Graph Embeddings and Spectral Methods

- weighted graphs: terminology and representations
- graph Laplacian and Dirichlet energy
- spectral graph embedding (scalar and vector)
- node ordering and graph partitioning

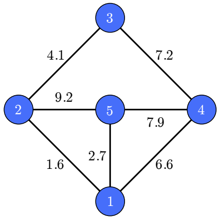
Graphs: Nodes and Edges

- A graph $G = (V, E)$ consists of:
  - a set of n *nodes* (or *vertices*) $V = \{1, \ldots, n\}$
  - a set of m *edges* (or *links*) $E = \{\{i, j\} \mid \text{nodes } i, j \text{ are connected}\}$
- Nodes i and j are *adjacent* (neighbors) if $\{i, j\} \in E$.
  - Neighbor set of i: $N(i) = \{j \mid \{i, j\} \in E\}$
  - *Degree* of node i: $d_i = |N(i)|$
- *Undirected graph*: $\{i, j\}$ is the same as $\{j, i\}$.

Weighted Graphs and Adjacency Matrix

- In a *weighted graph*, each edge $\{i, j\} \in E$ has a positive *weight* $W_{ij} > 0$.
  - $W_{ij} = W_{ji}$ (symmetric).
  - $W_{ij} = 0$ if $\{i, j\} \notin E$.
  - Diagonal entries $W_{ii} = 0$.
- The *weighted adjacency matrix* $W \in \mathbb{R}^{n \times n}$ completely specifies the graph.
  - $2m$ non-zero entries (for symmetric W).
- *Weighted degree* of node i: $d_i^{\mathrm{w}} = \sum_{\{i,j\} \in E} W_{ij}$.
  - In matrix notation: $\boldsymbol{d}^{\mathrm{w}} = W\mathbf{1}$.

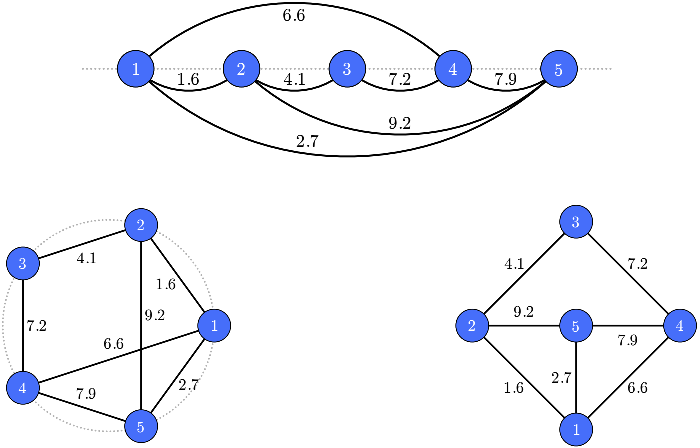
Example weighted graph



$$W = \begin{bmatrix} 0 & 1.6 & 0 & 6.6 & 2.7 \\ 1.6 & 0 & 4.1 & 0 & 9.2 \\ 0 & 4.1 & 0 & 7.2 & 0 \\ 6.6 & 0 & 7.2 & 0 & 7.9 \\ 2.7 & 9.2 & 0 & 7.9 & 0 \end{bmatrix}$$

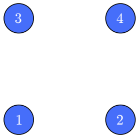
- $n = 5$ nodes, $m = 7$ edges
- Weighted degrees: $d^{\mathrm{w}} = (10.9, 14.9, 11.3, 21.7, 19.8)$

Example graph drawing styles

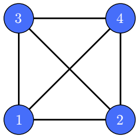


Some named graphs

- An *empty* graph has no edges, $i.e.$, $E = \emptyset$.



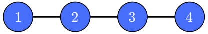
- A *full* or *complete* graph has an edge between every pair of nodes.



Some named graphs

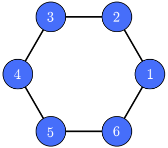
- A *chain* graph P_n is a graph with n nodes arranged in a line. Adjacency matrix is tridiagonal, $e.g.$for unweighted P_4

$$W = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



- A *cycle* graph C_n. Similar to a path, but endpoints are connected.

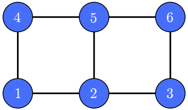
$$W = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$



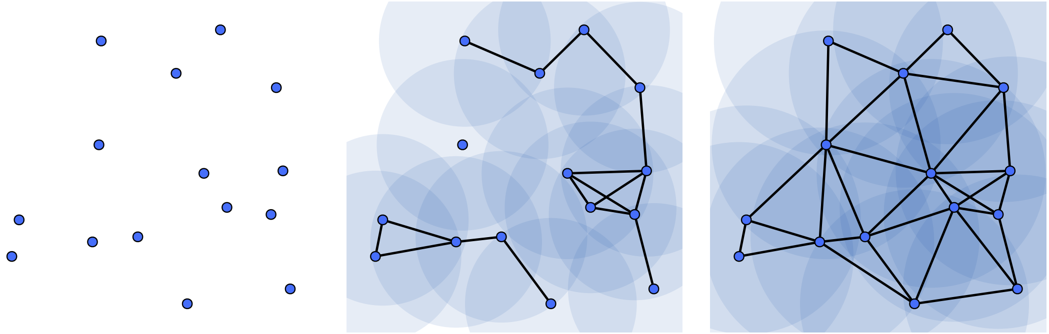
Some named graphs

- A *mesh* or *grid* graph

$$W = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

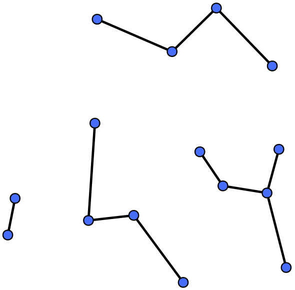


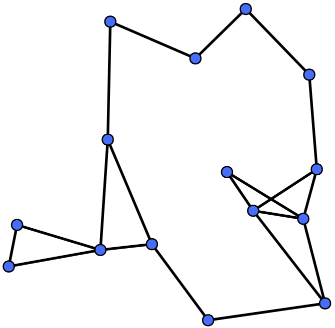
Geometric graphs



- in some applications, we create a graph from a collection of vectors $x_i \in \mathbb{R}^n$
- We create an edge whenever $||x_i - x_j||_2 \leq d$, where d is less than a critical distance
- left $d = 0.3$, right $d = 0.4$

Nearest neighbor graphs



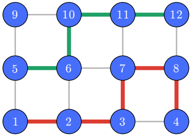


- we have an edge between i and j if i is among the k-nearest neighbors of j or vice versa.
- Here k is a parameter that we choose.
- When $k = 1$ the graph is called the nearest neighbor graph. Left $k = 1$, right $k = 2$

Choosing a method

- the choice of method (and parameters) depends on the final application
- all methods share the same basic idea
- edges of the graph indicate that nodes are 'similar', with higher weight indicating a higher degree of similarity.
- small $||x_i - x_j||_2$ indicates that nodes i and j are similar

Graph Connectivity and Paths



- A *path* of length L: sequence of nodes $i_1, \ldots, i_{L+1}$ where $\{i_j, i_{j+1}\} \in E$.
- Nodes i and j are *pathwise connected* if a path exists between them.
- A graph is *connected* if every pair of nodes is pathwise connected.
- Powers of unweighted adjacency matrix: $(W^L)_{ij}$ is number of paths of length L between i, j.
- The i, j entry of the matrix

$$Z = I + W + W^2 + \cdots + W^{n-1}$$

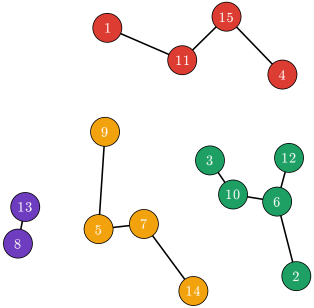
gives the number of paths of length at most $n - 1$ between nodes i and j.

Connected components

- a graph partitions the nodes into groups of mutually pathwise connected nodes.
- that is, we have subsets of nodes $G_1, \ldots, G_K \subseteq \{1, \ldots, n\}$ with

$$G_i \cap G_j = \emptyset \text{ for } i \neq j, \qquad G_1 \cup \cdots \cup G_K = \{1, \ldots, n\}.$$

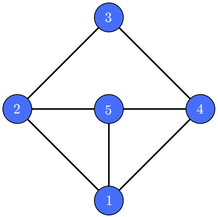
- Within each group of nodes, every node is pathwise connected to every other one

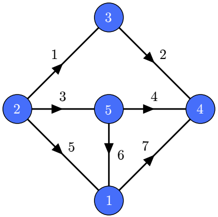


Incidence matrix (directed graphs)

- For an undirected graph, assign arbitrary directions to edges to form a *network*.
- The $n \times m$ *incidence matrix* A has entries:

$$A_{ij} = \begin{cases} 1 & \text{edge } j \text{ points to node } i \\ -1 & \text{edge } j \text{ points from node } i \\ 0 & \text{otherwise} \end{cases}$$



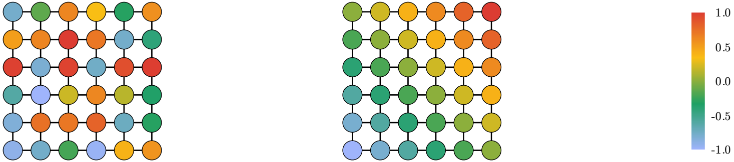


Node potentials and Dirichlet energy

- Assign a scalar value x_i to each node i: *node potentials* $x \in \mathbb{R}^n$.
- *Dirichlet energy* $D(x)$ measures smoothness of x across the graph.

$$D(x) = \frac{1}{2} \sum_{i,j=1}^{n} W_{ij}(x_i - x_j)^2$$

- Small $D(x)$ means $x_i \approx x_j$ for adjacent nodes (especially with large W_{ij}).



The Graph Laplacian Matrix

- The Dirichlet energy is a quadratic form

$$D(x) = x^{\mathsf{T}} L x$$

- L is the *Laplacian matrix*: $L = D - W$.
  - $D = \mathrm{diag}(d^{\mathsf{w}})$ is the diagonal matrix of weighted degrees.
  - Entries: $L_{ii} = d_i^{\mathsf{w}}$, $L_{ij} = -W_{ij}$ for $i \neq j$.
- L is symmetric and positive semi-definite (PSD).
  - Not positive definite (PD), since $L\mathbf{1} = 0$ (hence $D(\mathbf{1}) = 0$).

Laplacian matrix

let's establish $L = D - W$

$$
\begin{aligned}
\mathcal{D}(x) &= (1/2)\sum_{i,j=1}^{n} W_{ij}(x_i - x_j)^2 \\
&= (1/2)\sum_{i,j=1}^{n} W_{ij}(x_i^2 - 2x_i x_j + x_j^2) \\
&= (1/2)\sum_{i=1}^{n}\left(\sum_{j=1}^{n} W_{ij}\right) x_i^2 - \sum_{i,j=1}^{n} W_{ij} x_i x_j + (1/2)\sum_{j=1}^{n}\left(\sum_{i=1}^{n} W_{ij}\right) x_j^2 \\
&= x^T D x - x^T W x.
\end{aligned}
$$

we use that fact that the first and last sums are both equal to $\sum_{i=1}^{n} d_i x_i^2$.

Laplacian from Incidence Matrix

- let w be the vector of edge weights.
- the Laplacian can also be defined using the incidence matrix A

$$L = A\text{diag}(w)A^\mathsf{T}$$

- this definition is independent of the arbitrary edge orientations chosen for A.
- multiplication by A^T gives a vector of potential differences
- when $w = \mathbf{1}$ then L is the *Gram matrix* of A^T

Nullspace of the Laplacian and connectivity

- If $Lx = 0$, then $D(x) = 0$, implying $x_i = x_j$ for all adjacent nodes.
- By extension, $x_i = x_j$ for all pathwise connected nodes.
- If the graph is connected:
$$\mathcal{N}(L) = \text{span}(\mathbf{1})$$
- $\mathbf{dim}\,\mathcal{N}(L) = 1$. Smallest eigenvalue $\lambda_1 = 0$, with eigenvector $\mathbf{1}$.
- If the graph is disconnected with K components:
$$\mathbf{dim}\,\mathcal{N}(L) = K$$
- Number of zero eigenvalues of L equals number of connected components.

Scalar spectral embedding problem

- Assign node potentials $x \in \mathbb{R}^n$ (an *embedding*) to minimize Dirichlet energy.
- *Smoothness*: adjacent nodes should have similar values (small $|x_i - x_j|$).
- Constraints needed to prevent trivial or arbitrary solutions:
  - *Centering*: $\mathbf{1}^\mathsf{T} x = 0$ (mean of potentials is zero, due to shift invariance of $D(x)$).
  - *Scaling*: $||x||_2^2 = n$ (RMS value of potentials is one, prevents $x = 0$).
- we would like to solve

$$
\begin{array}{ll}
\text{minimize} & x^\mathsf{T} L x \\
\text{subject to} & \mathbf{1}^\mathsf{T} x = 0 \\
& ||x||_2 = \sqrt{n}
\end{array}
$$

Eigendecomposition of the Laplacian

- eigenvalues of L are $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$.
- $\lambda_1 = 0$ has eigenvector $\mathbf{1}$.
- The second smallest eigenvalue λ_2 is the *Fiedler eigenvalue* (λ^{F}).
- Its associated eigenvector v^{F} (or v_2) is the *Fiedler eigenvector*.
- $\mathbf{1}^{\mathsf{T}} v^{\mathsf{F}} = 0$ and $||v^{\mathsf{F}}||_2 = 1$.

Scalar spectral embedding solution

- recall the optimization problem, where A is symmetric and $\lambda_1 < \lambda_2$

$$\begin{array}{ll} \text{minimize} & x^T A x \\ \text{subject to} & v_1^T x = 0 \\ & \|x\|_2 = 1, \end{array}$$

  where v_1 is an eigenvector associated with the smallest eigenvalue λ_1

- the normalized second smallest eigenvector v_2 is a solution

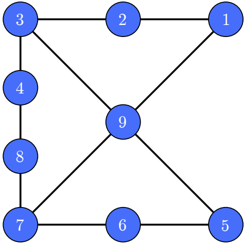
- for scalar spectral embedding, the solution is

$$x^{\text{se}} = \sqrt{n} v^{\text{F}}$$

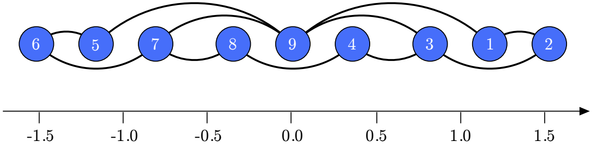
- x^{se} is the *spectral embedding* for the weighted graph.

- The optimal value of $D(x)$ is $n\lambda^{\text{F}}$. Small λ^{F} indicates a graph is 'almost disconnected'.

Example: scalar spectral embedding



The scalar spectral embedding is:

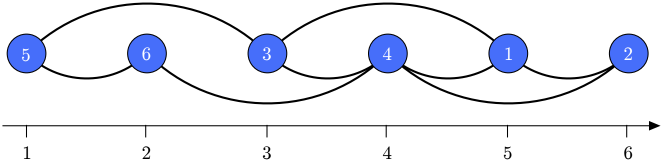


Applications: node ordering

- *Node ordering problem*: Assign integers $1, \ldots, n$ to nodes as new indices σ.
- Goal: edges connect nodes with nearby indices, especially for high weights.

$$\begin{array}{ll} \text{minimize} & \sigma^\mathsf{T} L \sigma \\ \text{subject to} & \sigma \in S_n \end{array}$$

- Exact solution is computationally hard ($n!$ permutations).
- *Approximate solution (spectral ordering)*: Sort entries of x^{se}.
- *Polishing*: Local search (swapping adjacent indices) to improve Dirichlet energy.

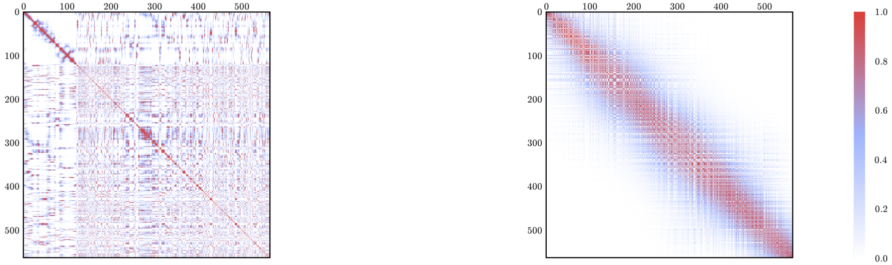


Applications: Permuting a correlation matrix

- given a correlation matrix C, create a graph, either connect based on a threshold, or use

$$W_{ij} = \left(\frac{C_{ij} + 1}{2}\right)^{\gamma}$$

- spectral ordering ensures that highly-correlated items are near each other
- application: LU or Cholesky solvers have reduced fill-in



Applications: Graph bisection

- *Node bisection problem*: Partition nodes into two groups A, B.
- Encode partition: $x_i = -1$ if $i \in A$, $x_i = 1$ if $i \in B$.
- *Balanced bisection*: $|A| = |B| = n/2 \implies \mathbf{1}^\mathsf{T} x = 0$.
- *Cut weight*: sum of weights of edges crossing the cut.

$$\begin{array}{ll} \text{minimize} & x^\mathsf{T} L x \\ \text{subject to} & x_i \in \{-1, 1\}, \text{ for } i = 1, \ldots, n \\ & \mathbf{1}^\mathsf{T} x = 0 \end{array}$$

- Exact solution is NP-hard.
- *Approximate solution (spectral bisection)*: Take x^{se}, assign nodes with smallest $n/2$ values to A, rest to B.

Vector Graph Embedding

- Assign a k-dimensional vector $x_i \in \mathbb{R}^k$ to each node i.
- Form an $n \times k$ matrix X, where rows are $x_i^\top$.
- Objective is to minimize the sum of squared differences between adjacent node vectors:

$$D(X) = \frac{1}{2} \sum_{i,j=1}^{n} W_{ij} ||x_i - x_j||_2^2$$

- This can be expressed in terms of the Laplacian: $D(X) = \textbf{trace}(X^\top L X)$.
- Constraints:
  - *Centering*: $X^\top \mathbf{1} = 0$ (mean of each component is zero).
  - *Standardization*: $\frac{1}{n} X^\top X = I$ (components are orthogonal and scaled).

Vector spectral embedding solution

- The columns of the optimal X are proportional to the k eigenvectors of L corresponding to the k smallest non-zero eigenvalues $(v_2, \ldots, v_{k+1})$.

$$\begin{bmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{bmatrix} \propto \begin{bmatrix} v_2 & \ldots & v_{k+1} \end{bmatrix}$$

- *Graph drawing*: $k = 2$ allows nodes to be plotted in a 2D plane based on their embedding vectors.