Applied Machine Learning

Machine Learning with Graphs

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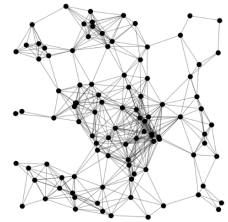
Learning objectives

- How to represent graph structured data
- Unsupervised learning with graphs
  - Community detection (clustering)
- Supervised learning with graphs
  - Node classification

Motivation

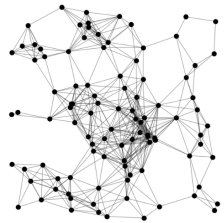


Our world is **complex** and analyzing interconnected data provides the much needed tools to study today's phenomena (e.g., online societies) and enables us to address the world's emerging problems (e.g., covid-19)

Complex Systems

- consists of many interconnected parts
- characterized by time-dependent interactions among their parts
- not an aggregation of their separate parts
- when looked at as a whole gives non trivial insights
- often interactions change states of parts, and the states of the parts change the networks of interactions

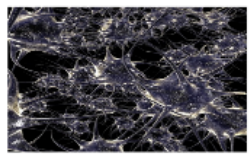
Motivation: applications



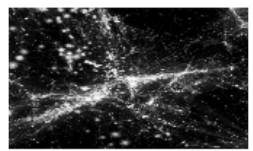
natural sciences: connections between atoms, molecules, cells, organisms and even the cosmic web

Chemistry

Biology

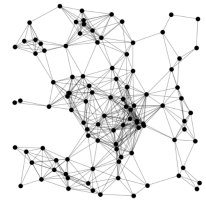


Physics



from a demo of galaxy networks

applied sciences: looking at compex system, as a whole, gives us non trivial insights and is necessary to understand these systems in many applications, e.e. in Medicine, law, even culinary (check this flavor network)



Representing Interconnected Data

we used independent **instances** as data in this course:

$$X = \begin{bmatrix} x^{(1)\top} \\ x^{(2)\top} \\ \vdots \\ x^{(N)\top} \end{bmatrix} = \begin{bmatrix} x_1^{(1)}, & x_2^{(1)}, & \cdots, & x_D^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(N)}, & x_2^{(N)}, & \cdots, & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D}$$

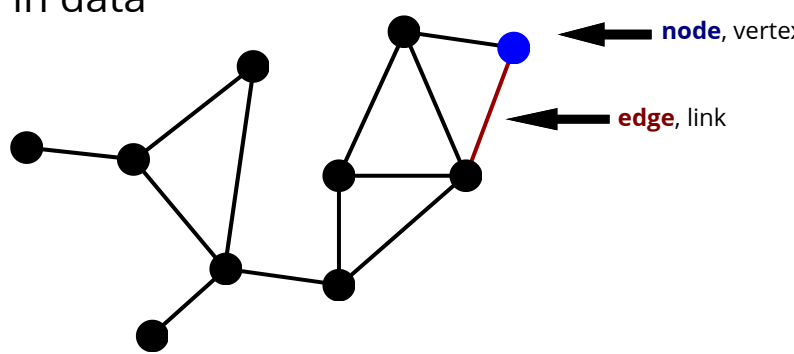
one instance

one feature

Graphs represent the relation between **instances** in data

the default representation

- variations: **simple**, weighted, directed, signed, multi-edges and multi-type nodes (heterogenous), attributed (nodes and or edges have feature vectors), dynamic (sequence of graphs), multilayer networks (multi-view), hypergraphs (beyond pairwise relations), etc.



Representing Graphs

Features Matrix

node features

$$X = \begin{bmatrix} x_1^{(1)}, & x_2^{(1)}, & \cdots, & x_D^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(N)}, & x_2^{(N)}, & \cdots, & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D}$$

one instance

one feature

Adjacency Matrix

connections between nodes

marginals of A are called **degree**

$d_i = \sum_j A_{ij}$

$$A = \begin{bmatrix} A_{11}, & A_{12}, & \cdots, & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1}, & A_{N2}, & \cdots, & A_{NN} \end{bmatrix} \in \mathbb{R}^{N \times N}$$

inlinks: all nodes linking to 1

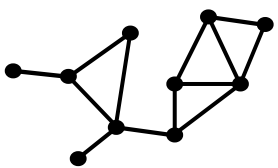
outlinks: all nodes node 2 links to

if unweighted then $\in \{0,1\}^{N \times N}$

Real world graphs are sparse (have lots of zeros) and we use sparse matrix representations to store them (only store non-zero values)

Representing Graphs

Adjacency Matrix



- person & friendship
- paper & citation
- cities & train tracks
- protiens & binding

$$A = \begin{bmatrix} A_{11}, & A_{12}, & \cdots, & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1}, & A_{N2}, & \cdots, & A_{NN} \end{bmatrix} \in \mathbb{R}^{N \times N}$$

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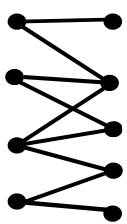
Incidence Matrix



often used to represent **bipartite** graphs

- actor & movies
- authors & papers
- metabolites & reactions
- words & documents
- two possible one mode projections: $B^\top B$, and $BB^\top$

$$B = \begin{bmatrix} A_{11}, & A_{12}, & \cdots, & A_{1M} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1}, & A_{N2}, & \cdots, & A_{NM} \end{bmatrix} \in \mathbb{R}^{N \times M}$$

all edges node 1 belongs to

edges, or second set of nodes

nodes: all nodes edge 2 links

if unweighted then $\in \{0,1\}^{N \times M}$

Representing Graphs

Laplacian Matrix

$$\in \mathbb{R}^{N \times N}$$

$$L = D - A$$

diagonal degree matrix

$$A = \begin{bmatrix} A_{11}, & A_{12}, & \cdots, & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1}, & A_{N2}, & \cdots, & A_{NN} \end{bmatrix} \in \mathbb{R}^{N \times N}$$

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if unweighted then $\in \{0,1\}^{N \times N}$

Eigenvalues of Graph laplacian tells us about the connectivity of the graph

- e.g. number of zero eigenvalues is the number of connected components
- second-smallest eigenvalue of L is called Algebraic connectivity or Fiedler value
- **Signs of values in Fiedler eigenvector** (associated to Fiedler eigenvalue) tell us how to partition the graph into two components by breaking least edges, i.e. **minimum cut** solution

$$L = \begin{bmatrix} d_1, & -A_{12}, & \cdots, & -A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ -A_{N1}, & -A_{N2}, & \cdots, & d_N \end{bmatrix} \in \mathbb{R}^{N \times N}$$

sums to zero

sums to zero

Representing Graphs

Adjacency Matrix

connections between nodes

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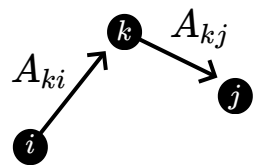
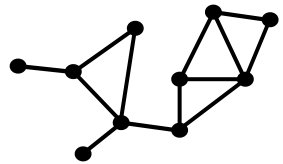
Powers of A

- A^2 : # of walks with length two
  - If undirected, number of common neighbors
  - what is A^2_{ii}?
- A^3 : # of walks with length three
  - what is A^3_{ii}?
  - if undirected, $Tr(A^3)/6$ gives the number of triangles
  - we compute number of triangles more effectively from eigenvalues of A as $\frac{1}{6}\sum_i \lambda_i^3$, since if λ is eigenvalue of A then λ^p is eigenvalue of A^p
  - real world graphs usually have a lot of triangles, e.g. friends of friends are friends



Degree distribution



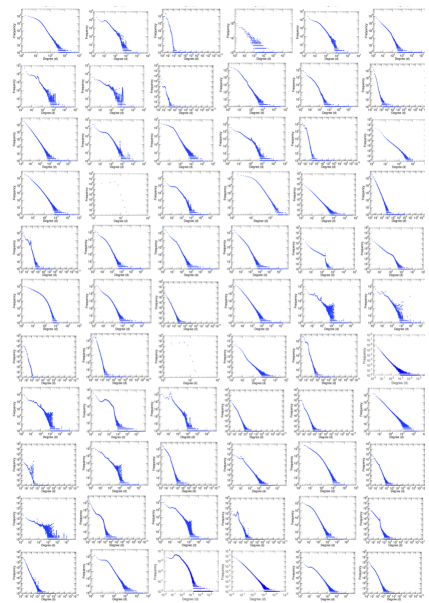
- marginals of A are called **degree**
  - $d_i = \sum_j A_{ij}$
  - if directed, ($A_{ij} = 1$ there is an edge from node j to i) we have
    - column-wise and row-wise marginals as indegree and out degree of nodes
    - $d_i^{in} = \sum_j A_{ij}$, and $d_i^{out} = \sum_j A_{ji}$
- $\sum_i \sum_j A_{ij}$
  - total number of edges (if directed), or twice that if undirected

$$A = \begin{bmatrix} A_{11}, & A_{12}, & \cdots, & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1}, & A_{N2}, & \cdots, & A_{NN} \end{bmatrix}$$

inlinks

outlinks

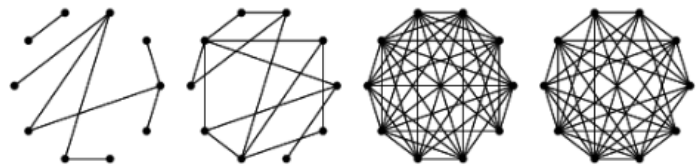
- **degree distribution:** how many nodes of degree k are in the graph
  - is often heavy tailed in real world networks (there are few nodes with very high degree & many with very small degree)
- degree distribution is plotted in log-log and a line could give a goof fit
  - $ln(p(d)) = -\alpha ln(d) + ln(c) \Rightarrow p(d) = cd^{-\alpha}$: powerlaw distribution
- often referred to as being **scale-free** since
  - $p(\lambda d) = \lambda^{-\alpha} c d^{-\alpha}$



example degree distributions

Real-world v.s. random graphs

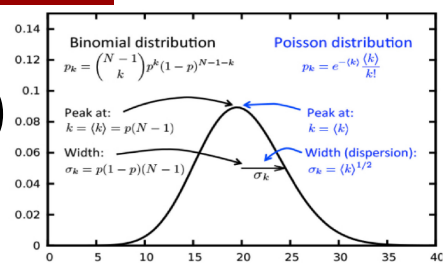
Erdös-Rényi Model (ER) graphs



- basis of random graph theory
- simple model that results in small-world graphs
- parameters: ER(n, p) or ER(n, m)
  - n: number of nodes
  - p: probability of an edge between any two nodes
  - m: number of edges
- generation: all edges are equally likely so toss n(n-1)/2 coins

Degree distribution:

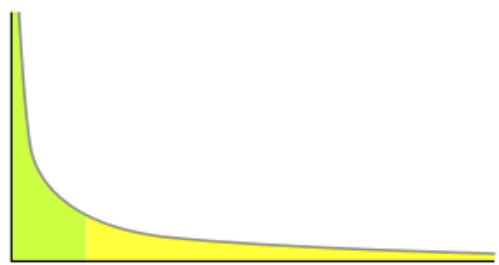
$p(d)$



d

compare with real world graphs which have a heavy tail

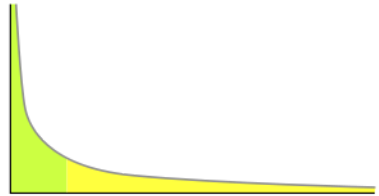
$p(d)$



d

Powerlaws

a common distribution

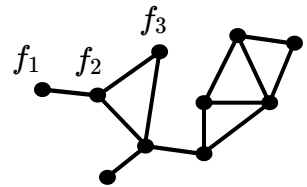


- Income follow a Pareto distribution
  - few individuals earned most of the money & majority earned small amounts
  - in the US 1% of the population earns a disproportionate 15% of the total US income
  - 80/20 rule (Pareto principle): a general rule of thumb
    - e.g. 20 percent of the code has 80 percent of the errors
- Zipf's law
  - distribution of words ranked by their frequency in a random text corpus is approximated by a power-law distribution
  - the second item occurs approximately 1/2 as often as the first, and the third item 1/3 as often as the first, and so on

preferential attachment which results in scale-free graphs

- node is connected to existing nodes with $p(i) \propto d_i$

Spectral clustering



consider function f that maps vertices to a value

$$f = (f_1, f_2, \dots f_N) \in \mathbb{R}^N \Rightarrow f^\top L f = \frac{1}{2} \sum_{ij} A_{ij} (f_i - f_j)^2$$

measures how much the value of f is smooth over edges, i.e. the difference of values for connecting nodes

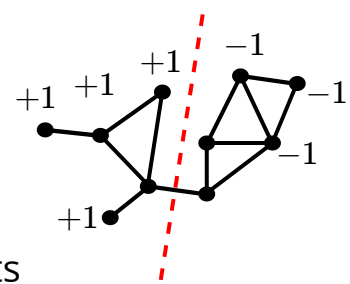
How to cluster? Find f that give smoothest results, i.e, minimizes this

$$f_i \in \{+1, -1\} \text{ and } \sum_i f_i = 0$$

relaxed

$$f_i \in \mathbb{R} \text{ and } \sum_i f_i^2 = N \Rightarrow \min f^\top L f = N \lambda_1$$

Courant Fisher Minmax Theorem



- second smallest eigenvalue ⇒ sparsest cut
- signs of corresponding **eigenvector** ⇒ cluster assignments

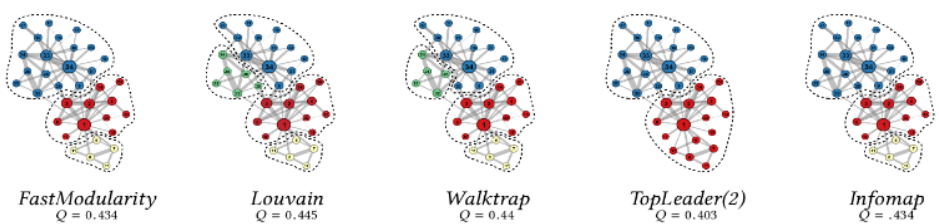
more than 2 clusters? use k-means on top k eigenvectors (each node is represented with k features)

read more here

Clustering Graphs

Better choices for graphs:

- modularity optimization
  - number of links between them is more than chance, examples: FastModularity, **Louvain**
    the best default
- random walk based
-
  - Within them a random walk is more likely to trap, e.g. Walktrap
- compression based
  - Coding gives efficient compression of any random walk, e.g. Infomap
- centroid based
  - follow their closest leader e.g. TopLeader



Clustering Graphs

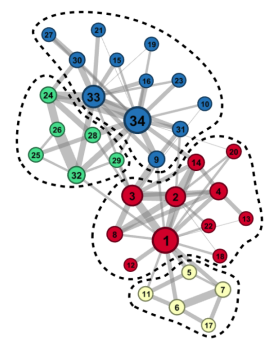
- Modularity optimization
  - number of links between them is more than chance
  - e_{ij}: fraction of edges between cluster i and j, and $a_i = \sum_j e_{ij}$

$$Q = \sum_i (e_{ii} - a_i^2) = Tr(e) - ||e^2||_1$$

here $||e^2||_1 = \sum_{ij} e_{ij}^2$

example

$$e = \begin{bmatrix} 0.71 & 0.35 & 0.06 & 0. \\ 0.22 & 0.3 & 0.22 & 0. \\ 0.065 & 0.35 & 0.59 & 0.4 \\ 0. & 0. & 0.12 & 0.6 \end{bmatrix}$$



optimize with an agglomerative hierarchical clustering

- merge two cluster that give the highest gain in Q

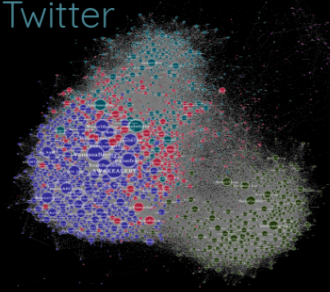
$$\Delta Q = 2(e_{ij} - a_i a_j)$$

FastModularity

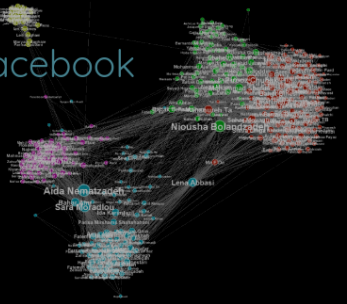
uses this with heap based data structure ⇒ O(m log n)

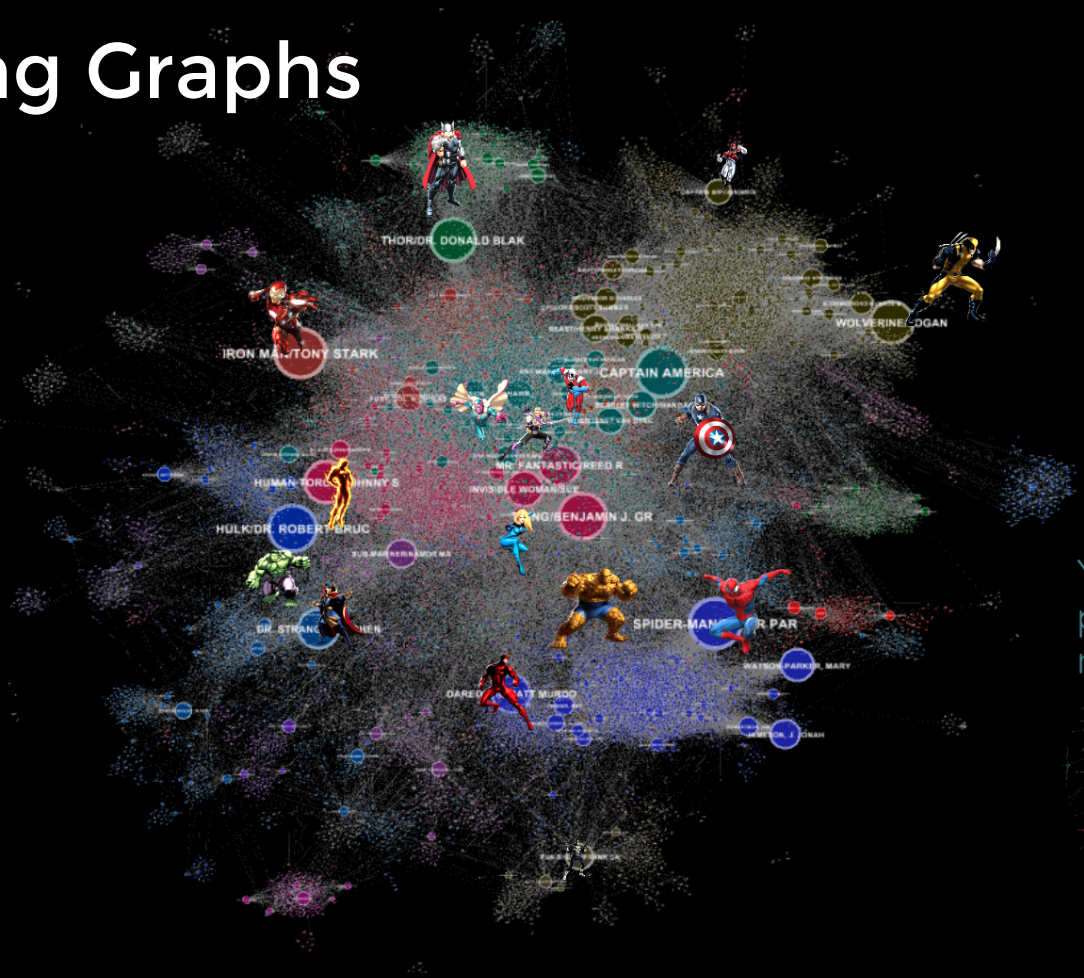
Clustering Graphs

Twitter

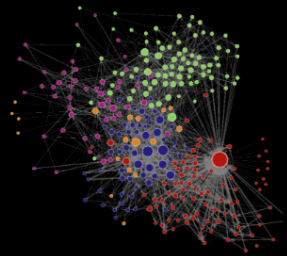


Facebook

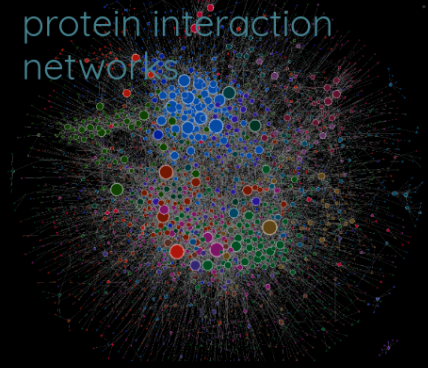




C. elegans
neural network



Yeast protein
protein interaction
networks

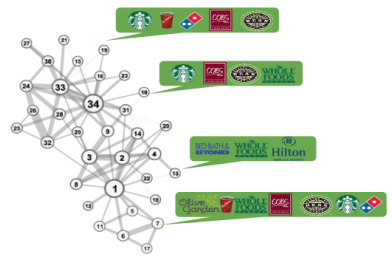


Attributed Graphs

Individual characteristics or activity (attributes) & relations (graph)

characteristics

age, occupation, salary, sex, etc.



activity & interest

check-ins, page-likes, group memberships, movies

Interplay between attributes and relations, a positive feedback loop derived by two social theories:

- **social selection**
  - similarity of individuals' characteristics motivates them to form relations
- **social influence**
  - characteristics of individuals may be affected by the characteristics of their relations
    - your neighbours' attributes can reveal yours

inductive bias: homophily

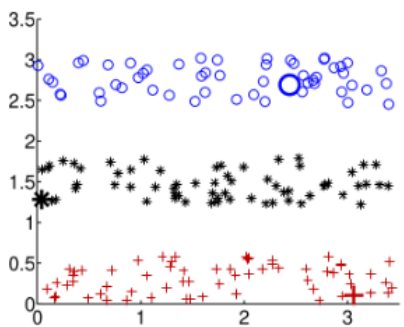
birds of the same feather flock together

Node classification

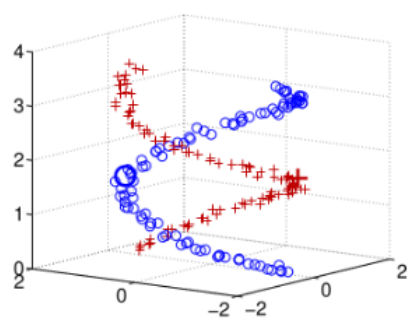
Label Propagation Algorithm

label = mean (scalar) & mode (categorical) of your neighbors

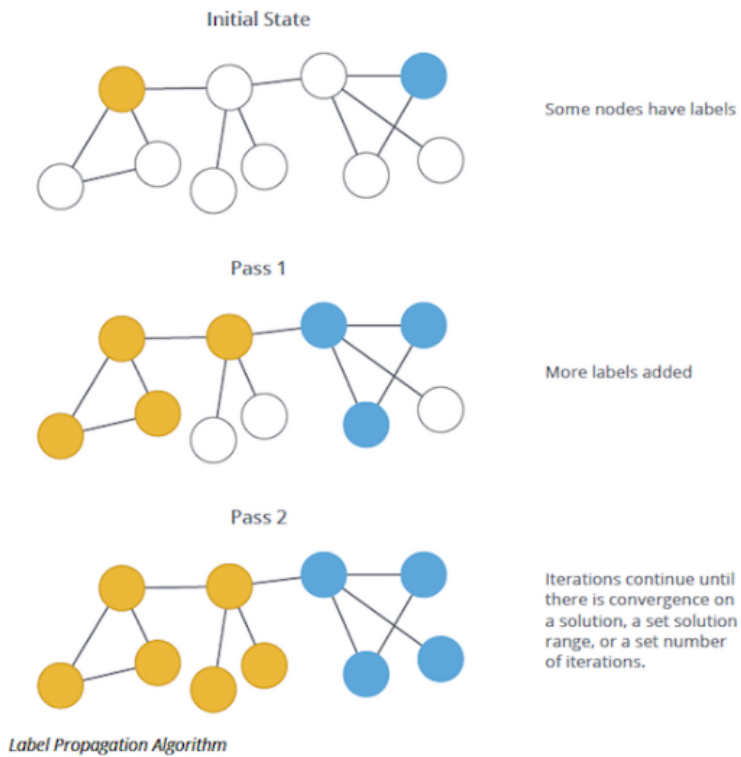
proposed for semi-supervised classification of iid data by defining a fully connected distance graph



(a) 3-Bands

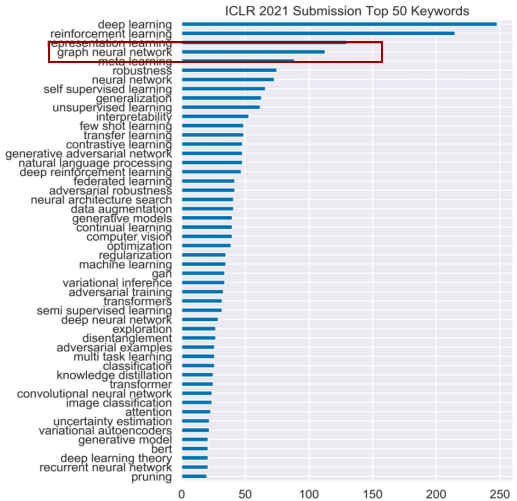


(b) Springs



Label Propagation Algorithm

Graph Representation Learning



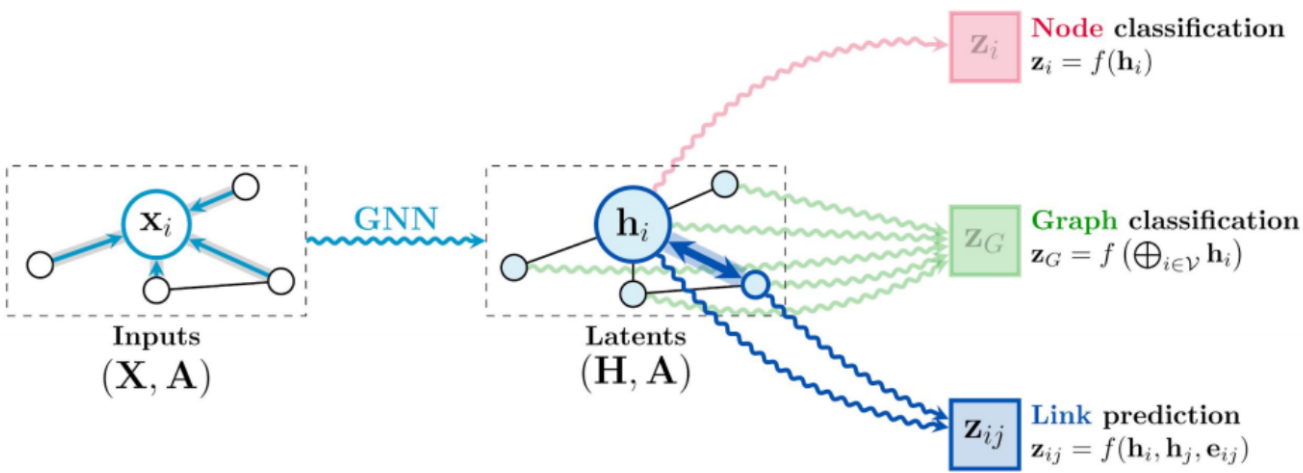
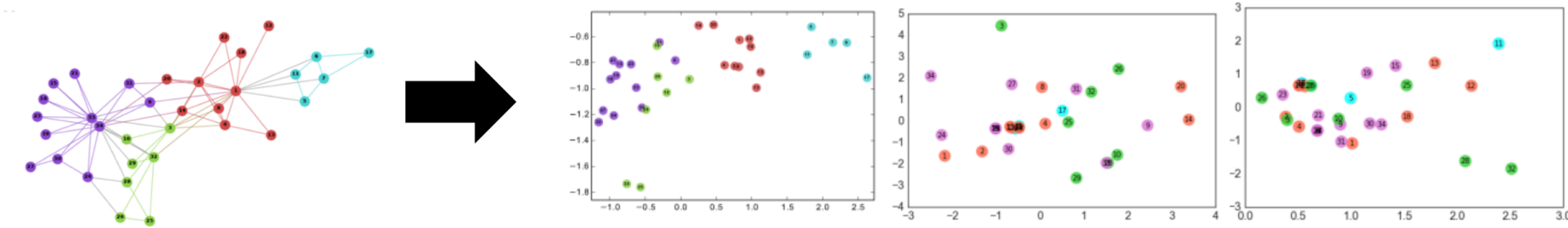


Image form https://www.youtube.com/watch?v=uF53xsT7mjc , also recommended to watch:
https://www.youtube.com/watch?v=8owQBFAHw7E

Graph Representation Learning

embed the graph in vector space $G \rightarrow \mathbb{R}^{N \times D}$

distance in the embedded space ⇒ link prediction
decision boundaries in the embedded space ⇒ node classification



(a) Output: DeepWalk (e) Output: LE (f) Output: SVD

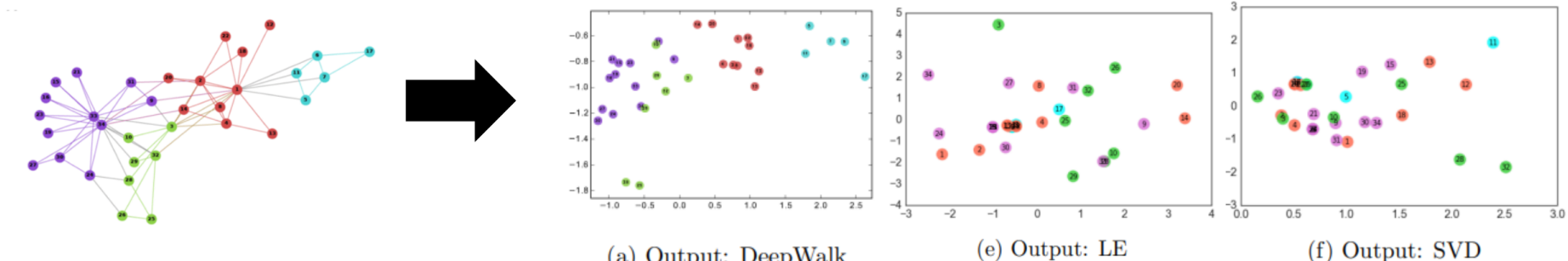
See A Tutorial on Network Embeddings, 2018

Graph Representation Learning

embed the graph in vector space $G \rightarrow \mathbb{R}^{N \times D}$ $h_i : i \in G \rightarrow \mathbb{R}^D$

Preserves the edge structure based on cross-entropy loss:

$$\sum_{(i,j)\in E} \log \sigma(h_i^\top h_j) + \sum_{(i,j)\notin E} \log(1 - \sigma(h_i^\top h_j))$$



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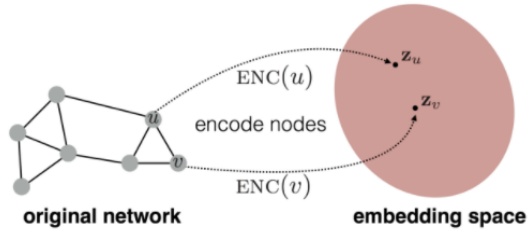
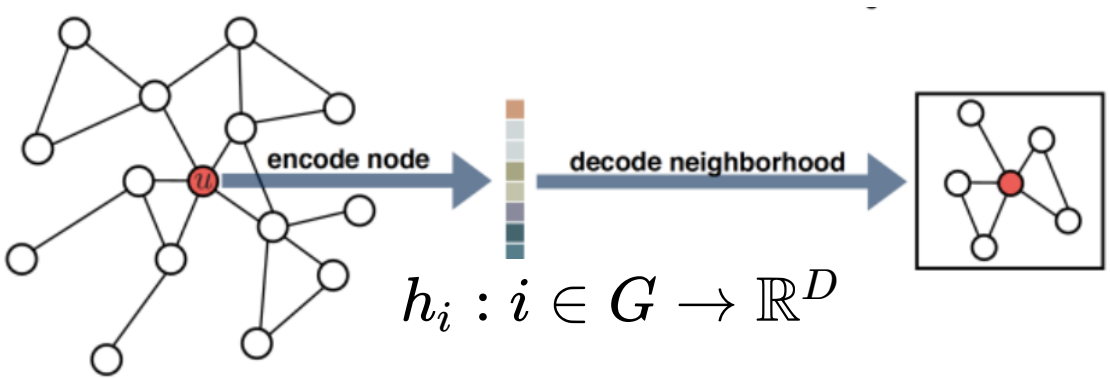
This can be trained unsupervised, and puts connected nodes closeby
Deepwalk, node2vec and LINE redefine this based on nodes that co-occur in a (short) random walk

See https://petar-v.com/talks/GNN-Wednesday.pdf
https://www.cs.mcgill.ca/~wlh/grl_book/files/GRL_Book-Chapter_3-Node_Embeddings.pdf

An Encoder-Decoder Perspective



Encoder gives low dimensional embedding that summarizes the graph position and structure in local neighbourhood
Decoder reconstructs this neighbourhood given the embedding of the node



$$h_i : i \in G \rightarrow \mathbb{R}^D$$

$$\mathcal{L} = \sum_{i,j} l(DEC(h_i, h_j), S(i,j))$$

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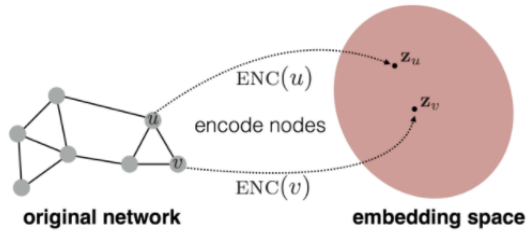

$$\mathcal{L} = \sum_{i,j} l(DEC(h_i, h_j), S(i, j))$$

Method	Decoder	Similarity measure	Loss function
Lap. Eigenmaps	$\|\mathbf{z}_u - \mathbf{z}_v\|_2^2$	general	$\text{DEC}(\mathbf{z}_u, \mathbf{z}_v) \cdot \mathbf{S}[u, v]$

- learn embeddings for each node such that the inner product between the learned embedding vectors approximates some deterministic measure of node similarity
- gives identical to the solution for spectral clustering, i.e. d smallest eigenvectors of the Laplacian

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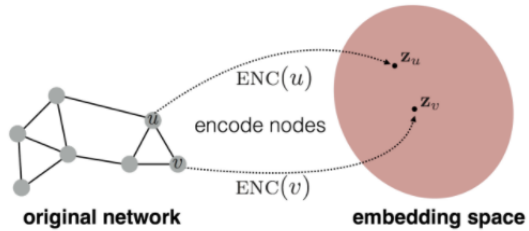
Shallow embedding algorithms



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Graph Fact.	$\mathbf{z}_u^\top \mathbf{z}_v$	$\mathbf{A}[u,v]$	$\|\text{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
GraRep	$\mathbf{z}_u^\top \mathbf{z}_v$	$\mathbf{A}[u,v], ..., \mathbf{A}^k[u,v]$	$\|\text{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
HOPE	$\mathbf{z}_u^\top \mathbf{z}_v$	general	$\|\text{DEC}(\mathbf{z}_u, \mathbf{z}_v) - \mathbf{S}[u,v]\|_2^2$
DeepWalk	$\frac{e^{\mathbf{z}_u^\top \mathbf{z}_v}}{\sum_{k \in \mathcal{V}} e^{\mathbf{z}_u^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v\|u)$	$-\mathbf{S}[u,v] \log(\text{DEC}(\mathbf{z}_u, \mathbf{z}_v))$
node2vec	$\frac{e^{\mathbf{z}_u^\top \mathbf{z}_v}}{\sum_{k \in \mathcal{V}} e^{\mathbf{z}_u^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v\|u)$ (biased)	$-\mathbf{S}[u,v] \log(\text{DEC}(\mathbf{z}_u, \mathbf{z}_v))$

matrix-factorization

$\mathcal{L} \approx \|\mathbf{Z}\mathbf{Z}^\top - \mathbf{S}\|_2^2,$

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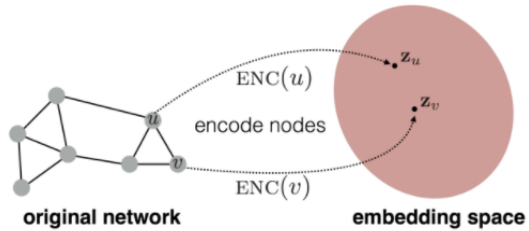
Shallow embedding algorithms



$$\mathcal{L} = \sum_{i,j} l(DEC(h_i, h_j), S(i, j))$$

Limitations of Shallow Embeddings:

- No parameter sharing ⇒ less scalable
- Ignores features or attributes

Read more:
A Tutorial on Network Embeddings, 2018 &
Representation Learning on Graphs, 2017 &
GLR book's chapter on node embedding, 2020

Instead use graph neural networks, more complex encoders, which work based on feature propagation

- Number of parameters doesn't grow with graph size but feature dimension
- Naturally incorporates node features

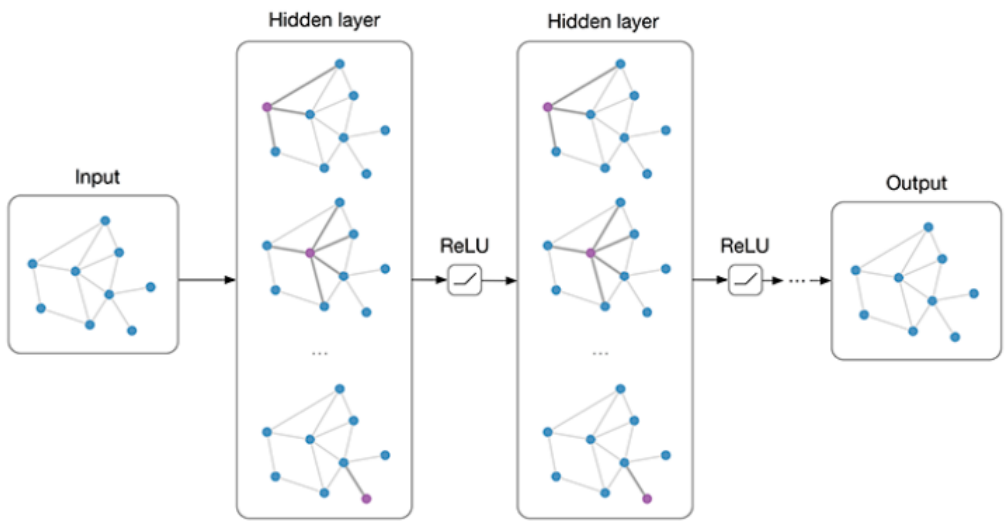
Graph Neural Networks

Use the local neighbourhood similar to convolution on images

$$H^{l+1} = \phi(AH^lW^l)$$

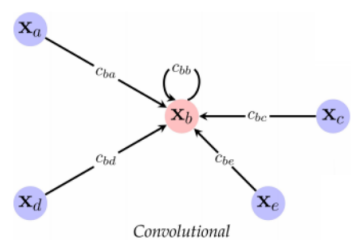
$$H^{l+1} = \phi(\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}}H^lW^l)$$

$$\hat{A} = A + I$$



Multi-layer Graph Convolutional Network (GCN) with first-order filters.

$$h_i^{l+1} = \phi(\sum_{j \in \mathcal{N}(i)} \frac{1}{c_{ij}} h_j^l W^l)$$



GCN (Kipf & Welling, ICLR'17)

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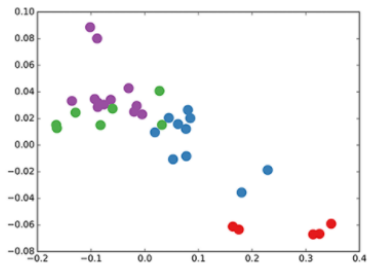
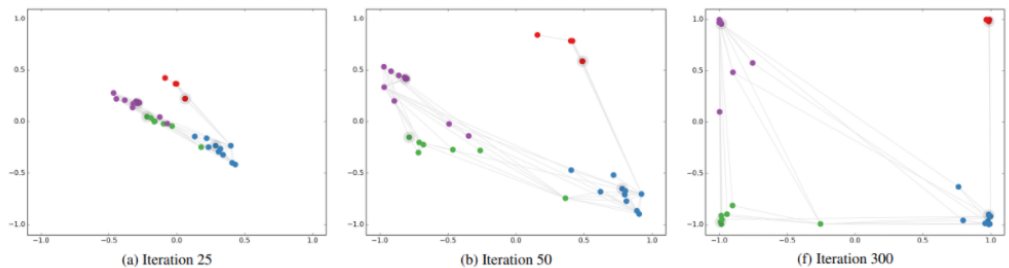


$X = I$



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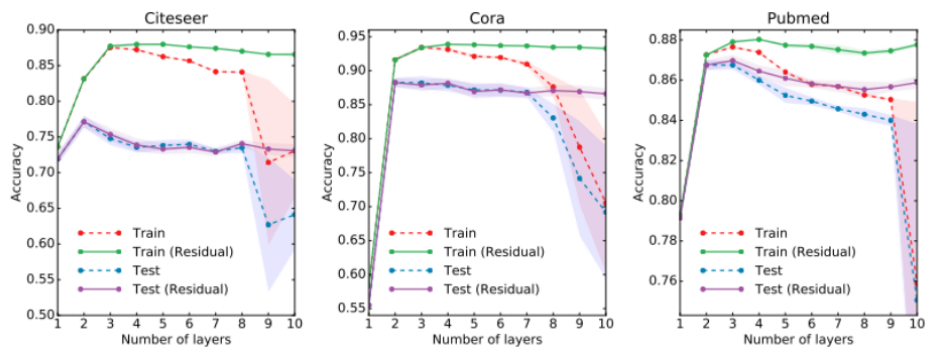

Summary

- graphs are everywhere
- real world graphs have special patterns
- graphs are represented with matrices
- unsupervised: graph clustering partitions the nodes in a graph
- supervised: Node classification, Link prediction
- Shallow and deep models for graphs