COMPSCI 589
Lecture 17: Hierarchical Clustering and K-Means

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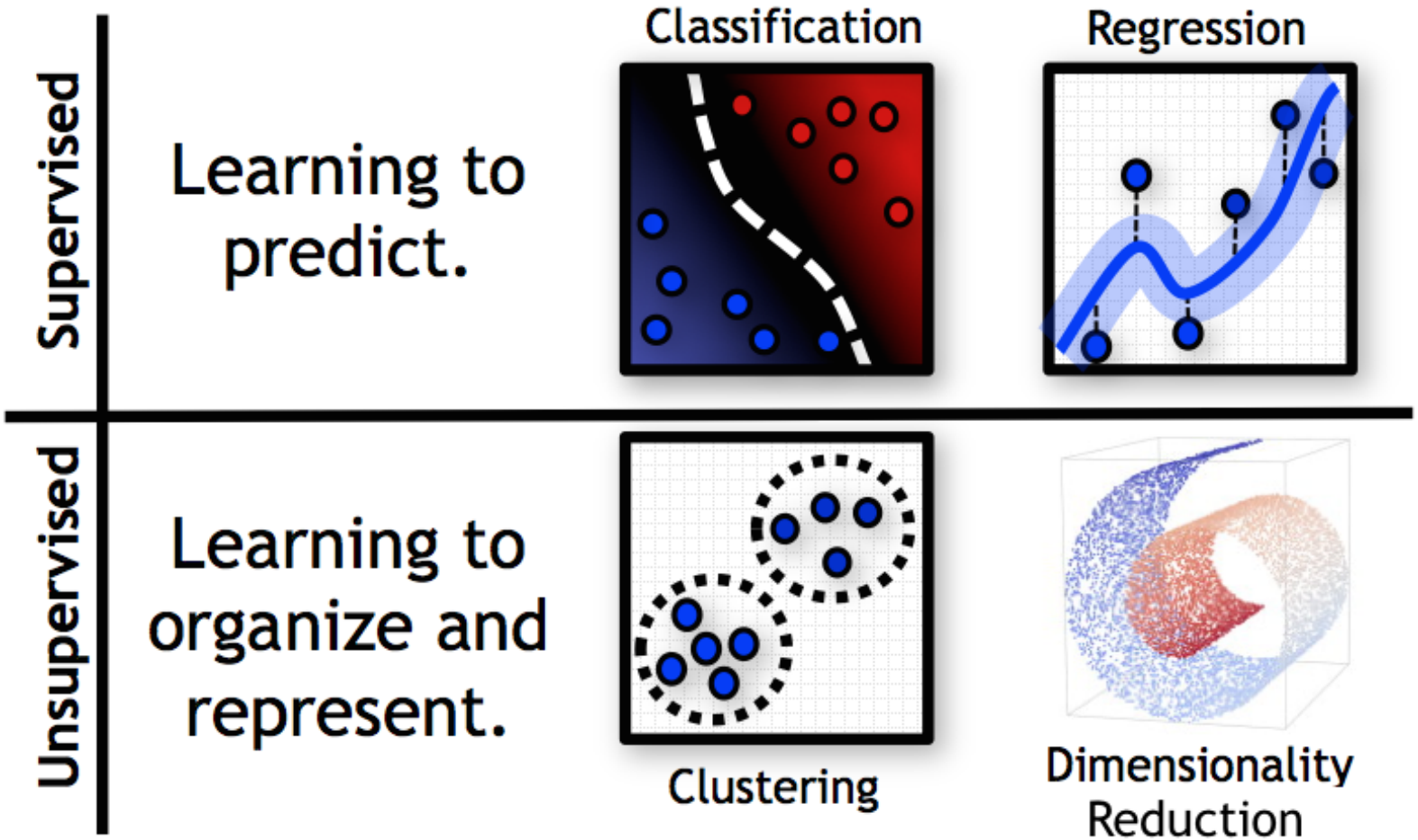
Views on Machine Learning

Mitchell (1997): "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Substitute "training data D" for "experience E."

Machine Learning Tasks



The Classification Task

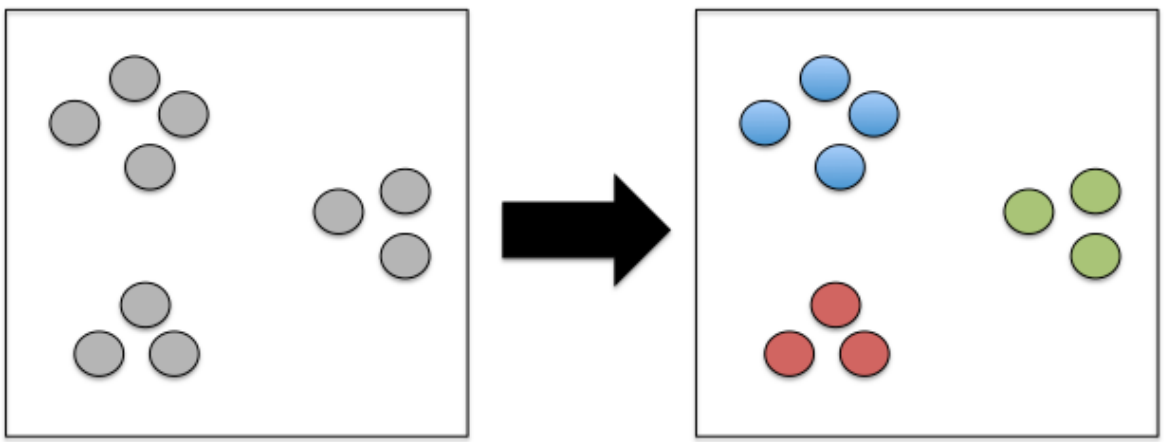
Definition: The Classification Task

Given a feature vector $\mathbf{x} \in \mathbb{R}^D$ that describes an object that belongs to one of C classes from the set $\mathcal{Y}$, predict which class the object belongs to.

The Clustering Task

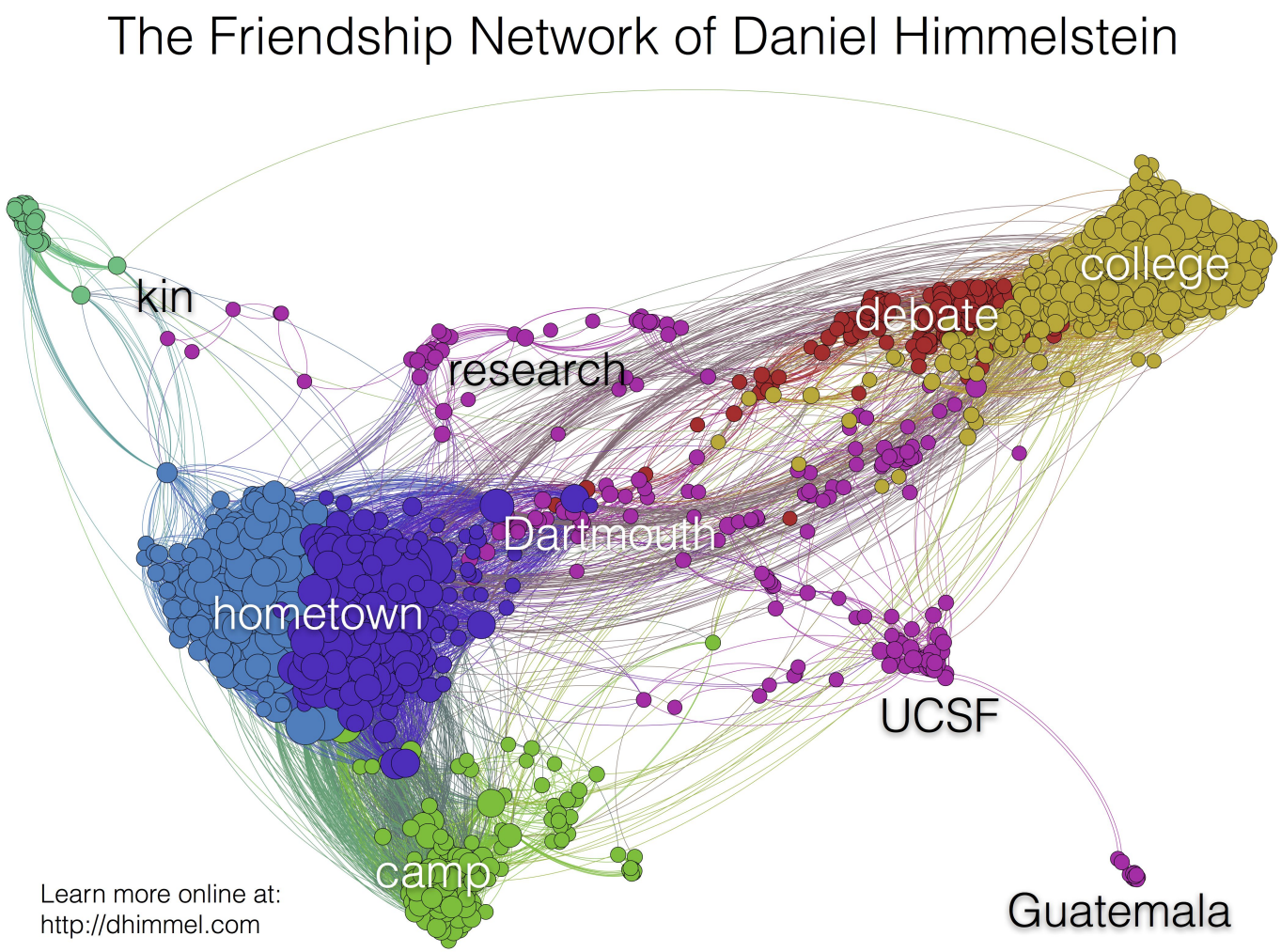
Definition: The Clustering Task

Given a collection of data cases $\mathbf{x}_i \in \mathbb{R}^D$, partition the data cases into groups such that the data cases within each partition are more similar to each other than they are to data cases in other partitions.

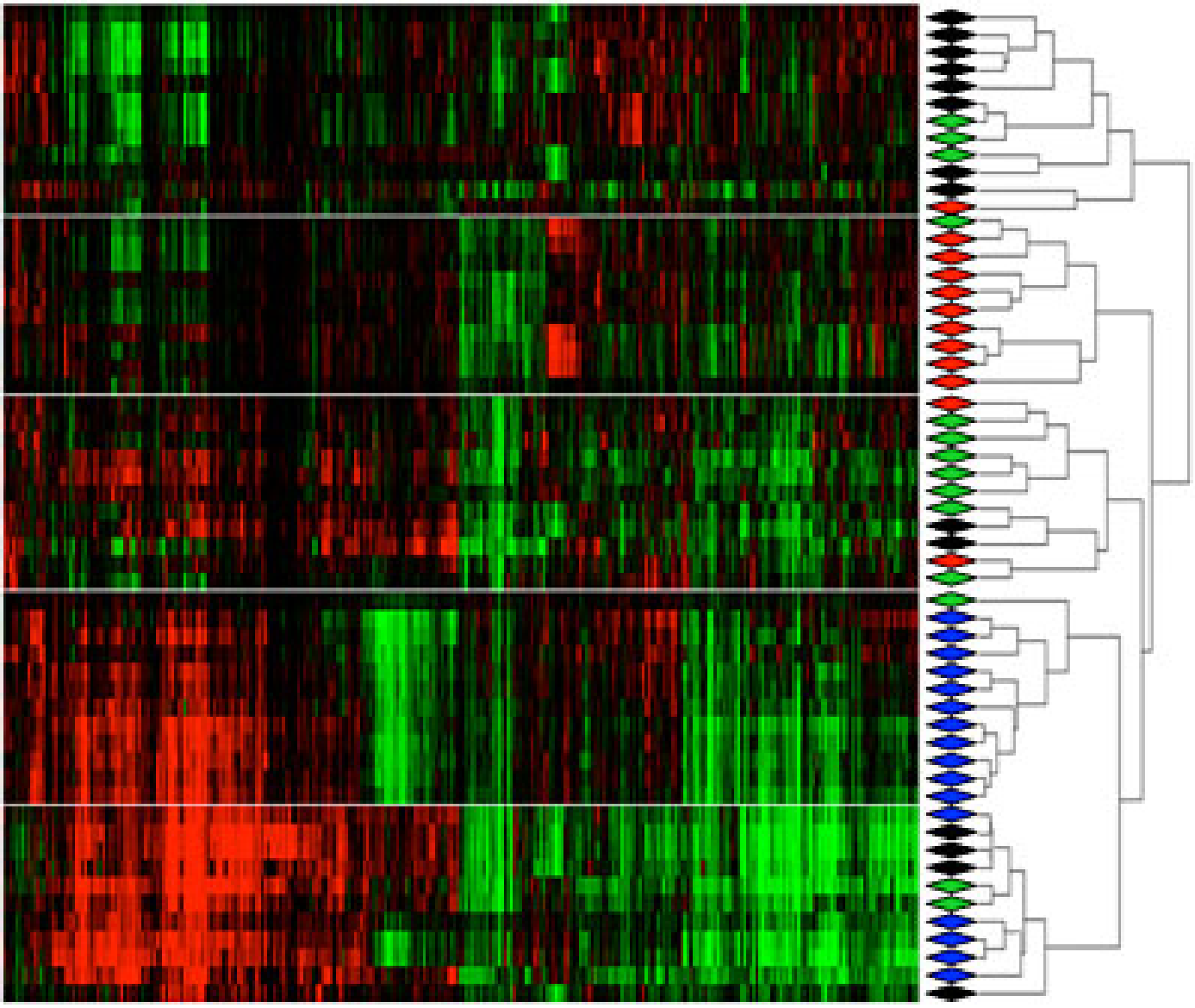


Examples: Market Segmentation

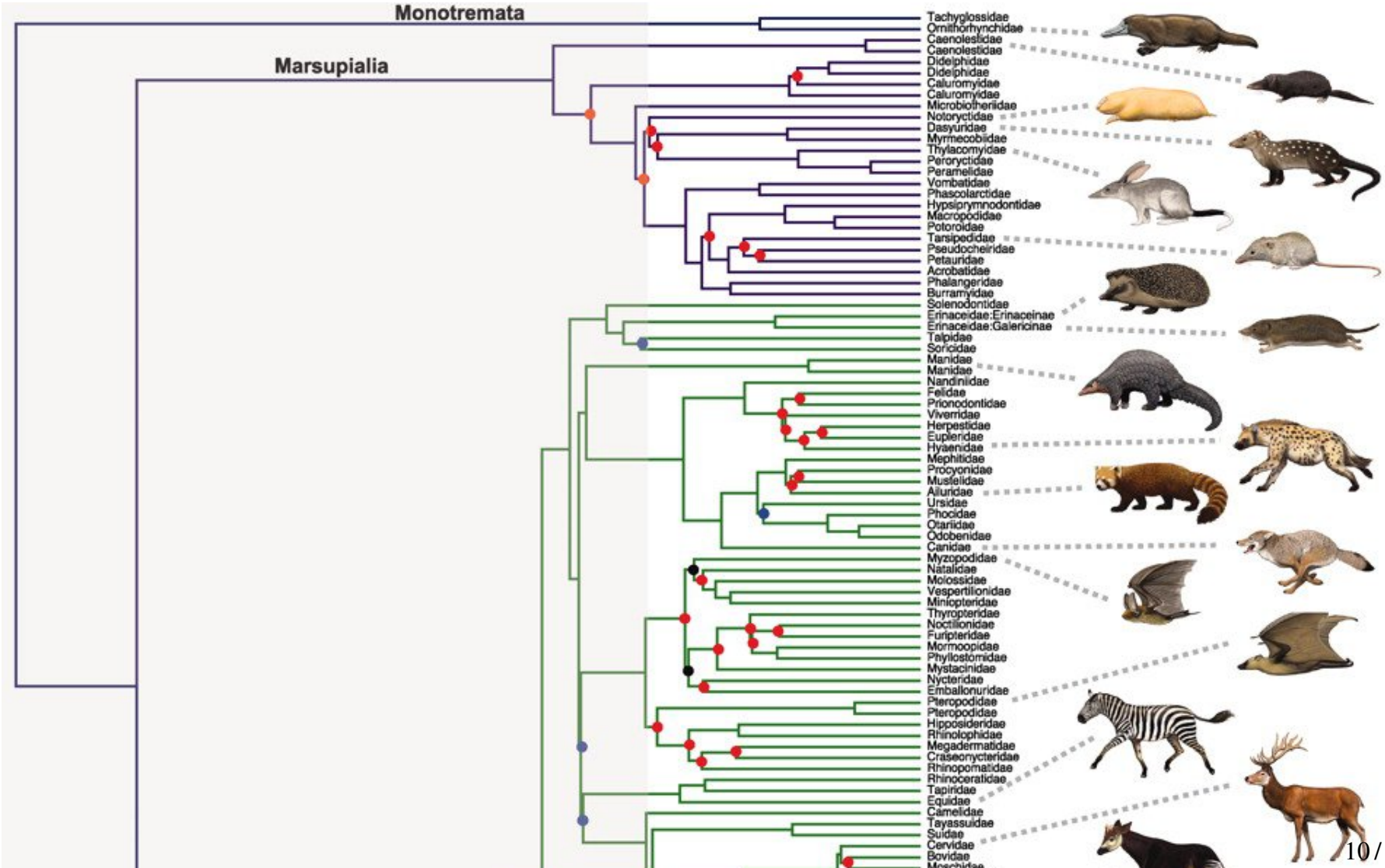
Examples: Community Detection



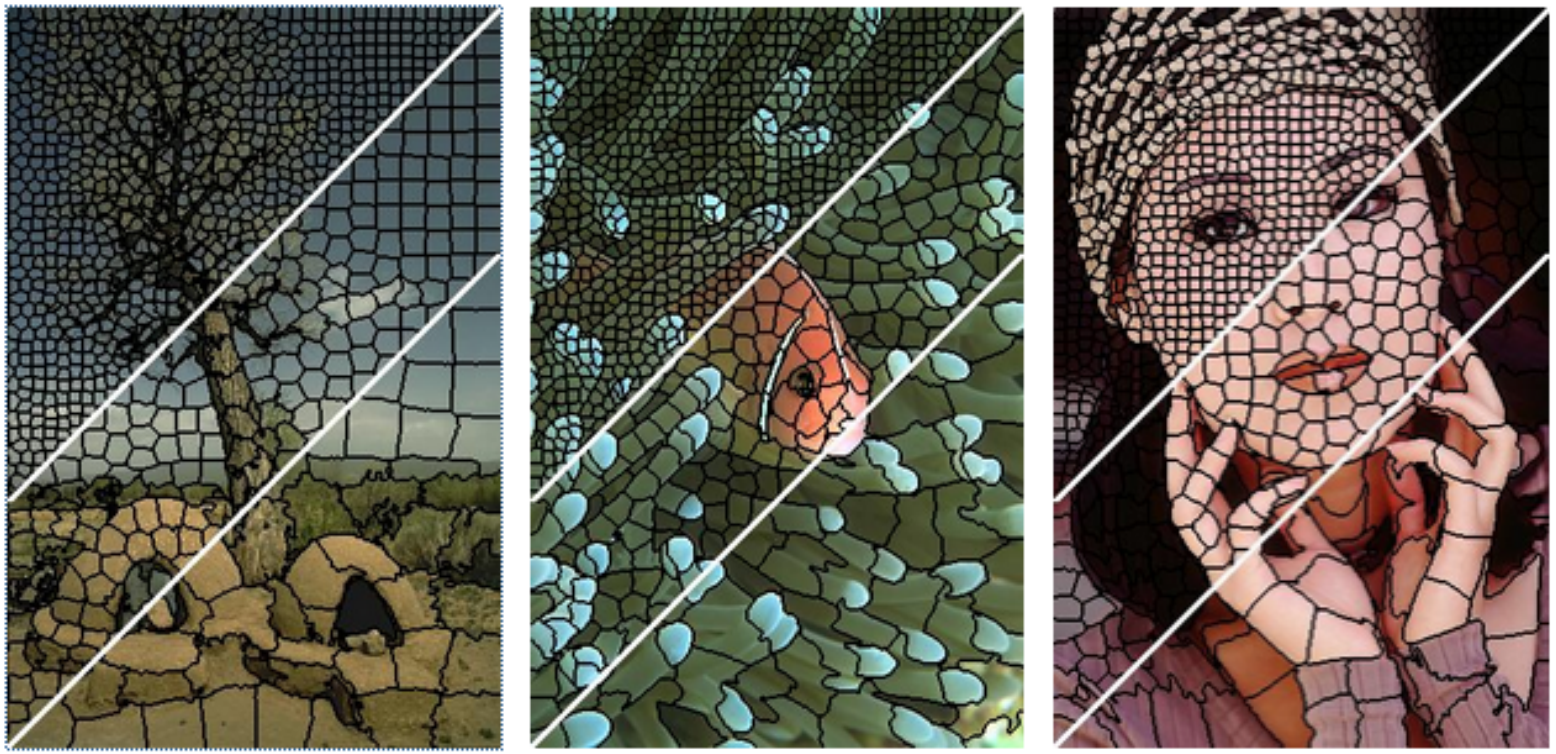
Examples: Gene Expression



Examples: Phylogenetic Trees



Examples: Super Pixels



Defining a Clustering

- Suppose we have N data cases $\mathcal{D} = \{\mathbf{x}_i\}_{i=1:N}$.
- A clustering of the N cases into K clusters is a partitioning of $\mathcal{D}$ into K mutually disjoint subsets $\mathcal{C} = \{C_1, ..., C_K\}$ such that $C_1 \cup ... \cup C_K = \mathcal{D}$.

Exhaustive Clustering

- Suppose we have a function $S(\mathcal{C})$ that takes a partitioning $\mathcal{C}$ of the data set D and returns a score with lower scores indicating better clusterings.
- The optimal clustering according to S is simply given by

$$\arg\min_{\mathcal{C}} \quad S(\mathcal{C})$$

- **Question:** What is the complexity of exhaustive clustering?

Number of Clusterings

- The total number of clusterings of a set of N elements is the Bell number B_N where $B_0 = 1$ and $B_{n+1} = \sum_{k=0}^{n} \binom{n}{k} B_k$.
- The first few Bell numbers are: 1, 1, 2, 5, 15, 52, 203, 877, 4140, 21147, 115975, 678570, 4213597, 27644437, 190899322, ...
- The complexity of exhaustive clustering scales with B_N and is thus computationally totally intractable for general scoring functions.
- We will need either approximation algorithms or scoring functions with special properties.

Hierarchical Agglomerative Clustering

- Hierarchical Clustering methods are a family of greedy tree-based clustering methods.
- Hierarchical Agglomerative Clustering (HAC) is the most popular member of this family.
- It begins with all data cases assigned to their own clusters, and then greedily and recursively merges the pair of clusters that is optimal with respect to a given criteria.

Distance and Linkage Functions

- Like KNN, HAC need to be supplied with a function for computing the distance between two data cases. This is often taken to be Euclidean distance, but could be any distance function.
- To merge clusters, HAC also needs what is called a linkage function for measuring the distance between clusters.
- Linkage functions can differ significantly in their computational complexity and the clusterings they produce.

Examples of Linkage Functions

Linkage	*Description*
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *largest* of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *smallest* of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the *average* of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable *inversions*.

The Hierarchical Agglomerative Clustering Algorithm

Algorithm 10.2 *Hierarchical Clustering*

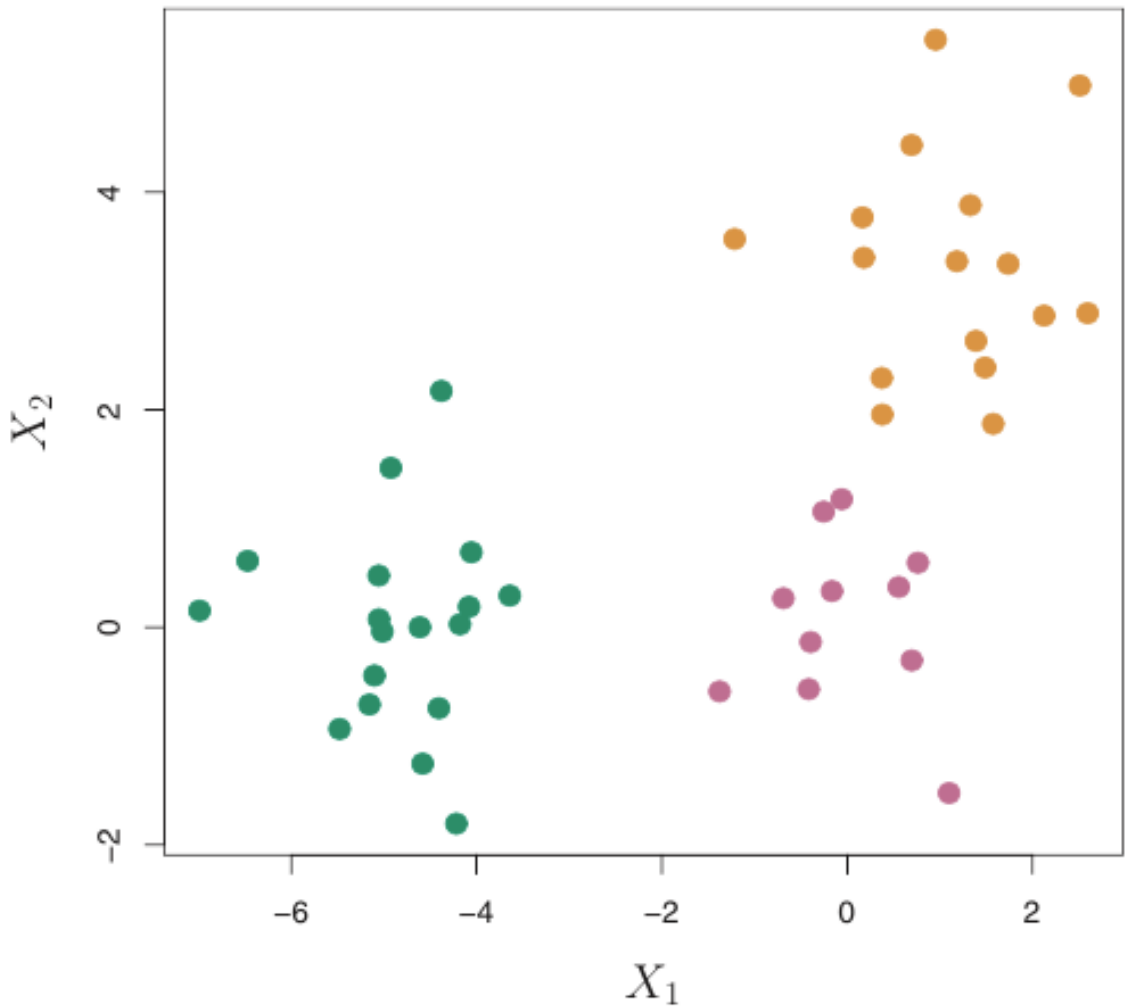
1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.

2. For $i = n, n-1, \ldots, 2$:

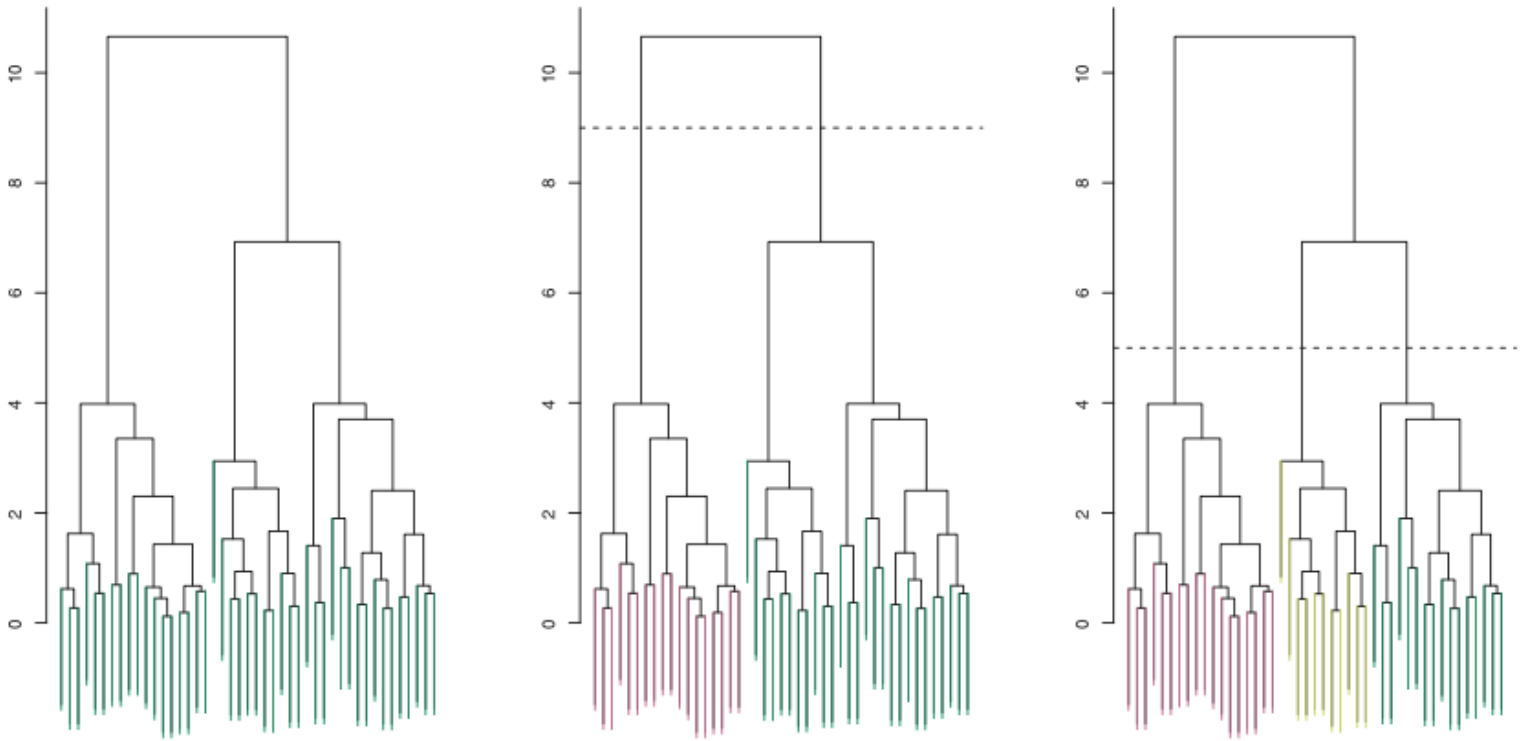
   (a) Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.

   (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Example: Data



Example: Dendrograms



Issues

- We need to have a good notion of similarity for the results of cluster analysis to be meaningful at all.
- As with KNN, pre-processing like re-scaling/normalizing features can completely change the results.
- Further, we need to slect between the different linkage functions.
- We need some way to determine the "right" number of clusters to focus on. We want to cluster on salient differences between data cases, not noise.
- This procedure is not able to nicely handle noise observations that are different from each other and from the rest of the data that do belong to valid clusters.
- All of these issues mean we need to be cautious in interpreting the results of clustering. It should be the starting point for an exploratory data analysis, not the end point.

The K-Means Algorithm

- The K-Means algorithm is an iterative optimization algorithm for clustering that alternates between two steps.
- The algorithm maintains a set of K cluster centroids or prototypes μ_k that represent the average (mean) feature vector of the data cases in each cluster.
- In the first step, the distance between each data case and each prototype is computed, and each data case is assigned to the nearest prototype.
- In the second step, the prototypes are updated to the mean of the data cases assigned to them.

The K-Means Algorithm

Algorithm 10.1 *K-Means Clustering*

1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.

2. Iterate until the cluster assignments stop changing:

   (a) For each of the K clusters, compute the cluster *centroid*. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.

   (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).

The K-Means Algorithm

Suppose we let z_i indicate which cluster $\mathbf{x}_i$ belongs to and $\mu_k \in \mathbb{R}^D$ be the cluster centroid/prototype for cluster k. The two main steps of the algorithm can then be expressed as follows:

1. $z_i = \arg\min_k ||\mu_k - \mathbf{x}_i||_2^2$
2. $\mu_k = \frac{\sum_{i=1}^N [z_i = k]\mathbf{x}_i}{\sum_{i=1}^N [z_i = k]}$

The K-Means Objective

- The K-Means algorithm attempts to minimize the sum of the within-cluster variation over all clusters (also called the within-cluster sum of squares):

$$\mathcal{C}^* = \arg\min_{\mathcal{C}} \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{\mathbf{x}_i, \mathbf{x}_j \in C_k} ||\mathbf{x}_i - \mathbf{x}_j||_2^2$$

- Note that this objective function has many, many local optima in general, each corresponding to a different clustering of the data.
- K-Means produces a non-increasing sequence of objective function values and is guaranteed to converge to some local optima. Finding the global optimum is not computationally tractable.

Initialization

- Because K-Means finds a local optimum, it can be highly sensitive to initialization.
- It is common to perform multiple random re-starts of the algorithm and take the clustering with the minimal total variation.
- Common initializations include setting the initial centers to be randomly selected data cases, setting the initial partition to a random partition, and selecting centers using a "furthest first"-style heuristic (more formally known as K-Means++).
- It often helps to initially to run with $K\log(K)$ clusters, then merge clusters to get down to K and run the algorithm from that initialization.

Issues

- Only works with Euclidean distance. An alternate version based on Manhattan distance exists and is called the K-medians algorithm.
- Pre-processing like re-scaling/normalizing features can completely change the results.
- We need some way to determine the "right" number of clusters to focus on. We want to cluster on salient differences between data cases, not noise.
- The run time is $O(NKT)$ where T is the number of iterations to convergence of the total variation. T is often small (like 20), but examples can be constructed that require an exponential number of steps to converge.
- Results in a hard assignment of data cases to clusters, which may be a problem if there are outliers.