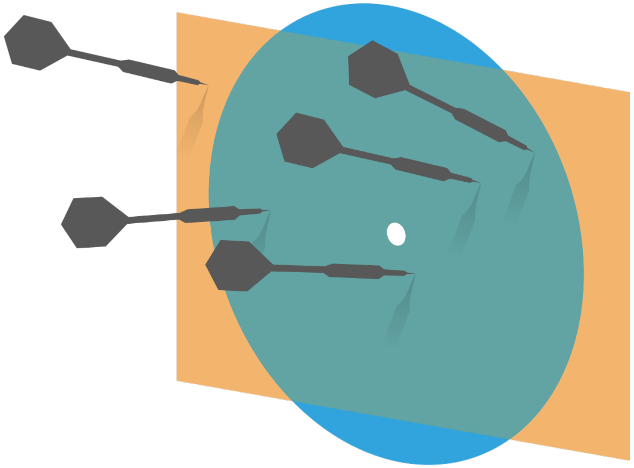
Probability and Statistics for Computer Science



Credit: wikipedia

"Unsupervised learning is arguably more typical of human and animal learning…"--- Kelvin Murphy, former professor at UBC

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 12.1.2021

Last time

- Curse of dimensions
- Unsupervised learning
- Clustering

Q. Is k-means clustering deterministic?

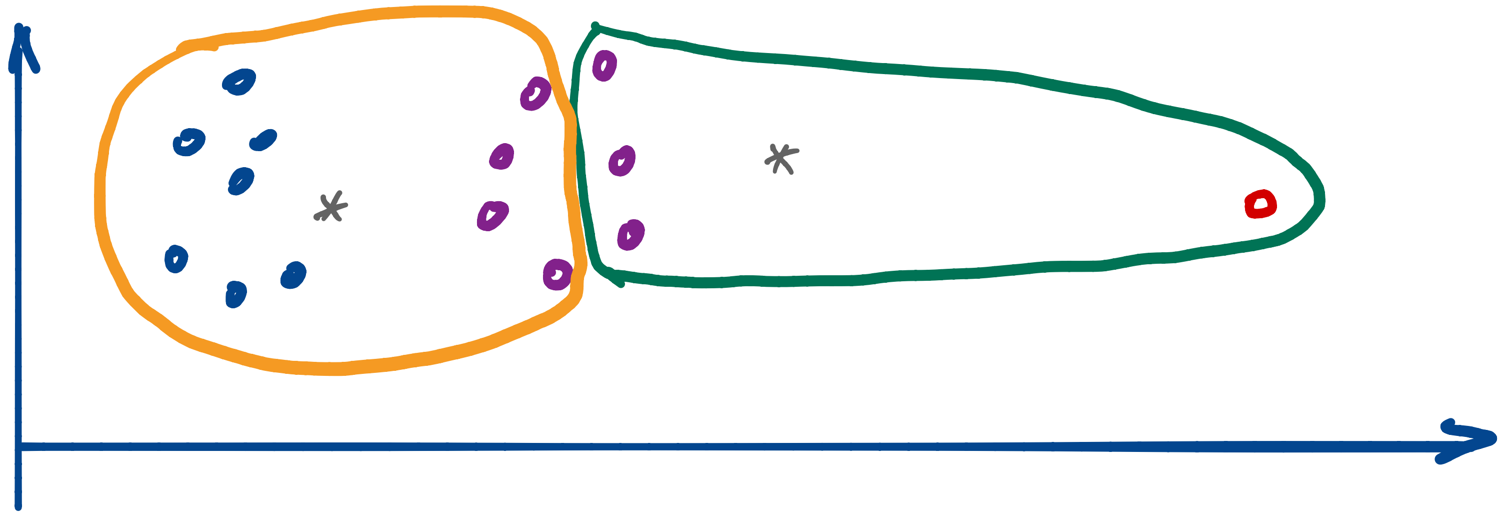
A. Yes
B. No

Some issues with k-means clustering

- Sensitive to outlier
- Sensitive to the seeds (centroids)

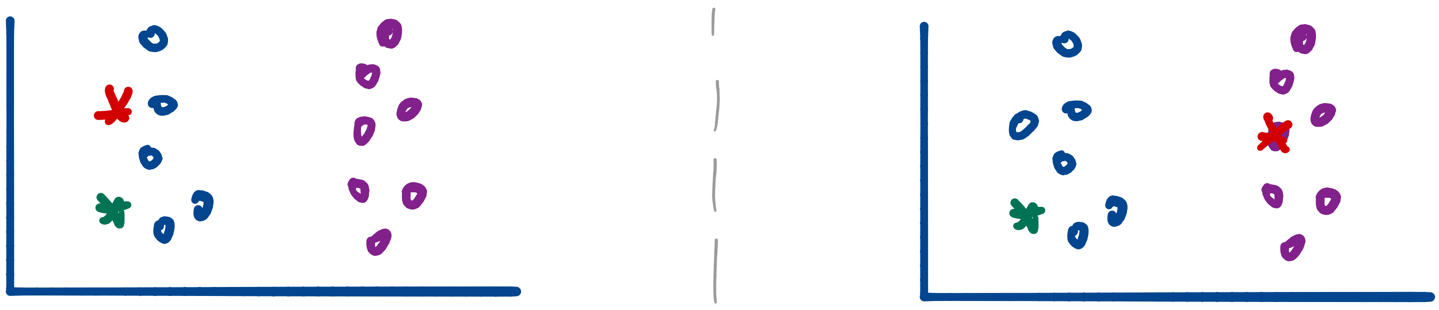
Some issues with k-means clustering

- Sensitive to outlier: example



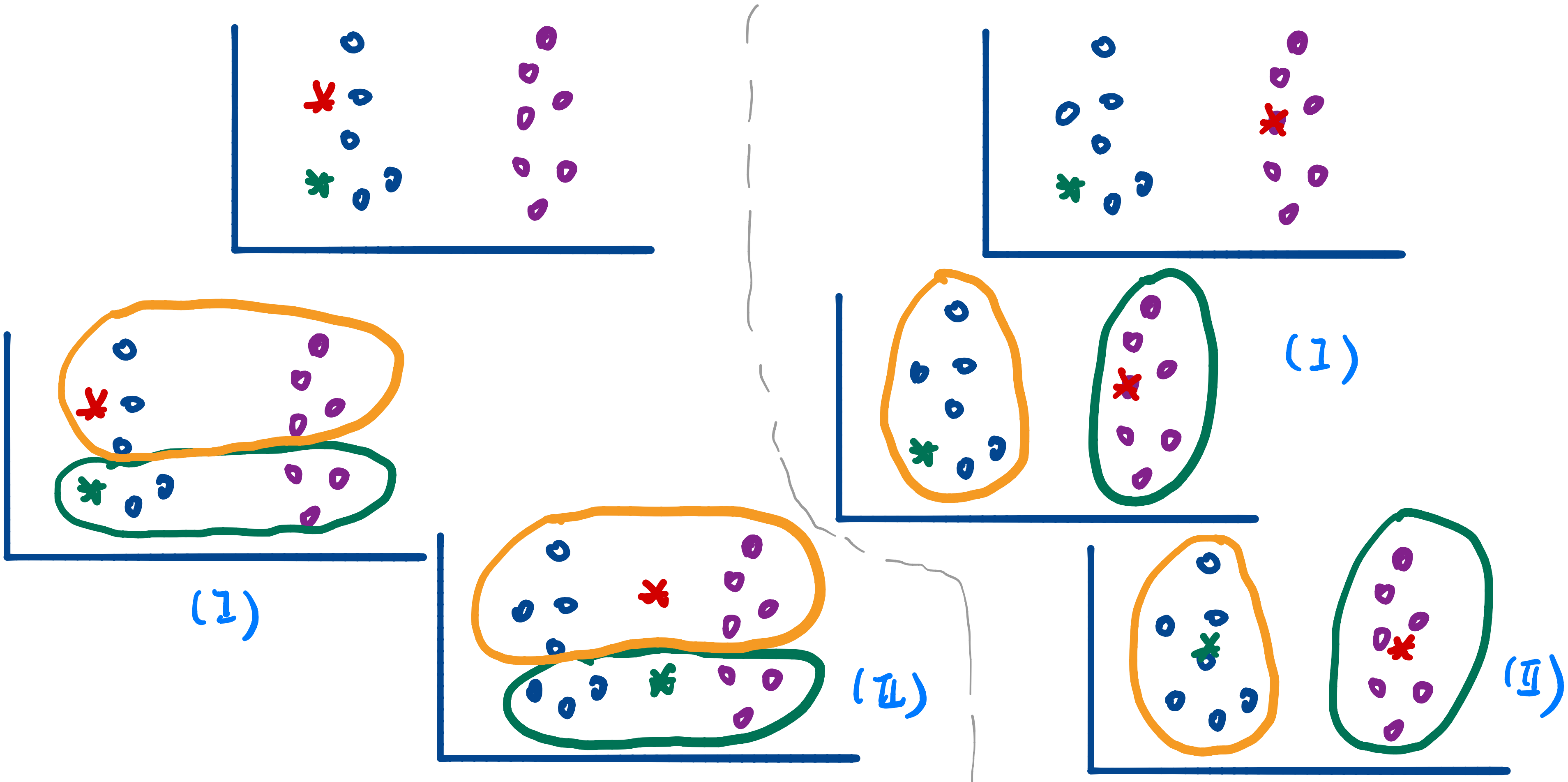
Some issues with k-means clustering

- Sensitive to the seeds (example)



Some issues with k-means clustering

- Sensitive to the seeds (example)



Objectives

* Application of Clustering
  Cluster Center Histogram

* Spectral Clustering

K-means clustering example: Portugal consumers

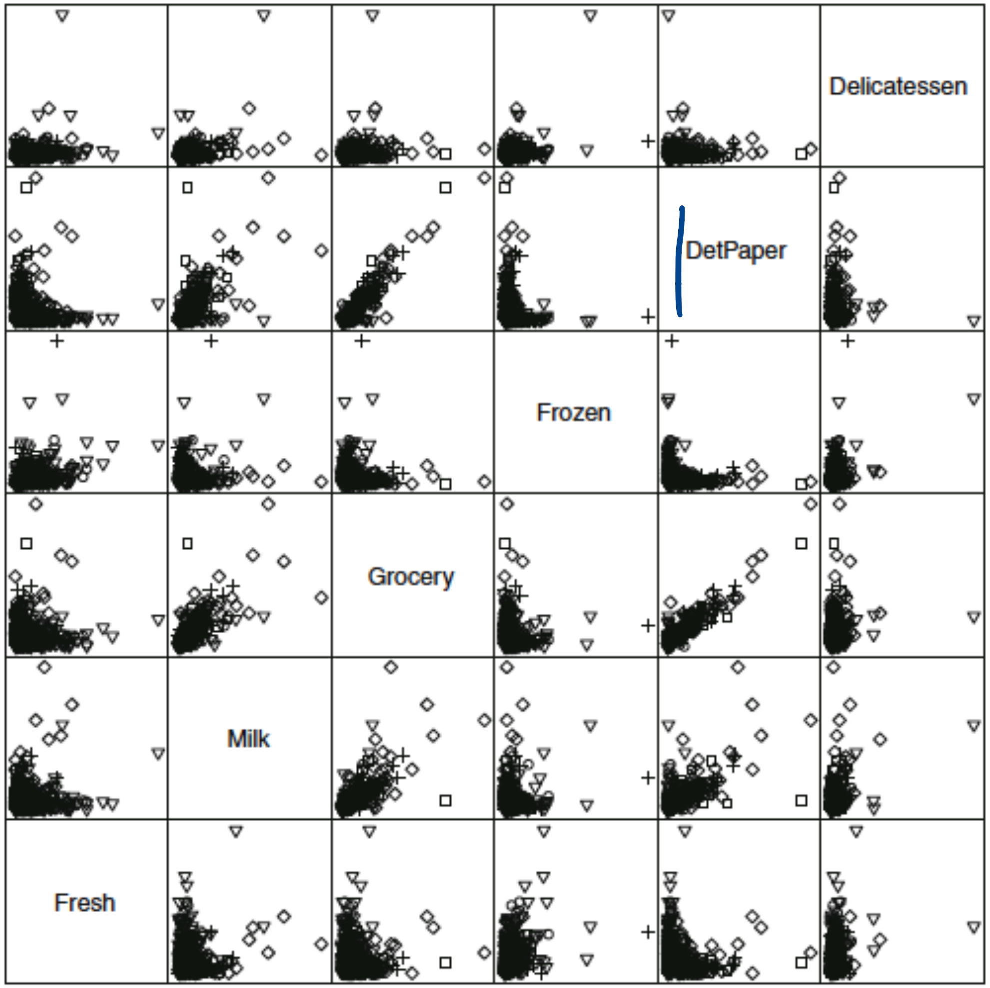
- The dataset consists of the annual grocery spending of 440 customers
- Each customer's spending is recorded in 6 features:
  - fresh food, milk, grocery, frozen, detergents/paper, delicatessen
- Each customer is labeled by: 6 labels in total
  - Channel (Channel 1 & 2) (Horeca 298, Retail 142)
  - Region (Region 1, 2 &3) (Lisbon 77, Oporto 47, Other 316)

Lisbon, Portugal

Oporto, Portugal

Visualization of the data

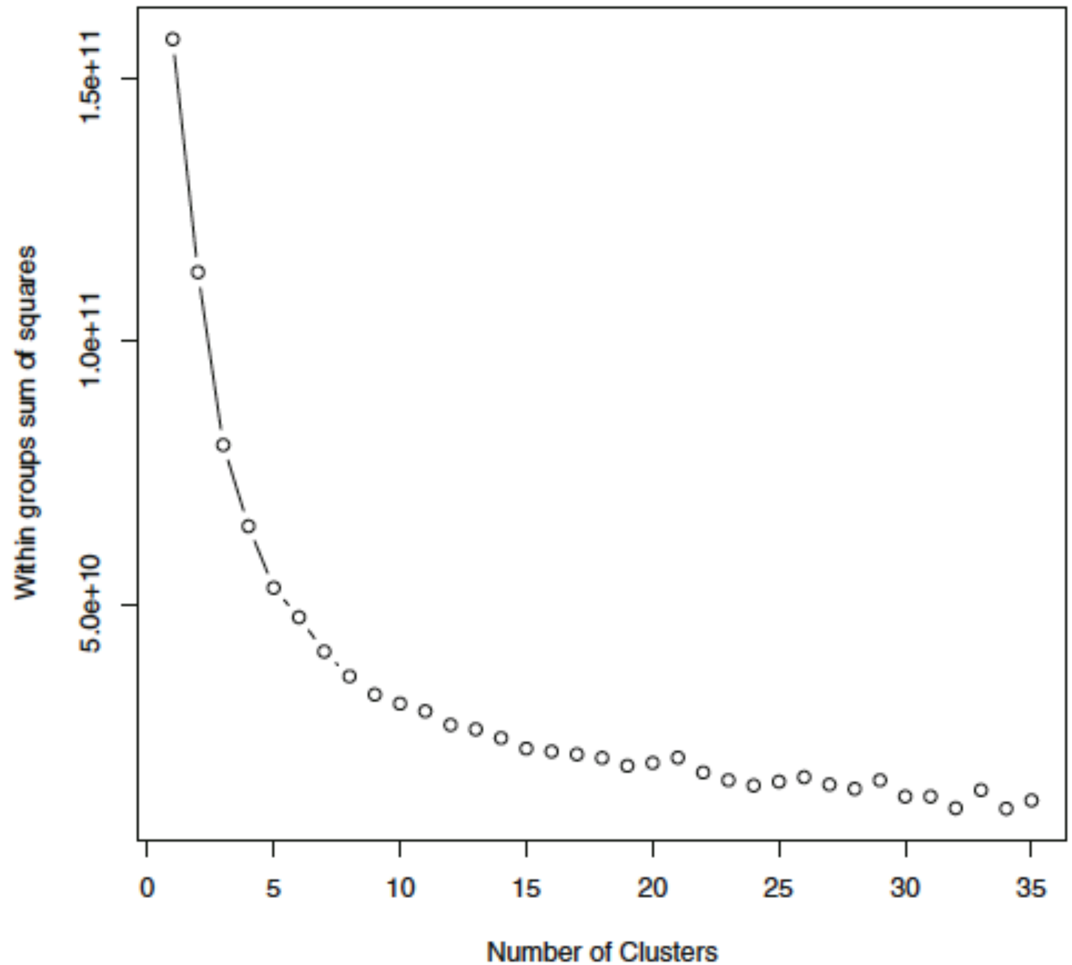
- Visualize the data with scatter plots
- We do see that some features are correlated.
- But overall we do not see significant structure or groups in the data.



Scatter Plot Matrix

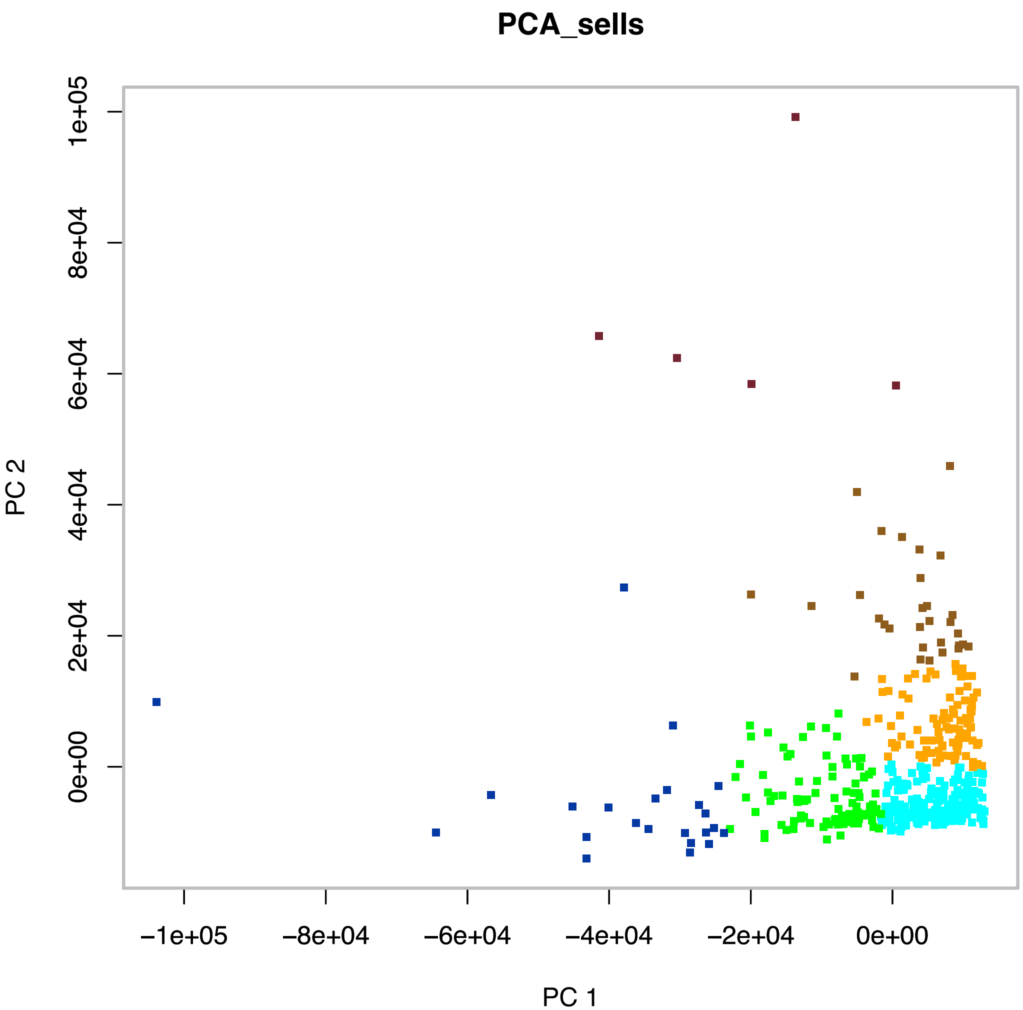
Do kmeans and choose k through the cost function

It's good to pick a **k** around the knee:
I choose 6 for it matches the number of labels



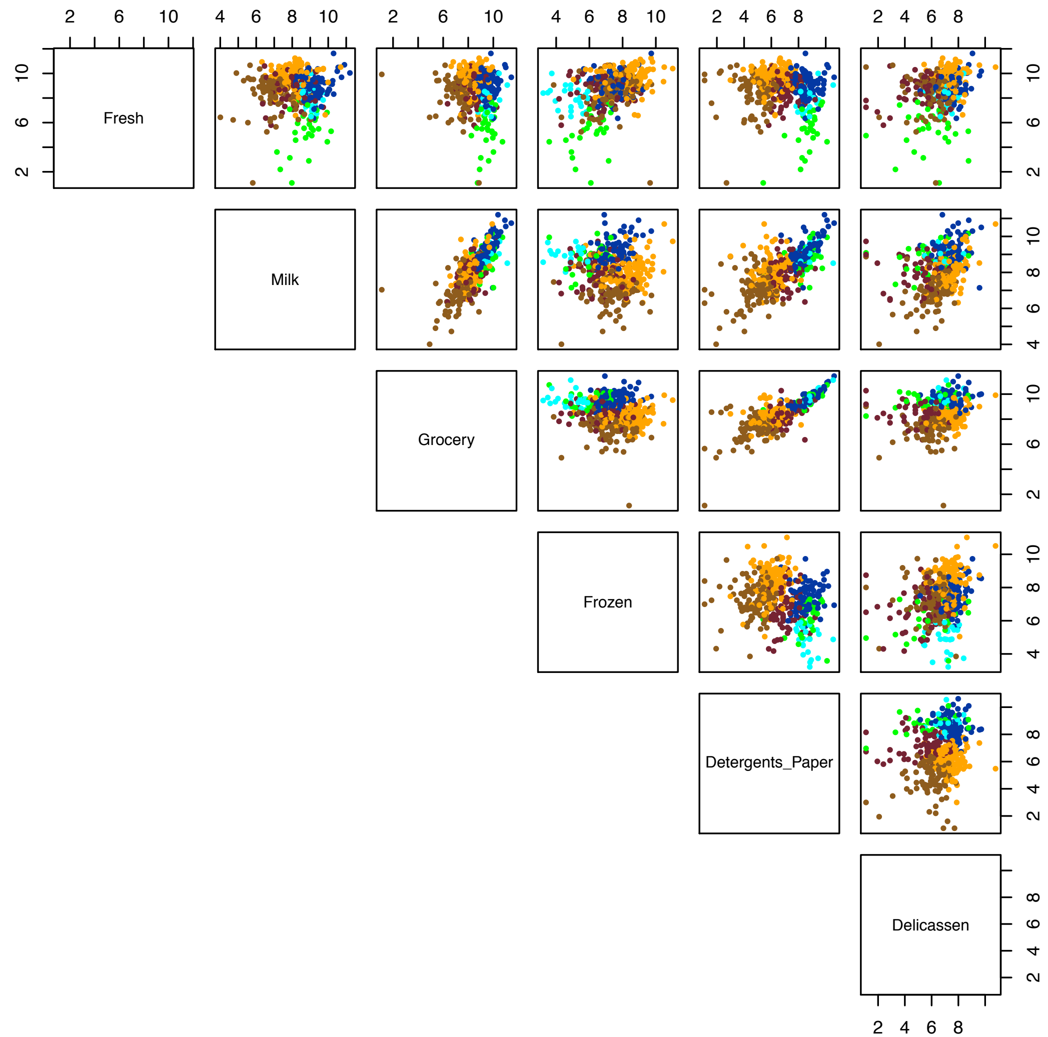
Visualization of the data (PCA)

- PCA does show some separation. **Colors are the clusters**
- Data points show large range of dynamics!



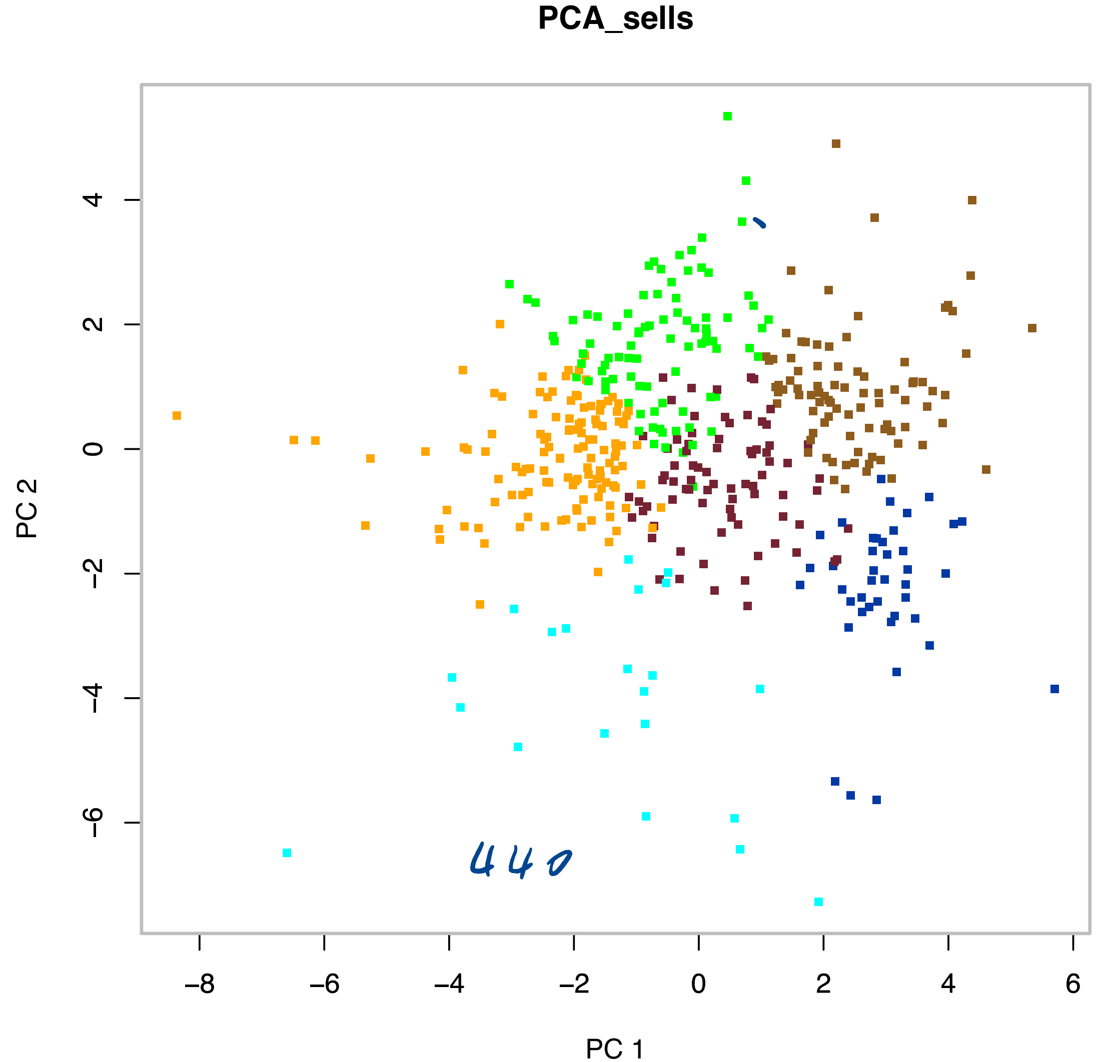
Do log transform of the data

- Log transform the data
- Do scatter plot matrix after the log transform
- Do the kmeans and color the clusters identified by k-means



PCA after log transformation: Clusters

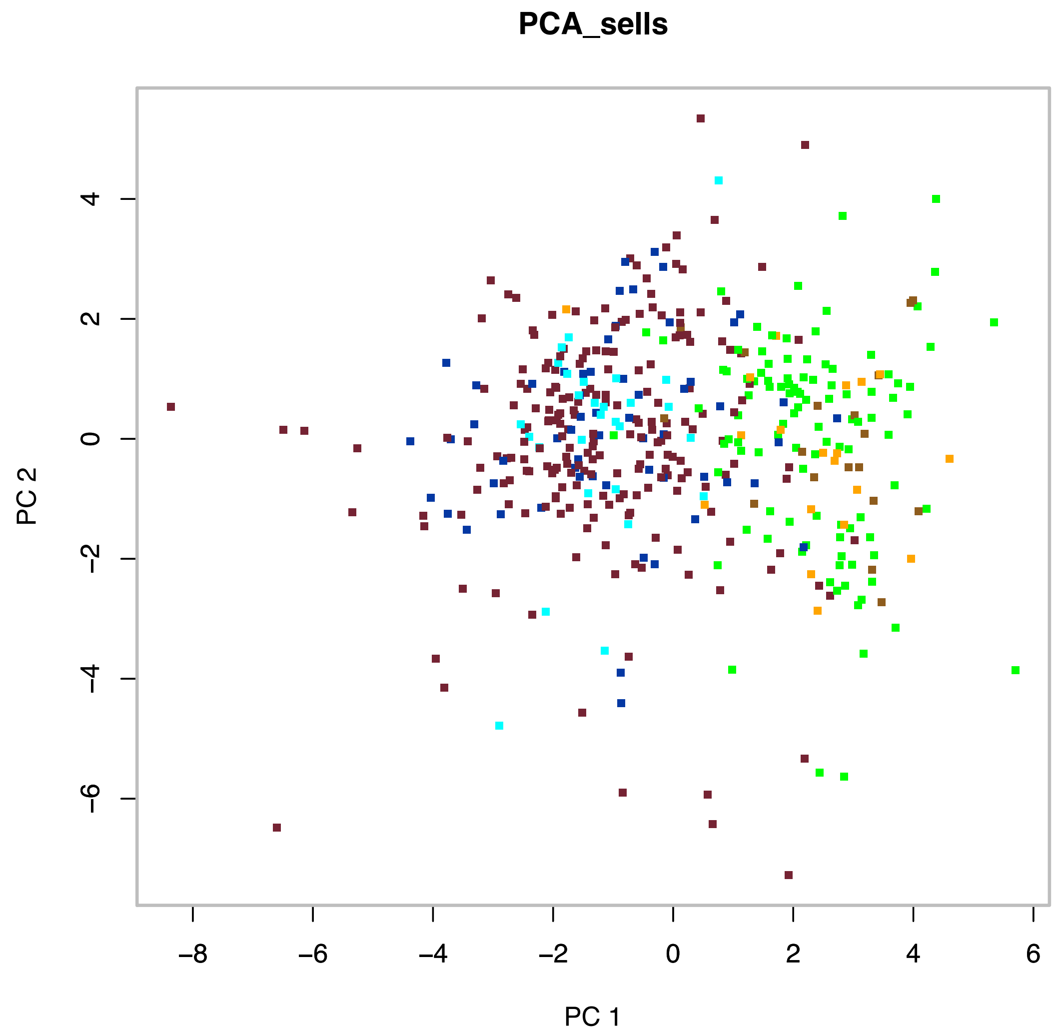
Colors show the **clusters** identified by k-means



PCA after log transformation

Colors show the **Channel-region labels**

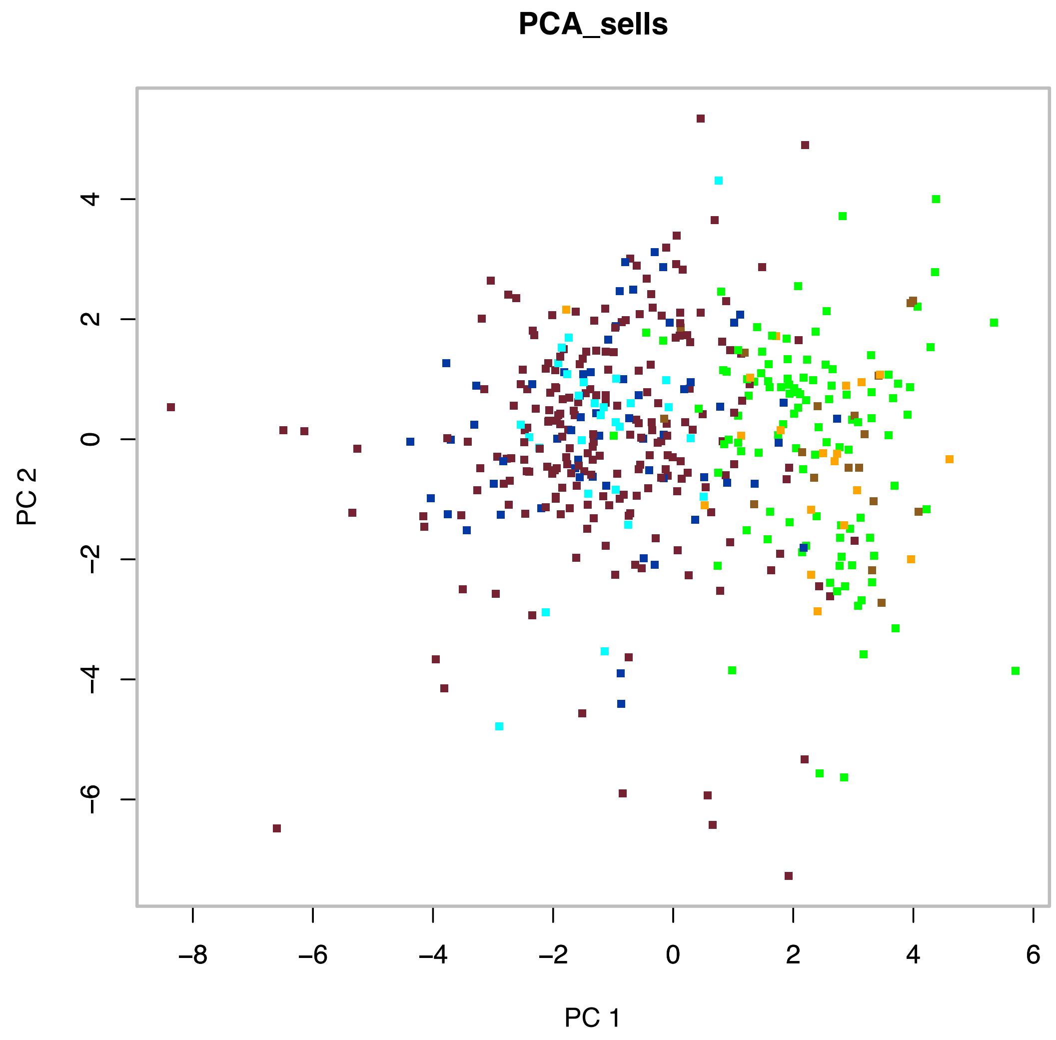
What does this tell us?



PCA after log transformation

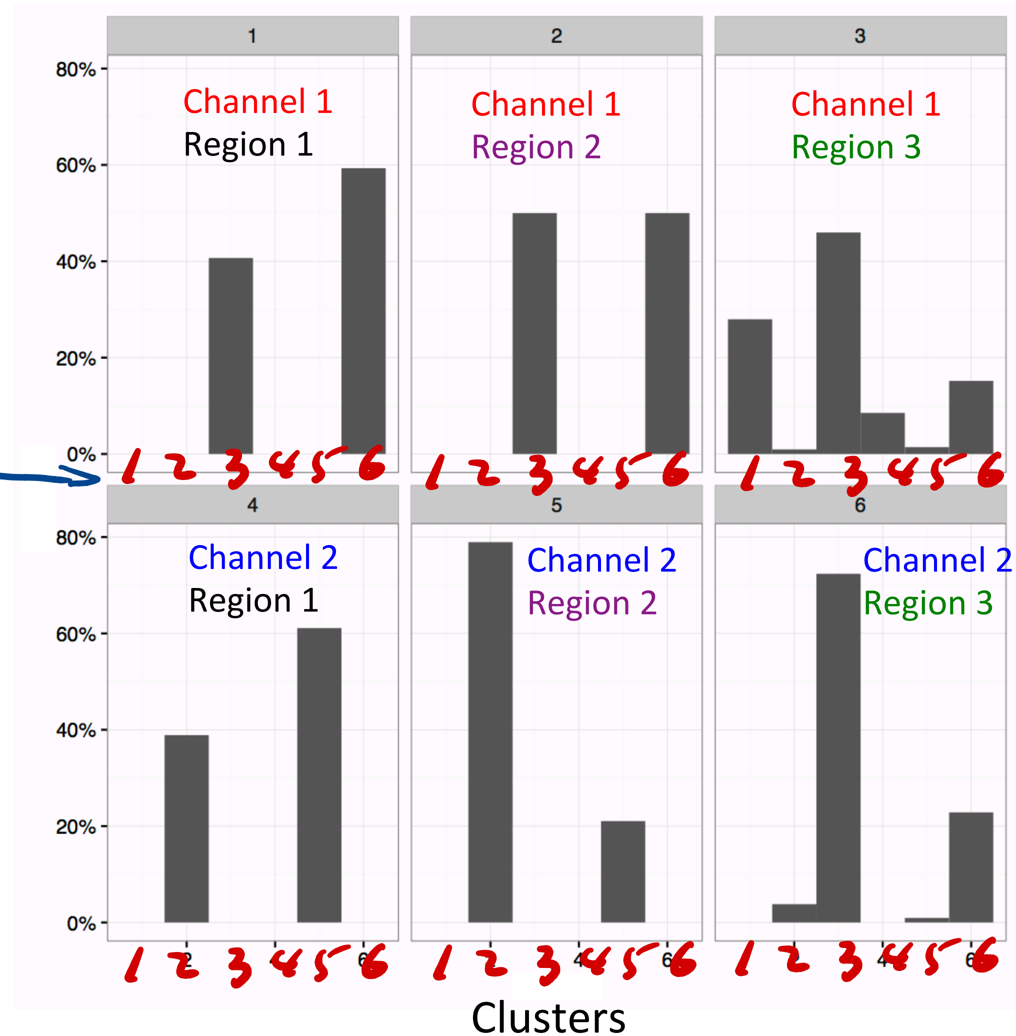
Colors show the **Channel-region labels**

Channels differ a lot



Cluster center histogram of the Portugal grocery spending data

- For each channel/ region, we make a histogram of customers that map to each of the **6 cluster centers.**



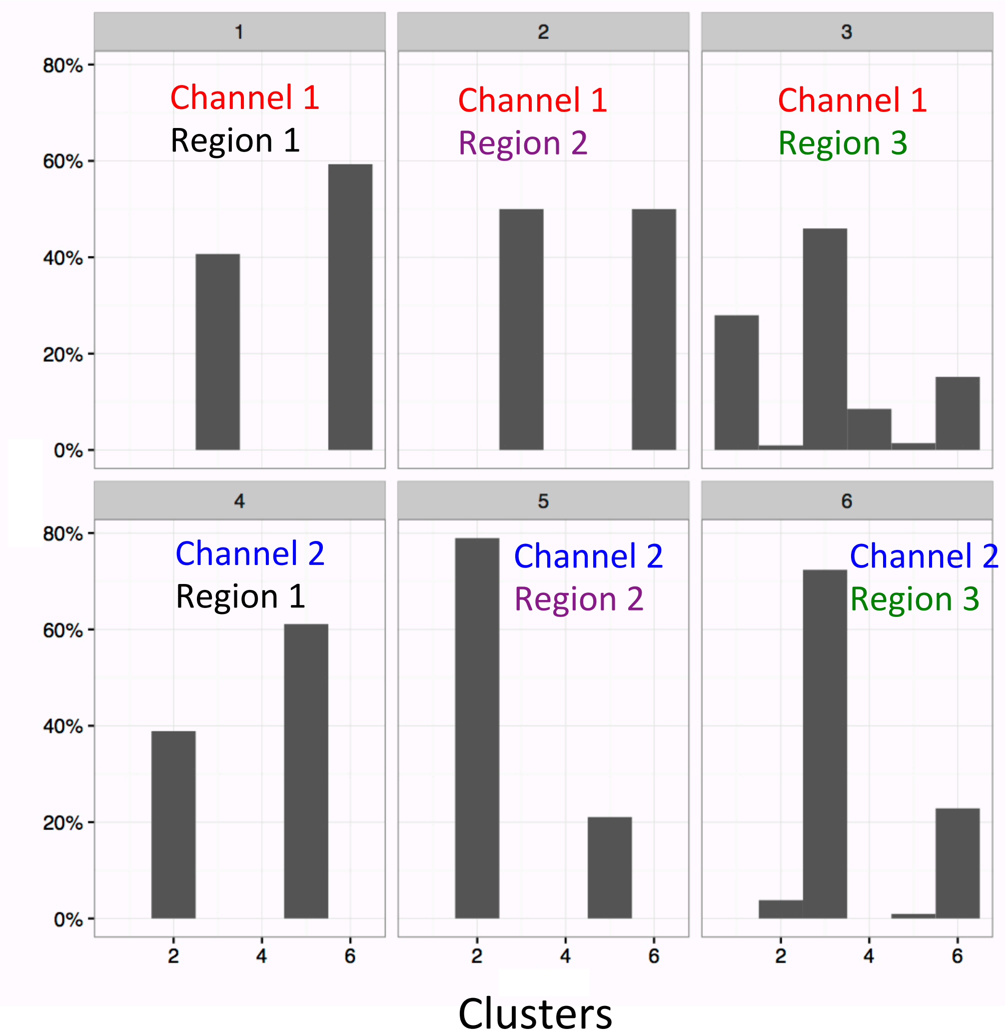
- **What do you see?**

Channel1: Horeca
Channel2: Retail

Region1: Lisbon
Region2: Oporto
Region3: Other

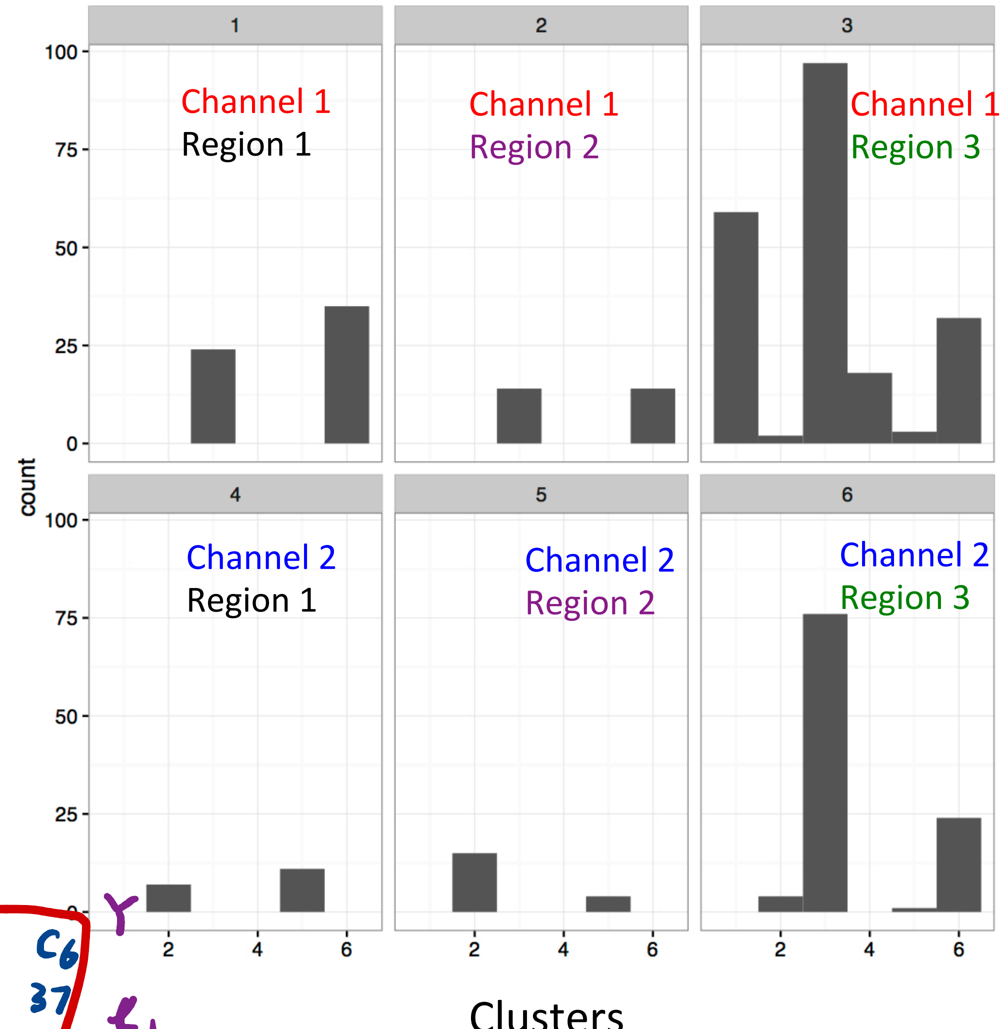
Cluster center histogram of the Portugal grocery spending data

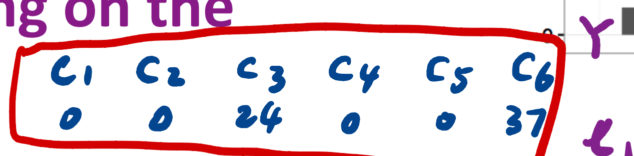
- For each channel/ region, we make a histogram of customers that map to each of the 6 cluster centers.
- **Channels are significantly different!**
- **Region 3 is special**
- **Is it enough to plot the percentage?**



Cluster center histogram of the Portugal grocery spending data

- For each channel/ region, we make a histogram of customers that map to each of the 6 cluster centers.
- **Channels are significantly different!**
- **Region 3 is special**
- **Count matters depending on the purpose**





Q. What can we do with cluster center histograms?

A. investigate the feature patterns of data groups

B. Classify new data with the cluster center histograms.

C. Both A and B.

Review at home

Vector Quantization for classifying data of varying size

- The classifiers usually assume that each feature vector has the same number of entries.
- Many datasets in fact have items of different size
  - Images usually have different numbers of pixels
  - Audio signals (and other time series) usually have different durations
- We will use **vector quantization** to map variable length data to fixed-length feature vectors using **cluster center histogram**.

Review at home

Pattern vocabulary: conceptual example

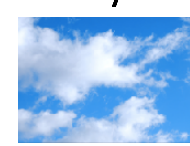
- Suppose we want to classify images into beach or prairie
- We can slice each images into 10 by 10 subsets (data entry of length 100)
- Then cluster the pieces, use the cluster center histograms to train and classify

Sand

Water

Grass

Sky



Credit: Prof. David. Varodayan

Review at home

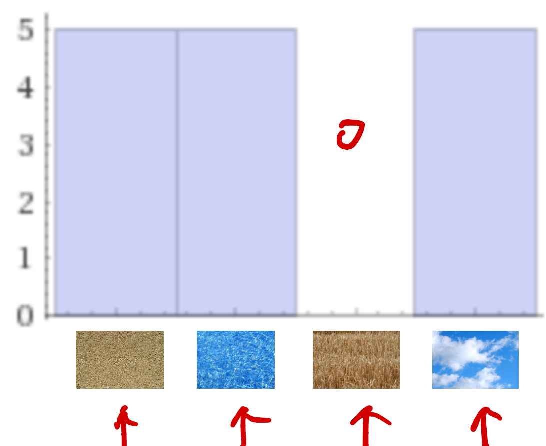
Generate fixed-length feature vectors : conceptual example

- Slice the images into 10 by 10 pixel subsets
- Do clustering on all the subsets from the training images
- Assign each subset to the nearest cluster centers (in k clusters/patterns)
- For each image, produce the counts with respect to each cluster center and form a feature vector of dimension k

M is # label

K = 4

K is # of clusters



$$\boldsymbol{x}_i = \begin{bmatrix} 5 \\ 5 \\ 0 \\ 5 \end{bmatrix}$$

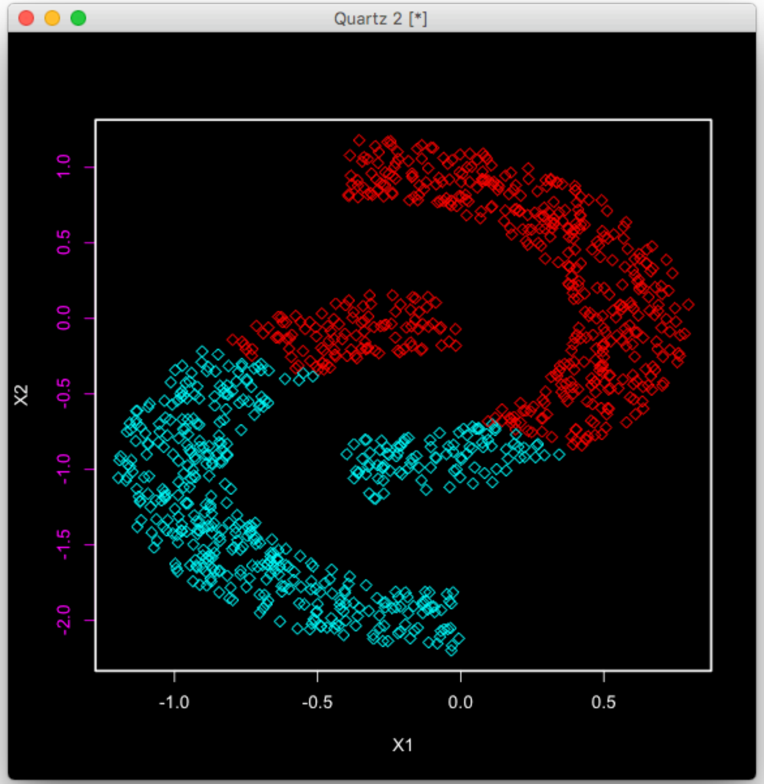
Credit: Prof. David. Varodayan

Spectral clustering

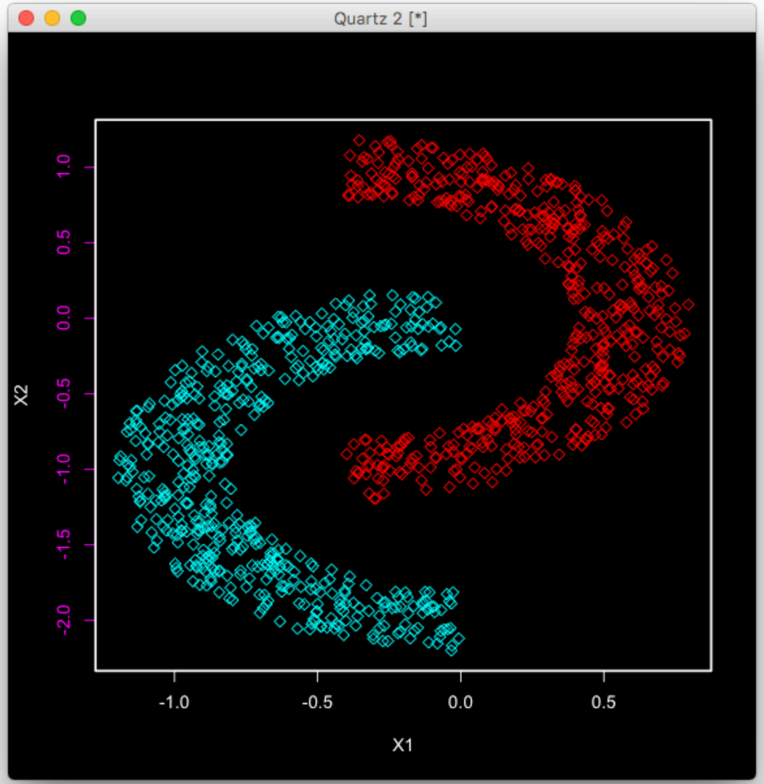
K-means is limited

- K-means fails in the **Two-moon** problem

K-means result



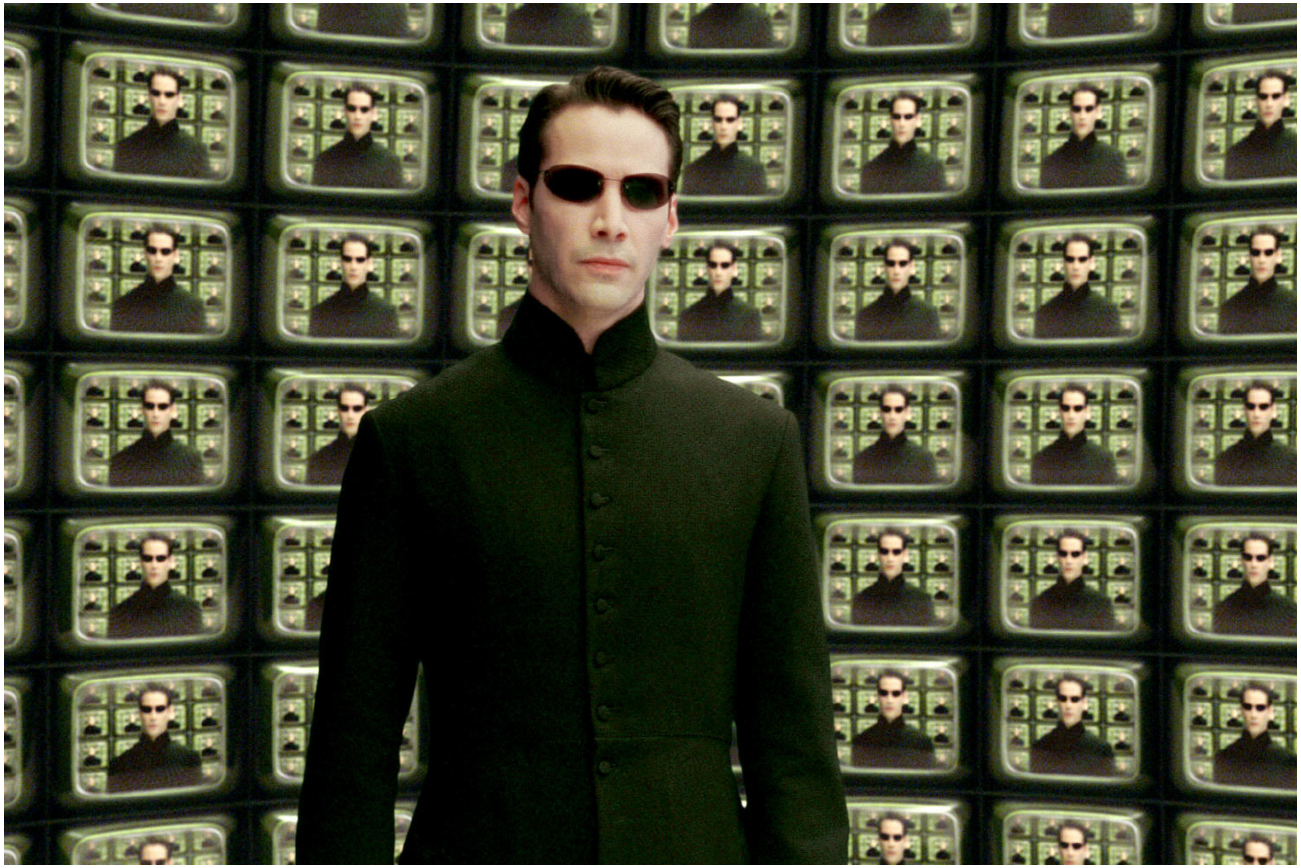
Expected result



Spectral Clustering

- **Theoretical basis**
  - The Graph Representation
  - The Adjacency Matrix
  - Graph cut
  - The Laplacian Matrix
  - The properties of Laplacian that point to the solution

Again it's about Matrix !



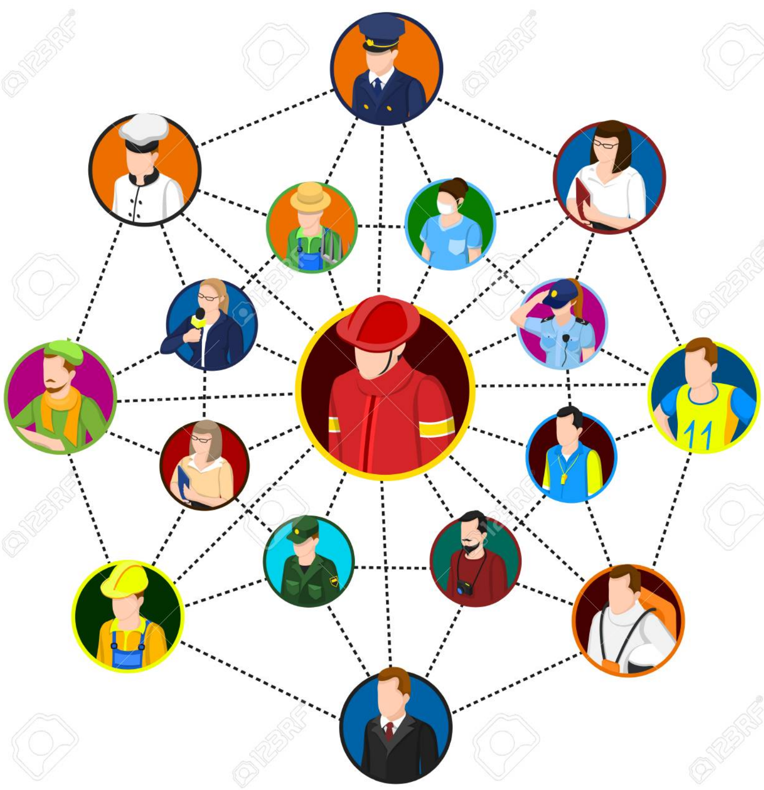
Spectral Clustering

- **Theoretical basis**
  - ***The Graph Representation***

Introduction of Graph

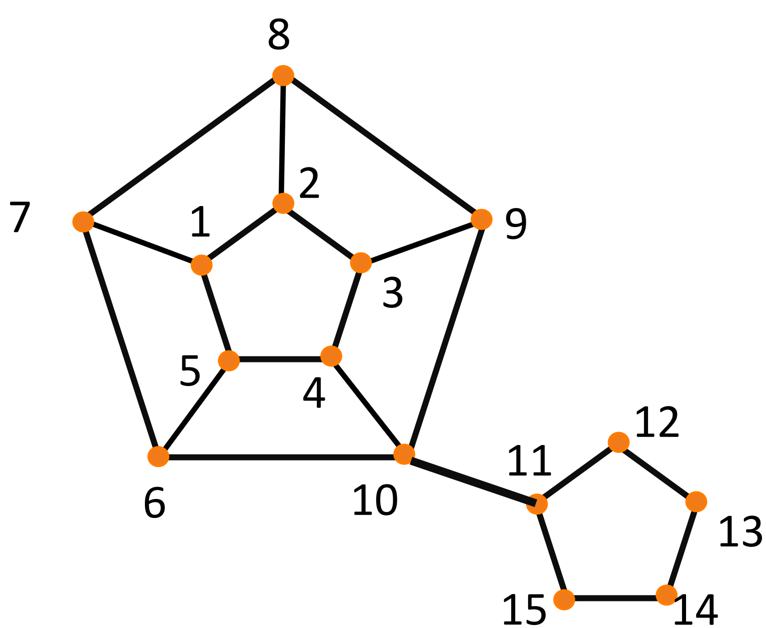
- Real world data often needs graph
- Strength

A graph model of Social network data



Graph in terms of Mathematics

- The graph is a set G(V, E)
- V is the set of vertices



15 vertices, 21 edges

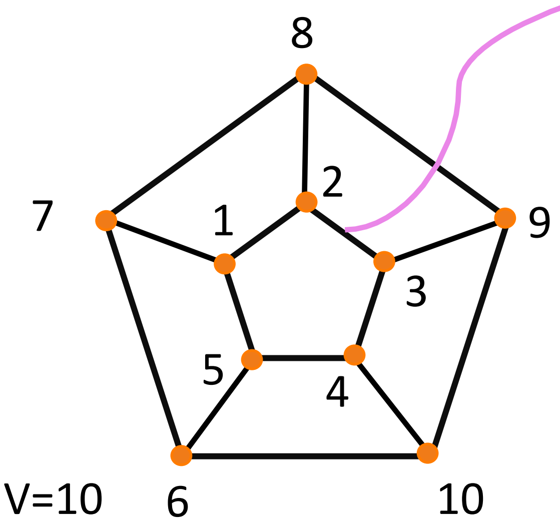
- E is the set of edges, showing the relationship between pair of vertices

Spectral Clustering

- **Theoretical basis**
  - The Graph Representation
  - ***The Adjacency Matrix***

Graph data in the format of matrix

These 10 geometric data points can be represented with an *undirected* Graph and then numerically written as a matrix



V=10
E=15

N=10

Adjacency Matrix*: W $\{\omega_{ij}>=0\}$

	1	2	3	4	5	6	7	8	9	10
1	0	1	0	0	1	0	1	0	0	0
2	1	0	1	0	0	0	0	1	0	0
3	0	1	0	1	0	0	0	0	1	0
4	0	0	1	0	1	0	0	0	0	1
5	1	0	0	1	0	1	0	0	0	0
6	0	0	0	0	1	0	1	0	0	1
7	1	0	0	0	0	1	0	1	0	0
8	0	1	0	0	0	0	1	0	1	0
9	0	0	1	0	0	0	0	1	0	1
10	0	0	0	1	0	1	0	0	1	0

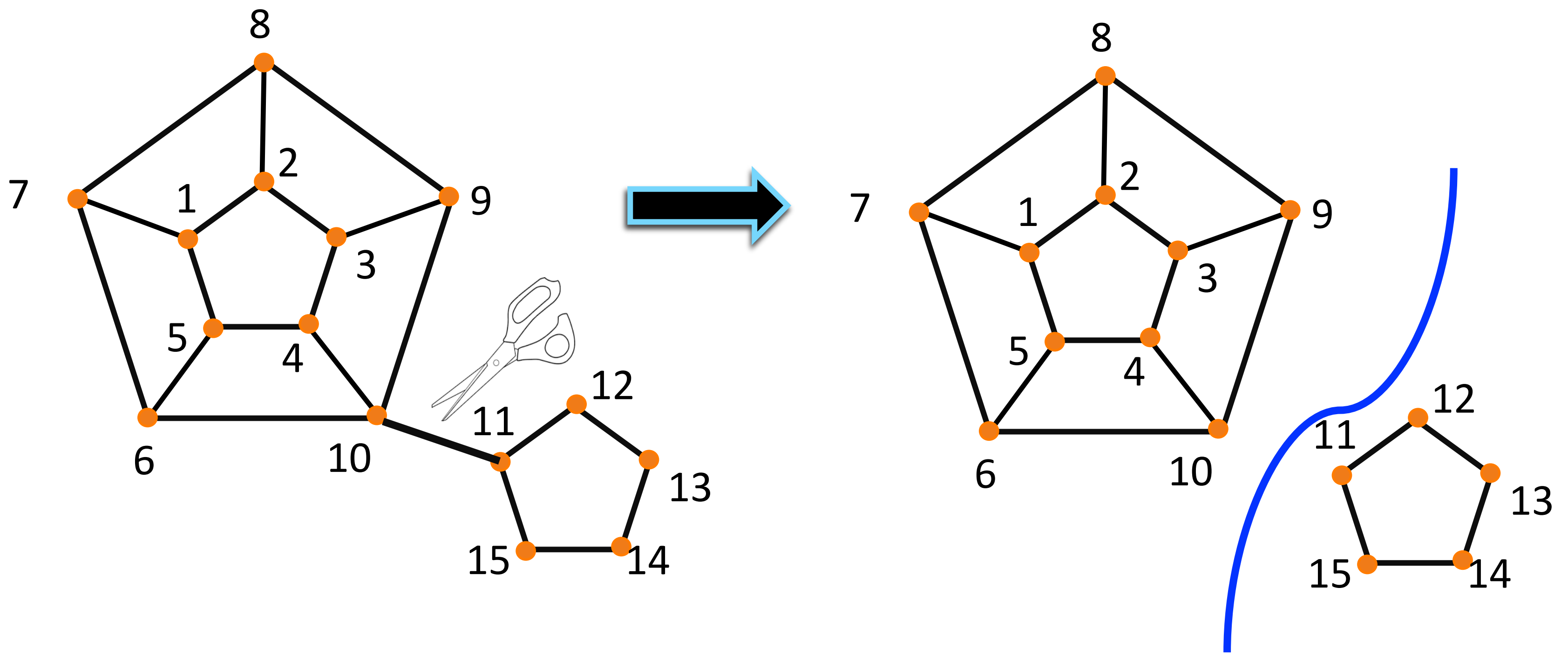
* Some people prefer "Similarity matrix"

Spectral Clustering

- **Theoretical basis**
  - The Graph Representation
  - The Adjacency Matrix
  - ***Graph cut***

Spectral Clustering emerged from Graph-cut

- Clusters are learned via min-Cut of the Graph



Spectral Clustering vs Graph-cut

- Spectral clustering is equivalent to the Graph-cut

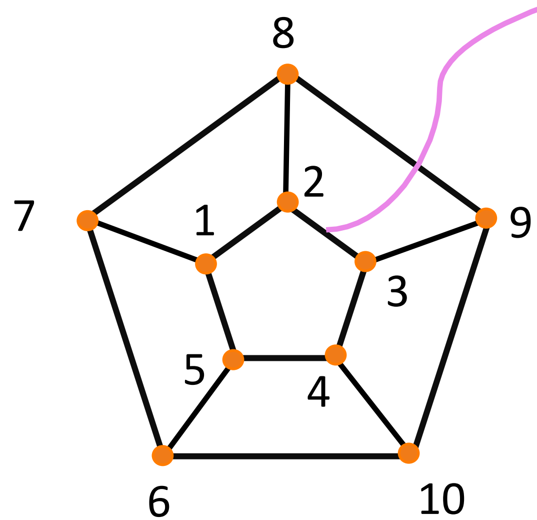
  Finding clusters is to solve **an Eigenvalue problem** using **Graph's Laplacian matrix**

Spectral Clustering

- **Theoretical basis**
  - The Graph Representation
  - The Adjacency Matrix
  - Graph cut
  - ***The Laplacian Matrix***

Graph data in the format of matrix

The weights ω_{ij} of the edges stored in the matrix of the graph can be **any non-negative values**



N=10

Adjacency Matrix: W $\{\omega_{ij}>=0\}$

	1	2	3	4	5	6	7	8	9	10
1	0	1	0	0	1	0	1	0	0	0
2	1	0	1	0	0	0	0	1	0	0
3	0	1	0	1	0	0	0	0	1	0
4	0	0	1	0	1	0	0	0	0	1
5	1	0	0	1	0	1	0	0	0	0
6	0	0	0	0	1	0	1	0	0	1
7	1	0	0	0	0	1	0	1	0	0
8	0	1	0	0	0	0	1	0	1	0
9	0	0	1	0	0	0	0	1	0	1
10	0	0	0	1	0	1	0	0	1	0

Transform Adjacency Matrix W into Graph Laplacian Matrix L

- $\mathbf{L = D - W}$

$$\mathbf{D}_{ij} = \begin{cases} \sum_k \omega_{ik}, & i=j \\ 0, & i \neq j \end{cases}$$

Adjacency Matrix: W $\{\omega_{ij}\}$

	1	2	3	4	5	6	7	8	9	X
1	0	1	0	0	1	0	1	0	0	0
2	1	0	1	0	0	0	0	1	0	0
3	0	1	0	1	0	0	0	0	1	0
4	0	0	1	0	1	0	0	0	0	1
5	1	0	0	1	0	1	0	0	0	0
6	0	0	0	0	1	0	1	0	0	1
7	1	0	0	0	0	1	0	1	0	0
8	0	1	0	0	0	0	1	0	1	0
9	0	0	1	0	0	0	0	1	0	1
X	0	0	0	1	0	1	0	0	1	0

Laplacian Matrix: L $\{L_{ij}\}$

	1	2	3	4	5	6	7	8	9	X
1	3	-1	0	0	-1	0	-1	0	0	0
2	-1	3	-1	0	0	0	0	-1	0	0
3	0	-1	3	-1	0	0	0	0	-1	0
4	0	0	-1	3	-1	0	0	0	0	-1
5	-1	0	0	-1	3	-1	0	0	0	0
6	0	0	0	0	-1	3	-1	0	0	-1
7	-1	0	0	0	0	-1	3	-1	0	0
8	0	-1	0	0	0	0	-1	3	-1	0
9	0	0	-1	0	0	0	0	-1	3	-1
X	0	0	0	-1	0	-1	0	0	-1	3

Q. What properties do you see in L matrix?

symmetric

Adjacency Matrix: **W** $\{\omega_{ij}\}$

	1	2	3	4	5	6	7	8	9	X
1	0	1	0	0	1	0	1	0	0	0
2	1	0	1	0	0	0	0	1	0	0
3	0	1	0	1	0	0	0	0	1	0
4	0	0	1	0	1	0	0	0	0	1
5	1	0	0	1	0	1	0	0	0	0
6	0	0	0	0	1	0	1	0	0	1
7	1	0	0	0	0	1	0	1	0	0
8	0	1	0	0	0	0	1	0	1	0
9	0	0	1	0	0	0	0	1	0	1
X	0	0	0	1	0	1	0	0	1	0

Laplacian Matrix: **L** $\{L_{ij}\}$

	1	2	3	4	5	6	7	8	9	X
1	3	-1	0	0	-1	0	-1	0	0	0
2	-1	3	-1	0	0	0	0	-1	0	0
3	0	-1	3	-1	0	0	0	0	-1	0
4	0	0	-1	3	-1	0	0	0	0	-1
5	-1	0	0	-1	3	-1	0	0	0	0
6	0	0	0	0	-1	3	-1	0	0	-1
7	-1	0	0	0	0	-1	3	-1	0	0
8	0	-1	0	0	0	0	-1	3	-1	0
9	0	0	-1	0	0	0	0	-1	3	-1
X	0	0	0	-1	0	-1	0	0	-1	3

Spectral Clustering

- **Theoretical basis**
    - The Graph Representation
    - The Adjacency Matrix
    - Graph cut
    - The Laplacian Matrix
    - ***The properties of Laplacian that point to the solution***

Laplacian Matrix L's properties

- $\mathbf{L = D - W}$

$$D_{ij} = \begin{cases} \sum_k \omega_{ik}, & i=j \\ 0, & i \neq j \end{cases}$$

Laplacian Matrix: **L** ($\{L_{ij}\}$)

	1	2	3	4	5	6	7	8	9	X
1	3	-1	0	0	-1	0	-1	0	0	0
2	-1	3	-1	0	0	0	0	-1	0	0
3	0	-1	3	-1	0	0	0	0	-1	0
4	0	0	-1	3	-1	0	0	0	0	-1
5	-1	0	0	-1	3	-1	0	0	0	0
6	0	0	0	0	-1	3	-1	0	0	-1
7	-1	0	0	0	0	-1	3	-1	0	0
8	0	-1	0	0	0	0	-1	3	-1	0
9	0	0	-1	0	0	0	0	-1	3	-1
X	0	0	0	-1	0	-1	0	0	-1	3

Properties (I—III)

(I) Symmetric

(II) Row Sums = 0

(III) Quadratic form

$f'Lf = \frac{1}{2} \sum_{ij} \omega_{ij}(f_i - f_j)^2 >= 0$

f is any nonzero vector

→ Semi positive defi.

$\lambda_i \geq 0$

Energy function

Laplacian Matrix L's properties (p4)

- $L = D - W$
- $L\,x = \lambda\,x$

$$D_{ij} = \begin{cases} \sum_k \omega_{ik}, & i=j \\ 0, & i \neq j \end{cases}$$

Property (IV):
Positive semi-definite

All $\lambda_i >= 0$, while there is **at least one eigenvalue $\lambda_0 = 0$ s.t. $u_0 = \{\underbrace{1, 1 \ldots 1}_{n}\}$ constant vector**

Laplacian Matrix L's properties (p5)

- $L = D - W$
- $L x = \lambda x$

$$D_{ij} = \begin{cases} \sum_k \omega_{ik}, & i=j \\ 0, & i \neq j \end{cases}$$

Property (V):

# of zero valued λ_i is equal to the number of disconnected components in the graph

↓

clusters

Review at home

Proof of Laplacian Matrix L's property V

Prove: # of zero valued λ_i = the number of disconnected components of the graph

Def. Let the number of eigenvalues $\boldsymbol{\lambda_i=0}$ be **k**

(a) If **k** =1, the null space ($Lf_{ns} = \boldsymbol{\lambda_1} f_{ns} =0$) has dimension = 1, given we know u_s={1,1…1} is a special solution in this space, all vectors should be f_{ns} = C{u_s}, and C is any nonzero constant real number

Review at home

Proof of Laplacian Matrix L's property V

i) If the graph has only one connected component **ξ** and its energy is 0, then $f' L f = \frac{1}{2} \sum \omega_{ij}(f_i - f_j)^2 = 0$

Then all $f_i = C$ for all vertices within **ξ** ,

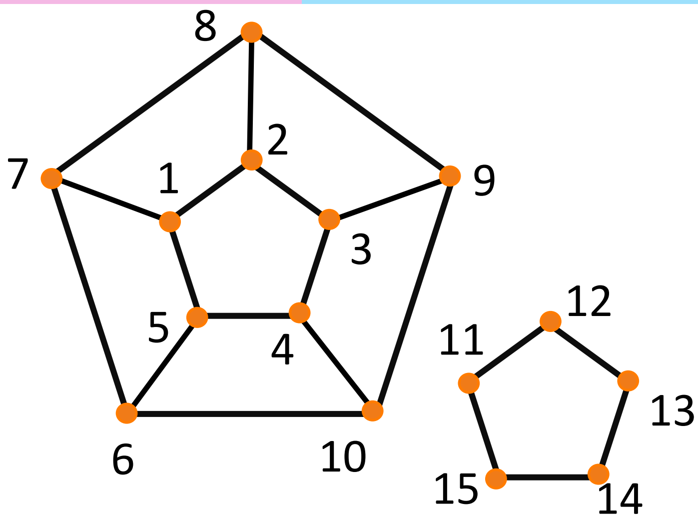
consistent with $f_{ns} = C\{u_s\}$

ii) If the graph has more than one connected component, ie there are 2 separate ones

The Laplacian can be written as $\begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix}$

Review at home

Proof of Laplacian Matrix L's property V



Is this hypothesis true? The graph has two disjoint parts and the graph's null space includes only constant vectors?

Not True. If there are 2 parts, we can construct another vector $\tilde{f}$

$$\tilde{f} = \begin{bmatrix} c \\ \vdots \\ c \\ 0 \\ \vdots \\ 0 \end{bmatrix} \begin{matrix} \left.\vphantom{\begin{matrix} c \\ \vdots \\ c \end{matrix}}\right\} |L_1| \\ \left.\vphantom{\begin{matrix} 0 \\ \vdots \\ 0 \end{matrix}}\right\} |L_2| \end{matrix}$$

Satisfies
$L\tilde{f} = 0$ and $\tilde{f}'L\tilde{f} = 0$

$$f_{ns} = \begin{bmatrix} c \\ \vdots \\ c \\ \vdots \\ c \end{bmatrix} \Big\} |L|$$

Then $\tilde{f}$ and f_{ns} are not colinear

$\Rightarrow$ The dimension of null space is 2

$\Rightarrow$ **contradiction**

Review at home

Proof of Laplacian Matrix L's property V

(b) In the same line of reasoning, we can prove for **k** >1, **k** is still the number of disconnected components.

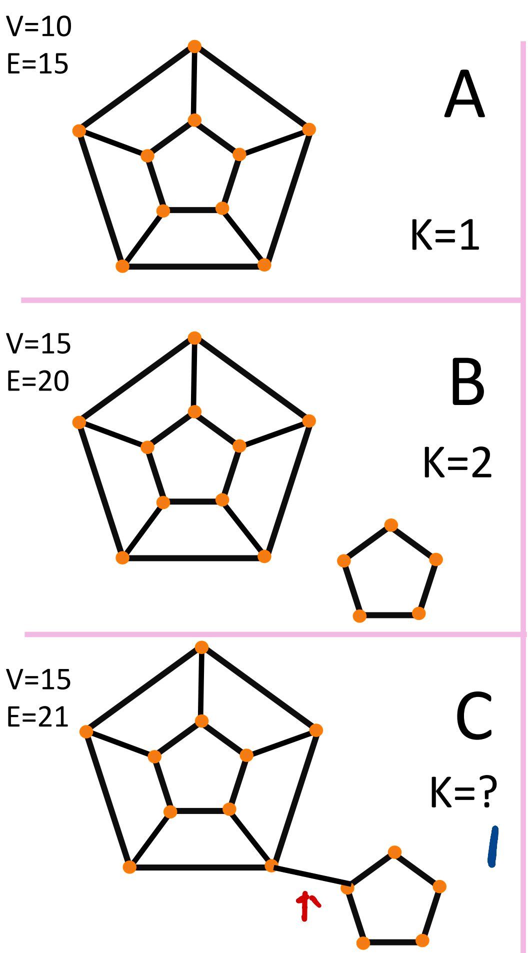
We can see:
When k>1, the Laplacian can be written as shown

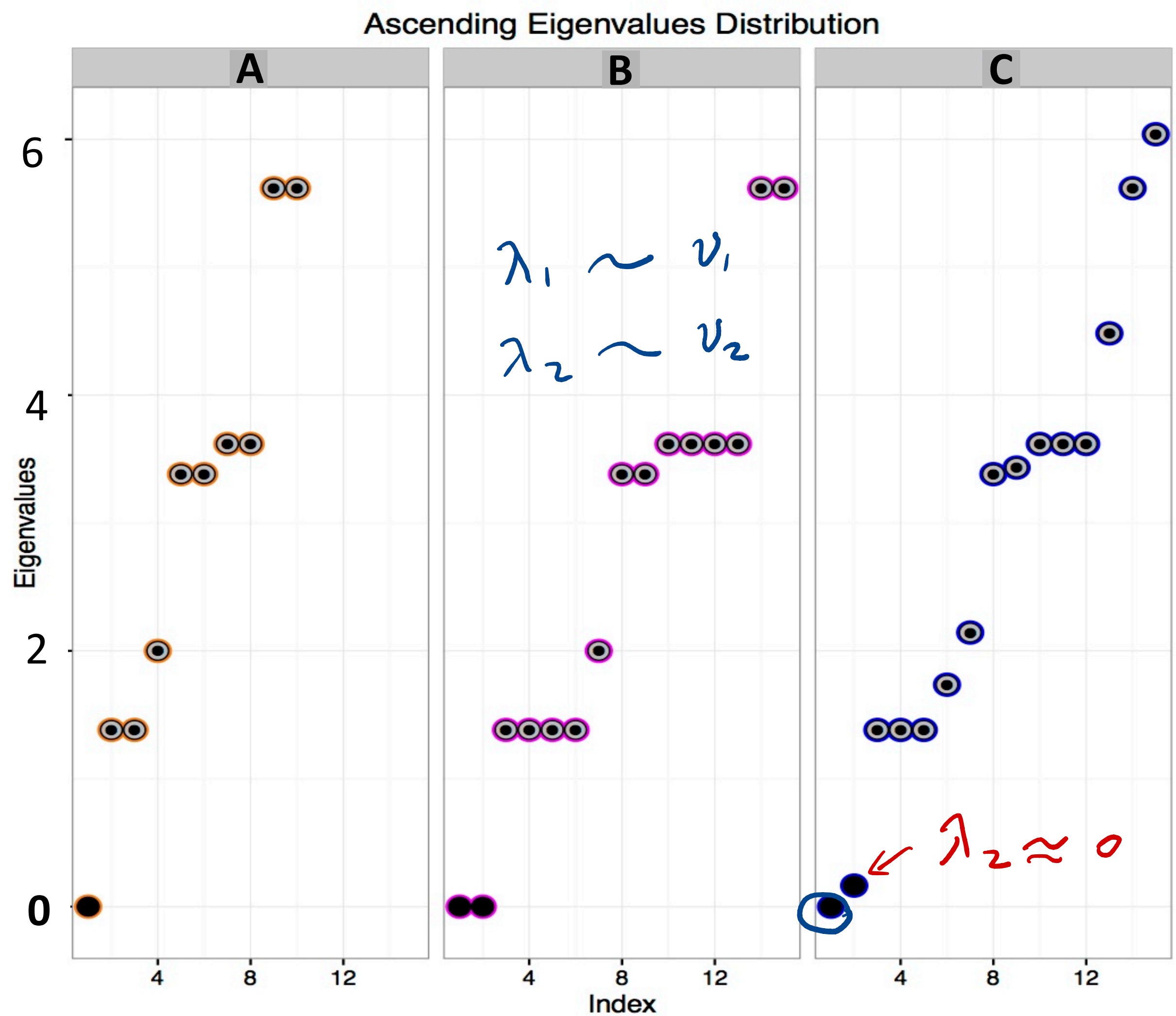
$$L = \begin{pmatrix} L_1 & & & 0 \\ & L_2 & & \\ & & \ddots & \\ 0 & & & L_k \end{pmatrix}$$

where the eigenvectors u_i for the zero valued λ_i are piecewise constant.

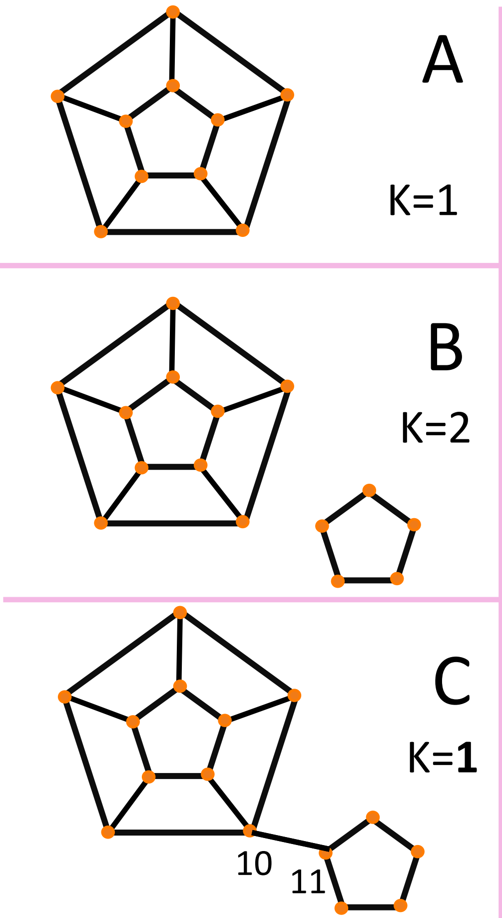
Proof is solved# → Solution for clustering

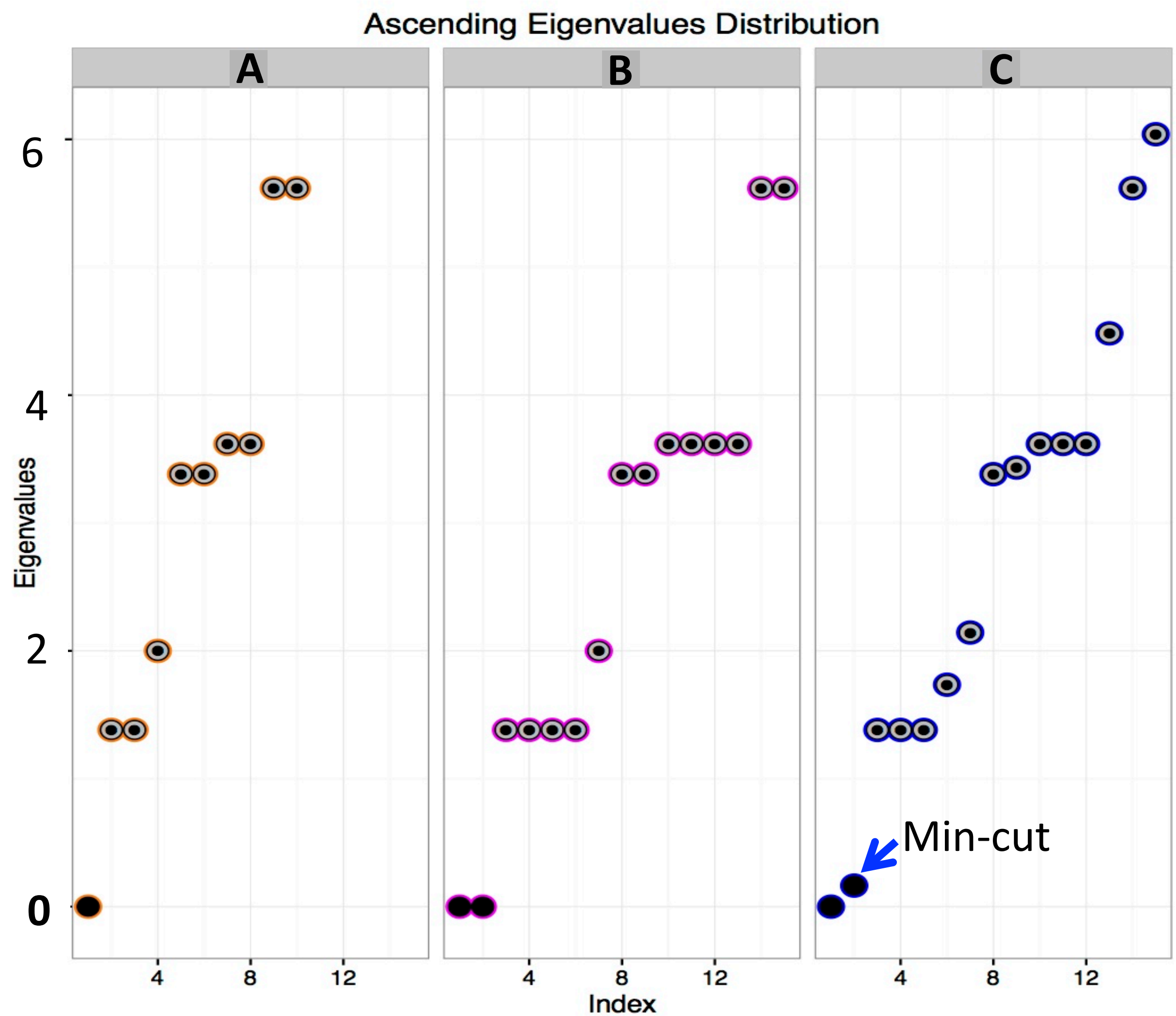
Eigenvalue distributions of three examples



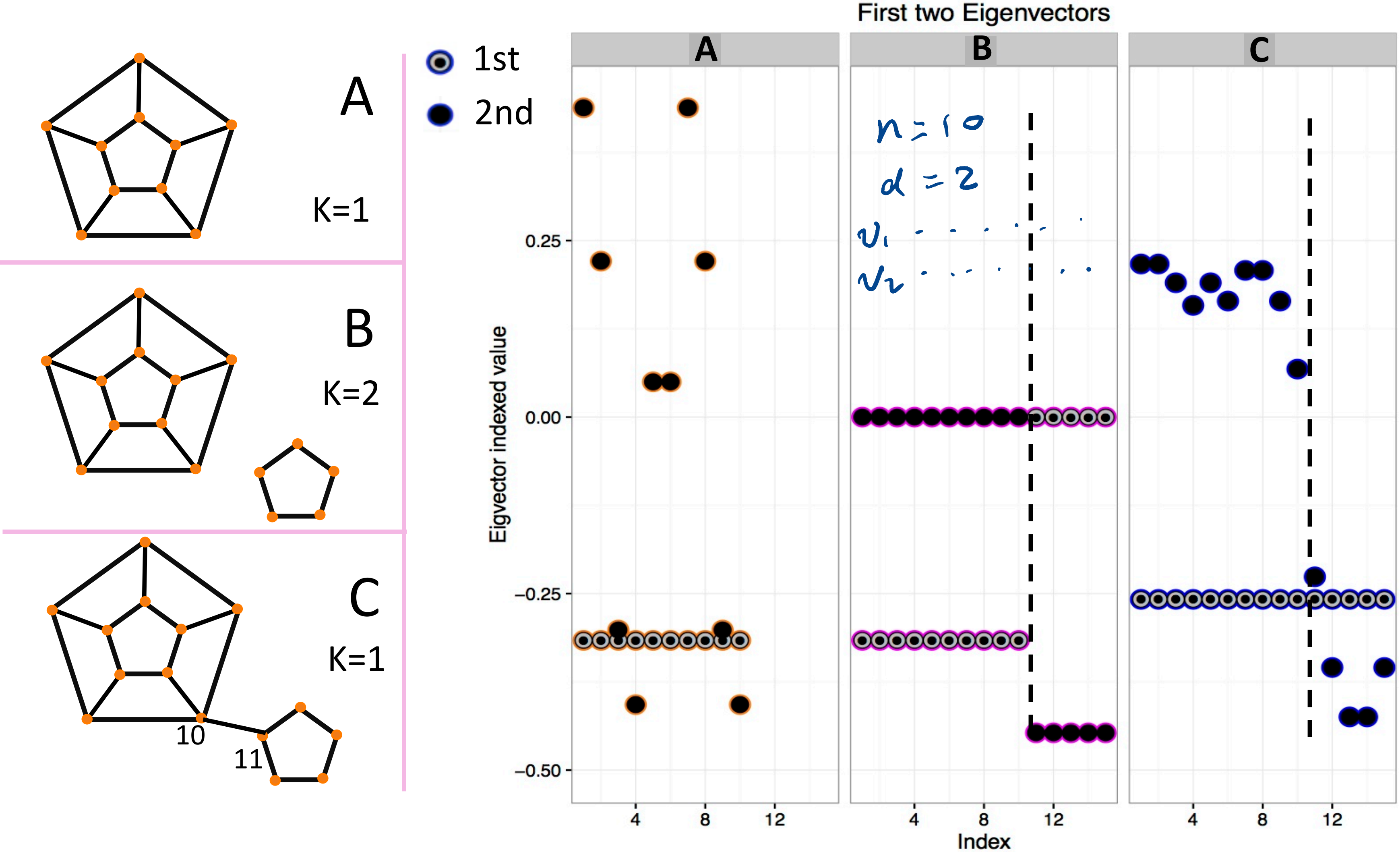


Eigenvalue distributions of three examples





First two Eigenvectors of three examples



Discussion

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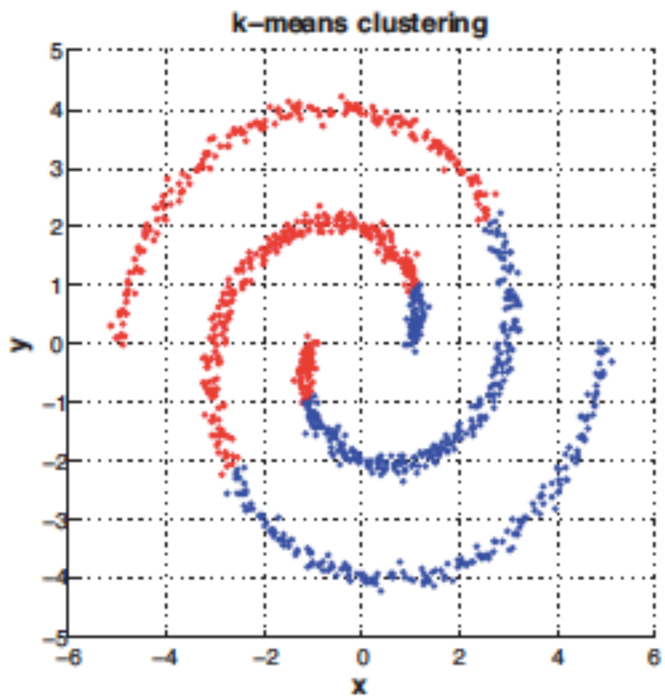
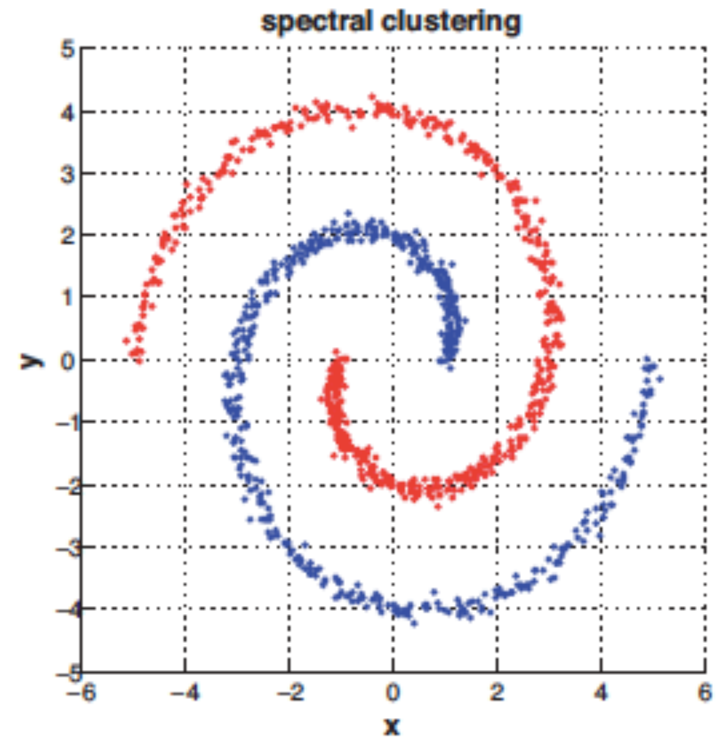
  i) Graph representation kept the topological relationship btw data

  ii) Eigenvectors are piecewise constant in the ideal cases, which are easy to cluster

Some Spectral clustering results



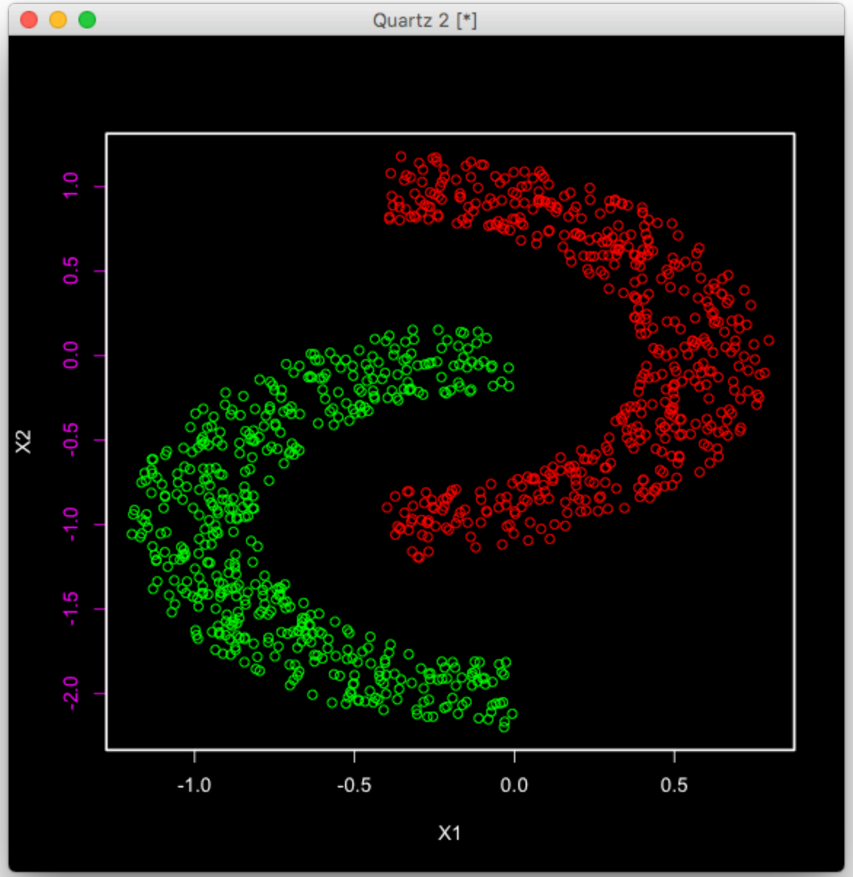
(a)



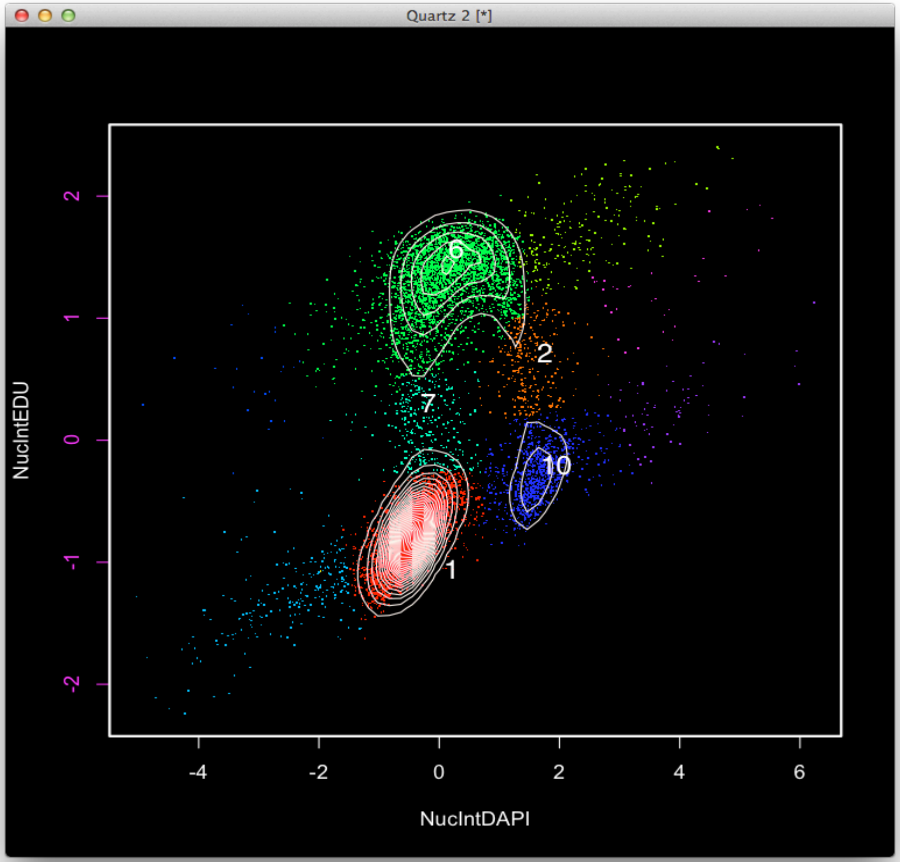
(b)

Some Spectral clustering results

Two-Moons



Cell Cycle phases



Conclusion of Spectral Clustering

Given # of zero valued λ_i = the number of disconnected components of the graph, we can *approximately* **use the first k number of eigenvectors to cluster the data into k clusters.**

The intuition: The singularities of the graph's Laplacian correspond to the # of clusters in the graph.

Assignments

- Finish Chapter 12 of the textbook
- Next time: Markov chain

Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. "Probability and Statistical Inference"
- Kelvin Murphy, "Machine learning, A Probabilistic perspective"

See you next time

See You!