Introduction to Spectral Graph Theory and Graph Clustering

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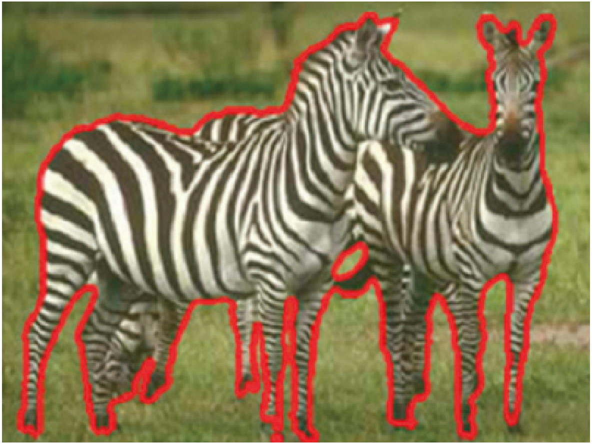
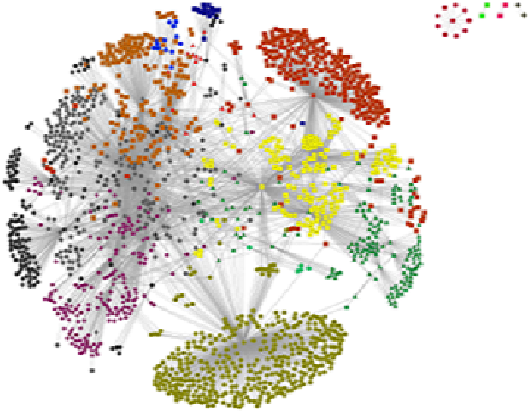
Motivation

Image partitioning in computer vision



Motivation

Community detection in network analysis



Outline

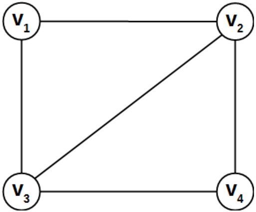
I. Graph and graph Laplacian
   - Graph
   - Weighted graph
   - Graph Laplacian

II. Graph clustering
   - Graph clustering
   - Normalized cut
   - Spectral clustering

I.1 Graph

An (undirected) **graph** is a pair $G = (V, E)$, where

- $\{v_i\}$ is a set of vertices;
- E is a subset of $V \times V$.



Remarks:

- An edge is a pair $\{u, v\}$ with $u \neq v$ (no self-loop);
- There is at most one edge from u to v (simple graph).

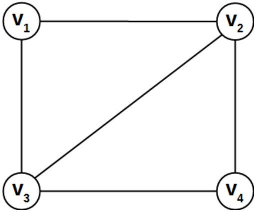
I.1 Graph

- For every vertex $v \in V$, the **degree** $d(v)$ of v is the number of edges adjacent to v:

$$d(v) = |\{u \in V | \{u, v\} \in E\}|.$$

- Let $d_i = d(v_i)$, the **degree matrix**

$$D = D(G) = \mathrm{diag}(d_1, \ldots, d_n).$$

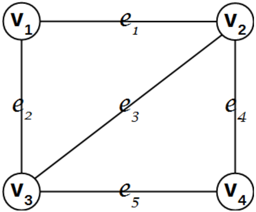


$$D = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

I.1 Graph

- Given a graph $G = (V, E)$, with $|V| = n$ and $|E| = m$, the **incidence matrix** $\tilde{D}(G)$ of G is an $n \times m$ matrix with

$$\tilde{d}_{ij} = \left\{ \begin{array}{ll} 1, & \text{if } \exists k \text{ s.t. } e_j = \{v_i, v_k\} \\ 0, & \text{otherwise} \end{array} \right) .$$

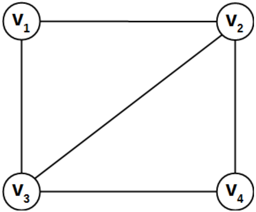


$$\tilde{D}(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} \begin{array}{c} \begin{array}{ccccc} e_1 & e_2 & e_3 & e_4 & e_5 \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix} \end{array}$$

I.1 Graph

- Given a graph $G = (V, E)$, with $|V| = n$ and $|E| = m$, the **adjacency matrix** $A(G)$ of G is a symmetric $n \times n$ matrix with

$$a_{ij} = \begin{cases} 1, & \text{if } \{v_i, v_j\} \in E \\ 0, & \text{otherwise} \end{cases} .$$



$$A(G) = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

I.2 Weighted graph

A **weighted graph** is a pair $G = (V, W)$ where

- $V = \{v_i\}$ is a set of vertices and $|V| = n$;
- $W \in \mathbb{R}^{n \times n}$ is called *weight matrix* with

$$w_{ij} = \begin{cases} w_{ji} \geq 0 & i \neq j \\ 0 & i = j \end{cases} .$$

The **underlying graph** of G is $\widehat{G} = (V, E)$ with

$$E = \{\{v_i, v_j\} | w_{ij} > 0\}.$$

- If $w_{ij} \in \{0, 1\}$, $W = A$, the adjacency matrix of $\widehat{G}$.
- Since $w_{ii} = 0$, there is no self-loops in $\widehat{G}$.

I.2 Weighted graph

- For every vertex $v_i \in V$, the **degree** $d(v_i)$ of v_i is the sum of the weights of the edges adjacent to v_i:

$$d(v_i) = \sum_{j=1}^{n} w_{ij}.$$

- Let $d_i = d(v_i)$, the **degree matrix**

$$D = D(G) = \text{diag}(d_1, \ldots, d_n).$$

Remark:
Let $\boldsymbol{d} = \text{diag(D)}$ and denote $\mathbf{1} = (1, \ldots, 1)^T$, then $\boldsymbol{d} = W\mathbf{1}$.

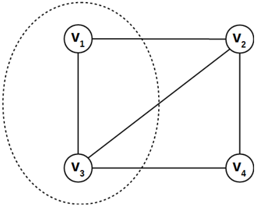
I.2 Weighted graph

- Given a subset of vertices $A \subseteq V$, we define the **volume** $\text{vol}(A)$ by

$$\text{vol}(A) = \sum_{v_i \in A} d(v_i) = \sum_{v_i \in A} \sum_{j=1}^{n} w_{ij}.$$

Remarks:

- If $\text{vol}(A) = 0$, all the vertices in A are isolated.
- Example:



If $A = \{v_1, v_3\}$, then

$$\begin{aligned}\text{vol}(A) &= d(v_1) + d(v_3)\\ &= (w_{12} + w_{13}) + \\ &\quad (w_{31} + w_{32} + w_{34})\end{aligned}$$

I.2 Weighted graph

- Given two subsets of vertices $A, B \subseteq V$, we define the **links** links(A, B) by

$$\text{links}(A, B) = \sum_{v_i \in A, v_j \in B} w_{ij}.$$

Remarks:

- A and B are not necessarily distinct;
- Since W is symmetric, links$(A, B) = $ links(B, A);
- vol$(A) = $ links(A, V).

I.2 Weighted graph

- The quantity $\mathrm{cut}(A)$ is defined by

$$\mathrm{cut}(A) = \mathrm{links}(A, V - A).$$

- The quantity $\mathrm{assoc}(A)$ is defined by

$$\mathrm{assoc}(A) = \mathrm{links}(A, A).$$

Remarks:

- $\mathrm{cut}(A)$ measures how many links escape from A;
- $\mathrm{assoc}(A)$ measures how many links stay within A;
- $\mathrm{cut}(A) + \mathrm{assoc}(A) = \mathrm{vol}(A)$.

I.3 Graph Laplacian

Given a weighted graph $G = (V, W)$, the (graph) **Laplacian** L of G is defined by

$$L = D - W.$$

where D is the degree matrix of G.

Remark

- $D = \text{diag}(W \cdot \mathbf{1})$.

I.3 Graph Laplacian

Properties of Laplacian

1. $x^T L x = \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(x_i - x_j)^2$ for $\forall x \in \mathbb{R}^n$.
2. $L \geq 0$ if $w_{ij} \geq 0$ for all i, j;
3. $L \cdot \mathbf{1} = \mathbf{0}$;
4. If the underlying graph of G is connected, then

$$0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_n;$$

5. If the underlying graph of G is connected, then the dimension of the nullspace of L is 1.

I.3 Graph Laplacian

Proofs:

Property 1. Since $L = D - W$, we have

$$\begin{aligned}
x^T L x &= x^T D x - x^T W x \\
&= \sum_{i=1}^{n} d_i x_i^2 - \sum_{i,j=1}^{n} w_{ij} x_i x_j \\
&= \frac{1}{2} \Big(\sum_{i}^{n} d_i x_i^2 - 2 \sum_{i,j=1}^{n} w_{ij} x_i x_j + \sum_{j=1}^{n} d_j x_j^2 \Big) \\
&= \frac{1}{2} \Big(\sum_{i,j=1}^{n} w_{ij} x_i^2 - 2 \sum_{i,j=1}^{n} w_{ij} x_i x_j + \sum_{i,j=1}^{n} w_{ij} x_j^2 \Big) \\
&= \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (x_i - x_j)^2.
\end{aligned}$$

I.3 Graph Laplacian

Property 2.

- Since $L^T = D - W^T = D - W = L$, L is symmetric.
- Since $x^T Lx = \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(x_i - x_j)^2$ and $w_{ij} \geq 0$ for all i, j, we have $x^T Lx \geq 0$.

Property 3.

$$L \cdot \mathbf{1} = (D - W)\mathbf{1} = D\mathbf{1} - W\mathbf{1} = \boldsymbol{d} - \boldsymbol{d} = \mathbf{0}.$$

Property 4 and **Property 5** skip for now, see §2.2 of [Gallier'14].

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II.1 Graph clustering

k-**way partitioning:** given a weighted graph $G = (V, W)$, find a partition $A_1, A_2, \ldots, A_k$ of V, such that

- $A_1 \cup A_2 \cup \ldots \cup A_k = V$;
- $A_1 \cap A_2 \cap \ldots \cap A_k = \varnothing$;
- for any i and j, the edges between (A_i, A_j) have low weight and the edges within A_i have high weight.

If $k = 2$, it is a *two-way partitioning*.

II.1 Graph clustering

- Recall: (two-way) cut:

$$\mathsf{cut}(A) = \mathsf{links}(A, \bar{A}) = \sum_{v_i \in A, v_j \in \bar{A}} w_{ij}$$

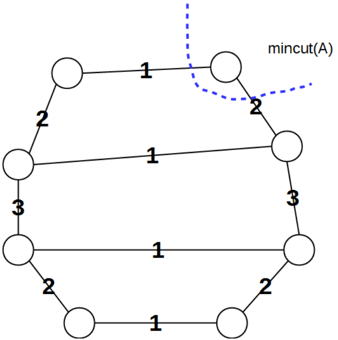
where $\bar{A} = V - A$.

II.1 Graph clustering problems

The **mincut** is defined by

$$\min \mathsf{cut}(A) = \min \sum_{v_i \in A, v_j \in \bar{A}} w_{ij}.$$

In practice, the mincut easily yields unbalanced partitions.



$$\min \mathsf{cut}(A) = 1 + 2 = 3;$$

II.2 Normalized cut

The **normalized cut**[1] is defined by

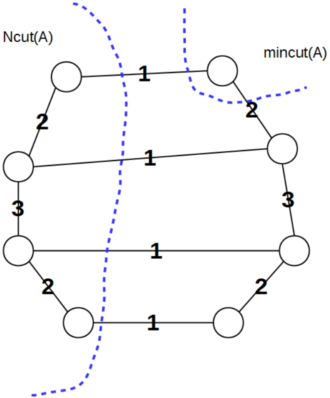
$$\mathsf{Ncut}(A) = \frac{\mathsf{cut}(A)}{\mathsf{vol}(A)} + \frac{\mathsf{cut}(\bar{A})}{\mathsf{vol}(\bar{A})}.$$

[1] Jianbo Shi and Jitendra Malik, 2000

II.2 Normalized cut

Minimal Ncut:

$$\min \mathsf{Ncut}(A).$$



$$\min \mathsf{Ncut}(A) = \frac{4}{3+6+6+3} + \frac{4}{3+6+6+3} = \frac{4}{9}.$$

II.2 Normalized cut

1. Let $x = (x_1, \ldots, x_n)$ be the *indicator vector*, such that

$$x_i = \begin{cases} 1 & \text{if } v_i \in A \\ -1 & \text{if } v_i \in \bar{A} \end{cases} .$$

2. Then
   $(\mathbf{1}+x)^T D(\mathbf{1}+x) = 4\sum_{v_i \in A} d_i = 4 \cdot \mathrm{vol}(A)$;
   $(\mathbf{1}+x)^T W(\mathbf{1}+x) = 4\sum_{v_i \in A, v_j \in A} w_{ij} = 4 \cdot \mathrm{assoc}(A)$.
   $(\mathbf{1}+x)^T L(\mathbf{1}+x) = 4 \cdot (\mathrm{vol}(A) - \mathrm{assoc}(A)) = 4 \cdot \mathrm{cut}(A)$;
   and
   $(\mathbf{1}-x)^T D(\mathbf{1}-x) = 4\sum_{v_i \in \bar{A}} d_i = 4 \cdot \mathrm{vol}(\bar{A})$;
   $(\mathbf{1}-x)^T W(\mathbf{1}-x) = 4\sum_{v_i \in \bar{A}, v_j \in \bar{A}} w_{ij} = 4 \cdot \mathrm{assoc}(\bar{A})$.
   $(\mathbf{1}-x)^T L(\mathbf{1}-x) = 4 \cdot (\mathrm{vol}(\bar{A}) - \mathrm{assoc}(\bar{A})) = 4 \cdot \mathrm{cut}(\bar{A})$.
   (Please verify it after class.)

II.2 Normalized cut

3. Ncut(A) can now be written as

$$\begin{aligned}\text{Ncut}(A) &= \frac{1}{4}\left(\frac{(\mathbf{1}+x)^T L(\mathbf{1}+x)}{k\mathbf{1}^T D\mathbf{1}} + \frac{(\mathbf{1}-x)^T L(\mathbf{1}-x)}{(1-k)\mathbf{1}^T D\mathbf{1}}\right) \\ &= \frac{1}{4}\cdot\frac{((\mathbf{1}+x)-b(\mathbf{1}-x))^T L((\mathbf{1}+x)-b(\mathbf{1}-x))}{b\mathbf{1}^T D\mathbf{1}}.\end{aligned}$$

   where $k = \text{vol}(A)/\text{vol}(V)$, $b = k/(1-k)$ and $\text{vol}(V) = \mathbf{1}^T D\mathbf{1}$.

4. Let $y = (\mathbf{1}+x) - b(\mathbf{1}-x)$, we have

$$\text{Ncut}(A) = \frac{1}{4}\cdot\frac{y^T L y}{b\mathbf{1}^T D\mathbf{1}}$$

   where

$$y_i = \begin{cases} 2 & \text{if } v_i \in A \\ -2b & \text{if } v_i \in \bar{A} \end{cases}.$$

II.2 Normalized cut

5. Since $b = k/(1-k) = \mathsf{vol}(A)/\mathsf{vol}(\bar{A})$, we have

$$\frac{1}{4}y^T D y = \sum_{v_i \in A} d_i + b^2 \sum_{v_i \in \bar{A}} d_i = \mathsf{vol}(A) + b^2 \mathsf{vol}(\bar{A})$$
$$= b(\mathsf{vol}(\bar{A}) + \mathsf{vol}(A)) = b\mathbf{1}^T D\mathbf{1}.$$

In addition,

$$y^T D\mathbf{1} = y^T \boldsymbol{d} = 2 \cdot \sum_{v_i \in A} d_i - 2b \cdot \sum_{v_i \in \bar{A}} d_i$$
$$= 2 \cdot \mathsf{vol}(A) - 2b \cdot \mathsf{vol}(\bar{A}) = 0$$

II.2 Normalized cut

6. The **minimal normalized cut** is to solve the following **binary optimization**:

$$
\begin{aligned}
y = \arg\min_{y} \quad & \frac{y^T L y}{y^T D y} \\
s.t. \quad & y(i) \in \{2, -2b\} \\
& y^T D \mathbf{1} = 0
\end{aligned}
\tag{1}
$$

7. Relaxation

$$
\begin{aligned}
y = \arg\min_{y} \quad & \frac{y^T L y}{y^T D y} \\
s.t. \quad & y \in \mathbb{R}^n \\
& y^T D \mathbf{1} = 0
\end{aligned}
\tag{2}
$$

II.2 Normalized cut

Variational principle

- Let $A, B \in \mathbb{R}^{n \times n}$, $A^T = A$, $B^T = B > 0$ and $\lambda_1 \leq \lambda_2 \leq \ldots \lambda_n$ be the eigenvalues of $Au = \lambda Bu$ with corresponding eigenvectors $u_1, u_2, \ldots, u_n$,
- then

$$\min_x \frac{x^T Ax}{x^T Bx} = \lambda_1 \ , \quad \arg\min_x \frac{x^T Ax}{x^T Bx} = u_1$$

  and

$$\min_{x^T Bu_1 = 0} \frac{x^T Ax}{x^T Bx} = \lambda_2 \ , \quad \arg \min_{x^T Bu_1 = 0} \frac{x^T Ax}{x^T Bx} = u_2.$$

- More general form exists.

II.2 Normalized cut

- For the matrix pair (L, D), it is known that $(\lambda_1, y_1) = (0, \mathbf{1})$.
- Therefore, by the variational principle, the relaxed minimal Ncut problem (2) is equivalent to finding the second smallest eigenpair (λ_2, y_2) of

$$Ly = \lambda Dy \tag{3}$$

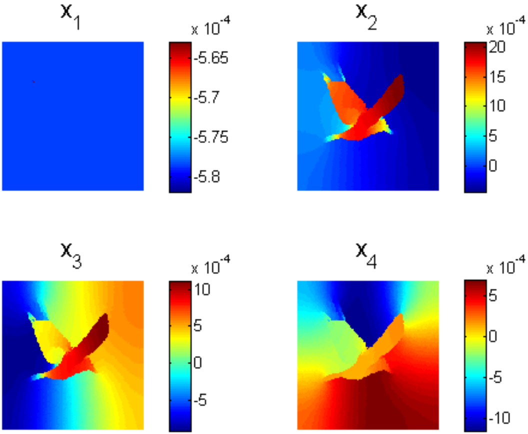
- L is extremely sparse and D is diagonal;
- Precision requirement for eigenvectors is low, say $\mathcal{O}(10^{-4})$.

II.2 Normalized cut

Image segmentation: original graph

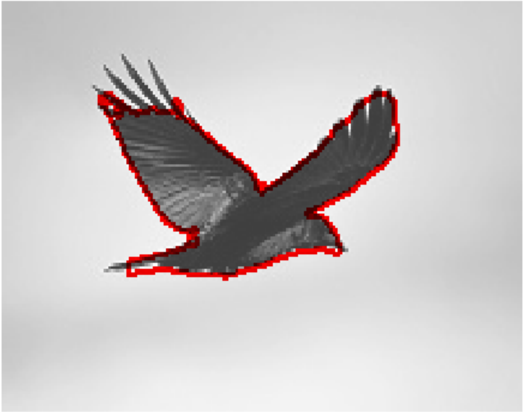
II.2 Normalized cut

Image segmentation: heatmap of eigenvectors



II.2 Normalized cut

Image segmentation $\min$ **Ncut**



Ncut remaining issues

- Once the indicator vector is computed, how to search the splitting point that the resulting partition has the minimal Ncut(A) value?
- How to use the extreme eigenvectors to do the k-way partitioning?

The above two problems are addressed in spectral clustering algorithm.

II.3 Spectral clustering

Spectral clustering algorithm [Ng et al, 2002]

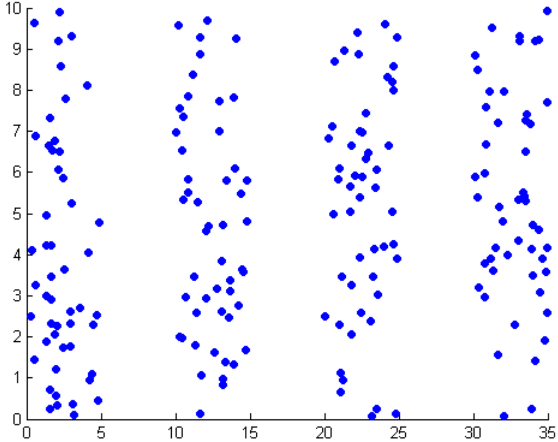
Given a weighted graph $G = (V, W)$,

1. *compute the normalized Laplacian* $L = D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}}$*;*
2. *find k eigenvectors $X = [x_1, \ldots, x_k]$ corresponding to the k smallest eigenvalues of L;*
3. *form $Y \in \mathbb{R}^{n \times k}$ by normalizing each row of X such that $Y(i,:) = X(i,;)/\|X(i,:)\|$;*
4. *treat each $Y(i,:)$ as a point, cluster them into k clusters via K-means with label $c_i = \{1, \ldots, k\}$.*

The label c_i indicates the cluster that v_i belongs to.

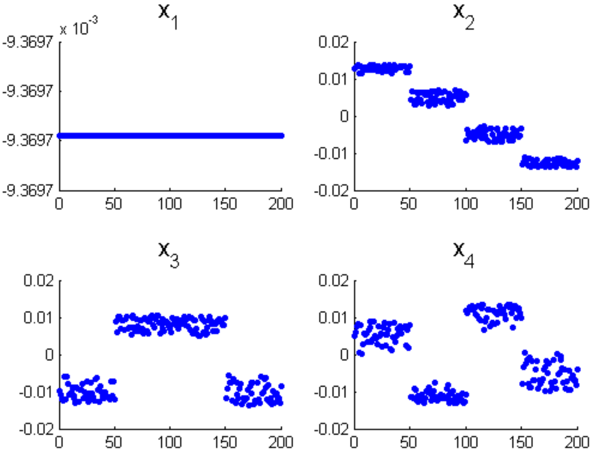
II.3 Spectral clustering

Synthetic example: original data



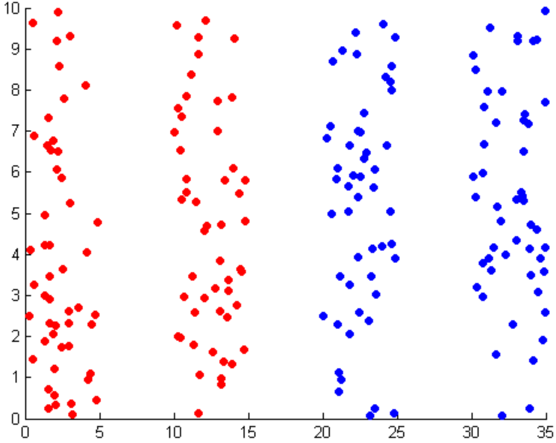
II.3 Spectral clustering

Synthetic example: computed eigenvectors



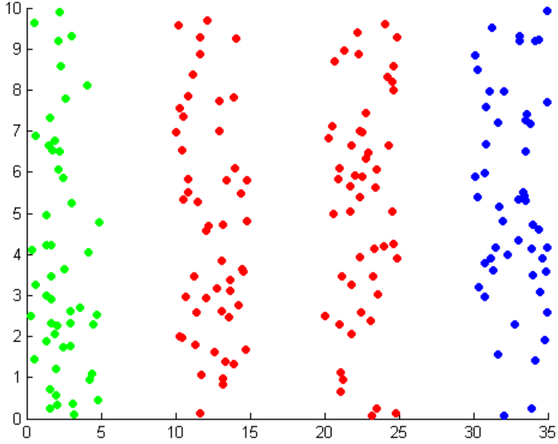
II.3 Spectral clustering

Synthetic example: 2-way clustering



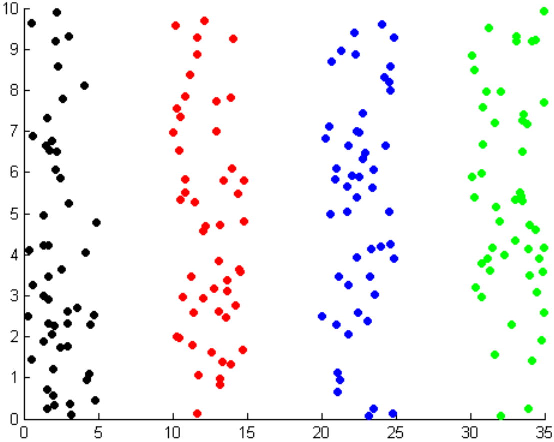
II.3 Spectral clustering

Synthetic example: 3-way clustering



II.3 Spectral clustering

Synthetic example: 4-way clustering



Further reading

1. Jean Gallier, *Notes on elementary spectral graph theory applications to graph clustering using normalized cuts*, 2013.
2. Jianbo Shi and Jitendra Malik, *Normalized cuts and image segmentation*, 2000.
3. Andrew Y Ng, Michael I. Jordan and Yair Weiss, *On spectral clustering: Analysis and an algorithm*, 2001