Automated Machine Learning on Graphs: A Survey

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Graphs are Ubiquitous

Biology Network

Social Network

Traffic Network
Graph Tasks

Link Prediction

Graph Classification

Node Classification

Images are from search engines
Graph Applications

Natural Language Processing

Reasoning

Computer Vision

Encoding Sentences with Graph Convolutional Networks for Semantic Role Labeling, EMNLP 2017
Neural Motifs: Scene Graph Parsing with Global Context, CVPR 2018
Learning by Abstraction: The Neural State Machine. NeurIPS 2019
Graph Applications

Structural Engineering

Physical Simulation

Drug Repurposing for Covid-19

Learning to Simulate and Design for Structural Engineering, *ICML 2020*

JAX, M.D. A Framework for Differentiable Physics, *NeurIPS 2020*

Network Medicine Framework for Identifying Drug Repurposing Opportunities for COVID-19, *arXiv 2020*
Graph in Industry

- Application scenario: recommendation, prediction, classification, anomaly detection, generation, etc.
- Many tech giants have developed their graph systems
  - Alibaba: Graph-Learn (AliGraph), Euler
  - Amazon: Deep Graph Library (DGL)
  - Baidu: Paddle Graph Learning (PGL)
  - DeepMind: Graph Nets
  - Facebook: PyTorch-BigGraph (PBG)
  - Tencent: Plato

……

Machine learning on graphs has important and diverse applications!
Machine Learning on Graphs

Peng Cui, Xiao Wang, Jian Pei, Wenwu Zhu. A Survey on Network Embedding. *IEEE TKDE, 2018.*

Ziwei Zhang, Peng Cui, Wenwu Zhu. Deep Learning on Graphs: A Survey. *IEEE TKDE, 2020.*
Network Embedding

- Learn vectorized representation of nodes
- Then apply classical vector-based machine learning algorithms
Graph Neural Network

- Design neural networks directly applicable for graphs for end-to-end learning
- Message-passing framework: nodes exchange messages along structures
Problems in Existing Graph Learning Methods

- Manually design architectures and hyper-parameters through trial-and-error
- Each task needs to be handled separately

Automated graph machine learning is critically needed!
A Glance of AutoML

Design ML methods → Design AutoML methods

Picture credit to Microsoft Azure Machine Learning AutoML
ML vs. AutoML

- Rely on expert knowledge
- Tedious trial-and-error
- Low tuning efficiency
- Limited by human design

- Free human out of the loop
- High optimization efficiency
- Discover & extract patterns and combinations automatically
Automated Graph Learning

- Automated Machine Learning on Graph
  - Graph Hyper-Parameter Optimization (HPO)
  - Graph Neural Architecture Search (NAS)

- The key: *Graph Structure!*

Various diverse graph structures may place complex impacts on graph HPO and graph NAS.
Challenge: Uniqueness of graph ML

Data

NN architecture

Search Space
- zeroize
- skip-connect
- 1×1 conv
- 3×3 conv
- 3×3 avg pool

predefined operation set

Linear: \( f(x_1, \ldots, x_n) = W_1 x_1 + \ldots + W_n x_n + b \),
Blending (element wise): \( f(z, x, y) = z \odot x + (1 - z) \odot y \),
Element wise product and sum,
Activations: Tanh, Sigmoid, and LeakyReLU.

G = (V, E)

Semi-Supervised Classification with Graph Convolutional Networks, *ICLR 2017*
NAS-Bench-201 Extending the Scope of Reproducible Neural Architecture Search, *ICLR 2020*
NAS-Bench-NLP Neural Architecture Search Benchmark for Natural Language Processing, *arXiv 2020*
Challenge: Complexity and diversity of graph tasks

- Link Prediction
- Community Detection
- Node Classification
- Network Distance
- Node Importance
- Graph Classification
- Graph Matching

Various graph properties

Various applications

Various domains

- No single method can perfectly handle all scenarios
Social Networks
- WeChat: 1.2 billion monthly active users (Sep 2020)
- Facebook: 2.8 billion active users (2020)

E-commerce Networks
- Millions of sellers, about 0.9 billion buyers, 10.6 trillion turnovers in China (2019)

Citation Networks
- 133 million authors, 277 million publications, 1.1 billion citations (AMiner, Feb 2021)

Challenge: how to handle billion-scale graphs?
Hyper-Parameter Optimization

- Goal: automatically find the optimal hyper-parameters
  
  Machine Learning Model

  Optimal Hyper-parameter Configuration

- Formulation: bi-level optimization

  \[
  \min_{\alpha \in \mathcal{A}} \mathcal{L}_{val}(\mathbf{W}^*(\alpha), \alpha) \\
  \text{s.t. } \mathbf{W}^*(\alpha) = \arg \min_{\mathbf{W}} \mathcal{L}_{train}(\mathbf{W}, \alpha)
  \]

- Challenge: each trial of the inner loop on graph is computationally expensive, especially for large-scale graphs
Transfer the **knowledge** about optimal hyper-parameters from sampled subgraphs to the original massive graph

Tu Ke, Jianxin Ma, Peng Cui, Jian Pei, and Wenwu Zhu. AutoNE: Hyperparameter optimization for massive network embedding. *KDD 2019.*
**Goal:** sample representative subgraphs that share similar properties with the original large-scale graph

**Challenge:** preserve diversity of the origin graph

**Method:** multi-start random walk strategy

- Supervised: nodes with different labels
- Unsupervised: from different discovered communities, e.g., a greedy algorithm that maximizes modularity
**Goal:** learn a vector representation for each subgraph so that knowledge can be transferred across different subgraphs

**Challenge:** learn comprehensive graph signatures

**Method:** NetLSD [Tsitsulin et al. KDD18]

Based on spectral graph theory, heat diffusion process on a graph

\[ h_t(G) = tr(H_t) = tr(e^{-tL}) = \sum_{j} e^{-t\lambda_j} \]
**Goal**: transfer knowledge about hyper-parameters in sampled subgraphs to the original large-scale graph

**Assumption**: two similar graphs have similar optimal hyper-parameter

**Method**: Gaussian Process based meta-learner

\[
\ln p(f \mid X) = - \frac{1}{2} f^T K(X, X)^{-1} f - \frac{1}{2} \ln \det(K(X, X)) + \text{constant}.
\]
Neural Architecture Search (NAS)

- Goal: automatically learn the best neural architecture

- Categorization
NAS for Graph Machine Learning

- Summary of NAS for graph ML

| Method           | Search space | Tasks | Search Strategy       | Performance Estimation | Other Characteristics       |
|------------------|--------------|-------|-----------------------|-------------------------|-----------------------------|
| GraphNAS [2020]  | ✓            | ✓     | Fixed                 | RNN controller + RL     | -                           |
| AGNN [2019]      | ✓ ✓           | ✓     | Fixed                 | Self-designed controller + RL | Inherit weights            |
| SNAG [2020a]     | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | RNN controller + RL     | Inherit weights            |
| PDNAS [2020c]    | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Differentiable          | Single-path one-shot       |
| POSE [2020]      | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Differentiable          | Single-path one-shot       |
| NAS-GNN [2020]   | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | -                           |
| AutoGraph [2020] | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | -                           |
| GeneticGNN [2020b]| ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | -                           |
| EGAN [2021a]     | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | One-shot                    |
| NAS-GCN [2020]   | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | -                           |
| LPGNAS [2020b]   | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Differentiable          | Single-path one-shot       |
| You et al. [2020b]| ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Random search           | -                           |
| SAGS [2020]      | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Self-designed algorithm | -                           |
| Peng et al. [2020]| ✓ ✓ ✓ ✓       | ✓     | Fixed                 | CEM-RL [2019]           | One-shot                    |
| GNAS[2021]       | ✓ ✓ ✓ ✓       | ✓     | Various               | Differentiable          | One-shot+meta learning      |
| AutoSTG[2021]    | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Differentiable          | One-shot                    |
| DSS[2021]        | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Differentiable          | One-shot                    |
| SANE[2021b]      | ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | One-shot                    |
| AutoAttend[2021b]| ✓ ✓ ✓ ✓       | ✓     | Fixed                 | Evolutionary algorithm  | Cross-layer attention       |

Table 1: A summary of different NAS methods for graph machine learnings.
Graph NAS Search Space

- Message-passing framework of GNNs
  \[ m_i^{(l)} = \text{AGG}^{(l)} \left( \left\{ a_{ij}^{(l)} W^{(l)} h_i^{(l)}, \forall j \in \mathcal{N}(i) \right\} \right) \]
  \[ h_i^{(l+1)} = \sigma \left( \text{COMBINE}^{(l)} \left[ m_i^{(l)}, h_i^{(l)} \right] \right), \]
- \( h_i^{(l)} \): the representation of node \( v_i \) in the \( l^{th} \) layer
- \( m_i^{(l)} \): the received message of node \( v_i \) in the \( l^{th} \) layer

- Micro search space:
  - Aggregation function \( \text{AGG}(\cdot) \): mean, max, sum, etc.
  - Combining function \( \text{COMBINE}(\cdot) \): CONCAT, SUM, MLP, etc.
  - Aggregation weights \( a_{ij} \) and attention heads
  - Non-linearity \( \sigma(\cdot) \): Sigmoid, ReLU, tanh, etc.
  - Dimensionality

| Type             | Formulation                     |
|------------------|---------------------------------|
| CONST            | \( a_{ij}^{\text{const}} = 1 \) |
| GCN              | \( a_{ij}^{\text{GCN}} = \frac{1}{\sqrt{|\mathcal{N}(i)||\mathcal{N}(j)|}} \) |
| GAT              | \( a_{ij}^{\text{GAT}} = \text{LeakyReLU}(\text{ATT}(W_a [h_i, h_j])) \) |
| SYM-GAT          | \( a_{ij}^{\text{SYM}} = a_{ij}^{\text{GAT}} + a_{ij}^{\text{GAT}} \) |
| COS              | \( a_{ij}^{\text{COS}} = \cos(W_a h_i, W_a h_j) \) |
| LINEAR           | \( a_{ij}^{\text{LINEAR}} = \tanh(\text{sum}(W_a h_i + W_a h_j)) \) |
| GENE-LINEAR      | \( a_{ij}^{\text{GENE-LINEAR}} = \tanh(\text{sum}(W_a h_i + W_a h_j)) \) |

Neural message passing for quantum chemistry. *ICML, 2017.*
Graph Neural Architecture Search, *IJCAI 2020.*
Graph NAS Search Space

- Macro search space: how to arrange different layers
- Residual connection, dense connection, etc.

Formulation:

$$H^{(l)} = \sum_{j < l} F_{jl} \left( H^{(j)} \right)$$

- $F_{jl}$: connectivity pattern from $j^{th}$ to the $l^{th}$ layer
- ZERO (not connecting), IDENTITY (residual connection), MLP, etc.
Graph NAS Search Space

- Other search spaces
  - Pooling methods: $h_G = \text{POOL}(H)$
    - Aggregate node-level representation into graph-level representation
  - Hyper-parameters: similar to HPO for graphs
    - Number of layers, number of epochs, optimizer, dropout rate, etc.
  - Spaces for specific tasks:
    - E.g., spatial-temporal graph operators

![Diagram of Graph NAS Search Space](image)
**Graph NAS Search Strategy**

- Most previous general NAS search strategies can be directly applied
  - Controller (e.g., RNN) + Reinforcement learning (RL)
  - Evolutionary
  - Differentiable

- Controller samples architecture (e.g., as a sequence)
- RL feedback rewards (e.g., validation performance) to update the controller
Graph NAS Search Strategy

- Most previous general NAS search strategies can be directly applied
  - Controller (e.g., RNN) + Reinforcement learning (RL)
  - Evolutionary
  - Differentiable

- Need to define how to sample parents, generate offspring, and update populations
- E.g., remove the worst individual (Real, et al., 2017), remove the oldest individual (Real, et al., 2018), or no remove (Liu, et al., 2018)
Graph NAS Search Strategy

- Most previous general NAS search strategies can be directly applied
  - Controller (e.g., RNN) + Reinforcement learning (RL)
  - Evolutionary
  - Differentiable

- Generate a super-network to combine operations of the search space
- Continuous relaxation to make the model differentiable

DARTS: Differentiable Architecture Search, ICLR 2019
Graph NAS Performance Estimation

- Low-fidelity training
  - Reduce number of epochs
  - Reduce training data: sample subgraphs as in HPO

- Inheriting weights
  - Challenge: parameters in graph ML (e.g., GNNs) are unlike other NNs
  - E.g., constraints by AGNN (Zhou et al., 2019)
    - Same weight shapes
    - Same attention and activation functions

- Weight sharing in differentiable NAS with one-shot model
AutoML library on Graph

- Graph related
  - PyTorch geometric
  - DGL Deep Graph Library
  - Paddle Graph Learning
  - PyTorch BigGraph
  - graph-learn

- AutoML related
  - AutoKeras
  - Neural Network Intelligence
  - HYPEROPT
  - H2O AutoML
  - TPOT
Introduction – AutoGL

- We design the world’s first autoML framework & toolkit for machine learning on graphs.

AutoGL

Open source

Easy to use

Flexible to be extended

https://mn.cs.Tsinghua.edu.cn/AutoGL
https://github.com/THUMNLab/AutoGL
Modular Design

- Key modules:
  - AutoGL Dataset: manage graph datasets
  - AutoGL Solver: a high-level API to control the overall pipeline

- Five functional modules:
  - Auto Feature Engineering,
  - Neural Architecture Search,
  - Hyper-parameter Optimization
  - Model Training
  - Auto Ensemble
Neural Architecture Search

Algorithms
- Random
- One-Shot
- RL
- ENAS
- Darts
- Vanilla RL
- GraphNAS
- Macro
- Micro

Search Space
- GraphNAS
- Single Path

AutoGL Solver

Auto Ensemble
Hyper-Parameter Optimization

Data → AutoGL Dataset → Auto Feature Engineering → Neural Architecture Search → Hyper-Parameter Optimization → Model Training → Auto Ensemble

Hyper-Parameter Optimization

General-Purpose

Random | Bayes
Grid | CAMES
Anneal | TPE

Graph Aware

AutoNE
Model Training

Trainer
• Learning rate
• Epochs
• Optimizer
• Loss
• Early Stopping
...

Model
• Forward
• Ops & Architectures
• Dropout & Hidden
...

Currently supported models
- Node classification
  - GCN
  - GAT
  - GraphSAGE
- Link Prediction
- Graph classification
  - TopKPool
  - GIN
Ensemble

Stacking

Voting

Meta-learner

AutoGL Solver

Auto Ensemble

Auto Feature Engineering

Neural Architecture Search

Hyper-Parameter Optimization

Model Training

Data

AutoGL Dataset
### Example Results

#### Table 1: The results of node classification

| Model   | Cora      | CiteSeer  | PubMed    |
|---------|-----------|-----------|-----------|
| GCN     | 80.9 ± 0.7| 70.9 ± 0.7| 78.7 ± 0.6|
| GAT     | 82.3 ± 0.7| 71.9 ± 0.6| 77.9 ± 0.4|
| GraphSAGE| 74.5 ± 1.8| 67.2 ± 0.9| 76.8 ± 0.6|
| AutoGL  | **83.2 ± 0.6**| **72.4 ± 0.6**| **79.3 ± 0.4**|

#### Table 2: The results of graph classification

| Model             | MUTAG      | PROTEINS   | IMDB-B     |
|-------------------|------------|------------|------------|
| Top-K Pooling     | 80.8 ± 7.1 | 69.5 ± 4.4 | 71.0 ± 5.5 |
| GIN               | 82.7 ± 6.9 | 66.5 ± 3.9 | 69.1 ± 3.7 |
| AutoGL            | **87.6 ± 6.0**| **73.3 ± 4.4**| **72.1 ± 5.0**|

#### Table 3: The results of different HPO methods for node classification

| Method | Trials | GCN     | GAT     | GCN     | GAT     | GCN     | GAT     |
|--------|--------|---------|---------|---------|---------|---------|---------|
|        |        | Cora    |         | CiteSeer|         | PubMed  |         |
| None   |        | 80.9 ± 0.7| 82.3 ± 0.7| 70.9 ± 0.7| 71.9 ± 0.6| 78.7 ± 0.6| 77.9 ± 0.4|
| random | 1      | 81.0 ± 0.6| 81.4 ± 1.1| 70.4 ± 0.7| 70.1 ± 1.1| 78.3 ± 0.8| 76.9 ± 0.8|
|        | 10     | 82.0 ± 0.6| 82.5 ± 0.7| 71.5 ± 0.6| **72.2 ± 0.7**| 79.1 ± 0.3| 78.2 ± 0.3|
|        | 50     | 81.8 ± 1.1| **83.2 ± 0.7**| 71.1 ± 1.0| 72.1 ± 1.0| **79.2 ± 0.4**| 78.2 ± 0.4|
| TPE    | 1      | 81.8 ± 0.6| 81.9 ± 1.0| 70.1 ± 1.2| 71.0 ± 1.2| 78.7 ± 0.6| 77.7 ± 0.6|
|        | 10     | 82.0 ± 0.7| 82.3 ± 1.2| 71.2 ± 0.6| 72.1 ± 0.7| 79.0 ± 0.4| **78.3 ± 0.4**|
|        | 50     | **82.1 ± 1.0**| 83.2 ± 0.8| **72.4 ± 0.6**| 71.6 ± 0.8| 79.1 ± 0.6| 78.1 ± 0.4|
AutoGL Plans

Incoming new features:

- DGL backend
- More large-scale graph support
  - E.g., sampling, distributed, etc.
- More graph tasks
  - E.g., heterogenous graphs, spatial-temporal graphs, etc.

Warmly welcome all feedbacks and suggestions!

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Overview of Our Representative Works

Our roadmap for automated machine learning on graphs

AutoGL HPO

AutoNE

Scalability

e-AutoGR

Scalability +
Explainability

AutoGL NAS

AutoAttend

Attention

GASSO

Graph Structure

AutoGL Tool and Library
Summary and Future Directions

- Machine Learning on Graphs
- Automate Graph Machine Learning
  - Graph HPO
  - Graph NAS
- AutoGL Platform

Open Problems:
- Graph models for AutoML
  - E.g., regard each NN as a Directed Acyclic Graph (DAG)
  - E.g., using GNNs as surrogate models in model performance prediction
- Robustness and explainability
- Hardware-aware models
- Comprehensive evaluation protocols
Thanks!

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