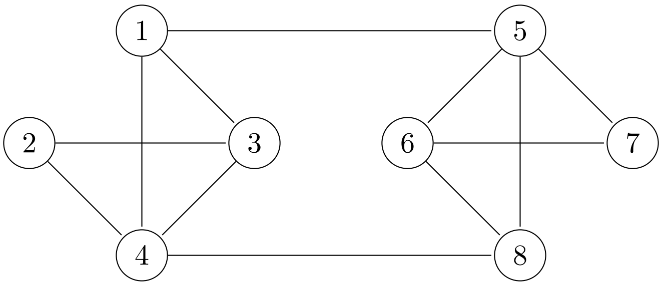
Exercise 1 (Spectral Clustering) 0 points

Consider the following graph $G = (V, E)$ with node set $V = \{1, \ldots, 8\}$.



Let $s\colon \{1, \ldots, 8\}^2 \to \mathbb{R}_{\geq 0}$ be the similarity measure that is defined by

$$s(v, w) = \begin{cases} 1 & \text{if } v = w, \\ 1 & \text{if } (v, w) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

We want to cluster the vertices of this graph using spectral clustering methods. Solve the following tasks.

a) Compute the Laplacian L of the similarity matrix S associated with s.

b) Compute the two smallest eigenvalues λ_1 and λ_2 of L along with corresponding eigenvectors $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^8$.

Hint: Use a computer to solve this task. Your solution should be sufficiently precise but needs not be exact. Round your final values to three decimal places.

c) What is special about the eigenpair belonging to the smallest eigenvalue of L? Justify your answer.

d) Plot the points $\big((\mathbf{u}_1)_i, (\mathbf{u}_2)_i\big)$ for all $i = 1, \ldots, 8$.

e) Using your plot from part d), discuss which clustering of V is returned by the Spectral Clustering algorithm on S with $k = 2$.

Solution:

a) The similarity matrix is

$$S = \begin{pmatrix} 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \end{pmatrix}.$$

The matrix D is

$$D = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}.$$

The Laplacian L is

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

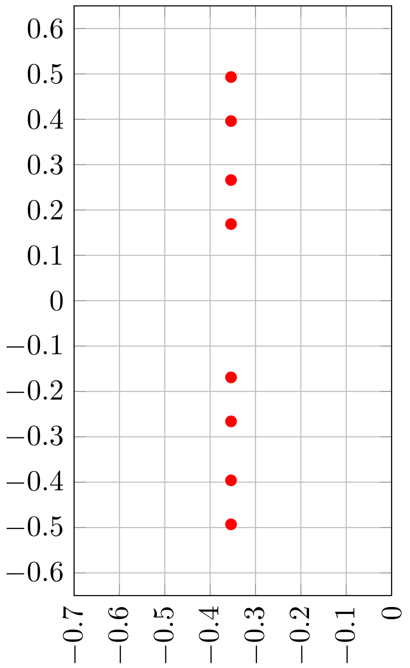
b) The two smallest eigenvalues are $\lambda_1 = 0$ and $\lambda_2 \approx 0.657$. The corresponding normalised eigenvectors are

$$\mathbf{u}_1 \approx \begin{pmatrix} -0.354 \\ -0.354 \\ -0.354 \\ -0.354 \\ -0.354 \\ -0.354 \\ -0.354 \\ -0.354 \end{pmatrix} \quad \text{and} \quad \mathbf{u}_2 \approx \begin{pmatrix} 0.169 \\ 0.493 \\ 0.396 \\ 0.266 \\ -0.266 \\ -0.396 \\ -0.493 \\ -0.169 \end{pmatrix}$$

Hint: See part c).

c) By construction of the Laplacian, the smallest eigenvalue is *always* 0 with eigenvector $\frac{1}{\sqrt{n}} \cdot \mathbf{1}$. Numerical methods for b) may return a very small negative eigenvalue due to imprecision, but this is not possible, since L is always positive semi-definite.

d)



e) Clustering the points from d) with 2-means (and a suitable initialization) will return two clusters that correspond to the clustering $\{\{1,2,3,4\},\{5,6,7,8\}\}$ of the graph.

Exercise 2 (Naive DNF Counting) **1+4+5=10 points**

We consider the following naive rejection sampling algorithm for counting the number μ of satisfying DNF assignments:

1. For some m, independently sample m assignment $\alpha_1, \dots, \alpha_m$ for the n variables, uniformly at random from the 2^n possible assignments

2. For each i, let $y_i := \begin{cases} 1 & \text{if satisfing assigment,} \\ 0 & \text{else} \end{cases}$

3. Return $\hat{\mu} = \frac{2^n}{m} \sum_{i=1}^m y_i$ as the estimate.

a) Determine the minimum number of samples that is needed to return an estimate that deviates from μ by at most ε with a probability of $1 - \delta$, using Lemma 6.1.

b) Improve the bound computed in (a) to $m \geq \frac{2^{n-1} \ln(2/\delta)}{\varepsilon^2}$. Proof your result.

Hint: You can follow the general idea of the proof of Lemma 6.1 in the lecture.

c) Assume μ can be bounded by some polynomial $\alpha(n)$. Show that even after sampling $2^{n/2}$ assignments the probability of finding even a single satisfying assignment is exponentially small in n.

Hint: The following inequality may be useful for achieving the desired bound (you may use it without showing it to hold):

$$1 + \alpha x \leq (1 + \alpha)^x \qquad \text{for all } x \geq 1 \text{ and } \alpha \geq -1. \tag{1}$$

Solution:

a) We have $b = \max \left\{ |f(\omega)| \middle| \omega \in \Omega \right\} = \max_{y \in \{0,1\}} 2^n y = 2^n$ and thus we get

$$m \geq \frac{2^n \ln(2/\delta)}{\varepsilon^2}.$$

b) Let $X_i := 2^n y_i$ and $X = \sum_{i=1}^m X_i$. Note that

$$\mu = \mathrm{E}(X_i) = \frac{1}{m} \mathrm{E}(X).$$

Since $\mathrm{rg}(X_i) \in [0, 2^n]$, by Lemma 6.2 we have

$$\Pr\left(|\hat{\mu} - \mu| \geq \varepsilon \right) = \Pr\left(|X - m\mu| \geq \varepsilon m \right) \leq 2 \exp\left(-\frac{2\varepsilon^2}{2^n} m \right).$$

With $m \geq \frac{2^{n-1}\ln(2/\delta)}{\varepsilon^2}$, we have

$$\frac{\varepsilon^2}{2^{n-1}} m \geq \ln\left(\frac{2}{\delta}\right)$$

and thus

$$2\exp\left(-\frac{\varepsilon^2}{2^{n-1}} m\right) \leq 2\exp\left(-\ln\left(\frac{2}{\delta}\right)\right) = \delta.$$

Thus we can improve the bound to $m \geq \frac{2^{n-1}\ln(2/\delta)}{\varepsilon^2}$.

c) The probability that a uniformly at random drawn assignment is satisfying is $a := \frac{\alpha(n)}{2^n}$. We know from the lecture that RS accepts in at most k rounds with probability $1-(1-a)^k$. Thus for $k = 2^{n/2}$ we get

$$\begin{aligned} 1-(1-a)^{2^{n/2}} &\overset{(1)}{\leq} 1-(1-a2^{n/2}) \\ &= a2^{n/2} = \frac{2^{n/2}\alpha(n)}{2^n} = \alpha(n)2^{-n/2}. \end{aligned}$$

For an arbitrary polynomial $\alpha(n)$ this value is exponentially small in n.

Exercise 3 (Symmetric Markov Chains) **5 points**

A Markov chain $\mathcal{Q}$ is called *symmetric* if its transition matrix Q is symmetric.

Show that there exists a unique probability vector $\boldsymbol{\pi} \in \mathbb{R}^{1\times n}$ such that $\boldsymbol{\pi}$ is the stationary distribution of $\mathcal{Q}$ for all connected, symmetric Markov chains $\mathcal{Q}$ with state space $[n]$.

Solution:

Let $Q \in \mathbb{R}^{n\times n}$ be the transition matrix of a connected, symmetric Markov chain $\mathcal{Q}$. Then $Q = Q^\mathsf{T}$. Since Q is stochastic, the column entries in each row sum to 1: $\sum_{j\in[n]} q_{i,j} = 1$ for all $i \in [n]$. Since Q is symmetric, the same holds for the columns of Q: $\sum_{i\in[n]} q_{i,j} = 1$ for all $j \in [n]$.

Now let $\mathbf{x} := (1, \dots, 1) \in \mathbb{R}^{1\times n}$. Then for all $j \in [n]$ we have $(\mathbf{x}Q)_j = \sum_{i\in[n]} 1 \cdot q_{i,j} = 1$, i. e. $\mathbf{x}Q = \mathbf{x}$.

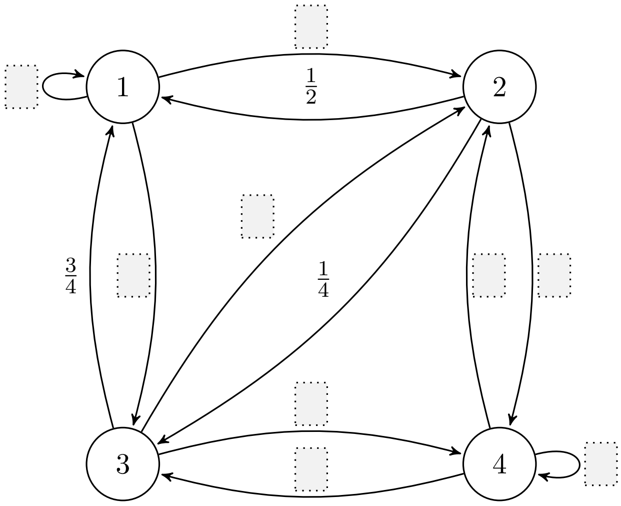
Define $\boldsymbol{\pi} = \frac{\mathbf{x}}{n} = \left(\frac{1}{n}, \dots, \frac{1}{n}\right) \in \mathbb{R}^{1\times n}$. Then $\boldsymbol{\pi}$ is a probability vector and

$$\boldsymbol{\pi}Q = \tfrac{1}{n}\mathbf{x}Q = \tfrac{1}{n}\mathbf{x} = \boldsymbol{\pi}.$$

Since $\mathcal{Q}$ is connected, $\boldsymbol{\pi}$ is unique with this property by Theorem 6.9 of the lecture. Thus, $\boldsymbol{\pi}$ is the unique stationary distribution of every symmetric, connected Markov chain with state space $[n]$.

Exercise 4 (Completing Markov Chains) **5 points**

Consider the following incomplete graphical representation of a Markov chain with 4 states. Therein, all missing edges have probability 0.



Fill in the gaps in the graphical representation such that the stationary distribution of the Markov chain becomes $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3, \pi_4) = \left(\frac{1}{2}, \frac{1}{12}, \frac{1}{4}, \frac{1}{6}\right)$ where π_i denotes the probability of being in state i. Justify your solution.

Hint: You may use Lemma 6.11 to solve this exercise.

Solution:

We use the equations $\pi_i q_{ij} = \pi_j q_{ji}$ for all $i, j \in [4]$ from Lemma 6.11 of the lecture and the equations $q_{i1} + q_{i2} + q_{i3} + q_{i4} = 1$ for all $i \in [4]$.

State 1:

- The equality $\pi_1 q_{12} = \pi_2 q_{21}$ yields $\frac{1}{2} \cdot q_{12} = \frac{1}{12} \cdot \frac{1}{2}$, so $q_{12} = \frac{1}{12}$.
- The equality $\pi_1 q_{13} = \pi_3 q_{31}$ yields $\frac{1}{2} \cdot q_{13} = \frac{1}{4} \cdot \frac{3}{4}$, so $q_{13} = \frac{3}{8}$.
- The equality $q_{11} + q_{12} + q_{13} + q_{14} = 1$ yields $q_{11} + \frac{1}{12} + \frac{3}{8} + 0 = 1$, so $q_{11} = \frac{13}{24}$.

State 2:

- The equality $q_{21} + q_{22} + q_{23} + q_{24} = 1$ yields $\frac{1}{2} + 0 + \frac{1}{4} + q_{24} = 1$, so $q_{24} = \frac{1}{4}$.

State 3:

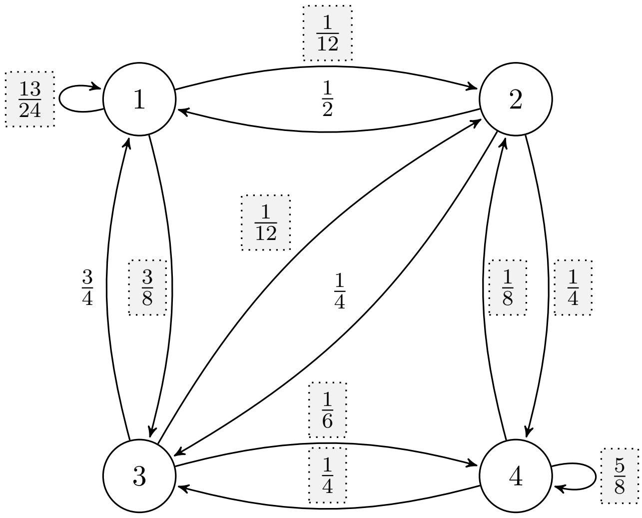
- The equality $\pi_2 q_{23} = \pi_3 q_{32}$ yields $\frac{1}{12} \cdot \frac{1}{4} = \frac{1}{4} \cdot q_{32}$, so $q_{32} = \frac{1}{12}$.
- The equality $q_{31} + q_{32} + q_{33} + q_{34} = 1$ yields $\frac{3}{4} + \frac{1}{12} + q_{33} + 0 = 1$, so $q_{34} = \frac{2}{12} = \frac{1}{6}$.

State 4:

- The equality $\pi_2 q_{24} = \pi_4 q_{42}$ yields $\frac{1}{12} \cdot \frac{1}{4} = \frac{1}{6} \cdot q_{42}$, so $q_{42} = \frac{1}{8}$.

- The equality $\pi_3 q_{34} = \pi_4 q_{43}$ yields $\frac{1}{4} \cdot \frac{1}{6} = \frac{1}{6} \cdot q_{43}$, so $q_{43} = \frac{1}{4}$.
- The equality $q_{41} + q_{42} + q_{43} + q_{44} = 1$ yields $0 + \frac{1}{8} + \frac{1}{4} + q_{44} = 1$, so $q_{44} = \frac{5}{8}$.

Note that with these definitions, Q is a well-defined transition matrix. The resulting Markov chain $\mathcal{Q}$ is depicted below.



Since Q and $\boldsymbol{\pi}$ fulfill the conditions of Lemma 6.11, $\boldsymbol{\pi}$ is the stationary distribution of $\mathcal{Q}$. Note that Q was derived using a system of 9 linear independent equations in 9 variables. Thus Q is the unique solution that satisfies Lemma 6.11.