Statistical Data Analysis

Dr. Jana de Wiljes

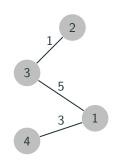
11. Januar 2022

Universität Potsdam

What is a graph (formally)?

The objects on the following slides will play a major role in this course.

- $G = (V, E, \omega)$, where $V \neq \emptyset$ is a set (called the **vertex set**), $E \subset \binom{V}{2} = \{\{u, v\} : u, v \in V\}$ (called the **edge set**) and $\omega : E \to \mathbb{R}^+$, is called a (weighted) graph
- usually we choose (or rename) $V = \{1, 2, \dots, n\} \text{ and use the notations } ij = \{i, j\} \text{ for } \{i, j\} \in E \text{ and } \omega_{ij} = \omega(ij)$
- for every i ∈ V define
 N(i) := {j ∈ V : ij ∈ E}, called the
 neighbourhood of i (in G); elements of
 N(i) are called neighbours of i (those elements are adjacent to i)



$$w(23) = 1,$$

 $N(4) = \{1\},$
 $d(1) = |\{3,4\}| = 2$

Graph classes

Well known graph classes are:

- the **path graph** P_n has vertex set $\{1, 2, ..., n\}$ and edge set $\{\{1, 2\}, \{2, 3\}, ..., \{n 1, n\}\}$
- the **cycle graph** C_n has vertex set $\{1, 2, ..., n\}$ and edge set $\{\{1, 2\}, \{2, 3\}, ..., \{n 1, n\}, \{n, 1\}\}$
- the complete graph K_n consists of n vertices which are all adjacent to each other
- the **complete bipartite graph** $K_{m,n}$ has two sets V_1 and V_2 of vertices of sizes m and n, such that the edge set consists of all possible edges between V_1 and V_2

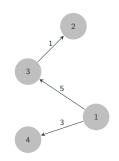
A set of vertices in a graph which are all adjacent to each other (they **induce** a complete (sub)graph), is called **clique**.

The graph $K_{1,n}$ is called a **star**.

What is a digraph (formally)?

Edges can have a direction.

- $G = (V, E, \omega)$, where $V \neq \emptyset$ is a set, $E \subset V \times V$ (this is sometimes also called the **set of arcs**) and $\omega : E \to \mathbb{R}^+$, is called a **(weighted) digraph**
- for (i, j) ∈ E the vertex i is called predecessor of j and j is called successor of i
- similar notation simplifications as before
- N⁺(i) := {j ∈ V : (i, j) ∈ E} is the out-neighbourhood of i,
 N⁻(i) := {j ∈ V : (j, i) ∈ E} is the in-neighbourhood of i
- $d^+(i) := |N^+(i)|$ is the **out-degree** of i and $d^-(i) := |N^-(i)|$ is the **in-degree** of i



$$N^{-}(3) = \{1\},\$$

 $N^{+}(4) = \emptyset,\$
 $d^{+}(1) = 2,\$
 $d^{-}(2) = 1$

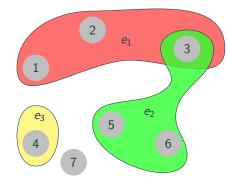
Example of a multigraph

It is sometimes necessary to allow multiple edges between two vertices or a **loop** (a self-edge). In that case we use the term **multigraph**.

What is a hypergraph (formally)?

Sometimes more than two vertices need to form an edge (certain real life situations' have this property).

- natural generalisation is a hypergraph H = (V, E), where
 - $V \neq \emptyset$ is (also) a set, but
 - E can be an arbitrary subset (the elements are called hyperedges) of the power set P(V)
- if all hyperedges are of the same size r, then H is called r-uniform



Storing graphs

Certain matrices and lists can be associated with a graph (we will see more examples later).

affinity matrix W(G):

$$w_{ij} = \begin{cases} \omega_{ij} & \text{if } \{i,j\} \in E, \\ 0 & \text{else.} \end{cases}$$

- adjacency matrix A(G): special case of W(G), where $w_{ij} = 1$ for all $ij \in E$.
- adjacency list:
 - associate list to every vertex containing its neighbours
 - call list of these lists adjacency list of the graph (treated differently in the literature)
 - not very useful for mathematical arguments
 - especially useful (for storing) when A(G) is sparse

All the above constructions are valid for directed graphs.

How to transform a digraph into a graph?

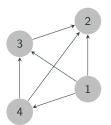
Consider the following three approaches.

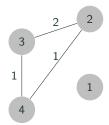
- ignore the directions
- carry out cocitation coupling
 - existence of common predecessors induce edges
 - weights are naturally given by number of common predecessors
- carry out bibliographic coupling
 - existence of common successors induce edges
 - weights are naturally given by number of common successors

Cocitation coupling

A (undirected) graph is constructed via:

- ullet cocitation c_{ij} of $i,j\in V$ is the number of common predecessors of i and j
- the **cocitation network** has vertex set V and an edge between i and j iff $c_{ij} > 0$
- ullet it is also possible to obtain a weighted graph with weights c_{ij}
- note that $c_{ij} = \sum_{k=1}^{n} a_{ki} a_{kj}$, therefore $C = A^{T} A$

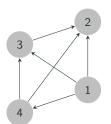


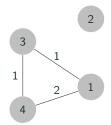


Bibliographic coupling

A (undirected) graph is constructed via:

- **bibliographic coupling** b_{ij} of $i, j \in V$ is the number of common successors of i and j
- the **bibliographic coupling network** has vertex set V and an edge between i and j iff $b_{ii} > 0$
- ullet it is also possible to obtain a weighted graph with weights b_{ij}
- note that $b_{ij} = \sum_{k=1}^{n} a_{ik} a_{jk}$, therefore $B = AA^{T}$





How to transform a hypergraph into a graph?

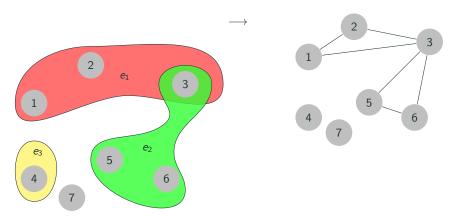
The following constructions are standard.

- clique expansion
 - the vertex set is *V*
 - each hyperedge e is replaced by an edge for every pair of vertices in e
 - this construction yields cliques for every hyperedge
- star expansion
 - vertex set is $V \cup E$
 - edge between u and e iff $u \in e$
 - every hyperedge corresponds to a star
- there are more...

Clique expansion

The clique expansion $G^{x} = (V^{x}, E^{x})$ is constructed from H = (V, E) via:

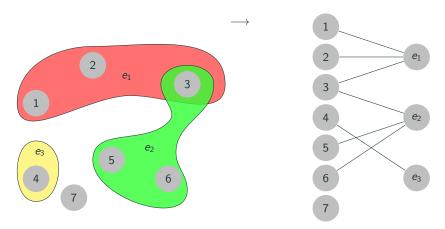
- $V^{\times} = V$
- $E^{\times} = \{\{i,j\} : \exists e \in E \text{ with } i,j \in e\}$



Star expansion

The star expansion $G^* = (V^*, E^*)$ is constructed from H = (V, E) via:

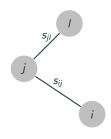
- $V^* = V \cup E$
- $E^* = \{\{i, e\} : i \in e, e \in E\}$



What if data without network structure is given?

Solution: Build your own graph!

- given a set of data points x₁, x₂..., x_n and some notion of similarity¹s_{ij} ≥ 0 between all pairs of data points x_i and x_j
- build graph G = (V, E), where the vertex i represents the data point x_i, so
 V = {1, 2, ..., n}
- $\{i,j\} \in E \text{ if } s_{ij} > 0$
- edge weight $\omega_{ij} = s_{ij}$ (edge weights represent similarities)
- G is called similarity graph (although with this particular choice of edges it is often referred to as the fully connected graph)



graph for $\{x_i, x_j, x_l\}$ with $s_{ij}, s_{jl} > 0$ and $s_{il} = 0$

The ε -neighbourhood graph

The ε -neighbourhood graph is constructed as follows:

- vertices are data points
- fix some $\varepsilon > 0$
- ullet connect all vertices whose similarities are smaller than arepsilon
- \bullet since ε is usually small, values of existing edges are roughly of the same scale
- hence usually unweighted

The (mutual) k-nearest neighbour graph

The *k*-nearest neighbour graph is constructed as follows:

- vertices are data points
- fix some k > 0
- connect i to the k nearest (w.r.t. s_{ij}) k vertices via an edge starting at i
- obtain an undirected graph by ignoring the directions

The **mutual** *k*-**nearest neighbour graph** is constructed as follows:

- vertices are data points
- fix some k
- connect i to the k nearest (w.r.t. s_{ij}) k vertices via an edge starting at i
- obtain an undirected graph by deleting all non symmetric edges

Graph Partitioning and Community

Detection

Difference

Graph Partitioning (GP)

- partition vertices into given number of groups
- sizes of groups are (roughly) fixed
- many edges inside groups, few edges between groups
- goal: dividing network into smaller more manageable pieces
- example:
 - numerical solution of network processes on a parallel computer

Community Detection (CD)

- partition vertices into groups
- sizes of groups are not fixed
- many edges inside groups, few edges between groups
- goal: understanding structure of a network
- examples:
 - collaboration
 - related web pages

Why is partitioning hard?

Problem

Partition vertex set into two parts (graph bisection).

n vertices into parts of sizes n_1 and n_2 ($n_1 + n_2 = n$):

- $\frac{n!}{n_1!n_2!}$ possibilities (half of it if order is ignored and $n_1=n_2$)
- using Stirling's formula $n! \approx \sqrt{2\pi n} (n/e)^n$ we get

$$\frac{n!}{n_1! n_2!} \approx \frac{n^{n+1/2}}{n_1^{n_1+1/2} n_2^{n_2+1/2}}$$

• for a balanced partition $(n_1 \approx n_2)$:

roughly
$$\frac{2^{n+1}}{\sqrt{n}}$$
 possibilities

Therefore, exhausitive search is usually unfeasible.

Arbitrary number of classes

Methods for graph bisection can be generalised (other ways are possible):

- number of vertices: n
- number of classes: k
- define $I = k 2^{\lfloor \log_2 k \rfloor}$
- for r = 1, ..., I (ascending order) apply graph bisection method with

$$n_1^{(r)} = n - \frac{r \cdot n}{k}$$
 and $n_2^{(r)} = \frac{n}{k}$

- apply (equally sized) graph bisection $\lfloor \log_2 k \rfloor$ times to the $n \frac{l \cdot n}{k}$ vertices in the large class
- results in k classes of (almost) same size $\frac{n}{k}$

Graph cuts

Given a graph $G = (V, E, \omega)$.

• for disjoint $A, B \subset V$ define the *cut size*

$$\operatorname{cut}(A,B) = \sum_{i \in A, j \in B} \omega_{ij}$$

• for a partition $A = A_1, A_2, \dots, A_k$ define

$$\operatorname{cut}(A_1, A_2, \dots, A_k) = \sum_{i=1}^k \operatorname{cut}(A_i, \overline{A}_i)$$

• basic problem: find A minimizing cut (A_1, A_2, \dots, A_k)

Types of methods (usually heuristics)

Local

- Kernighan-Lin algorithm
- Fiduccia-Mattheyses algorithm
- ...

Global

- Spectral clustering
- ...

Kernighan-Lin algorithm

The algorithm (Kernighan and Lin in 1970) works as follows:

Algorithmus (H)

Graph G = (V, E), positive integers n_1, n_2 Choose random partition V_1, V_2 of V with $|V_1| = n_1$ no pair of unused vertices exists minPair $\leftarrow \sum \omega_{ii} + 1$ $i \in V_1, j \in V_2$, neither i nor j has been swapped before $\operatorname{cut}((V_1 \setminus \{i\}) \cup \{j\}, (V_2 \setminus \{j\}) \cup \{i\}) \leq \min \operatorname{Pair} \operatorname{\textit{minPair}}$ $\leftarrow \operatorname{cut}((V_1 \setminus \{i\}) \cup \{i\}, (V_2 \setminus \{i\}) \cup \{i\}) \ i_0 \leftarrow i, i_0 \leftarrow i$ $V_1 = (V_1 \setminus \{i_0\}) \cup \{j_0\}, V_2 = (V_2 \setminus \{j_0\}) \cup \{i_0\} \text{ (swap } i_0 \text{ and } j_0)$ Pick partition (from the different V_1, V_2) with smallest cut size Partition V_1, V_2 of V Partition vertex set into two parts (Kernighan & Lin)

Runtime of Kernighan-Lin algorithm

At first glance we get:

- $0 \le \min\{n_1, n_2\} \le \frac{n}{2} \leadsto \mathcal{O}(n)$ swaps (worst case)
- $\frac{n}{2} \cdot \frac{n}{2}$ of considered pairs per swap (worst case)
- cut size change (swap *i* and *j*):

$$\sum_{v \in N(i) \cap V_1} \omega_{iv} + \sum_{v \in N(j) \cap V_2} \omega_{jv} - \sum_{v \in N(i) \cap V_2} \omega_{iv} - \sum_{v \in N(j) \cap V_1} \omega_{jv} + \omega_{ij}$$

- evaluating this expression costs $\mathcal{O}(m/n)$, where m=|E|, if stored in adjacency list
- \rightsquigarrow runtime is $\mathcal{O}(m \cdot n^2)$ for one (!) round

Notes on the Kernighan-Lin algorithm

- swapping every round avoids local minima
- usually the algorithm is repeated several times with last output as input
- first partition is random → sometimes algorithm is started more than once to get other (hopefully better) results
- convergence rate unknown
- for larger number of classes (i.e. $k \ge 3$) optimum might not be reached if applied
- Generalisation to hypergraphs: Fiduccia-Mattheyses algorithm

Spectral clustering

- mathematical foundation by Donath & Hoffman and Fiedler in 1973
- applications in various fields/for various problems
 - image segmentation
 - educational data mining
 - entity resolution
 - speech separation
 - ...

Laplacian matrix (and another graph definition)

The degree matrix D(G) is given by

$$d_{ij} = \begin{cases} \sum_{I \in N(i)} w_{iI} & \text{if } i = j, \\ 0 & \text{else.} \end{cases}$$

Laplacian matrix:

$$L(G) = D(G) - W(G)$$

We also need:

$$\operatorname{vol}(A) = \sum_{ij \in E, i,j \in A} \omega_{ij} \text{ for } A \subset V \text{ (no double counting!)}$$

Spectral clustering and graph cuts

Clustering corresponds to finding cuts in graphs (see next slides; other interpretations possible), there are (usually) two types:

- RatioCut (balanced by number of vertices in each cluster)
- NCut (balanced by sum of edge weights in each cluster)

Formalization of RatioCut and NCut

- RatioCut $(A_1, A_2, \dots, A_k) = \sum_{i=1}^k \frac{\operatorname{cut}(A_i, \overline{A}_i)}{|A_i|}$
 - $\sum_{i=1}^{k} (1/|A_i|)$ is minimized if all A_i have the same size
 - hence minimizing RadioCut balances clusters by their number of vertices (as desired)
- $\mathsf{NCut}(A_1, A_2, \dots, A_k) = \sum_{i=1}^k \frac{\mathsf{cut}(A_i, \overline{A}_i)}{\mathsf{vol}(A_i)}$
 - $\sum_{i=1}^{k} (1/\text{vol}(A_i))$ is minimized if all $\text{vol}(A_i)$ coincide
 - hence minimizing NCut balances clusters by their edge weights (as desired)
- · corresponding optimization problems are NP hard
- spectral clustering is a way to solve relaxed versions of those problems

Useful properties of the Laplacian

Proposition: The Laplacian matrix L (= D - W) satisfies the following properties:

i For every vector $f \in \mathbb{R}^n$ we have

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

- ii L is symmetric and positive semi-definite.
- iii The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector.
- iv L has n non-negative, real-valued eigenvalues $0=\lambda_1\leq \lambda_2\leq \cdots \leq \lambda_n.$

Useful properties of the Laplacian

Proof:

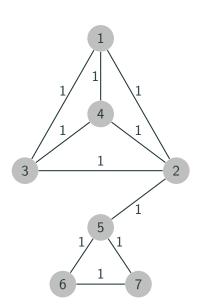
i By the definition of d_i ,

$$f^{T}Lf = f^{T}Df - f^{T}Wf = \sum_{i=1}^{n} d_{i}f_{i}^{2} - \sum_{i,j=1}^{n} f_{i}f_{j}w_{ij}$$

$$= \frac{1}{2} \left(\sum_{i=1}^{n} d_{i}f_{i}^{2} - 2 \sum_{i,j=1}^{n} f_{i}f_{j}w_{ij} + \sum_{j=1}^{n} d_{j}f_{j}^{2} \right) = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij}(f_{i} - f_{j})^{2}.$$

- ii The symmetry of L follows directly from the symmetry of W and D. The positive semi-definiteness is a direct consequence of Part (i), which shows that $f^T L f \geq 0$ for all $f \in \mathbb{R}^n$.
- iii All eigenvalues are real (symmetric matrix). The rest follows easily from Part (ii) and the defining equation of eigenvalues.
- iv This is a direct consequence of (i)-(iii).

Graph cuts and spectral clustering



$$f^{T}Lf = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2$$

Connectivity

Proposition: The number of connected components of a graph is equal to the multiplicity of the first eigenvalue (which is 0) of the graph Laplacian matrix.

Goal is to solve

$$\min_{A\subset V}\mathsf{RatioCut}(A,\overline{A})$$

Reformulation: for $A \subset V$ define $f = (f_1, \dots, f_n) \in \mathbb{R}^n$ (some kind of indicator vector) via

$$f_i = \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A, \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \in \overline{A}. \end{cases}$$

It can be shown that

$$f^T L f = |V| \cdot \mathsf{RatioCut}(A, \overline{A})$$

Proof:

$$2f^{T}Lf = \sum_{i,j=1}^{n} w_{ij} (f_{i} - f_{j})^{2}$$

$$= \sum_{i \in A, j \in \overline{A}} w_{i,j} \left(\sqrt{\frac{|\overline{A}|}{|A|}} + \sqrt{\frac{|A|}{|\overline{A}|}} + \sum_{i \in \overline{A}, j \in A} w_{i,j} \left(-\sqrt{\frac{|\overline{A}|}{|A|}} - \sqrt{\frac{|A|}{|\overline{A}|}} \right)^{2}$$

$$= 2 \operatorname{cut}(A, \overline{A}) \left(\frac{|\overline{A}|}{|A|} + \frac{|A|}{|\overline{A}|} + 2 \right)$$

$$= 2 \operatorname{cut}(A, \overline{A}) \left(\frac{|A| + |\overline{A}|}{|A|} + \frac{|A| + |\overline{A}|}{|\overline{A}|} \right)$$

$$= 2|V| \cdot \operatorname{RatioCut}(A, \overline{A})$$

Further, f is orthogonal to 1:

$$\sum_{i=1}^n f_i = \sum_{i \in A} \sqrt{\frac{|\overline{A}|}{|A|}} - \sum_{i \in \overline{A}} \sqrt{\frac{|A|}{|\overline{A}|}} = |A| \sqrt{\frac{|\overline{A}|}{|A|}} - |\overline{A}| \sqrt{\frac{|A|}{|\overline{A}|}} = 0.$$

Finally

$$||f||^2 = \sum_{i=1}^n f_i^2 = |A| \frac{|\overline{A}|}{|A|} + |\overline{A}| \frac{|A|}{|\overline{A}|} = |\overline{A}| + |A| = n.$$

Hence the minimization problem is equivalent to

$$\min_{A \subset V} f^T L f$$

subject to the given f.

This problem is NP-hard since the solution vector only takes two particular values.

Relaxing this problem is possible:

$$\min_{f \in \mathbb{R}^n} f^T L f \text{ subject to } f \perp 1, ||f|| = \sqrt{n}$$

The Rayleigh-Ritz theorem (see e.g. Strang - Linear algebra and its applications) gives the solution of this problem via an eigenvector corresponding to the second smallest eigenvalue of L.

Remark: Solution has to be transformed!

Special case (k = 2) of unnormalized spectral clustering

Algorithmus (H)

Weight matrix (or any similarity matrix) $S \in \mathbb{R}^{n \times n}$ Construct similarity graph G Compute L(G) Compute Eigenvectors X_1 and X_2 of L(G) Build $U \in \mathbb{R}^{n \times 2}$ with X_1 and X_2 as columns Rows of U are $y_1, y_2, \ldots, y_n \in \mathbb{R}^2$ Cluster y_1, y_2, \ldots, y_n into Clusters C_1 and C_2 (k-means) Clusters $A_1 = \{j : y_j \in C_1\}$ and $A_2 = \{j : y_j \in C_2\}$ Unnormalized spectral clustering (k = 2)

Relaxation of RatioCut for k > 2 (sketch)

• Define k indicator vectors $h_j = (h_{1,j}, h_{2,j}, \dots, h_{n,j})^T$ via

$$h_{i,j} = \begin{cases} 1/\sqrt{|A_j|} & \text{if } v_i \in A_j, \\ 0 & \text{else} \end{cases}$$

- Matrix $H \in \mathbb{R}^{n \times k}$ with columns h_1, h_2, \dots, h_k is orthogonal
- We have $h_i^T L h_i = \frac{\text{cut}(A_i, \overline{A_i})}{|A_i|}$ and $h_i^T L h_i = (H^T L H)_{ii}$
- Together this yields RatioCut $(A_1, A_2, \dots, A_k) = \operatorname{tr}(H^T L H)$
- Hence the minimum of RatioCut (A_1, A_2, \dots, A_k) can be approximated by solving (the relaxed version)

$$\min_{H \in \mathbb{R}^{n \times k}} \operatorname{tr}(H^T L H)$$
 subject to $H^T H = I$

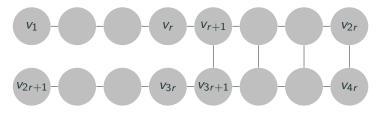
General case of unnormalized spectral clustering

Algorithmus (H)

Weight matrix (or any similarity matrix) $S \in \mathbb{R}^{n \times n}$, number k of clusters Construct similarity graph G Compute L(G) Compute Eigenvectors X_1, X_2, \ldots, X_k of L(G) Build $U \in \mathbb{R}^{n \times k}$ with X_1, X_2, \ldots, X_k as columns Rows of U are $y_1, y_2, \ldots, y_n \in \mathbb{R}^k$ Cluster y_1, y_2, \ldots, y_n into Clusters C_1, C_2, \ldots, C_k (k-means) Clusters A_1, A_2, \ldots, A_k with $A_i = \{j : y_j \in C_i\}$ Unnormalized spectral clustering

Notes on spectral clustering

- faster $(\mathcal{O}(mn))$ or $\mathcal{O}(n^2)$ for the eigenvector calculation) than Kernighan-Lin
- quality of approximated solution can be arbitrarily far from exact solution (cockroach graphs for k=2)



- other relaxations possible (and probably useful)
- any other clustering algorithm may be used instead of k-means

Computing eigenvalues

- find roots of characteristic polynomial (computationally expensive)
- power method: iterate (with any starting vector $X_{(0)}$)

$$X_{(I)} = A^I X_{(0)}$$

- power method converges to eigenvector X corresponding to (w.r.t. absolute value) largest eigenvalue
- power method is fast but
 - method does not work if $X_{(0)}$ is orthogonal to X (can be avoided by choosing all entries of $X_{(0)}$ to be positive, since X has only entries of same sign)
 - entries of X_(I) become large during the iterative process (renormalization helps)
 - When are we done? (option is to start with two different vectors)

Computational complexity of the power method

Two aspects:

- complexity of one multiplication
- required number of multiplications

First aspect:

- n^2 multiplications if stored in adjacency matrix
- less if matrix is stored in adjacency lists and matrix is sparse
 - compute

$$\sum_{j\in N(i)} X_{(I)_j}$$

which gives the *i*-th entry of $X_{(l+1)}$

• therefore a total of

$$\sum_{i} d(i) = 2m$$

operations (m being the number of edges in the graph)

Computational complexity of the power method

Second aspect:

- it can be shown that this is $\mathcal{O}(n)$
- we will come back to this

Total computational complexity is $\mathcal{O}(mn)$, which means

- $\mathcal{O}(n^2)$ if graph is sparse
- $\mathcal{O}(n^3)$ if graph is dense

→ use adjacency list

Computing other eigenvalues

We have

$$(\lambda_n I - L)X_i = (\lambda_n - \lambda_i)X_i$$

hence eigenvalues are reversed for matrix $\lambda_n I - L$

 \leadsto smallest eigenvalue can be calculated with power method

Computing other eigenvalues

Trick to compute second largest eigenvalue:

- X_n normalised eigenvector corresponding to largest eigenvalue λ_n
- choose starting vector X and define

$$Y = X - (X_n^T X) X_n$$

we have

$$X_i^T Y = \begin{cases} 0 & \text{if } i = n, \\ X_i^T X & \text{otherwise} \end{cases}$$

therefore

$$Y = \sum_{i=1}^{n-1} c_i X_i$$

where $c_i = X_i^T Y$

 \rightsquigarrow use Y as starting vector for power method

Compute all eigenvalues and eigenvectors

Combining methods for given (symmetric) matrix A with eigenvectors X_i and eigenvalues λ_i :

- Find orthogonal matrix Q with $B = Q^T A Q$ being a tridiagonal matrix
 - $Q^T X_i$ is eigenvector of B
 - B can be found efficiently, e.g. by Householder algorithm or Lancosz algorithm
- compute eigenvalues and eigenvectors of B
 - these give eigenvalues and eigenvectors of A
 - can be done using for example the QL algorithm