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# GraphGAN: Graph Representation Learning with Generative Adversarial Nets

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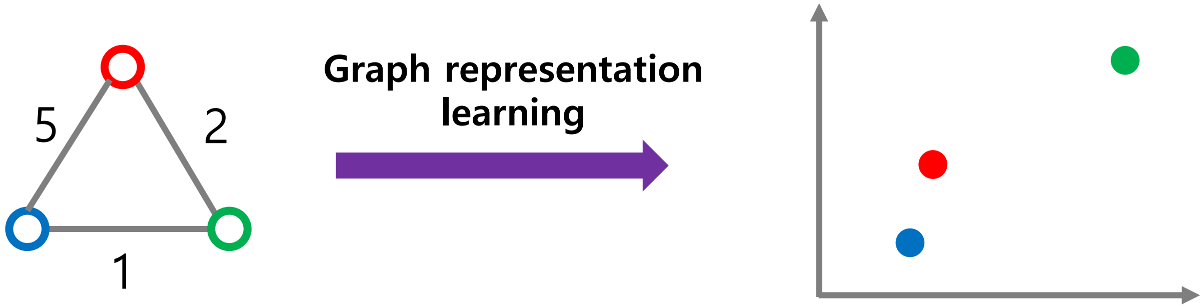
# Background (1/3)

- **Graph representation learning** tries to embed each node of a graph into a low-dimensional vector space, which preserves the structural similarities or distances among the nodes in the original graph

- Also known as **network embedding / graph embedding / graph feature learning**



# Background (2/3)

- **Graph representation learning** can benefit a wide range of real-world applications:
  - Link prediction (Gao, Denoyer, and Gallinari, CIKM 2011)
  - Node classification (Tang, Aggarwal, and Liu, SDM 2016)
  - Recommendation (Yu et al., WSDM 2014)
  - Visualization (Maaten and Hinton, JMLR 2008)
  - Knowledge graph representation (Lin et al., AAAI 2015)
  - Clustering (Tian et al., AAAI 2014)
  - Text embedding (Tang, Qu, and Mei, KDD 2015)
  - Social network analysis (Liu et al., IJCAI 2016)

# Background (3/3)

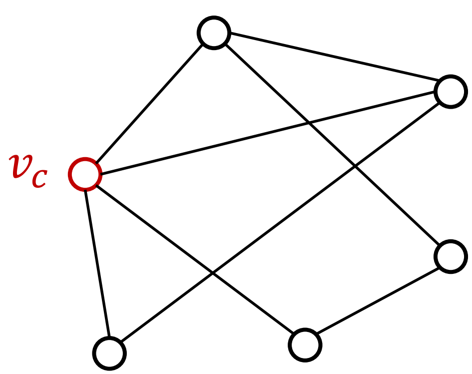
- Researchers have examined applying representation learning methods to various types of graphs:
  - Weighted graphs (Grover and Leskovec, KDD 2016)
  - Directed graphs (Zhou et al., AAAI 2017)
  - Signed graphs (Wang et al., SDM 2017)
  - Heterogeneous graphs (Wang et al., WSDM 2018)
  - Attributed graphs (Huang, Li, and Hu, WSDM 2017)

- Several prior works also try to preserve specific properties during the learning process:
  - Global structures (Wang, Cui, and Zhu, KDD 2017)
  - Community structures (Wang et al., AAAI 2017)
  - Group information (Chen, Zhang, and Huang, CIKM 2016)
  - Asymmetric transitivity (Ou et al., KDD 2016)

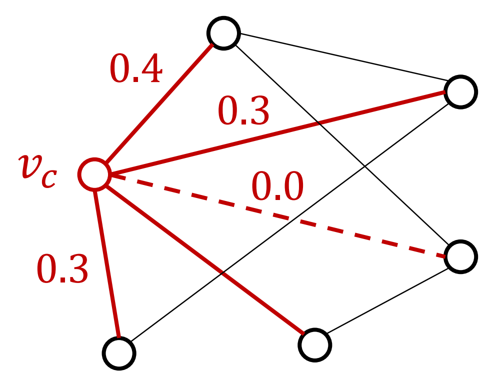
# Motivation (1/3)

## Generative Model

- Generative graph representation learning model assumes an **underlying true connectivity distribution** $p_{true}(v|v_c)$ for each vertex $v_c$
  - Similar to GMM and LDA
  - The edges can be viewed as observed samples generated by $p_{true}(v|v_c)$
  - Vertex embeddings are learned by maximizing the likelihood of edges
  - E.g., DeepWalk (KDD 2014) and node2vec (KDD 2016)




*Original graph*

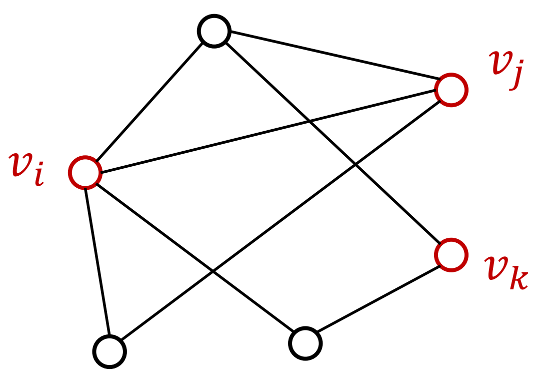



$p_{true}(v|v_c)$

# Motivation (2/3)

## Discriminative Model

- Discriminative graph representation learning model aim to learn a **classifier** for predicting the existence of edges directly
  - Consider two vertices $v_i$ and $v_j$ jointly as features
  - Predict the probability of an edge existing between them, i.e., $p(edge|v_i, v_j)$
  - E.g., SDNE (KDD 2016) and PPNE (DASFAA, 2017)




$$p(edge|v_i, v_j) = 0.8$$

$$p(edge|v_i, v_k) = 0.3$$

……

# Motivation (3/3)

## G + D ?

- Generative and discriminative models are two sides of the same coin
- LINE (WWW 2015) has tried to combine these two objectives
- Generative adversarial nets (GAN) have received a great deal of attention
  - GAN designs a game-theoretical minimax game to combine G and D
  - GAN achieves success in various applications:
    - image generation (Denton et al., NIPS 2015)
    - sequence generation (Yu et al., AAAI 2017)
    - dialogue generation (Li et al., arXiv 2017)
    - information retrieval (Wang et al., SIGIR 2017)
    - domain adaption (Zhang, Barzilay, and Jaakkola, arXiv 2017)

- We propose **GraphGAN**, a framework that unifies generative and discriminative thinking for graph representation learning

# The Minimax Game

- $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, $\mathcal{V} = \{v_1, \dots, v_V\}$, $\mathcal{E} = \{e_{ij}\}_{i,j=1}^{V}$
- $\mathcal{N}(v_c)$: set of neighbors of $v_c$
- $p_{true}(v_c)$: underlying true connectivity distribution for $v_c$

- The objective of GraphGAN is to learn the following two models:
  - $G(v|v_c; \theta_G)$ which tries to approximate $p_{true}(v_c)$
  - $D(v, v_c; \theta_D)$ which aims to discriminate the connectivity for the vertex pair $(v, v_c)$

- The two-player minimax game:

$$\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^{V} \Big( \mathbb{E}_{v \sim p_{\mathrm{true}}(\cdot|v_c)} \big[ \log D(v, v_c; \theta_D) \big] + \mathbb{E}_{v \sim G(\cdot|v_c; \theta_G)} \big[ \log \big(1 - D(v, v_c; \theta_D)\big) \big] \Big) \tag{1}$$

# Implementation & Optimization of D

$$\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^{V} \Big( \mathbb{E}_{v \sim p_{\text{true}}(\cdot|v_c)} \big[ \log D(v, v_c; \theta_D) \big] + \mathbb{E}_{v \sim G(\cdot|v_c;\theta_G)} \big[ \log \big( 1 - D(v, v_c; \theta_D) \big) \big] \Big) \tag{1}$$

- Implementation of D:

$$D(v, v_c; \theta_D) = \sigma(\mathbf{d}_v^\top \mathbf{d}_{v_c}) = \frac{1}{1 + \exp(-\mathbf{d}_v^\top \mathbf{d}_{v_c})}, \tag{2}$$

where $\mathbf{d}_v, \mathbf{d}_{v_c} \in \mathbb{R}^k$ are the k-dimensional vectors of $v$ and $v_c$ for D

- Gradient of $V(G, D)$ w.r.t $\theta_D$:

$$\nabla_{\theta_D} V(G, D) = \begin{cases} \nabla_{\mathbf{d}_v, \mathbf{d}_{v_c}} \log D(v, v_c; \theta_D), & if\ v \sim p_{\text{true}}; \\ \nabla_{\mathbf{d}_v, \mathbf{d}_{v_c}} \big( 1 - \log D(v, v_c; \theta_D) \big), & if\ v \sim G. \end{cases} \tag{3}$$

# Optimization of G

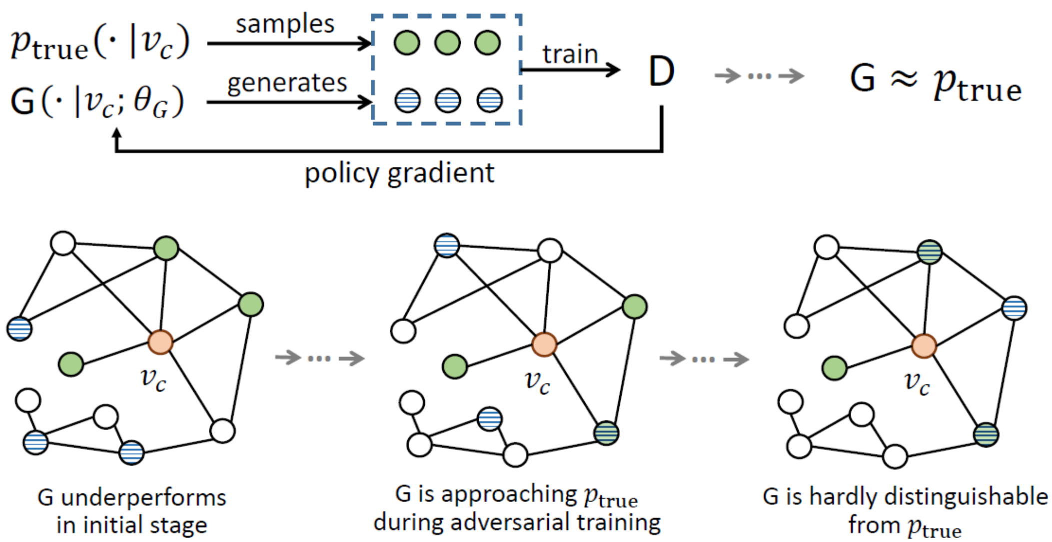
$$\min_{\theta_G}\max_{\theta_D} V(G,D) = \sum_{c=1}^{V}\Big(\mathbb{E}_{v\sim p_{\text{true}}(\cdot|v_c)}\big[\log D(v,v_c;\theta_D)\big] + \mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\log\big(1-D(v,v_c;\theta_D)\big)\big]\Big) \tag{1}$$

- Gradient of $V(G,D)$ w.r.t $\theta_G$ (policy gradient):

$$\begin{aligned}
&\nabla_{\theta_G} V(G,D) \\
=&\nabla_{\theta_G}\sum_{c=1}^{V}\mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\log\big(1-D(v,v_c;\theta_D)\big)\big] \\
=&\sum_{c=1}^{V}\sum_{i=1}^{N}\nabla_{\theta_G}G(v_i|v_c;\theta_G)\log\big(1-D(v_i,v_c;\theta_D)\big) \\
=&\sum_{c=1}^{V}\sum_{i=1}^{N}G(v_i|v_c;\theta_G)\nabla_{\theta_G}\log G(v_i|v_c;\theta_G)\log\big(1-D(v_i,v_c;\theta_D)\big) \\
=&\sum_{c=1}^{V}\mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\nabla_{\theta_G}\log G(v|v_c;\theta_G)\log\big(1-D(v,v_c;\theta_D)\big)\big].
\end{aligned} \tag{4}$$

# GraphGAN Framework

$$\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^{V} \Big( \mathbb{E}_{v \sim p_{\text{true}}(\cdot|v_c)} \big[ \log D(v, v_c; \theta_D) \big] + \mathbb{E}_{v \sim G(\cdot|v_c;\theta_G)} \big[ \log \big(1 - D(v, v_c; \theta_D)\big) \big] \Big) \tag{1}$$



# Implementation of G

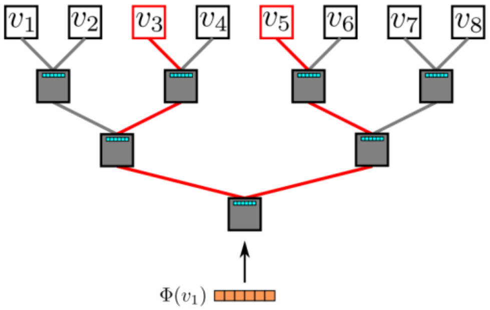
- Softmax?
  - Computationally inefficient
  - Graph-structure-unaware

$$G(v|v_c;\theta_G) = \frac{\exp(\mathbf{g}_v^\top \mathbf{g}_{v_c})}{\sum_{v \neq v_c} \exp(\mathbf{g}_v^\top \mathbf{g}_{v_c})}$$

where $\mathbf{g}_v, \mathbf{g}_{v_c} \in \mathbb{R}^k$ are the k-dimensional vectors of $v$ and $v_c$ for G

- Hierarchical softmax?
  - Graph-structure-unaware

$$p(w|w_I) = \prod_{j=1}^{L(w)-1} \sigma\left( [\![ n(w,j+1) = \mathrm{ch}(n(w,j)) ]\!] \cdot {v'_{n(w,j)}}^\top v_{w_I} \right)$$




- Negative sampling?
  - Not a valid probability distribution
  - graph-structure-unaware

$$\log \sigma({v'_{w_O}}^\top v_{w_I}) + \sum_{i=1}^{k} \mathbb{E}_{w_i \sim P_n(w)} \left[ \log \sigma(-{v'_{w_i}}^\top v_{w_I}) \right]$$

# Graph Softmax (1/5)

## Objectives

- The design of graph softmax should satisfy the following three properties:
  - **Normalized**: The generator should produce a valid probability distribution, i.e., $\sum_{v \neq v_c} G(v|v_c;\theta_G) = 1$
  - **Graph-structure-aware**: The generator should take advantage of the structural information of a graph
  - **Computationally efficient**: The computation of $G(v|v_c;\theta_G)$ should only involve a small number of vertices in the graph

# Graph Softmax (2/5)

## Design

- **Breadth First Search** (BFS) on $\mathcal{G}$ from every vertex $v_c$
  - **BFS-tree** $T_c$ rooted at $v_c$
- For a given vertex $v$ and one of its neighbors $v_i \in \mathcal{N}_c(v)$, the **relevance probability** of $v_i$ given $v$ as

$$p_c(v_i|v) = \frac{\exp(\mathbf{g}_{v_i}^\top \mathbf{g}_v)}{\sum_{v_j \in \mathcal{N}_c(v)} \exp(\mathbf{g}_{v_j}^\top \mathbf{g}_v)}, \quad (6)$$

  where $\mathcal{N}_c(v)$ is the set of neighbors of $v$ in $T_c$

- **Graph softmax**

$$G(v|v_c;\theta_G) \triangleq \left(\prod_{j=1}^{m} p_c(v_{r_j}|v_{r_{j-1}})\right) \cdot p_c(v_{r_{m-1}}|v_{r_m}), \quad (7)$$

  given the unique path from $v_c$ to $v$ in tree $T_c$: $P_{v_c \to v} = (v_{r_0}, v_1, \ldots, v_{r_m})$, where $v_{r_0} = v_c$ and $v_{r_0} = v$

# Graph Softmax (3/5)

## Design

### ❑ Graph softmax

$$G(v|v_c;\theta_G) \triangleq \left(\prod_{j=1}^{m} p_c(v_{r_j}|v_{r_{j-1}})\right) \cdot p_c(v_{r_{m-1}}|v_{r_m}), \qquad (7)$$

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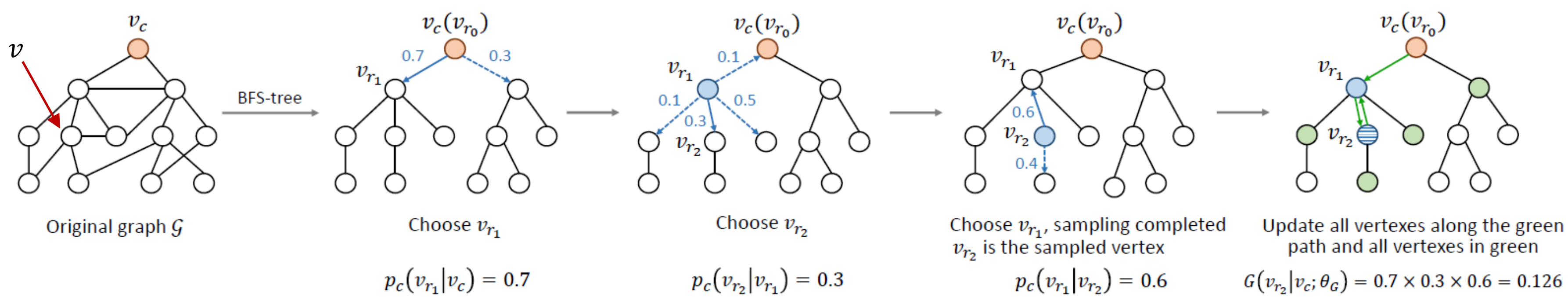


# Graph Softmax (4/5)

## Properties

- $\sum_{v \neq v_c} G(v|v_c;\theta_G) = 1$ in graph softmax
- In graph softmax, $G(v|v_c;\theta_G)$ decreases exponentially with the increase of the shortest distance between $v$ and $v_c$ in original graph $\mathcal{G}$
- In graph softmax, calculation of $G(v|v_c;\theta_G)$ depends on $O(d \log V)$ vertices, where $d$ is average degree of vertices and $V$ is the number of vertices in graph $\mathcal{G}$

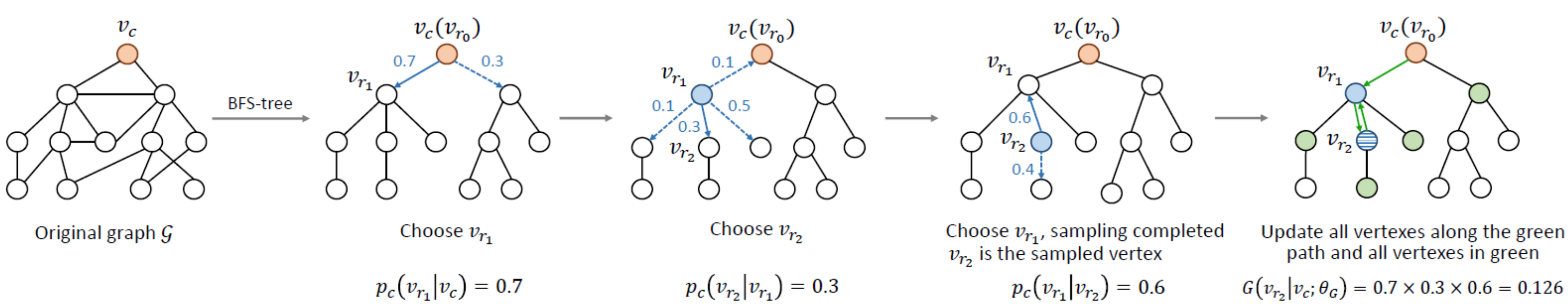
# Graph Softmax (5/5)

## Generating Strategy

**Algorithm 1** Online generating strategy for the generator

**Input:** BFS-tree $T_c$, representation vectors $\{\mathbf{g}_i\}_{i \in \mathcal{V}}$
**Output:** generated sample $v_{gen}$

$v_{pre} \leftarrow v_c$, $v_{cur} \leftarrow v_c$;
**while true do**
  Randomly select $v_i$ proportionally to $p_c(v_i|v_{cur})$ in Eq. (6);
  **if** $v_i = v_{pre}$ **then**
    $v_{gen} \leftarrow v_{cur}$;
    **return** $v_{gen}$
  **else**
    $v_{pre} \leftarrow v_{cur}$, $v_{cur} \leftarrow v_i$;
  **end if**
**end while**



# GraphGAN Algorithm

**Algorithm 2** GraphGAN framework

**Input:** dimension of embedding $k$, size of generating samples $s$, size of discriminating samples $t$

**Output:** generator $G(v|v_c;\theta_G)$, discriminator $D(v, v_c;\theta_D)$

Initialize and pre-train $G(v|v_c;\theta_G)$ and $D(v, v_c;\theta_D)$;<br>
Construct BFS-tree $T_c$ for all $v_c \in \mathcal{V}$;<br>
**while** GraphGAN not converge **do**<br>
    **for** G-steps **do**<br>
        $G(v|v_c;\theta_G)$ generates $s$ vertices for each vertex $v_c$ according to Algorithm 1;<br>
        Update $\theta_G$ according to Eq. (4), (6) and (7);<br>
    **end for**<br>
    **for** D-steps **do**<br>
        Sample $t$ positive vertices from ground truth and $t$ negative vertices from $G(v|v_c;\theta_G)$ for each vertex $v_c$;<br>
        Update $\theta_D$ according to Eq. (2) and (3);<br>
    **end for**<br>
**end while**<br>
**return** $G(v|v_c;\theta_G)$ and $D(v, v_c;\theta_D)$

# Experiments (1/3)

## Datasets

- arXiv-AstroPh: 18,772 vertices and 198,110 edges
- arXiv-GrQc: 5,242 vertices and 14,496 edges
- BlogCatalog: 10,312 vertices, 333,982 edges and 39 labels
- Wikipedia: 4,777 vertices, 184,812 edges and 40 labels
- MovieLens-1M: 6,040 users and 3,706 movies

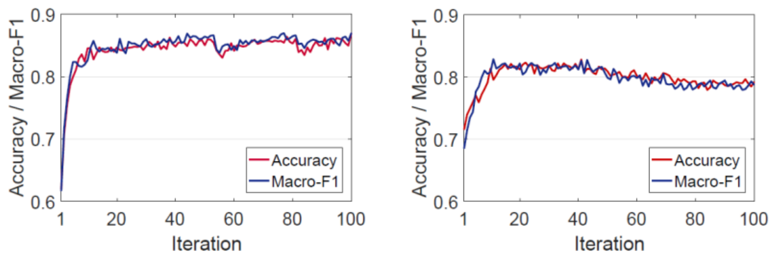
## Baselines

- DeepWalk (KDD 2014)
- LINE (WWW 2015)
- Node2vec (KDD 2016)
- Struc2vec (KDD 2017)

# Experiments (2/3)

## Link Prediction

- Learning curves




(a) Generator (b) Discriminator

Fig. 4: Learning curves of the generator and the discriminator of GraphGAN on arXiv-GrQc in link prediction.

- Results

TABLE 1: Accuracy and Macro-F1 on arXiv-AstroPh and arXiv-GrQc in link prediction.

| Model | arXiv-AstroPh | | arXiv-GrQc | |
|---|---|---|---|---|
| | Accuracy | Macro-F1 | Accuracy | Macro-F1 |
| DeepWalk | 0.841 | 0.839 | 0.803 | 0.812 |
| LINE | 0.820 | 0.814 | 0.764 | 0.761 |
| Node2vec | 0.845 | 0.854 | 0.844 | 0.842 |
| Struc2vec | 0.821 | 0.810 | 0.780 | 0.776 |
| GraphGAN | **0.855** | **0.859** | **0.849** | **0.853** |

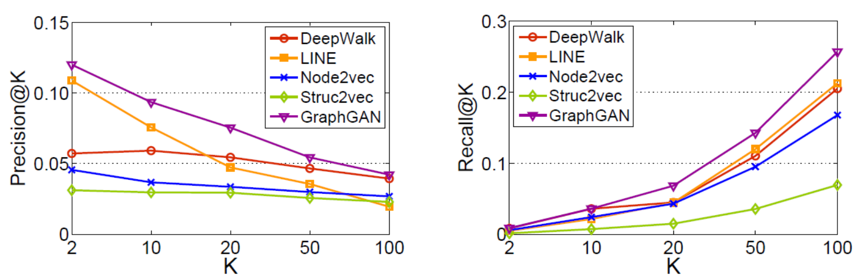
# Experiments (3/3)

## Node Classification

TABLE 2: Accuracy and Macro-F1 on BlogCatalog and Wikipedia in node classification.

| Model | BlogCatalog | | Wikipedia | |
|---|---|---|---|---|
| | Accuracy | Macro-F1 | Accuracy | Macro-F1 |
| DeepWalk | 0.225 | 0.214 | 0.194 | 0.183 |
| LINE | 0.205 | 0.192 | 0.175 | 0.164 |
| Node2vec | 0.215 | 0.206 | 0.191 | 0.179 |
| Struc2vec | 0.228 | 0.216 | 0.211 | 0.190 |
| GraphGAN | **0.232** | **0.221** | **0.213** | **0.194** |

## Recommendation




(a) Precision@K (b) Recall@K

Fig. 5: Precision@K and Recall@K on MovieLens-1M in recommendation.

# Summary

- We propose **GraphGAN**, a novel framework that unifies generative and discriminative thinking for graph representation learning
  - Generator $G(v|v_c)$ tries to fit $p_{true}(v|v_c)$ as much as possible
  - Discriminator $D(v, v_c)$ tries to tell whether an edge exists between $v$ and $v_c$

- G and D act as two players in a **minimax game**:
  - G tries to produce the most indistinguishable "fake" vertices under guidance provided by D
  - D tries to draw a clear line between the ground truth and "counterfeits" to avoid being fooled by G

- We propose **graph softmax** as the implementation of G
  - Graph softmax overcomes the limitations of softmax and hierarchical softmax
  - Graph softmax satisfies the properties of **normalization**, **graph structure awareness** and **computational efficiency**

# Q & A

**Thanks!**

Visit https://hwwang55.github.io/files/2018-AAAI-GraphGAN.pdf for full paper