN	×	×	✓
	SAGE [15]	SAGE-SUM/-MEAN/-MAX/-LSTM	×	✓	✓
human- designed	GAT [30]	GAT, GAT-SYM/-COS/ -LINEAR/-GEN-LINEAR	×	×	✓
	GIN [33]	MLP	×	×	✓
	LGCN [11]	CNN	×	×	✓
	GeniePath [21]	GeniePath	×	✓	✓
	JK-Network [34]	depends on the base GNN.	✓	✓	✓
NAS	SANE	learned combination of aggregators	✓	✓	

Search Space

More explanations on node aggregator

GNN models	Symbol in the paper	Key explanations
GCN [15]	GCN	$ F_N^l(v) = \sum_{u \in \widetilde{N}(v)} \left(\operatorname{degree}(v) \cdot \operatorname{degree}(u) \right)^{-1/2} \cdot \mathbf{h}_u^{l-1}. $
GraphSAGE [15]	SAGE-MEAN, SAGE-MAX, SAGE-SUM, SAGE-LSTM	Apply mean, max, sum, or LSTM operation to $\{\mathbf{h}_u u\in\widetilde{N}(v)\}$.
	GAT	Compute attention score: $\mathbf{e}_{uv}^{gat} = \text{Leaky_ReLU}(\mathbf{a}[\mathbf{W}_{u}\mathbf{h}_{u} \mathbf{W}_{v}\mathbf{h}_{v}]).$
	GAT-SYM	$\mathbf{e}_{uv}^{sys} = \mathbf{e}_{uv}^{gat} + \mathbf{e}_{vu}^{gat}$.
GAT [30]	GAT-COS	$\mathbf{e}_{uv}^{cos} = \langle \mathbf{W}_{u} \mathbf{h}_{u}, \mathbf{W}_{v} \mathbf{h}_{v} \rangle.$
	GAT-LINEAR	$\mathbf{e}_{uv}^{lin} = \tanh(\mathbf{W}_{u}\mathbf{h}_{u} + \mathbf{W}_{v}\mathbf{h}_{v}).$
	GAT-GEN-LINEAR	$\mathbf{e}_{uv}^{gen-lin} = \mathbf{W}_G \tanh(\mathbf{W}_u \mathbf{h}_u + \mathbf{W}_v \mathbf{h}_v).$
GIN [33]	MLP	$F_N^l(v) = \text{MLP}\bigg((1+\epsilon^{l-1})\cdot\mathbf{h}_v^{l-1} + \sum_{u\in N(v)}\mathbf{h}_u^{l-1}\bigg).$
LGCN [11]	CNN	Use 1-D CNN as the aggregator.
GeniePath [21]	GeniePath	Composition of two aggregators, one is GAT, and the other is LSTM-based one.
JK-Network [34]		Depending on the base above GNN.

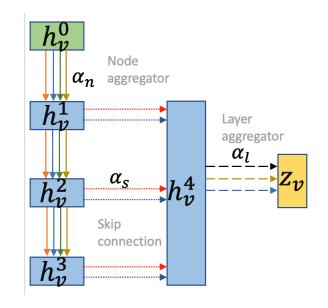
Differentiable search algorithm

- Supernet (DAG)
 - Continuous relaxation
 - Mixed OPs

$$\bar{o}^{(i,j)}(x) = \sum_{o \in O} \frac{\exp(\boldsymbol{\alpha}_o^{(i,j)})}{\sum_{o' \in O} \exp(\boldsymbol{\alpha}_{o'}^{(i,j)})} o(x)$$

Computation process

$$\begin{split} \mathbf{h}_{v}^{(l)} &= \sigma \bigg(\mathbf{W}_{n}^{(l)} \cdot \bar{o}_{n}(\{\mathbf{h}_{u}^{(l-1)}, \forall u \in \widetilde{N}(v)\}) \bigg) \\ \mathbf{H}_{v}^{K+1} &= \left[\bar{o}_{s}(\mathbf{h}_{v}^{1}), \cdots, \bar{o}_{s}(\mathbf{h}_{v}^{K}) \right] \\ \mathbf{z}_{v} &= \bar{o}_{l}\left(\mathbf{H}_{v}^{K+1} \right) \end{split}$$



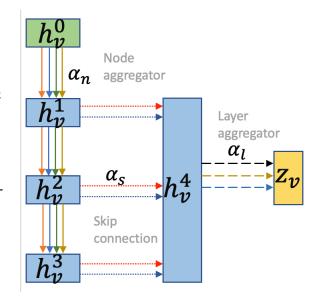
Differentiable search algorithm

• Search $\{\alpha_n, \alpha_s, \alpha_l\}$

DEFINITION 1 (SANE PROBLEM). Formally, the general paradigm of SANE is to solve a bi-level optimization problem:

$$\min_{\boldsymbol{\alpha} \in \mathcal{A}} \mathcal{L}_{val}(\boldsymbol{w}^*(\boldsymbol{\alpha}), \boldsymbol{\alpha}), \text{ s.t. } \boldsymbol{w}^*(\boldsymbol{\alpha}) = \arg\min_{\boldsymbol{w}} \mathcal{L}_{train}(\boldsymbol{w}, \boldsymbol{\alpha}), \quad (6)$$

where \mathcal{L}_{train} and \mathcal{L}_{val} are the training and validation loss, respectively. $\boldsymbol{\alpha}$ represent a network architecture, where $\boldsymbol{\alpha} = \{\boldsymbol{\alpha}_n, \boldsymbol{\alpha}_s, \boldsymbol{\alpha}_l\}$ and $\boldsymbol{w}^*(\boldsymbol{\alpha})$ the corresponding weights after training.



- Derive architecture
 - Choose the OP with the largest weight.

$$o^{(i,j)} = \operatorname{arg\,max}_{o \in O} \alpha_o^{(i,j)}$$

Differentiable search algorithm

• Gradient-based optimization.

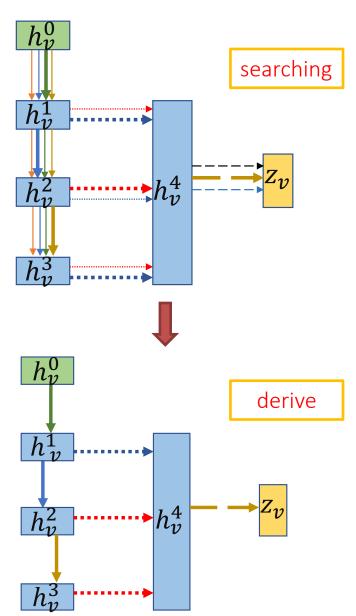
$$\nabla_{\alpha} \mathcal{L}_{val}(\mathbf{w}^*(\alpha), \alpha) \approx \nabla_{\alpha} \mathcal{L}_{val}(\mathbf{w} - \xi \nabla_{\mathbf{w}} \mathcal{L}_{train}(\mathbf{w}, \alpha), \alpha)$$

Algorithm 1 SANE - Search to Aggregate NEighborhood.

Require: The search space \mathcal{F} , the number of top architectures k, the epochs for search T.

Ensure: The *k* searched architectures \mathcal{A}_k .

- 1: **while** $t = 1, \dots, T$ **do**
- 2: Compute the validation loss \mathcal{L}_{val} ;
- Update α_n , α_s and α_l by gradient descend rule Eq. (7) with Eq. (3), (4) and (5) respectively;
- 4: Compute the training loss \mathcal{L}_{train} ;
- Update weights **w** by descending $\nabla_{\mathbf{w}} \mathcal{L}_{train}(\mathbf{w}, \boldsymbol{\alpha})$ with the architecture $\boldsymbol{\alpha} = [\boldsymbol{\alpha}_n, \boldsymbol{\alpha}_s, \boldsymbol{\alpha}_l]$;
- 6: end while
- 7: Derive the final architecture based on the trained $\{\alpha_n, \alpha_s, \alpha_l\}$;



Transfer learning for large graphs

- Sample a smaller graph.
- Search in the smaller graph.
- Transfer to the large graph

Algorithm 2 Transferable SANE.

Require: The search space \mathcal{F} , the number of top architectures k, the epochs for search T, the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$.

Ensure: The k searched architectures \mathcal{A}_k and corresponding test performance on \mathcal{G} .

- 1: Compute the PageRank values for nodes in \mathcal{V} , denoted as \mathbf{p} ;
- 2: /*The detail of the sampling method is the RPN in [18]*/
- 3: Sample N, $N = 15\% |\mathcal{V}|$ nodes \mathcal{V}_s , according to the PageRank vector \mathbf{p} ;
- 4: Construct a proxy graph $\mathcal{G}_{proxy} = (\mathcal{V}_s, \mathcal{E}_s)$, with $\mathcal{E}_s = \{e_{uv} | \forall e_{uv} \in \mathcal{E} \text{ and } u \in \mathcal{V}_s, v \in \mathcal{V}_s\}$.
- 5: Obtain $\{\alpha_n, \alpha_s, \alpha_l\}$ by SANE (Algorithm 1) on \mathcal{G}_{proxy} , given \mathcal{F}, k, T , obtain the best k architecture.
- 6: Re-train the architecture $\{\alpha_n, \alpha_s, \alpha_l\}$ on \mathcal{G} , and return the test performance.

- Task
 - Node classification
 - Transducive/inductive/transfer

Datasets

Task	Datasets	N	Е	F	С
	Cora	2,708	5,278	1,433	7
transductive	CiteSeer	3,327	4,552	3,703	6
	PubMed	19,717	44,324	500	3
inductive	PPI	56,944	818,716	121	50
transfer	Reddit	232,965	57,307,946	602	50

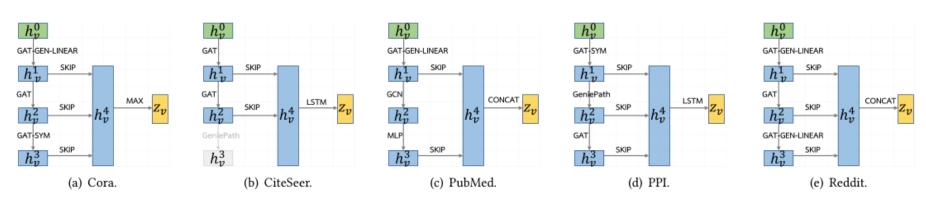
- Performance comparison
 - Human-designed architectures
 - NAS approaches

	Methods	Cora	Transductive CiteSeer	PubMed	Inductive PPI
	Methods	Cora	Citeseei	rubivieu	rrı
	GCN	0.8811 (0.0101)	0.7666 (0.0202)	0.8858 (0.0030)	0.6500 (0.0000)
	GCN-JK	0.8820 (0.0118)	0.7763 (0.0136)	0.8927 (0.0037)	0.8078(0.0000)
	GraphSAGE	0.8741 (0.0159)	0.7599 (0.0094)	0.8834 (0.0044)	0.6504 (0.0000)
	GraphSAGE-JK	0.8841 (0.0015)	0.7654 (0.0054)	0.8942 (0.0066)	0.8019 (0.0000)
Human-designed	GAT	0.8719 (0.0163)	0.7518 (0.0145)	0.8573 (0.0066)	0.9414 (0.0000)
architectures	GAT-JK	0.8726 (0.0086)	0.7527 (0.0128)	0.8674 (0.0055)	0.9749 (0.0000)
arcintectures	GIN	0.8600 (0.0083)	0.7340 (0.0139)	0.8799 (0.0046)	0.8724 (0.0002)
	GIN-JK	0.8699 (0.0103)	0.7651 (0.0133)	0.8878 (0.0054)	0.9467 (0.0000)
	GeniePath	0.8670 (0.0123)	0.7594 (0.0137)	0.8846 (0.0039)	0.7138 (0.0000)
	GeniePath-JK	0.8776 (0.0117)	0.7591 (0.0116)	0.8868 (0.0037)	0.9694 (0.0000)
	LGCN	0.8687 (0.0075)	0.7543 (0.0221)	0.8753 (0.0012)	0.7720 (0.0020)
	Random	0.8594 (0.0072)	0.7062 (0.0042)	0.8866(0.0010)	0.9517 (0.0032)
	Bayesian	0.8835 (0.0072)	0.7335 (0.0006)	0.8801(0.0033)	0.9583 (0.0082)
NAS approaches	GraphNAS	0.8840 (0.0071)	0.7762 (0.0061)	0.8896 (0.0024)	0.9692 (0.0128)
	GraphNAS-WS	0.8808 (0.0101)	0.7613 (0.0156)	0.8842 (0.0103)	0.9584 (0.0415)
one-shot NAS	SANE	0.8926 (0.0123)	0.7859 (0.0108)	0.9047 (0.0091)	0.9856 (0.0120)

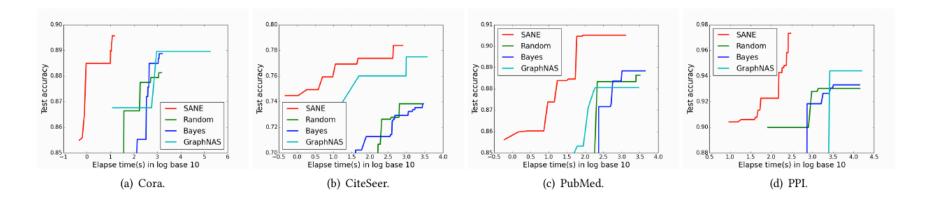
Transferred learning

	Methods	Reddit
Human-designed architectures	GraphSAGE GraphSAGE-JK	0.9379 (0.0003) 0.9421 (0.0005)
NAS approaches	Random Bayesian GraphNAS GraphNAS-WS	0.9284 (0.0005) 0.9379 (0.0002) 0.9432 (0.0004) 0.9418 (0.0010)
one-shot NAS	SANE	0.9528 (0.0008)

Searched architectures



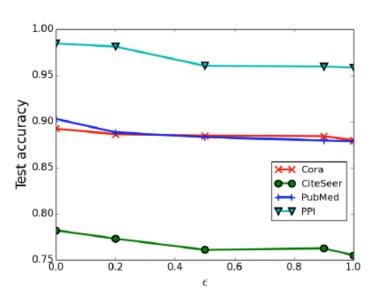
The test accuracy w.r.t. search time(s)



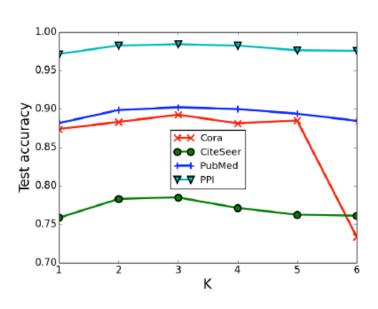
• The total time (s) of running once of each model.

	transductive task			inductive task
	Cora	CiteSeer	PubMed	PPI
Random	1,500	2,694	3,174	13,934
Bayesian	1,631	2,895	4,384	14,543
GraphNAS	3,240	3,665	5,917	15,940
SANE	14	35	54	298

- Ablation study
 - The influence of differentiable search
 - The influence of K
- The test accuracy w.r.t. different ϵ and K for transductive and inductive tasks.



(a) Random explore: ϵ .



(b) Number of GNN layers: K.

Discussion

Conclusion

- Novel and Effective search space
- Differentiable search algorithm
- Transfer learning in large graphs

Future work

- More advanced one-shot NAS approaches
 - NASP, ASNG-NAS, etc.
- Other graph-based tasks
 - Graph-based recommendation

Automated GNN for Recommendation

- How to construct the graphs?
 - Multiple graphs, bipartite graphs, heterogeneous graph?

- How to define neighbors beyond aggregation schemas?
 - Neighbors of different types
 - Rich side information
 - Neighbors in different hops
 - Higher-order relations

- How to address the scalability problem ?
 - Billion-scale graph in reality.

Summary

GNN is naturally suitable for recommendation

 Automated machine learning can obtain dataspecific GNN architectures.

Automated GNN can further improve recommendation.

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Q&A

Thank You! ©