

One Week Online Workshop on Statistics and Machine Learning in Practice
Brahmananda Keshab Chandra College

SPECTRAL CLUSTERING

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INDIAN STATISTICAL INSTITUTE
JULY 29, 2020

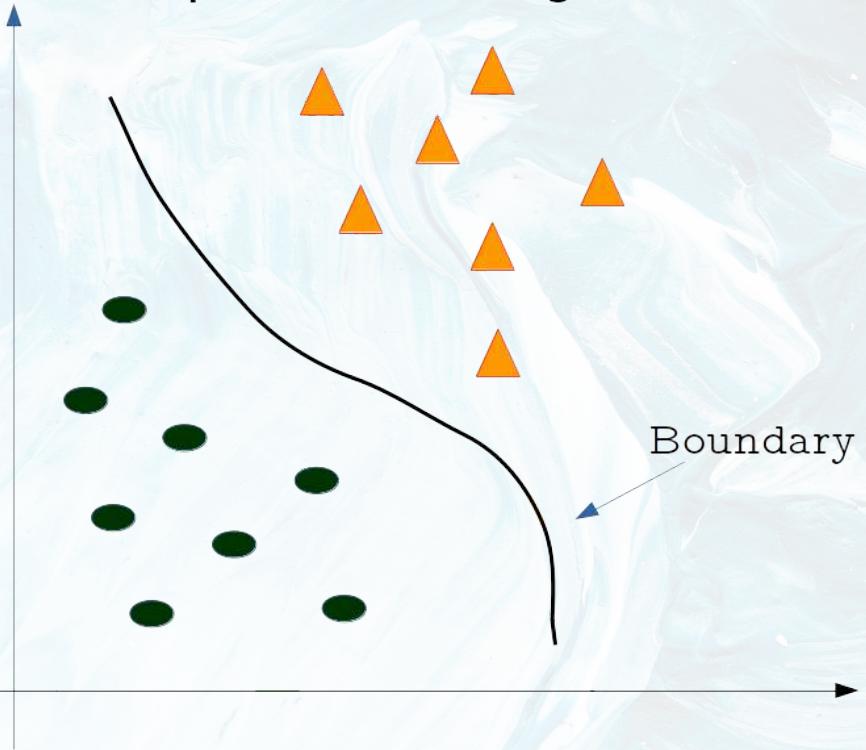
CLUSTERING

The study of natural groupings in data

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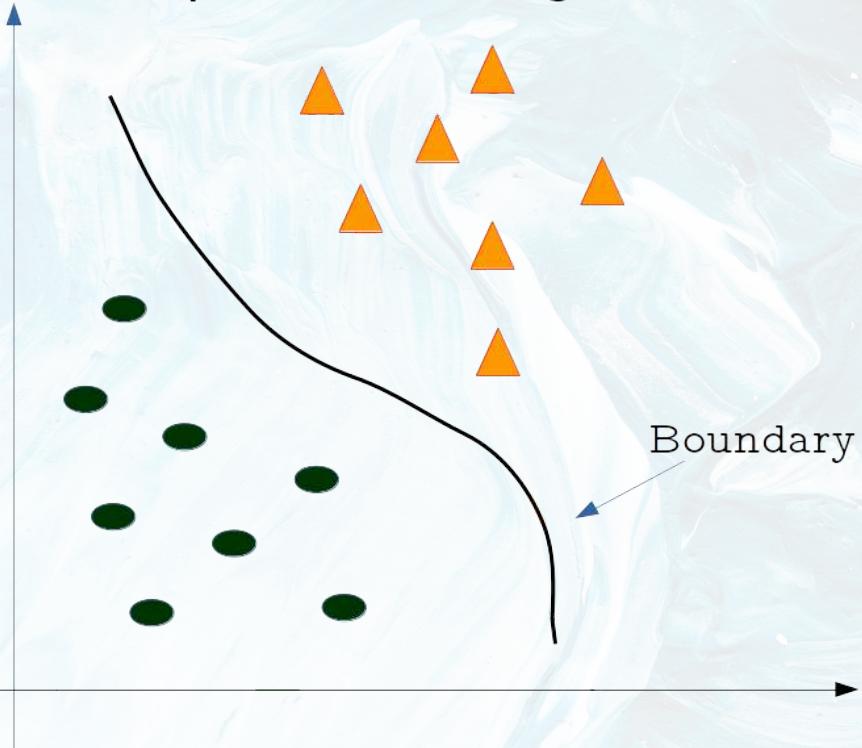
Supervised Learning



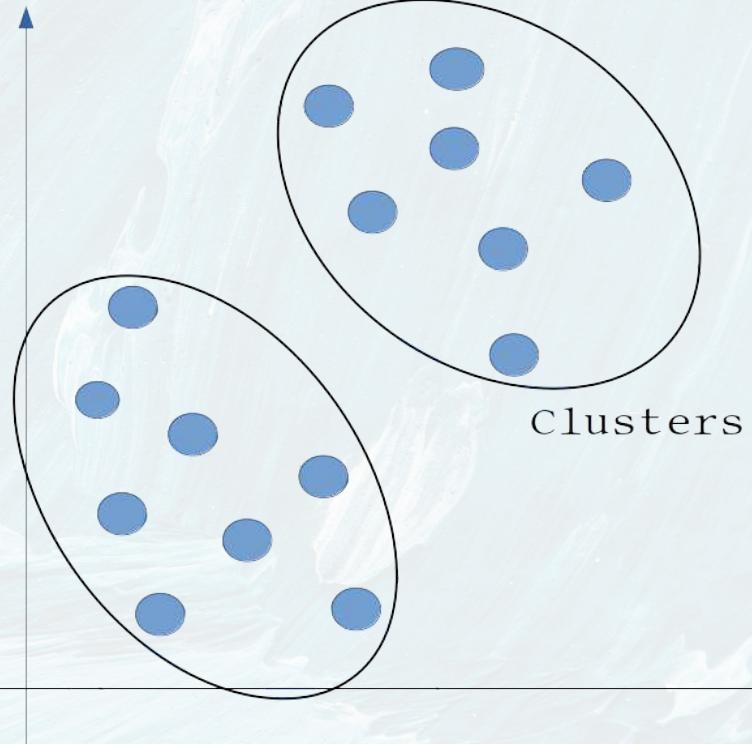
CLUSTERING

The study of natural groupings in data

Supervised Learning



Unsupervised Learning



CLUSTERING: Applications

Grouping similar news articles

https://www.indiatoday.in/news.html

60%

NEWS

INDIA

Rajasthan crisis: Governer under pressure from BJP, says Congress

- Over 3,300 coronavirus patients 'untraceable' in Bengaluru amid spike in cases
- Covid bed occupancy coming down, few people need hospitalisation now: Kejriwal
- Coronavirus in India: Bodies of Covid patients burnt in open in Patna
- Watch | India battles Covid-19
- Kargil Vijay Diwas: From Rajnath Singh to Rahul Gandhi, leaders pay tribute to brave martyrs
- Prressman House: The building at the heart of Maharashtra's political diversity
- Kolkata: Ambulance driver demands Rs 9,200 from coronavirus patients for 6-km journey to hospital

Movies

AR Rahman: A gang in Bollywood is spreading false rumours about me

- Rajkummar Rao gets emotional watching old film
- Varun Dhawan's 'Jabariya Jodi' vs Akshay Kumar's 'Jawaani Jaaneman': Which movie is better?
- The Akhtars on nepotism and celebrity culture
- Sonu Sood on e-Mind Rocks 2020: I wasn't

SPORTS

IPL 2020's knock-on effect on UAE economy will be huge: Kumar Sangakkara

- It was about changing the momentum of innings: Stuart Broad on his 33-ball fifty
- Have never thought of bringing the ODI style of play in Test cricket: Gautam Gambhir
- England vs West Indies: Broad's Assertion put hosts on top in the contest
- Racism a topical and burning issue for Indians and Sri Lankans: Kumar Sangakkara
- Ganguly has an astute cricket brain, he will be a fair ICC chief: Sangakkara
- If MS Dhoni thinks he can still win matches for India, he should play: Gautam Gambhir
- What's done is done: Irfan Pathan lashes out at Steve Bucknor over 2008 howlers

TRENDING NEWS

Dr PK Mahanandi: The untouchable boy who became art advisor for Swedish government

- Lund University has had enough of Indians on Facebook
- Carryminati's YouTube account hacked, hacker asks for bitcoin donations
- Adorable video of elephant playing with its human friend goes viral

sports cluster

Covaxin enters human trials at AIIMS: All you need to know

Rajasthan crisis explained in 10 point: From Pilot, Gehlot to ED and Malinga

SUGGESTED STORIES

WATCH RIGHT NOW

Watch: Hyderabad's Osmania Hospital once again flooded after heavy rain

Assam floods: Nearly 27 people affected, 91 killed in deluge

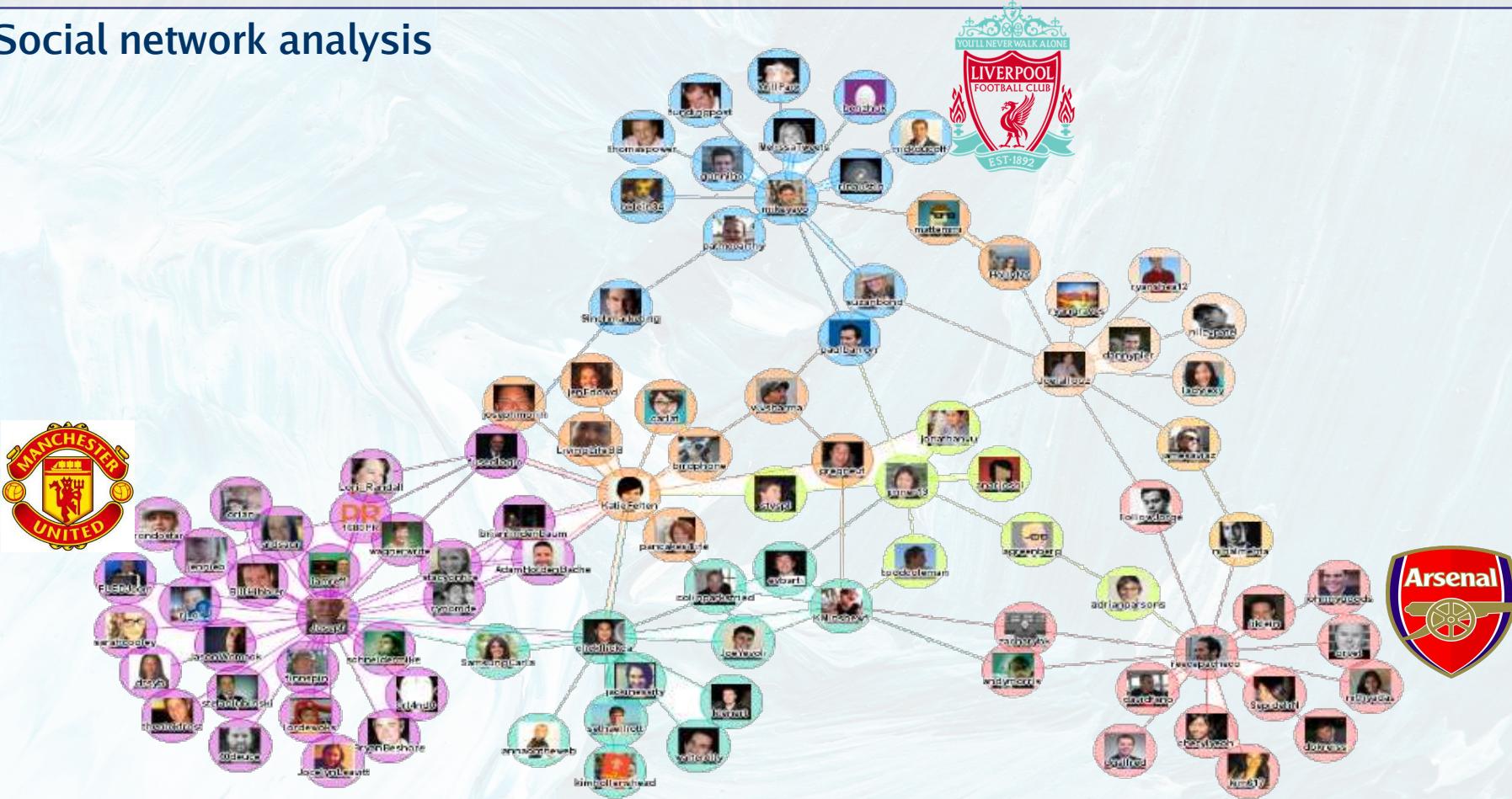
Don't buy it from black market: Delhi CM Kejriwal on Operation Plasma Bazaar | EXCLUSIVE

WATCH: India's coronavirus tally exceeds 12 lakh

Why not Manesar hotel: Chidambaram asks ED after raids on Ashok Gehlot's brother

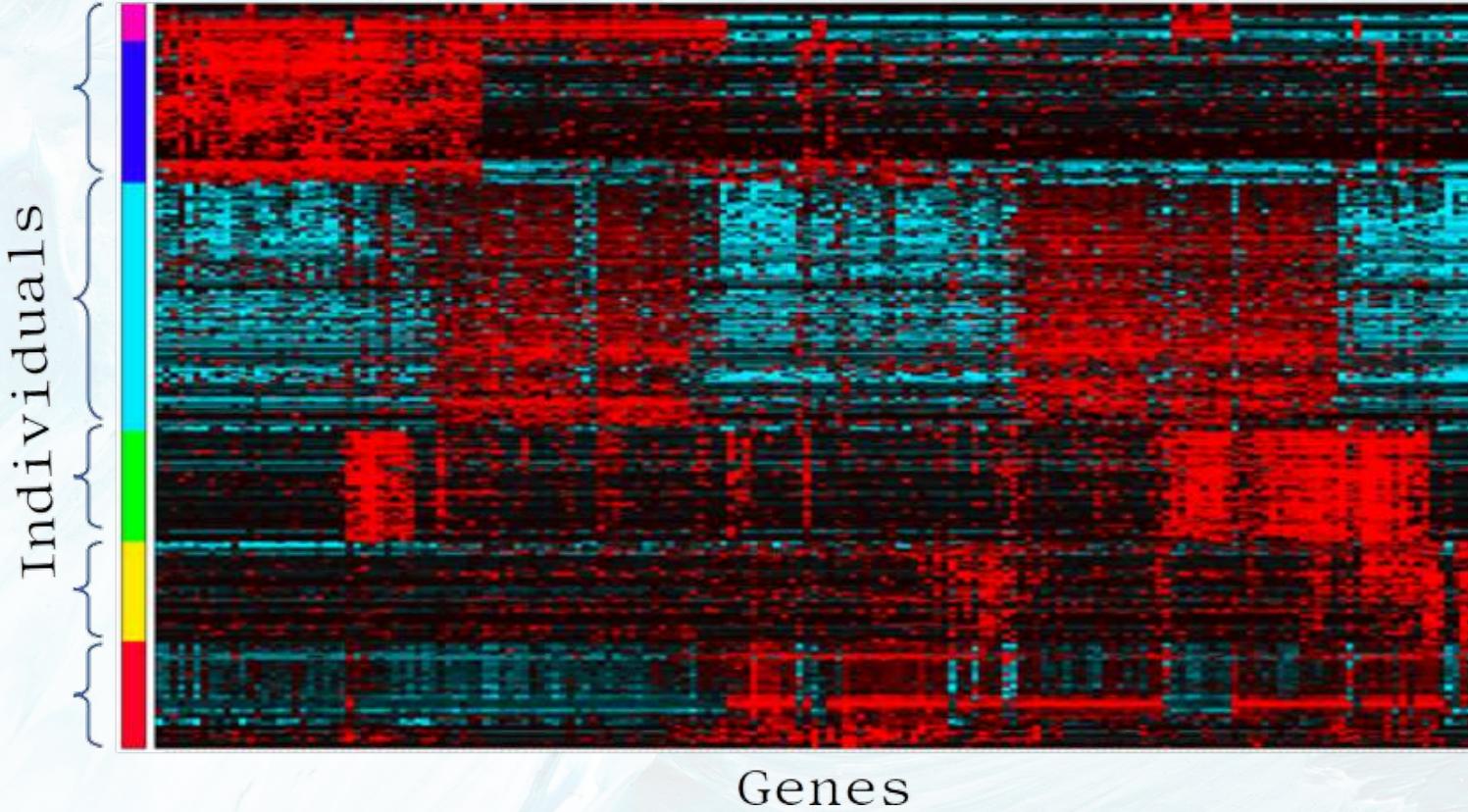
CLUSTERING: Applications

Social network analysis



CLUSTERING: Applications

Bioinformatics: Identifying disease subtypes, patient groups



CLUSTERING: Applications

Image segmentation



FEATURE-SPACE VS GRAPH CLUSTERING

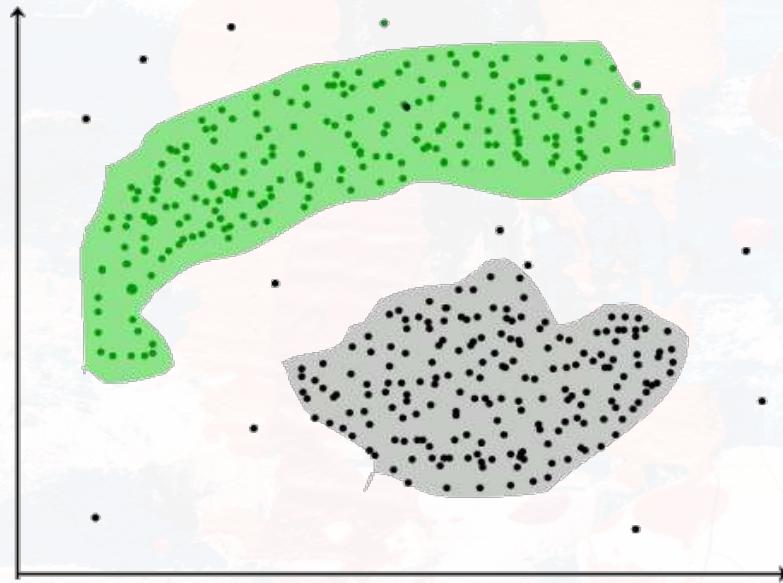
Feature-space: k -Means Clustering

$$\mathbf{X} \in \Re^{n \times d} \quad n \text{ samples, } d \text{ features}$$

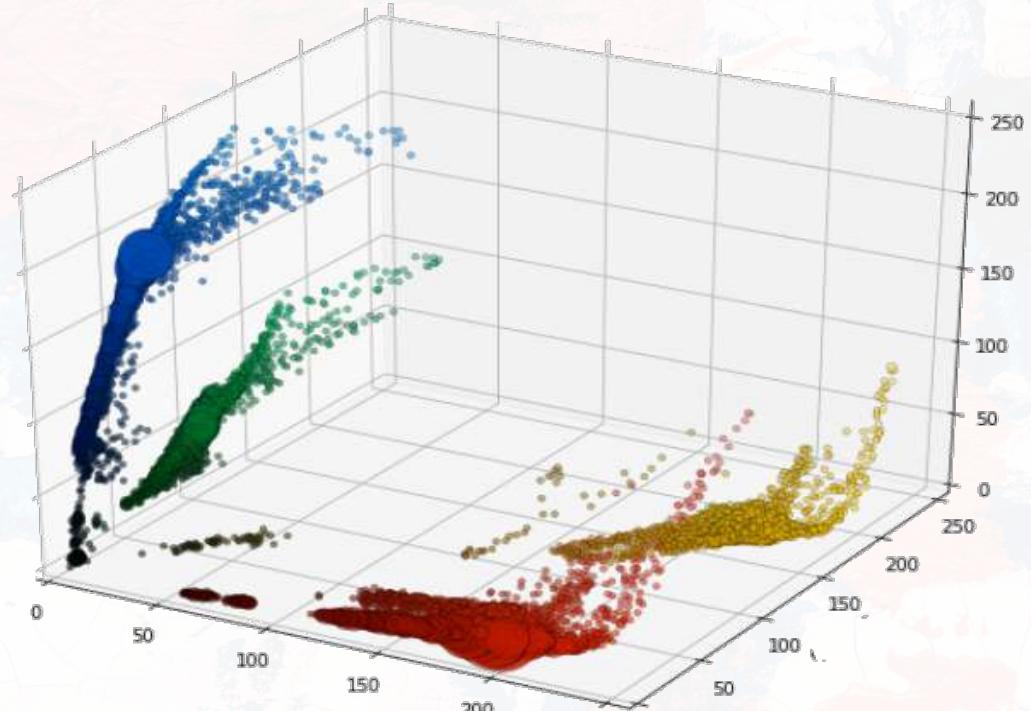
FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space: k -Means Clustering

$$\mathbf{X} \in \Re^{n \times d} \quad n \text{ samples, } d \text{ features}$$



2 Dimensions



3 Dimensions

FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space: k -Means Clustering

- But, what about high dimensions?

Disease subtyping: ~1,000 samples ~20,000 genes

Object recognition: 1024x1024 images -> ~1M pixels

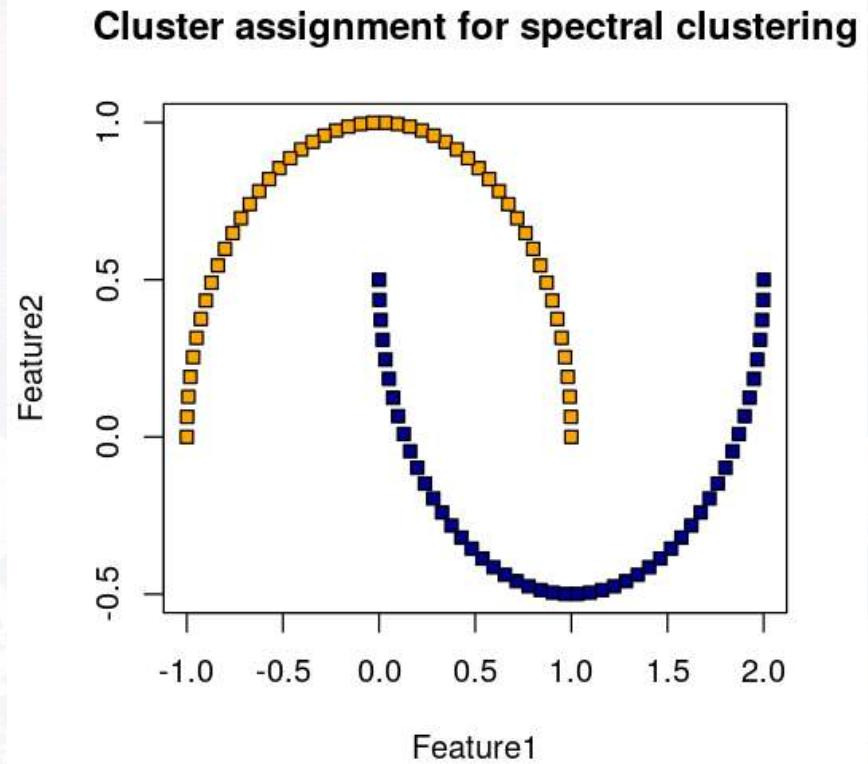
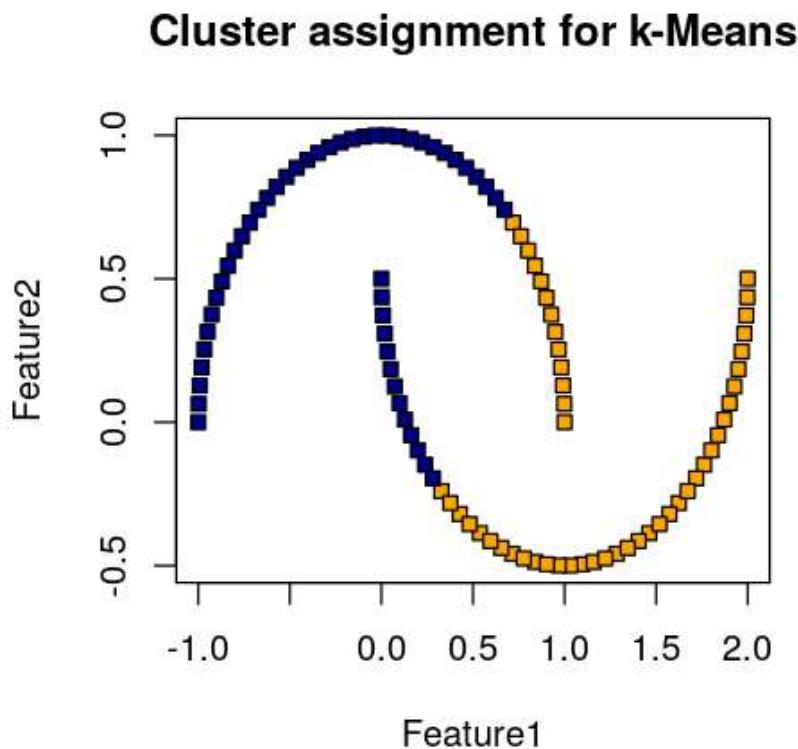
FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space: k -Means Clustering

- But, what about high dimensions?
 - Disease subtyping: ~1,000 samples ~20,000 genes
 - Object recognition: 1024x1024 images -> ~1M pixels
- In such high dimensions:
 - Data becomes geometrically sparse
 - Distance between nearby points roughly same as distance between far away points

FEATURE-SPACE VS GRAPH CLUSTERING

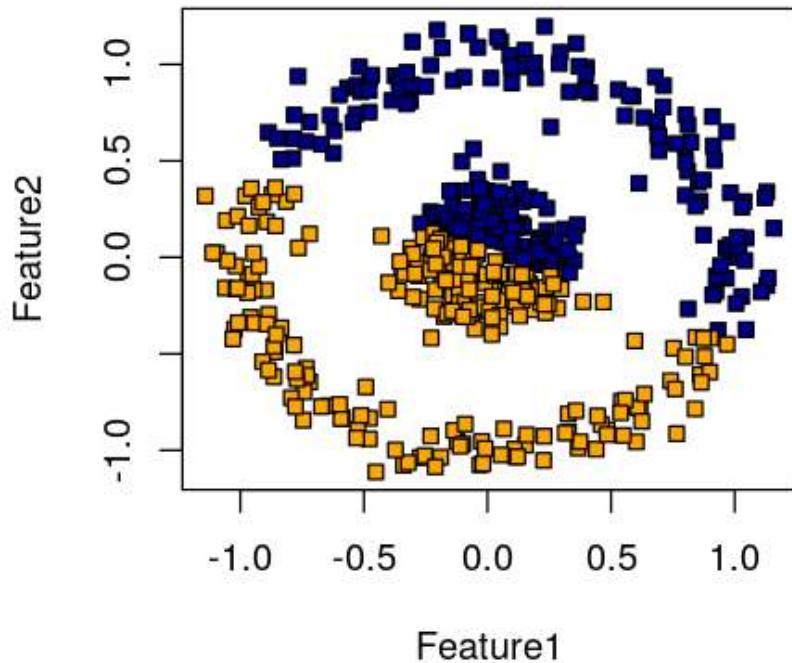
Handling non-linearity



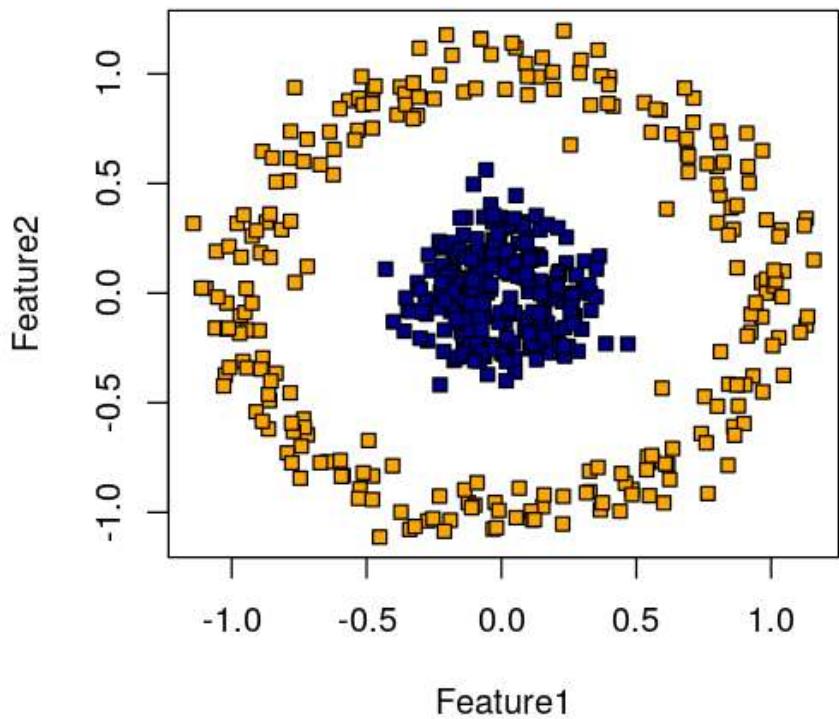
FEATURE-SPACE VS GRAPH CLUSTERING

Handling non-linearity

Cluster assignment for k-Means

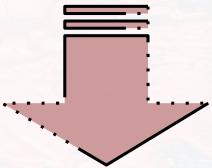


Cluster assignment for spectral clustering



FEATURE-SPACE VS GRAPH CLUSTERING

FEATURE-SPACE BASED REPRESENTATION



GRAPH BASED REPRESENTATION

FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space

$$\mathbf{X} \in \Re^{n \times d}$$

Samples: n

Features/Dimension: d

Graph

FEATURE-SPACE VS EIGENSPACE CLUSTERING

Feature-space

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

Samples: n

Features/Dimension: d

$$\kappa(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$



Gaussian similarity kernel

Graph

$$\mathbf{W} \in \mathbb{R}^{n \times n}$$

Pairwise
similarity
matrix

FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

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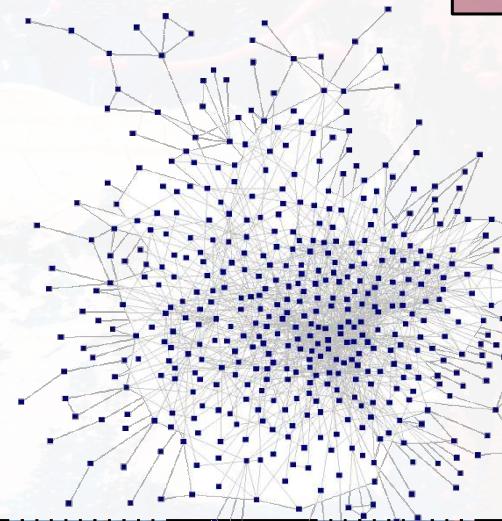


Gaussian similarity kernel

Graph

$$\mathbf{W} \in \mathbb{R}^{n \times n}$$

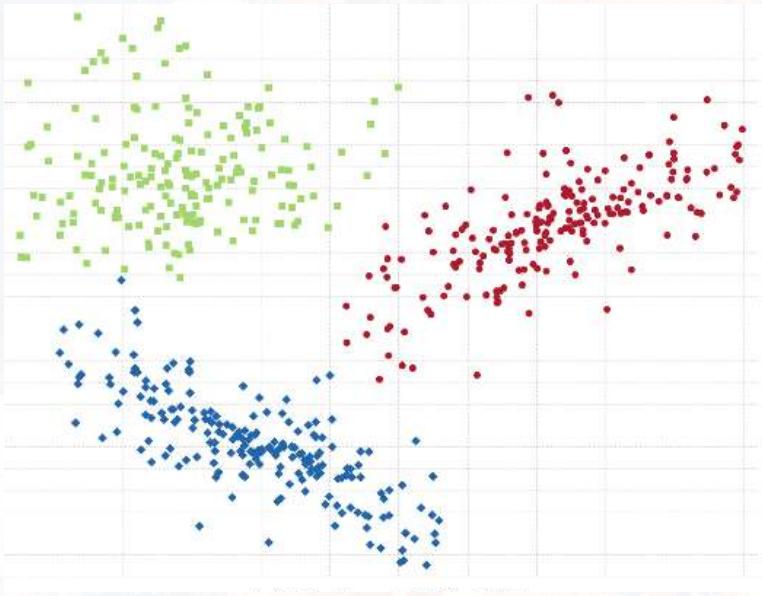
Pairwise
similarity
matrix



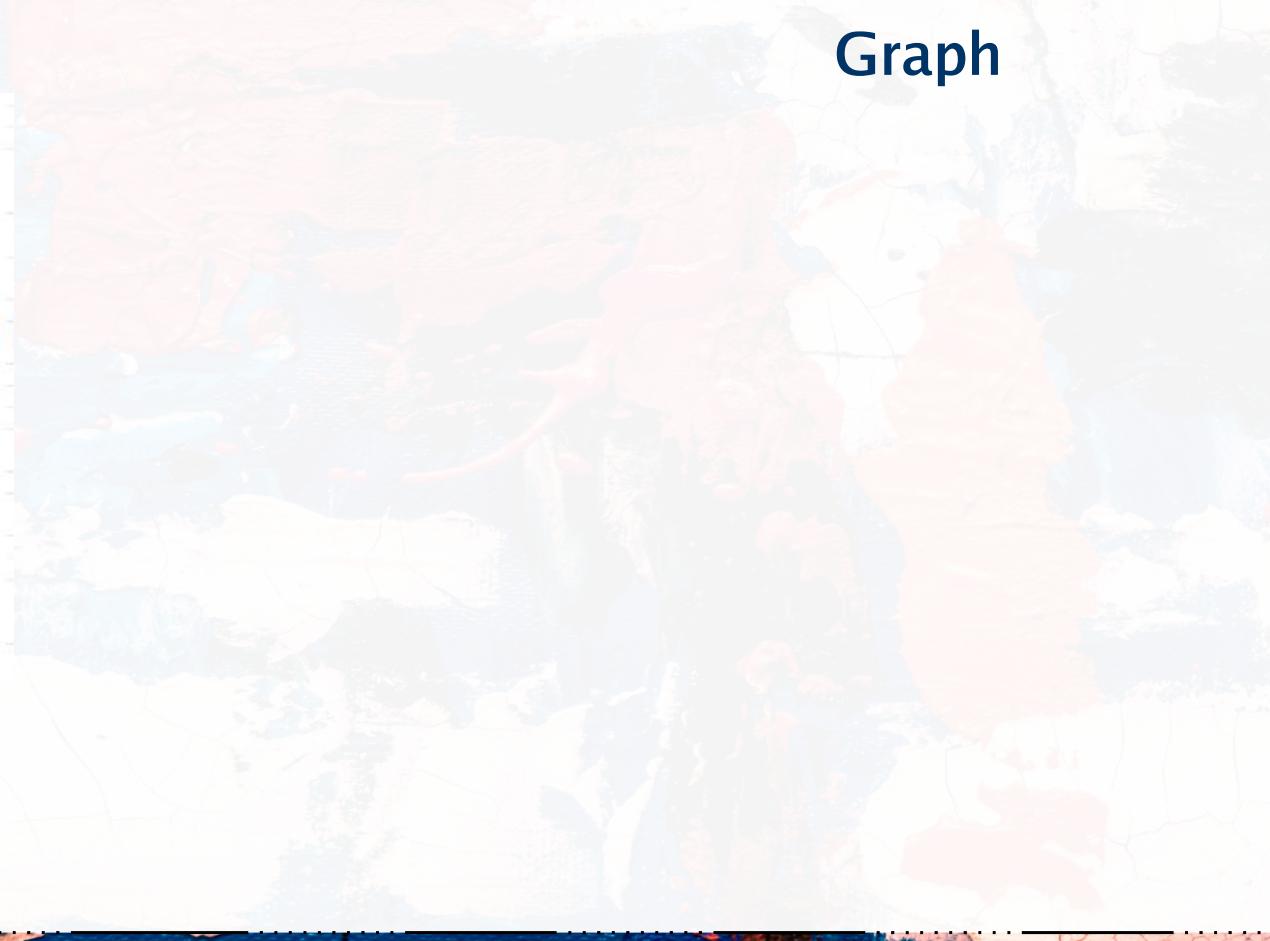
\mathbf{G}
weighted
adjacency

FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space



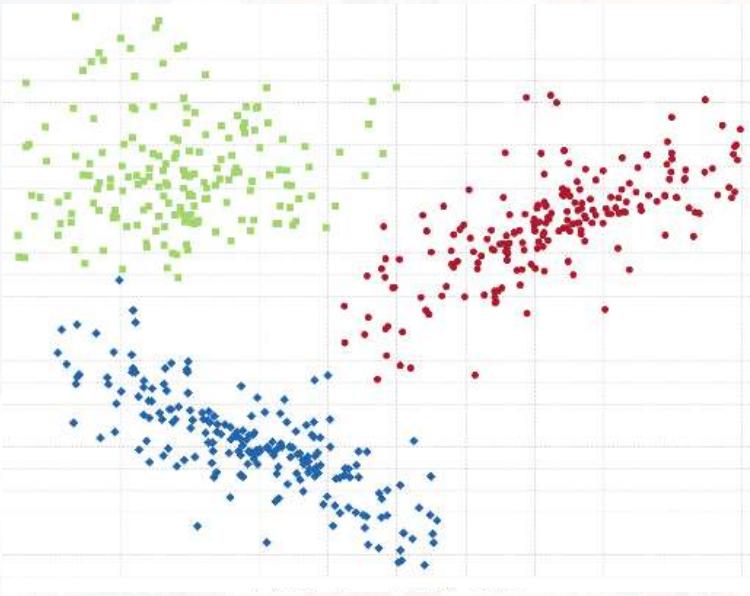
Graph



Clusters in dataset

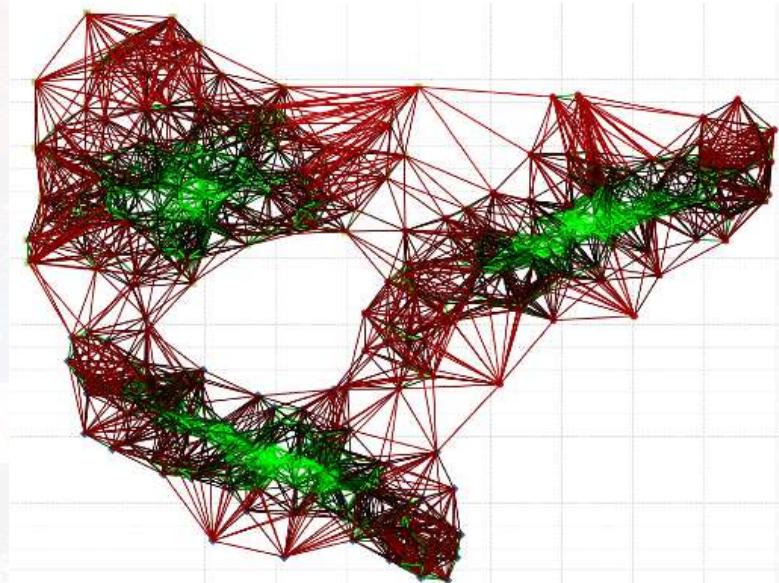
FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space



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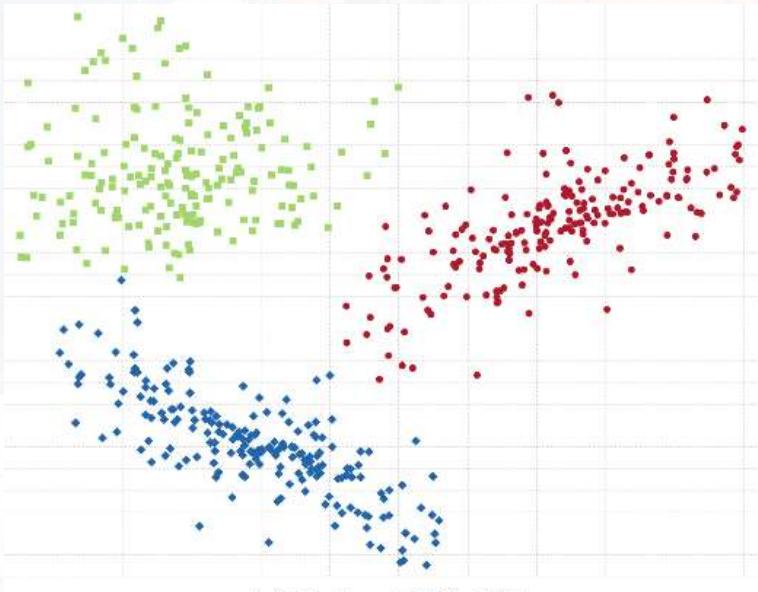
Graph



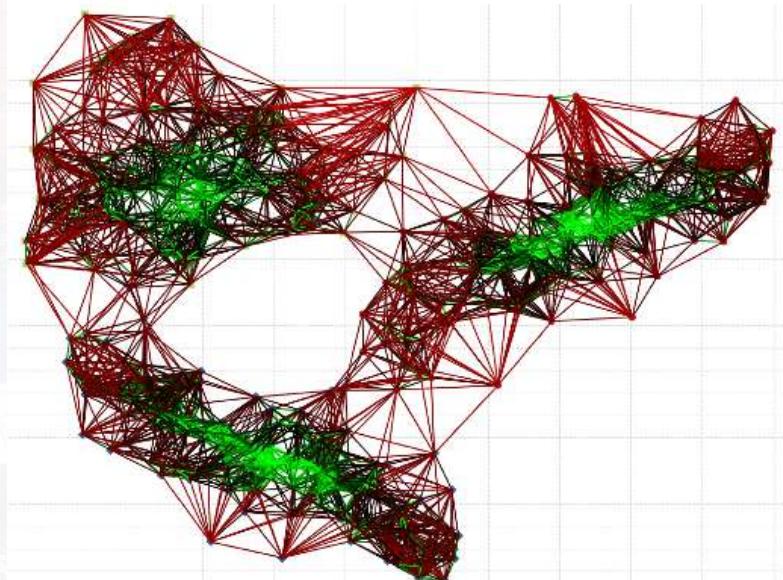
Strongly connected
components in graph

FEATURE-SPACE VS GRAPH CLUSTERING

Feature-space



Graph



Graph-cut problem

$$\text{minimize} \sum_{j=1}^k \sum_{i \in \mathcal{C}_j} \left\| x_i - \frac{1}{|\mathcal{C}_j|} \sum_{t \in \mathcal{C}_j} x_t \right\|_2^2$$

THE GRAPH-CUT

Find a k-way partition of graph such that:

Edges between different components have very low weight

(points in different clusters are dissimilar)

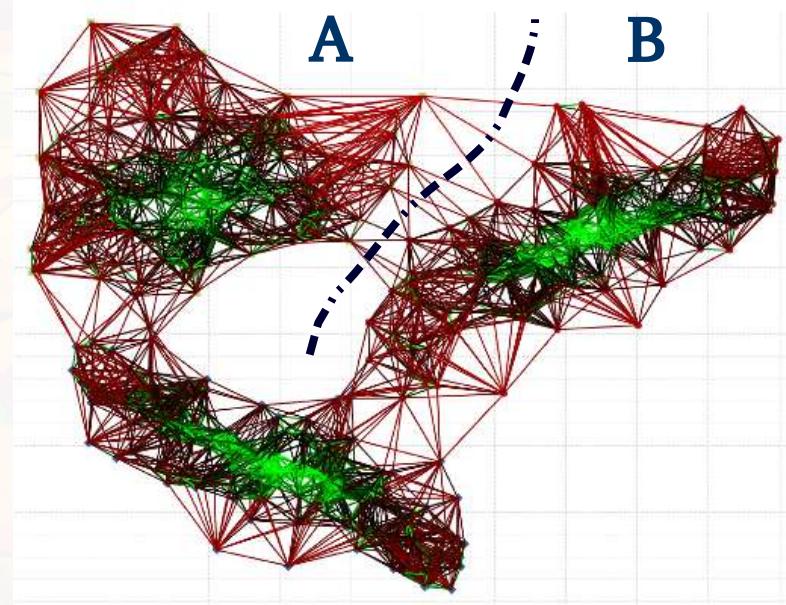
Edges within a component have high weight

(points within same cluster are similar)

THE GRAPH-CUT

$$\mathbf{W} = [w_{ij}]_{n \times n}$$

$$\text{cut } W(A, B) := \sum_{i \in A, j \in B} w_{ij}$$



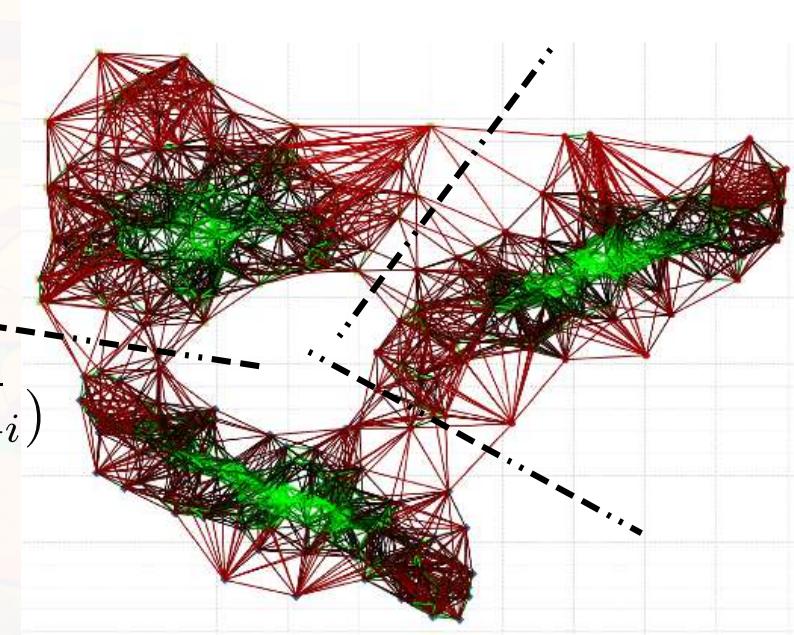
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k-way cut:

$$\text{minimize } \text{cut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k W(A_i, \bar{A}_i)$$



THE GRAPH-CUT

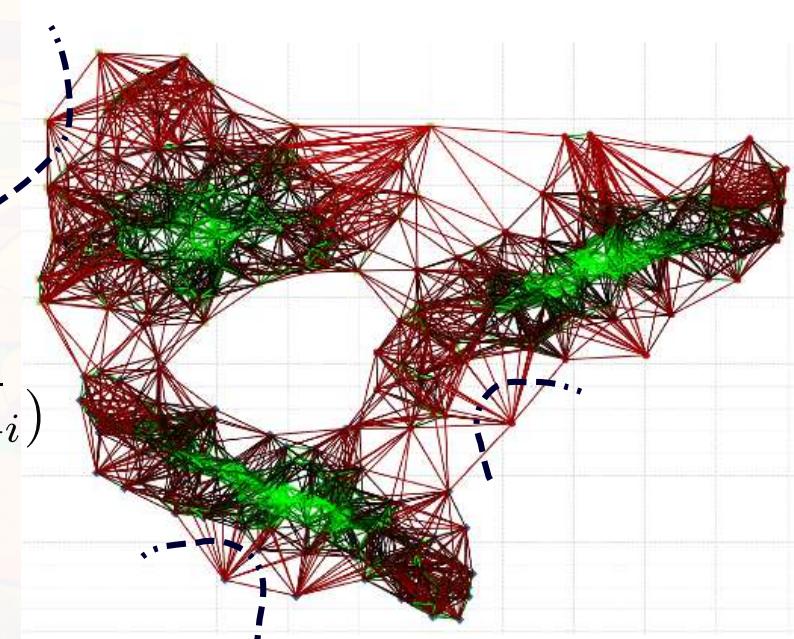
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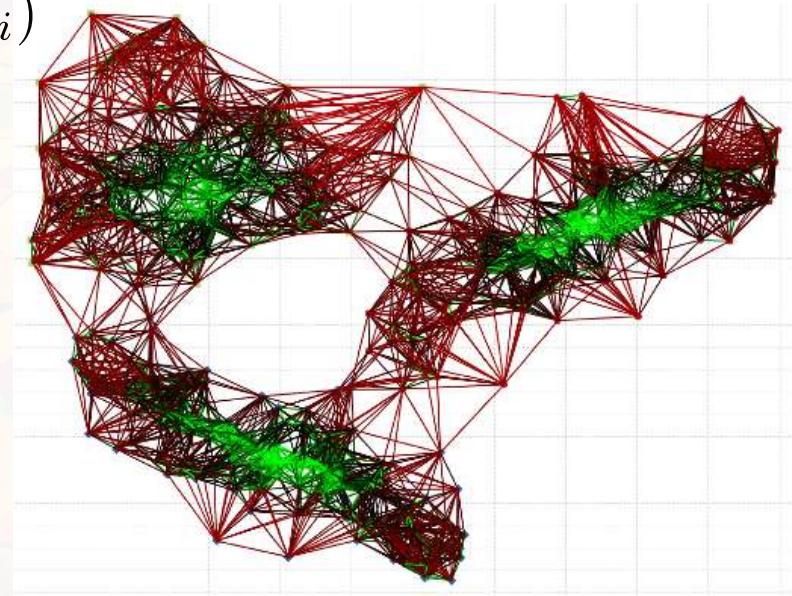
- In many cases, mincut simply separates individual vertices from rest of the graph



THE GRAPH-CUT

$$\text{minimize } \text{cut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k W(A_i, \bar{A}_i)$$

Explicitly request subsets
to be “reasonably large”



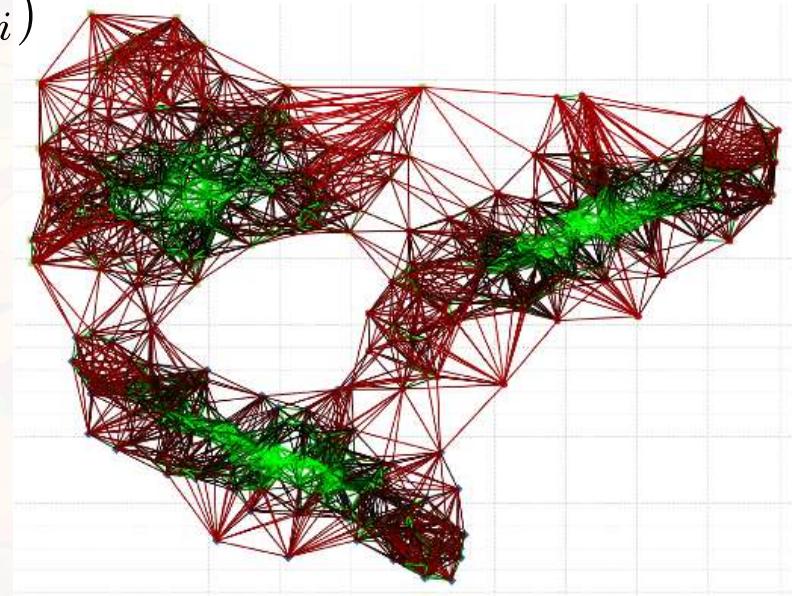
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$$\text{degree of vertex } v_i: d_i = \sum_{j=1}^n w_{ij}$$

$$\text{size of subset: } \text{vol}(A_i) := \sum_{i \in A} d_i$$



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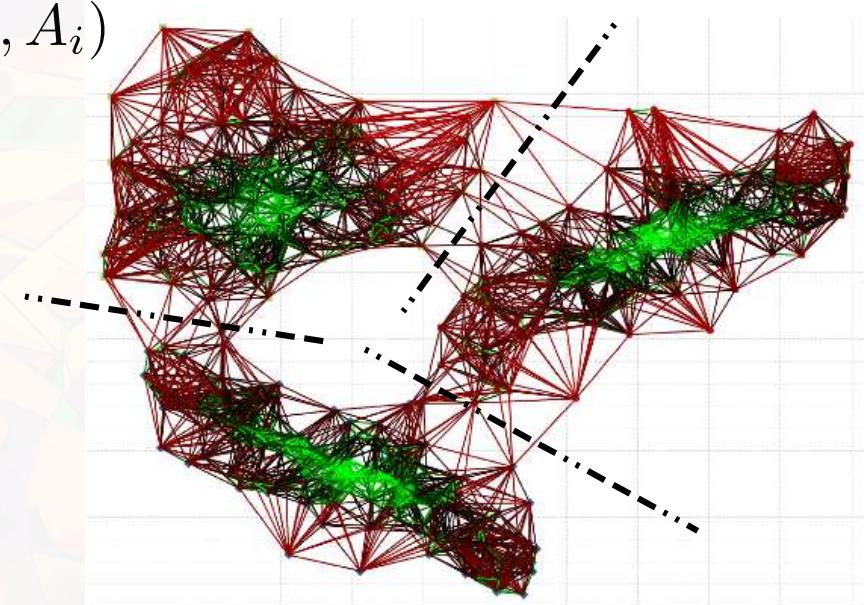
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Normalized cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$



SOLVING THE GRAPH-CUT

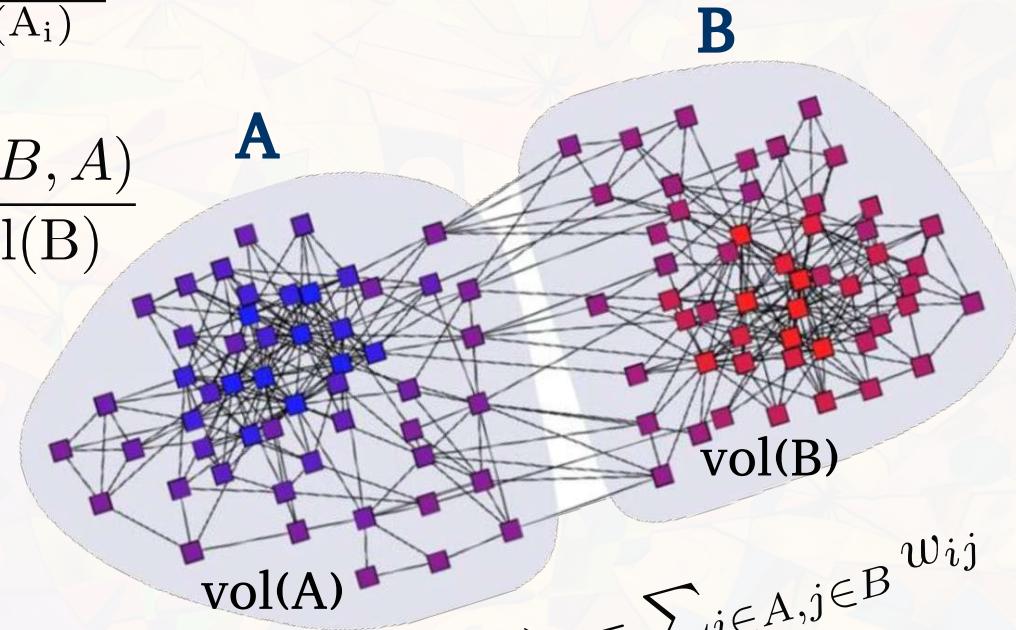
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Solving 2-way cut

$$\text{minimize } \text{Ncut}(A, B) := \frac{W(A, B)}{\text{vol}(A)} + \frac{W(B, A)}{\text{vol}(B)}$$



$$W(A, B) := \sum_{i \in A, j \in B} w_{ij}$$

SOLVING THE GRAPH-CUT

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$

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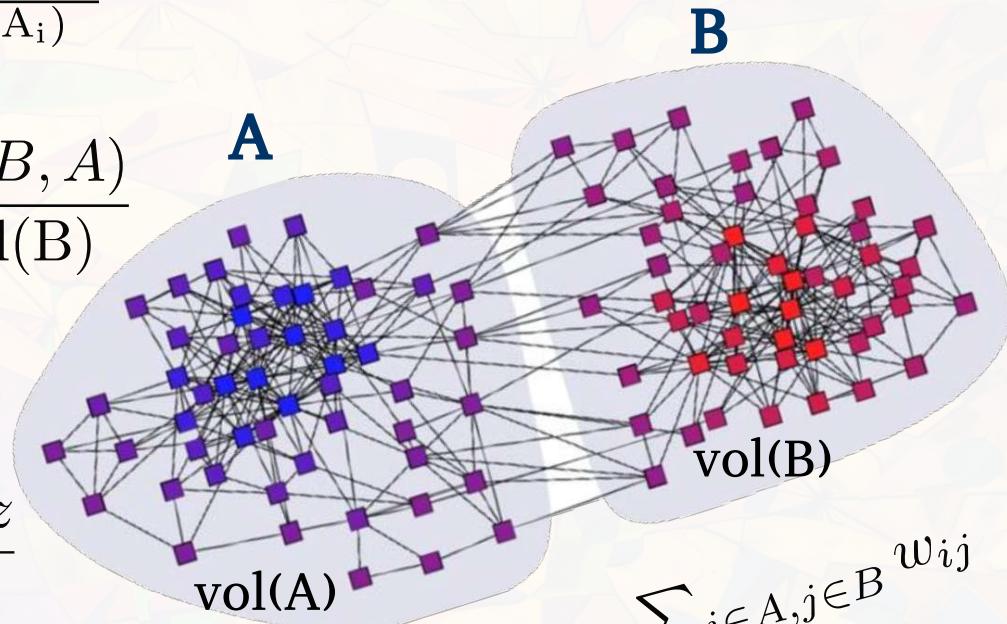
$$\text{minimize } \text{Ncut}(A, B) := \frac{W(A, B)}{\text{vol}(A)} + \frac{W(B, A)}{\text{vol}(B)}$$



Reduces to

$$\underset{z \in \mathbb{R}^n}{\text{minimize}} \frac{z^T \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}} z}{z^T z}$$

$$\text{such that } z^T (\mathbf{D}^{\frac{1}{2}} \mathbf{1}) = 0$$



SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}} z}{z^T z}$$

such that $\mathbf{z}^T \left(\mathbf{D}^{\frac{1}{2}} \mathbf{1} \right) = 0$

SOLVING THE GRAPH-CUT

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$$\text{such that } z^T \left(\mathbf{D}^{\frac{1}{2}} \mathbf{1} \right) = 0$$

\mathbf{W} =Pairwise-similarity matrix of size $n \times n$

$$\mathbf{D} = \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{bmatrix} \text{ Degree matrix}$$

SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T D^{-\frac{1}{2}} (D - W) D^{-\frac{1}{2}} z}{z^T z}$$

such that $z^T (D^{\frac{1}{2}} \mathbf{1}) = 0$

The normalized graph Laplacian

$$L = D^{-\frac{1}{2}} (D - W) D^{-\frac{1}{2}}$$

SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}} z}{z^T z}$$

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The normalized graph Laplacian

$$\mathbf{L} = \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}}$$

- Symmetric positive semi-definite

$$v^T \mathbf{L} v \geq 0, \forall v \in \Re^n, v \neq \mathbf{0}$$

all the eigenvalues are ≥ 0

- $\mathbf{D}^{\frac{1}{2}} \mathbf{1}$ is an eigenvector of \mathbf{L} with eigenvalue 0

SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}} z}{z^T z}$$

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Rayleigh quotient:

Let A be a real symmetric matrix
Constraint: v is orthogonal to $j-1$
smallest eigenvectors v_1, \dots, v_{j-1} , the

$$\text{quotient } \frac{v^T A v}{v^T v}$$

is minimized by next smallest
eigenvector v_j and eigenvalue λ_j

SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T \mathbf{D}^{-\frac{1}{2}} (\mathbf{D} - \mathbf{W}) \mathbf{D}^{-\frac{1}{2}} z}{z^T z}$$

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The normalized graph Laplacian

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- $\mathbf{D}^{\frac{1}{2}} \mathbf{1}$ is an eigenvector of \mathbf{L} with eigenvalue 0

Minimized by:
second smallest eigenvector
of \mathbf{L} and its eigenvalue

SOLVING THE GRAPH-CUT

$$\underset{z \in \Re^n}{\text{minimize}} \frac{z^T \mathbf{L} z}{z^T z} \text{ such that } z^T \left(\mathbf{D}^{\frac{1}{2}} \mathbf{1} \right) = 0$$

SOLVING THE GRAPH-CUT

$$\underset{z \in \mathbb{R}^n}{\text{minimize}} \frac{z^T \mathbf{L} z}{z^T z} \text{ such that } z^T (\mathbf{D}^{\frac{1}{2}} \mathbf{1}) = 0$$

Eigen decomposition $\mathbf{L} = U \Sigma U^T$

$$\begin{bmatrix} \sqrt{d_1} & | & | & | \\ \vdots & u_2 & u_3 & \dots & u_n \\ \sqrt{d_n} & | & | & | \end{bmatrix} \quad \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

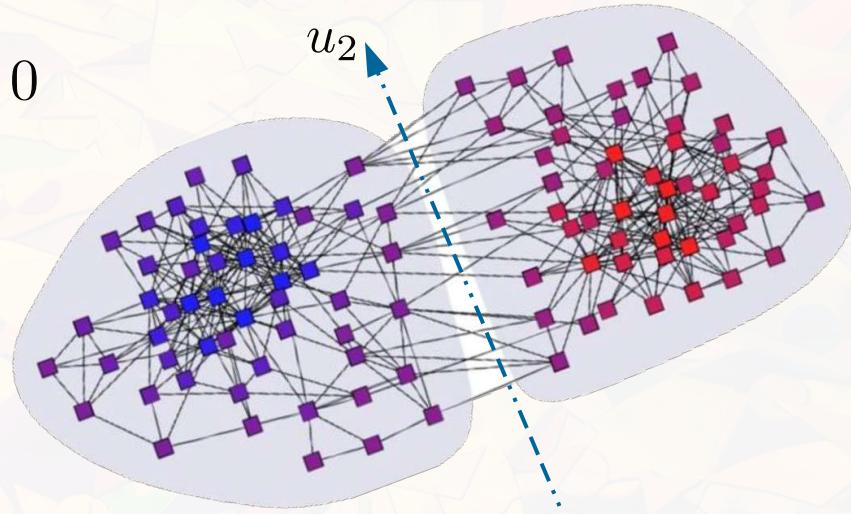

(arranged in
ascending order)

SOLVING THE GRAPH-CUT

$$\underset{z \in \mathbb{R}^n}{\text{minimize}} \frac{z^T \mathbf{L} z}{z^T z} \text{ such that } z^T (\mathbf{D}^{\frac{1}{2}} \mathbf{1}) = 0$$

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SOLVING THE GRAPH-CUT

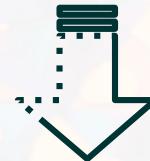
Solving k-way cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$

SOLVING THE GRAPH-CUT

Solving k-way cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$



$$\text{minimize } \text{trace}(U^T \mathbf{L} U)$$

such that $U \in \Re^{n \times k}, U^T U = \mathbf{I}_k$

SOLVING THE GRAPH-CUT

Solving k-way cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$



$$\text{minimize } \text{trace}(U^T \mathbf{L} U)$$

$$\text{such that } U \in \Re^{n \times k}, U^T U = \mathbf{I}_k$$

$$= \sum_{i=1}^k \lambda_i(\mathbf{L}) \quad [\text{Ky-Fan theorem}]$$

U^* = Eigenvectors corresponding to
k smallest eigenvalues of \mathbf{L}

SOLVING THE GRAPH-CUT

Solving k-way cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$



$$\text{minimize } \text{trace}(U^T \mathbf{L} U)$$

such that $U \in \Re^{n \times k}$, $U^T U = \mathbf{I}_k$

Eigen decomposition $\mathbf{L} = U \Sigma U^T$

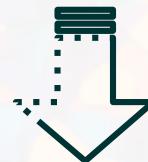


$$\begin{bmatrix} | & | & & | & & | \\ u_1 & u_2 & \dots & u_k & u_{k+1} & \dots & u_n \\ | & | & & | & & | \end{bmatrix}$$


SOLVING THE GRAPH-CUT

Solving k-way cut

$$\text{minimize } \text{Ncut}(A_1, A_2, \dots, A_k) := \sum_{i=1}^k \frac{W(A_i, \bar{A}_i)}{\text{vol}(A_i)}$$

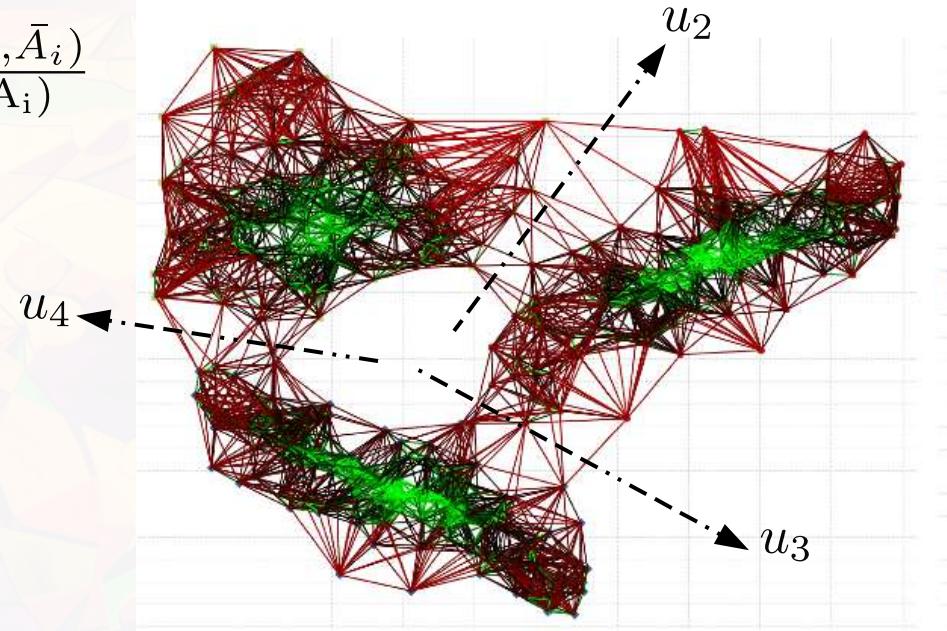


$$\text{minimize } \text{trace}(U^T \mathbf{L} U)$$

such that $U \in \Re^{n \times k}$, $U^T U = \mathbf{I}_k$

Eigen decomposition $\mathbf{L} = U \Sigma U^T$

$$\begin{bmatrix} | & | & & | & & | \\ u_1 & u_2 & \dots & u_k & u_{k+1} & \dots & u_n \\ | & | & & | & & | \end{bmatrix}$$

SPECTRAL CLUSTERING

Why the word “Spectral”?

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- Derived from “spectrum”

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- Here, clustering solutions are obtained from eigenvalues and eigenvectors of some matrix \mathbf{L}
- Clustering using *spectrum of \mathbf{L}*

“Spectral Clustering”!

SPECTRAL CLUSTERING ALGORITHM

Normalized spectral clustering by Ng, Jordan, and Weiss (2002)

Input Similarity matrix \mathbf{W} , number of clusters k .

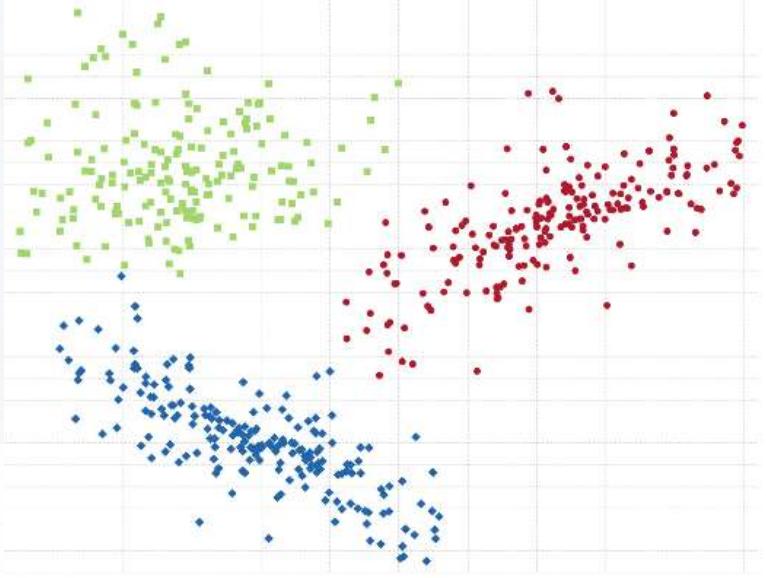
Output Clusters A_1, \dots, A_k .

1. Construct degree matrix \mathbf{D} and normalized Laplacian $\mathbf{L} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{D} - \mathbf{W})\mathbf{D}^{-\frac{1}{2}}$
2. Find eigenvectors $U = [u_1 \dots u_k]$ corresponding to k smallest eigenvalues of matrix \mathbf{L} .
3. Perform clustering on the rows of U using k -means algorithm.

Return clusters A_1, \dots, A_k from k -means clustering.

SPECTRAL CLUSTERING

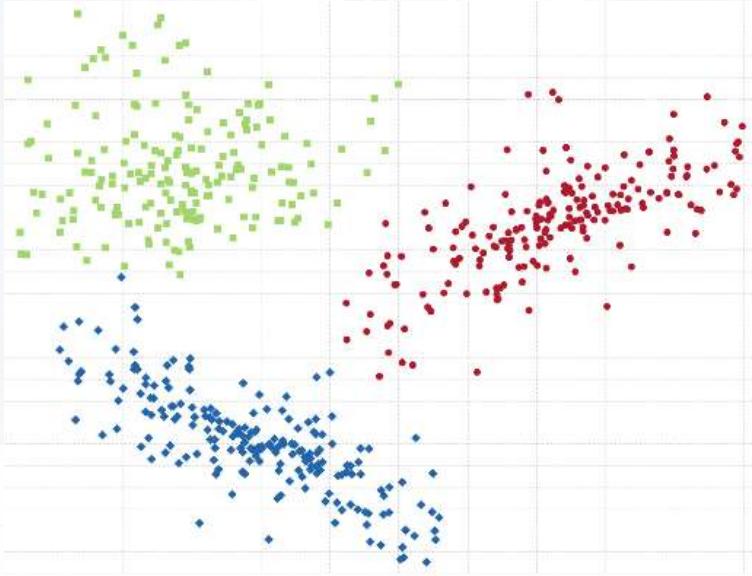
Feature-space



$$\mathbf{X} \in \Re^{n \times d}$$

SPECTRAL CLUSTERING

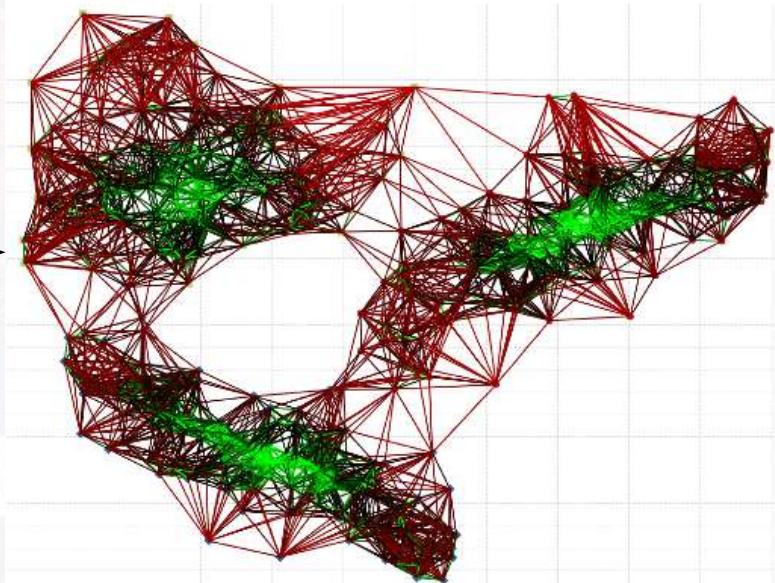
Feature-space



$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

similarity
measure

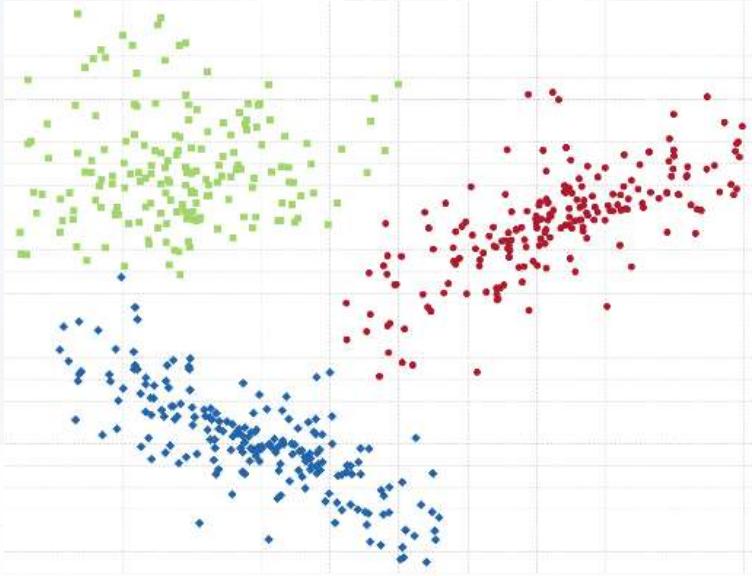
Graph



$$\mathbf{W} \text{ and Laplacian } \mathbf{L} \in \mathbb{R}^{n \times n}$$

SPECTRAL CLUSTERING

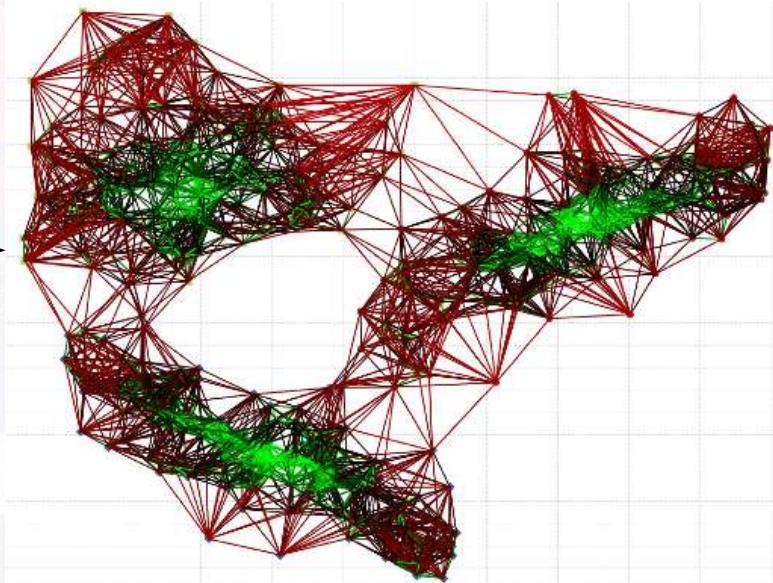
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$$\mathbf{W} \text{ and Laplacian } \mathbf{L} \in \mathbb{R}^{n \times n}$$

k – means clustering on low-rank $\mathbf{U} \leftarrow$ Eigenvectors $\mathbf{U} \in \mathbb{R}^{n \times k}$

SPECTRAL CLUSTERING

We will study the performance of spectral clustering in lab session.

T H A N K Y O U