Clustering

Predictive Analytics

Acknowledgments

These slides draw upon and adapt selected materials by:

- **Fragkiskos D. Malliaros** (CentraleSupélec, Université Paris–Saclay, France)

Unsupervised learning (clustering)

Supervised vs. Unsupervised Learning

Supervised learning

- We have labeled examples
- Given those examples, learn a model that can generalize to unseen examples
- Key tasks:
  - Classification
  - Regression

Unsupervised learning

- The data is unlabeled
- Given the data, learn a model that identifies structure in the data (and generalize to new data)
- Key task:
  - Clustering

What is Cluster Analysis?

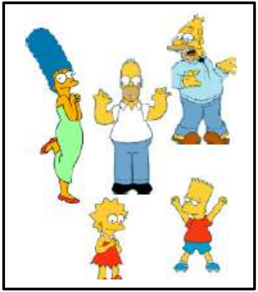
- Cluster: a collection of data objects
  - Similar (or related) to one another within the same group
  - Dissimilar (or unrelated) with objects in other groups

- Cluster analysis (or clustering)
  - Finding similarities between data according to the characteristics of the data and …
  - … grouping similar data objects into clusters

- Typical applications
  - As a stand-alone tool to get further insights about the data
  - As a preprocessing step for other algorithms

Any Natural Grouping?

Clustering is subjective



Simpson's family

School employees

Females

Males

Slide by Eamonn Keogh, UCR

What is a Good Clustering?

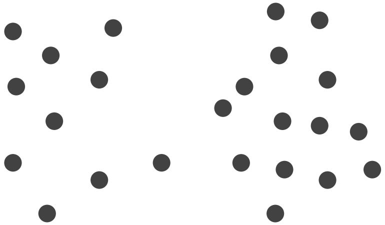
- Good clusters have:
  - High intra-cluster similarity: cohesive within clusters
  - Low inter-cluster similarity: distinctive between clusters

- The quality of a clustering method depends on
  - The similarity measure used by the method
  - Its ability to discover some or all of the hidden patterns

Recall the distance and similarity measures covered in kNN classification

Goals of Clustering

- Group objects that are similar into clusters: classes that are unknown beforehand



Goals of Clustering

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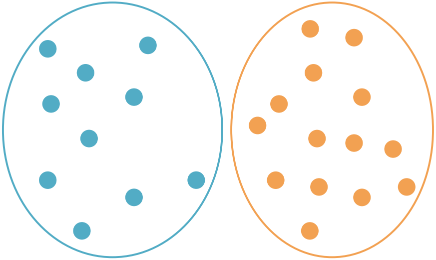
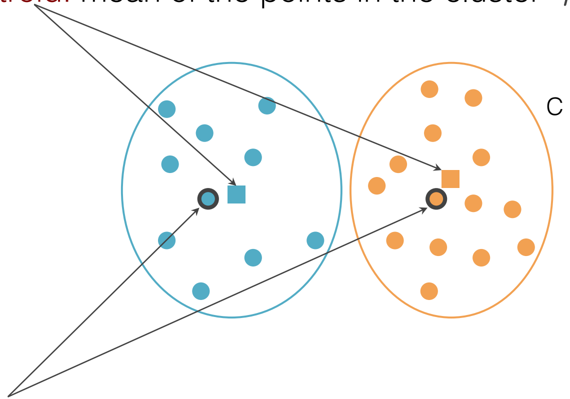


Applications of Clustering

- Understand general characteristics of the data
- Visualize the data
- Infer some properties of a data point based on how it relates to other data points
- Examples
  - Find subtypes of diseases
  - Visualize protein families
  - Find categories among images
  - Find patterns in financial transactions
  - Detect communities in social networks
  - Find users with similar interests (e.g., Netflix, Amazon)

Cluster Centroids and Medoids

- Centroid: mean of the points in the cluster $\mu = \frac{1}{|C|} \sum_{x \in C} x$



- Medoid: point in the cluster that is closest to the centroid

$$m = \arg\min_{x \in C} d(x, \mu)$$

Cluster Evaluation

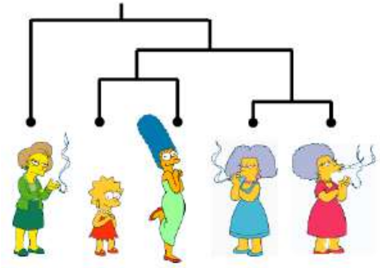
- Clustering is unsupervised
- There is no ground truth. How do we evaluate the quality of a clustering algorithm?
- Based on the shape of the clusters:
  - Points within the same cluster should be nearby/similar and points far from each other should belong to different clusters
- Based on the stability of the clusters:
  - We should get the same results if we remove some data points, add noise, etc.
- Based on domain knowledge
  - The clusters should "make sense"

Major Clustering Approaches

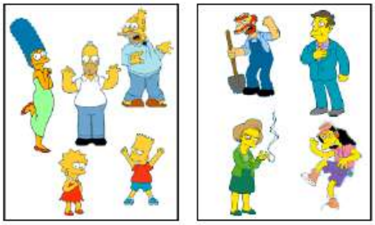
- Partitioning approach
  – Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  – Typical methods: k-means, k-medoids
- Hierarchical approach
  – Create a hierarchical decomposition of the set of data (or objects) using some criterion
  – Typical methods: Diana, Agnes, BIRCH, CHAMELEON
- Density-based approach
  – Based on connectivity and density functions
  – Typical methods: DBSCAN, OPTICS, DenClue
- Grid-based approach
  – Based on a multiple-level granularity structure
  – Typical methods: STING, WaveCluster, CLIQUE

Hierarchical vs. Partitional

Hierarchical



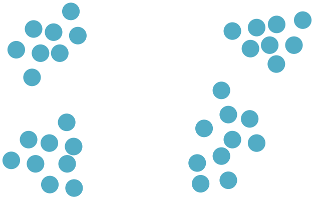
Partitional



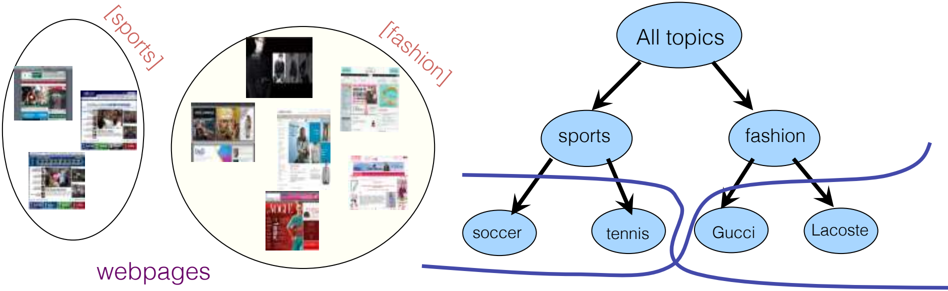
Hierarchical clustering

Hierarchical Clustering

- Group data over a variety of possible scales, in a multi-level hierarchy



Hierarchical Clustering (2/2)



- A hierarchy might be more natural
- Different users might care about different levels of granularity or even prunings

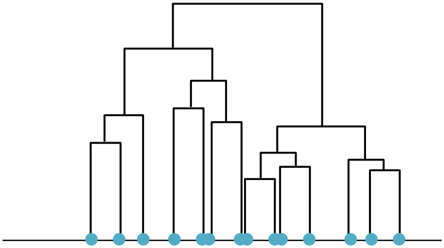
Construction

- Agglomerative approach (bottom-up)
  - Start with each element in its own cluster
  - Iteratively join neighboring clusters

- Divisive approach (top-down)
  - Start with all elements in the same cluster
  - Iteratively separate into smaller clusters

Dendrogram

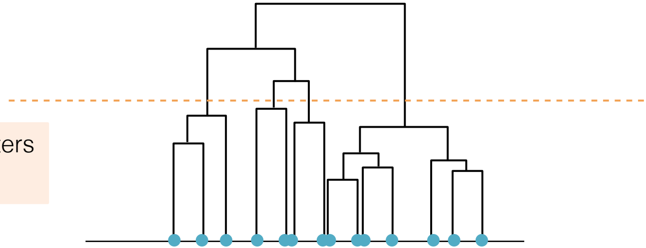
- The results of a hierarchical clustering algorithm are presented in a dendogram



Dendrogram

- The results of a hierarchical clustering algorithm are presented in a dendogram

How many clusters do I have?



Dendrogram

- The results of a hierarchical clustering algorithm are presented in a dendogram

Hierarchical Clustering

- Advantages
  - No need to pre-define the number of clusters
  - Interpretability
- Drawbacks
  - Computational complexity
  - Must decide at which level of the hierarchy to split
  - Lack of robustness (unstable)

k-means clustering

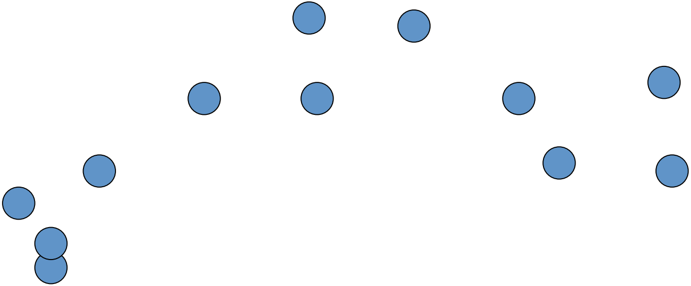
k-means Algorithm – The Idea

Most well-known and popular clustering algorithm:

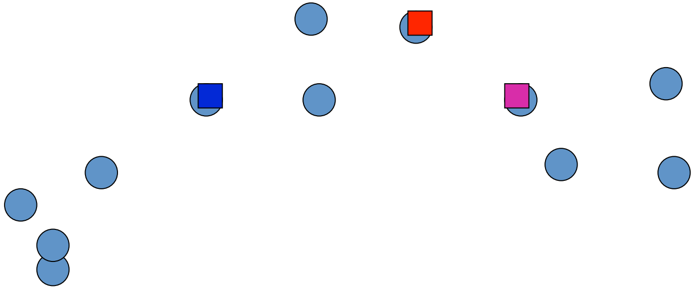
1. Start with some initial cluster centers

2. Iterate:
   - Assign each example to closest center
   - Recalculate centers as the mean of the points in a cluster

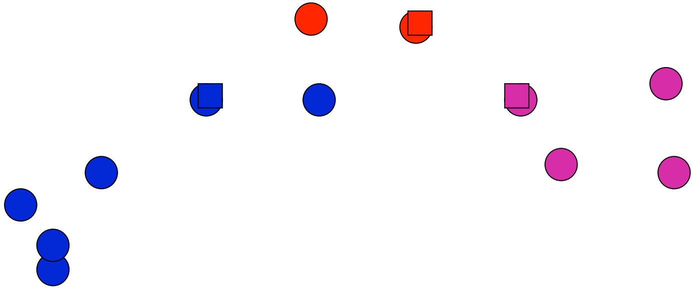
k-means: An Example



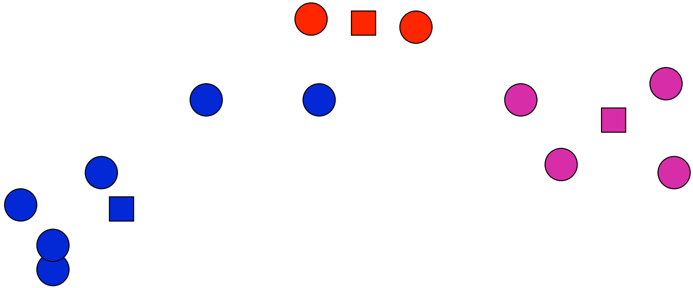
k-means: Initialize Centers Randomly



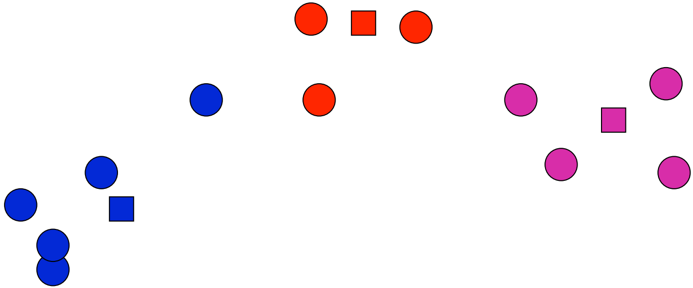
k-means: Assign Points to Nearest Center



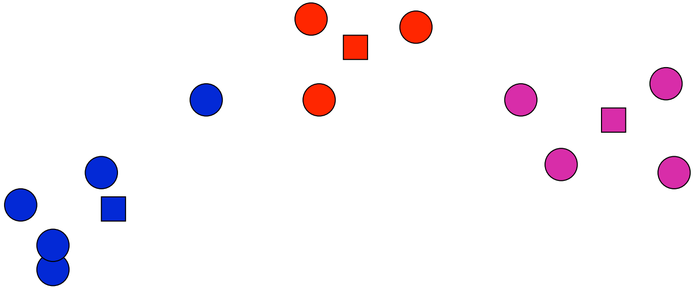
k-means: Readjust Centers



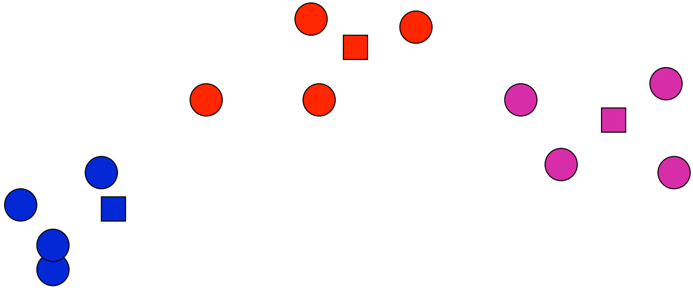
k-means: Assign Points to Nearest Center



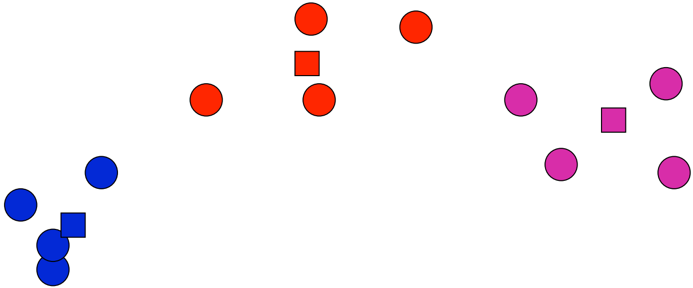
k-means: Readjust Centers



k-means: Assign Points to Nearest Center

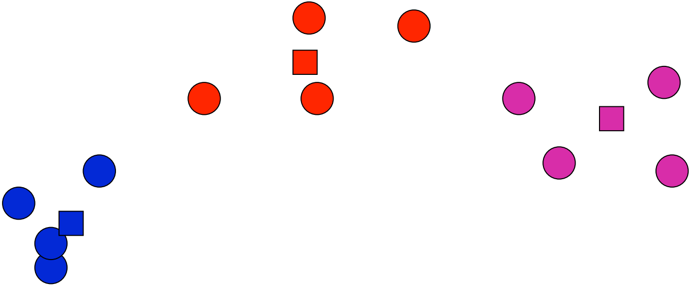


k-means: Readjust Centers



k-means: Assign Points to nearest Center

No changes: Done



Test demo at: http://stanford.edu/class/ee103/visualizations/kmeans/kmeans.html

k-means Clustering – Objective Function

- Minimize the intra-cluster variance
  - Within-cluster sum of squares

$$\mathrm{Var}_{\mathrm{in}}(C) = \frac{1}{|C|} \sum_{x \in C} ||x - \mu_C||^2$$

For a cluster C

$$V = \sum_{k=1}^{K} \sum_{x \in C_k} \frac{1}{|C_k|} ||x - \mu_{C_k}||^2$$

For all clusters

- What will this partition of the space look like?

k-means Clustering – Objective Function

- Minimize the intra-cluster variance
  - Within-cluster sum of squares

$$\mathrm{Var}_{\mathrm{in}}(C) = \frac{1}{|C|} \sum_{x \in C} ||x - \mu_C||^2$$

For a cluster C

$$V = \sum_{k=1}^{K} \sum_{x \in C_k} \frac{1}{|C_k|} ||x - \mu_{C_k}||^2$$

For all clusters

- For each cluster, the points in that cluster are those that are closest to its centroid than to any other centroid

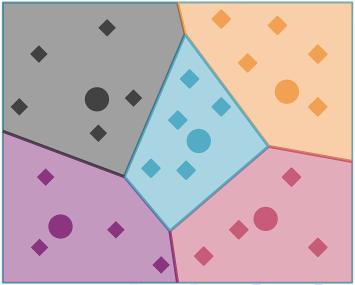
k-means Clustering – Objective Function

- Minimize the intra-cluster variance
  - Within-cluster sum of squares

$$\mathrm{Var}_{\mathrm{in}}(C) = \frac{1}{|C|} \sum_{x \in C} ||x - \mu_C||^2$$ For a cluster C

$$V = \sum_{k=1}^{K} \sum_{x \in C_k} \frac{1}{|C_k|} ||x - \mu_{C_k}||^2$$ For all clusters

- Voronoi tesselation



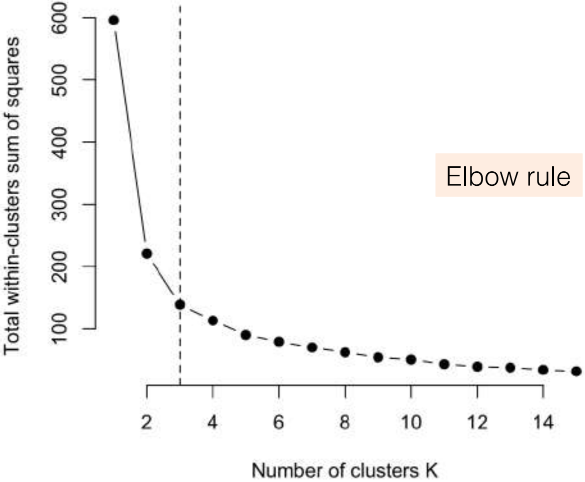
- Optimal solution: hard problem

Lloyd's Algorithm for k-means

- k-means cannot be easily optimized

- We adopt a greedy strategy (Lloyd's Algorithm)
  - Partition the data into k clusters at random
  - Compute the centroid of each cluster
  - Assign each point to the cluster of the centroid centroid
  - Repeat until cluster membership converges

How to Select k?



Elbow rule

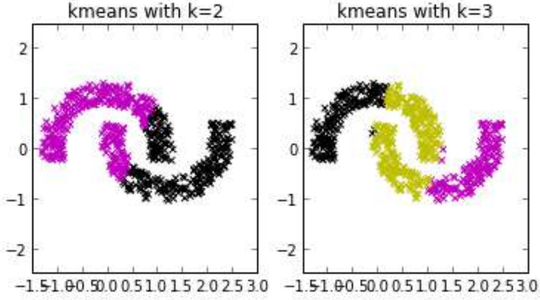
Summary of k-means

- Advantages
  - Computational time is linear: $\mathcal{O}(npkt)$ t: number of iterations
  - Easily implementable

compute kn distances
in p dimensions

- Drawbacks
  - Need to select k (user-defined parameter)
  - Sensitivity to noise and outliers
  - Non-deterministic (stochastic)
    - Different solutions with each iteration
  - The clusters are forced to have “spherical” (convex) shapes

Example



Source: https://pafnuty.wordpress.com/

Improving k-means: k-means++

- The quality of the solution depends on the initialization
- Rationale behind random initialization
  - Choosing a random assignment may lead the algorithm to a good local minimum

- Another approach: k-means++ [Arthurs and Vassilvitskii '07]
  1. Select a random point and declare it centroid c_1
  2. For all remaining data points x_j compute distance $d(x_j, c_1)$
  3. Select a random point with probability proportional to $d(x_j, c_1)^2$ and set it as c_2
     - This will give a point far enough from c_1
  4. Repeat steps 2 and 3 for all centroids k

scikit-learn

http://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

http://scikit-learn.org/stable/auto_examples/cluster/
plot_kmeans_digits.html#sphx-glr-auto-examples-cluster-plot-kmeans-digits-py

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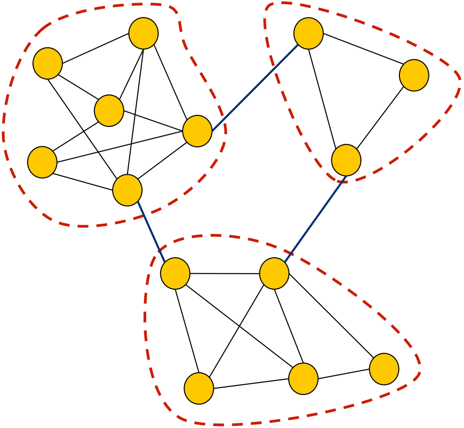
Spectral clustering

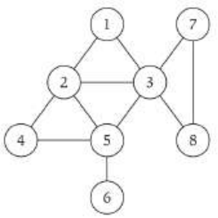
Clustering Structure in Graphs



How to discover the clustering structure?

Graph Representation: Adjacency Matrix

- A graph can be represented by the adjacency matrix A
  - Matrix of size $n \times n$, where $n=|V|$ is the number of nodes
  - $A_{ij} > 0$, if i and j are connected
  - $A_{ij} = 0$, if i and j are not connected
  - In case of **unweighted** graphs, $A_{ij} = 1$, if (i, j) is an edge of the graph
  - Space proportional to n^2



Undirected graph

Node indexing

Node indexing

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

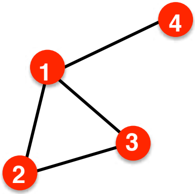
Adjacency matrix

Graph Representation: Laplacian Matrix

- Let G = (V, E) be a graph. Then, the Laplacian matrix is defined as

$$\mathbf{L}_{ij} = \begin{cases} k_i & \text{if } i = j \\ -1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

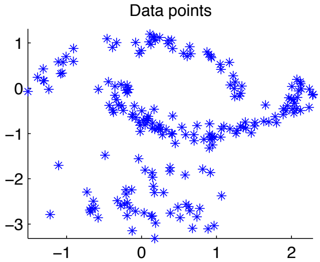
- Diagonal degree matrix D, where $D_{ii} = k_i$ (node degrees)



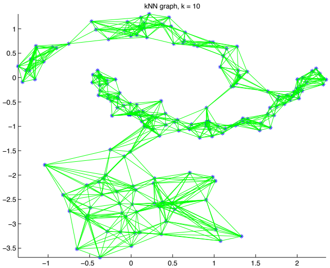
$$\mathbf{L} = \mathbf{D} - \mathbf{A} = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

Clustering Non-Graph Data

- Apply graph clustering algorithms on data with no inherent graph structure (e.g., points in a d-dimensional Euclidean space)
- How?
  1. Construct a similarity graph based on the topological relationships and distances between data points (e.g., kNN graph)
  2. Then, the problem of clustering the set of data points is transformed to a graph clustering problem



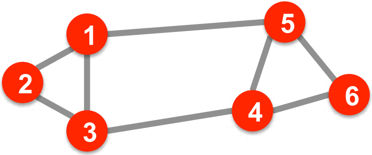
Similarity graph (e.g., kNN)



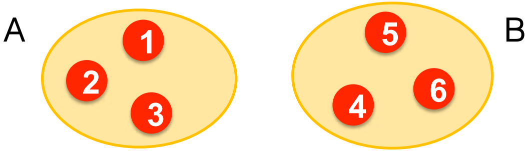
[von Luxburg '07], [Shi and Malik '00], [Ng, Jordan, Weiss '02]

Graph Partitioning (1/2)

- Undirected graph $G=(V, E)$



- Bi-partitioning task:
  - Divide nodes into two disjoint groups A, B

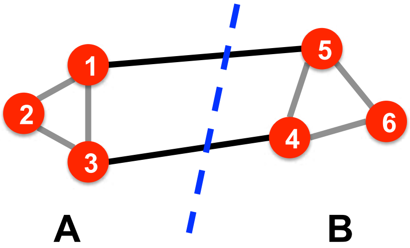


Questions:

- How can we define a good partition of G ?
- How can we efficiently identify such a partition?

Graph Partitioning (2/2)

- What makes a good partition?
  - Maximize the number of within-group connections
  - Minimize the number of between-group connections

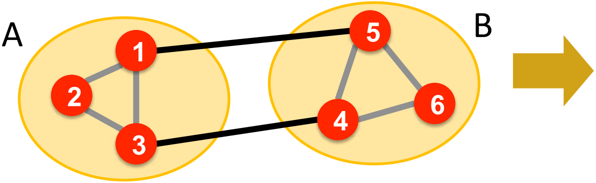


Graph Cuts

- Express partitioning objectives as a function of the edge cut of the partition
- Cut: Set of edges across two groups:

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

Two partitions, A and B



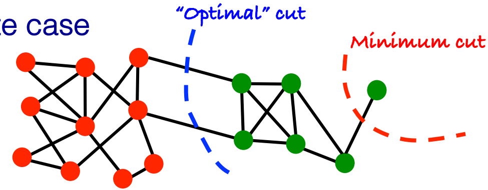
$$\text{cut}(A, B) = 2$$

Graph Cut Criterion for Clustering

- Criterion: Minimum-cut
  - Minimize the weight of connections between groups

$$\arg\min_{A,B} \; \mathrm{cut}(A, B)$$

- Degenerate case



Problem

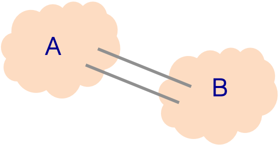
- Not satisfactory partition – often isolated nodes
- Does not consider internal cluster connectivity

Ratio Cut

Normalize cut by the size of the groups

$$\text{ratio-cut}(A,B) = \frac{\text{cut}(A,B)}{|A|} + \frac{\text{cut}(A,B)}{|B|}$$

Size of A and B



Internal group connectivity is not taken into account

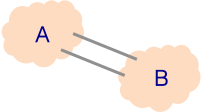
Normalized Cut

- Criterion: Normalized cut
  - Connectivity between groups relative to the density of each group

$$\text{normalized-cut}(A, B) = \frac{\text{cut}(A, B)}{\text{vol (A)}} + \frac{\text{cut}(A, B)}{\text{vol (B)}}$$

  - Vol(A): total weighted degree of the nodes in A, i.e., $\sum_{i \in A} k_i$

- Why use this criterion?
  - It produces more balanced partitions

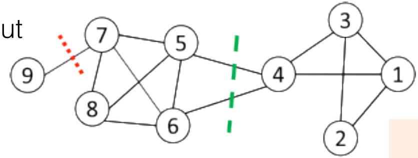


- How do we efficiently find a good partition?
  - Computing the optimal cut is NP-hard

[Shi and Malik '97]

Ratio Cut vs. Normalized Cut (1/2)

Red is Min-Cut



$$\text{ratio-cut}(A, B) = \frac{\text{cut}(A, B)}{|A|} + \frac{\text{cut}(A, B)}{|B|}$$

$$\text{normalized-cut}(A, B) = \frac{\text{cut}(A, B)}{\text{vol (A)}} + \frac{\text{cut}(A, B)}{\text{vol (B)}}$$

Ratio-Cut(Red) = 1/1 + 1/8 = 1.125

Ratio-Cut(Green) = 2/5 + 2/4 = 0.9

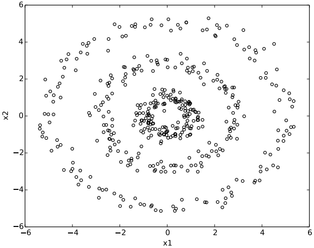
Lower value is better

Normalized-Cut(Red) = 1/1 + 1/26 = 1.03

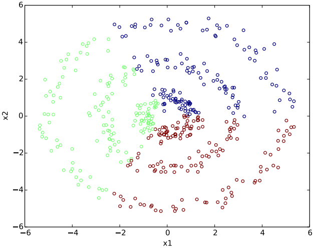
Normalized-Cut(Green) = 2/12 + 2/16 = 0.29

Normalized is even better
for Green due to density

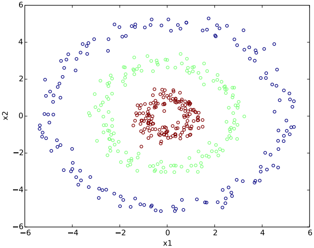
Spectral Clustering vs. k-Means



- 2-dimensional points
- Find k=3 clusters



k-means



spectral clustering

scikit-learn

http://scikit-learn.org/stable/modules/clustering.html#spectral-clustering

http://scikit-learn.org/stable/auto_examples/cluster/
plot_cluster_comparison.html

Comparison (scikit-learn)