

Machine Learning on graphs. Structural Graph Embeddings

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Network Science



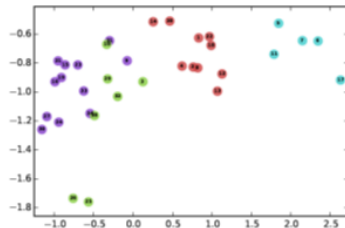
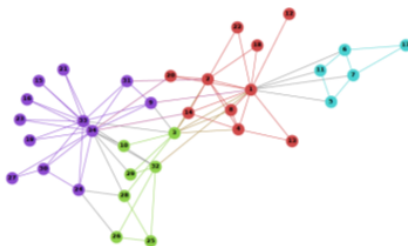
- Node classification (attribute inference)
- Link prediction (missing/hidden links inference)
- Community detection (clustering nodes in graph)
- Graph visualization (cluster projections)

1 Graph Embeddings

- Problem statement
- Structural graph embeddings (simple models)
- Structural graph embeddings (mixed-hop models)
- Structural graph embeddings (with attributes)

Graph Embeddings

- Necessity to automatically select features
- Reduce domain- and task- specific bias
- Unified framework to vectorize network
- Preserve graph properties in vector space
- Similar nodes \rightarrow close embeddings

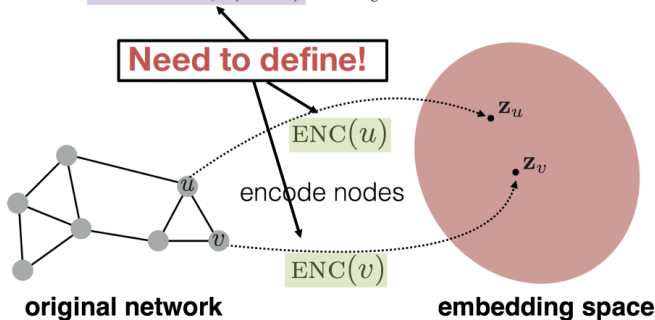


¹<http://snap.stanford.edu/proj/embeddings-www/>

Graph Embeddings

- Define **Encoder**
- Define **Similarity**/graph feature to preserve graph properties
- Define similarity/distance in the embedding space
- **Optimize** loss to fit embedding with similarity computed on graph

Goal: $\text{similarity}(u, v) \approx \mathbf{z}_v^\top \mathbf{z}_u$



Structural Graph Embeddings

- Embedding look-up (each node - separate vector)
- Different similarity measures (adjacency, common neighbours, distances, exact function, etc.)
- Quadratic optimization for MSE loss
- Fast models via random walks

First-order Proximity

- Similarity between u and v is A_{uv}
- MSE Loss
- Variant of Matrix Decomposition

The diagram illustrates the MSE loss formula for graph proximity. The loss \mathcal{L} is shown in a red box. It is equal to the sum over all node pairs $(u, v) \in V \times V$ of the squared difference between the embedding similarity $\mathbf{z}_u^\top \mathbf{z}_v$ and the weighted adjacency matrix element $\mathbf{A}_{u,v}$. The components are color-coded and labeled with arrows:

- \mathcal{L} (red box): loss (what we want to minimize)
- $\sum_{(u,v) \in V \times V}$ (green box): sum over all node pairs
- $\mathbf{z}_u^\top \mathbf{z}_v$ (purple box): embedding similarity
- $\mathbf{A}_{u,v}$ (blue box): (weighted) adjacency matrix for the graph

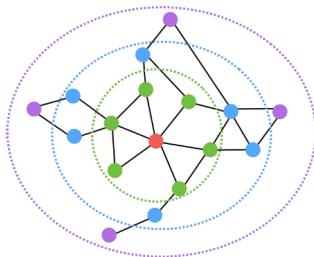
$$\mathcal{L} = \sum_{(u,v) \in V \times V} \|\mathbf{z}_u^\top \mathbf{z}_v - \mathbf{A}_{u,v}\|^2$$

from Leskovec et al., 2018

- Pros:
 - Use SGD for scalable optimization
 - Matrix factorization (SVD) or decomposition (QR) may be applicable
- Cons:
 - Quadratic complexity
 - Large embeddings space
 - No indirect graph properties are preserved

Multi-order Proximity

- Similarity of neighborhoods of u and v via indices or k -hop paths
- Direct optimization of exact similarity metric

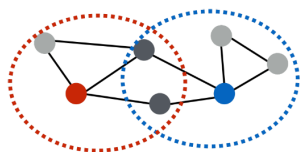


- **Red:** Target node
- **Green:** 1-hop neighbors
 - \mathbf{A} (i.e., adjacency matrix)
- **Blue:** 2-hop neighbors
 - \mathbf{A}^2
- **Purple:** 3-hop neighbors
 - \mathbf{A}^3

$$\mathcal{L} = \sum_{(u,v) \in V \times V} \|\mathbf{z}_u^\top \mathbf{z}_v - \mathbf{A}_{u,v}^k\|^2$$

Multi-order Proximity

- Similarity score S_{uv} as Jaccard/Common Neighbours, etc. (HOPE)



$$\mathcal{L} = \sum_{(u,v) \in V \times V} \left\| \boxed{\mathbf{z}_u^\top \mathbf{z}_v} - \boxed{S_{u,v}} \right\|^2$$

embedding similarity

multi-hop network similarity (i.e., any neighborhood overlap measure)

- Weighted k-hop paths with different k (GraRep)

$$\tilde{\mathbf{A}}_{i,j}^k = \max \left(\log \left(\frac{(\mathbf{A}_{i,j}/d_i)}{\sum_{l \in V} (\mathbf{A}_{l,j}/d_l)^k} \right)^k - \alpha, 0 \right)$$

node degree

constant shift

from Leskovec et al., 2018

- Even worse complexity

Random Walks

- Similarity between u and v is probability to co-occur on a random walk
- Sample each vertex u neighborhood $N_R(u)$ (multiset) by short random walks via strategy R
- Optimize similarity considering independent neighbor samples via MLE (remind Word2Vec)

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

from Leskovec et al., 2018

- $P(v|z_u)$ is approximated via softmax over similarity $z_u^T \cdot z_v$

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log \left(\frac{\exp(\mathbf{z}_u^\top \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^\top \mathbf{z}_n)} \right)$$


- Problem in second Σ over all nodes
- Hard to find optimal solution

Negative Sampling

- Use *Negative Sampling* to approximate denominator

$$\log \left(\frac{\exp(\mathbf{z}_u^\top \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u^\top \mathbf{z}_n)} \right)$$

random distribution
over all nodes

$$\approx \log(\sigma(\mathbf{z}_u^\top \mathbf{z}_v)) - \sum_{i=1}^k \log(\sigma(\mathbf{z}_u^\top \mathbf{z}_{n_i})), n_i \sim P_V$$


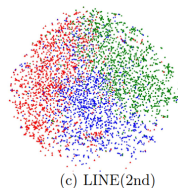
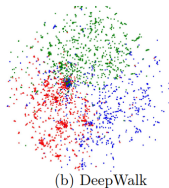
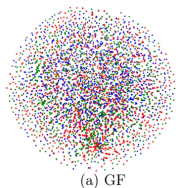
from Leskovec et al., 2018

- Sample in proportion to node degree
- Experiment with k to impact negative prior and robustness
- No need to sample non-connected edges — same as random

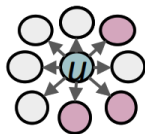
- Finite unbiased random walks (DeepWalk)
- 1-hops & 2-hops for half of the embedding, arbitrary random walks for the second half of the embedding (LINE)
- Diffusion for sampling (Diff2Vec)
- Biased random walks combining BFS and DFS (Node2Vec)

DeepWalk & LINE

- DeepWalk: Unbiased random walks with fixed length and number
- LINE: Combination of first-order and second-order proximity aggregation via concatenation



- BFS samples local neighborhood, DFS goes for global features



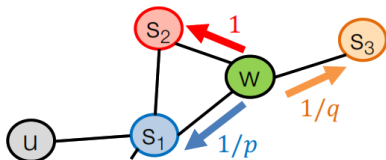
BFS:



DFS:

- Two parameters p and q to control sampling
- Second order Markov process

- Parameters are multiplied by edge weights and normalized for random walk probabilities

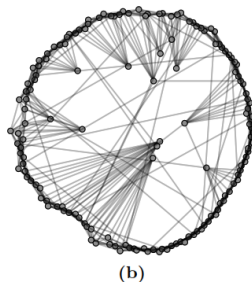
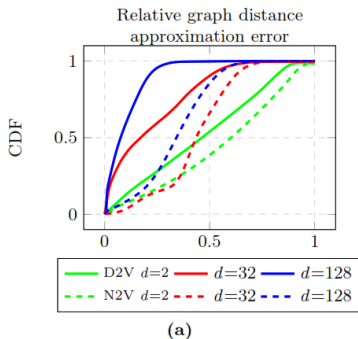


$1/p, 1/q, 1$ are
unnormalized
probabilities

p, q model transition probabilities

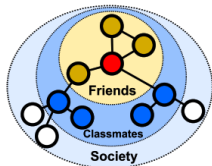
- p ... return parameter
- q ... "walk away" parameter

- Sample node according to supervised diffusion
- Efficient initialization and [possibility to control clustering parameters]

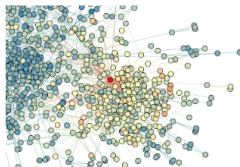


Grarep & Walklets

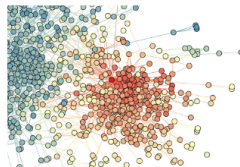
- Grarep: Approximate normalized A^k efficiently
- Walklets: approximate attention over k -distance neighbors



(a) A student (in red) is a member of several increasing larger social communities.

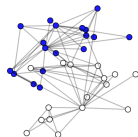


(b) WALKLETS Fine Representation

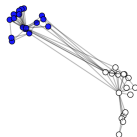


(c) WALKLETS Coarse Representation

- GEMSEC model cluster information adding regularization term over community labels given number of classes
- parameter γ balance cluster error and cluster structure given model hyper-parameters



(a) DeepWalk



(b) GEMSEC

$$\mathcal{L} = \underbrace{\sum_{v \in V} \left[\ln \left(\sum_{u \in V} \exp(f(v) \cdot f(u)) \right) - \sum_{n_i \in N_S(v)} f(n_i) \cdot f(v) \right]}_{\text{Embedding cost}} + \underbrace{\gamma \cdot \sum_{v \in V} \min_{c \in C} \|f(v) - \mu_c\|_2}_{\text{Clustering cost}} \quad (5)$$

- Modularized Nonnegative Matrix Factorization (M-NMF) incorporates first-second order proximity together with community structure.
- $S = S_1 + \eta S_2$, S_i goes for i -th order proximity.
- C represents community structure.
- H represents nodes community labels.
- B stands for $\left(A_{ij} - \frac{k_i k_j}{2m}\right)$ matrix in modularity function.
- U is our embedding.

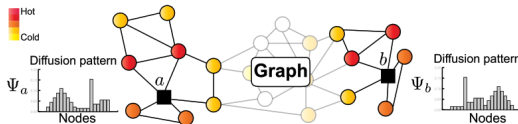
$$\min_{\mathbf{M}, \mathbf{U}, \mathbf{H}, \mathbf{C}} \|\mathbf{S} - \mathbf{M}\mathbf{U}^T\|_F^2 + \alpha \|\mathbf{H} - \mathbf{U}\mathbf{C}^T\|_F^2 - \beta \text{tr}(\mathbf{H}^T \mathbf{B} \mathbf{H})$$
$$s.t., \mathbf{M} \geq 0, \mathbf{U} \geq 0, \mathbf{H} \geq 0, \mathbf{C} \geq 0, \text{tr}(\mathbf{H}^T \mathbf{H}) = n,$$

- HOPE is specific asymmetric transitivity preserving graph embedding.
- Asymmetric similarity measures can be formulated as $S = M_g^{-1} M_l$.
- Katz index refers to $M_g = I - \beta A$, $M_l = \beta A$.
- Rooted PageRank can be stated as
 $M_g = I - \alpha P$, $M_l = (1 - \alpha)P$, $P = D^{-1}A$.
- Common neighbors is represented by $M_g = I$, $M_l = A^2$.
- Adamic-Adar with $M_g = I$, $M_l = ADA$.
- Generalized SVD and directly estimate matrices M_g and M_l .

- Structural Deep Network Embedding (SDNE) uses autoencoder via Laplacian eigenmaps.
- Watch Your Step: Learning Node Embeddings via Graph Attention - attention on random walks aggregation without use on inference
- Metapath2vec adapts random walks on heterogeneous networks
- Discriminative Deep Random Walk (DDRW) includes label regularization to incorporate classification task

Diffusion Wavelets for Structural Similarity

- GraphWave learns heat wavelet diffusion patterns. Nodes with similar neighbors will have similar GraphWave embeddings.
- $O(|E|)$ performance



VERSE for Structural Similarity

- VERSE uses conditional probability not on the embedding, but on the similarity rank.
- $O(|E|)$ performance

$$\begin{aligned} \text{sim}_E(v, \cdot) &= \frac{\exp(W_v W^\top)}{\sum_{i=1}^n \exp(W_v \cdot W_i)} \\ \mathcal{L} &= - \sum_{v \in V} \text{sim}_G(v, \cdot) \log(\text{sim}_E(v, \cdot)) \\ \mathcal{L}_{NCE} &= \sum_{\substack{u \sim \mathcal{P} \\ v \sim \text{sim}_G(u, \cdot)}} \left[\log \Pr_W(D = 1 | \text{sim}_E(u, v)) + \right. \\ &\quad \left. s \mathbb{E}_{\tilde{v} \sim Q(u)} \log \Pr_W(D = 0 | \text{sim}_E(u, \tilde{v})) \right] \end{aligned}$$

Short conclusion for structural Graph Embeddings

- Random walks are powerful tool for fast network embedding
- Proximity-aware embeddings, random walks can be modeled in terms of each other (and even deep neural networks !)
- complexity and space are important to choose the embedding model
- provided models are used for transductive learning only, inductive learning require additional regularizations and local optimizations
- large graphs are hard to fit with handcrafted sampling strategies
- no clear way to support features

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