Chapter 5

Decompositions for Combinatorial Structures

Part I: Spectral methods

Background:
Eigendecompositions

Eigenvectors and values

- Let $\boldsymbol{A} \in \mathbb{R}^{n \times n}$
  - $\boldsymbol{v} \in \mathbb{R}^{n}$ is an **eigenvector** of $\boldsymbol{A}$ if $\boldsymbol{Av} = \lambda \boldsymbol{v}$
  - If $\boldsymbol{Av} = \lambda \boldsymbol{v}$, λ is an **eigenvalue** associated to $\boldsymbol{v}$
    - If there are k eigenvectors $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, …, $\boldsymbol{v}_k$ s.t. $\boldsymbol{Av}_i = \lambda \boldsymbol{v}_i$ for all i, then λ has (algebraic) **multiplicity** of k
    - n-by-n matrix has n eigenvectors and n eigenvalues (counting the multiplicity)
      - Some can be complex

Spectrum of a matrix

- The **characteristic polynomial** of $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is $p_{\boldsymbol{A}}(\lambda) = \det(\boldsymbol{A} - \lambda \boldsymbol{I})$
  - The roots of $p_{\boldsymbol{A}}(\lambda)$ are the eigenvalues of $\boldsymbol{A}$
    - I.e. $p_{\boldsymbol{A}}(\lambda) = 0 \Leftrightarrow \lambda$ is an eigenvalue of $\boldsymbol{A}$
  - The collection of the eigenvalues of $\boldsymbol{A}$ is called the **spectrum** of $\boldsymbol{A}$

Eigendecomposition

- The **eigendecomposition** of symmetric $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{\mathsf{T}}$
  - $\boldsymbol{Q}$ is orthogonal and has the eigenvectors as its columns
  - $\boldsymbol{\Lambda}$ is diagonal with the eigenvalues
  - The symmetry of $\boldsymbol{A}$ is sufficient but not necessary

Properties of eigendecomposition

- $\boldsymbol{A}\boldsymbol{A}^T = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T\boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{U}^T = \boldsymbol{U}\boldsymbol{\Sigma}^2\boldsymbol{U}^T$
- $\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{\Sigma}^2\boldsymbol{V}^T$
- If $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T$ then trace($\boldsymbol{A}$) = trace($\boldsymbol{\Lambda}$) = $\sum_i \lambda_i$
- The rank of $\boldsymbol{A}$ is the number of non-zero eigenvalues

Positive seminefinite matrix

- Matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is **positive semidefinite** if $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \geq 0$ for any $\boldsymbol{x} \in \mathbb{R}^n$
  - $\boldsymbol{A}$ is **positive definite** if the inequality is strict for any non-zero $\boldsymbol{x}$
- If $\boldsymbol{A} = \boldsymbol{B}\boldsymbol{B}^T$ for some $\boldsymbol{B} \in \mathbb{R}^{n \times m}$, $\boldsymbol{A}$ is positive semidefinite
- If $\boldsymbol{A}$ is positive semidefinite, all its eigenvalues are non-negative

Graphs and matrices

Combinatorial structures

- We consider matrices that correspond to some **combinatorial object**
  - E.g. graph or set system
- The matrices can be binary-valued, integer-valued, or real-valued
- We use continuous and discrete decomposition methods to learn about the latent structures of these object

Fundamental matrices of graphs

- A graph $G = (V, E)$ can be represented by its **adjacency matrix *A***
  - $a_{ij} = 1$ if $\{v_i, v_j\} \in E$, o/w 0
- Or by its **incidence matrix *P***
  - $p_{ij} = 1$ if $e_j \in E$ starts from v_i, $p_{ij} = -1$ if $e_j \in E$ ends in v_i, and 0 o/w
  - Edges in undirected graphs can be oriented arbitrarily
- $a_{ii} = 0$ (no self-loops)

Similarity matrix

- The **similarity matrix** ***S*** of n elements is n-by-n symmetric nonnegative matrix
  - s_{ij} is the similarity between i and j
  - 0s at diagonal
- Can be interpret as a weighted adjacency matrix of a (complete) **similarity graph**

Which similarity?

- Any distance metric (suitable for data) can be used as the similarity measure
  - sim($\boldsymbol{x}$, $\boldsymbol{y}$) = M – $||\boldsymbol{x} - \boldsymbol{y}||$ where M is the maximum distance
    - Euclidean, Hamming, Jaccard, mutual information, Hellinger, …
- Often the similarities are scaled to emphasize high similarity (and de-emphasize low similarity)
  - **Gaussian kernel** is common:
    Ksim($\boldsymbol{x}$, $\boldsymbol{y}$) = $\exp\{-||\boldsymbol{x} - \boldsymbol{y}||^2/(2\sigma^2)\}$

Sparsifying similarity graphs

- Similarity graphs are complete
  - But often we only need pairwise similarities of quite similar elements
- To sparsify the similarity graph, we can remove edges between dissimilar pairs
  - This sets the corresponding values in the matrix to 0

Getting non-complete graphs

- How to decide when vertices are too dissimilar?
- In **ϵ-neighbour graphs** we add an edge between two vertices that are within distance ϵ to each other
  - Usually the resulting graph is considered unweighted as all weights would be roughly similar
- In **k-nearest neighbour graphs** we connect two vertices if one is within the k nearest neighbours of the other
  - In **mutual k-nearest neighbour graph** we only connect two vertices if they're both in each other's k nearest neighbours

Which similarity graph?

- With ϵ-graphs choosing the parameter is hard
  - No single correct answer if different clusters have different internal similarities
- k-nearest neighbours can connect points with different similarities
  - But far-away high density regions become unconnected
- The mutual k-nearest neighbours is somewhat in between
  - Good for detecting clusters with different densities
- General recommendation: start with k-NN
  - Others if data supports that

Even More Matrices

- The (weighted) adjacency matrix $\boldsymbol{A}$ has the weight of edge (i, j) at position a_{ij}
- The **degree matrix $\boldsymbol{\Delta}$** of a graph is a diagonal n-by-n matrix with the (weighted) degree of vertex i at position $\Delta_{ii} = d_i$
  - $\Delta_{ii} = d_i = \sum_j a_{ij}$
- The **normalized adjacency matrix $\boldsymbol{M}$** is the adjacency matrix where in every row i all values are divided by d_i
  - Every row sums up to 1
  - $\boldsymbol{M} = \boldsymbol{\Delta}^{-1}\boldsymbol{A}$

Graph Laplacians

- The **Laplacian matrix *L*** of a graph is the adjacency matrix subtracted from the degree matrix

$$\boldsymbol{L} = \boldsymbol{\Delta} - \boldsymbol{A} = \begin{pmatrix} \sum_{j \neq 1} a_{1,j} & -a_{1,2} & \cdots & -a_{1,n} \\ -a_{2,1} & \sum_{j \neq 2} a_{2,j} & \cdots & -a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n,1} & -a_{n,2} & \cdots & \sum_{j \neq n} a_{n,j} \end{pmatrix}$$

- The Laplacian is symmetric and positive semi-definite
  - Undirected graphs
  - Has n real, non-negative, orthogonal eigenvalues

    $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_n \geq 0$

The normalized, symmetric Laplacian

- The **normalized, symmetric Laplacian matrix** $\boldsymbol{L}^s$ of a graph is defined as

$$\boldsymbol{\Delta}^{-1/2}\boldsymbol{L}\boldsymbol{\Delta}^{-1/2} = \boldsymbol{I} - \boldsymbol{\Delta}^{-1/2}\boldsymbol{A}\boldsymbol{\Delta}^{-1/2} = \begin{pmatrix} \frac{\sum_{j\neq 1} a_{1,j}}{\sqrt{d_1 d_1}} & -\frac{a_{1,2}}{\sqrt{d_1 d_2}} & \cdots & -\frac{a_{1,n}}{\sqrt{d_1 d_n}} \\ -\frac{a_{2,1}}{\sqrt{d_2 d_1}} & \frac{\sum_{j\neq 2} a_{2,j}}{\sqrt{d_2 d_2}} & \cdots & -\frac{a_{2,n}}{\sqrt{d_2 d_n}} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{a_{n,1}}{\sqrt{d_n d_1}} & -\frac{a_{n,2}}{\sqrt{d_n d_2}} & \cdots & \frac{\sum_{j\neq n} a_{n,j}}{\sqrt{d_n d_n}} \end{pmatrix}$$

  - Also positive semi-definite

- The **normalized, asymmetric Laplacian** $\boldsymbol{L}^a$ (a.k.a **random walk Laplacian**) is $\boldsymbol{L}^a = \boldsymbol{\Delta}^{-1}\boldsymbol{L}$

Spectral clustering

von Luxburg 2007 Skillicorn chapter 4

Clustering as Graph Cuts

- A **cut** of a connected graph $G = (V, E)$ divides the set of vertices into two partitions S and $V \setminus S$ and removes the edges between them
  - Cut can be expressed by giving the set S
  - Or by giving the cut set $F = \{(v, u) \in E : |\{v, u\} \cap S| = 1\}$
- Graph cut clusters graph's vertices into two clusters
- A k**-way** cut cuts the graph into k disjoint set of vertices $C_1, C_2, \ldots, C_k$ and removes the edges between them

What is a good cut?

- Just any cut won’t cut it
- In **minimum cut** the goal is to find any set of vertices such that cutting them from the rest of the graph requires removing the least number of edges
  - Least sum of weights for weighted graphs
- The minimum cut can be found in polynomial time
  - The max-flow min-cut theorem
- But minimum cut isn’t very good for clustering purposes

What cuts would cut it? (1)

- We want a cut that penalizes imbalanced cluster sizes
- In **ratio cut**, the goal is to minimize the ratio of the weight of the edges in the cut set and the size of the clusters C_i
- Let $W(A, B) = \sum_{i \in A, j \in B} w_{ij}$
  - w_{ij} is the weight of edge (i, j)

$$\text{RatioCut} = \sum_{i=1}^{k} \frac{W(C_i, V \backslash C_i)}{|C_i|}$$

What cuts would cut it? (2)

- The **volume** of a set of vertices A is the weight of all edges connected to A
  - $vol(A) = W(A, V) = \sum_{i \in A, j \in V} w_{ij}$
- In **normalized cut** we measure the size of C_i not by $|C_i|$ but by $vol(C_i)$

$$\text{NormalizedCut} = \sum_{i=1}^{k} \frac{W(C_i, V \backslash C_i)}{vol(C_i)}$$

Finding optimal RatioCut or NormalizedCut is NP-hard

Clusterings and matrices redux

- Recall that we can express a clustering using a binary cluster assignment matrix
- Let the i-th column of this matrix be $\boldsymbol{c}_i$
  - Clusters are disjoint so $\boldsymbol{c}_i^T \boldsymbol{c}_j = 0$
  - Cluster has $\boldsymbol{c}_i^T \boldsymbol{c}_i = ||\boldsymbol{c}_i||^2$ elements
- We can get the $vol(C_i)$ and $W(C_i, V)$ using $\boldsymbol{c}_i$'s
  - $vol(C_i) = \sum_{j \in C_i} d_j = \sum_{r=1}^{n} \sum_{s=1}^{n} c_{ir} \boldsymbol{\Delta}_{rs} c_{is} = \boldsymbol{c}_i^T \boldsymbol{\Delta} \boldsymbol{c}_i$
  - $W(C_i, C_i) = \sum_{r \in C_i} \sum_{s \in C_i} a_{rs} = \boldsymbol{c}_i^T \boldsymbol{A} \boldsymbol{c}_i$
  - $W(C_i, V \setminus C_i) = W(C_i, V) - W(C_i, C_i) = \boldsymbol{c}_i^T (\boldsymbol{\Delta} - \boldsymbol{A}) \boldsymbol{c}_i$
    $= \boldsymbol{c}_i^T \boldsymbol{L} \boldsymbol{c}_i$

Cuts using matrices

$$\text{RatioCut} = \sum_{i=1}^{k} \frac{W(C_i, V \setminus C_i)}{|C_i|} = \sum_{i=1}^{k} \frac{\boldsymbol{c}_i^T \boldsymbol{L} \boldsymbol{c}_i}{\|\boldsymbol{c}_i\|^2}$$

$$\text{NormalizedCut} = \sum_{i=1}^{k} \frac{W(C_i, V \setminus C_i)}{vol(C_i)} = \sum_{i=1}^{k} \frac{\boldsymbol{c}_i^T \boldsymbol{L} \boldsymbol{c}_i}{\boldsymbol{c}_i^T \boldsymbol{\Delta} \boldsymbol{c}_i}$$

Finding approximate cuts

- Re-writing the objective functions doesn’t make them any easier
  - The complexity comes from the binary clustering assignments
- Relax!
  - Let $\boldsymbol{c}_i$’s take any real value
- Relaxed RatioCut:

$$J_{rc}(\mathcal{C}) = \sum_{i=1}^{k} \frac{\boldsymbol{c}_i^T \boldsymbol{L} \boldsymbol{c}_i}{\|\boldsymbol{c}_i\|^2} = \sum_{i=1}^{k} \left(\frac{\boldsymbol{c}_i}{\|\boldsymbol{c}_i\|} \right)^T \boldsymbol{L} \left(\frac{\boldsymbol{c}_i}{\|\boldsymbol{c}_i\|} \right) = \sum_{i=1}^{k} \boldsymbol{u}_i^T \boldsymbol{L} \boldsymbol{u}_i$$

  - $\boldsymbol{u}_i = \boldsymbol{c}_i / ||\boldsymbol{c}_i||$ i.e. the unit vector in the direction of $\boldsymbol{c}_i$

Solving the relaxed version

- We want to minimize the function J_{rc} over $\boldsymbol{u}_i$'s
  - We have a constraint that $\boldsymbol{u}_i^T \boldsymbol{u}_i = 1$
- To solve, derive w.r.t. $\boldsymbol{u}_i$'s and find the roots
  - Add Lagrange multipliers to incorporate the constraints:

$$\frac{\partial}{\partial \boldsymbol{u}_i}\left(\sum_{i=1}^{k} \boldsymbol{u}_i^T \boldsymbol{L} \boldsymbol{u}_i + \sum_{i=1}^{k} \lambda_i (1 - \boldsymbol{u}_i^T \boldsymbol{u}_i)\right) = 0$$

- Hence, $\boldsymbol{L}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$
  - $\boldsymbol{u}_i$ is an eigenvector of $\boldsymbol{L}$ corresponding to the eigenvalue λ_i

Which eigenvectors to choose

- We know that $\boldsymbol{L}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$
  - Hence $\lambda_i = \boldsymbol{u}_i^T \boldsymbol{L}\boldsymbol{u}_i$
- As we're minimizing the sum of $\boldsymbol{u}_i^T \boldsymbol{L}\boldsymbol{u}_i$'s we should choose the $\boldsymbol{u}_i$'s corresponding to the k smallest eigenvalues
  - They are our relaxed cluster indicators
- Note that we know that $\lambda_n = 0$ and that the corresponding eigenvector is $(n^{-1/2}, n^{-1/2}, \ldots, n^{-1/2})$ (the graph is connected!)
  - No help on clustering...

The Fiedler vector and value

- The **Fiedler value** f of graph G = (V, E) is the second-smallest eigenvalue λ_{n-1} of $\boldsymbol{L}_G$
  - The **Fiedler vector** is the corresponding eigenvector
- If we want to remove minimum number of vertices s.t. we cut the graph, we have to remove at least f vertices
- The **edge boundary** ∂U of subset $U \subseteq V$ is

  $\partial U = \{(u, v) \in E : u \in U, v \notin U\}$
  - $|\partial U| \geq f|U||V \setminus U|/n$

$W(U, V \setminus U)$ for unweighted graphs

Normalized cut and choice of Laplacians

- For normalized cut similar procedure shows that we should select the k smallest eigenvectors of $\boldsymbol{L}^s$ (or $\boldsymbol{L}^a$) instead of $\boldsymbol{L}$
- Which one we should choose?
  - Both ratio and normalized cut aim at minimizing intra-cluster similarity
  - But only normalized cut considers inter-cluster similarity
    ⇒ Either $\boldsymbol{L}^s$ or $\boldsymbol{L}^a$
- The asymmetric Laplacian is better
  - With symmetric one further normalization is needed

Spectral clustering

- To do the clustering, we need to move our real-valued eigenvectors $\boldsymbol{u}_i$ to binary cluster indicator vectors
- First, create a matrix $\boldsymbol{U}$ with $\boldsymbol{u}_i$'s as its columns
  - Optionally, normalize the rows to sum up to 1 (esp. if using $\boldsymbol{L}^s$)
- Cluster the rows of this matrix using k-means (or any other clustering method)

Computational complexity

- Solving the eigenvectors is $O(n^3)$ in general or $O(n^2)$ if the similarity graph has as many edges as vertices
- The k-means on the $\boldsymbol{U}$ matrix takes $O(tnk^2)$
  - t is the number of iterations in k-means

Spectral clustering pseudo-code

Assume connected graph

Algorithm 16.1: Spectral Clustering Algorithm

Spectral Clustering $(\mathbf{D}, k)$:

1 Compute the similarity matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ ← Sparsify if needed

2 **if** *ratio cut* **then** $\mathbf{B} \leftarrow \mathbf{L}$

3 **else if** *normalized cut* **then** $\mathbf{B} \leftarrow \mathbf{L}^s$ or $\mathbf{L}^a$

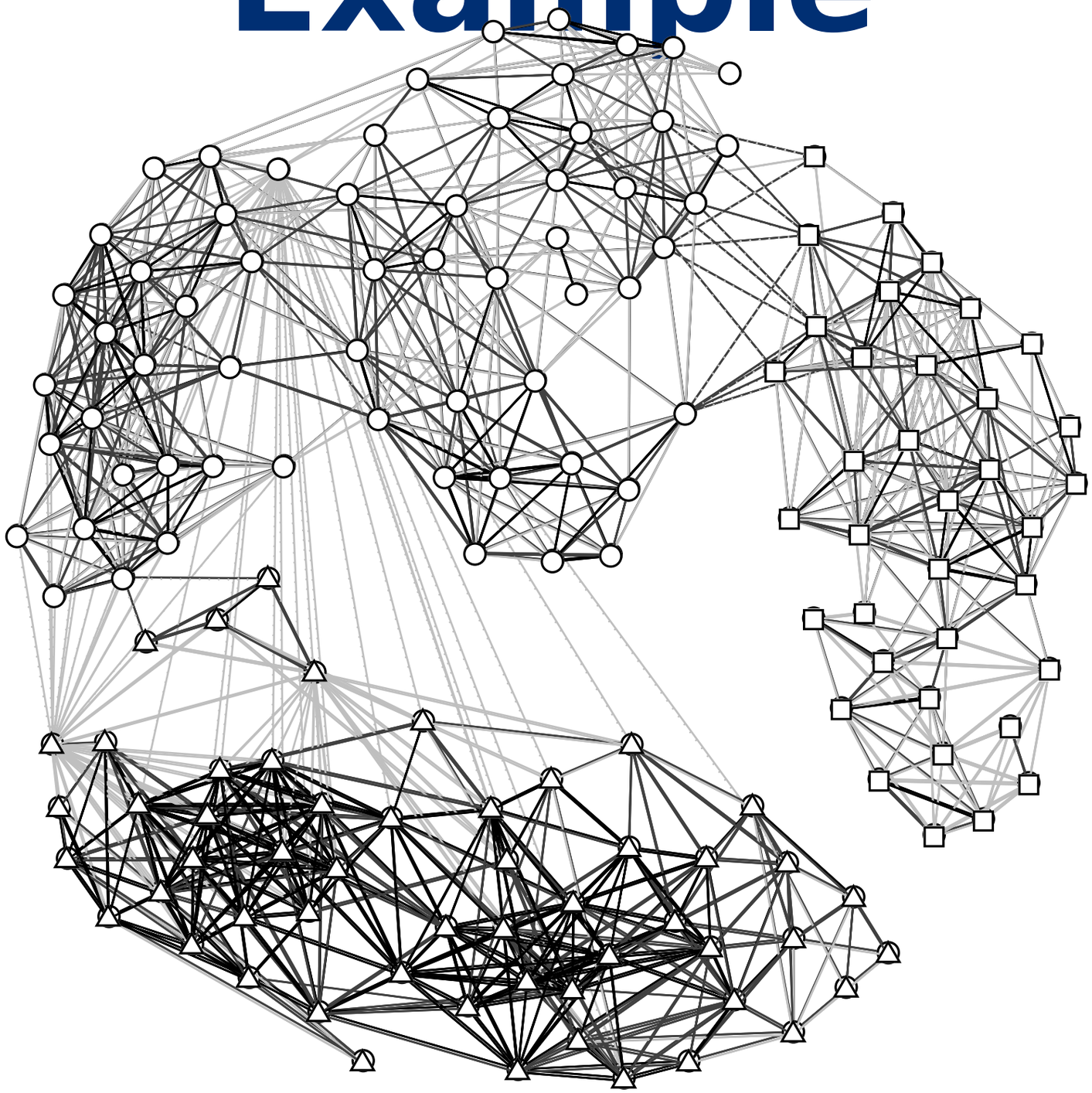
4 Solve $\mathbf{B}\mathbf{u}_i = \lambda_i \mathbf{u}_i$ for $i = n, \ldots, n-k+1$, where $\lambda_n \leq \lambda_{n-1} \leq \cdots \leq \lambda_{n-k+1}$

5 $\mathbf{U} \leftarrow \begin{pmatrix} \mathbf{u}_n & \mathbf{u}_{n-1} & \cdots & \mathbf{u}_{n-k+1} \end{pmatrix}$

6 $\mathbf{Y} \leftarrow$ normalize rows of $\mathbf{U}$ using (16.19)

7 $\mathcal{C} \leftarrow \{C_1, \ldots, C_k\}$ via K-means on $\mathbf{Y}$

Example



ZM Figures 16.1 and 16.4

Is spectral clustering optimal?

- Spectral clustering is not always a good approximation of the graph cuts
  - In so-called cockroach graphs, spectral clustering always horizontally, when optimal is to cut vertically
  - Approximation ratio of $O(n)$