### Spectral clustering

Lecture 2 Spectral clustering: from confusion to clarity

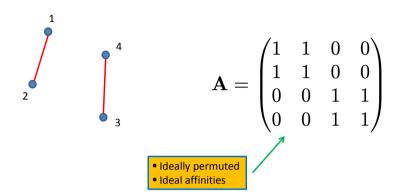
### Indicator vectors

• Each cluster has an indicator vector, represented by a binary vector that contains "1" for points in the cluster and "0" otherwise:

$$\mathbf{c}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{c}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

### A simple example

• Two ideal clusters, with two points each



### A simple example

• Clearly, we can decompose **A** as

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

$$\mathbf{c_1} \text{ and } \mathbf{c_2}$$

$$\mathbf{A} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 & 1 \end{pmatrix}$$

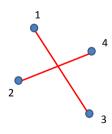
### Eigensystem of A

• An eigenvalue decomposition of **A** gives

$$\label{eq:normalized eigenvectors} \begin{aligned} \text{normalized eigenvectors} &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \\ \text{corresponding eigenvalues} &= \begin{pmatrix} 2 & 2 & 0 & 0 \end{pmatrix} \end{aligned}$$

### Permutations of A

• Two ideal cluster, with two points each



$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}$$

### Initial idea

- To each cluster there is a non-zero eigenvalue in A
  - Number of clusters = number of non-zero eigenvalues in A
- To each such eigenvalue/cluster, the corresponding normalized eigenvector is a scaled version of the corresponding indicator vector

### Eigensystem of permuted A

• An eigenvalue decomposition of **A** gives

$$\mbox{normalized eigenvectors} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$
 
$$\mbox{corresponding eigenvalues} = \begin{pmatrix} 2 & 2 & 0 & 0 \end{pmatrix}$$

Initial idea holds: permutations of the points carries over to permutations of the elements of the eigenvectors

### Eigensystem of permuted A

- The goal of spectral clustering is to determine the permutation of **A** that turns it into a block diagonal form
- This is done by analyzing the eigensystem of A

A glitch (I)

- In this case: the non-zero eigenvalues are equal
  - Any linear combination of the first two eigenvectors is also an eigenvector of the same eigenvalue
  - Any small perturbation of **A** can make a large change in the eigenvectors
  - Eigenvectors will not correspond to the indicator vectors

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### A glitch (I)

$$\mathbf{A} = \begin{pmatrix} 1 & 0.99 & 0.01 & 0.02 \\ 0.99 & 1 & 0.01 & 0.03 \\ 0.01 & 0.01 & 1 & 0.98 \\ 0.02 & 0.03 & 0.98 & 1 \end{pmatrix}$$
 Again ideally but with soil b

Again ideally ordered but with some noise

proximate numerical values



$$\text{normalized eigenvectors} = \begin{pmatrix} 0.53 & -0.46 & -0.28 & 0.65 \\ 0.54 & -0.46 & 0.27 & -0.65 \\ 0.46 & 0.54 & -0.65 & -0.27 \\ 0.47 & 0.53 & 0.65 & 0.27 \end{pmatrix}$$

$$\text{corresponding eigenvalues} = \begin{pmatrix} 2.02 & 1.95 & 0.02 & 0.01 \end{pmatrix}$$

### A glitch (I)

- It is still the case the there are two dominant eigenvalues, corresponding to the two separate clusters
- But the corresponding eigenvectors do not directly reveal the points of each cluster
  - A linear combination of them, however, will!

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### Fixing the glitch (I)

• Define, for *n* points and *k* clusters:

 $\mathbf{U} = n \times k$  matrix containing the normalized eigenvectors of the k largest eigenvalues of  $\mathbf{A}$  in its columns

Each row in U corresponds to a data point

### Fixing the glitch (I)

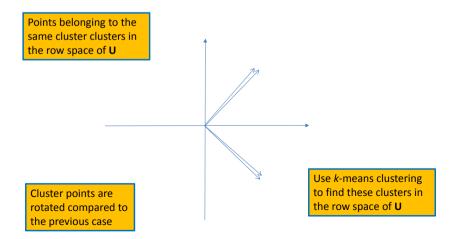
• In the last numerical example:

= U

We notice that rows of **U** corresponding to the same cluster are approximately equal

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### Fixing the glitch (I)



### A clustering algorithm, (I)

- Assume *n* points and *k* clusters
- Compute  $n \times n$  affinity matrix **A**
- Compute the eigensystem of A
- There should be *k* non-zero eigenvalues
- Set U to hold the corresponding normalized eigenvectors in its columns
- Apply k-means clustering on the row space of
   U to find the k clusters

### An observation (I)

- The **self-affinity** of each point is a constant value found in the diagonal of **A**
- Changing this constant means adding a term to **A** that is proportional to the identity matrix:

$$A' = A + \alpha I$$

### An observation (I)

- In the literature it is common to set the self-affinity to zero
  - All diagonal elements of **A** are zero
- The phrase
   "k eigenvalues of A are non-zero"
   should then be replaced by
   "k eigenvalues of A are large"

### An observation (I)

• A and A' have the same eigenvectors but their eigenvalues differ:

$$\mathbf{A'}_{\mathsf{k}} = \lambda_k + \alpha \qquad \qquad \mathbf{A'} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Same eigenvectors as before

With  $\alpha$  = -1

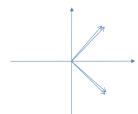
corresponding eigenvalues =  $\begin{pmatrix} 1 & 1 & -1 & -1 \end{pmatrix}$ 

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### An observation (II)

In the previous numerical example:

 Not only are the row vectors of U for points in different clusters distinct, they are orthogonal



• This is not a coincidence!

### An observation (II)

• Assuming that the k largest eigenvalues of  $\mathbf{A}$  are approximately equal (to  $\lambda$ ):

$$\mathbf{A} + \alpha \mathbf{I} = \lambda \mathbf{U} \mathbf{U}^\mathsf{T}$$



The inner product of rows from different clusters correspond to zero affinity in an ideal **A** 

In the ideal case: rows in **U** belonging to different clusters must be orthogonal

- But not necessarily of unit length!
- We will return to this later on!

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### A clustering algorithm (II)

- Assume *n* points and *k* clusters
- Compute  $n \times n$  affinity matrix **A** (0 in diagonal!)
- Compute eigensystem of A
- There should be *k* "large" eigenvalues which are approximately equal
- Set U to hold the corresponding normalized eigenvectors in its columns
- Apply k-means clustering on the row space of U to find the k clusters

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### An observation (III)

- Using the "larger" or "significant" eigenvalues of A can be replaced with "equal to zero" or "close-to-zero" eigenvalues of related matrices
- We need to modify A accordingly
- Leads to the Laplacian L of A, and we do clustering based on the eigensystem of L instead of A

### Degree matrix

• We define

**D** = diagonal matrix  $\{d_{ii}\}$ where  $d_{ii}$  = sum of row/column i in **A** 

as the degree matrix of A

### A simple example

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix} \qquad \mathbf{D} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

$$\mathbf{D} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

$$\mathbf{c}_1 = \left(egin{array}{c} 1 \ 1 \ 0 \ 0 \ 0 \end{array}
ight) \quad \mathbf{c}_2 = \left(egin{array}{c} 0 \ 0 \ 1 \ 1 \ 1 \end{array}
ight)$$

The indicator vectors are

Laplacian

Formally, we define

$$L = D - A$$

as the Laplacian of A

• The indicator vectors are eigenvectors also of L, with eigenvalue 0

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### Properties of L

In the ideal case:

- L has the same eigenvectors as A and D
- L has eigenvalues = 0 for the indicator vectors In general (also with noise):

$$\mathbf{u}^T \mathbf{L} \ \mathbf{u} = \frac{1}{2} \sum_{i,j=1}^n a_{ij}^{\prime} (u_i - u_j)^2$$

L is positive semi-definite!

### Properties of L

In the general case (also with noise):

- Positive semi-definite
- Sum along rows/columns of **L** vanishes
- There is always one eigenvalue = 0 in L
- Corresponding eigenvector = is 1 (constant 1)
  - 1 is the sum of all indicator vectors!

### Properties of L

#### In the ideal case

- L has a block structure,
  - Non-zero blocks representing fully connected components
  - Zero blocks representing unconnected components

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### Properties of L

#### From this follows:

- If u is a cluster indicator vector ⇒
   u is an eigenvector of L with eigenvalue 0
- If u is an eigenvector of L with eigenvalue 0 ⇒
  u is a linear combination of the cluster indicator
  vectors

#### From this follows:

- 1. The number of eigenvalues = 0 in  $\mathbf{L}$  is = k (k= number of clusters)
- 2. The corresponding eigenvectors span the space of indicator vectors

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# A clustering algorithm (III) Unnormalized spectral clustering

- Assume *n* points and *k* clusters
- Compute  $n \times n$  affinity matrix **A**
- Compute **D**, and compute **L** = **D A**
- Compute eigensystem of L
- There should be *k* "zero" eigenvalues
- Set **U** to hold the corresponding normalized eigenvectors in its columns
- Apply k-means clustering on the row space of U to find the k clusters

### Fiedler's method for k = 2

- The Laplacian **L** has always (even for noisy data) an eigenvalue  $\lambda_1 = 0$
- Corresponding eigenvector e<sub>1</sub> is 1
- If k = 2, there should be a second eigenvalue
   = 0, or at least close to zero
- Corresponding eigenvector denoted e<sub>2</sub>
- The row space of {e<sub>1</sub>, e<sub>2</sub>} should form clusters in two orthogonal directions

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### Fiedler's method for k = 2

- Consequently, the signs of the elements in e<sub>2</sub>
   must be indicators of the two classes
- For example:
  - "+" means class 1
  - "-" means class 2
- We don't really need **e**<sub>1</sub>
- Only the signs of the elements in **e**<sub>2</sub>
  - **e**<sub>2</sub> is often referred to as the *Fiedler vector*

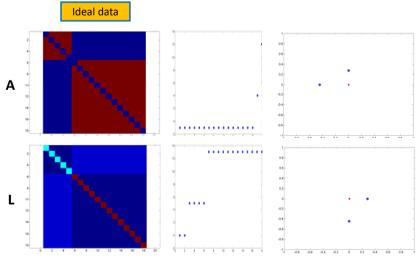
### An observation (IV)

- Should we do clustering on **A** or on **L**?
- For ideal data
  - full connections internally in each component
  - no connects between components
     there is, in general, no difference in the result
- For non-ideal data, (= in practice) the results differ
  - Often: clustering based on L is better!

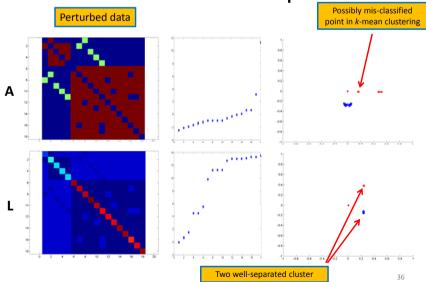
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### A numerical example







### **Analysis**

- It can be shown that the clustering on A is equivalent to solving the mincut problem of the corresponding graph [see von Luxburg]
- Prefers to cut fewer edges, even if they have higher affinity, than more edges even when each has lower affinity
- In our example: there is a risk of cutting the edge between point 1 and the rest of the points in the first cluster

### **Analysis**

- It can be shown that the clustering on L is for k = 2 approximates the solution of the Ratio-cut problem of the corresponding graph [see von Luxburg]
- Normalizes the cost of a cut with the number of vertices of each sub-graph
- In our example: reduces the risk of cutting the edge between point 1 and the rest of the points in the first cluster

## A glitch (II)

- The last clustering algorithm works well for arbitrary k, but assumes that the number of points in each cluster,  $n_k$ , is approximately equal
- Otherwise, eigenvalues which are "zero" and "non-zero" may mix in the data of real data

### A simple example

• An ideal **A** with k = 2 and  $n_1$  and  $n_2$  points in each cluster

### A simple example

• Eigensystem of A

$$\mathbf{c}_1 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad \mathbf{c}_2 = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \begin{matrix} n_1 \\ \vdots \\ n_2 \\ n_2 \\ \end{matrix}$$

$$\mathbf{corresponding eigenvalues} = \begin{pmatrix} n_1 - 1 & n_2 - 1 & -1 & \dots & -1 \end{pmatrix}$$

### A simple example

### A simple example

• Eigensystem of **D** 

$$\mathbf{c}_{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \mathbf{c}_{2} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{1}$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{c}_{2} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{2}$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{2}$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{2}$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{1} - 1 \qquad \qquad n_{1} - 1 \qquad \qquad n_{2} - 1 \qquad \qquad n_{2}$$

### A simple example

• Eigensystem of **L** 

$$\mathbf{c}_{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \mathbf{c}_{2} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{1}$$

$$\begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 0 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad n_{2}$$

$$\begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 0 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \end{pmatrix} \qquad \qquad \begin{pmatrix} \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1} \\ \vdots \\ \mathbf{c}_{1}$$

### A glitch (II)

- For this example:
  - There are 2 eigenvalues approximately = 0
  - There are  $n_1$  1 eigenvalues approximately =  $n_1$
  - There are  $n_2$  1 eigenvalues approximately =  $n_2$
- If  $n_2 >> n_1$  and with sufficiently noisy data:
  - The first two types of eigenvalues can mix
  - Also their eigenvectors will mix
  - Poor clustering performance

## Fixing the glitch (II)

- There are (at least) two ways of fixing this glitch, where both normalize the Laplacian L before computing the eigensystem:
  - Normalized spectral clustering according to Shi & Malik (2000) [Not covered here!]
    - Based on EVD of  $\mathbf{L}_{rw} = \mathbf{D}^{-1}\mathbf{L}$
  - Normalized spectral clustering according to Ng et al (2002) [Next!]

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### Fixing the glitch (II)

• We define a normalized Laplacian as

$$L_{\text{sym}} = D^{-1/2} L D^{-1/2}$$

 Referred to as the normalized symmetric Laplacian

### Fixing the glitch (II)

- **L**<sub>sym</sub> is symmetric, and (in the ideal case):
  - Diagonal elements in  $\mathbf{L}_{sym}$  are all = 1
  - Off-diagonal elements sum to -1 along row and columns
  - Same number of eigenvalues = 0 as L
  - Same block structure as L
  - Same eigenvectors as L
  - An non-zero eigenvalue  $n_k$  in **L** becomes  $n_k / (n_k 1)$  in  $\mathbf{L}_{\text{sym}}$

### Fixing the glitch (II)

- The cluster indicator vectors are eigenvectors also of L<sub>sym</sub>, with eigenvalues = 0
- We can consider the eigensystem of **L**<sub>sym</sub> instead!
- Better separation between "zero" and "nonzero" eigenvalues

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### A glitch (III)

A simple example with three ideal clusters

- $n_1$ ,  $n_2$ ,  $n_3$  points each
- The indicator vectors c<sub>1</sub>, c<sub>2</sub>, c<sub>3</sub> are eigenvectors of L<sub>sym</sub> with eigenvalue 0
- Normalized to unit norm they become

$$\hat{\mathbf{c}}_{1} = \begin{pmatrix} 1/\sqrt{n_{1}} \\ \vdots \\ 1/\sqrt{n_{1}} \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \hat{\mathbf{c}}_{2} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1/\sqrt{n_{2}} \\ \vdots \\ 1/\sqrt{n_{2}} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \hat{\mathbf{c}}_{3} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1/\sqrt{n_{3}} \\ \vdots \\ 1/\sqrt{n_{3}} \\ \vdots \\ 1/\sqrt{n_{3}} \end{pmatrix} \begin{bmatrix} n_{1} \\ n_{2} \\ \vdots \\ n_{3} \\ \vdots \\ 1/\sqrt{n_{3}} \end{bmatrix}$$

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### A glitch (III)

- In the practical case, these is some noise and the three eigenvectors if L<sub>sym</sub> corresponding to eigenvalue "zero" are linear combinations of the previous vectors
  - Normalized linear combinations!
  - Correspond to rotations of the previous vectors
  - Therefore we do k-means clustering on the row space of **U** to find the clusters
  - If  $n_1$ ,  $n_2$ ,  $n_3$  are of different magnitudes:
    - Clusters with many points are found close to the origin
    - (Why?)

### Fixing the glitch (III)

- We normalize the rows of U before the final k-means clustering
- The resulting rows lie on a unit hyper-sphere
- This leads to a better separation of the clusters in the row space of U
- We return to the issue of clustering points on a sphere in the following lecture

# A clustering algorithm (IV) Ng et al (2002)

- Assume *n* points and *k* clusters
- Compute  $n \times n$  affinity matrix **A**, and its **D**
- Compute L = D A
- Compute  $L_{sym} = D^{-1/2} L D^{-1/2}$
- ullet Compute eigensystem of  ${f L}_{
  m sym}$
- There should be *k* "zero" eigenvalues
- Set **U** to hold the corresponding normalized eigenvectors in its columns
- Set **T** = **U** but with each row normalized to unit norm
- Apply k-means clustering on the row space of T to find the k clusters

### Does it matter with algorithm we use?

- The unnormalized algorithm is attractive since it is simple, but
  - Use it only when you know that the clusters have the same order of points
- The two normalized methods (S-M & Ng) are approximately of the same order of additional computations
  - Von Luxburg suggests S-M before Ng method
  - In practice Ng's method appears to work as well

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### Summary

- 3 basic algorithms for spectral clustering
  - Unnormalized: **L u** =  $\lambda$  **u**
  - Shi-Malik
    - Solve:  $\mathbf{L}_{rw} \mathbf{u} = \lambda \mathbf{u}$ , where  $\mathbf{L}_{rw} = \mathbf{D}^{-1} \mathbf{L}$
  - Ng, et al:
    - Solve:  $\mathbf{L}_{\text{sym}} \mathbf{u} = \lambda \mathbf{u}$  , where  $\mathbf{L}_{\text{sym}} = \mathbf{D}^{-1/2} \mathbf{L} \mathbf{D}^{-1/2}$
- Spectral properties of A, D, L
  - Relations to the cluster indicator vectors