



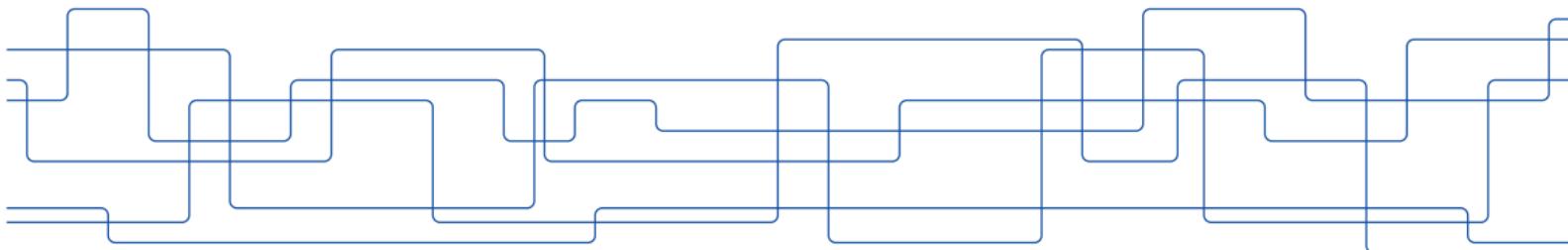
DD2434 Machine Learning, Advanced Course

Module 4 : learning with graphs

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overview of module 4

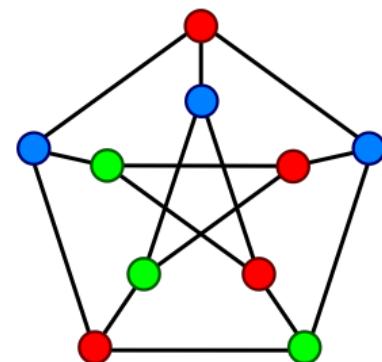
- ▶ introduction to mining and learning with graphs
- ▶ spectral graph theory
- ▶ spectral graph clustering
- ▶ graph embeddings

reading material

- ▶ von Luxburg. A tutorial on spectral clustering
- ▶ Hamilton. Graph representation learning (chapters 1, 2, 3, and 5)

graphs: a simple but universal model

- ▶ graph: $G = (V, E)$, set of vertices: V , set of edges: E
- ▶ vertices or nodes : represent entities
- ▶ edges or links: represent pairwise relations between entities
- ▶ basic model can be enriched with considering directions, weights, labels, timestamps, etc., on vertices and edges
- ▶ graphs are used to model many real-world datasets

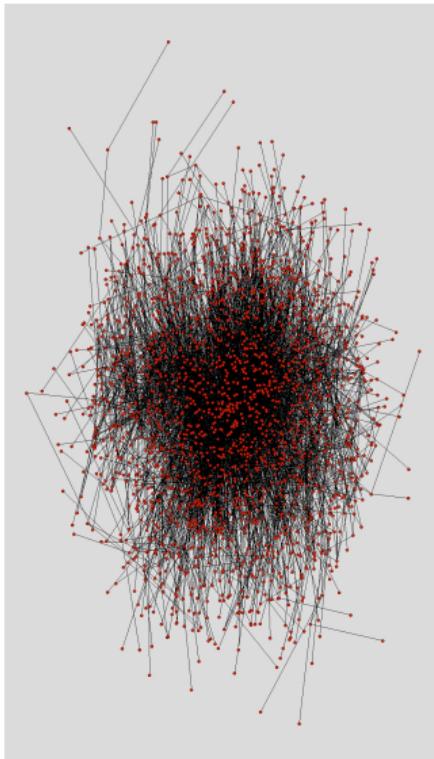


types of networks

- ▶ social networks
- ▶ knowledge and information networks
- ▶ technology networks
- ▶ biological networks

social networks

- ▶ nodes represent **individuals**
- links denote **social interactions**
 - ▶ networks of acquaintances
 - ▶ collaboration networks
 - ▶ actor networks
 - ▶ co-authorship networks
 - ▶ director networks
 - ▶ phone-call networks
 - ▶ **e-mail** networks
 - ▶ IM networks
 - ▶ sexual networks

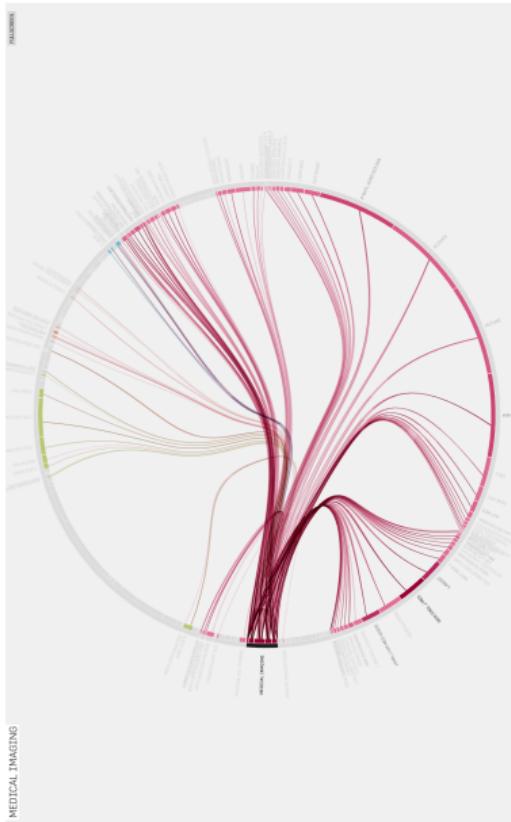


knowledge and information networks

- ▶ nodes store **information items**

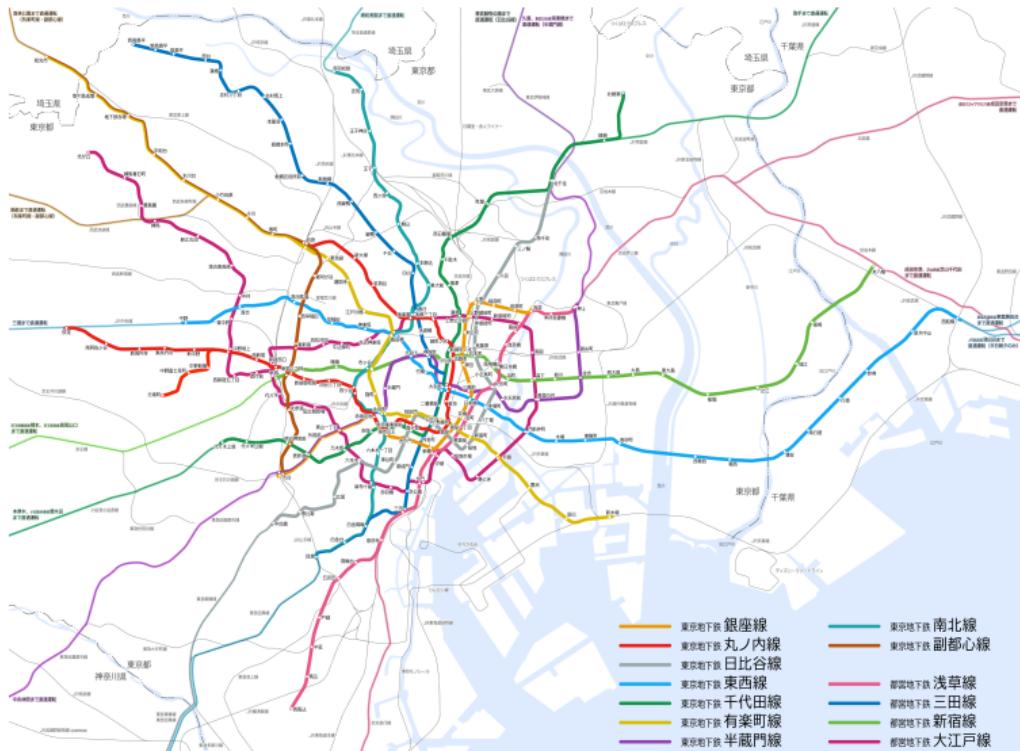
links **associate** information between items

- ▶ **citation** network (directed acyclic)
- ▶ the web (directed)
- ▶ word networks
- ▶ networks of trust (directed)
- ▶ software graphs (directed)
- ▶ home page/blog networks (directed)
- ▶ peer-to-peer networks
- ▶ bluetooth networks

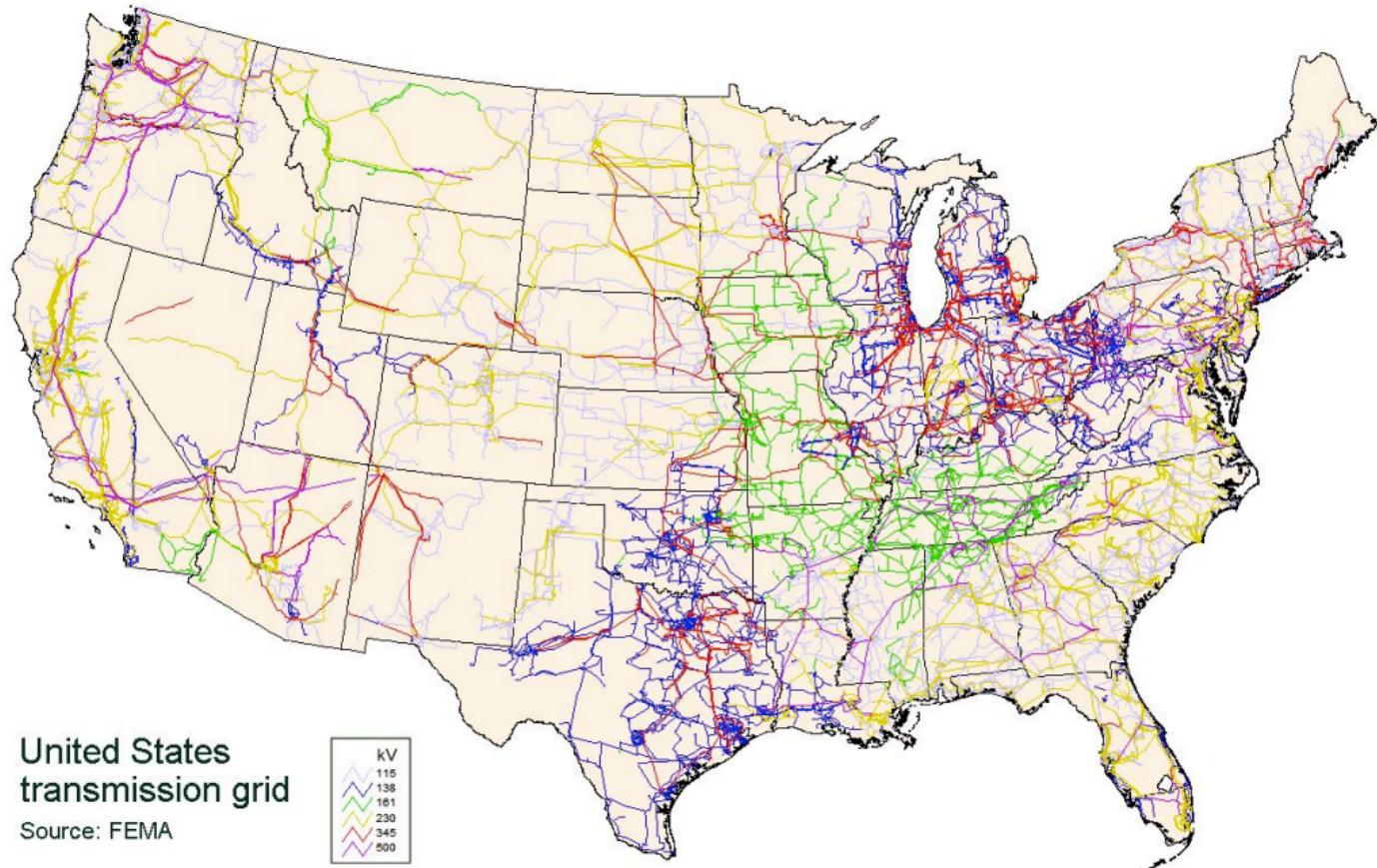


technological networks

- ▶ networks built for distribution of a commodity
 - the internet, power grids, telephone networks, airline networks, transportation networks

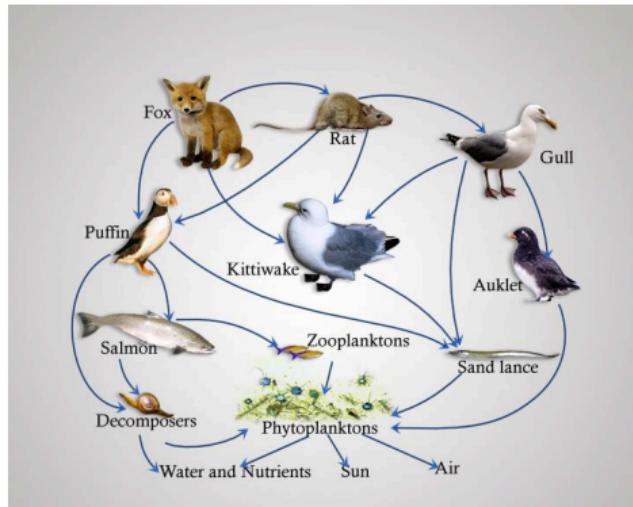
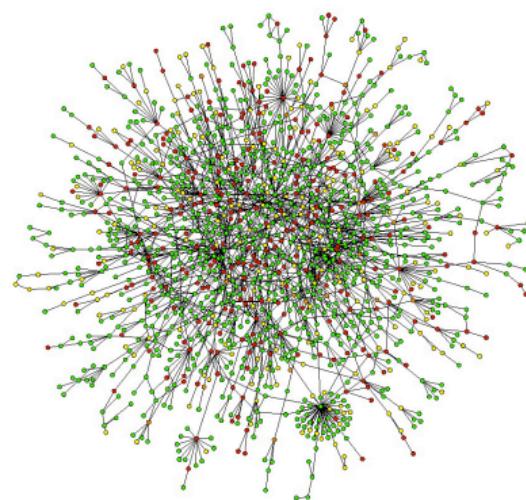


US power grid



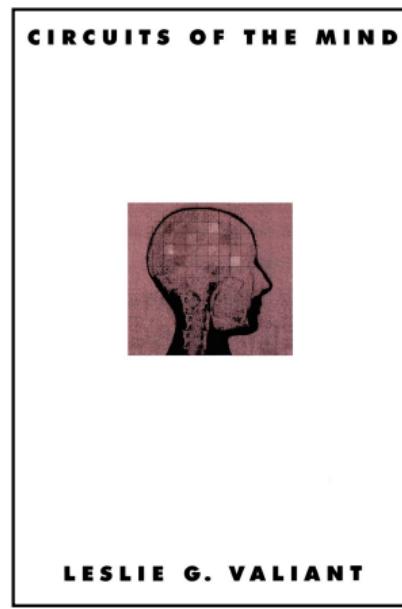
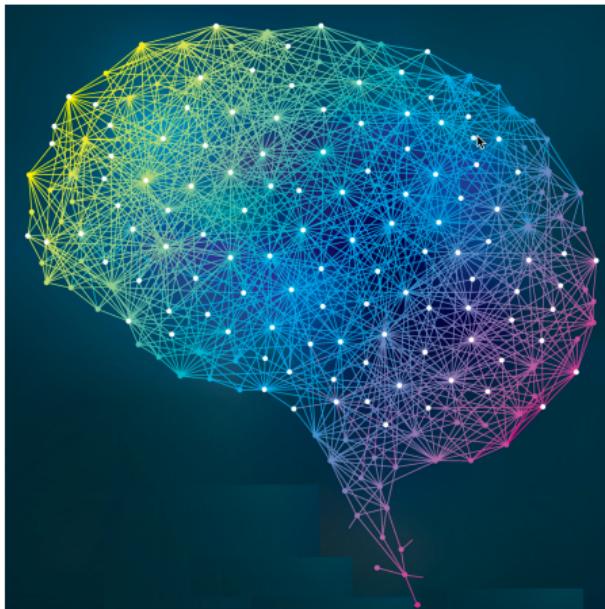
biological networks

- ▶ biological systems represented as networks
 - ▶ protein-protein interaction networks
 - ▶ gene regulation networks
 - ▶ gene co-expression networks
 - ▶ metabolic pathways
 - ▶ the food web
 - ▶ neural networks



brain network

- ▶ human brain can be modeled as a complex network
 - how do neurons and neuronal structures connect and communicate?



network science

- ▶ the world is full with networks
- ▶ what are the research questions to consider?
 - understand their **topology** and measure their **properties**
 - study **evolution** and **dynamics**
 - create realistic **models**
 - design algorithms for **learning** and making **predictions** on network data

properties of real-world networks

diverse collections of graphs arising from different phenomena

are there typical patterns ? **yes !**

- ▶ static networks

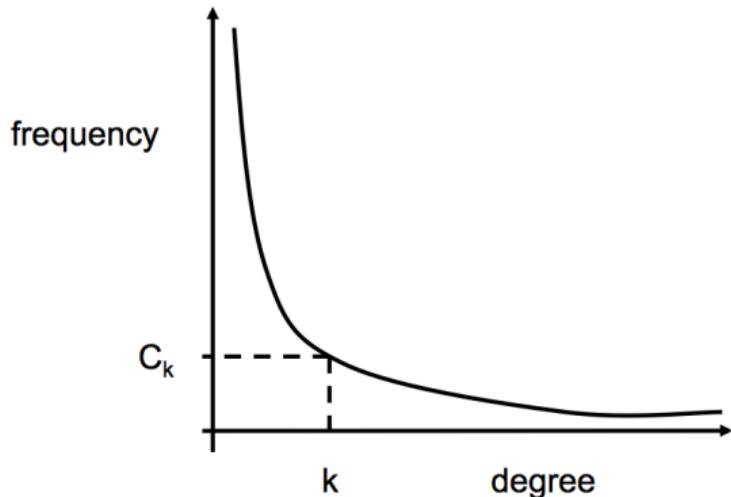
- heavy tails
- clustering coefficients
- communities
- small diameters

- ▶ time-evolving networks

- densification
- shrinking diameters

degree distribution

- ▶ C_k = number of vertices with degree k



- ▶ **problem** : find the probability distribution that fits best the observed data

power-law degree distribution

- ▶ C_k = number of vertices with degree k , then

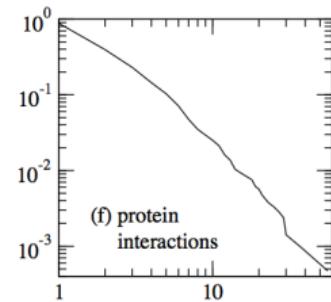
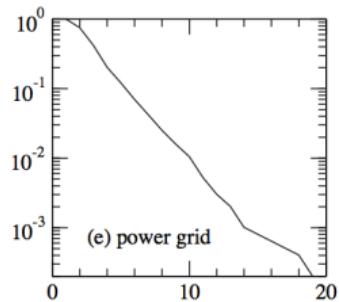
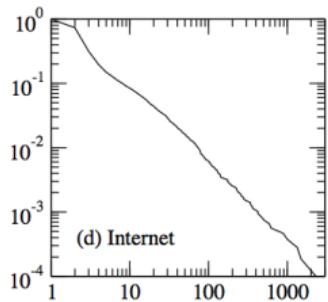
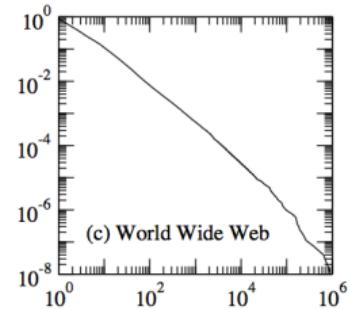
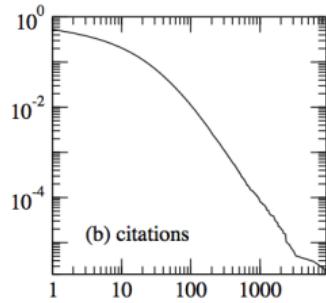
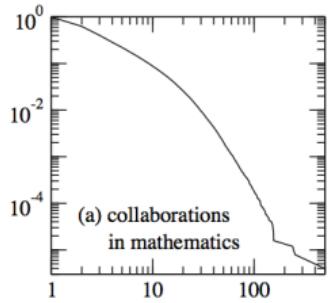
$$C_k = c k^{-\gamma}$$

with $\gamma > 1$, or

$$\ln C_k = \ln c - \gamma \ln k$$

- ▶ plotting $\ln C_k$ versus $\ln k$ gives a straight line with slope $-\gamma$
- ▶ **heavy-tail distribution** : there is a non-negligible fraction of nodes that have very high degrees (hubs)
- ▶ **scale free** : average is not informative

power-law degree distribution



power-laws in a wide variety of networks

very different from Erdős-Rényi random graphs

clustering coefficients

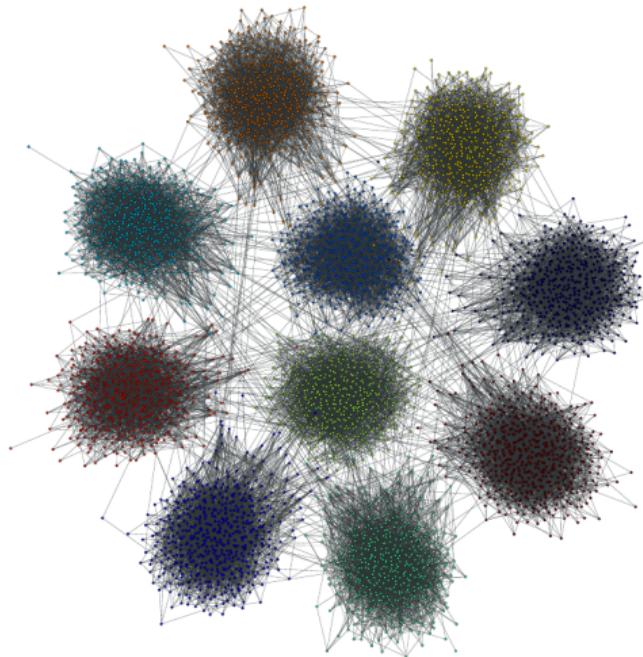
- ▶ a proposed measure to capture local clustering is graph transitivity

$$T(G) = \frac{3 \times \{\text{number of triangles in the network}\}}{\{\text{number of connected triples of vertices}\}}$$

- ▶ captures “transitivity of clustering”
- ▶ if u is connected to v and
 v is connected to w , it is also likely that
 u is connected to w

community structure

informal definition of community: a set of vertices densely connected to each other and sparsely connected to the rest of the graph



artificial communities: <http://projects.skewed.de/graph-tool/>

community structure

- ▶ Leskovec et al. study community structure in an collection of real-world networks
- ▶ introduce the [network community profile \(NCP\)](#) plot
- ▶ characterizes the best possible community over a range of scales

community structure

important findings of Leskovec et al.

1. up to certain size k_0 (~ 100 vertices) there are good cuts
 - as the size increases so does the quality of the community
2. at the size k_0 we observe the best possible community
 - such communities are typically connected to the remainder with a single edge
3. above the size k_0 the community quality decreases
 - this is because they blend in and gradually disappear

small-world phenomena

small worlds : graphs with short paths



- ▶ Stanley Milgram (1933-1984)
- ▶ conducted a number of famous sociology experiments
- ▶ obedience to authority (1963)
- ▶ small-world experiment (1967)
 - we live in a small-world

for criticism on the small-world experiment, see “*Could It Be a Big World After All? What the Milgram Papers in the Yale Archives Reveal About the Original Small World Study*” by Judith Kleinfeld

small-world experiments

- ▶ letters were handed out to people in Nebraska to be sent to a target in Boston
- ▶ people were instructed to pass on the letters to someone they knew on *first-name basis*
- ▶ the letters that reached the destination (64 / 296) followed paths of length around 6
- ▶ *six degrees of separation* (term due to John Guare)

see also :

- the Kevin Bacon game
- the Erdős number

small diameter

proposed measures

- ▶ **diameter** : largest shortest-path over all pairs
- ▶ **effective diameter** : upper bound of the shortest path of 90% of the pairs of vertices
- ▶ **average shortest path** : average of the shortest paths over all pairs of vertices
- ▶ **characteristic path length** : median of the shortest paths over all pairs of vertices
- ▶ **hop-plots** : plot of $|N_h(u)|$, the number of neighbors of u at distance at most h , as a function of h

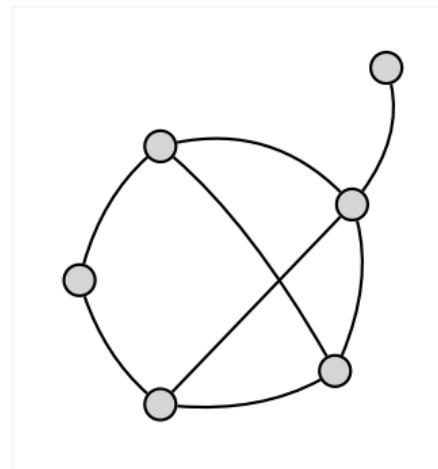
mining and learning with graphs

typical problems

- graph clustering and community detection
- node classification
- link prediction
- link classification

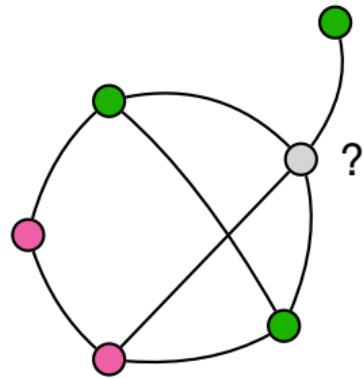
node classification

- ▶ use information about graph attributes and graph structure to make predictions about **node labels**



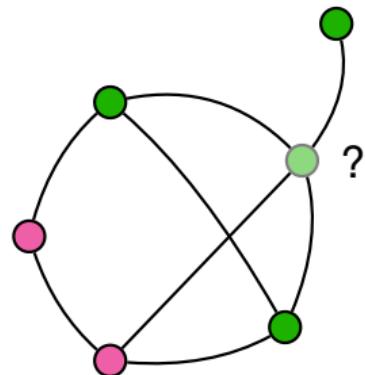
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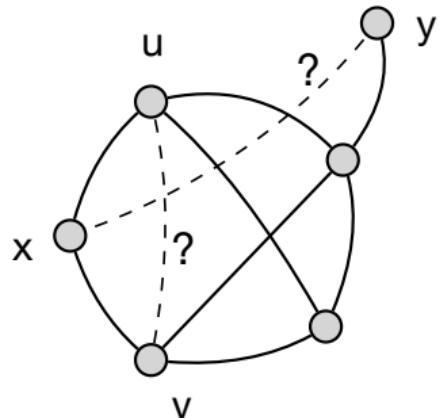
node classification

- ▶ use information about graph attributes and graph structure to make predictions about **node labels**



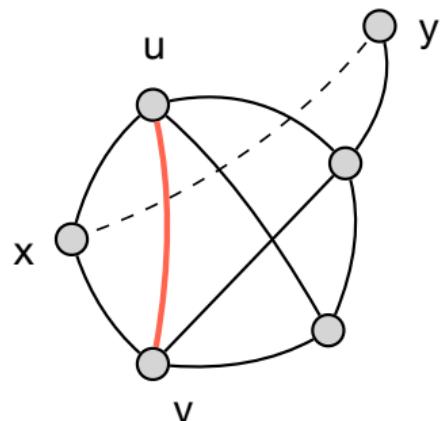
link prediction

- ▶ use information about graph attributes and graph structure to make predictions about new links



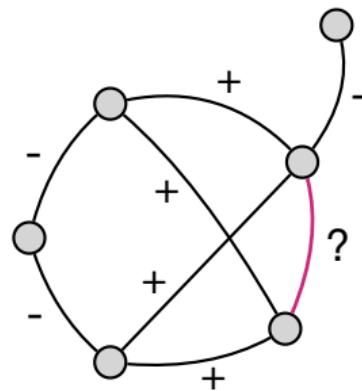
node classification

- ▶ use information about graph attributes and graph structure to make predictions about new links



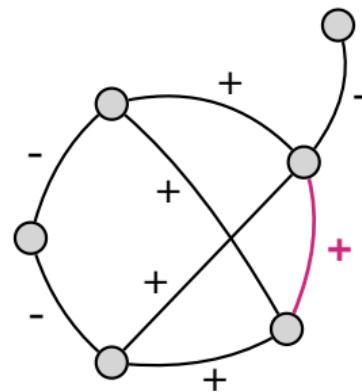
link classification

- ▶ use information about graph attributes and graph structure to make predictions about **link labels**



node classification

- ▶ use information about graph attributes and graph structure to make predictions about **link labels**



summary and discussion

- ▶ many real-world data can be modeled as graphs, simple or with attributes
- ▶ graphs across different application domains have structural similarities
- ▶ many machine learning problems can be formulated in the graph setting

spectral graph theory

objective:

- ▶ view the adjacency (or related) matrix of a graph with a **linear algebra** lens
- ▶ identify connections between **spectral properties** of such a matrix and **structural properties** of the graph
 - connectivity
 - bipartiteness
 - cuts
 - ...
- ▶ spectral properties = eigenvalues and eigenvectors
- ▶ in other words, what does the eigenvalues and eigenvectors of the adjacency (or related) matrix tell us about the graph?

once again, eigenvalues and eigenvectors

- ▶ consider a real $n \times n$ matrix \mathbf{A} , i.e., $\mathbf{A} \in \mathbb{R}^{n \times n}$
- ▶ $\lambda \in \mathbb{C}$ is an **eigenvalue** of \mathbf{A} if there exists $\mathbf{x} \in \mathbb{C}^n$, $\mathbf{x} \neq \mathbf{0}$ such that

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

such a vector \mathbf{x} is called **eigenvector** of \mathbf{A} corresponding to eigenvalue λ

- ▶ alternatively,

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0} \quad \text{or} \quad \det(\mathbf{A} - \lambda\mathbf{I}) = 0$$

it follows that \mathbf{A} has n eigenvalues (possibly complex and possibly with multiplicity > 1)

once again, eigenvalues and eigenvectors

- ▶ consider a real and symmetric $n \times n$ matrix \mathbf{A}
(e.g., the adjacency matrix of an undirected graph)

then

- eigenvalues are real and eigenvectors are orthogonal
- ▶ \mathbf{A} is positive semi-definite if $\mathbf{x}^T \mathbf{A} \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$
- ▶ a symmetric positive semi-definite real matrix has real and non negative eigenvalues

variational characterization of eigenvalues

- ▶ consider a real and symmetric $n \times n$ matrix \mathbf{A}
 - the eigenvalues $\lambda_1, \dots, \lambda_n$ of \mathbf{A} can be ordered

$$\lambda_1 \leq \dots \leq \lambda_n$$

- ▶ the eigenvalues satisfy the following minimax principles w.r.t. Rayleigh quotient

$$\lambda_n = \max_{\mathbf{x} \neq 0} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

$$\lambda_1 = \min_{\mathbf{x} \neq 0} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq 0 \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \quad \text{and "so on" for the other eigenvalues}$$

- ▶ very useful way to think about eigenvalues

background: eigenvalues and eigenvectors

- ▶ the inverse holds, i.e.,

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{ij} A_{ij} x_i x_j}{\sum_i x_i^2}$$

and if \mathbf{x} is an “optimal vector”, then \mathbf{x} is eigenvector of λ_1

- optimal vector: $\arg \min$ of the expression above

- ▶ similarly

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{ij} A_{ij} x_i x_j}{\sum_i x_i^2}$$

and if \mathbf{x} is an “optimal vector”, then \mathbf{x} is eigenvector of λ_2

- optimal vector: $\arg \min$ of the expression above

spectral graph analysis

- ▶ apply the eigenvalue characterization for graphs
- ▶ consider $G = (V, E)$ an undirected and d -regular graph
 - regular graph is used w.l.o.g. for simplicity of expositions
- ▶ question: which matrix to consider?
 - the adjacency matrix \mathbf{A} of the graph
 - some matrix \mathbf{B} so that $\mathbf{x}^T \mathbf{B} \mathbf{x}$ is related to a structural property of the graph
- ▶ let \mathbf{A} be the adjacency matrix of G ; define the Laplacian matrix of G as

$$\mathbf{L} = \mathbf{I} - \frac{1}{d} \mathbf{A} \quad \text{or} \quad \mathbf{L}_{ij} = \begin{cases} 1 & \text{if } i = j \\ -1/d & \text{if } (i, j) \in E, i \neq j \\ 0 & \text{if } (i, j) \notin E, i \neq j \end{cases}$$

spectral graph analysis

- ▶ for the Laplacian matrix $\mathbf{L} = \mathbf{I} - \frac{1}{d} \mathbf{A}$, we can show that (proof left as exercise)

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{d} \sum_{(u,v) \in E} |x_u - x_v|^2$$

here, x_u is the coordinate of the vector \mathbf{x} that corresponds to vertex $u \in V$

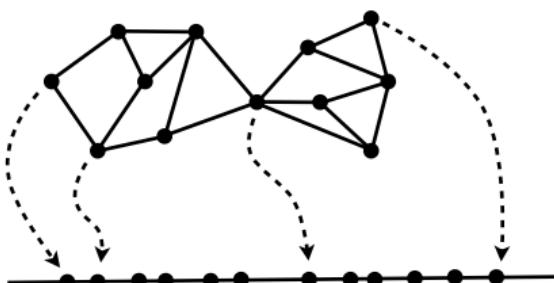
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$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{d} \sum_{(u,v) \in E} |x_u - x_v|^2$$

here, x_u is the coordinate of the vector \mathbf{x} that corresponds to vertex $u \in V$

- vector \mathbf{x} is seen as a 1-dimensional embedding
 - i.e., mapping the vertices of the graph onto the real line



the smallest eigenvalue

apply the eigenvalue characterization theorem for \mathbf{L}

- ▶ what is λ_1 ?

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{L} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- ▶ observe that $\lambda_1 \geq 0$
- ▶ can it be $\lambda_1 = 0$?
- ▶ **yes**: take \mathbf{x} to be the constant vector

the second smallest eigenvalue

apply the eigenvalue characterization theorem for \mathbf{L}

- ▶ what is λ_2 ?

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq 0 \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T \mathbf{L} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq 0 \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- ▶ can it be $\lambda_2 = 0$?
- ▶ $\lambda_2 = 0$ if and only if the graph is **disconnected**
 - map the vertices of each connected component to a different constant

the k -th smallest eigenvalue

- ▶ alternative characterization for λ_k

$$\lambda_k = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x} \in \mathbb{S}_{k-1}^\perp}} \max \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- ▶ $\lambda_k = 0$ if and only if the graph has at least k connected components

where

- \mathbb{S}_k : space spanned by k independent vectors
- \mathbb{S}_k^\perp : space orthogonal to \mathbb{S}_k

the largest eigenvalue

- ▶ what about λ_n ?

$$\lambda_n = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{L} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- ▶ consider a **boolean** version of this problem
 - restrict mapping to $\{-1, +1\}$
 - mapping of vertices to $\{-1, +1\}$ corresponds to a **graph cut** S

$$\lambda_n \geq \max_{\mathbf{x} \in \{-1, +1\}^n} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

‘ \geq ’ because $\mathbf{x} \in \{-1, +1\}^n$ is more restricted case

the largest eigenvalue

- ▶ consider the graph cut S defined by the mapping of vertices to $\{-1, +1\}$, then:

$$\begin{aligned}\lambda_n &\geq \max_{x \in \{-1, +1\}^n} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\ &= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{d n} \\ &= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{2 |E|} \\ &= \frac{2 \text{maxcut}(G)}{|E|}\end{aligned}$$

where, $E(S, T)$ is the number of edges between $S, T \subseteq V$

- ▶ it follows that if G is bipartite then $\lambda_n \geq 2$
 - because if G is bipartite, there exists S that cuts all edges

the largest eigenvalue

- ▶ on the other hand

$$\begin{aligned}\lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\ &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{2d \sum_{u \in V} x_u^2 - \sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2} \\ &= 2 - \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2}\end{aligned}$$

- ▶ first note that $\lambda_n \leq 2$
- ▶ $\lambda_n = 2$ if and only if there is \mathbf{x} such that $x_u = -x_v$ for all $(u, v) \in E$
- ▶ $\lambda_n = 2$ if and only if G has a bipartite connected component

summary so far

- ▶ eigenvalues and structural properties of G :
 - $\lambda_2 = 0$ if and only if G is disconnected
 - $\lambda_k = 0$ if and only if G has at least k connected components
 - $\lambda_n = 2$ if and only if G has a bipartite connected component

robustness

- ▶ how **robust** are these results ?
- ▶ for instance, what if $\lambda_2 = \epsilon$?
 - is the graph **G** almost disconnected ?
i.e., does it have **small cuts** ?
- ▶ or, what if $\lambda_n = 2 - \epsilon$?
 - does it have a component that is “close” to bipartite ?

the second eigenvalue

we can rewrite the expression for λ_2 as

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{d \sum_{u \in V} x_u^2} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\frac{1}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{2n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

where V^2 is the set of ordered pairs of vertices

why?

$$\sum_{(u,v) \in V^2} (x_u - x_v)^2 = 2n \sum_v x_v^2 - 2 \sum_{u,v} x_u x_v = 2n \sum_v x_v^2 - 2 \left(\sum_u x_u \right)^2$$

$$\text{and } \sum_u x_u = 0 \text{ since } \mathbf{x}^T \mathbf{x}_1 = 0$$

the second eigenvalue

we can further rewrite the expression for λ_2 as follows:

note that we change the argument over which we take \min

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\frac{1}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{2n} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

why?

because for any \mathbf{y} that is not a constant vector,

and having $\mathbf{y}^T \mathbf{x}_1 = \sum_u y_u = s \neq 0$,

the vector $\mathbf{x} = \mathbf{y} - s/n$ achieves the same value

and it satisfies $\mathbf{x}^T \mathbf{x}_1 = \sum_u x_u = 0$ and $\mathbf{x} \neq \mathbf{0}$

the second eigenvalue

we can further rewrite the expression for λ_2 as follows:

note that we change the argument over which we take \min

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\frac{1}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{2n} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

why?

so, for any non-constant \mathbf{y} that minimizes the r.h.s. ratio

there is an \mathbf{x} (with $\mathbf{x}^T \mathbf{x}_1 = 0$ and $\mathbf{x} \neq \mathbf{0}$) that minimizes the l.h.s. ratio

(notice that since \mathbf{x} subtracts the constant s/n from \mathbf{y} the ratios are the same, as the constant s/n cancels out inside the differences)

the second eigenvalue

we can now write

$$\lambda_2 = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{nd} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{n^2} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\mathbb{E}_{(u,v) \in E} [(x_u - x_v)^2]}{\mathbb{E}_{(u,v) \in V^2} [(x_u - x_v)^2]}$$

consider again **discrete version** of the problem, $x_u \in \{0, 1\}$

$$\min_{\substack{\mathbf{x} \in \{0,1\}^n \\ \mathbf{x} \text{ non const}}} \frac{\mathbb{E}_{(u,v) \in E} [(x_u - x_v)^2]}{\mathbb{E}_{(u,v) \in V^2} [(x_u - x_v)^2]} = \min_{S \subseteq V} \frac{n}{d} \frac{E(S, \bar{S})}{|S| |\bar{S}|} = usc(G)$$

where $usc(G)$ is the **uniform sparsest cut** of G defined as

$$usc(G) = \min_{S \subseteq V} \frac{n}{d} \frac{E(S, \bar{S})}{|S| |\bar{S}|}$$

uniform sparsest cut

- ▶ it can be shown that

$$\lambda_2 \leq usc(G) \leq \sqrt{8\lambda_2}$$

- ▶ the first inequality holds because λ_2 is a **relaxation** to **usc**
- ▶ the second inequality is constructive :
 - ▶ if x is an eigenvector of λ_2
 - then there is some $t \in V$ such that the cut $(S, V \setminus S) = (\{u \in V \mid x_u \leq x_t\}, \{u \in V \mid x_u > x_t\})$ has cost $usc(S) \leq \sqrt{8\lambda_2}$

conductance

- ▶ **conductance**: another popular measure for cuts
- ▶ the conductance of a set $S \subseteq V$ is defined as

$$\phi(S) = \frac{E(S, V \setminus S)}{d|S|}$$

- ▶ it expresses the probability to “move out” of S by following a random edge from S
- ▶ we are interested in sets of small conductance
- ▶ the conductance of the graph G is defined as

$$\phi(G) = \min_{\substack{S \subseteq V \\ 0 \leq |S| \leq |V|/2}} \phi(S)$$

Cheeger's inequality

- ▶ Cheeger's inequality:

$$\frac{\lambda_2}{2} \leq \frac{usc(G)}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}$$

⇒ conductance is small if and only if λ_2 is small

- ▶ the two leftmost inequalities are “easy” to show
- ▶ the first follows by the definition of relaxation
- ▶ the second follows by

$$\frac{usc(S)}{2} = \frac{n}{2d} \frac{E(S, V \setminus S)}{|S||V \setminus S|} \leq \frac{E(S, V \setminus S)}{d|S|} = \phi(S)$$

since $|V \setminus S| \geq n/2$

generalization to non-regular graphs

- ▶ $G = (V, E)$ is undirected and non-regular
- ▶ let d_u be the degree of vertex u
- ▶ define \mathbf{D} to be a diagonal matrix whose u -th diagonal element is d_u
- ▶ the *normalized Laplacian matrix* of G is defined

$$\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2} \mathbf{A} \mathbf{D}^{-1/2}$$

or

$$\mathbf{L}_{uv} = \begin{cases} 1 & \text{if } u = v \\ -1/\sqrt{d_u d_v} & \text{if } (u, v) \in E, u \neq v \\ 0 & \text{if } (u, v) \notin E, u \neq v \end{cases}$$

generalization to non-regular graphs

- with the *normalized Laplacian* the eigenvalue expressions become (e.g., λ_2)

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \langle \mathbf{x}, \mathbf{x}_1 \rangle_D = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{\sum_{u \in V} d_u x_u^2}$$

where we use weighted inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_D = \sum_{u \in V} d_u x_u y_u$$

summary

- ▶ eigenvalues and structural properties of G :
 - $\lambda_2 = 0$ if and only if G is disconnected
 - $\lambda_k = 0$ if and only if G has at least k connected components
 - $\lambda_n = 2$ if and only if G has a bipartite connected component
 - small λ_2 if and only if G is “almost” disconnected (small conductance)

discussion

- ▶ deep connections between spectral properties of appropriately-defined matrices and structural properties of a graph
- ▶ spectral analysis provides a means to embed the graph nodes into low-dimensional Euclidean spaces
- ▶ spectral embeddings can be used to solve a number of different learning problems on graphs
- ▶ many other state-of-the-art embeddings are known, going beyond spectral analysis