Automated Learning from Graph-Structured Data

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https://quanmingyao.github.io/AutoML.github.io/acml21-tutorial.html



Tutorial Outline

1. What is Automated Machine Learning (AutoML)
   - Background on technical tools from machine learning
2. Automated Graph Neural Networks (GNN)
   - Explore neural architecture search for GNN
3. Automated Knowledge Graph (KG) Embedding
   - Explore AutoML for KG Embedding

Schedule at a Glance

Time	Event
00-45 minutes	**Part 1**: An introduction to Automated Machine Learning (AutoML)
	Speaker: Quanming Yao
45-90 minutes	**Part 2**: Automated Graph Neural Networks (GNN)
	Speaker: Huan Zhao
90-135 minutes	**Part 3**: Automated Knowledge Graph (KG) Embedding
	Speaker: Yongqi Zhang
135-150 minutes	**Part 4**: Discussion

Automated Learning from Graph-Structured Data

Part 2: Automated Graph Neural Network

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Nov. 17th 2021

Outline

- Background
  - Graph neural network (GNN)
  - Neural architecture search (NAS)
- Graph neural architecture search
  - Reinforcement learning based search
  - Differentiable architecture search
- Conclusion

Graph-based applications

Search Engine

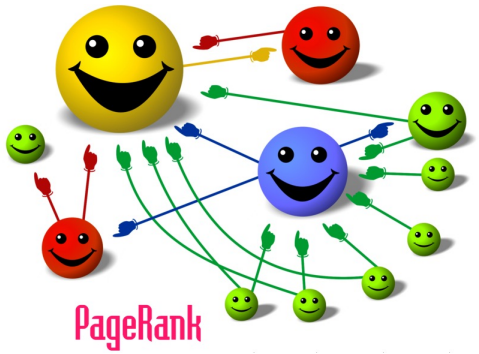


Image Credit: Wikipedia

Recommendation

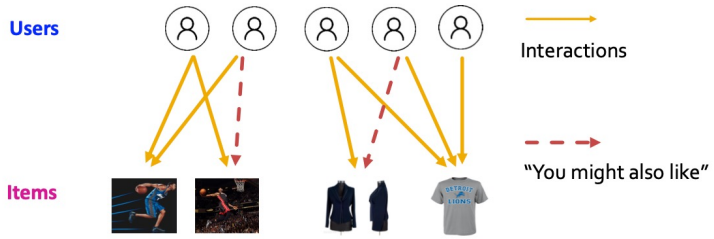


Image Credit: Jure Stanford CS224

Social Network

Image Credit: Shreyansh@Medium

biomedicine

A protein chain acquires its native 3D structure

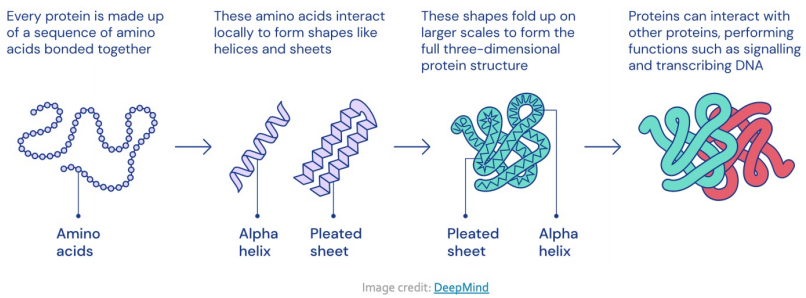
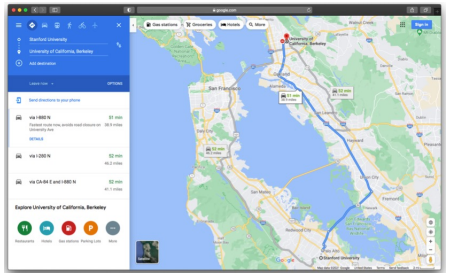


Image Credit: Jure Stanford CS224

Traffic prediction



- **Nodes:** Road segments
- **Edges:** Connectivity between road segments

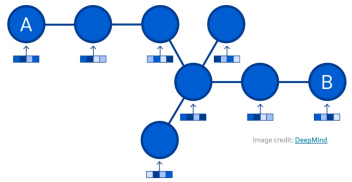


Image Credit: Jure Stanford CS224

Chip Design

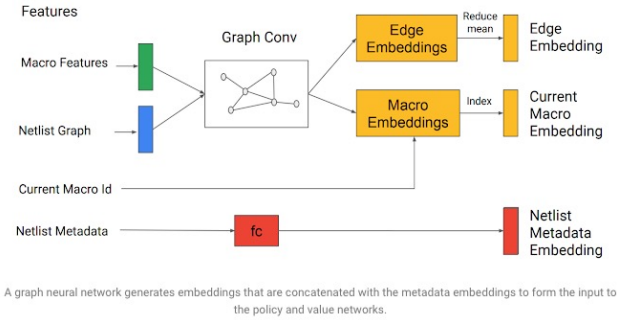
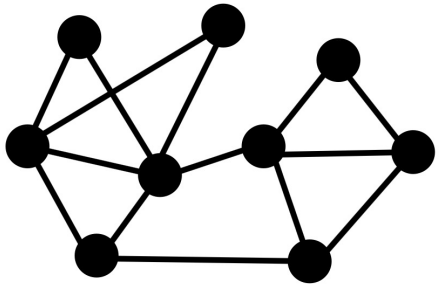
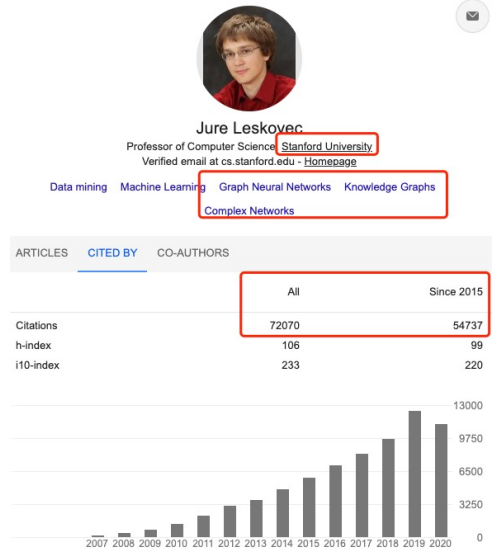


Image Credit: Google Blog

Graph is an universal language for describing and analyzing entities with relations/interactions.



Graph



Prof. Jure Leskovec in Stanford CS224

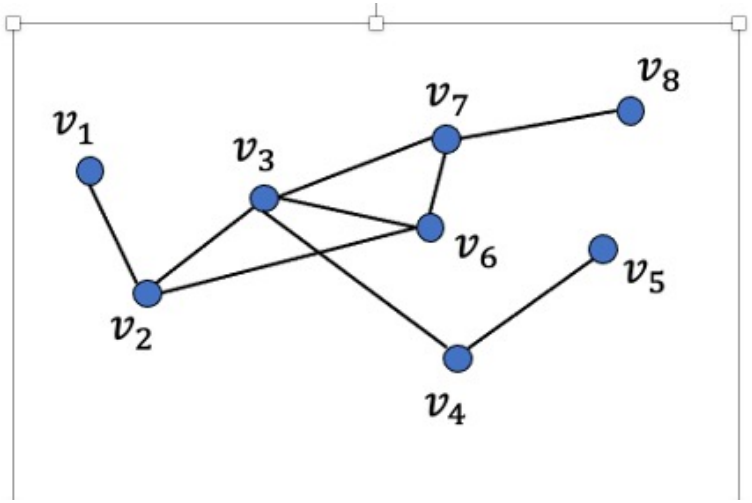
Basic definitions of Graph

- Node set $\mathcal{V}$
- Edge set $\mathcal{E}$
- Adjacency Matrix A
- Neighbor set

$$N(v) = \{u \in \mathcal{V} | (v, u) \in \mathcal{E}\}$$

- Feature Matrix

$$\mathbf{X} \in \mathbb{R}^{N \times d}$$



Adjacency Matrix: $A[i,j] = 1$ if v_i is adjacent to v_j
$A[i,j] = 0$, otherwise

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$\boldsymbol{A}$

Image Credit: Ma et al. @KDD 2020

Graph Neural Networks (GNN)

- GNNs have been new state-of-the-art (SOTA) for graph-based tasks.

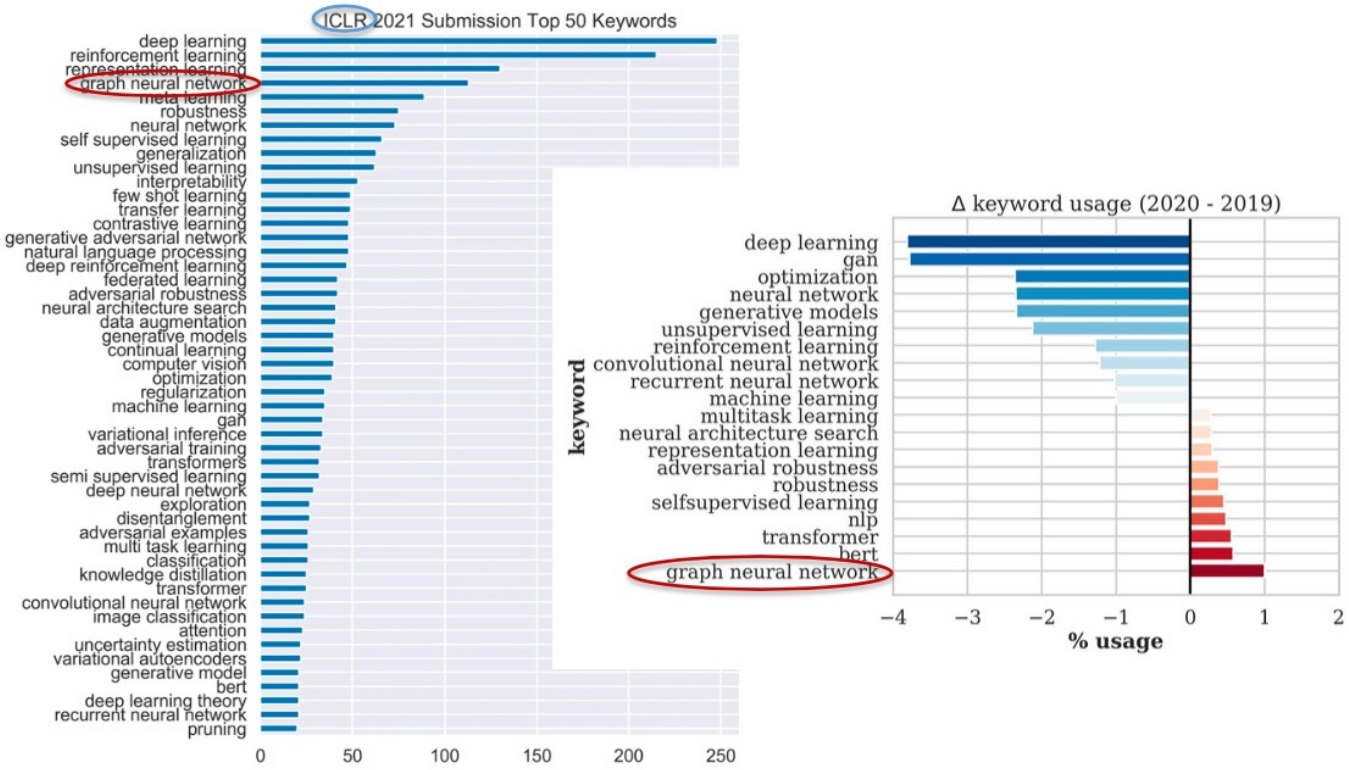


Image Credit: Xavier Bresson

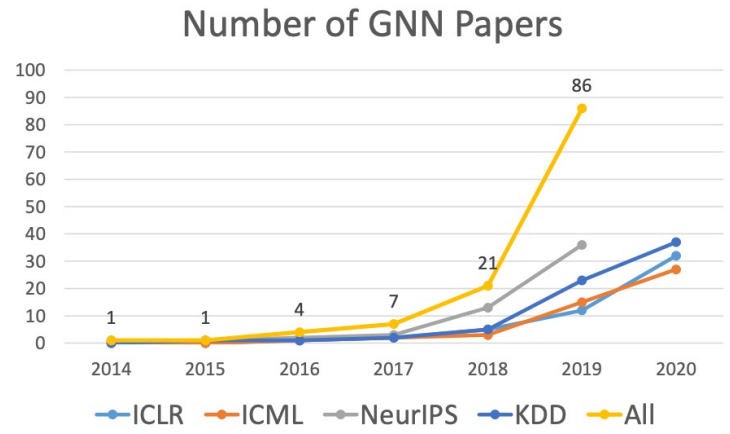


Image Credit: Tecent AI Lab

Illustrative architecture of GNN

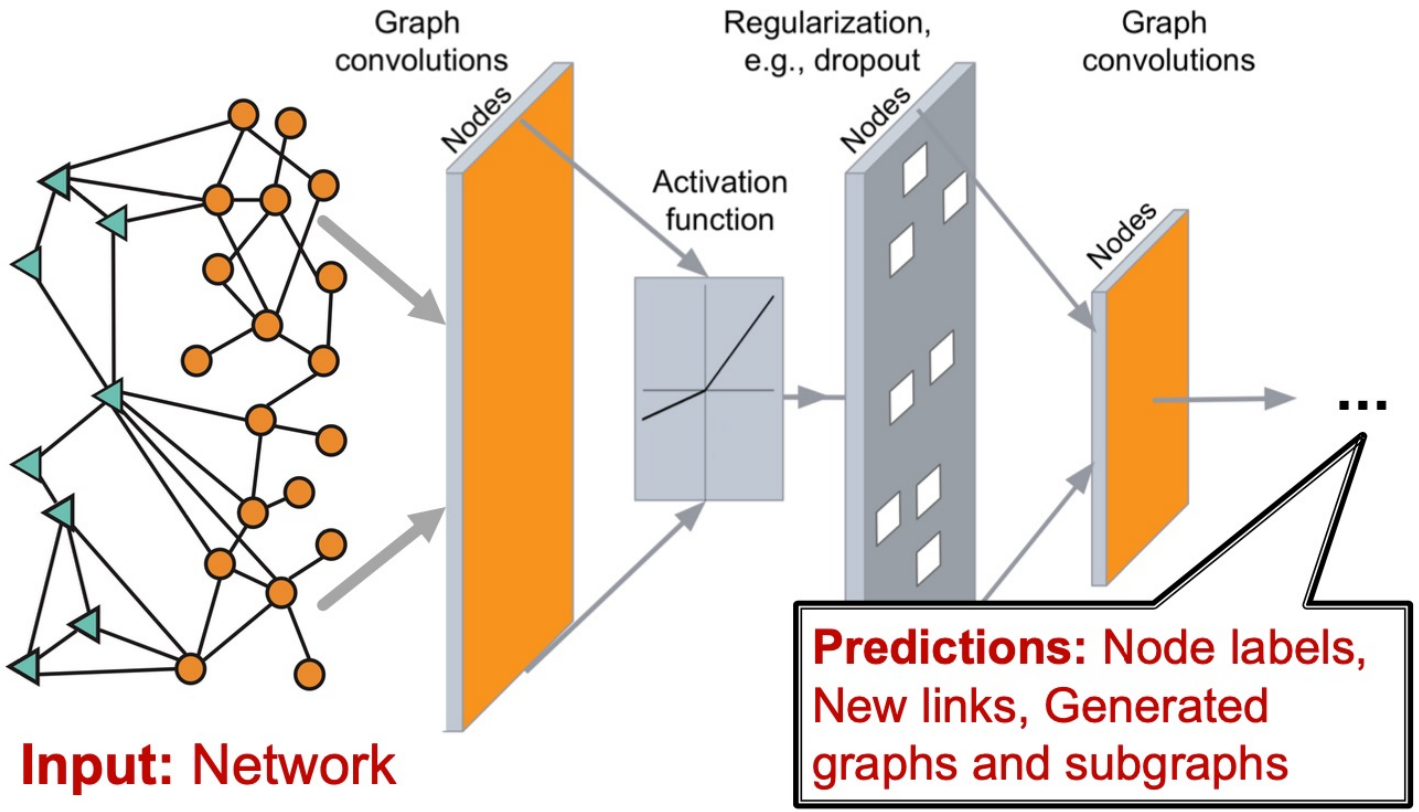


Image Credit: Jure Stanford CS224

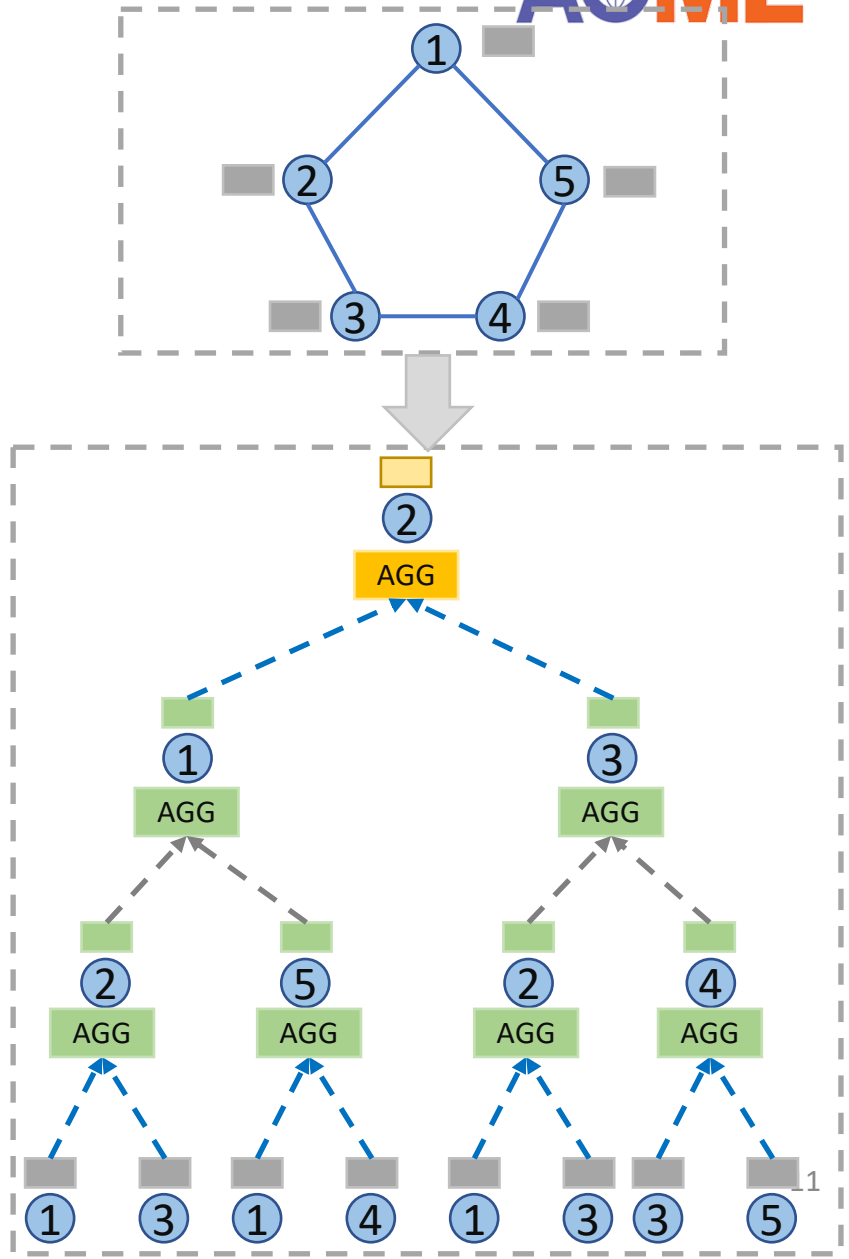
GNN

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

Self contained Neighborhood

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

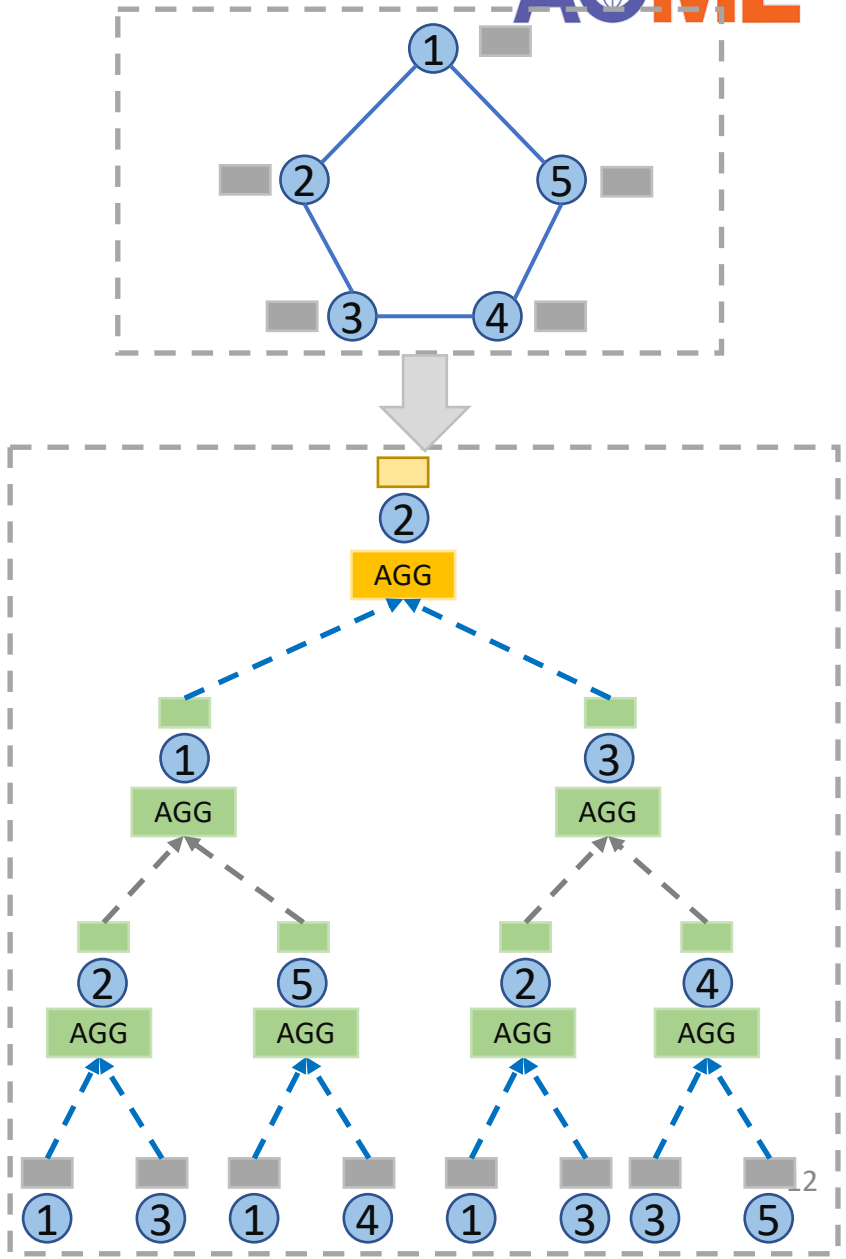
- Variants of GNN
  - GCN: normalized sum aggregator
  - GraphSAGE: MEAN, MAX, SUM, LSTM
  - GAT: Attention aggregator
  - GIN: Multi-Layer Perceptrons (MLP)



GNN

- Message passing framework
  - Instantiate existing GNN models. [Zhao et al. 2021]

GNN models	Symbol in the paper	Key explanations
GCN [14]	GCN	$F_N^l(v) = \sum_{u \in \widetilde{N}(v)} \left(\text{degree}(v) \cdot \text{degree}(u)\right)^{-1/2} \cdot \mathbf{h}_u^{l-1}$
GraphSAGE [3]	SAGE-MEAN, SAGE-MAX, SAGE-SUM	Apply mean, max, or sum operation to $\{\mathbf{h}_u \vert u \in \widetilde{N}(v)\}$.
GAT [4]	GAT	Compute attention score: $\mathbf{e}_{uv}^{gat} = \text{Leaky\_ReLU}\left(\mathbf{a}\left[\mathbf{W}_u\mathbf{h}_u \vert\vert \mathbf{W}_v\mathbf{h}_v\right]\right)$.
	GAT-SYM	$\mathbf{e}_{uv}^{sys} = \mathbf{e}_{uv}^{gat} + \mathbf{e}_{vu}^{gat}$.
	GAT-COS	$\mathbf{e}_{uv}^{cos} = \langle \mathbf{W}_u\mathbf{h}_u, \mathbf{W}_v\mathbf{h}_v \rangle$.
	GAT-LINEAR	$\mathbf{e}_{uv}^{lin} = \tanh\left(\mathbf{W}_u\mathbf{h}_u + \mathbf{W}_v\mathbf{h}_v\right)$.
	GAT-GEN-LINEAR	$\mathbf{e}_{uv}^{gen-lin} = \mathbf{W}_G \tanh\left(\mathbf{W}_u\mathbf{h}_u + \mathbf{W}_v\mathbf{h}_v\right)$.
GIN [16]	GIN	$F_N^l(v) = \text{MLP}\left((1+\epsilon^{l-1}) \cdot \mathbf{h}_v^{l-1} + \sum_{u \in N(v)} \mathbf{h}_u^{l-1}\right)$.
LGCN [15]	CNN	Use 1-D CNN as the aggregator, equivalent to a weighted summation aggregator.
GeniePath [18]	GeniePath	Composition of GAT and LSTM-based aggregators



Zhao et al. Search to aggregate neighborhood for graph neural networks. ICDE 2021

Design Space for GNN [You et al. 2020]

- The performance of GNN models vary
  - Combinations of 12 key design dimensions.
  - 315,000 instances

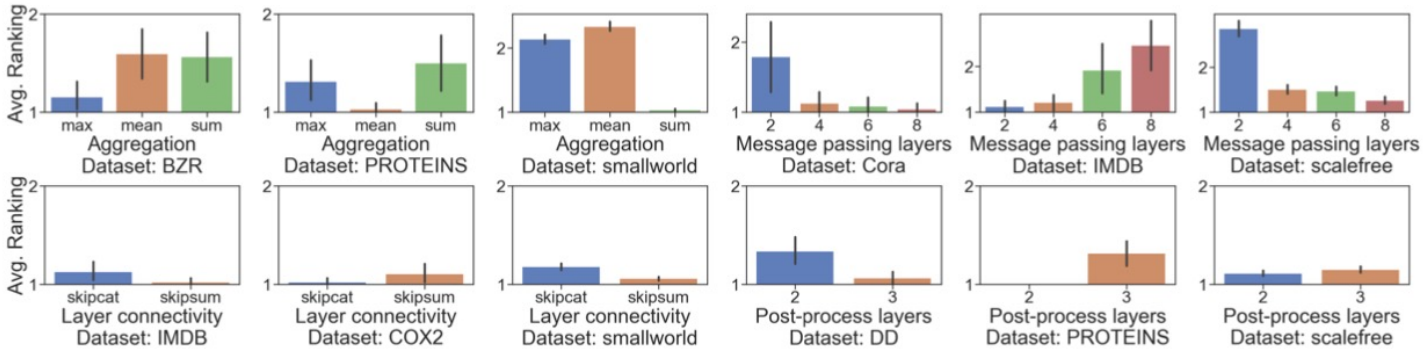
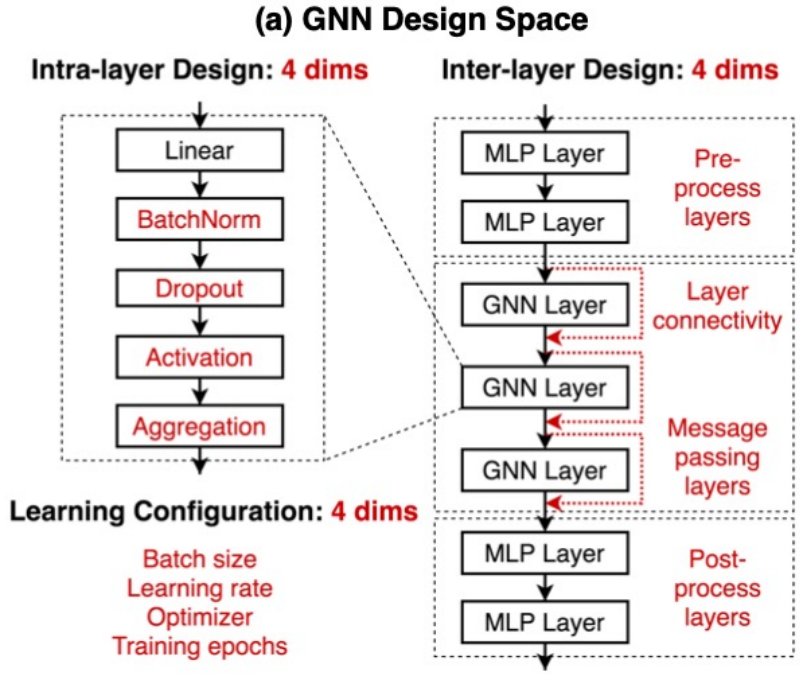


Figure 4: **Ranking analysis for GNN design choices over different GNN tasks**. Lower is better. Preferable design choices greatly vary across GNN tasks.



Batch Normalization	Dropout	Activation	Aggregation
True, False	False, 0.3, 0.6	ReLU, PReLU, Swish	Mean, Max, Sum

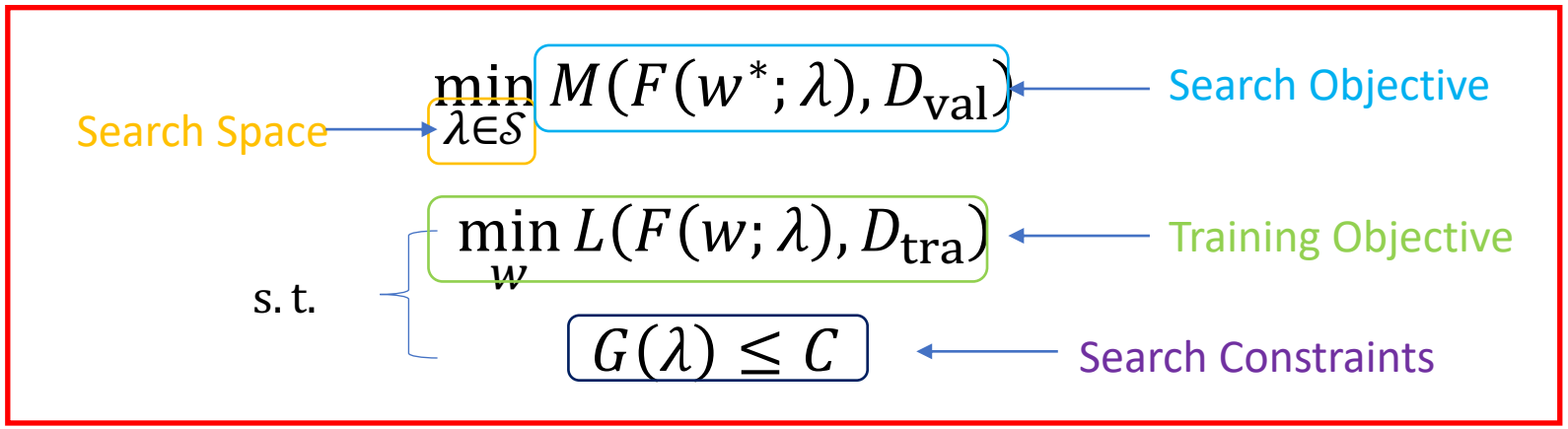
Layer connectivity	Pre-process layers	Message passing layers	Post-precess layers
Stack, Skip-Sum, Skip-Cat	1, 2, 3	2, 4, 6, 8	1, 2, 3

Batch size	Learning rate	Optimizer	Training epochs
16, 32, 64	0.1, 0.01, 0.001	SGD, Adam	100, 200, 400

Neural architecture search for graph neural network

Neural Architecture Search

- Explore the possibility of automatically searching for unexplored architectures beyond human-designed ones.
- A bi-level optimization problem
  - Derive a search space based on domain knowledge
  - Search objective is usually validation performance
  - Training objective usually comes from classical learning models
  - Search constraint is usually resource budgets

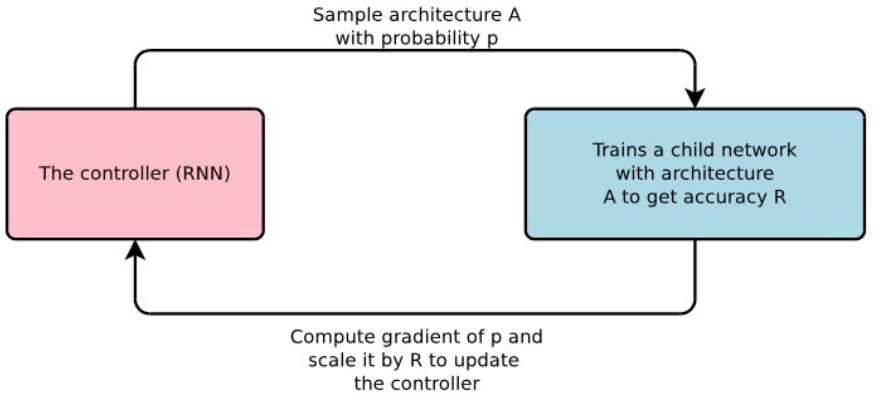


Zoph et al. Neural Architecture Search with Reinforcement Learning. ICLR 2017

Two representative approaches

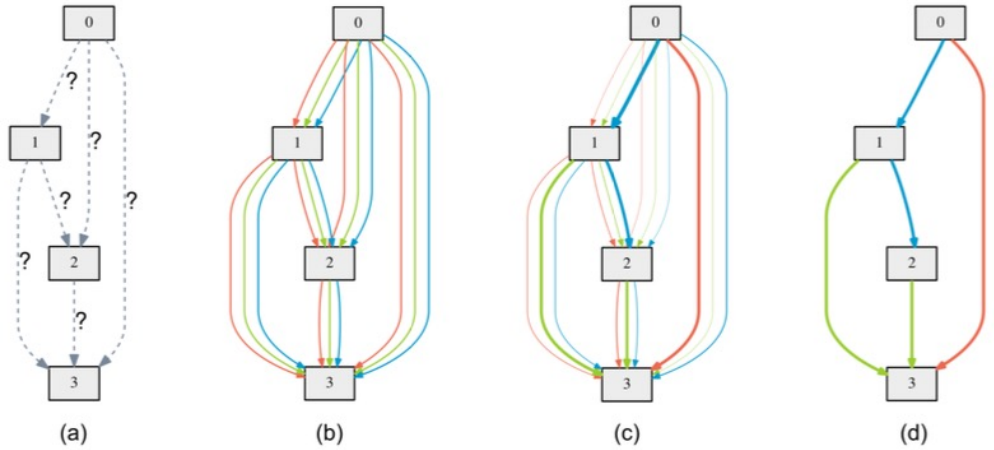
- Stand alone (Reinforcement learning)
  - An RNN controller to sample a candidate architecture
  - Train till convergency
  - Update the RNN controller by the validation accuracy

NASNet [Zoph et al. 2017]



- One-shot (Differentiable architecture search)
  - Train a supernet including all candidate architectures
  - Derive a chidnet from the supernet as the search architecture

DARTS [Liu et al. 2017]

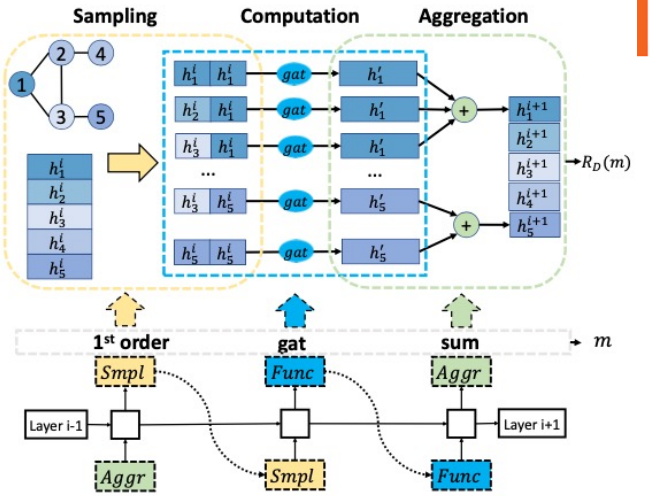


Zoph et al. Neural Architecture Search with Reinforcement Learning. ICLR 2017
Liu et al. Darts: Differentiable architecture search. ICLR 2019

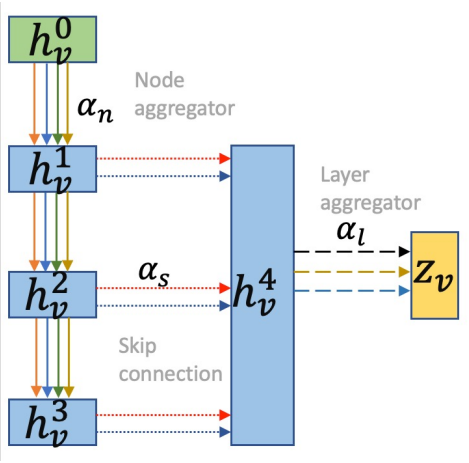
NAS for GNN

- Two representative approaches
  - Search for task-specific GNN architectures.
- GraphNAS [Gao et al. 2020]
  - Reinforcement learning based method
- SANE [Zhao et al. 2021]
  - Differentiable architecture search

GraphNAS [Gao et al. 2020]



SANE [Zhao et al. 2021]



Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020
Zhao et al. Search to aggregate neighborhood for graph neural networks. ICDE 2021

GraphNAS [Gao et al. 2020]

- A first graph neural architecture search.
  - Search for combination of GNN layers
- A customized search space and RL based search algorithm.
- SOTA performance in various settings.
  - Semi-supervised
  - Supervised

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

GraphNAS [Gao et al. 2020]

- Operations in the search space
  - Neighbor sampling $Smpl$
  - Message computation $Func$
  - Message aggregation $Aggr$
  - Multi-head and readout $Read$
  - Activation function σ
  - Number of multi-head k
  - Output dimension d

- An exemplar GNN layer

$$[first\_order, gat, sum, concat, 8, 16, elu]$$

Operators	**Values**
$Smpl$	$first\_order$
$Func$	$e_{uv}h_u$
$Aggr$	sum, $mean$, max, mlp
$Read$	avg, for the last layer $concat$, otherwise
activate function σ	$sigmoid$, $tanh$, $relu$, $identity$, $softplus$, $leaky\_relu$, $relu6$, elu
multi-head k	1, 2, 4, 6, 8, 16
output dimension d	8, 16, 32, 64, 128, 256, 512

Table 1: Operators of search space $\mathcal{M}$

e_{uv}	**Values**
const	$e_{uv}^{con} = 1$
gcn	$e_{uv}^{gcn} = 1/\sqrt{d_u d_v}$
gat	$e_{uv}^{gat} = leaky\_relu((W_l * h_u + W_r * h_v))$
sym-gat	$e_{uv}^{sym} = e_{vu}^{gat} + e_{uv}^{gat}$
cos	$e_{uv}^{cos} =< W_l * h_u, W_r * h_v >$
linear	$e_{uv}^{lin} = tanh(sum(W_l * h_u))$
gene-linear	$e_{uv}^{gan} = W_a * tanh(W_l * h_u + W_r * h_v)$

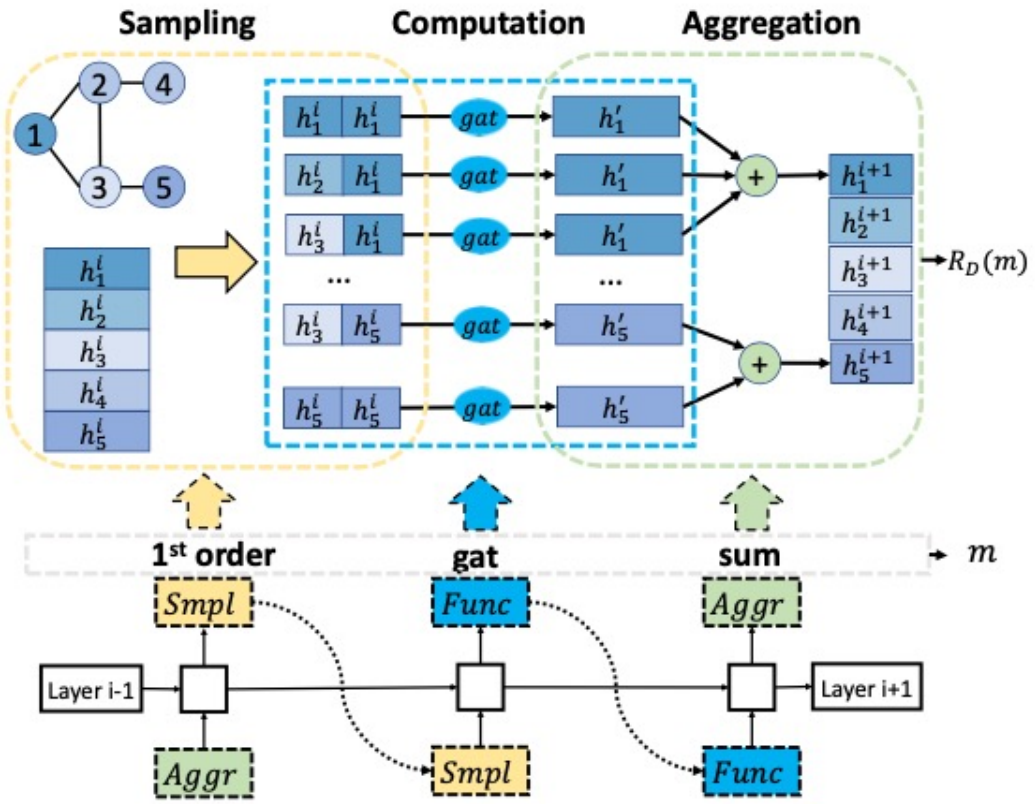
Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

GraphNAS [Gao et al. 2020]

- K-layer GNN
  - List of strings

$$[\ first\_order, gcn, sum, concat, 1, 16, relu,$$
$$first\_order, gat, sum, avg, 8, 16, elu\ ].$$

- Size of the search space
  - $9{,}408^L$
  - 8×10^7 When $L = 2$



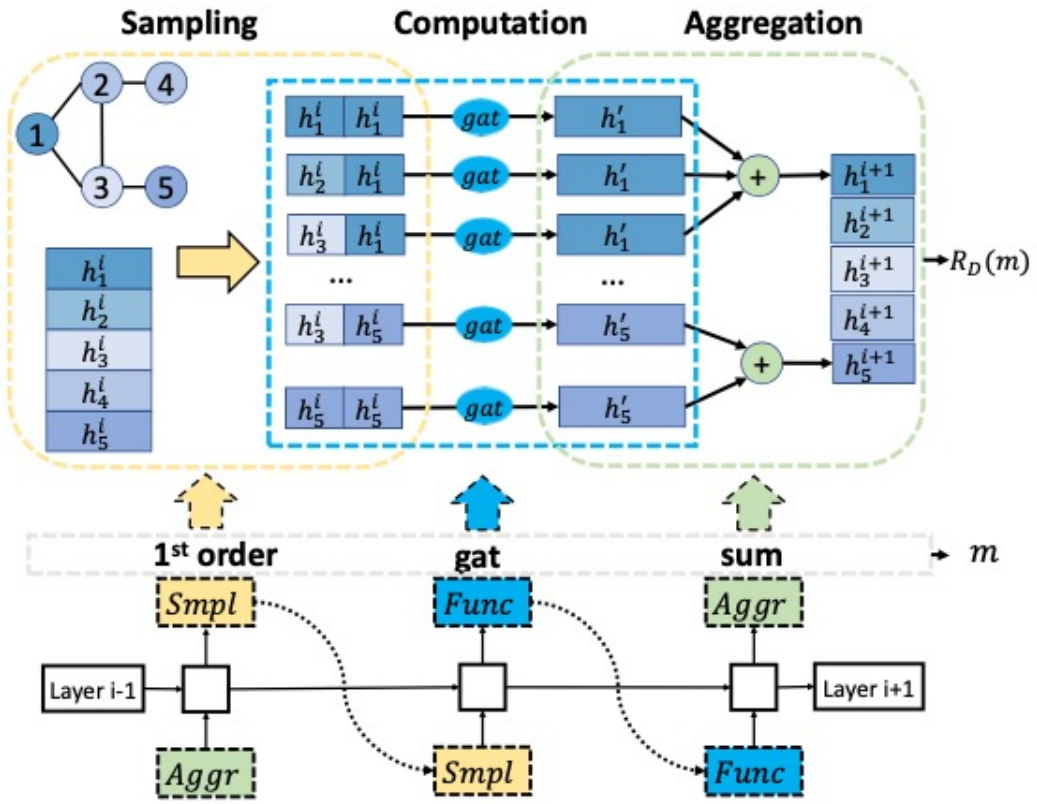
Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

GraphNAS [Gao et al. 2020]

- Search algorithm
  - A RNN controller samples an architecture
  - Training till convergency
  - Update RNN controller based on the validation accuracy

- Search Objective

$$m^* = \arg\max_{m \in \mathcal{M}} \mathbb{E}[R_D(m)].$$



Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

GraphNAS [Gao et al. 2020]

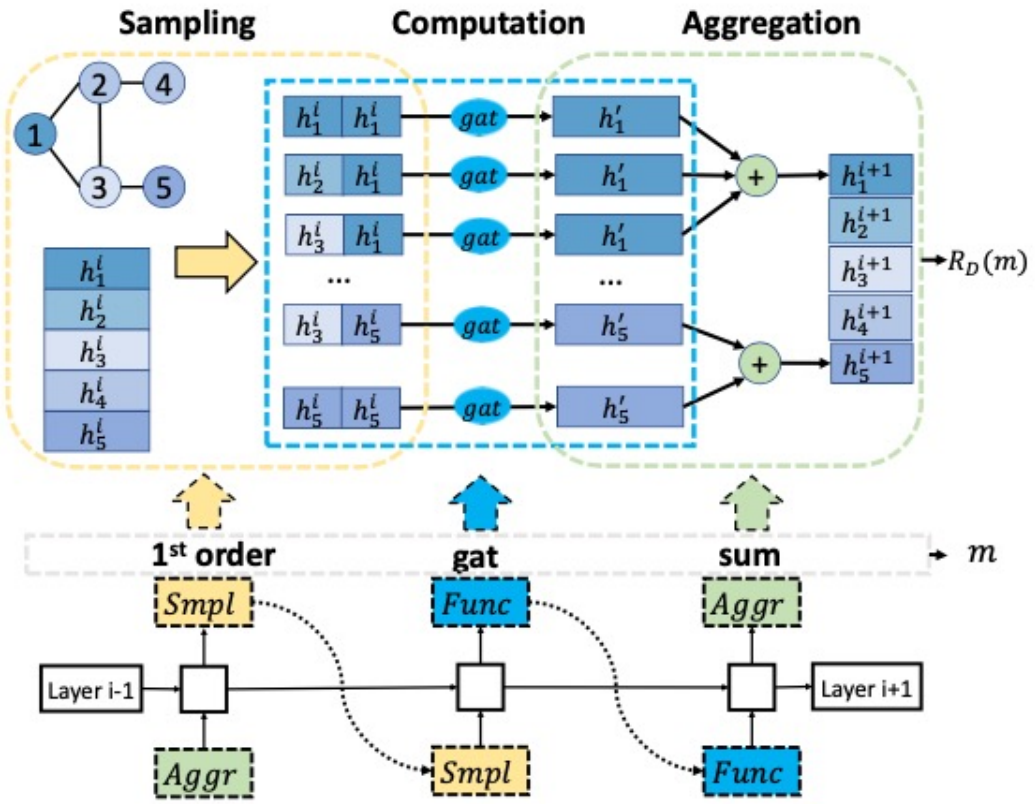
- Search Objective

$$m^* = \arg\max_{m \in \mathcal{M}} \mathbb{E}[R_D(m)].$$

- Policy gradient

$$\nabla_\theta \mathbb{E}_{P(m_{1:T};\theta)}[R]$$
$$= \sum_{t=1}^{T} \mathbb{E}_{P(m_{1:T};\theta)}[\nabla_\theta log P(m_t | m_{t-1:1}; \theta)(R - b)]$$

  - $m_{1:T}$: a list of operators with length T
  - θ : the parameters of the RNN controller



Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

GraphNAS [Gao et al. 2020]

- How to build deeper GNNs.
  - Recall the size is $9{,}408^L$
  - Extremely expensive when L is large

- Avoid exponential growth of search space
  - Three constraints
    - Independency of each layer
    - Reduce some operators
    - User different message functions for multi-head
- A DAG to represent each GNN layer
  - Five nodes
    - two input(1,2), two intermediate(3,4), one output(5)

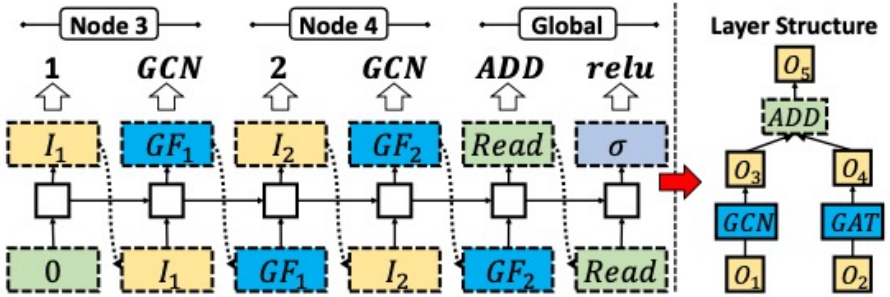


Figure 2: An illustration of GraphNAS constructing a single GNN layer at the right-hand side. The layer has two input states O_1 and O_2, two intermediate states O_3 and O_4, and an output state O_5. The controller at the left-hand side samples O_2 from $\{O_1, O_2, O_3\}$ and take O_2 as the input of O_4, and then samples GAT for processing O_2. The output state $O_5 = relu(O_3 + O_4)$ collects information from O_3 and O_4, and the controller assigns a readout operator add and an activation operator $relu$ for O_5. As a result, this layer can be described as a list of operators: [1,gcn, 2, gat, add, $relu$].

$$O_{out} = \sigma(Read(O_i|3 \leqslant i \leqslant B+2)),$$

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

Experiments

- Datasets
  - Three benchmark ones.
- Task
  - Node classification
- Settings
  - Semi-supervised
    - 20 training, 500 validation, 100 test
  - Supervised
    - 500 validation, 500 test, rest training
  - Supervised with randomly split
  - Transfer learning

N, E, F and C denote the number of "Nodes", "Edges", "Features" and "Classes", respectively.

Dataset	N	E	F	C
Cora	2,708	5,278	1,433	7
CiteSeer	3,327	4,552	3,703	6
PubMed	19,717	44,324	500	3

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

Experiments

- Results
  - SOTA on all datasets.
    - GraphNAS-R: randomly search algorithm
    - GraphNAS-S: simple variant with only one computational node in each layer.

	Cora			Citeseer			Pubmed		
	semi	sup	rand	semi	sup	rand	semi	sup	rand
GCN	81.4±0.5	90.2±0.0	88.3±1.3	70.9±0.5	80.0±0.3	77.2±1.7	79.0±0.4	87.8±0.2	88.1±1.4
GAT	83.0±0.7	89.5±0.3	87.2±1.1	72.5±0.7	78.6±0.3	77.1±1.3	79.0±0.3	86.5±0.6	87.8±1.4
ARMA	82.8±0.6	89.8±0.1	88.2±1.0	72.3±1.1	79.9±0.6	76.7±1.5	78.8±0.3	88.1±0.2	88.7±1.0
APPNP	83.3±0.1	90.4±0.2	87.5±1.4	71.8±0.4	79.2±0.4	77.3±1.6	80.2±0.2	87.4±0.3	88.2±1.1
HGCN	79.8±1.2	89.7±0.4	87.7±1.1	70.0±1.3	79.2±0.5	76.9±1.3	78.4±0.6	88.0±0.5	88.0±1.6
GraphNAS-R	83.3±0.4	90.0±0.3	88.5±1.0	73.4±0.4	81.1±0.3	76.5±1.3	79.0±0.4	90.7±0.6	90.3±0.8
GraphNAS-S	81.4±0.6	90.1±0.3	88.5±1.0	71.7±0.6	79.6±0.5	77.5±2.3	79.5±0.5	88.5±0.2	88.5±1.1
GraphNAS	**83.7±0.4**	**90.6±0.3**	**88.9±1.2**	**73.5±0.3**	**81.2±0.5**	**77.6±1.5**	**80.5±0.3**	**91.2±0.3**	**91.1±1.0**

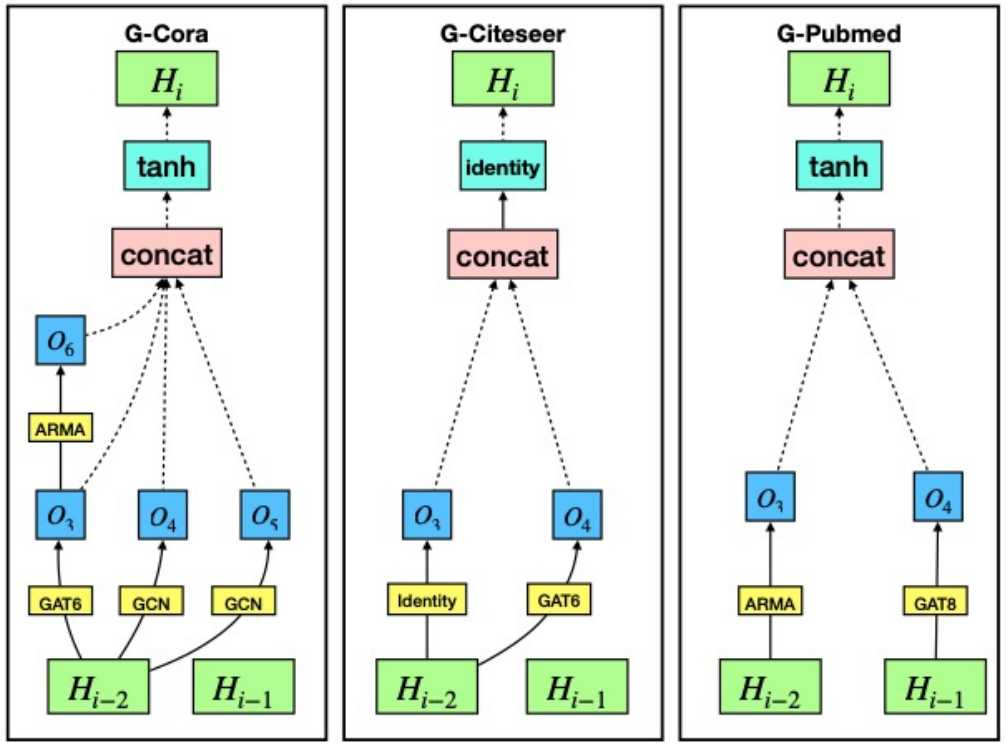
Table 3: Node classification results *w.r.t.* accuracy, where "semi" stands for semi-supervised learning experiments, "sup" for supervised learning experiments and "rand" for supervised learning experiments with randomly split data.

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

Experiments

- Searched architectures

Figure 5: An example of the graph neural architectures designed by GraphNAS on the supervised learning task. The architecture *G-Cora* designed by GraphNAS on Cora is $[1, gat\_6, 1, gcn, 1, gcn, 3, arma, tanh, concat]$, the architecture *G-Citeseer* designed by GraphNAS on Citeseer is $[1, identity, 1, gat\_6, identity, concat]$, and the architecture *G-Pubmed* designed by GraphNAS on Pubmed is $[2, gat\_8, 1, arma, tanh, concat]$.



Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

Experiments

- More Results
  - Transfer learning
  - Influence of search epochs.

Model	CS	Physics	Computers	Photo
GCN	95.5±0.3	98.3±0.2	88.0±0.6	95.4±0.3
GAT	95.5±0.3	98.1±0.2	89.1±0.6	95.6±0.3
ARMA	95.4±0.2	**98.5±0.1**	86.1±1.0	94.8±0.8
APPNP	95.6±0.2	**98.5±0.1**	89.8±0.4	95.8±0.3
GraphNAS	**97.1±0.2**	**98.5±0.2**	**92.0±0.4**	**96.5±0.4**

Table 4: Transferring architectures designed by GraphNAS on the citation networks to the other four datasets

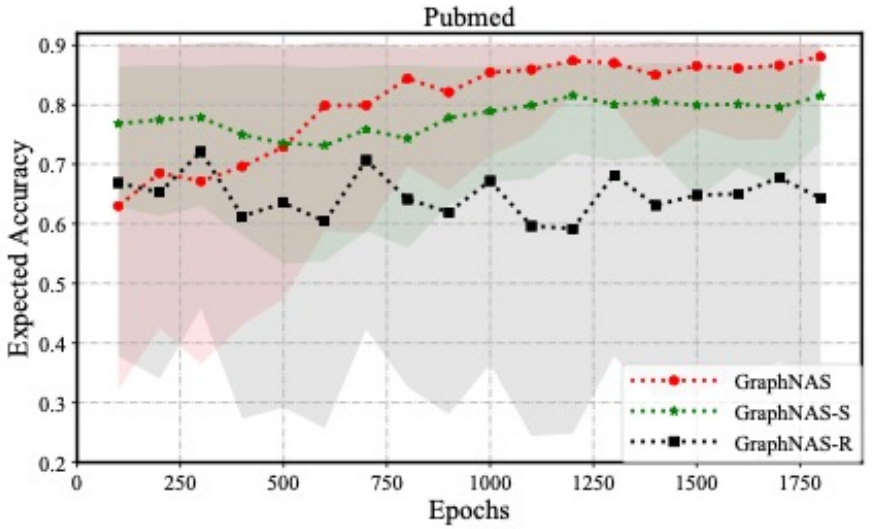


Figure 4: Comparisons *w.r.t.* the number of search epochs on Pubmed. The expected accuracy of the architecture designed by GraphNAS raises with the search epochs. GraphNAS outperforms Simple-NAS after 500 epochs.

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

Quick Summary

- A first graph neural network architecture search by RL
- Effective but expensive due to "trial-and-error" manner
  - Stand alone
- More efficient search algorithm is needed
  - One-shot

Gao et al. GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. IJCAI 2020

SANE [Zhao et al. 2021]

- Search to Aggregate Neighborhood (SANE) for graph neural networks
  - Differentiable architecture search
  - A research work from our group.

- A more compact search space only search for node and layer aggregation functions
  - The expressive ability of GNNs mainly rely on the aggregation function[Hu et al. 2019]
  - The intermediate layers can further improve the expressive ability [Xu et al. 2018]

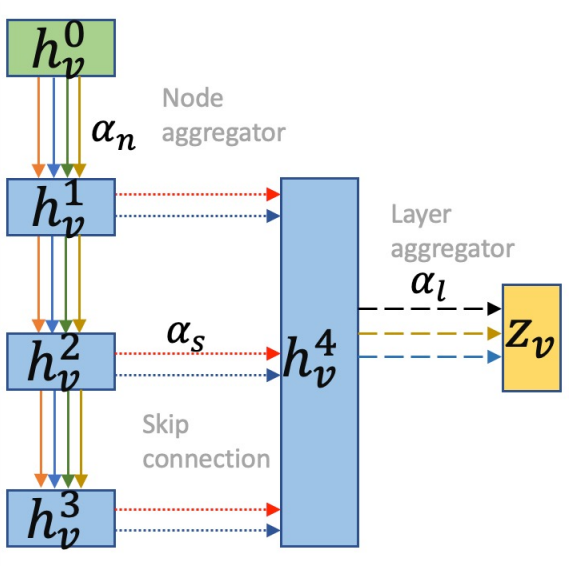
- SOTA performance

Zhao et al. Search to aggregate neighborhood for graph neural networks. ICDE 2021
Hu et al. How Powerful are Graph Neural Networks? ICLR 2019
Xu et al. Representation Learning on Graphs with Jumping Knowledge Networks. ICML 2018

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
human-designed	GCN [17]	GCN	×	×	✓
	SAGE [15]	SAGE-SUM/-MEAN/-MAX/-LSTM	×	✓	✓
	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	✓	✓	

Zhao et al. Search to aggregate neighborhood for graph neural networks. ICDE 2021

Search Space

- More explanations on node aggregator

GNN models	Symbol in the paper	Key explanations
GCN [15]	GCN	$F_N^l(v) = \sum_{u \in \widetilde{N}(v)} \left(\text{degree}(v) \cdot \text{degree}(u)\right)^{-1/2} \cdot \mathbf{h}_u^{l-1}$.
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 [30]	GAT	Compute attention score: $\mathbf{e}_{uv}^{gat} = \text{Leaky\_ReLU}\left(\mathbf{a}\left[\mathbf{W}_u\mathbf{h}_u \| \mathbf{W}_v\mathbf{h}_v\right]\right)$.
	GAT-SYM	$\mathbf{e}_{uv}^{sys} = \mathbf{e}_{uv}^{gat} + \mathbf{e}_{vu}^{gat}$.
	GAT-COS	$\mathbf{e}_{uv}^{cos} = \langle \mathbf{W}_u\mathbf{h}_u, \mathbf{W}_v\mathbf{h}_v \rangle$.
	GAT-LINEAR	$\mathbf{e}_{uv}^{lin} = \tanh\left(\mathbf{W}_u\mathbf{h}_u + \mathbf{W}_v\mathbf{h}_v\right)$.
	GAT-GEN-LINEAR	$\mathbf{e}_{uv}^{gen-lin} = \mathbf{W}_G \tanh\left(\mathbf{W}_u\mathbf{h}_u + \mathbf{W}_v\mathbf{h}_v\right)$.
GIN [33]	MLP	$F_N^l(v) = \text{MLP}\left((1+\epsilon^{l-1}) \cdot \mathbf{h}_v^{l-1} + \sum_{u \in N(v)} \mathbf{h}_u^{l-1}\right)$.
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.

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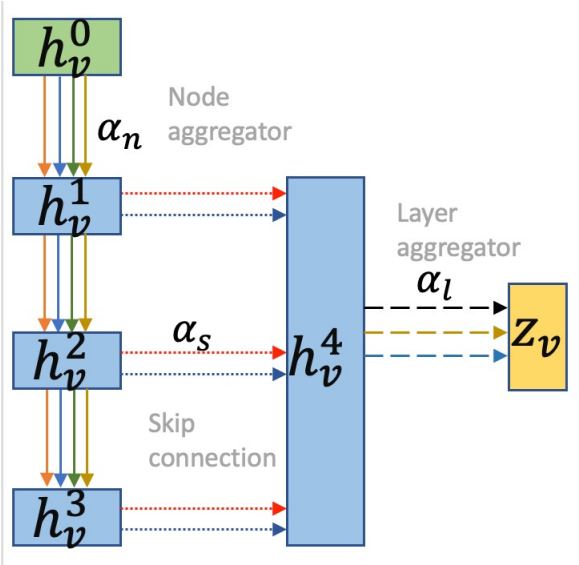
Differentiable search algorithm

- 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

$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}_n^{(l)} \cdot \bar{o}_n(\{\mathbf{h}_u^{(l-1)}, \forall u \in \widetilde{N}(v)\})\right)$$

$$\mathbf{H}_v^{K+1} = \left[\bar{o}_s(\mathbf{h}_v^1), \cdots, \bar{o}_s(\mathbf{h}_v^K)\right]$$

$$\mathbf{z}_v = \bar{o}_l\left(\mathbf{H}_v^{K+1}\right)$$

Zhao et al. Search to aggregate neighborhood for graph neural networks. ICDE 2021

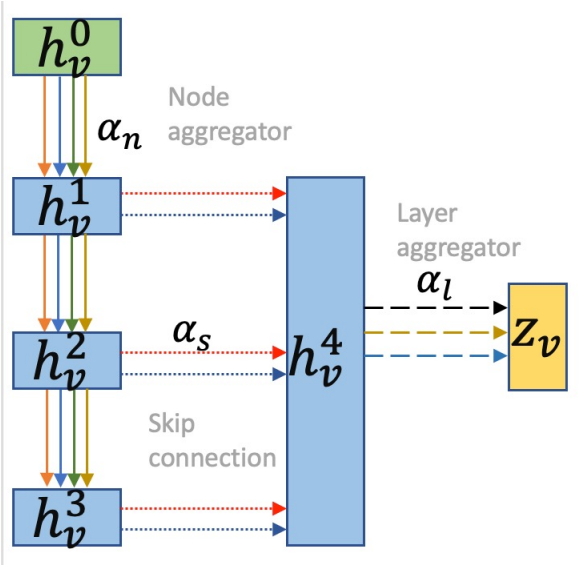
Differentiable search algorithm

- 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.

$$o^{(i,j)} = \arg\max_{o \in O} \boldsymbol{\alpha}_o^{(i,j)}$$

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Differentiable search algorithm

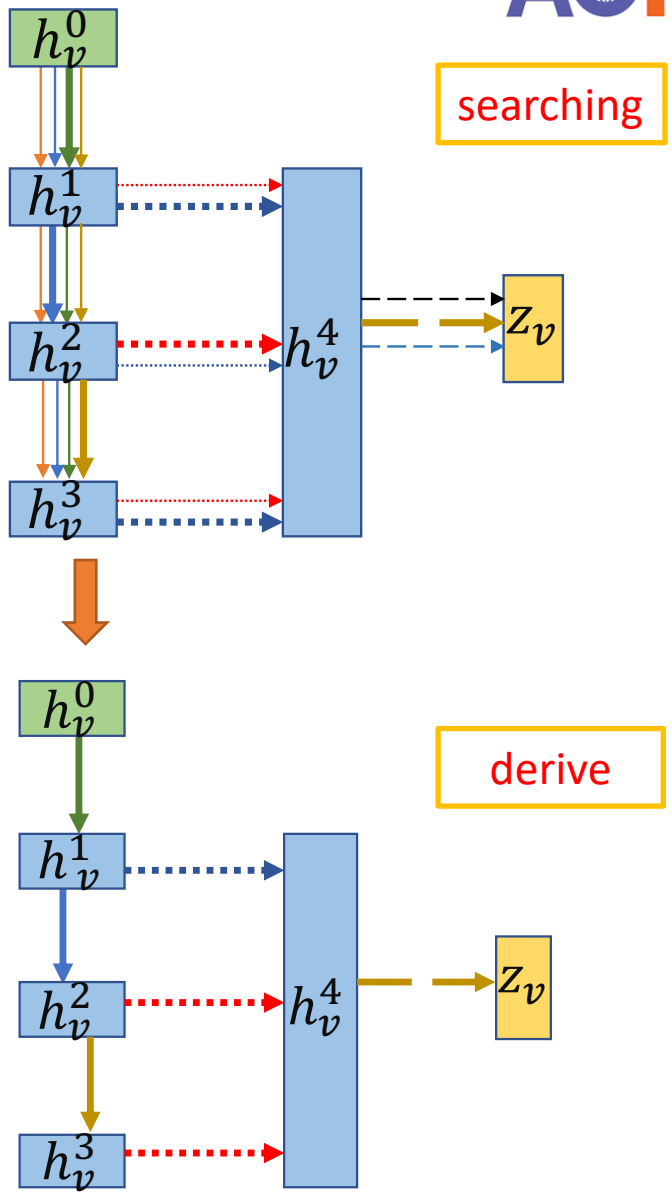
- Gradient-based optimization.

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

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** $t = 1, \cdots, T$ **do**
2: Compute the validation loss $\mathcal{L}_{val}$;
3: Update $\boldsymbol{\alpha}_n$, $\boldsymbol{\alpha}_s$ and $\boldsymbol{\alpha}_l$ by gradient descend rule Eq. (7) with Eq. (3), (4) and (5) respectively;
4: Compute the training loss $\mathcal{L}_{train}$;
5: Update weights $\mathbf{w}$ 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 $\{\boldsymbol{\alpha}_n, \boldsymbol{\alpha}_s, \boldsymbol{\alpha}_l\}$;



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Experiments

- Datasets

Task	Dataset	N	E	F	C
Transductive	Cora	2,708	5,278	1,433	7
	CiteSeer	3,327	4,552	3,703	6
	PubMed	19,717	44,324	500	3
Inductive	PPI	56,944	818,716	121	50

- Task
  - Node classification
- Settings
  - Supervised
  - Transductive and Inductive

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Experiments

- Performance comparison
  - Human-designed architectures
  - NAS approaches

		Transductive			Inductive
	Methods	Cora	CiteSeer	PubMed	PPI
Human-designed architectures	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)
	GAT	0.8719 (0.0163)	0.7518 (0.0145)	0.8573 (0.0066)	0.9414 (0.0000)
	GAT-JK	0.8726 (0.0086)	0.7527 (0.0128)	0.8674 (0.0055)	0.9749 (0.0000)
	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)
NAS approaches	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)
	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)**

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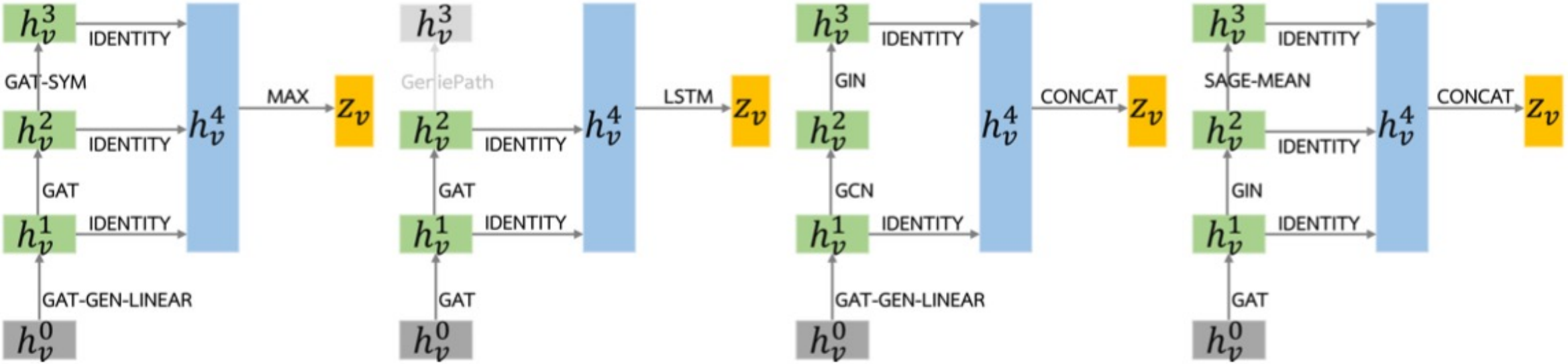
Experiments

- Searched architectures



(a) Cora. (b) CiteSeer. (c) PubMed. (d) PPI.

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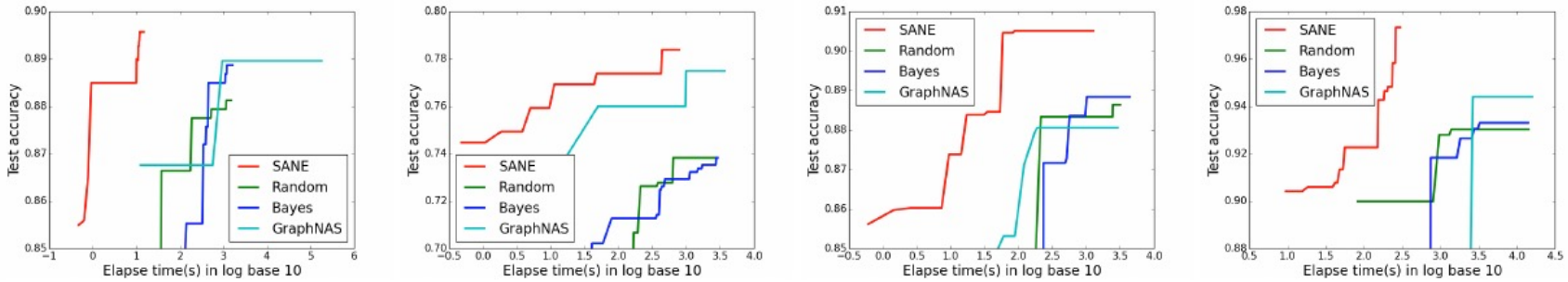
Experiments

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



(a) Cora. (b) CiteSeer. (c) PubMed. (d) PPI.

- 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

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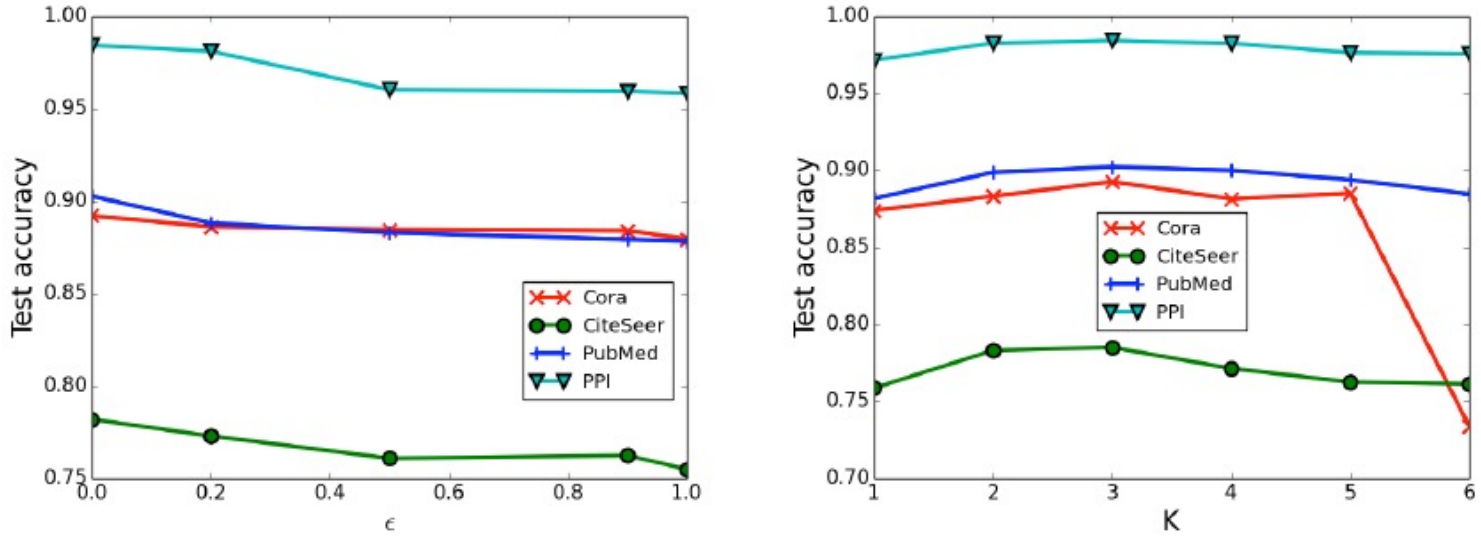
Experiments

- 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.

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Quick Summary

- SANE shows potential to obtain SOTA GNN architectures more efficiently.

- Comparisons
  - GraphNAS
    - More accurate evaluation on the child model
    - Computationally expensive
  - SANE
    - More efficient
    - Not that robust.

- More following works can be checked in [Zhang et al. 2021] .

Summary

- NAS show great potential in explore data-specific GNN architectures.
- Differentiable architecture search tends to be better than RL based method.
- Future work
  - Large-scale Graph Architecture search
    - Open Graph Benchmark (OGB)
  - Different types of graphs
    - Heterogeneous graph / hypergraphs / dynamic graphs
  - More challenging settings
    - Heterophily/adversary/noisy

References

- Semi-supervised classification with graph convolutional networks. ICLR 2017
- Inductive representation learning on large graphs. NeurIPS 2017
- Graph attention networks. ICLR 2018
- Representation Learning on Graphs with Jumping Knowledge Networks. ICML 2018
- Adaptive Stochastic Natural Gradient Method for One-Shot Neural Architecture Search. ICML 2019
- GraphNAS: Graph Neural Architecture Search with Reinforcement Learning. ICDE 2021
- Auto-GNN: Neural Architecture Search of Graph Neural Networks. Arxiv 2019
- DARTS: DIFFERENTIABLE ARCHITECTURE SEARCH. ICLR 2019
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- Simplifying Architecture Search for Graph Neural Network. CIKM-CSSA 2020
- Search to aggregate neighborhood for graph neural networks. ICDE 2021
- Design Space for Graph Neural Networks. NeurIPS 2020
- Policy-GNN: Aggregation Optimization for Graph Neural Networks. KDD 2020
- Taking Human out of Learning Applications: A Survey on Automated Machine Learning. Arxiv 2018
- Zhang et al. Automated Machine Learning on Graphs: A Survey. IJCAI 2021

Next Works

Research Topic

Automated Learning from Graph Structured Data

Manage topic | Submit your abstract | Submit your manuscript | Participate

Special Issue in: **Frontiers in artificial intelligence**

Jointly hold by: Quanming Yao, Huan Zhao

Rex Ying, and Xia Hu

Overview | Articles | Authors | Impact

Your submission is welcome!

About this Research Topic

Machine learning is an important technique to learn from graph structured data (GSD). However, since it is knowledge- and labor-intensive to pursue good learning performance, humans are heavily involved in every aspect of learning from GSD. Examples are property prediction for molecular graphs, product recommendations from heterogeneous information networks, and logical queries from knowledge base. To make machine learning techniques easier to apply and reduce the demand for experienced human experts, automated machine learning (AutoML) has emerged as a hot topic with great interest. At the same time, a special type of deep network model has been recently proposed, called graph neural networks (GNNs), which capture the dependence of graphs via message passing between the nodes of graphs and allow learning from GSD in a more principled manner. Moreover, they allow learning from molecular dynamics and meteorological simulation, which further extend the classical scope of GSD.

However, again due to such diversities in GSD, there is no unitary GSD learning model that can perform consistently across different tasks and datasets. As a consequence, how to design adaptive methods to learn from GSD in a task-aware and data-specific manner is an important problem. Fortunately, there are emerging technical tools from machine learning communities that have the potential to solve the above problems. Examples are automated machine learning, neural architecture search, meta-learning, and learning to lean. These methods can all help generalize learning methods that can exhibit abilities to learn well across different datasets and tasks. Thus, by proposing this Research Topic, we hope to draw interest from both academia and industry, with the goal to push learning methods for GSD to the next level.

Submission Deadlines

19 December 2021	Abstract
17 February 2022	Manuscrip

Next Works

AH2: Automated Learning form Graph-Structured Data
Quanming Yao, Huan Zhao and Yongqi Zhang

Graph-structured data (GSD) is ubiquitous in real-life applications, which appears in many learning applications such as property prediction for molecular graphs, product recommendations from heterogeneous information networks, and logical queries from knowledge graphs. Recently, learning from graph-structured data has also become a research focus in the machine learning community. However, again due to such diversities in GSD, there are no universal learning models that can perform well and consistently across different learning applications based on graphs. In sharp contrast to this, convolutional neural networks work well on natural images, and transformers are good choices for text data. In this tutorial, we will talk about using automated machine learning (AutoML) as a tool to design learning models for GSD. Specifically, we will elaborate on what is AutoML, what kind of prior information from graphs can be explored by AutoML, and how insights can be generated from the searched models.

Quanming Yao

Tsinghua University

Dr. Quanming Yao is a tenure-track assistant professor at EE, Tsinghua University. He obtained his Ph.D. degree at the CSE of HKUST and was the founding leader of 4Paradigm INC's machine learning research team. He is a recipient of Forbes-30-Under-30 (China), Young Scientist Awards (HKIS), and Google Fellowship (machine learning).

Huan Zhao

4Paradigm

Dr. Huan Zhao is a senior researcher in 4Paradigm, leading the research on automated graph representation learning (AutoGraph) and real-world applications like retailing recommendation and bioinformatics. He has published various papers on top-tier venues like KDD, CIKM, AAAI, and TKDE. He obtained his Doctor Degree from HKUST in Jan. 2019.

Yongqi Zhang

4Paradigm

Dr. Yongqi Zhang is a senior researcher in 4Paradigm. He obtained the Ph.D. degree at CSE of HKUST. He has published many top-tier conference/journal papers as first-author in NeurIPS, ICDE, VLDB-J. His research interests focus on KG embedding and AutoML. He has been a reviewer for AAAI, IJCAI, CIKM and TKDE.

AAAI-22 Tutorial Forum

Thirty-Sixth Conference on Artificial Intelligence

February 23, 2022

Vancouver, BC, Canada

Our next stop

- more recent works will be included

Automated Learning from Graph-Structured Data

Part 2: Automated Graph Neural Network

Q&A

Code and slides can be accessed in my homepage

https://hzhaoaf.github.io/

Dr. Huan Zhao

Senior researcher, 4Paradigm