EECE 571F: Deep Learning with Structures

Lecture 6:
Unsupervised/Self-supervised Graph Representation Learning

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Course Scope

- Brief Intro to Deep Learning

- Geometric Deep Learning

  - Deep Learning Models for Sets and Sequences: Deep Sets & Transformers
  - Deep Learning Models for Graphs: Graph Convolution & Message Passing GNNs
  - Expressiveness & Generalizations of GNNs
  - Unsupervised/Self-supervised Graph Representation Learning

- Probabilistic Deep Learning

  - Deep Generative Models:
    Auto-regressive models, GANs, VAEs, Diffusion/Score based models
  - Discrete/Hybrid Latent Variable Models: RBMs, Latent Graph Models
  - Stochastic Gradient Estimation

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- In this lecture, we focus on methods that learn good node representations

  Given graphs (e.g., adjacency matrix A), the goal is to learn node representations X

  The learned X is useful for supervised fine-tuning, e.g., node classification

Unsupervised / Self-Supervised Learning

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- Reconstruction Loss (Auto-encoders)
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- Min-max Loss (Generative adversarial networks)

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DeepWalk [1] Node2Vec[2]

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Language Models

Model the probability of words given its context (e.g., a fixed-size window):

$$p(w_{i+1}|w_i, \cdots, w_{i-K})$$

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- One can use RNNs or CNNs to construct the probability
- The model can be learned via *maximum likelihood*

Skip-Gram Models

Model the probability of its context (e.g., a fixed-size window) given the word:

$$p(\{w_{i-k}, \cdots, w_{i-1}, w_{i+1}, \cdots, w_{i+k}\}|w_i) = \prod_{j \neq i, j \in \mathcal{N}_i} p(w_j|w_i)$$

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- The model only takes one word as input, thus being efficient
- Interpolation (context => word) vs. extrapolation (word => context)

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Words -> Nodes

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- Interpolation (context => word) vs. extrapolation (word => context)

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Words -> Nodes

How about edges?

Random Walks

A special Markov Chain

Starting at a node, one can randomly choose a neighboring node at a time to walk

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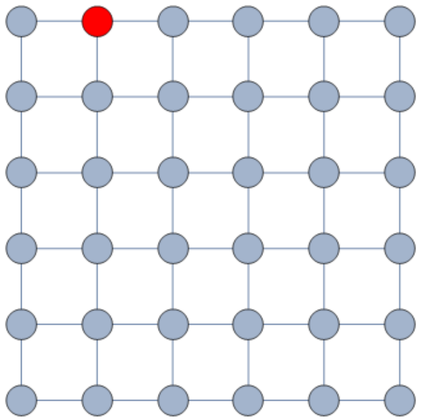


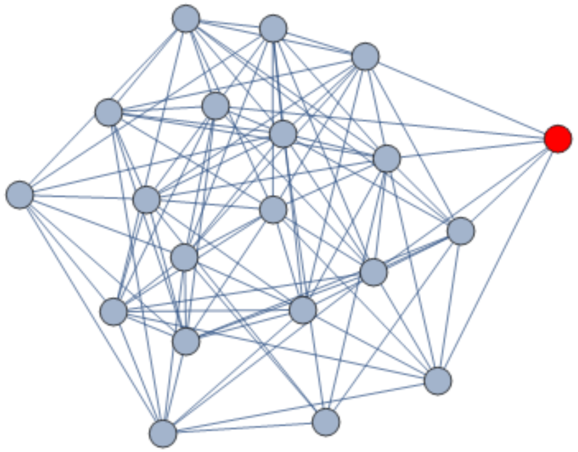
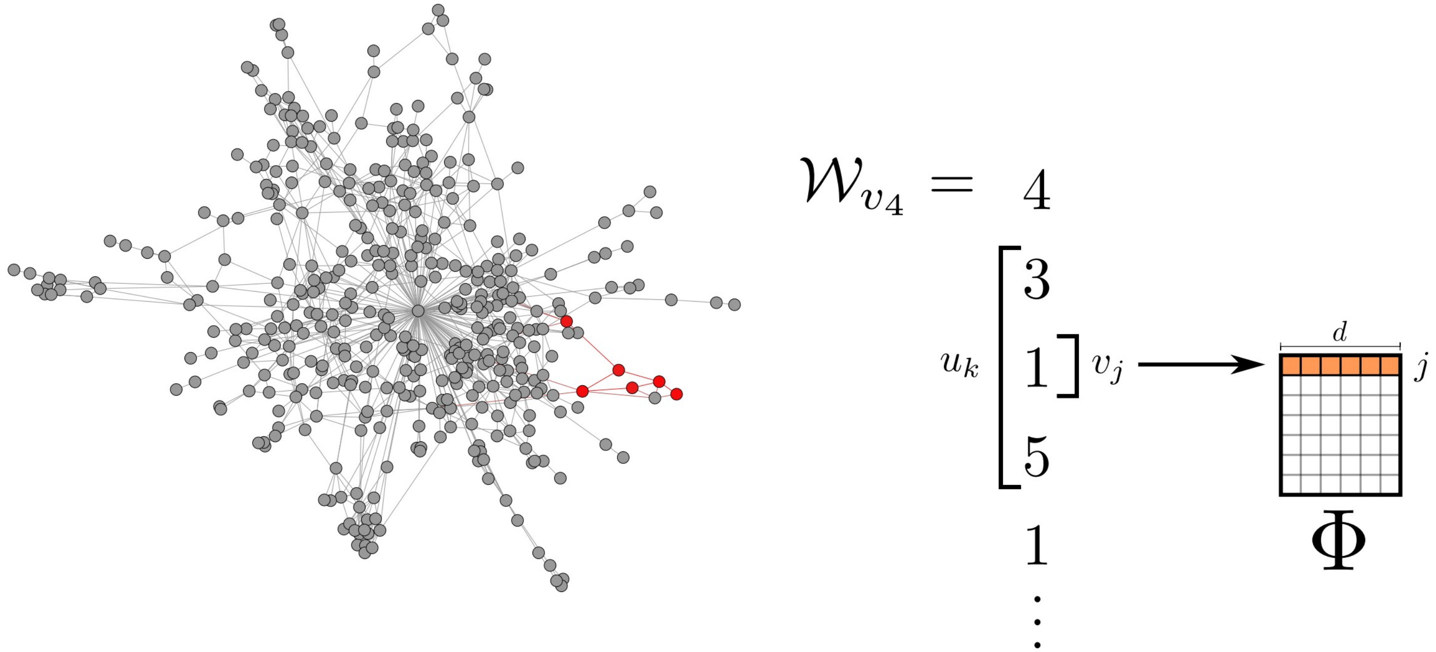


Image Credit: https://mathematica.stackexchange.com/questions/156626/generate-random-walk-on-a-graph

Deep Walks

Model the probability of context (random walks) given its word (vertex):



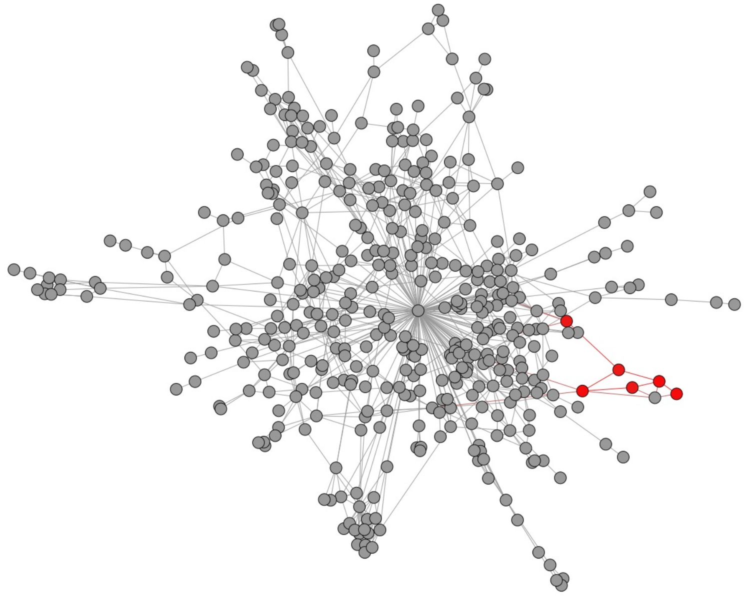
(a) Random walk generation. (b) Representation mapping.

Image Credit: [1]

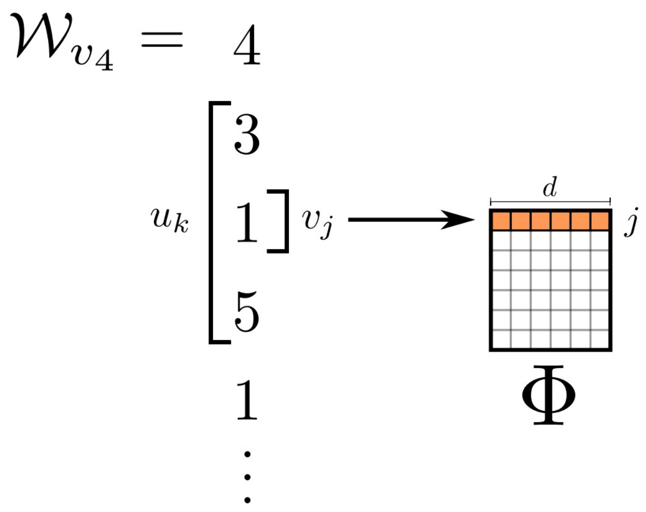
Deep Walks

Model the probability of context (random walks) given its word (vertex):

$$\max \quad \log p\Big(\{v_{i-w}, \cdots, v_{i-1}, v_{i+1}, \cdots, v_{i+w}\} \mid \Phi(v_i)\Big)$$



(a) Random walk generation.



(b) Representation mapping.

Image Credit: [1]

Deep Walks

Model the probability of context (random walks) given its word (vertex):

Algorithm 1 DEEPWALK(G, w, d, γ, t)

Input: graph $G(V, E)$
window size w
embedding size d
walks per vertex γ
walk length t
Output: matrix of vertex representations $\Phi \in \mathbb{R}^{|V| \times d}$

Initialization: Sample Φ from $\mathcal{U}^{|V| \times d}$
Build a binary Tree T from V
for $i = 0$ to γ **do**
    $\mathcal{O} = \text{Shuffle}(V)$
    for each $v_i \in \mathcal{O}$ **do**
        $\mathcal{W}_{v_i} = RandomWalk(G, v_i, \text{t})$
        SkipGram(Φ, $\mathcal{W}_{v_i}$, w)
    end for
end for

Image Credit: [1]

Deep Walks

Skip-Gram Algorithm

Algorithm 2 SkipGram(Φ, $\mathcal{W}_{v_i}$, w)

for each $v_j \in \mathcal{W}_{v_i}$ **do**
  for each $u_k \in \mathcal{W}_{v_i}[j - w : j + w]$ **do**
    $J(\Phi) = -\log \Pr(u_k \mid \Phi(v_j))$
    $\Phi = \Phi - \alpha * \frac{\partial J}{\partial \Phi}$
  end for
end for

Image Credit: [1]

Deep Walks

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  end for

end for

Conditional Independence

$$p(\{u_{j-w}, \cdots, u_{j-1}, u_{j+1}, \cdots, u_{j+w}\}|\Phi(v_j)) = \prod_{k \neq j, k \in \mathcal{N}_j} p(u_k|\Phi(v_j))$$

Image Credit: [1]

Deep Walks

Model the probability of context (random walks) given its word (vertex)

Construct probability using Softmax:

$$p(u_k = i | \Phi(v_j)) = \frac{\exp(w_i^T \Phi(v_j))}{\sum_{m=1}^{|V|} \exp(w_m^T \Phi(v_j))}$$

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One weight per vertex, i.e., a huge softmax on large graphs

Can we improve the efficiency?

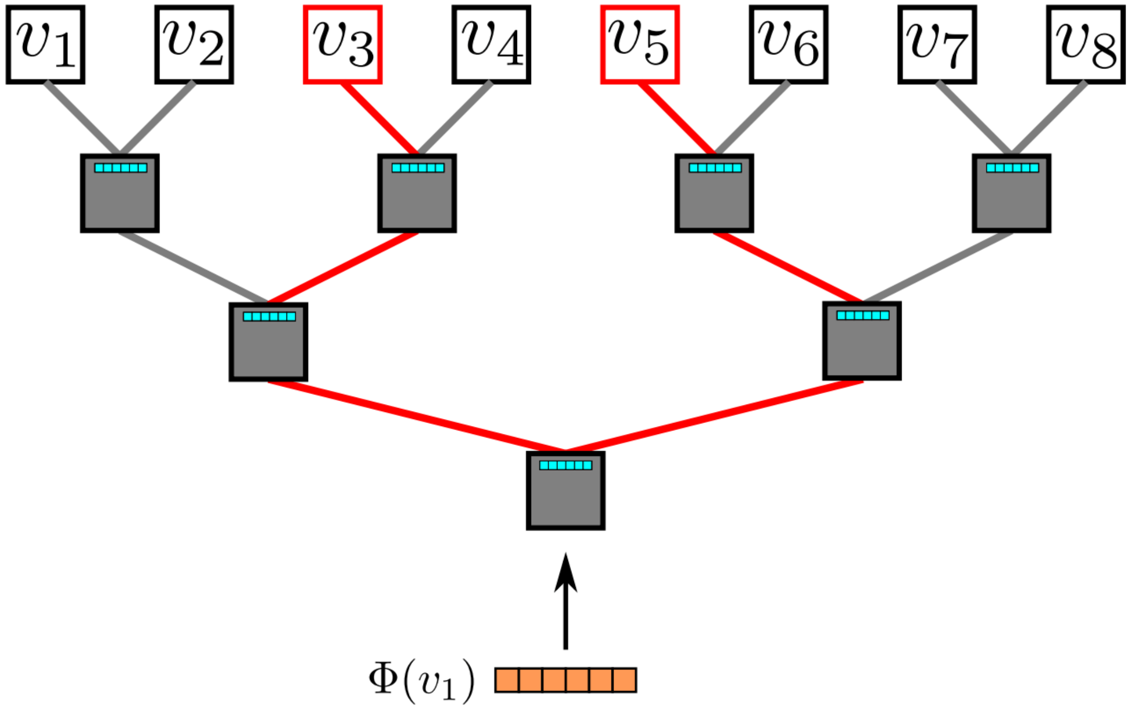
Image Credit: [1]

Deep Walks

Hierarchical Softmax

Build a binary tree over vocabulary (the set of all vertices)

$$p(u_k \mid \Phi(v_j)) = \prod_{l=1}^{\lceil \log |V| \rceil} p(b_l \mid \Phi(v_j))$$



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Deep Walks

Multi-Label Classification (BlogCatalog)

Two-stage pipeline: 1) learn node embeddings unsupervisedly; 2) learn node classifier supervisedly

	% Labeled Nodes	10%	20%	30%	40%	50%	60%	70%	80%	90%
Micro-F1(%)	DeepWalk	**36.00**	**38.20**	**39.60**	**40.30**	**41.00**	**41.30**	41.50	41.50	42.00
	SpectralClustering	31.06	34.95	37.27	38.93	39.97	40.99	**41.66**	**42.42**	**42.62**
	EdgeCluster	27.94	30.76	31.85	32.99	34.12	35.00	34.63	35.99	36.29
	Modularity	27.35	30.74	31.77	32.97	34.09	36.13	36.08	37.23	38.18
	wvRN	19.51	24.34	25.62	28.82	30.37	31.81	32.19	33.33	34.28
	Majority	16.51	16.66	16.61	16.70	16.91	16.99	16.92	16.49	17.26
Macro-F1(%)	DeepWalk	**21.30**	**23.80**	25.30	26.30	27.30	27.60	27.90	28.20	28.90
	SpectralClustering	19.14	23.57	**25.97**	**27.46**	**28.31**	**29.46**	**30.13**	**31.38**	**31.78**
	EdgeCluster	16.16	19.16	20.48	22.00	23.00	23.64	23.82	24.61	24.92
	Modularity	17.36	20.00	20.80	21.85	22.65	23.41	23.89	24.20	24.97
	wvRN	6.25	10.13	11.64	14.24	15.86	17.18	17.98	18.86	19.57
	Majority	2.52	2.55	2.52	2.58	2.58	2.63	2.61	2.48	2.62

Image Credit: [1]

Deep Graph InfoMax

Mutual Information between X and Y:

$$\begin{aligned}\mathrm{MI}(X, Y) &= \mathrm{KL}(p(X,Y) \| p(X)p(Y)) \\ &= \int\int p(X,Y) \log \frac{p(X,Y)}{p(X)p(Y)} dX dY\end{aligned}$$

Deep Graph InfoMax

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It quantifies the "amount of information" obtained about one random variable by observing the other random variable

The higher the mutual information => knowing one would give you more information about the other

Deep Graph InfoMax

How to estimate Mutual Information?

$$\begin{aligned}
\mathrm{MI}(X,Y) &= \mathrm{KL}(p(X,Y)\|p(X)p(Y)) \\
&= \int\int p(X,Y)\log\frac{p(X,Y)}{p(X)p(Y)}dXdY \\
&= \int\int p(X,Y)\log\frac{p(Y|X)}{p(Y)}dXdY \\
&= \mathbb{E}_{p(X,Y)}\left[\log\frac{p(Y|X)}{p(Y)}\right]
\end{aligned}$$

Deep Graph InfoMax

How to estimate Mutual Information?

Suppose we generate Y from a mixture distribution:

$$q(C=1) = q(C=0) = \frac{1}{2}$$
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Density Ratio Trick:

$$\frac{p(Y|X)}{p(Y)} = \frac{q(Y|C=1)}{q(Y|C=0)} = \frac{\frac{q(C=1|Y)q(Y)}{q(C=1)}}{\frac{q(C=0|Y)q(Y)}{q(C=0)}} = \frac{q(C=1|Y)}{q(C=0|Y)}$$

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Binary Classifier!

Deep Graph InfoMax

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Binary Classifier!

We only need samplers to train a classifier, no exact probability densities are required!

Deep Graph InfoMax

Given samples $Y, C \sim q(Y, C)$

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We build a classifier $q(C = 1|Y) \propto f_\theta(X, Y)$

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Minimize Binary Cross-entropy: $\min_q \quad -\frac{1}{N}\left(\sum_{Y,C} C \log q(C = 1|Y) + (1 - C) \log(1 - q(C = 1|Y))\right)$

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The optimal q is: $$q^*(C=1|Y) = \frac{\frac{p(Y|X)}{p(Y)}}{1+\frac{p(Y|X)}{p(Y)}}$$

Optimal Bayesian Classifier!

Deep Graph InfoMax

The optimal q is

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$$\mathcal{L}_{\mathrm{BCE}}(q) = -\mathbb{E}_{C,Y}\left[C \log q(C=1|Y) + (1-C)\log(1-q(C=1|Y))\right]$$

Deep Graph InfoMax

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Binary Cross-entropy: $$\mathcal{L}_{\mathrm{BCE}}(q) = -\mathbb{E}_{C,Y}\left[C\log q(C=1|Y) + (1-C)\log(1-q(C=1|Y))\right]$$

One can show [4] that $$\mathcal{L}_{\mathrm{BCE}}(q^*) \geq -\mathrm{MI}(X,Y)$$

One can also generalize this lower bound to multiple variables [4,5]

Deep Graph InfoMax

We want to learn node representations that capture global context information of the graph, i.e., maximize *local mutual information*

$$\mathcal{L} = \frac{1}{N+M}\left(\sum_{i=1}^{N}\mathbb{E}_{(\mathbf{X},\mathbf{A})}\left[\log \mathcal{D}\left(\vec{h}_i, \vec{s}\right)\right] + \sum_{j=1}^{M}\mathbb{E}_{(\widetilde{\mathbf{X}},\widetilde{\mathbf{A}})}\left[\log\left(1-\mathcal{D}\left(\vec{\widetilde{h}}_j, \vec{s}\right)\right)\right]\right)$$

- Graph input

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- Corrupted/Noisy graph input

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- Graph input
- Corrupted/Noisy graph input
- Node representation

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- Graph input
- Corrupted/Noisy graph input
- Node representation
- Graph representation

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- Graph input
- Corrupted/Noisy graph input
- Node representation
- Graph representation
- Discriminator / Binary classifier

Deep Graph InfoMax

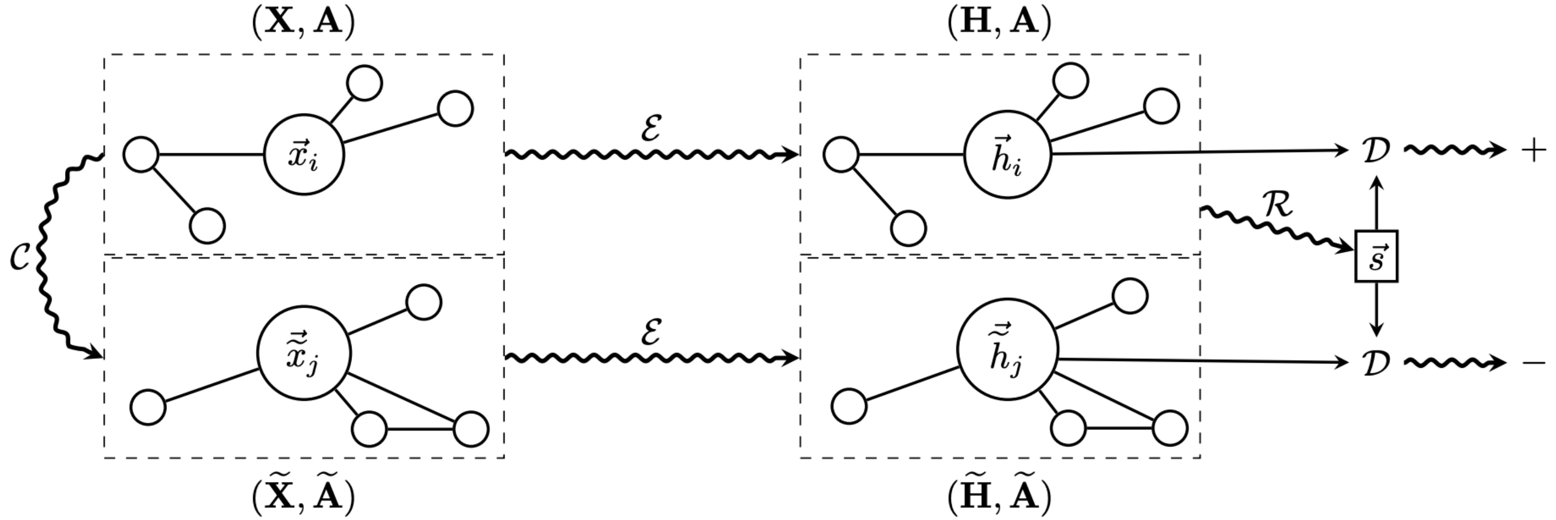
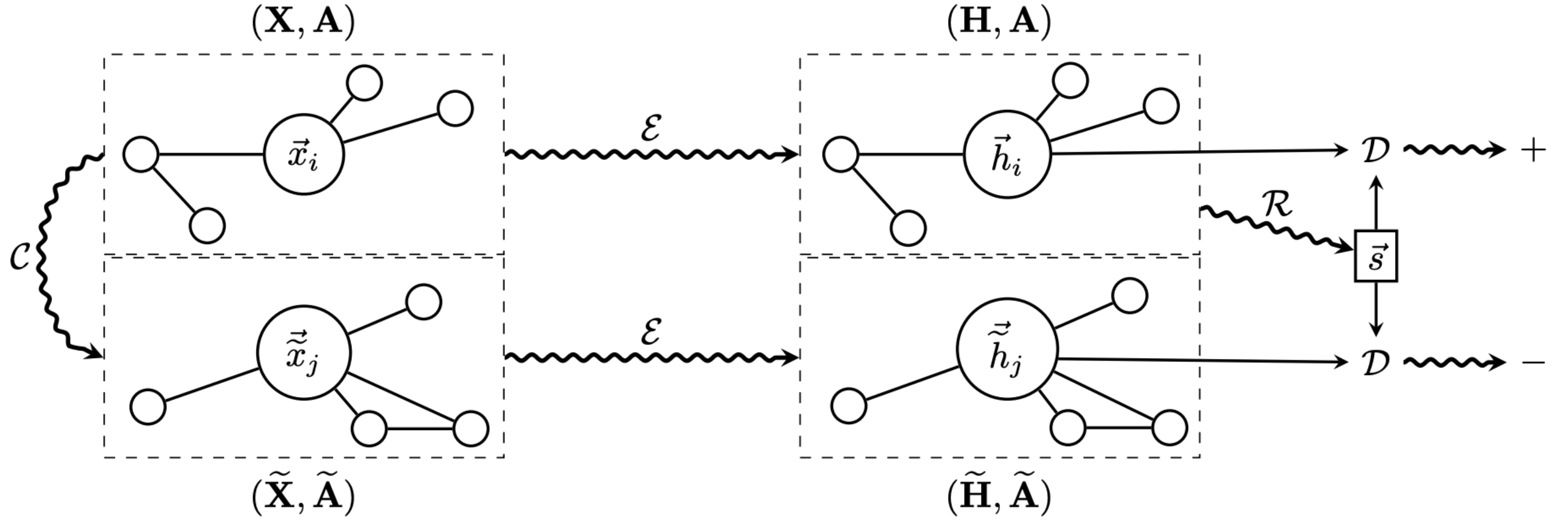


Image Credit: [3]

Deep Graph InfoMax



1. Sample a negative example by using the corruption function: $(\widetilde{\mathbf{X}}, \widetilde{\mathbf{A}}) \sim \mathcal{C}(\mathbf{X}, \mathbf{A})$.
2. Obtain patch representations, $\vec{h}_i$ for the input graph by passing it through the encoder: $\mathbf{H} = \mathcal{E}(\mathbf{X}, \mathbf{A}) = \{\vec{h}_1, \vec{h}_2, \ldots, \vec{h}_N\}$.
3. Obtain patch representations, $\vec{\widetilde{h}}_j$ for the negative example by passing it through the encoder: $\widetilde{\mathbf{H}} = \mathcal{E}(\widetilde{\mathbf{X}}, \widetilde{\mathbf{A}}) = \{\vec{\widetilde{h}}_1, \vec{\widetilde{h}}_2, \ldots, \vec{\widetilde{h}}_M\}$.
4. Summarize the input graph by passing its patch representations through the readout function: $\vec{s} = \mathcal{R}(\mathbf{H})$.
5. Update parameters of $\mathcal{E}$, $\mathcal{R}$ and $\mathcal{D}$ by applying gradient descent to maximize Equation 1.

Image Credit: [3]

Deep Graph InfoMax

If a huge graph is presented, sampling subgraphs is necessary

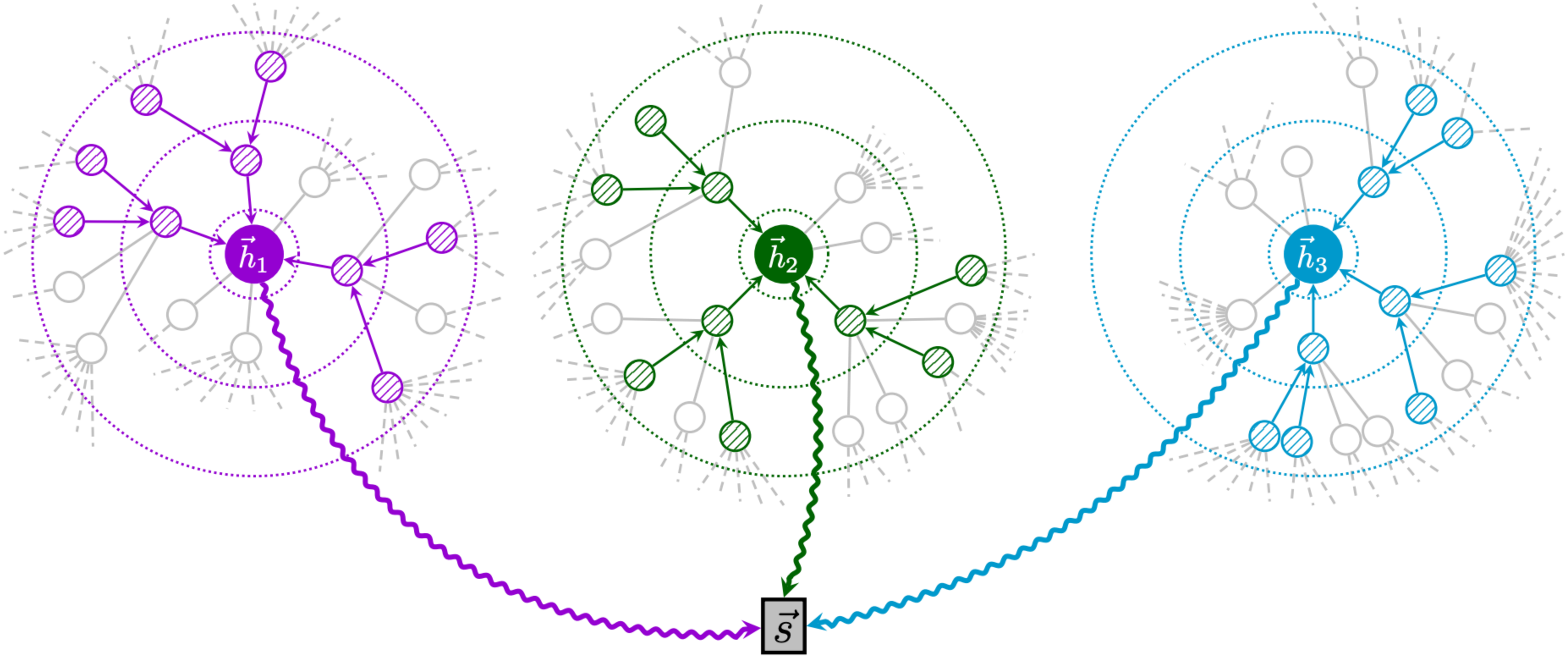


Image Credit: [3]

Deep Graph InfoMax

Transductive

Available data	Method	Cora	Citeseer	Pubmed
$\mathbf{X}$	Raw features	$47.9 \pm 0.4\%$	$49.3 \pm 0.2\%$	$69.1 \pm 0.3\%$
$\mathbf{A}, \mathbf{Y}$	LP (Zhu et al., 2003)	68.0%	45.3%	63.0%
$\mathbf{A}$	DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
$\mathbf{X}, \mathbf{A}$	DeepWalk + features	$70.7 \pm 0.6\%$	$51.4 \pm 0.5\%$	$74.3 \pm 0.9\%$
$\mathbf{X}, \mathbf{A}$	Random-Init (ours)	$69.3 \pm 1.4\%$	$61.9 \pm 1.6\%$	$69.6 \pm 1.9\%$
$\mathbf{X}, \mathbf{A}$	**DGI** (ours)	$\mathbf{82.3} \pm 0.6\%$	$\mathbf{71.8} \pm 0.7\%$	$\mathbf{76.8} \pm 0.6\%$
$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	GCN (Kipf & Welling, 2016a)	81.5%	70.3%	79.0%
$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%

Inductive

Available data	Method	Reddit	PPI
$\mathbf{X}$	Raw features	0.585	0.422
$\mathbf{A}$	DeepWalk (Perozzi et al., 2014)	0.324	—
$\mathbf{X}, \mathbf{A}$	DeepWalk + features	0.691	—
$\mathbf{X}, \mathbf{A}$	GraphSAGE-GCN (Hamilton et al., 2017a)	0.908	0.465
$\mathbf{X}, \mathbf{A}$	GraphSAGE-mean (Hamilton et al., 2017a)	0.897	0.486
$\mathbf{X}, \mathbf{A}$	GraphSAGE-LSTM (Hamilton et al., 2017a)	0.907	0.482
$\mathbf{X}, \mathbf{A}$	GraphSAGE-pool (Hamilton et al., 2017a)	0.892	0.502
$\mathbf{X}, \mathbf{A}$	Random-Init (ours)	0.933 ± 0.001	0.626 ± 0.002
$\mathbf{X}, \mathbf{A}$	**DGI** (ours)	$\mathbf{0.940} \pm 0.001$	$\mathbf{0.638} \pm 0.002$
$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	FastGCN (Chen et al., 2018)	0.937	—
$\mathbf{X}, \mathbf{A}, \mathbf{Y}$	Avg. pooling (Zhang et al., 2018)	0.958 ± 0.001	0.969 ± 0.002

Image Credit: [3]

SimCLR

Image Credit: https://ai.googleblog.com/2020/04/advancing-self-supervised-and-semi.html

SimCLR

Algorithm 1 SimCLR's main learning algorithm.

input: batch size N, constant τ, structure of f, g, $\mathcal{T}$.
for sampled minibatch $\{\boldsymbol{x}_k\}_{k=1}^N$ **do**
  for all $k \in \{1, \ldots, N\}$ **do**
    draw two augmentation functions $t \sim \mathcal{T}$, $t' \sim \mathcal{T}$
    # the first augmentation
    $\tilde{\boldsymbol{x}}_{2k-1} = t(\boldsymbol{x}_k)$
    $\boldsymbol{h}_{2k-1} = f(\tilde{\boldsymbol{x}}_{2k-1})$ # representation
    $\boldsymbol{z}_{2k-1} = g(\boldsymbol{h}_{2k-1})$ # projection
    # the second augmentation
    $\tilde{\boldsymbol{x}}_{2k} = t'(\boldsymbol{x}_k)$
    $\boldsymbol{h}_{2k} = f(\tilde{\boldsymbol{x}}_{2k})$ # representation
    $\boldsymbol{z}_{2k} = g(\boldsymbol{h}_{2k})$ # projection
  end for
  for all $i \in \{1, \ldots, 2N\}$ and $j \in \{1, \ldots, 2N\}$ **do**
    $s_{i,j} = \boldsymbol{z}_i^\top \boldsymbol{z}_j / (\|\boldsymbol{z}_i\| \|\boldsymbol{z}_j\|)$ # pairwise similarity
  end for
  define $\ell(i,j)$ **as** $\ell(i,j) = -\log \frac{\exp(s_{i,j}/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(s_{i,k}/\tau)}$
  $\mathcal{L} = \frac{1}{2N} \sum_{k=1}^{N} [\ell(2k-1, 2k) + \ell(2k, 2k-1)]$
  update networks f and g to minimize $\mathcal{L}$
end for
return encoder network $f(\cdot)$, and throw away $g(\cdot)$

Image Credit: [6]

SimCLR

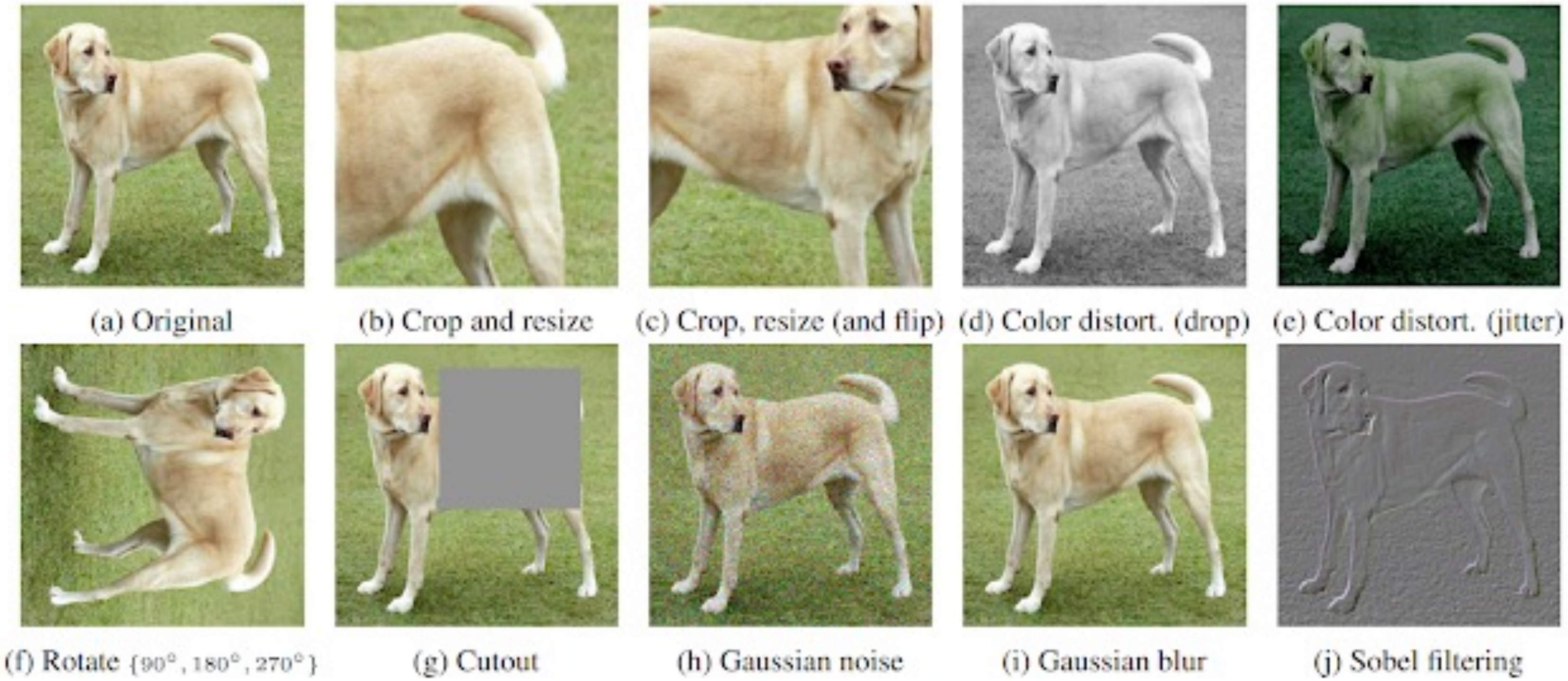


Image Credit: https://ai.googleblog.com/2020/04/advancing-self-supervised-and-semi.html

SimCLR

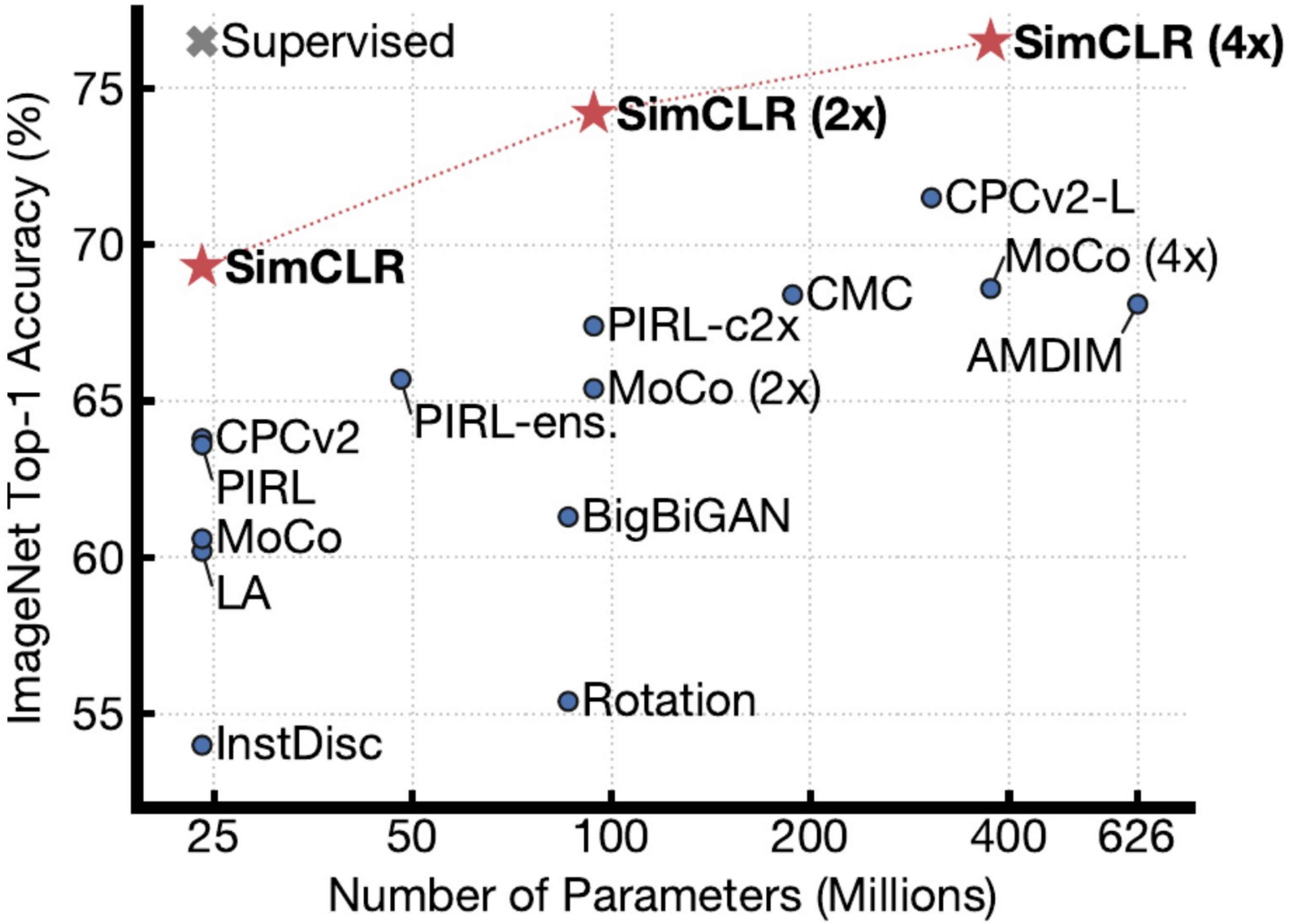


Image Credit: https://ai.googleblog.com/2020/04/advancing-self-supervised-and-semi.html

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Questions?