Laplacian Matrix for Dimensionality Reduction and Clustering

— Exercises without Solutions —

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These exercises complement my corresponding lecture notes, and there is a version with and one without solutions. The table of contents of the lecture notes is reproduced here to give an orientation when the exercises can be reasonably solved. For best learning effect I recommend to first seriously try to solve the exercises yourself before looking into the solutions.
More teaching material is available at https://www.ini.rub.de/PEOPLE/wiskott/Teaching/Material/.

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1 Introduction

2 Intuition

2.1 Heat diffusion analogy of Laplacian eigenmaps

2.2 Heat diffusion analogy of spectral clustering

2.3 Heat diffusion equation for connected heat reservoirs

2.4 Laplacian matrix

2.4.1 Exercise: Laplacian matrix is positive semi-definite

1. Create a small undirected graph with four vertices without loops and edge weights one and calculate its Laplacian.

2. For a directed graph $G = (V, E)$ without loops with vertices $V = \{v_1, ..., v_n\}$ and edges $E = \{e_1, ..., e_m\}$ (where edges are ordered pairs $e_i = (v_j, v_k)$ indicating a connection to node v_j from node v_k) the $n \times m$ incidence matrix $B = (b_{ij})$ is defined as:

$$b_{ij} := \begin{cases} +1 & \text{if } e_j = (v_i, v_x) \\ 0 & \text{if } v_i \notin e_j \\ -1 & \text{if } e_j = (v_x, v_i) \end{cases} \tag{1}$$

   with v_x being an arbitrary vertex. (Sometimes the transpose is defined as the incidence matrix.)

   Treat the undirected graph above as a directed graph, where the edges always go from the lower to the higher index vertex, and calculate its incidence matrix.

3. Show that $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{B}^T$. Argue also why this is generally the case, not only in this concrete example.

4. Show that $\boldsymbol{L} = \boldsymbol{M}\boldsymbol{M}^T$ also holds for a Laplacian matrix with weights not equal to $+1$, thus for a graph with general weighting of the edges, with an appropriately chosen matrix $\boldsymbol{M}$.

5. Prove that $\boldsymbol{L}$ is positive semi-definite.

2.5 Solution of the heat diffusion equation

2.5.1 Exercise: Eigenvectors and -values of the Laplacian matrix

Consider the Laplacian matrix

$$\boldsymbol{L} = \begin{pmatrix} a & -a & 0 \\ -a & a+b & -b \\ 0 & -b & b \end{pmatrix} \tag{1}$$

with $0 < a, b$.

1. Solve the ordinary eigenvalue problem $\boldsymbol{L}\boldsymbol{u}_i = \gamma_i \boldsymbol{u}_i$ for $i = 1, 2, 3$.

   Hint 1: A somewhat tedious calculation yields

$$0 \stackrel{!}{=} |\boldsymbol{L} - \gamma \boldsymbol{I}| = (a-\gamma)(a+b-\gamma)(b-\gamma) - (a-\gamma)b^2 - (b-\gamma)a^2 \tag{2}$$
$$\Longleftarrow \quad \gamma_2 = (a+b) - \sqrt{a^2 - ab + b^2} \tag{3}$$
$$\vee \quad \gamma_3 = (a+b) + \sqrt{a^2 - ab + b^2} \tag{4}$$

   You may take this for granted to also find γ_1 and $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, and $\boldsymbol{u}_3$.

   Hint 2: One can easily make hypotheses about $\boldsymbol{u}_2$ and $\boldsymbol{u}_3$ by looking at $\boldsymbol{L}$. Do not try to calculate them.

2.5.2 Exercise: Laplacian matrix for disconnected graphs

1. Show that a Laplacian matrix of a graph with N disconnected subgraphs, i.e. subgraphs that have no edges between them, has at least N eigenvectors with eigenvalue zero.
2. Argue why there are no more than N eigenvectors with eigenvalue zero.

   Hint: You may use the relation

$$\frac{1}{2}\sum_{ij}(u_i - u_j)^2 W_{ij} = \boldsymbol{u}^T \boldsymbol{L} \boldsymbol{u} \tag{1}$$

3. Do the results above also hold for the generalized eigenvalue equation

$$\boldsymbol{L}\boldsymbol{w} = \lambda \boldsymbol{D}\boldsymbol{w} \tag{2}$$

3 Formalism

3.1 Simple graphs

3.2 Matrix representation

3.3 Optimization problem

3.4 Associated eigenvalue problem

3.4.1 Exercise: Objective function of the Laplacian matrix

Given the Laplacian matrix

$$\boldsymbol{L} := \boldsymbol{D} - \boldsymbol{W} \tag{1}$$
$$\iff L_{ij} = D_{ii}\delta_{ij} - W_{ij} \tag{2}$$

with symmetric $W_{ij} = W_{ji}$ and

$$D_{ii} := \sum_j W_{ij} = \sum_j W_{ji} \tag{3}$$

Show that

$$\frac{1}{2}\sum_{i,j}(y_i - y_j)^2 W_{ij} = \boldsymbol{y}^T \boldsymbol{L} \boldsymbol{y} \tag{4}$$

3.4.2 Exercise: Generalized eigenvalue problem

Consider the generalized eigenvalue problem

$$\boldsymbol{A}\boldsymbol{u}_i = \lambda_i \boldsymbol{B}\boldsymbol{u}_i \tag{1}$$

with some real $N \times N$ matrices $\boldsymbol{A}$ and $\boldsymbol{B}$. The λ_i are the right-eigenvalues and the $\boldsymbol{u}_i$ are the (non-zero) right-eigenvectors. To find corresponding left-eigenvalues μ_i and left-eigenvectors $\boldsymbol{v}_i$, one has to solve the equation

$$\boldsymbol{v}_i^T \boldsymbol{A} = \mu_i \boldsymbol{v}_i^T \boldsymbol{B} \tag{2}$$

1. Show that left- and right-eigenvalues are identical.
2. Show that $\boldsymbol{v}_j^T \boldsymbol{A}\boldsymbol{u}_i = 0$ as well as $\boldsymbol{v}_j^T \boldsymbol{B}\boldsymbol{u}_i = 0$ for $\lambda_i \neq \lambda_j$.

   Hint: Consider (1) and (2) simultaneously with different eigenvalues.
3. Show that for symmetric $\boldsymbol{A}$ and $\boldsymbol{B}$ the right-eigenvectors are also left-eigenvectors.
4. Show that for symmetric $\boldsymbol{A}$ and $\boldsymbol{B}$ we have $\boldsymbol{u}_j^T \boldsymbol{A}\boldsymbol{u}_i = 0$ as well as $\boldsymbol{u}_j^T \boldsymbol{B}\boldsymbol{u}_i = 0$ for $\lambda_i \neq \lambda_j$.
5. For symmetric $\boldsymbol{A}$ and $\boldsymbol{B}$ it is convenient to normalize the eigenvectors such that $\boldsymbol{u}_i^T \boldsymbol{B}\boldsymbol{u}_i = 1$. Assume the eigenvectors form a basis, i.e. they are complete, and you want to represent an arbitrary vector $\boldsymbol{y}$ wrt this basis, i.e.

   $$\boldsymbol{y} = \sum_i \alpha_i \boldsymbol{u}_i \tag{3}$$

   Which constraint on the α_i follows from the constraint $\boldsymbol{y}^T \boldsymbol{B}\boldsymbol{y} = 1$?
6. Assume $\boldsymbol{A}$ and $\boldsymbol{B}$ are symmetric and you want to minimize (or maiximze) $\boldsymbol{y}^T \boldsymbol{A}\boldsymbol{y}$ under the constraint $\boldsymbol{y}^T \boldsymbol{B}\boldsymbol{y} = 1$. What is the solution?

   Hint: Use ansatz (3) and assume $\boldsymbol{u}_i^T \boldsymbol{B}\boldsymbol{u}_i = 1$.

3.4.3 Exercise: Eigenvectors of a graph with six nodes

Consider a graph with six nodes arranged in a 2×3 lattice with edges of weight 1 between direct neighbors, like the one shown in the figure.

Make an educated guess how the six eigenvectors of the corresponding Laplacian matrix might look.

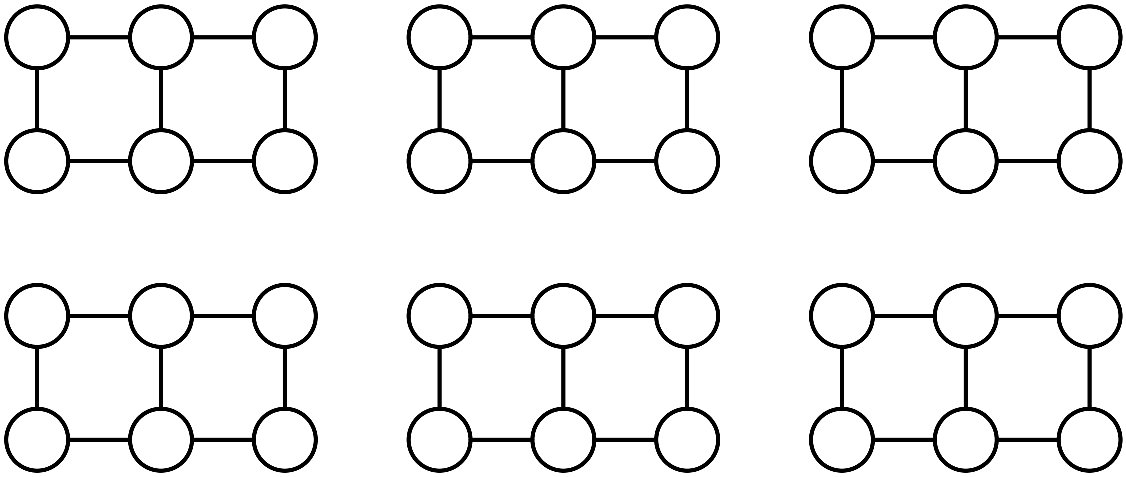

Figure: Graph with six nodes. Color the nodes red/blue or mark them with +/- according to the sign you give them. Nodes with value near zero stay empty.

3.4.4 Exercise: Example of Laplacian eigenmaps with three nodes

Given a connected graph with vertices v_i and undirected edges $e_k = (v_i, v_j)$ with symmetric positive weights W_{ij}, the goal of the Laplacian eigenmaps algorithm is to asign a value w_i to each vertex v_i to

$$\text{minimize} \quad \frac{1}{2}\sum_{i,j}(w_i - w_j)^2 W_{ij} \tag{1}$$

under the constraints

$$\begin{aligned} \boldsymbol{w}^T \boldsymbol{D}\mathbf{1} &= 0 \quad \text{(weighted zero mean)} && (2)\\ \text{and} \quad \boldsymbol{w}^T \boldsymbol{D}\boldsymbol{w} &= 1 \quad \text{(weighted unit variance)} && (3) \end{aligned}$$

where $\boldsymbol{D}$ is a diagonal matrix with

$$D_{ii} \;:=\; \sum_j W_{ij} = \sum_j W_{ji} \quad \text{(since } \boldsymbol{W} \text{ is symmetric)} \tag{4}$$

One can show that this is solved by the second eigenvector of the generalized eigenvalue equation

$$\boldsymbol{L}\boldsymbol{w} \;=\; \lambda \boldsymbol{D}\boldsymbol{w} \tag{5}$$

with the Laplacian matrix

$$\begin{aligned} \boldsymbol{L} &:= \boldsymbol{D} - \boldsymbol{W} && (6)\\ \iff \quad L_{ij} &= D_{ii}\delta_{ij} - W_{ij} && (7) \end{aligned}$$

Verify this statement for the graph with the following Laplacian matrix:

$$\boldsymbol{L} = \begin{pmatrix} a & -a & 0 \\ -a & a+b & -b \\ 0 & -b & b \end{pmatrix} \tag{8}$$

with $0 < a, b$. Proceed as follows.

1. Sketch the graph of the Laplacian matrix.
2. Solve the generalized eigenvalue problem $\boldsymbol{L}\tilde{\boldsymbol{w}}_i = \lambda_i \boldsymbol{D}\tilde{\boldsymbol{w}}_i$ for $i = 1, 2, 3$. The eigenvectors do not need to be normalized yet, that is done in the next step.
3. Check the eigenvectors whether they are consistent with constraint (2).
4. Scale the eigenvectors such that they become consistent with constraint (3).

   Hint: Use the notation $\boldsymbol{w}_i := \sigma_i \tilde{\boldsymbol{w}}_i$ with appropriate scaling factors σ_i (with $0 < \sigma_i$ to make it unique).
5. Any vector in $\boldsymbol{y} \in \mathbb{R}^3$ can be written as a linear combination of the three normalized eigenvectors, i.e.

$$\boldsymbol{y} = \sum_{i=1}^{3} \alpha_i \boldsymbol{w}_i \tag{9}$$

   Derive constraints on the α_i that follow if we impose constraints (2,3) on $\boldsymbol{y}$.
6. Find weights α_i that are consistent with constraints (2,3) and that minimize the objective function.
7. Plot the result of the Laplacian eigenmaps algorithm for this simple example, i.e. visualize the components of $\boldsymbol{w}_2$ and $\boldsymbol{w}_3$ in a 2D plot. Discuss, how the plot changes with a and b.

3.4.5 Exercise: Constraints of the Laplacian eigenmaps

In the Laplacian eigenmap algorithm, each vertex v_i of a graph with symmetric edge weights W_{ij} gets asigned a value w_i with the goal to

$$\text{minimize} \quad \frac{1}{2}\sum_{ij}(w_i - w_j)^2 W_{ij} \tag{1}$$

under the constraints

$$\begin{aligned} \boldsymbol{w}^T\boldsymbol{D}\boldsymbol{1} &= 0 \quad \text{(weighted zero mean)} && (2)\\ \text{and} \quad \boldsymbol{w}^T\boldsymbol{D}\boldsymbol{w} &= 1 \quad \text{(weighted unit variance)} && (3)\end{aligned}$$

One can show that

$$\frac{1}{2}\sum_{ij}(w_i - w_j)^2 W_{ij} = \boldsymbol{w}^T\boldsymbol{L}\boldsymbol{w} \tag{4}$$

where

$$\begin{aligned} L_{ij} &:= D_{ii}\delta_{ij} - W_{ij} && (5)\\ \text{with} \quad D_{ii} &:= \sum_j W_{ij} && (6)\end{aligned}$$

Show whether it is possibly to find an invertible linear coordinate transformation

$$\tilde{\boldsymbol{w}} = \boldsymbol{T}\boldsymbol{w} \tag{7}$$

such that the optimization problem simplifies to

$$\text{minimize} \quad \tilde{\boldsymbol{w}}^T\hat{\boldsymbol{L}}\tilde{\boldsymbol{w}} \tag{8}$$

under the constraints

$$\begin{aligned} \tilde{\boldsymbol{w}}^T\boldsymbol{1} &= 0 \quad \text{(zero mean)} && (9)\\ \text{and} \quad \tilde{\boldsymbol{w}}^T\tilde{\boldsymbol{w}} &= 1 \quad \text{(unit variance)} && (10)\end{aligned}$$

3.5 The role of the weighted normalization constraint

3.6 Symmetric normalized Laplacian matrix

3.6.1 Exercise: Eigenvectors and -values of the symmetric normalized Laplacian matrix

Consider the Laplacian matrix

$$\boldsymbol{L} = \begin{pmatrix} a & -a & 0 \\ -a & a+b & -b \\ 0 & -b & b \end{pmatrix} \tag{1}$$

with $0 < a, b$.

1. Calculate the symmetric normalized Laplacian matrix.
2. Solve the ordinary eigenvalue problem $\hat{\boldsymbol{L}}\hat{\boldsymbol{w}}_i = \lambda_i \hat{\boldsymbol{w}}_i$ for $i = 1, 2, 3$.

3.7 Random walk normalized Laplacian matrix +

3.8 Summary of mathematical properties

4 Algorithms

4.1 Similarity graphs

4.2 Laplacian eigenmaps (LEM)

4.2.1 Motivation

4.2.2 Objective

4.2.3 Algorithm

4.2.4 Sample applications

4.3 Locality preserving projections (LPP)

4.3.1 Linear LPP

4.3.2 Sample application

4.3.3 Nonlinear LPP

4.4 Spectral clustering

4.4.1 Objective

4.4.2 Algorithm

4.4.3 Sample application