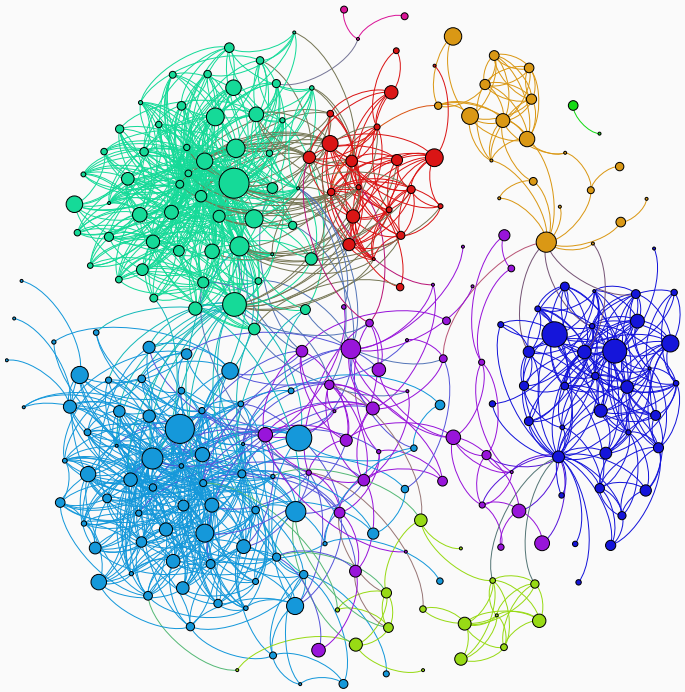
OUTLINE

1. Introduction
2. Basic Graph Notions
3. Graph Analysis
4. Learning in graphs

INTRODUCTION

Graph: collection of interconnected nodes

- Social networks

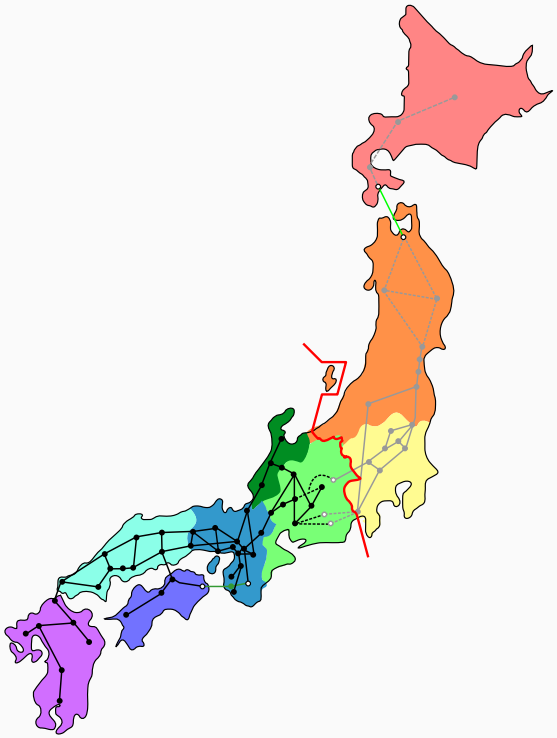


LinkedIn ego network

Credit: `http://allthingsgraphed.com`

Graph: collection of interconnected nodes

- Social networks
- Power grids



Japanese electrical network

Graph: collection of interconnected nodes

- Social networks
- Power grids
- Transportation networks

SNCF network

Credit: PouX / madcap, License: CC BY-SA 3.0

Graph: collection of interconnected nodes

- Social networks
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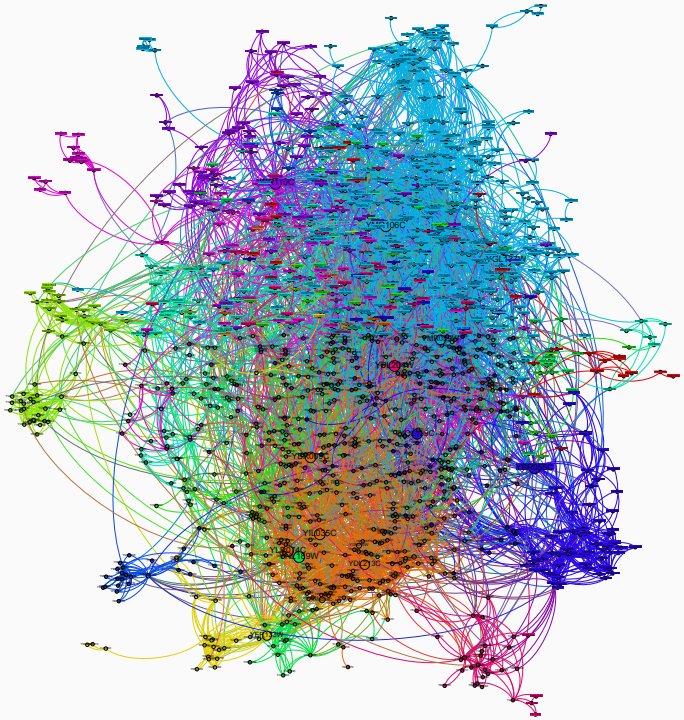
- Transportation networks
- Biological networks

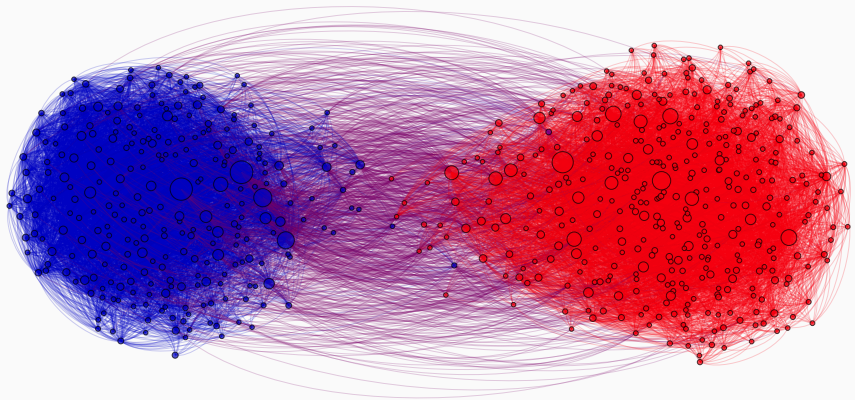


Protein-protein interaction network

Credit: `http://allthingsgraphed.com`

Graph: collection of interconnected nodes

- Social networks
- Power grids
- Transportation networks
- Biological networks
- Web pages



Hyperlinks between American political blogs
Credit: `http://allthingsgraphed.com`

Graph: collection of interconnected nodes

- Social networks
- Power grids
- Transportation networks
- Biological networks
- Web pages
- Graphs as an abstraction (e.g., similarity graphs)

Credit: Michal Valko

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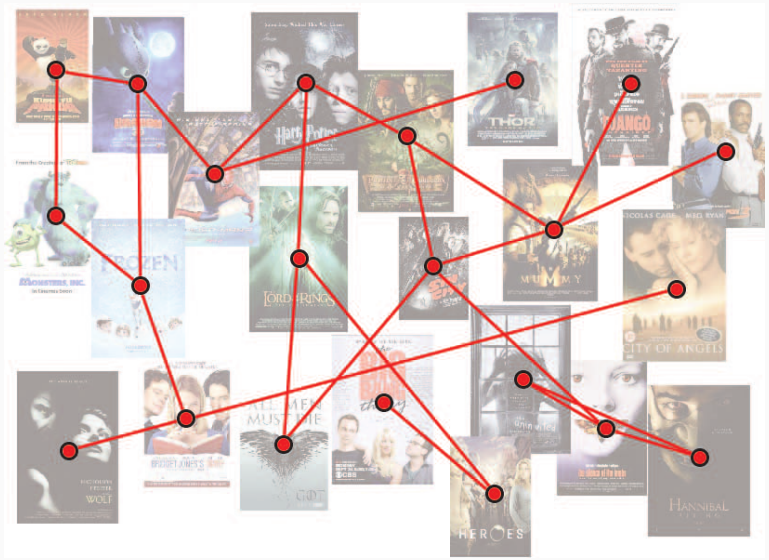


Credit: Michal Valko

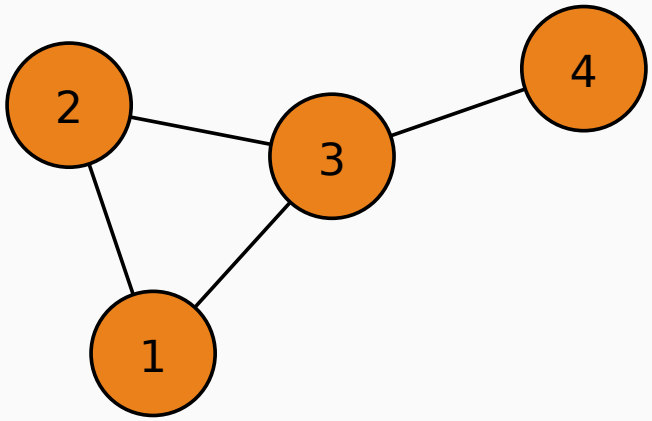
EXAMPLES OF RELEVANT TASKS

- Graph analysis (measuring networks)
  - Global study of connectivity and topology
  - Community detection
  - Identification of important (central) nodes
- Learning in graphs
  - Link prediction
  - Node classification
  - Graph embedding

BASIC GRAPH NOTIONS

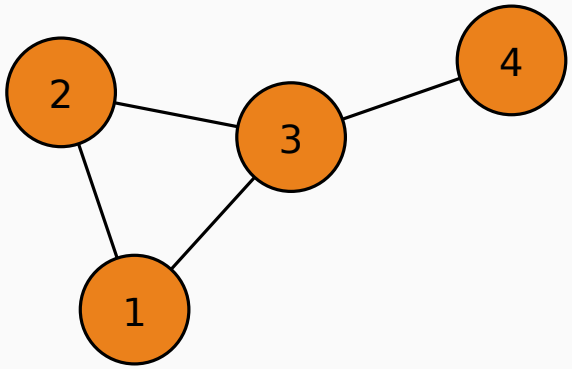
NOTATIONS

- A graph consists of a set of vertices (or nodes) and a set of edges
- More formally, a graph is denoted by $G = (V, E)$ where
  - $V = \{1, \ldots, n\}$ is the set of nodes
  - $E \subseteq V \times V$ is the set of edges
- An edge $(i, j) \in E$ links nodes i and j: we say they are adjacent or neighbors

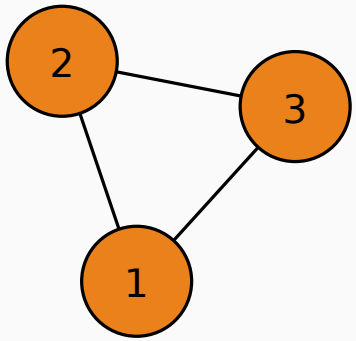


DEGREES

- The degree of a node is equal to its number of neighbors
- A graph is complete if there is an edge between every pair of vertices
- In a complete graph, all nodes thus have degree $n - 1$



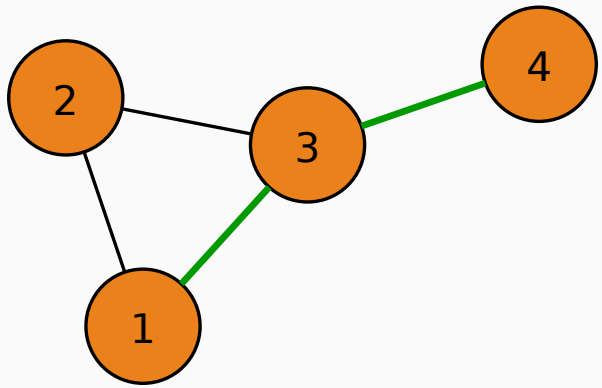
$d = [2, 2, 3, 1]$



$d = [2, 2, 2]$

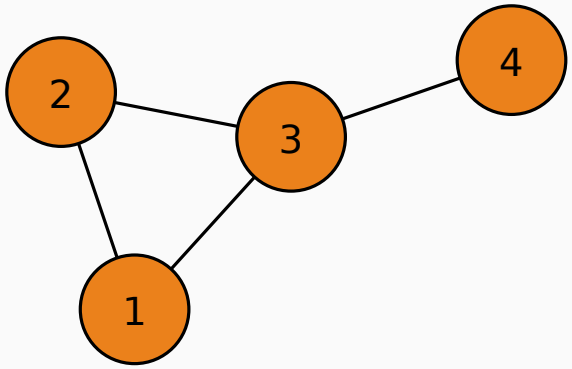
PATHS

- A path from node *i* to node *j* is a sequence of edges from *i* to *j*
- A cycle is a path that starts and ends at the same node
- The length of a path is the number of edges in the path
- A geodesic path is a shortest path between *i* and *j*
- The diameter of a graph is the length of the longest shortest path between any two nodes

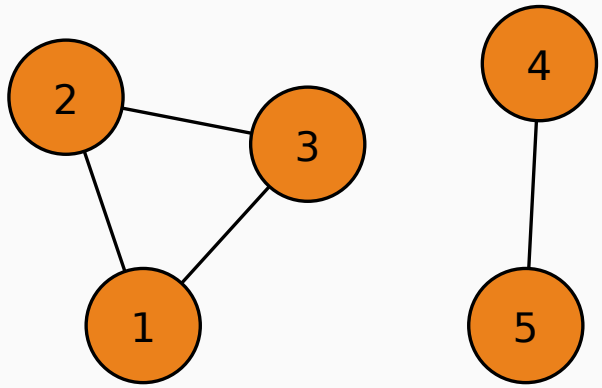


CONNECTIVITY

- All vertices which can be reached from each other by a path form a connected component
- A graph is connected if it has a single connected component



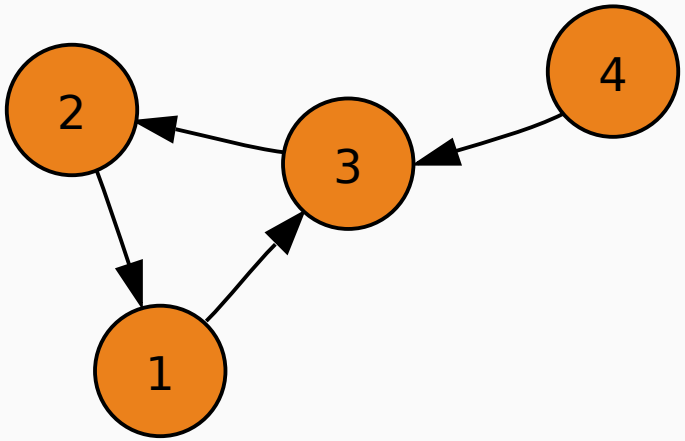
Connected graph



Graph with 2 connected components: $\{1, 2, 3\}$ and $\{4, 5\}$

DIRECTED GRAPH

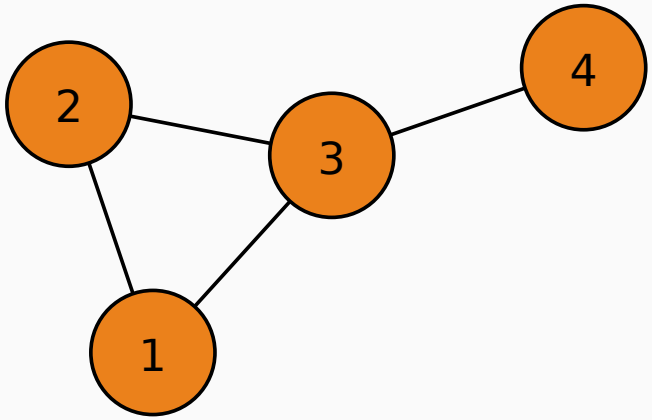
- Until now the graphs we considered were undirected
- In a directed graph, edges are ordered pairs
  - $(i, j) \in E$ points from i to j
  - In-degree of i: number of incoming edges to i
  - Out-degree of i: number of outgoing edges from i



$$d^{in} = [1, 1, 2, 0]^T$$
$$d^{out} = [1, 1, 1, 1]^T$$

COMPUTER REPRESENTATIONS

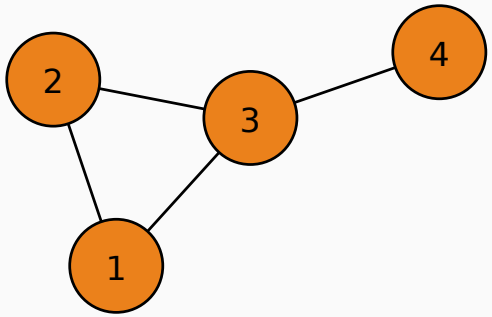
- Text representation: edge list



Corresponding file

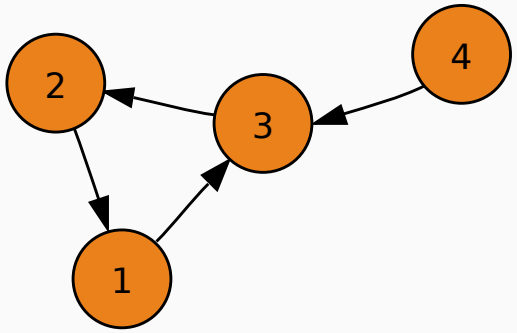
```
1 2
1 3
2 3
3 4
```

- Matrix representation: adjacency matrix $A \in \mathbb{R}^{n \times n}$
  - $A_{i,j} = 1$ if $(i, j) \in E$, else $A_{i,j} = 0$



$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

(symmetric)

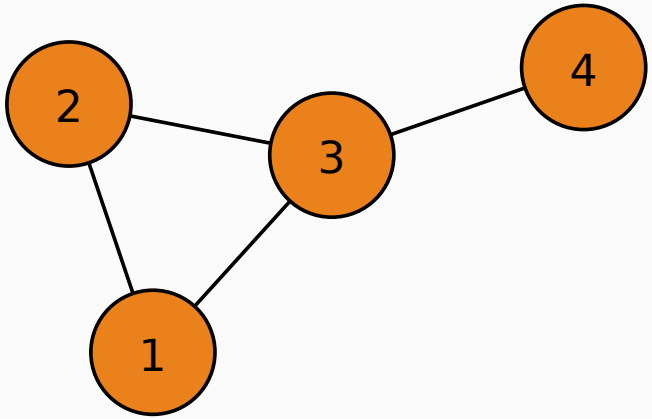


$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

(not symmetric)

COMPUTER REPRESENTATIONS

- Linked list representation: adjacency lists



Adjacency lists

```
1: 2 -> 3
2: 1 -> 3
3: 1 -> 2 -> 4
4: 3
```

- The best representation depends on available memory and algorithm of interest

RICHER GRAPHS

- Weighted edges (e.g., distance, similarity score)
- Labels on nodes and/or edges
- Feature vectors associated with nodes and/or edges
- ...

SOME CLASSIC GRAPH PROBLEMS AND ALGORITHMS

- Find shortest paths from a node to all others
  - Algorithm: Dijkstra
  - Time complexity (adjacency lists): $O(|E| + |V| \log(|V|))$
- Graph traversal (visit all nodes of the graph)
  - Algorithm: Depth-first search or breadth-first search
  - Time complexity: $O(|E| + |V|)$
  - Can be used to identify connected components
- Traveling Salesman Problem (TSP)
  - Algorithms: approximations and heuristics
  - Time complexity: NP-complete (exponential in graph size)
  - World TSP: `http://www.math.uwaterloo.ca/tsp/world/`

GRAPH ANALYSIS

FROM THE NETWORK TO INDIVIDUAL NODES

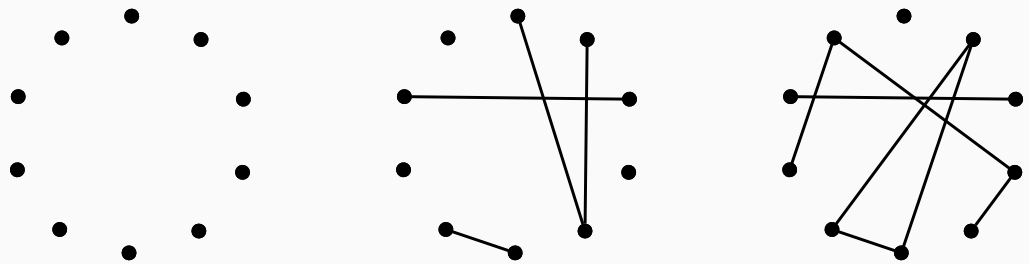
- We can analyze / measure the graph at different scales:
  - Global properties of the network
  - Communities (clusters of nodes)
  - Individual nodes
- In this part we will go from the global scale to the local scale

GLOBAL MEASURES OF NETWORKS

- Many descriptive measures are used to analyze the global properties of a network
  - Degree distribution
  - Clustering coefficient
  - “Small world” phenomena
  - ...
- We will illustrate some of them on two random graph models

ERDÖS–RÉNYI MODEL

- The Erdös–Rényi random graph model has two parameters
  - The number of nodes n
  - A probability $0 \leq p \leq 1$
- A random graph with n nodes is generated by drawing an edge between each pairs of nodes (i, j) independently with probability p
- This models graphs where nodes connect in a random and uniform way

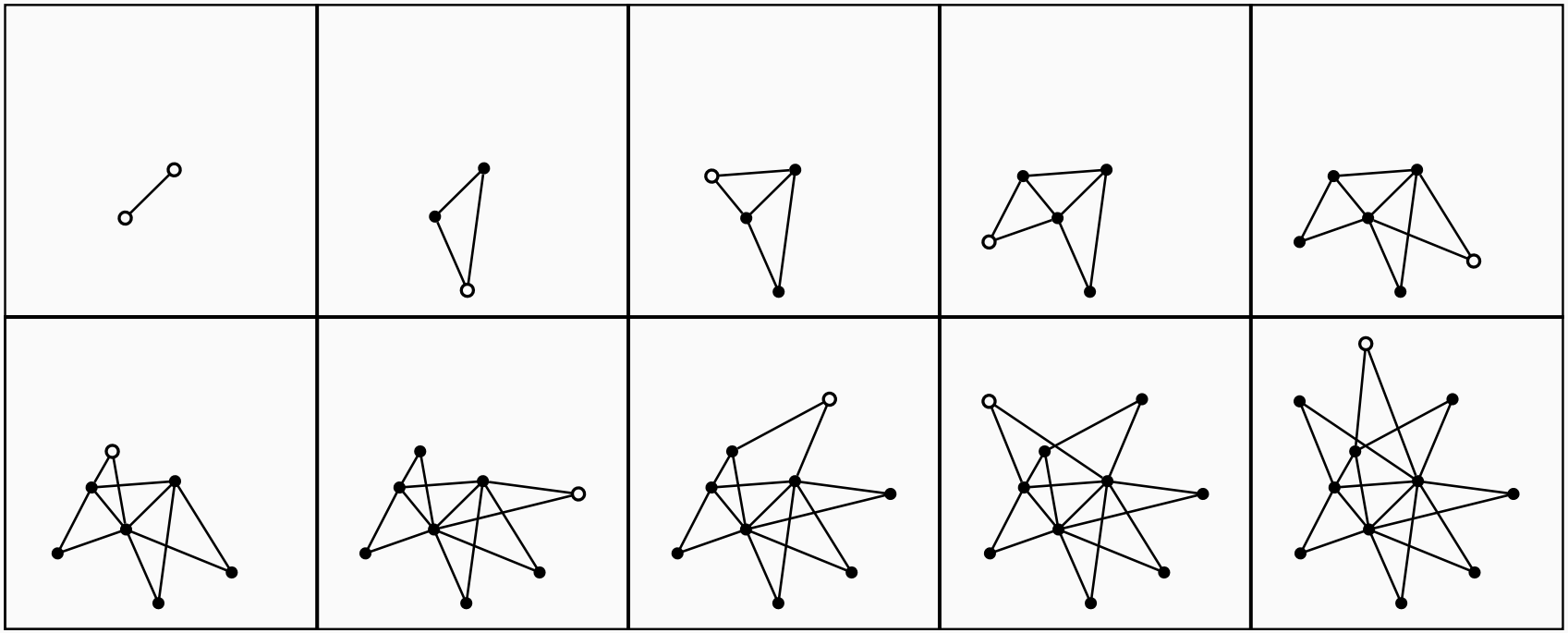


$p = 0$ $p = 0.1$ $p = 0.15$

BARABÁSI-ALBERT MODEL

- The Barabási-Albert random graph model has two parameters
  - An initial graph with n nodes
  - A probability $0 \leq p \leq 1$
- Nodes are added one at a time as follows
  1. With probability p, go to step 2, else go to step 3
  2. Connect new node to n existing nodes chosen uniformly at random
  3. Connect new node to n existing nodes with a probability proportional to their (in-)degree
- This models graphs with preferential attachment, often seen in real networks

BARABÁSI-ALBERT MODEL



DEGREE DISTRIBUTIONS

- Let p_k be the probability that a randomly selected node has degree k
- **Erdös–Rényi**: distribution of degree of a vertex is binomial

$$p_k = \binom{n-1}{k} p^k (1-p)^{n-1-k}$$

  - Highly concentrated around the mean
  - Probability of high degree nodes decreases exponentially fast

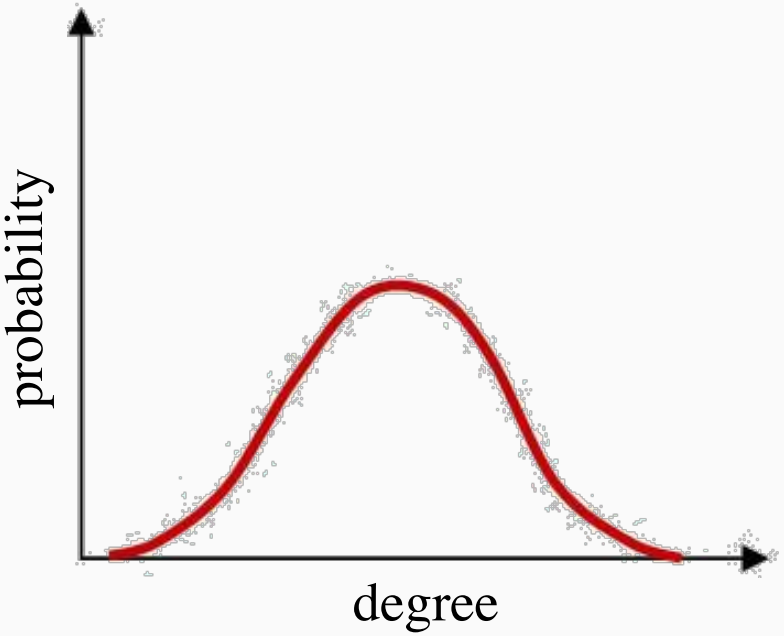
- **Barabási-Albert**: degree distribution follows a power law

$$p_k \propto k^{-\alpha}$$

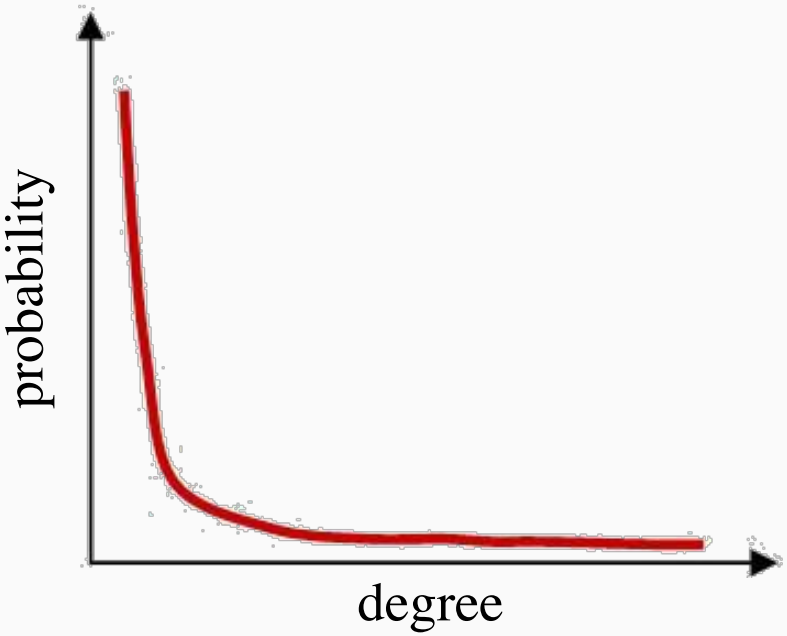
  - Heavy-tailed distribution: non-negligible fraction of high degree
  - Scale-free: average degree is not informative

DEGREE DISTRIBUTIONS

Erdös–Rényi

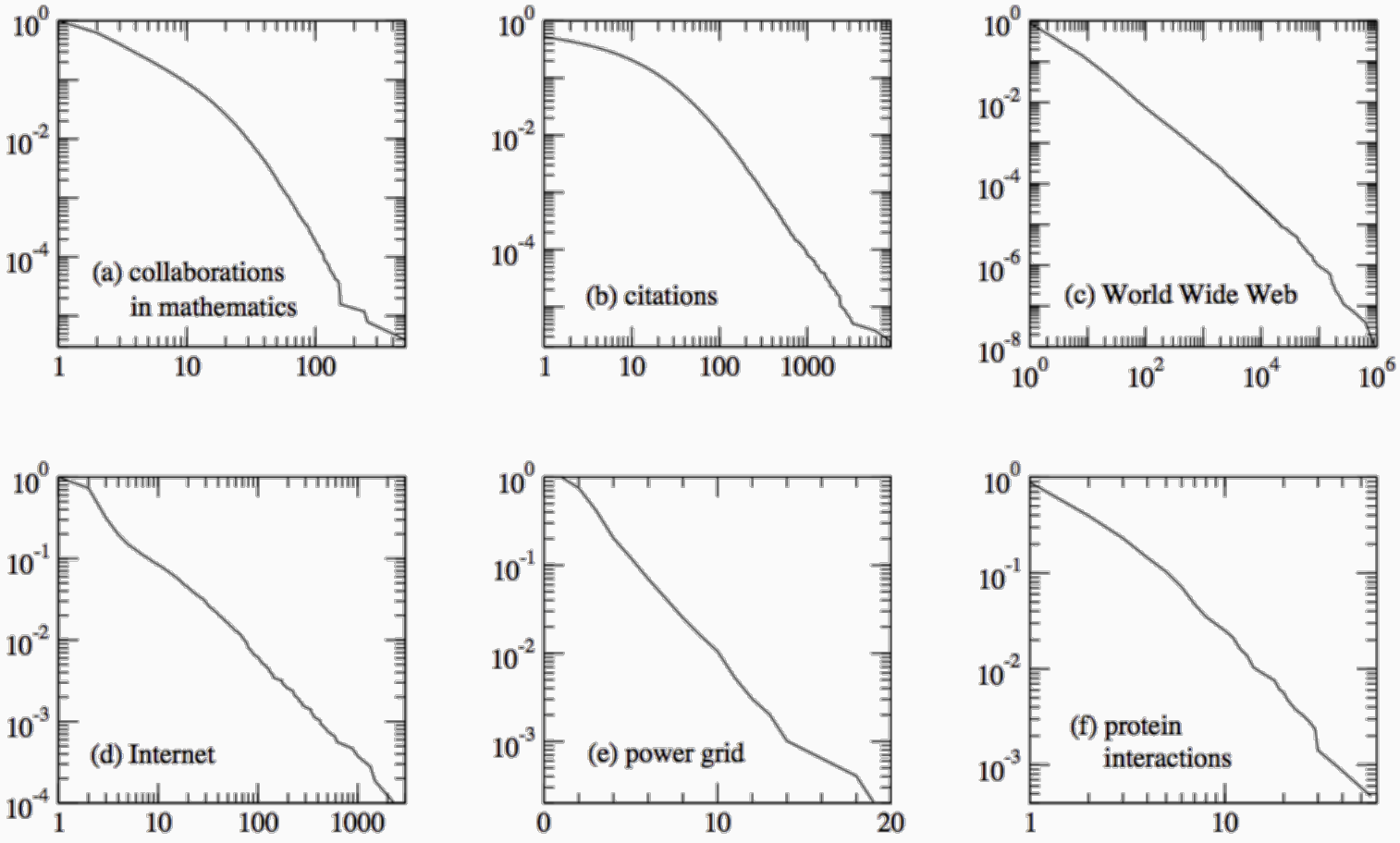


Barabási-Albert



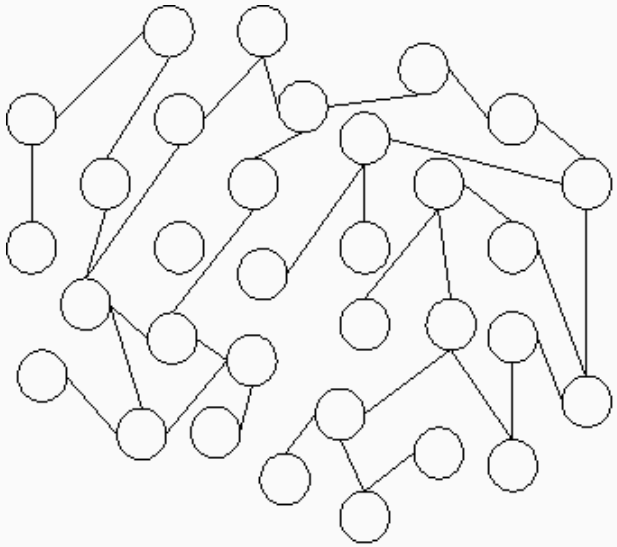
DEGREE DISTRIBUTIONS

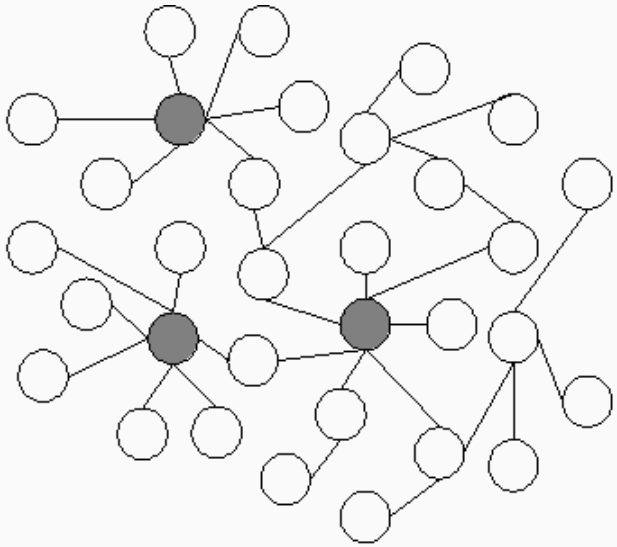
- Power law distributions give roughly a line in the log-log plot
- Many real networks have power law degree distributions



DEGREE DISTRIBUTIONS

- Which graph is uniformly random and which one is scale-free ?





MAXIMUM AND AVERAGE DEGREE

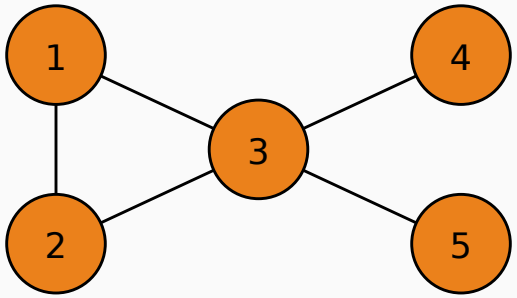
- Erdös–Rényi graphs
  - Average degree is np (in expectation)
  - Maximum degree highly concentrated around average degree
- For power law graphs (Barabási-Albert)
  - Average degree is a constant if $\alpha \geq 2$ (diverges if $\alpha < 2$)
  - Maximum degree is $O\left(n^{\frac{1}{\alpha-1}}\right)$

CLUSTERING COEFFICIENT

- A measure of how well nodes tend to cluster together
- The local clustering coefficient quantifies how close a node i and its neighbors are to being a complete graph

$$C_i = \frac{\text{triangles centered at node } i}{\text{triples centered at node } i}$$

- The global clustering coefficient $CC = \frac{1}{n}\sum_{i=1}^{n} C_i$ measures the density of triangles (local clusters) in the graph



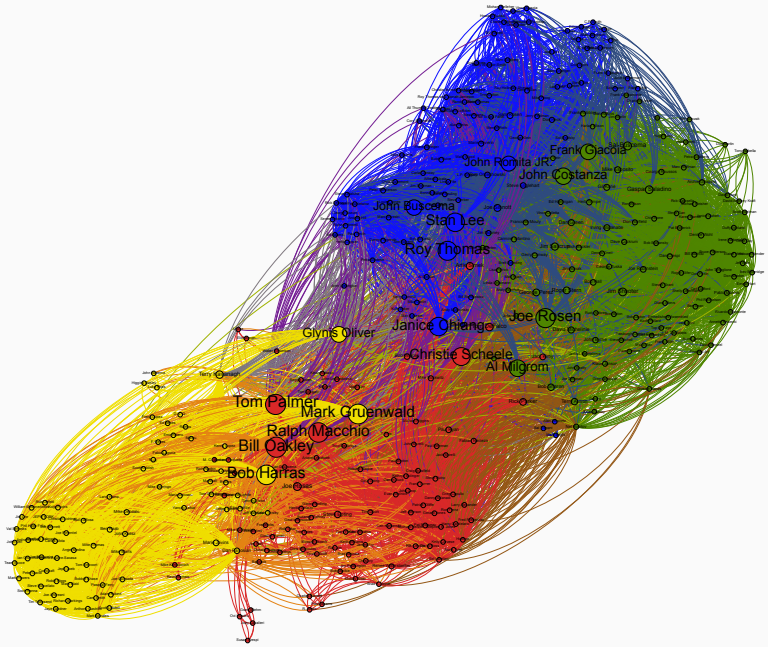
$$CC = \frac{1}{5}\left(1 + 1 + \frac{1}{6} + 0 + 0\right) = \frac{13}{30}$$

CLUSTERING COEFFICIENT

- For Erdös–Rényi random graphs, $\mathbb{E}[CC] = C_i = p$
  - Probability of two of your neighbors to also be neighbors is p, independently of the local structure
- For Barabási-Albert random graphs
  - CC approximately follows a power law in the number of nodes
  - Let $C(k)$ be the average clustering coefficient of nodes with degree k, then $C(k) \propto k^{-1}$ for Barabási-Albert
- More generally, a power law distribution for $C(k)$ indicates a hierarchical structure
  - Nodes with low degree are connected to other nodes in their community
  - Nodes with high degrees are linked to nodes in different communities

SMALL WORLD PHENOMENON

- Originates from Milgram's small world experiment in the 60's
- How to measure the small world phenomenon?
  - Average length of shortest paths
  - Diameter of the graph (longest shortest path)
  - Length distribution of all shortest paths
  - High clustering coefficient



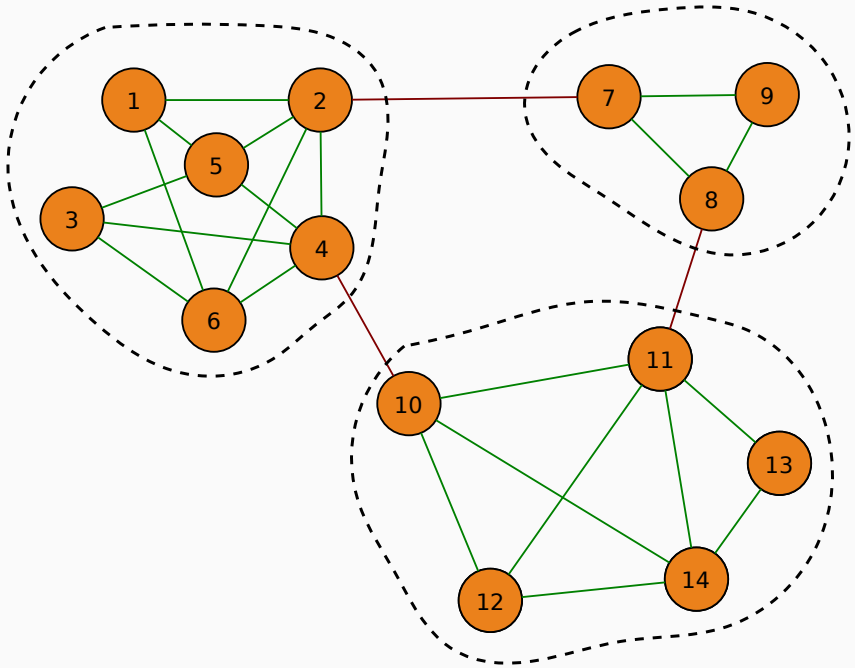
Marvel Comic Book Artist Collaboration Network from `http://allthingsgraphed.com`

COMMUNITY DETECTION

- We seek to partition the nodes of the graph into a set of groups (clusters) according to a certain quality criterion
- Applications: identify
  - social communities
  - clients with similar behavior
  - web pages about the same topic
  - proteins with strong interactions with each other
  - products frequently bought together
  - ...

WHAT IS A GOOD COMMUNITY?

- No universal definition: depends on the application and the network of interest
- General idea: a community is a set of nodes densely connected internally and/or sparsely connected externally



General approach to community detection

1. Define a quality criterion reflecting the desired properties of the communities
    - Many existing criteria (see next slide)
2. Design an algorithm to find the community optimizing the criterion
    - This is generally NP-difficult: for graphs with more than a few hundred nodes, only approximate solutions can be guaranteed

SOME QUALITY CRITERIA

Notations

n: number of nodes in the graph
m: number of edges in the graph
$S \subseteq V$: nodes in the community
n_S: number of nodes in S
m_S: number of edges in S
o_S: number of edges between S and $V \setminus S$

- Based on internal connections:
  - Internal density of edges: $\frac{m_S}{n_S(n_S-1)/2}$
  - Average internal degree: $\frac{2m_S}{n_S}$
- Based on external connections:
  - Expansion: $\frac{o_S}{n_S}$
  - Ratio cut: $\frac{o_S}{n_S(n-n_S)}$

SOME QUALITY CRITERIA

Notations

n: number of nodes in the graph
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$S \subseteq V$: nodes in the community
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m_S: number of edges in S
o_S: number of edges between S and $V \setminus S$

- Based on both internal and external connections:
  - Conductance: $\frac{o_S}{2m_S+o_S}$
  - Normalized cut: $\frac{o_S}{2m_S+o_S} + \frac{o_S}{2(m-m_S)+o_S}$
  - Modularity: $\frac{1}{4}(m_S - \mathbb{E}[m_S])$

ZOOM ON MODULARITY

- The expectation $\mathbb{E}[m_S]$ is computed with respect to a random process which preserves the degree of each node
  - Each edge is split into two parts (one on each node)
  - Each part is combined to another randomly
- Modularity is then equal to:

$$\frac{1}{2m} \sum_{i,j \in V} \left(A_{ij} - \frac{d_i d_j}{2m} \right) \mathbb{I}\{c_i = c_j\}$$

- Finding the communities maximizing the modularity requires to consider an exponential number of groups $\rightarrow$ very costly even for graphs with a few hundred nodes

LOUVAIN METHOD

- At the beginning, each node has its own community
- The algorithm alternates between two phases until convergence:

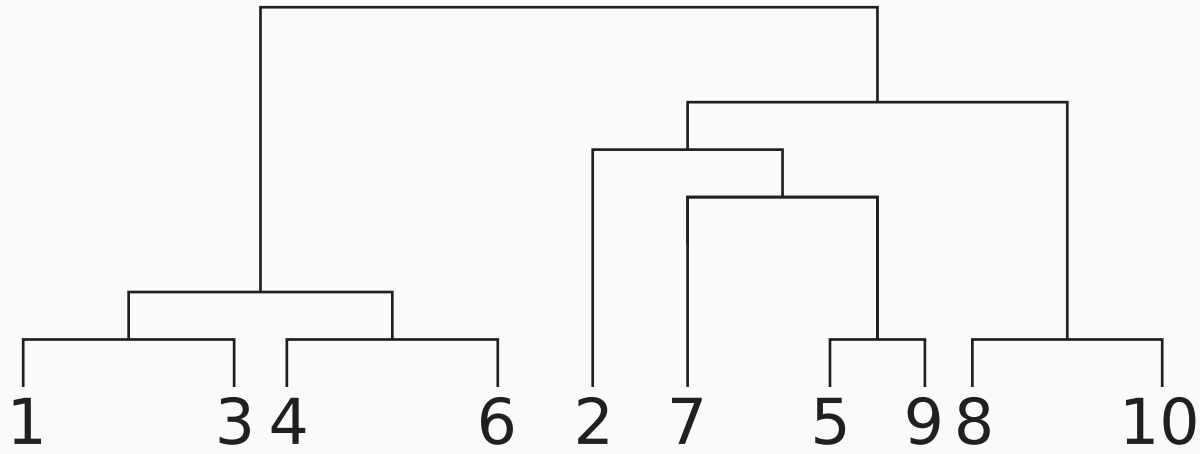
    1. **Optimize local modularity**
       For each node, we create a new community with the neighboring node maximizing the modularity. If no modularity improvement is possible, we keep the node alone.

    2. **Create a new weighted graph**
       The communities of phase 1 become the nodes of the graph. We create a self-loop on each community node weighted by the number of links within the community, and a link between pairs of communities weighted by the number of links between these communities.

- We obtain an approximate solution (no theoretical guarantee but good practical performance)

OTHER APPROACH: HIERARCHICAL CLUSTERING

- It is often relevant to analyze the community structure at different scales (cluster sizes)
- Goal: construct a hierarchy of clusters (represented as a dendrogram)



Hierarchical clustering: bottom-up approach

- In the bottom-up approach, we start with a cluster for each node (as in Louvain method)
- Greedy algorithm: at each iteration, we merge the two "closest" clusters
- We thus need to define a notion of dissimilarity between nodes and between sets of nodes

HIERARCHICAL CLUSTERING: DISTANCES

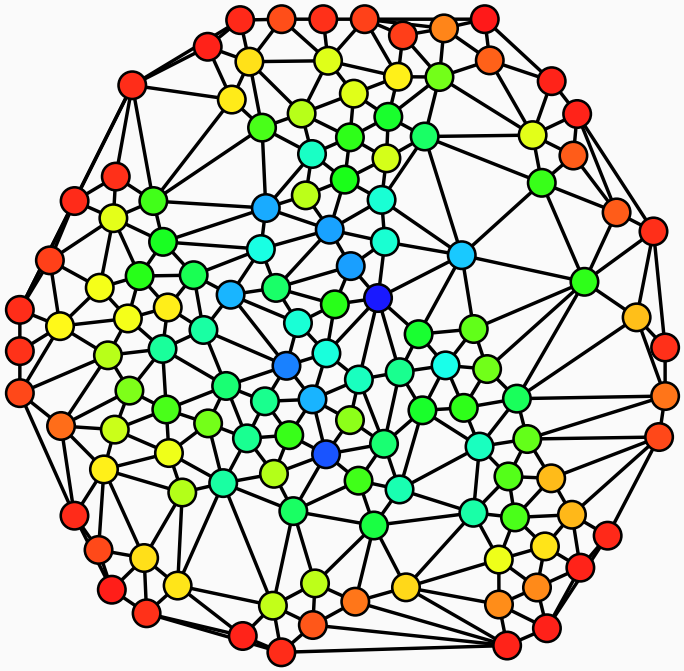
- A natural distance function $d(i, j)$ between 2 nodes i and j is the length of the shortest path between i and j
- Some popular dissimilarity measures between two clusters C_1 and C_2 (linkage criterion):
  - Minimum linkage: $D(C_1, C_2) = \min_{i \in C_1, j \in C_2} d(i, j)$
  - Maximum linkage: $D(C_1, C_2) = \max_{i \in C_1, j \in C_2} d(i, j)$
  - Average linkage: $D(C_1, C_2) = \frac{1}{|C_1||C_2|} \sum_{i \in C_1, j \in C_2} d(i, j)$
  - Centroid linkage: $D(C_1, C_2) = d(G_1, G_2)$ where G_1 and G_2 are the"centers" of C_1 and C_2

IDENTIFY CENTRAL NODES

- Goal: rank the nodes of the graph according to a centrality measure (importance)
- Applications: identify
  - influencers in a social network
  - important (“hub”) web pages
  - bottlenecks in transportation networks
  - products relevant for “loss leader” pricing strategies
  - ...

HOW TO DEFINE CENTRALITY ?

- Again, no universal definition
- Yet, a central notion: walks in graphs
  - A walk is a path which can go through the same node several times
  - Centrality measures vary with the type of walk considered and the way of counting them (number or length)



POPULAR CENTRALITY MEASURES

- Degree centrality: $C(x_i) = d_i$
  - Interpretation: number of walks of length 1 ending at node i
- Eigenvector centrality: $C(x_i) = v_i = \frac{1}{\lambda} \sum_{j=1}^{n} A_{ij} C(x_j)$
  - $\boldsymbol{v}$ satisfies $\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v}$ where λ is the largest eigenvalue of $\boldsymbol{A}$
  - Interpretation: number of walks of infinite length ending at node i
  - More importance given to nodes with well-connected neighbors
  - Google PageRank is a variant of eigenvector centrality

POPULAR CENTRALITY MEASURES

- Closeness centrality: $C(x_i) = \frac{1}{\sum_{j \neq i} d(i,j)}$
  - $d(i,j)$: length of shortest path between nodes i and j
  - Interpretation: inversely proportional to the sum of lengths of the shortest paths to other nodes
- Betweenness centrality: $C(x_i) = \sum_{j \neq i \neq k} \frac{\sigma_{jk}(i)}{\sigma_{jk}}$
  - σ_{jk}: number of shortest paths between j and k
  - $\sigma_{jk}(i)$: number of shortest paths between j and k going through i
  - Interpretation: number of times the node acts as a "bridge" between two nodes

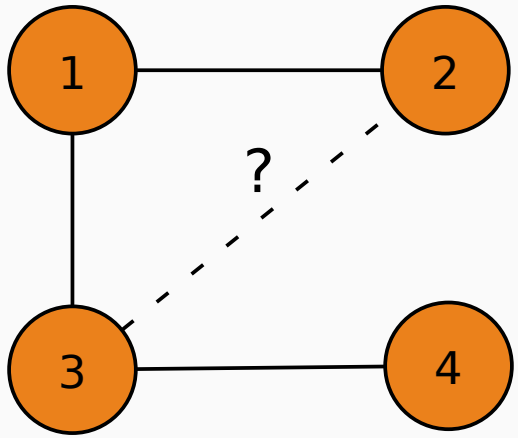
LEARNING IN GRAPHS

LEARNING IN GRAPHS

- So far we have focused on analyzing an observed graph
  - Global properties
  - Communities
  - Node centrality
- In this part we will learn from the observed graph to make predictions
- We will consider two tasks: link prediction and node labeling

LINK PREDICTION

- **Goal**: given a graph G, predict new edges
- These new edges can represent probable future interactions
  - E.g., two persons likely to become friend on Facebook
- They can also be missing edges (partially observed graph)
  - E.g., only a subset of protein-protein interactions are known
  - E.g., not all product combinations have been tried (to see whether they sell well together)



LINK PREDICTION: STANDARD APPROACH

- Use a similarity measure between pairs of nodes to rank potential edges
- Top-ranking edges are the more likely to be correct
- We can thus predict the top-k edges, or use a threshold
- This graph-based strategy can be easily combined with a content-based approach (when data is attached to nodes)

LINK PREDICTION: SIMILARITY SCORES

Notation

$\mathcal{N}(i)$: set of neighbors of node i

- Common neighbors: $S(i,j) = |\mathcal{N}(i) \cap \mathcal{N}(j)|$
- Jaccard coefficient: $S(i,j) = \frac{|\mathcal{N}(i) \cap \mathcal{N}(j)|}{|\mathcal{N}(i) \cup \mathcal{N}(j)|}$
  - Normalized version of common neighbors
- Adamic-Adar index: $S(i,j) = \sum_{k \in \mathcal{N}(i) \cap \mathcal{N}(j)} \frac{1}{\log |\mathcal{N}(k)|}$
  - More weight given to common neighbors of low degree
- Preferential attachment: $S(i,j) = |\mathcal{N}(i)| \cdot |\mathcal{N}(j)|$

LINK PREDICTION: SIMILARITY SCORES

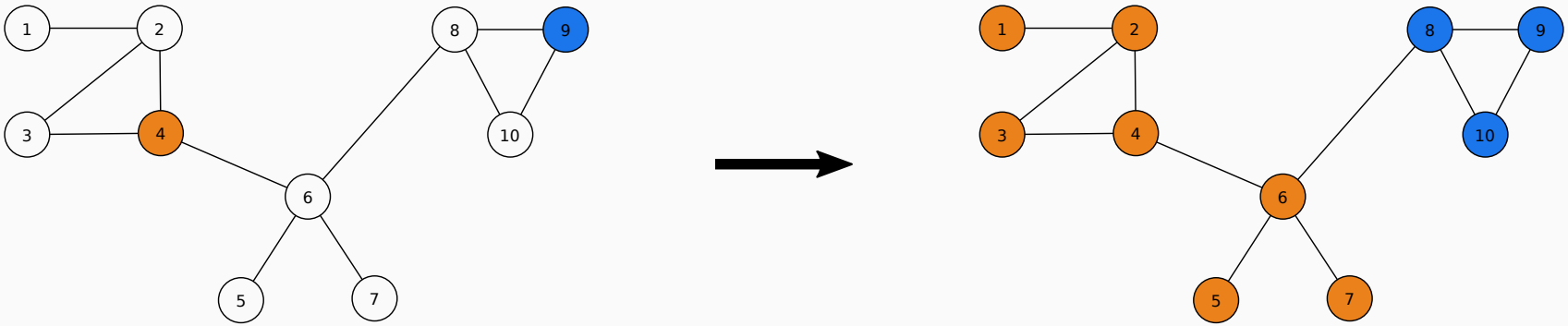
- Some similarity scores also use the community information when available
  - More weight given to neighbors from the same community
- Additional data attached to nodes can be easily integrated as part of the score
  - E.g., cosine similarity between node feature vectors
  - E.g., classifier trained to predict the presence of an edge from data at two nodes

LINK PREDICTION: EVALUATION

- How to evaluate the accuracy in link prediction and perform model selection?
- Practical approach: hide a subset of node pairs and predict based on the rest of the graph
- Performance measures:
  - Proportion correct predictions
  - Area under the ROC Curve (AUC): probability that an existing edge picked at random is ranked higher than a non-existing edge picked at random

NODE LABELING

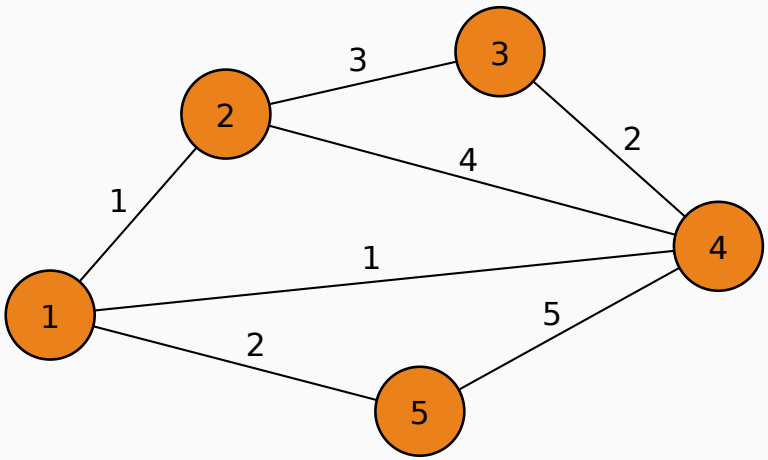
- **Goal**: given a graph where some nodes are labeled, predict missing node labels
- This is a semi-supervised learning problem
- **Central assumption**: correct labels are smooth on the graph
  - Classification: two neighbors tend to have the same label
  - Regression: two neighbors tend to have similar target values



GRAPH LAPLACIAN MATRIX

- For a graph $G = (V, E)$ we denote by

A	adjacency matrix
W	weight matrix
D	(diagonal) degree matrix
$L = D - W$	Laplacian matrix (symmetric)



$$L = \begin{pmatrix} 4 & -1 & 0 & -1 & -2 \\ -1 & 8 & -3 & -4 & 0 \\ 0 & -3 & 5 & -2 & 0 \\ -1 & -4 & -2 & 12 & -5 \\ -2 & 0 & 0 & -5 & 7 \end{pmatrix}$$

REFRESHER ON EIGENVECTORS AND EIGENVALUES

- Let $\boldsymbol{L} \in \mathbb{R}^{n \times n}$ symmetric matrix
- A vector $\boldsymbol{v} \in \mathbb{R}^n$ is an eigenvector of $\boldsymbol{L}$ of eigenvalue $\lambda \in \mathbb{R}$ if

$$\boldsymbol{L}\boldsymbol{v} = \lambda \boldsymbol{v}$$

- If $(\lambda_1, \boldsymbol{v}_1)$, $(\lambda_2, \boldsymbol{v}_2)$ are eigenpairs for $\boldsymbol{L}$ with $\lambda_1 \neq \lambda_2$ then $\boldsymbol{v}_1 \perp \boldsymbol{v}_2$, i.e., $\boldsymbol{v}_1^T \boldsymbol{v}_2 = 0$
- If $(\lambda, \boldsymbol{v}_1)$, $(\lambda, \boldsymbol{v}_2)$ are eigenpairs for $\boldsymbol{L}$, then $(\lambda, \boldsymbol{v}_1 + \boldsymbol{v}_2)$ is also en eigenpair
- The multiplicity of eigenvalue λ is the dimension of the space of eigenvectors corresponding to λ
- $\boldsymbol{L}$ has n eigenvalues (counting possible multiplicities)

- $\boldsymbol{L}$ is symmetric positive semi-definite (PSD) since for any $\boldsymbol{f} \in \mathbb{R}^n$

$$\begin{aligned}
\boldsymbol{f}^T \boldsymbol{L} \boldsymbol{f} &= \boldsymbol{f}^T \boldsymbol{D} \boldsymbol{f} - \boldsymbol{f}^T \boldsymbol{W} \boldsymbol{f} \\
&= \sum_i d_i f_i^2 - \sum_i \sum_j w_{i,j} f_i f_j = \sum_i \sum_j w_{i,j} f_i^2 - \sum_i \sum_j w_{i,j} f_i f_j \\
&= \frac{1}{2} \left(\sum_i \sum_j w_{i,j} f_i^2 - 2 \sum_i \sum_j w_{i,j} f_i f_j + \sum_i \sum_j w_{i,j} f_i^2 \right) \\
&= \frac{1}{2} \sum_i \sum_j w_{i,j} (f_i - f_j)^2 \geq 0
\end{aligned}$$

- Since $\boldsymbol{L}$ is PSD, its eigenvalues satisfy $0 \leq \lambda_1 \leq \cdots \leq \lambda_n$
- We can easily see that $(0, \mathbf{1}_n)$ is an eigenpair for $\boldsymbol{L}$

Theorem

The multiplicity of eigenvalue 0 *of* $\boldsymbol{L}$ *is equal to the number of connected components of the graph. The eigenspace of* 0 *is spanned by the components' indicators.*

Proof.

If $(0, \boldsymbol{f})$ is an eigenpair, then $0 = \frac{1}{2}\sum_{i,j} w_{i,j}(f_i - f_j)^2$, hence $\boldsymbol{f}$ is constant on each connected component. If there are k connected components, $\boldsymbol{L}$ is k-block-diagonal:

$$\boldsymbol{L} = \begin{bmatrix} \boldsymbol{L}_1 & & & \\ & \boldsymbol{L}_2 & & \\ & & \ddots & \\ & & & \boldsymbol{L}_k \end{bmatrix}$$

The spectrum of block-diagonal matrices is the union of the spectra of $\boldsymbol{L}_i$ (padded with zeros). The theorem follows from the fact that for $i = 1, \ldots, k$, $(0, \mathbf{1}_{|V_i|})$ is an eigenpair for $\boldsymbol{L}_i$, where V_i is the set of nodes in the i^{th} connected component. □

SMOOTHNESS OF A GRAPH FUNCTION

- A graph function is a vector $\boldsymbol{f} \in \mathbb{R}^n$ assigning values to nodes

$$\boldsymbol{f} : V \to \mathbb{R}$$

- The smoothness of a graph function is given by the quadratic form of the Laplacian

$$S_G(\boldsymbol{f}) = \boldsymbol{f}^T \boldsymbol{L} \boldsymbol{f} = \frac{1}{2} \sum_{i,j} w_{i,j} (f_i - f_j)^2$$

- When $S_G(\boldsymbol{f})$ is small, $\boldsymbol{f}$ does not vary much in high density regions of the graph

SYMMETRIC NORMALIZED LAPLACIAN

- We can also consider a symmetric normalized Laplacian matrix

$$L_{sym} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}$$

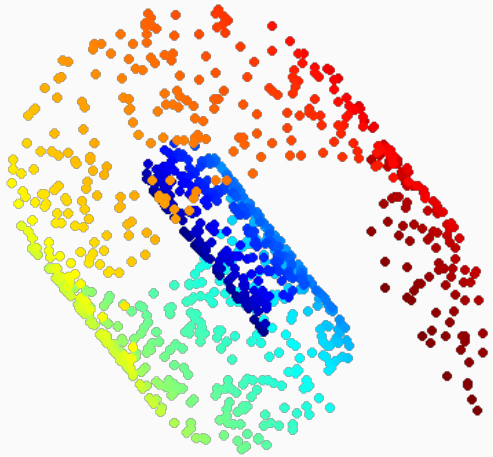
- Normalized variant of smoothness

$$f^T L_{sym} f = \frac{1}{2} \sum_{i,j} w_{i,j} \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \right)^2$$

- L_{sym} is also PSD, and $(0, D^{1/2} \mathbf{1}_n)$ is an eigenpair for L_{sym}

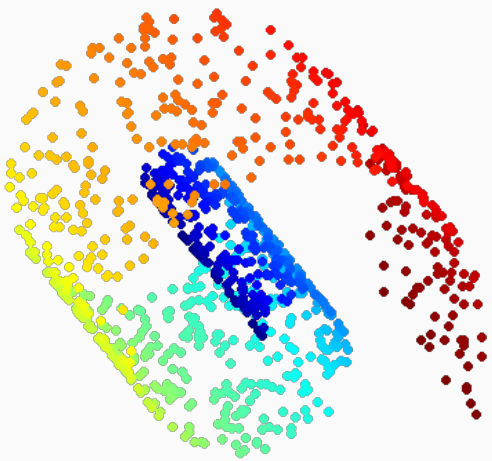
BEYOND EXPLICIT GRAPHS: DATA ON A MANIFOLD

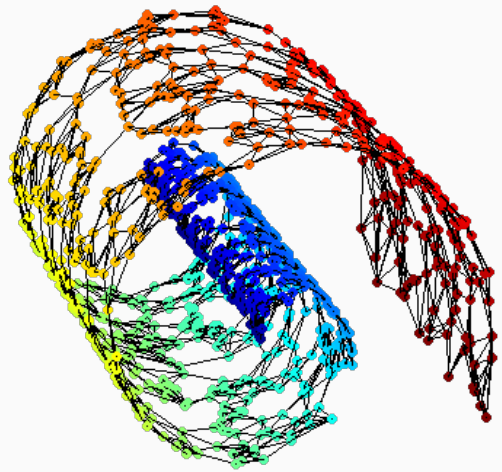
- There is a natural link between discrete representations (graphs) and continuous representations
- Metric space: distances between all points in the space are defined (e.g., Euclidean space)
- Manifold: every point has a neighborhood which is homeomorphic to the Euclidean space
  - Locally Euclidean (distance in small region is meaningful)
  - Global structure more complex (Euclidean distance between "distant" points is meaningless)



SIMILARITY GRAPHS AND MANIFOLD STRUCTURE

- Let $x_1, \ldots, x_n$ be a set of data points with similarity matrix S
  - $S_{i,j} \geq 0$: similarity score between x_i and x_j
  - Can use standard / handcrafted / learned similarity measure
- Similarity graph: $(x_i, x_j) \in E$ if $S_{i,j}$ large enough
- Such a graph can approximate the manifold structure!
- For this to work we must enforce locality (sparsify the graph)

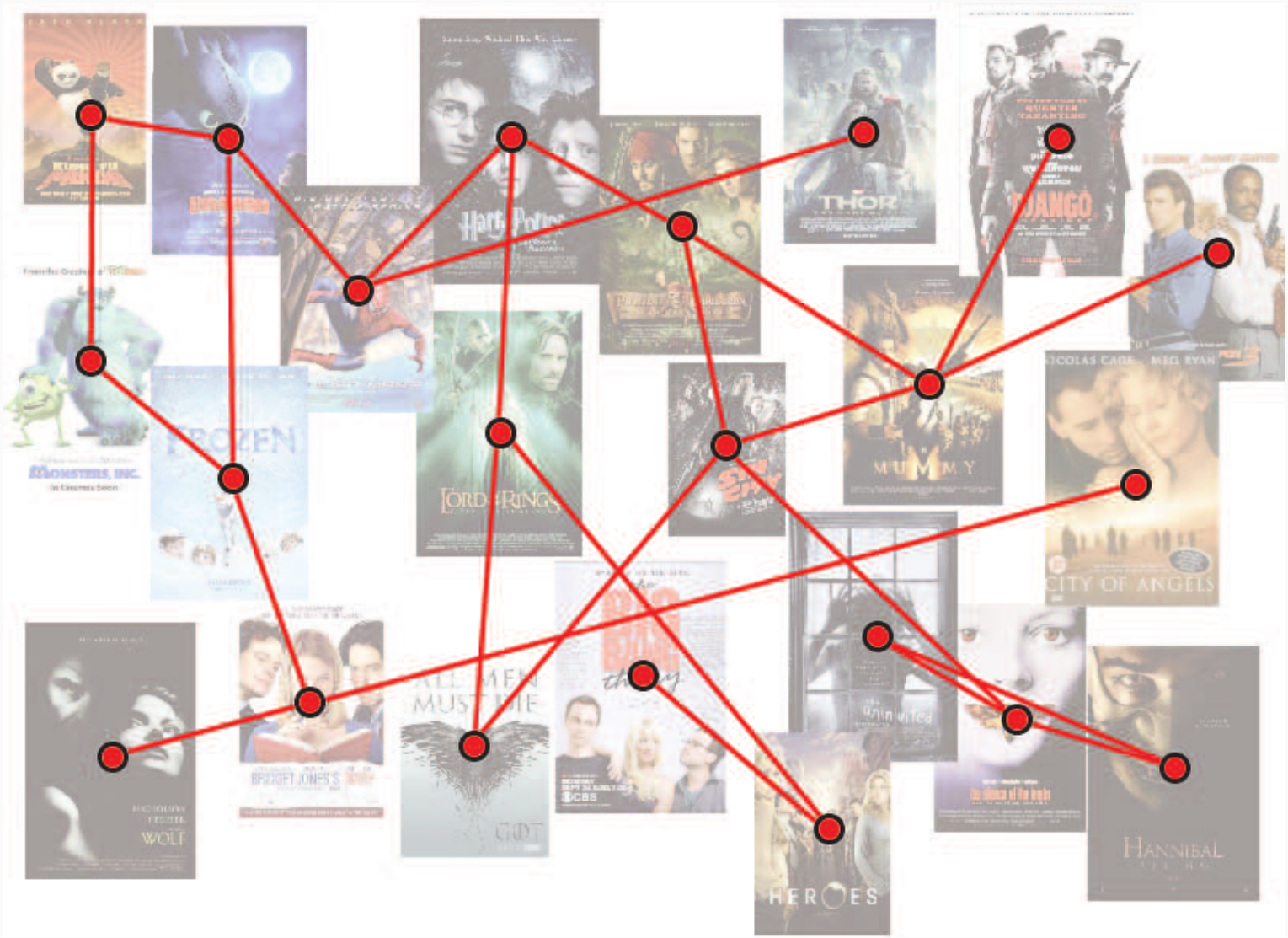




SPARSIFICATION OF SIMILARITY GRAPHS

- k-nearest neighbor graph
  - Connect i and j if x_i is among the k-nearest neighbors of v_j and/or x_j is among the k-nearest neighbors of v_i
- ϵ-neighborhood graph
  - Connect i and j if $S_{i,j}$ is larger than ϵ
- Exponential graph
  - Weight each edge $(i, j) \in V^2$ by $S_{i,j}$
  - Must use with fast-decaying similarity to enforce locality
  - Typical choice is the Gaussian kernel $S_{i,j} = \exp(-\gamma \|x_i - x_j\|^2)$
- Some issues
  - Little theoretical underpinning to guide graph construction
  - Must tune k, ϵ or γ to adjust locality
  - For efficiency reasons, we like to deal with sparse graphs

EXAMPLE: MOVIE SIMILARITY GRAPH



MANIFOLD REGULARIZATION

- Assume data lies on a nonlinear manifold $\mathcal{M} \subset \mathcal{X}$
- We want to learn a function $f : \mathcal{M} \to \mathbb{R}$ which varies smoothly in dense regions
- Natural choice is to enforce small gradient along $\mathcal{M}$ where the marginal probability density is large

$$\|f\|_I^2 = \int_{x \in \mathcal{M}} \|\nabla_{\mathcal{M}} f(x)\|^2 P(x) dx$$

- $P(x)$ is unknown but we can approximate it using n labeled/unlabeled points [Belkin et al., 2006]

$$\|f\|_I^2 \approx \frac{1}{n^2} \boldsymbol{f}^T \boldsymbol{L} \boldsymbol{f} = \frac{1}{2} \sum_{i,j} w_{i,j} (f_i - f_j)^2$$

under some conditions (appropriately scaled exponential graph)

MANIFOLD REGULARIZATION

- **Manifold regularization**: use the quadratic form of the Laplacian as regularizer for machine learning models
- Generic way to make use of unlabeled data in supervised learning algorithms $\rightarrow$ semi-supervised learning
- Smoothness assumption becomes the manifold assumption: points connected via a path through high density regions on the data manifold are likely to have a similar label
- Many successful algorithms: Laplacian eigenmaps, Laplacian SVMs, label propagation, online node labeling...

SEMI-SUPERVISED LABEL PROPAGATION: NOTATIONS

- Let $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_l, \boldsymbol{x}_{l+1}, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$
- We have labels $y_1, \ldots, y_l \in \{1, \ldots, C\}$ for the first l points
- Build exponential graph with $W_{i,j} = \exp(-\gamma \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2)$
- Define initial label matrix $\boldsymbol{Y} \in \mathbb{R}^{n \times C}$ such that

$$Y_{i,j} = \begin{cases} 1 & \text{if } \boldsymbol{x}_i \text{ has label } y_i = j \\ 0 & \text{otherwise} \end{cases}$$

- The algorithm will generate a prediction matrix $\boldsymbol{F} \in \mathbb{R}^{n \times C}$ from which we will predict the label of a node i using

$$\hat{y}_i = \arg\max_j F_{i,j}$$

SEMI-SUPERVISED LABEL PROPAGATION: FORMULATION

- The prediction matrix $\boldsymbol{F} \in \mathbb{R}^{n \times C}$ is the one minimizing the following objective function [Zhou et al., 2003]

$$\min_{\boldsymbol{F} \in \mathbb{R}^{n \times c}} \quad \frac{1}{2} \left(\underbrace{\sum_{i,j=1} w_{i,j} \left\| \frac{\boldsymbol{F}_i}{\sqrt{d_i}} - \frac{\boldsymbol{F}_j}{\sqrt{d_j}} \right\|^2}_{\text{smoothness term}} + \mu \underbrace{\sum_{i=1}^{n} \|\boldsymbol{F}_i - \boldsymbol{Y}_i\|^2}_{\text{fit known labels}} \right)$$

- Trade-off between two terms (ruled by $\mu \geq 0$)
  - Smoothing predictions with normalized Laplacian
  - Keeping accurate predictions for labeled points

SEMI-SUPERVISED LABEL PROPAGATION: SOLUTION

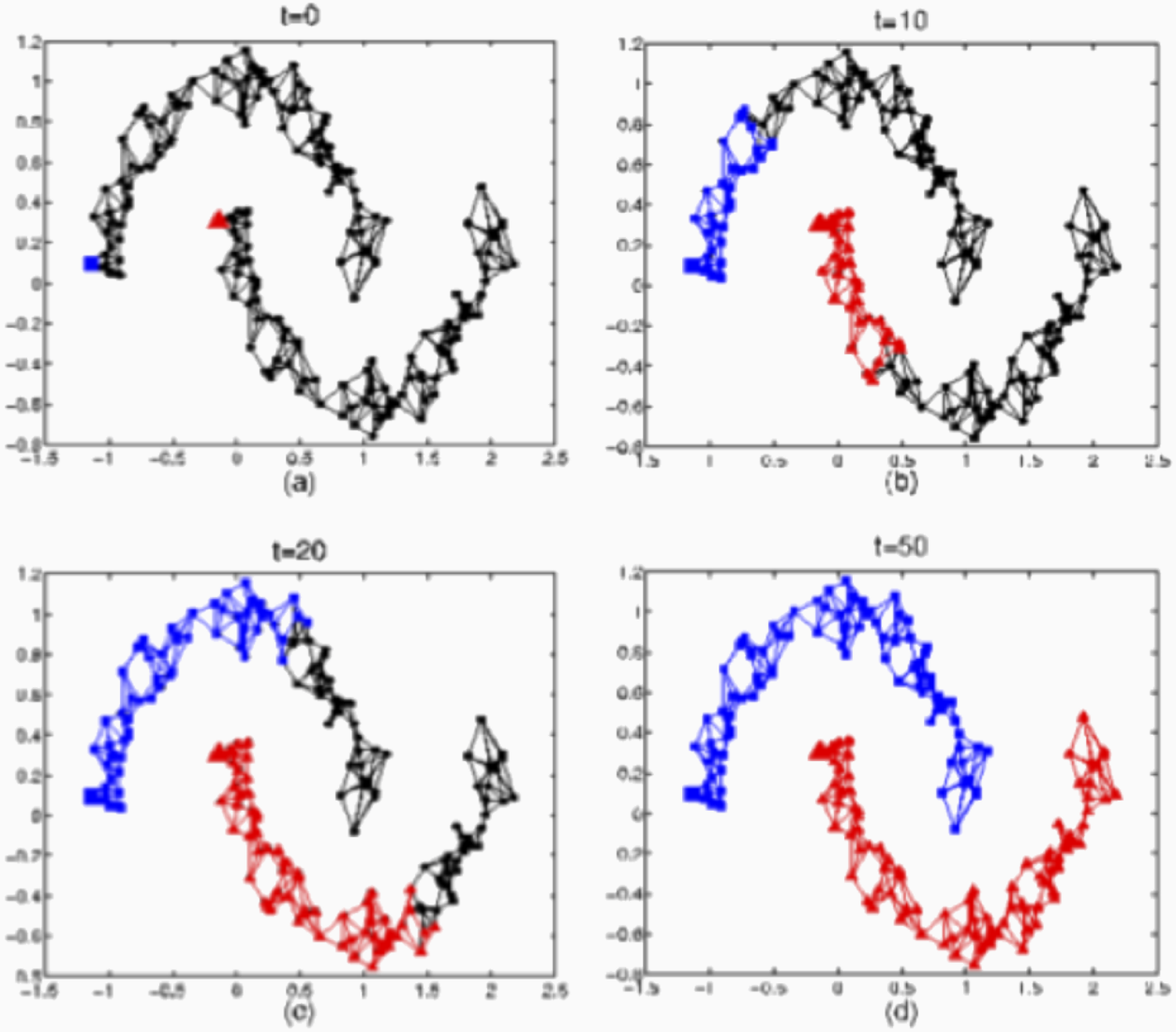
- The objective function is convex and quadratic, so there is a closed-form solution (found by setting the gradient to zero)

$$F^* = ((1-\alpha)I + L_{sym})^{-1}Y, \quad \text{with } \alpha = 1/(1+\mu)$$

- Inverting $(1-\alpha)I + L_{sym}$ is costly for large graphs
- Equivalent and cheaper iterative algorithm:
  1. Initialize $F(0) = Y$
  2. Iterate the following until convergence

$$F(t+1) = \alpha(I - L_{sym})F(t) + (1-\alpha)Y$$

Semi-supervised label propagation: illustration



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