Machine Learning (CS 181): 12. Clustering

David C. Parkes and Sasha Rush

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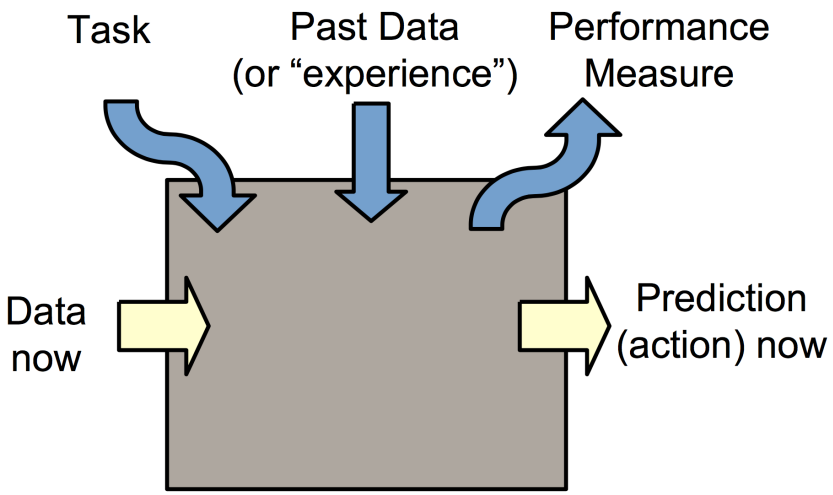
Supervised Learning

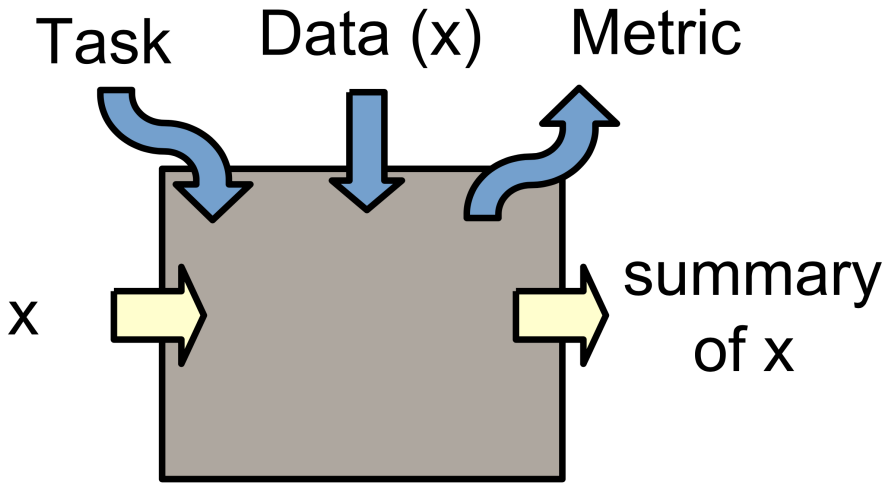
Data $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$



Solved via linear regression, logistic regression, Naive Bayes, neural nets, SVMs, etc.

Unsupervised Learning

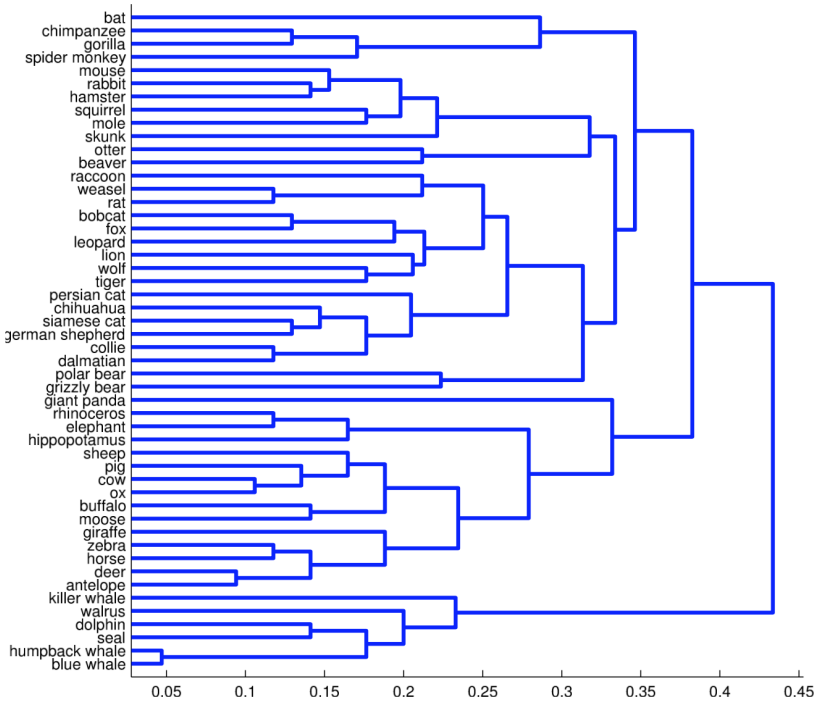
A different kind of task!



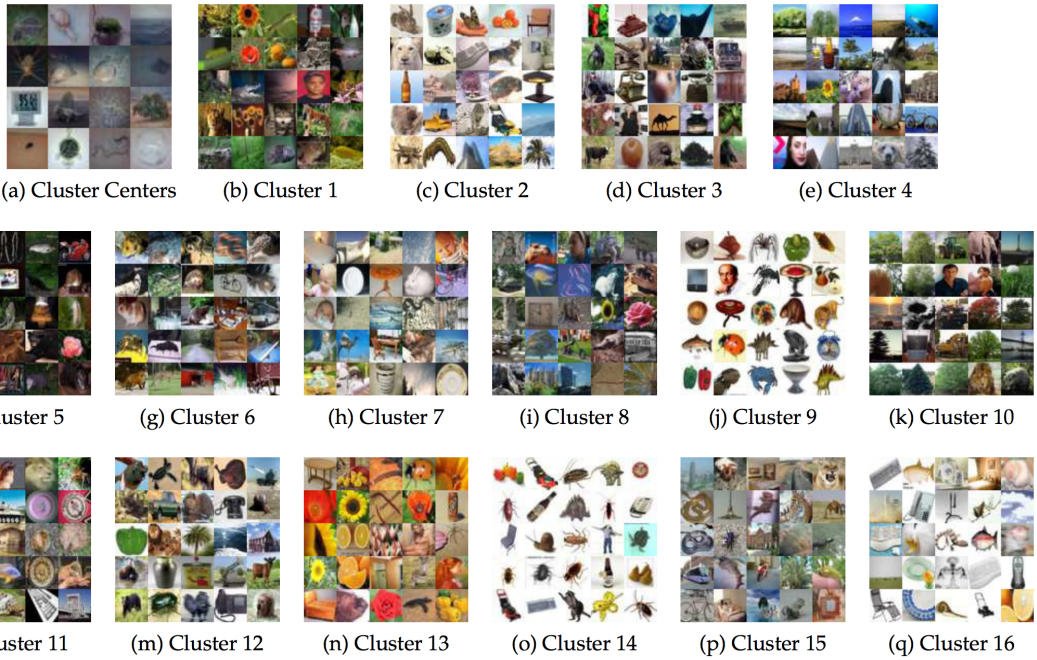
- Data $D = \{\mathbf{x}\}_{i=1}^{n}$. No target values.
- Typical goals: understand data, summarize data, identify concepts.

Application: Clustering Animals by Features

Data set of 50 animals, 85 binary features (e.g., longneck, water, smelly)



Application: Clustering Image Data

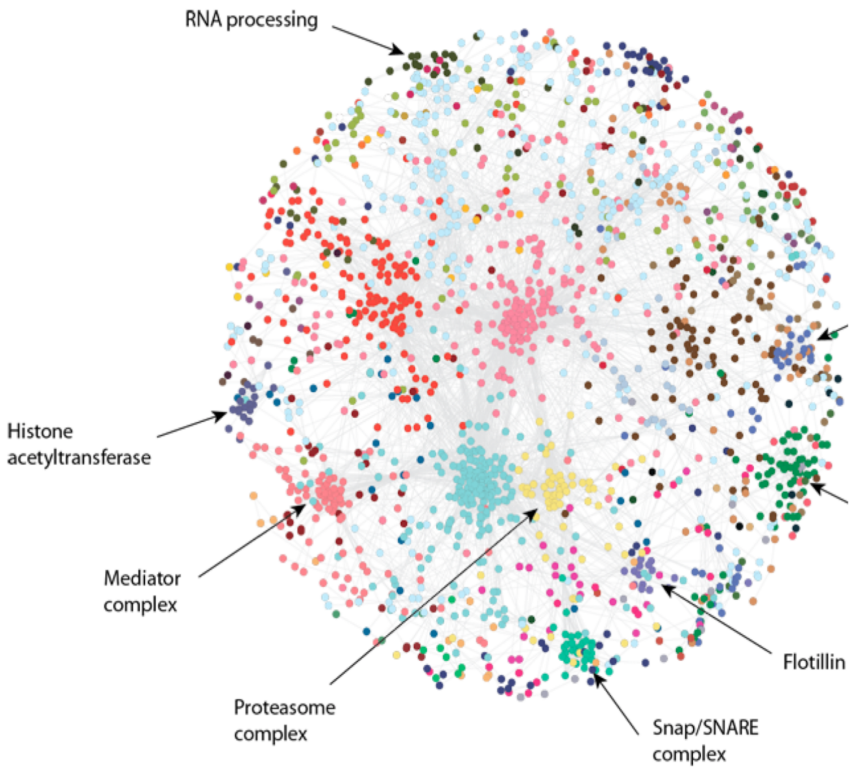


(a) Cluster Centers (b) Cluster 1 (c) Cluster 2 (d) Cluster 3 (e) Cluster 4

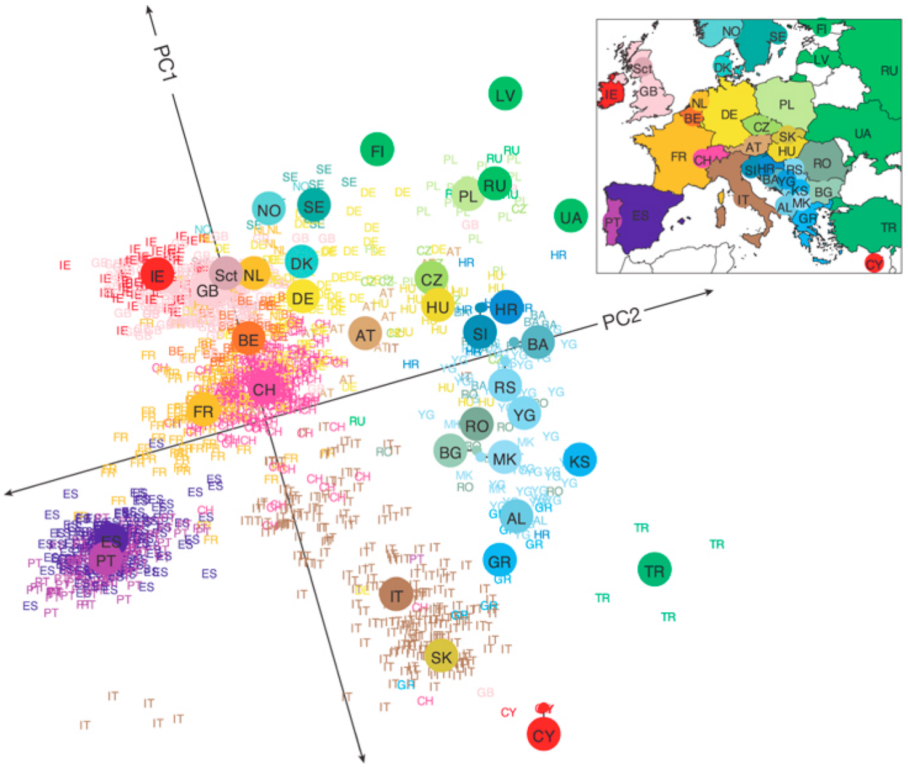
(f) Cluster 5 (g) Cluster 6 (h) Cluster 7 (i) Cluster 8 (j) Cluster 9 (k) Cluster 10

(l) Cluster 11 (m) Cluster 12 (n) Cluster 13 (o) Cluster 14 (p) Cluster 15 (q) Cluster 16

Clustering: Understanding Gene Regulation



Dimensionality Reduction: The European Gene Pool



Digital Humanities

Reconstructing Pompeian Households

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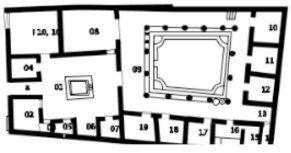
Abstract

A database of objects discovered in houses in the Roman city of Pompeii provides a unique view of ordinary life in an ancient city. Experts have used this collection to study the structure of Roman households, exploring the distribution and variability of tasks in architectural spaces, but such approaches are necessarily affected by modern cultural assumptions. In this study we present a data-driven approach to household archeology, treating it as an unsupervised labeling problem. This approach scales to large data sets and provides a more objective complement to human interpretation.

1 Introduction

Over the past century the goal of archeology has shifted from finding objects of artistic value to recon-

study. Only in the past few years has
jects, which are removed for conserva
upon excavation, been compiled and
by Allison [2]. This database, which
line,[1] contains more than 6000 artifact
in 30 architecturally similar "*atrium*
Pompeii. For each artifact, the dat
type from 240 typological categories
etc.) and a find location from 574 rooms. Allison has used data about artifacts in their original context to challenge many common assumptions about the function of particular types of object, the use of particular spaces, and the consistency of patterns of use across different houses.



	bronze casseruola
0.00036	door/chest/cupboard fitting
0.00035	glass bottle/flask/pyxis
0.00028	small glass bottle
0.00026	pottery jug
0.00024	bronze jug/jug fragment
0.00022	chest/cupboard fitting
0.00020	ceramic lamp
0.00018	jewelry
0.00016	pottery beaker/small vase
0.00015	coin
0.00013	pottery pot
	...
0.00010	table/table fittings/table base
0.00010	pottery jar/vase
0.00010	**bronze cooking pot/basin/pot/frag**

Conditional topic model (based on room features) on what topics (distributions over objects) will be found there.

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Clustering

- Simplest idea for discovering structure
- Find groups of similar examples:
  - For dimensionality reduction (project down to a few dimensions)
  - To understand the data
  - To preprocess a lot of unlabeled data, find concepts to use for supervised learning

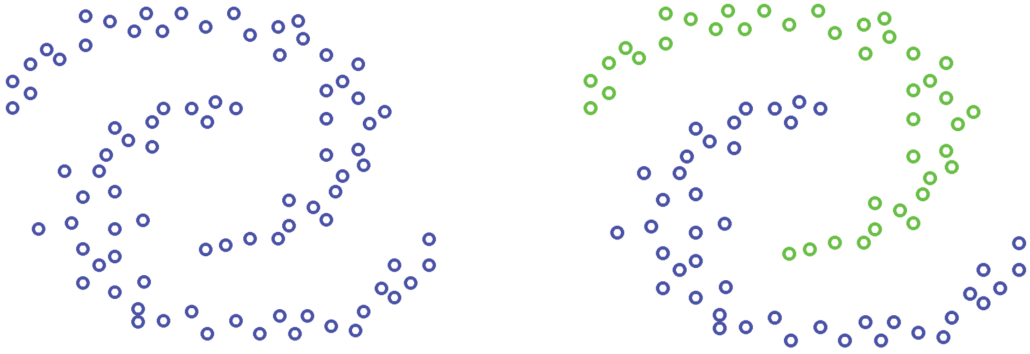
Today's lecture:

- K-means clustering
- Hierarchical Agglomerative Clustering (HAC)

Can also use *probabilistic methods*. But not this lecture!

Example 1: How Would You Cluster these Points?

Example 2: How Would You Cluster these Points?



The Clustering Problem

- Each example $\mathbf{x} \in \mathcal{X}$; often have $\mathbf{x} \in \mathbb{R}^m$. Data $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$
- Number of clusters K (may not be given)
- Typical output: assignment of each example to a cluster.
- $\mathbf{r}_i$ is the binary responsibility vector for example $\mathbf{x}_i$. A one-hot encoding ($r_{ik} = 1$ for assigned cluster, $r_{ik} = 0$ otherwise).

What is a good clustering?

- One where examples are "more similar" to other examples in their cluster than to examples in other clusters.
- But for what measure of similarity?
  - What is a measure of how close one example $\mathbf{x}$ is to another $\mathbf{x}'$?
  - What is a measure of how close one group of examples is to another?

For data in $\mathbb{R}^m$, a typical approach is ℓ_2 metric:

$$d(\mathbf{x}, \mathbf{x}') = ||\mathbf{x} - \mathbf{x}'|| = \sqrt{\sum_j (x_j - x'_j)^2}$$

Can also use specialized metrics; e.g., *edit distance* for strings or DNA sequences; the *Hamming distance* for bit vectors.

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The K-Means Objective

Defined for data in $\mathbb{R}^m$.

- Associate each cluster with a prototype $\boldsymbol{\mu}_k \in \mathbb{R}^m$, for $k \in \{1, \ldots, K\}$
- Make an assignment $\mathbf{r}_i$ of each example $\mathbf{x}_i$ to a cluster
- Objective: find prototypes and an assignment to minimize

$$\mathcal{L}(\mathbf{r}, \boldsymbol{\mu}) = \sum_{i=1}^{n} \sum_{k=1}^{K} r_{ik} ||\mathbf{x}_i - \boldsymbol{\mu}_k||,$$

where $||\mathbf{z}|| = \sqrt{\mathbf{z}^\top \mathbf{z}}$.

This is highly non-convex, with lots of local minima. (Also NP-hard).

K-Means Clustering Algorithm (Lloyd's algorithm)

1. Initialize prototypes $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ at random
2. Repeat until converged:
   - Step 1: Assign each example to the closest prototype (breaking ties in favor of current assignment)

$$\mathbf{r}_i := \arg \min_{k \in \{1,\ldots,K\}} ||\mathbf{x}_i - \boldsymbol{\mu}_k||$$

   - Step 2: For each k, set $\boldsymbol{\mu}_k$ to the centroid of assigned examples

$$\boldsymbol{\mu}_k := \frac{1}{n_k} \sum_{i=1}^{n} r_{ik} \mathbf{x}_i,$$

     where $n_k = \sum_i r_{ik}$.

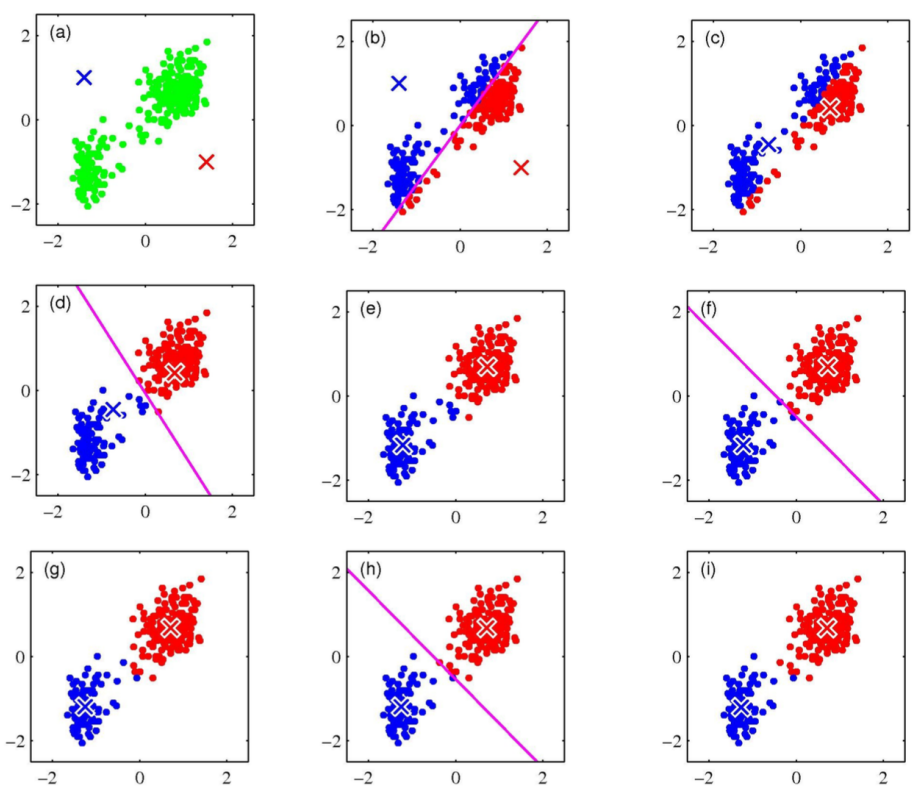
Typical to run this multiple times, with different initial conditions. (Can also first run on subset of the data.)

Example: Clustering Eruptions of the Old Faithful Geyser

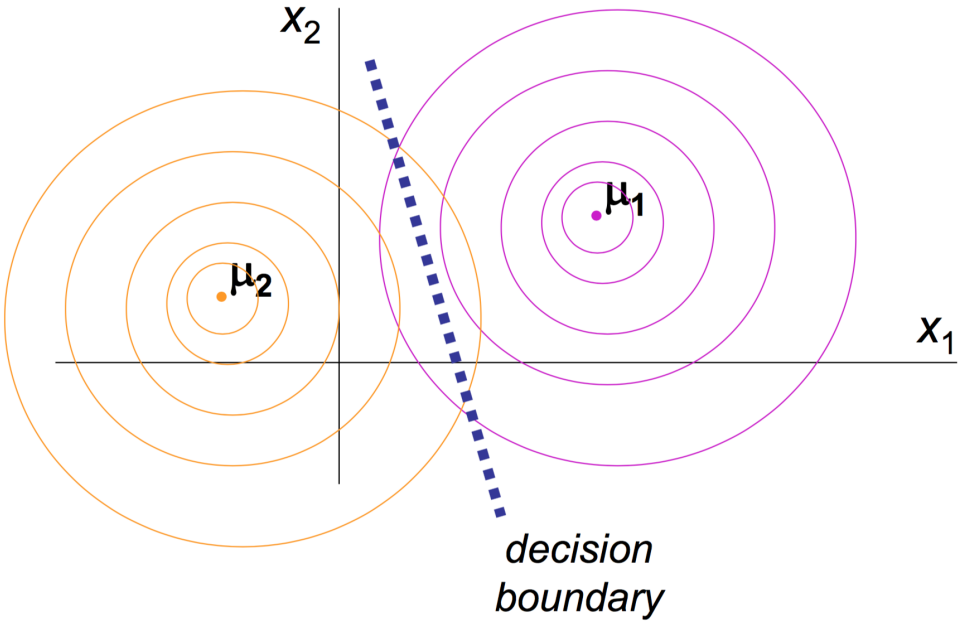
- Yellowstone National Park, Wyoming
- 272 data points
  - duration of eruption (y-axis)
  - duration to next eruption (x)
  - standardized

Typical to 'standardize' data for K-means. Pre-process:
$x'_{ij} = (x_{ij} - \mu_j)/\sigma_j$ where μ_j is mean of attribute j, σ_j is standard deviation of attribute j.

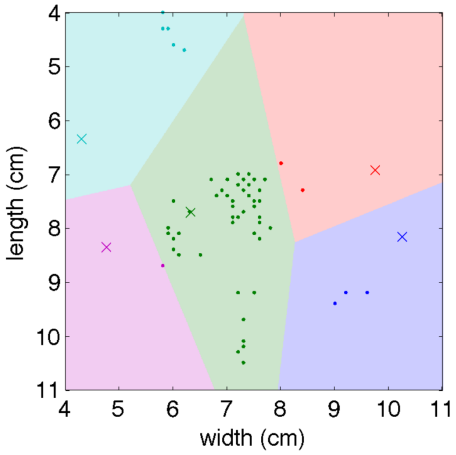
Example: K-Means on Old Faithful Eruptions (Bishop)



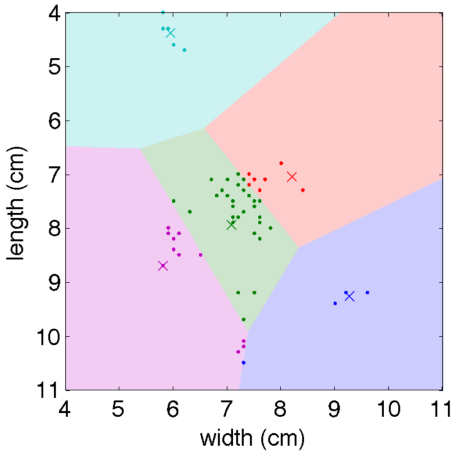
Note: Linear Decision Boundaries



Example: K-means on Oranges and Lemons (1 of 4)



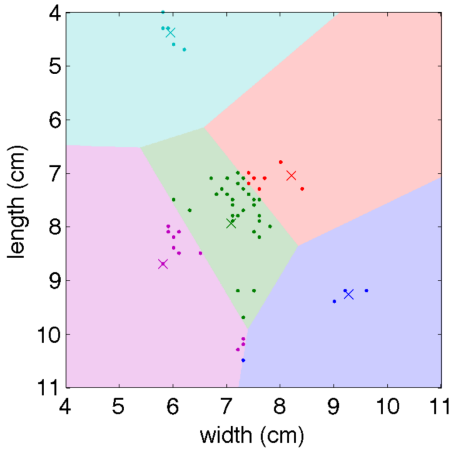
(a) Initialization



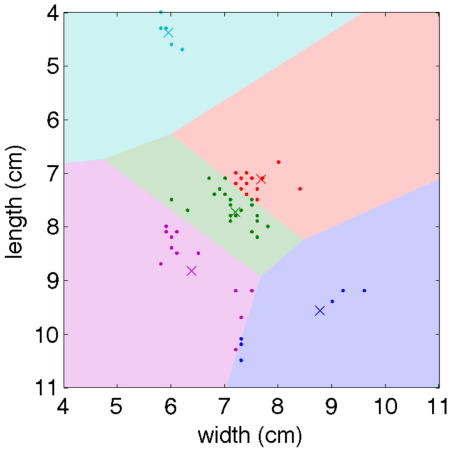
(b) Iteration 1

(R.Adams; $K = 5$, Iain Murray data)

Example: K-means on Oranges and Lemons (2 of 4)



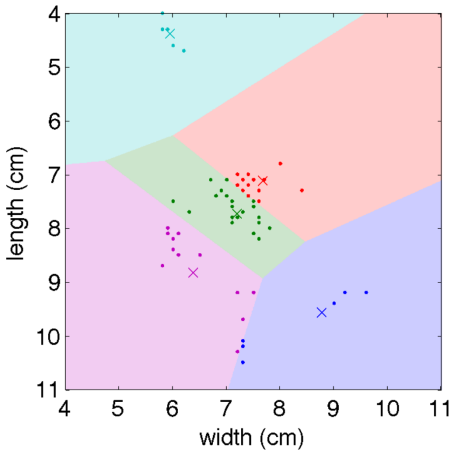
(b) Iteration 1



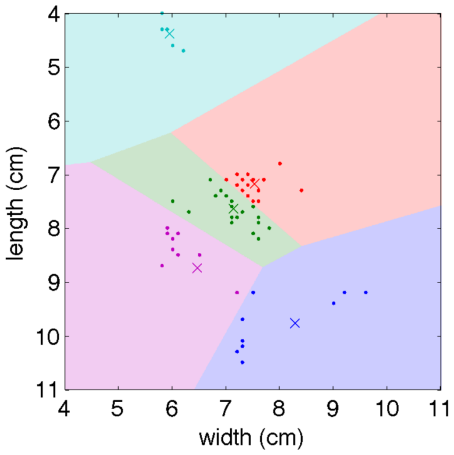
(c) Iteration 2

(R.Adams; $K = 5$, Iain Murray data)

Example: K-means on Oranges and Lemons (3 of 4)



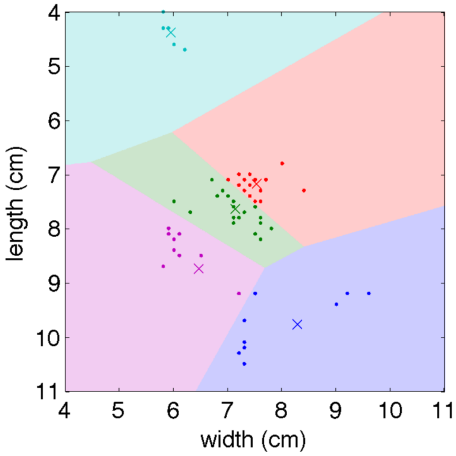
(c) Iteration 2



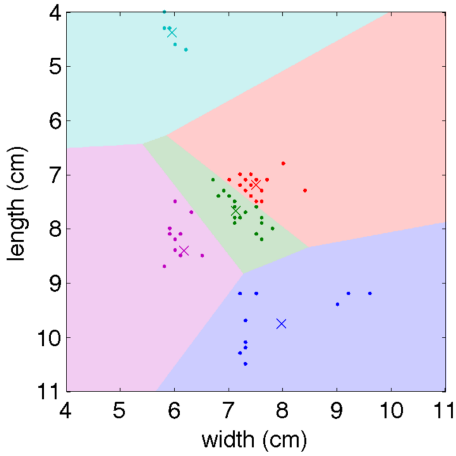
(d) Iteration 3

(R.Adams; $K = 5$, Iain Murray data)

Example: K-means on Oranges and Lemons (4 of 4)



(d) Iteration 3



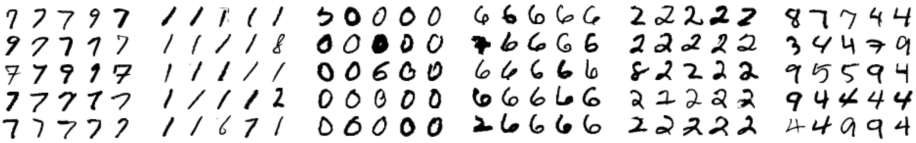
(e) Iteration 4

(R.Adams; $K = 5$, Iain Murray data)

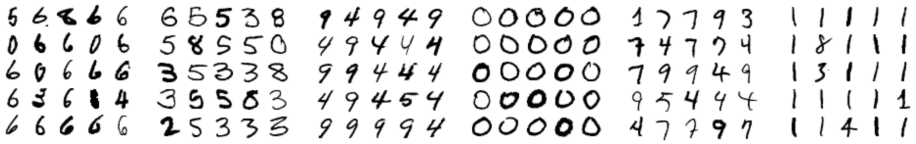
Example: K-means Clustering on Handwritten Digits

MNIST: 60,000 digits. 28 x 28 grayscale (0-255). Use Lloyd's algorithm, initialized via *k-means++* (a standard way to initialize.)

(a) Cluster Centers (b) Cluster 1 (c) Cluster 2 (d) Cluster 3 (e) Cluster 4



(f) Cluster 5 (g) Cluster 6 (h) Cluster 7 (i) Cluster 8 (j) Cluster 9 (k) Cluster 10

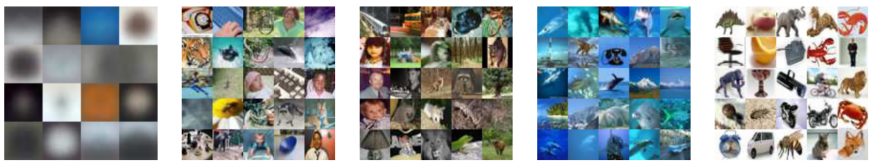


(l) Cluster 11 (m) Cluster 12 (n) Cluster 13 (o) Cluster 14 (p) Cluster 15 (q) Cluster 16

(R.Adams; $K = 16$. Clusters pick up on similar stroke patterns)

Example: K-means Clustering on Image Data

CIFAR-100 color. 50,000 images. 32 x 32 x 3 (RGB), each 0-255.



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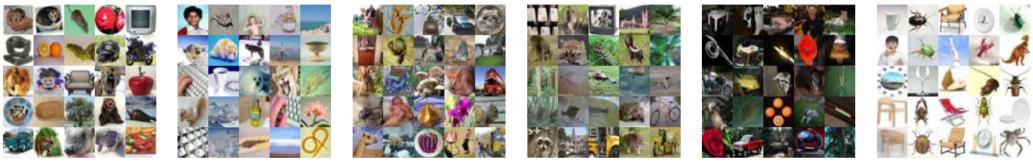

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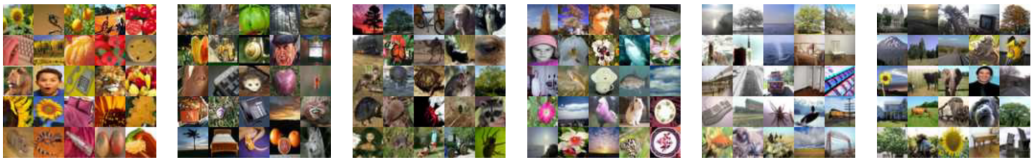

(l) Cluster 11 (m) Cluster 12 (n) Cluster 13 (o) Cluster 14 (p) Cluster 15 (q) Cluster 16

(R.Adams; $K = 16$. Clusters pick up on low-freq color variations)

Example: K-Means Clustering on Documents

30,991 articles from Grolier's Encyclopedia. Articles are represented via a count vector of most common words ($m = 15276$).

Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6
education	south	war	war	art	light
united	population	german	government	century	energy
american	north	british	law	architecture	atoms
public	major	united	political	style	theory
world	west	president	power	painting	stars
social	mi	power	united	period	chemical
government	km	government	party	sculpture	elements
century	sq	army	world	form	electrons
schools	deg	germany	century	artists	hydrogen
countries	river	congress	military	forms	carbon

Cluster 7	Cluster 8	Cluster 9	Cluster 10	Cluster 11	Cluster 12
energy	god	century	city	population	cells
system	world	world	american	major	body
radio	century	water	century	km	blood
space	religion	called	world	mi	species
power	jesus	time	war	government	cell
systems	religious	system	john	deg	called
television	steel	form	life	sq	plants
water	philosophy	united	united	north	animals
solar	science	example	family	south	system
signal	history	life	called	country	human

(R.Adams; $K = 12$, initialized with K-means++.)

Understanding Lloyd's Algorithm

Loss function:

$$\mathcal{L}(\{\mathbf{r}\}, \{\boldsymbol{\mu}\}) = \sum_{i=1}^{n} \sum_{k=1}^{K} r_{ik} ||\mathbf{x}_i - \boldsymbol{\mu}_k||$$

Solve this via coordinate descent. Alternate $\{\mathbf{r}_i\}$ and $\{\boldsymbol{\mu}_k\}$ updates.

- Step 1: $\{\mathbf{r}\}$ update. Fixing $\{\boldsymbol{\mu}\}$, minimize loss by assigning each example to the cluster that is closest.
- Step 2: $\{\boldsymbol{\mu}\}$ update. Fixing $\{\mathbf{r}\}$, work with squared distance, $\mathcal{L}(\boldsymbol{\mu}_k) = \sum_{i=1}^{n} r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top (\mathbf{x}_i - \boldsymbol{\mu}_k)$. We have:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_k} = -2 \sum_{i=1}^{n} r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k) = 0$$

$$\Leftrightarrow \quad \sum_{i=1}^{n} r_{ik} \mathbf{x}_i = \boldsymbol{\mu}_k \sum_{i=1}^{n} r_{ik} \qquad \Leftrightarrow \qquad \boldsymbol{\mu}_k = \frac{\sum_{i=1}^{n} r_{ik} \mathbf{x}_i}{\sum_{i=1}^{n} r_{ik}}$$

K-Means Clustering

- Simple, popular method.
- Parametric (effective number of parameters is mK, to define the cluster centroids).
- Not useful if linear decision boundaries fails.

Computational complexity:

- Assignment step is $O(nKm)$, since for each example need to compare to each center.
- Centroid update is $O(nm)$, since need to take average of different partitions of the data.
- $O(nKmT)$ time over T iterations (generally $T \ll n$)

A Simple Variant: The K-Medoids Algorithm

Rather than centroids, use actual examples as prototypes for each cluster.

1. Initialize prototypes $\mathbf{z}_1, \ldots, \mathbf{z}_K$ to random examples.
2. Repeat until converged:
   - Step 1: Assign each example to the closest prototype.
   - Step 2: For each k, set $\mathbf{z}_k$ to the example assigned to cluster k that minimizes the total distance to the examples assigned to cluster k.

Example: K-Medoids Clustering on Image data

CIFAR-100 data.

(a) Cluster Centers (b) Cluster 1 (c) Cluster 2 (d) Cluster 3 (e) Cluster 4

(f) Cluster 5 (g) Cluster 6 (h) Cluster 7 (i) Cluster 8 (j) Cluster 9 (k) Cluster 10

(l) Cluster 11 (m) Cluster 12 (n) Cluster 13 (o) Cluster 14 (p) Cluster 15 (q) Cluster 16

(R.Adams, $K = 16$)

Clustering: Additional Considerations

Setting K, the number of clusters:

- Smaller: may provide better interpretation
- Larger: useful if clustering is being used for feature extraction

No principled way to do this. A heuristic approach is to plot loss against K, and look for a "knee" in the plot.

Can be useful to add class labels: after clustering, it is common to want to associate a cluster with a name; e.g., by testing some examples and associating the cluster with the majority concept.

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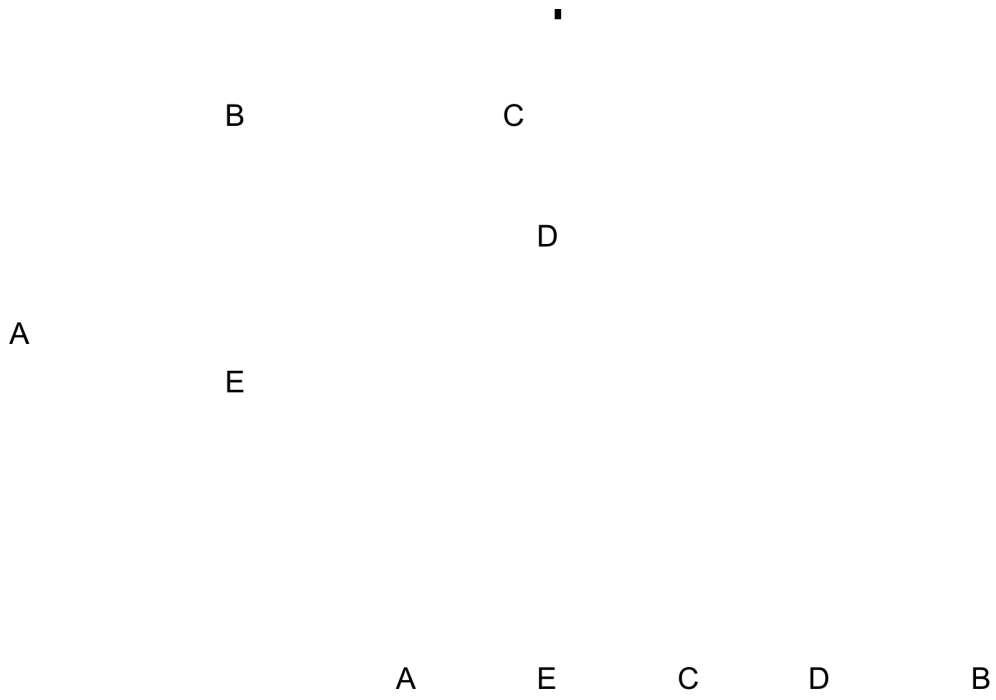
Hierarchical Agglomerative Clustering (HAC)

HAC will work by maintaining an 'active set' of clusters, and repeatedly merging clusters (forming a tree as it goes.)

Compared with K-Means:

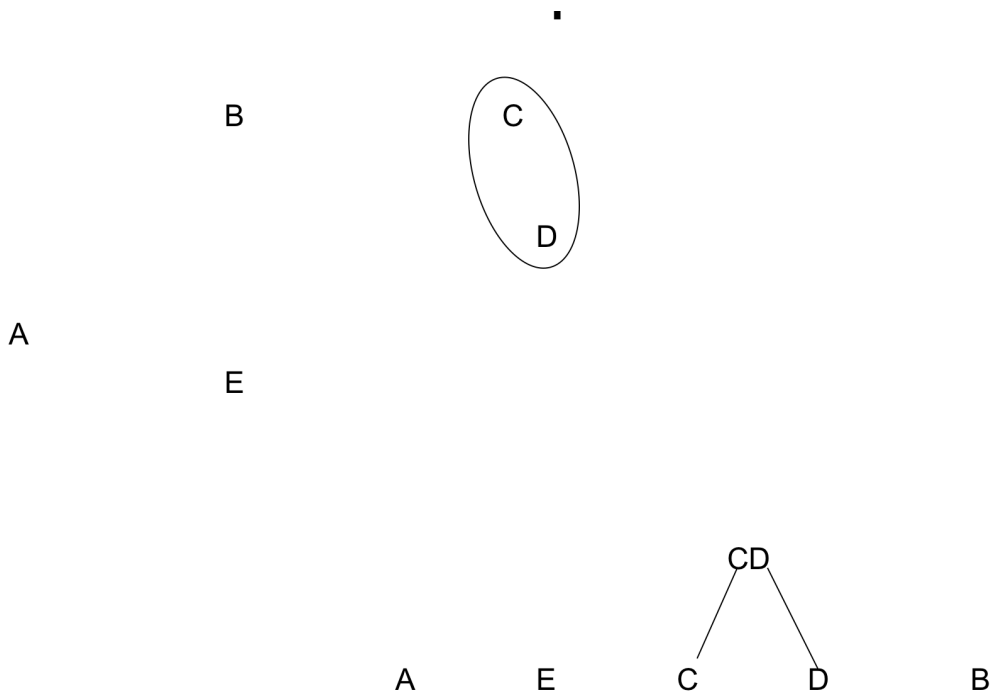
- Non parametric (instance based). Because of this, more flexible than K-means. Can generate arbitrary cluster shapes (can also over-fit!).
- Rather than a flat partition of data, it generates a hierarchy of clusters.
- No need to specify the number of clusters up front.
- Not randomized (this can be a problem with K-means.)

HAC Example (1 of 5)

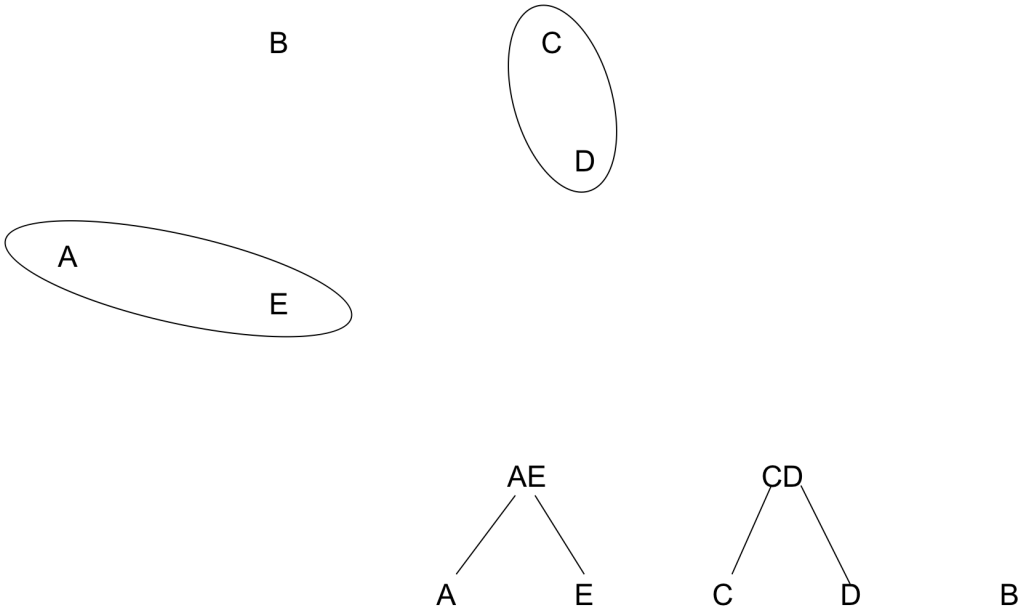


A E C D B

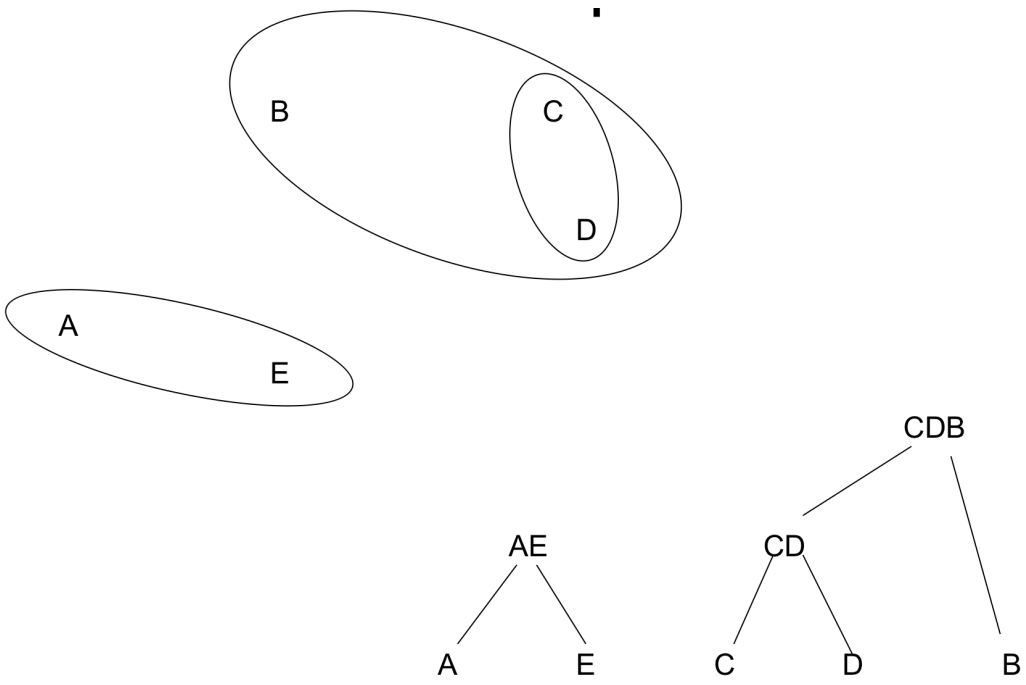
HAC Example (2 of 5)



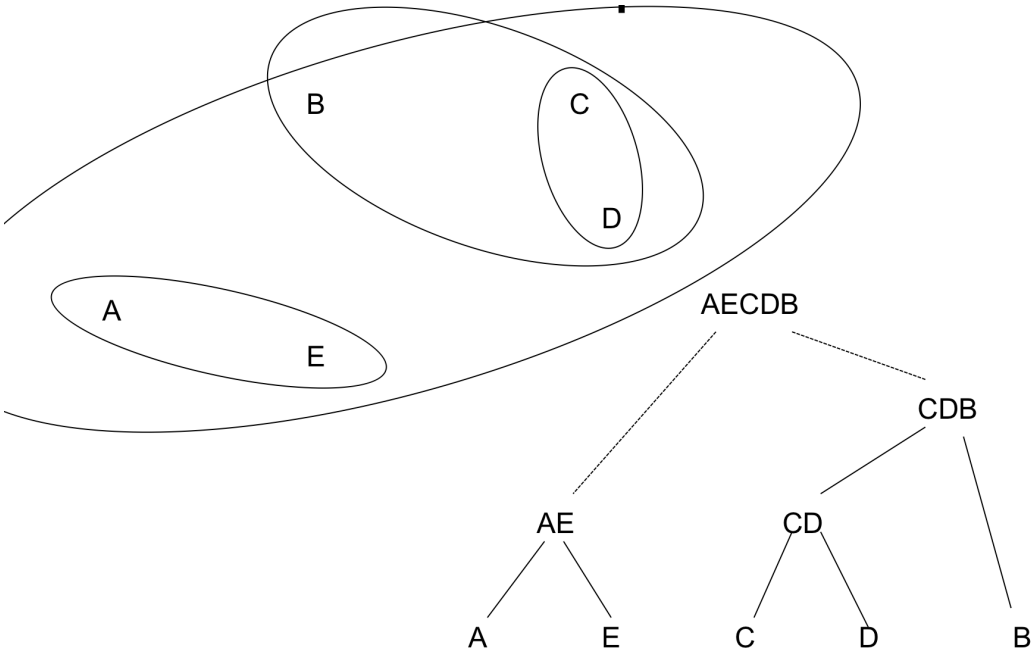
HAC Example (3 of 5)



HAC Example (4 of 5)



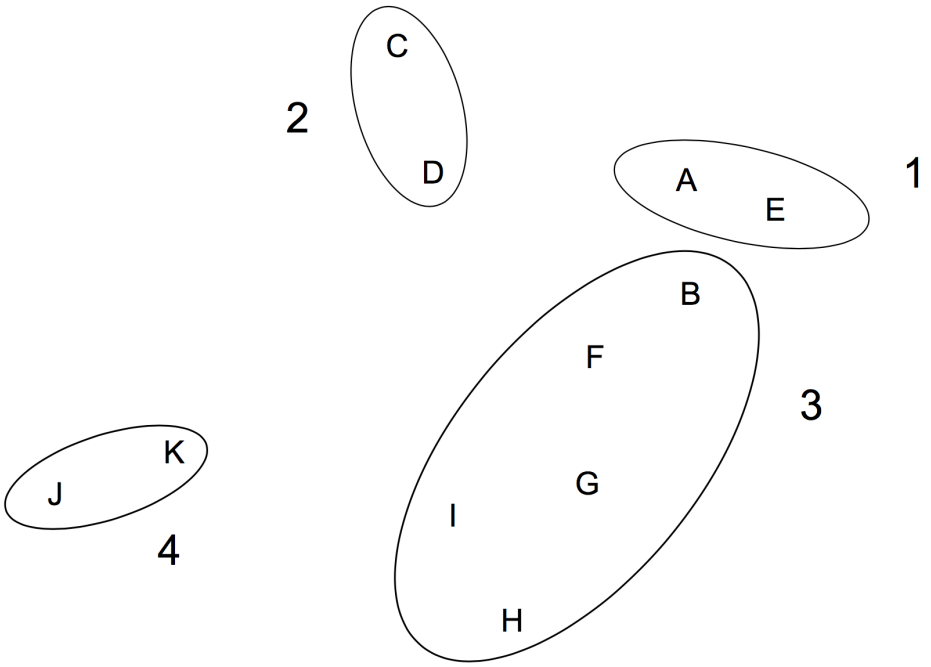
HAC Example (5 of 5)



HAC Algorithm

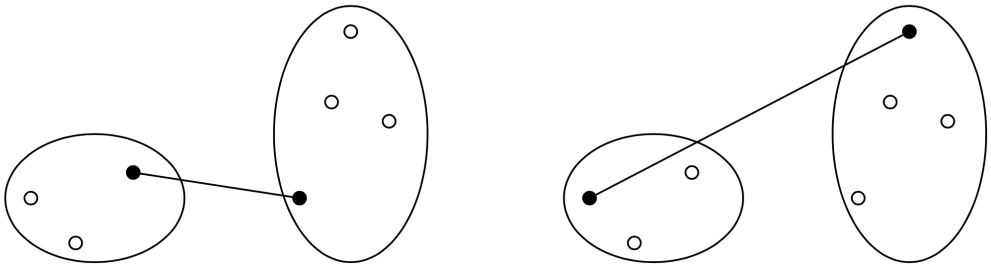
1. Start with each example in its own cluster.
2. Repeat until a single cluster:
   - Find the two "closest" clusters, and merge them.

What is closest to cluster {AE}?



Max? Min? Average? Centroid?

HAC: Min and Max Group Distances

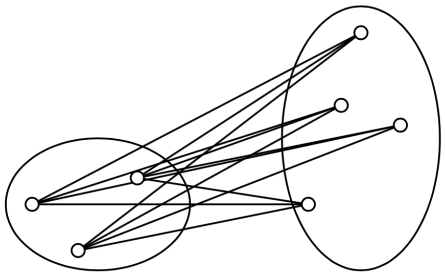


(a) min distance (b) max distance

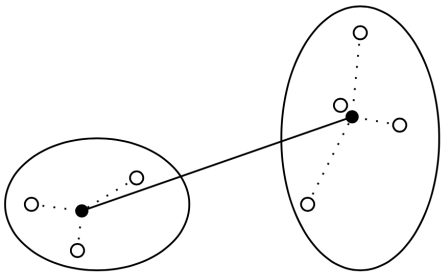
$$d_{\text{min}}(G, G') = \min_{\mathbf{x} \in G, \mathbf{x}' \in G'} ||\mathbf{x} - \mathbf{x}'||$$

$$d_{\text{max}}(G, G') = \max_{\mathbf{x} \in G, \mathbf{x}' \in G'} ||\mathbf{x} - \mathbf{x}'||$$

HAC: Average and Centroid Group Distances



(c) average distance

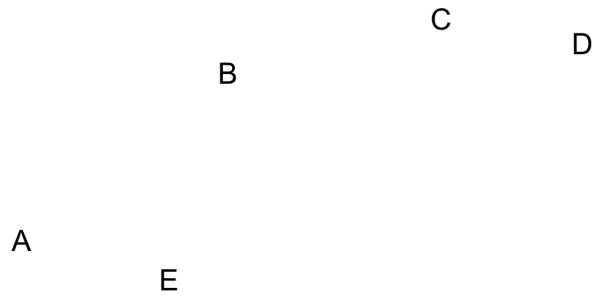


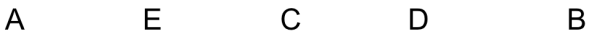
(d) centroid distance

$$d_{\text{avg}}(G, G') = \frac{1}{|G||G'|} \sum_{\mathbf{x} \in G, \mathbf{x}' \in G'} ||\mathbf{x} - \mathbf{x}'||$$

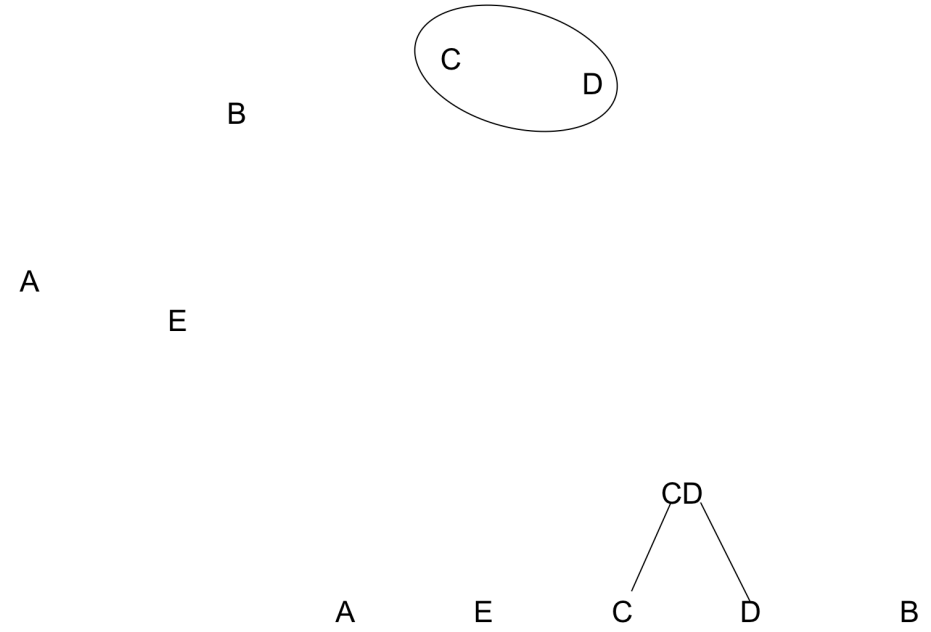
$$d_{\text{centroid}}(G, G') = ||\boldsymbol{\mu}_G - \boldsymbol{\mu}'_G||$$

Example: HAC with Min Distance (1 of 6)

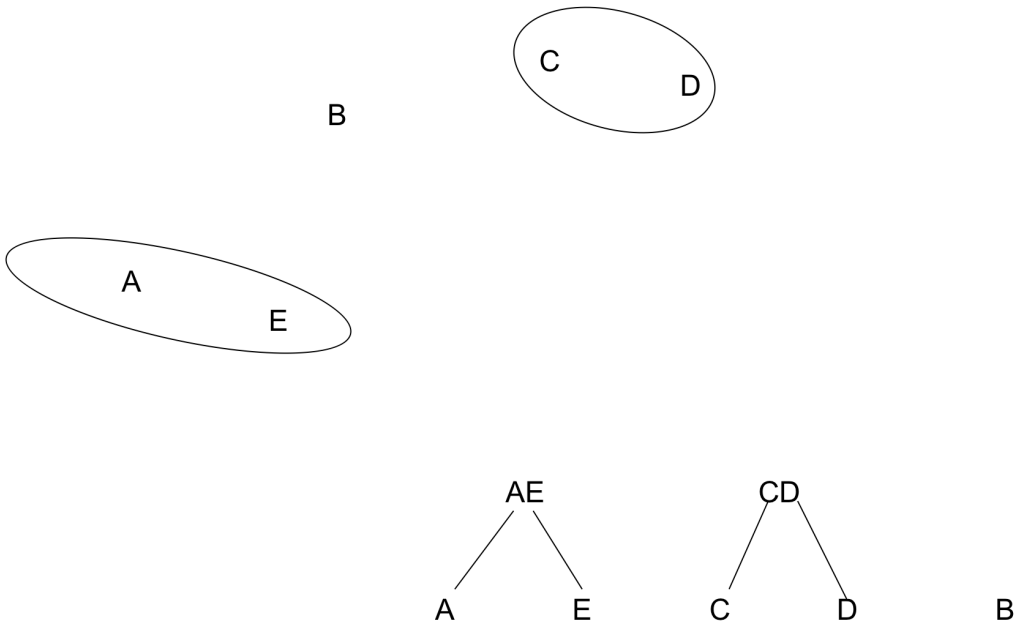




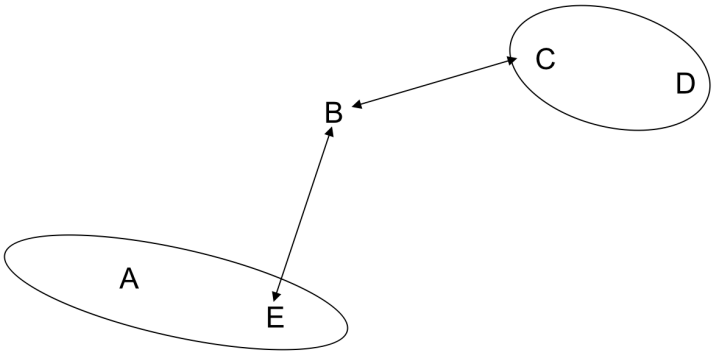
Example: HAC with Min Distance (2 of 6)

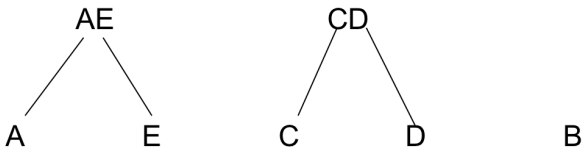


Example: HAC with Min Distance (3 of 6)

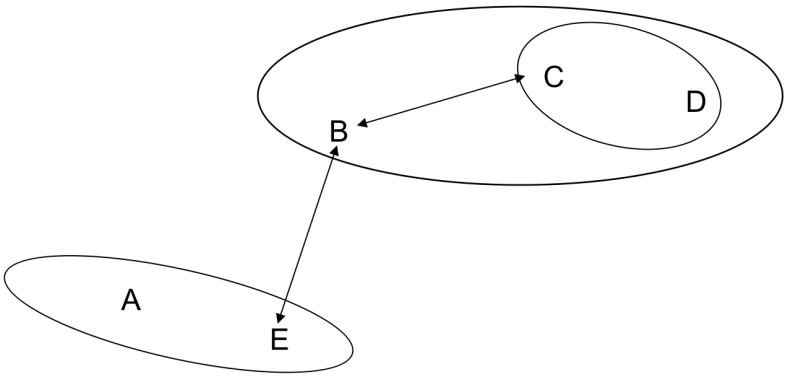


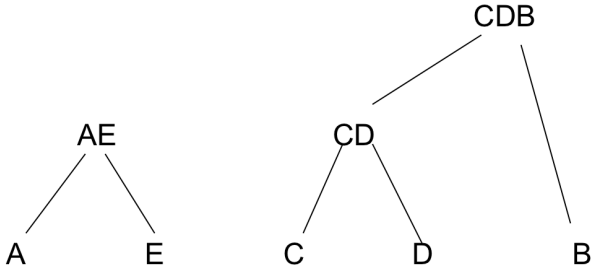
Example: HAC with Min Distance (4 of 6)



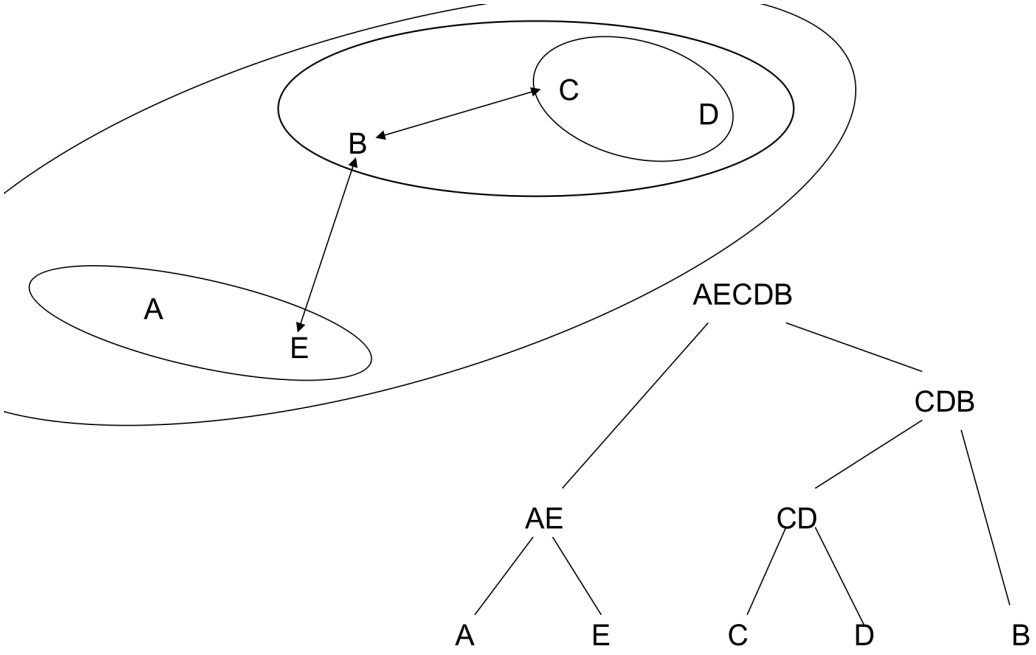


Example: HAC with Min Distance (5 of 6)

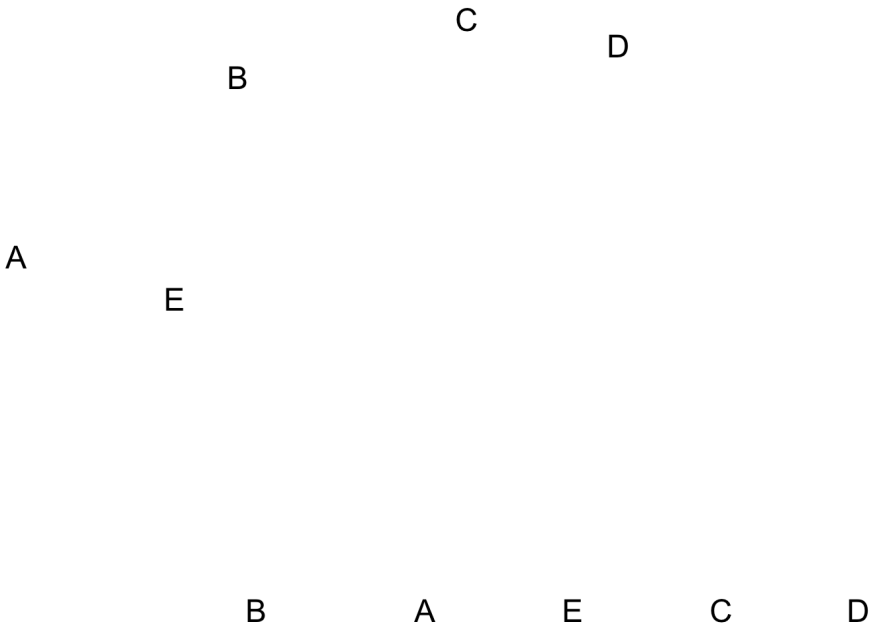




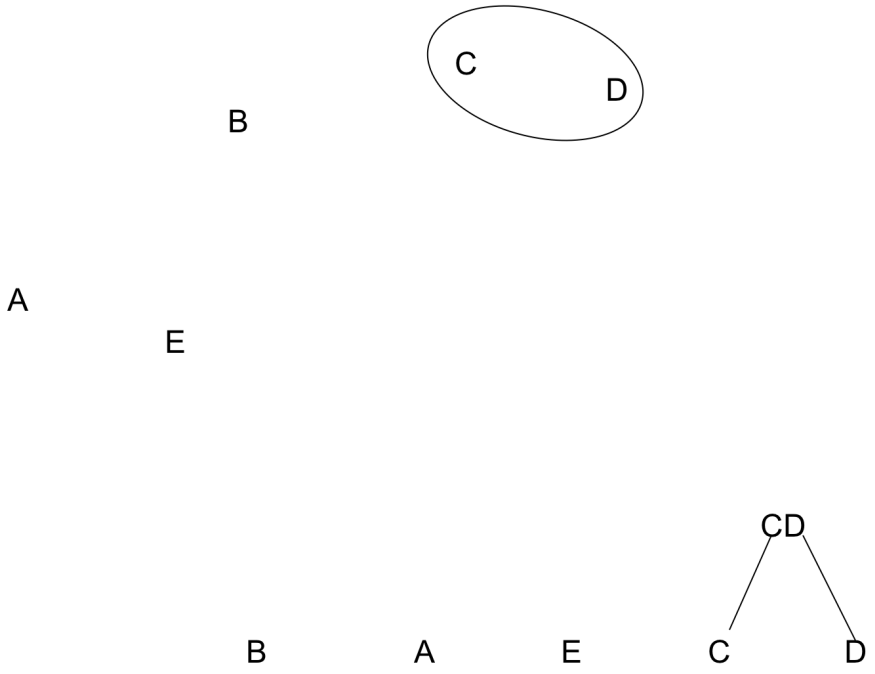
Example: HAC with Min Distance (6 of 6)



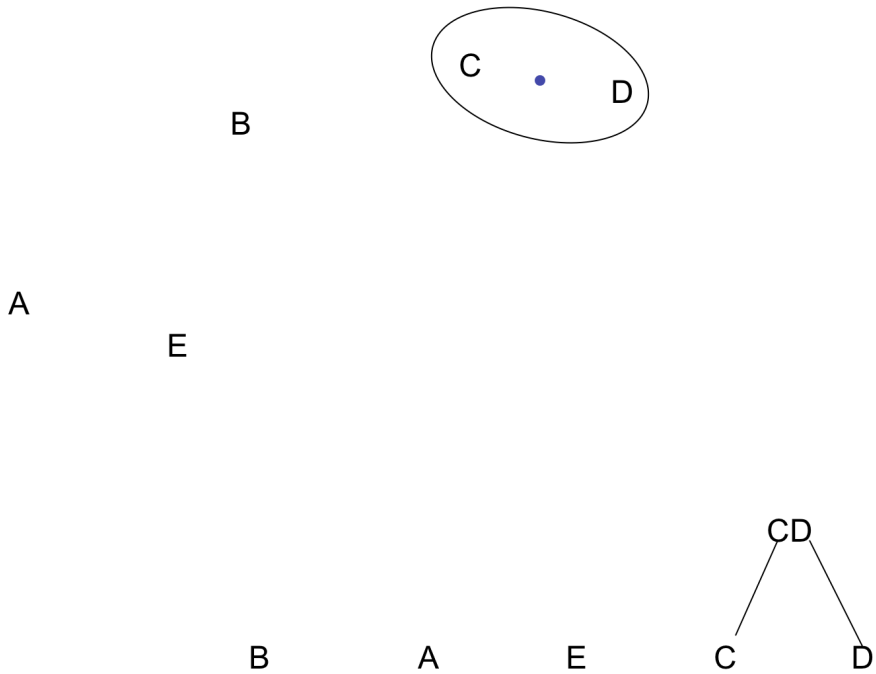
Example: HAC with Centroid Distance (1 of 7)



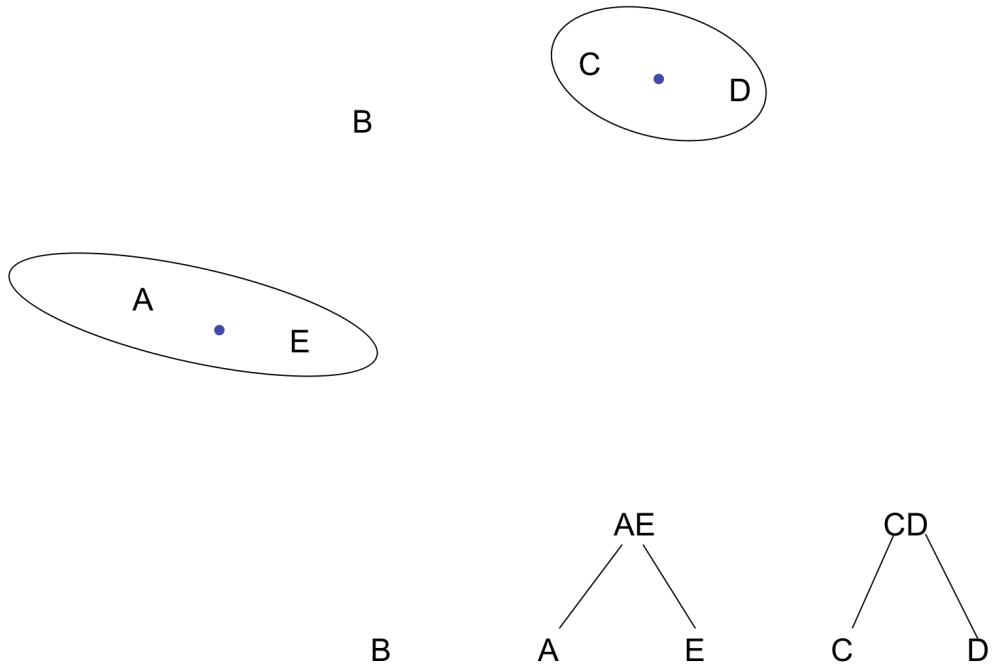
Example: HAC with Centroid Distance (2 of 7)



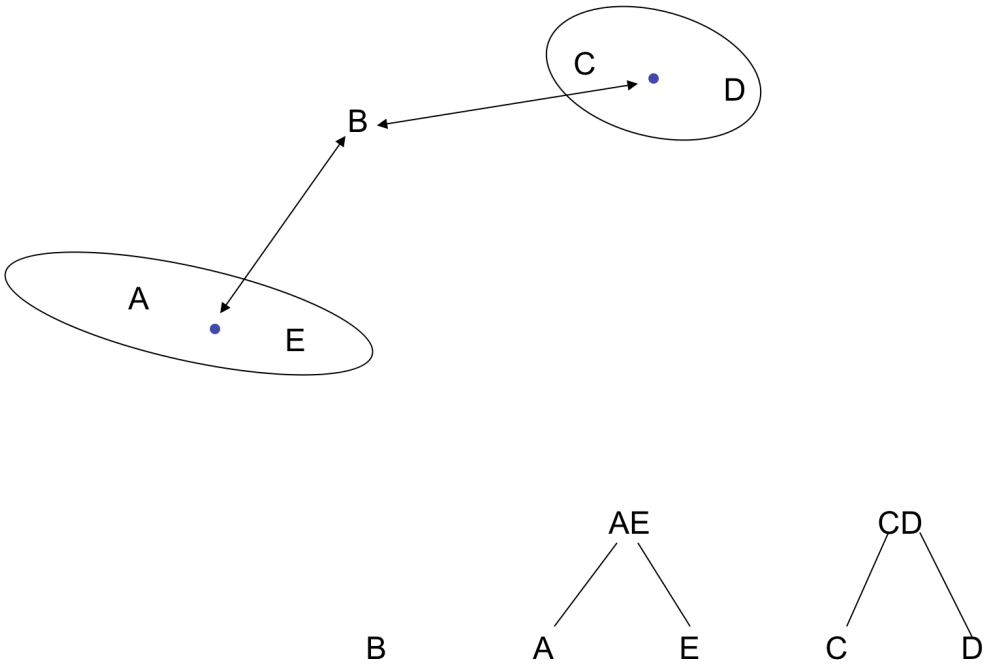
Example: HAC with Centroid Distance (3 of 7)



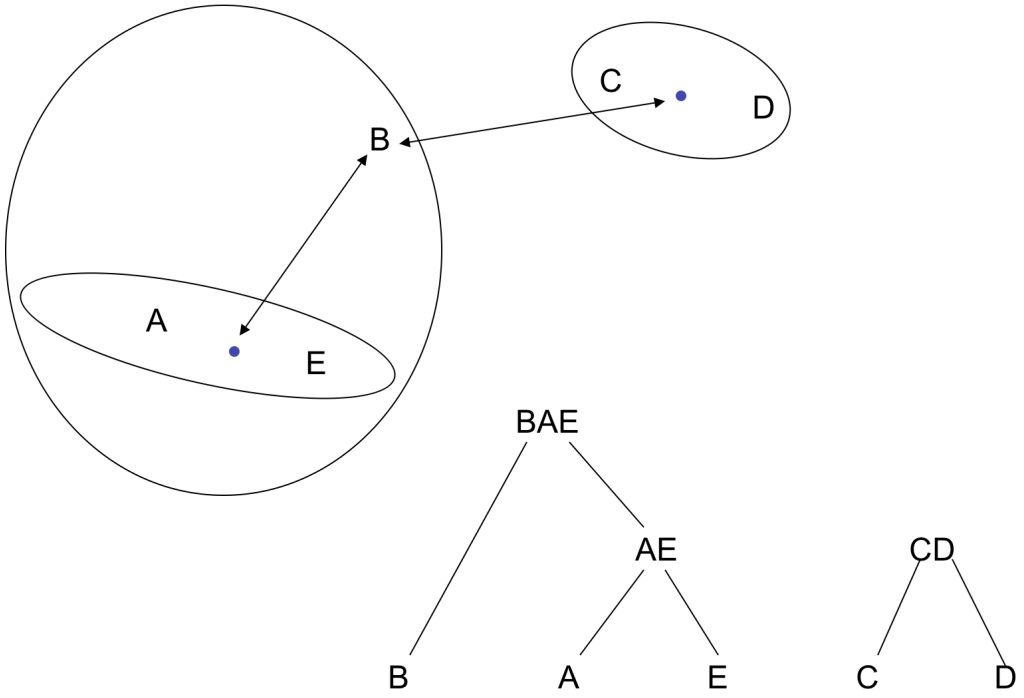
Example: HAC with Centroid Distance (4 of 7)



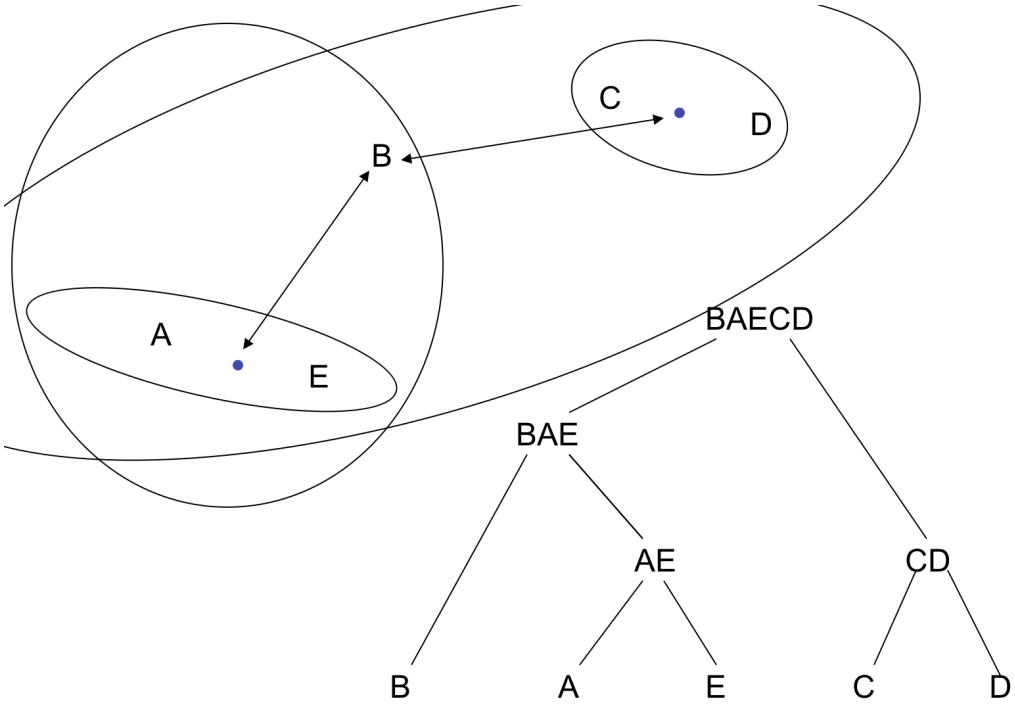
Example: HAC with Centroid Distance (5 of 7)



Example: HAC with Centroid Distance (6 of 7)



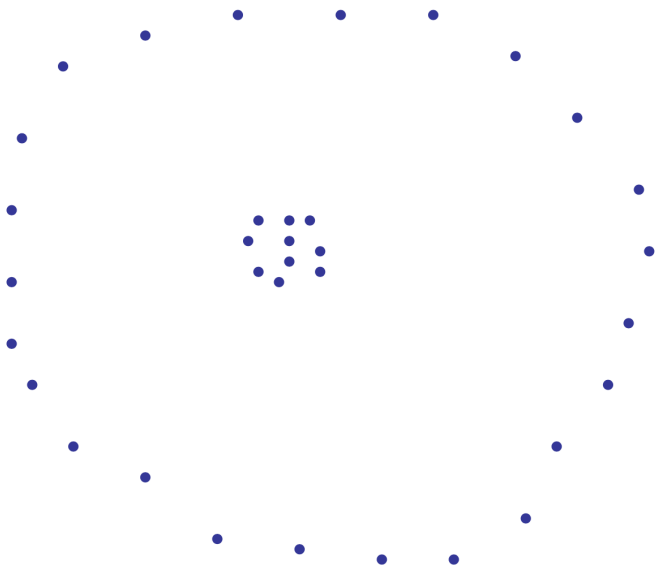
Example: HAC with Centroid Distance (7 of 7)



Comparing HAC Group Distance Criteria

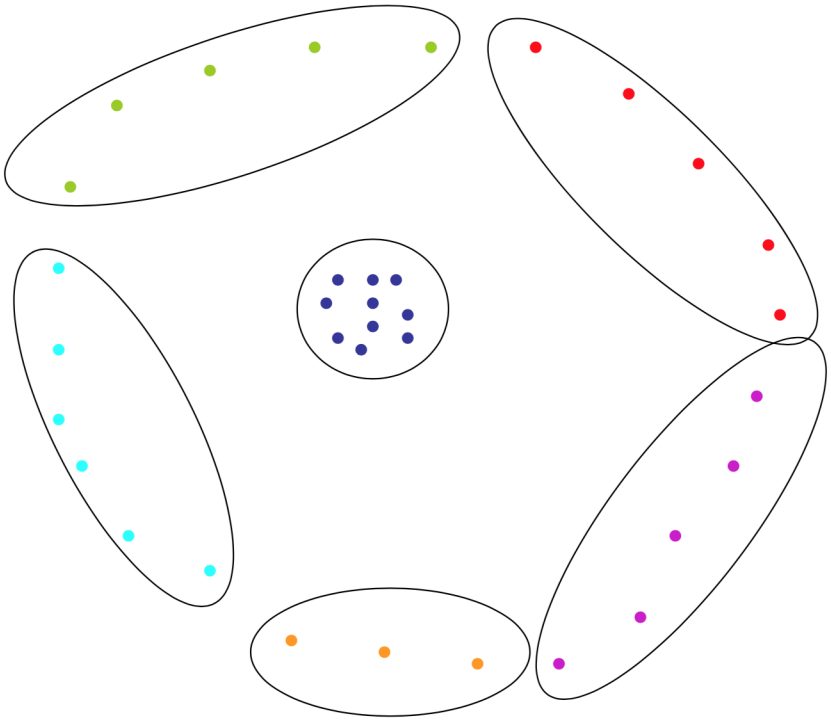
- Which distance will tend to merge large clusters with each other?
  A: min, because larger clusters are more likely to have a pair of examples that are close
- Which distance will tend to have a "chaining effect" and lead to long, stringy clusters?
  A: min, since only one distance has to be small.
- Which distance will tend to prefer compact clusters?
  A: max, since all distances have to be small to merge.
- The average and centroid distances are compromises, allowing some elongation but also preferring some compactness.

Simple HAC Example

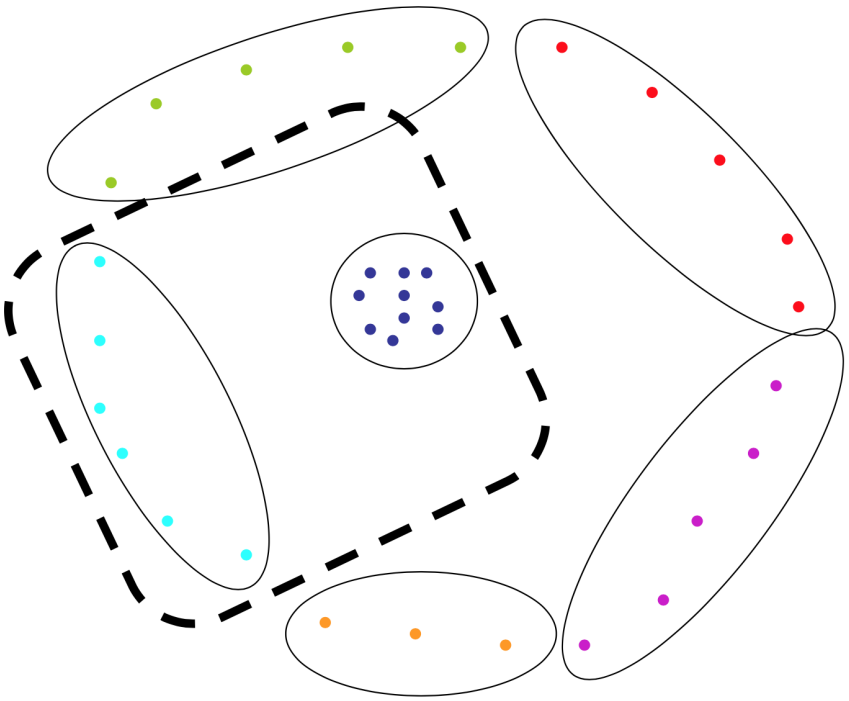


Which HAC distance will find the clusters? [A: min] What will max do?

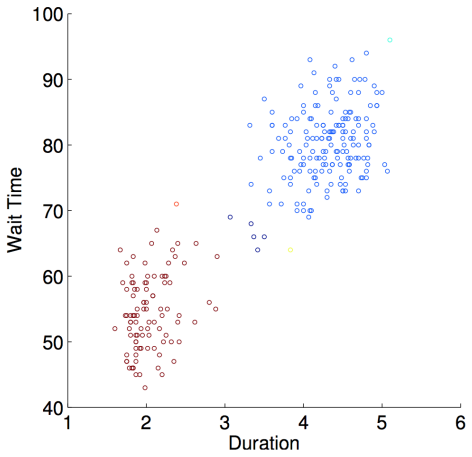
Simple HAC Example– Max (1 of 2)



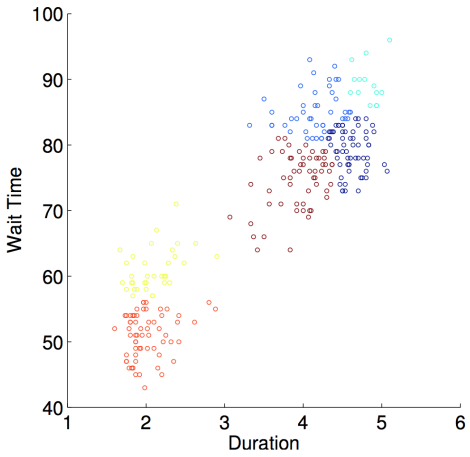
Simple HAC Example– Max (2 of 2)



Example: HAC on Old Faithful Eruptions (1 of 2)

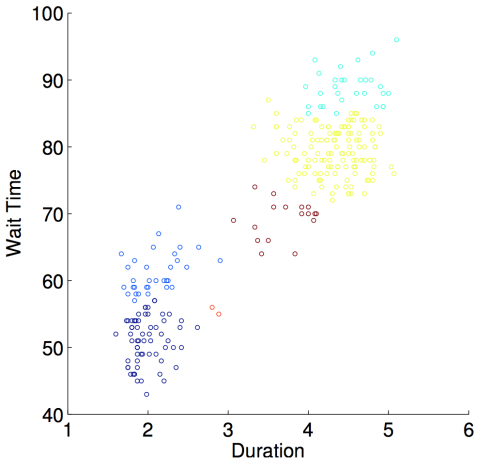


(a) min distance

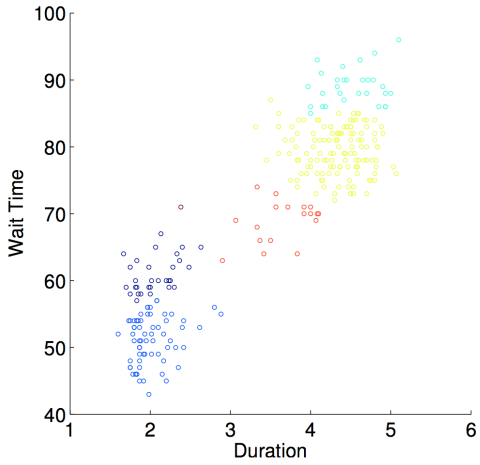


(b) max distance

Example: HAC on Old Faithful Eruptions (2 of 2)

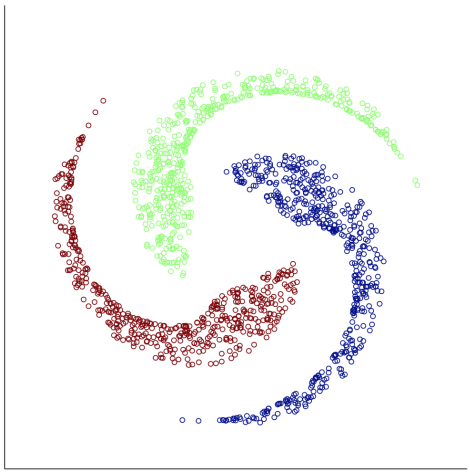


(c) average distance

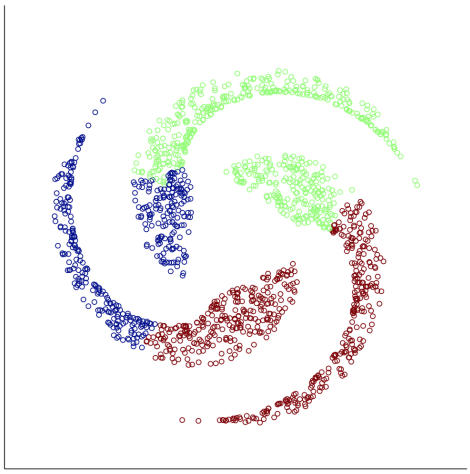


(d) centroid distance

Example: HAC Clustering on Pinwheel example (1 of 2)

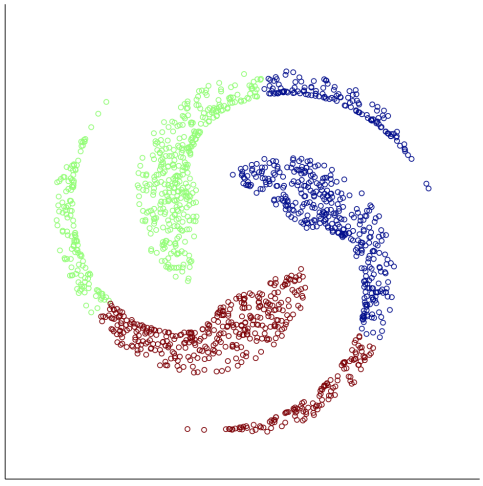


(a) min distance

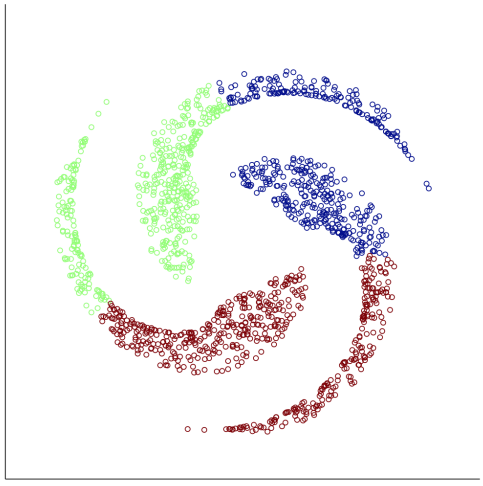


(b) max distance

Example: HAC Clustering on Pinwheel example (2 of 2)



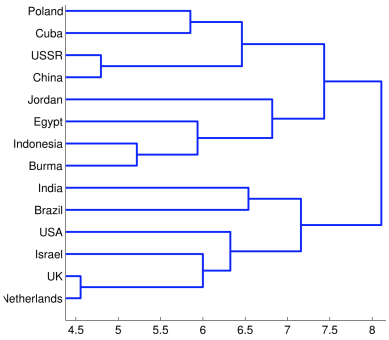
(c) average distance



(d) centroid distance

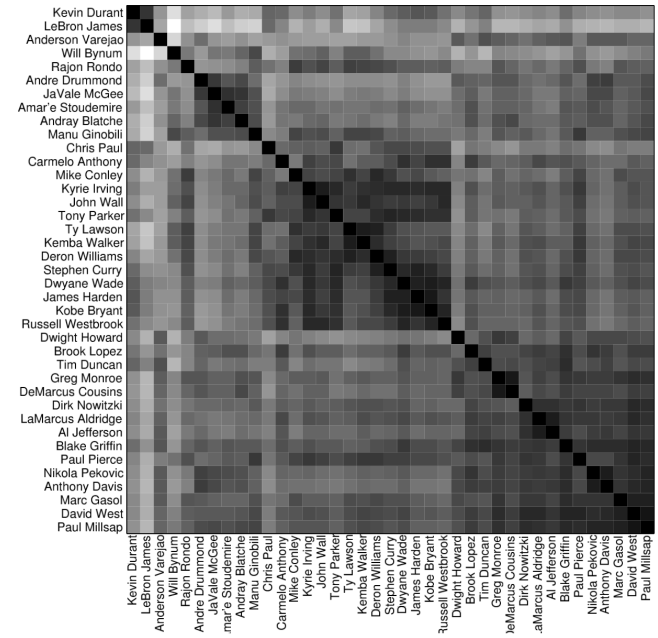
HAC: The Dendrogram Representation

- Shows examples along one axis (y-axis), distances along the other
- Shows the groups that have been joined together
- Indicate by the x-distance the distance between the two groups being merged
- A valid dendrogram requires these distances are monotonically increasing (guaranteed for all methods except centroid)



Application of HAC: Basketball Players (1 of 2)

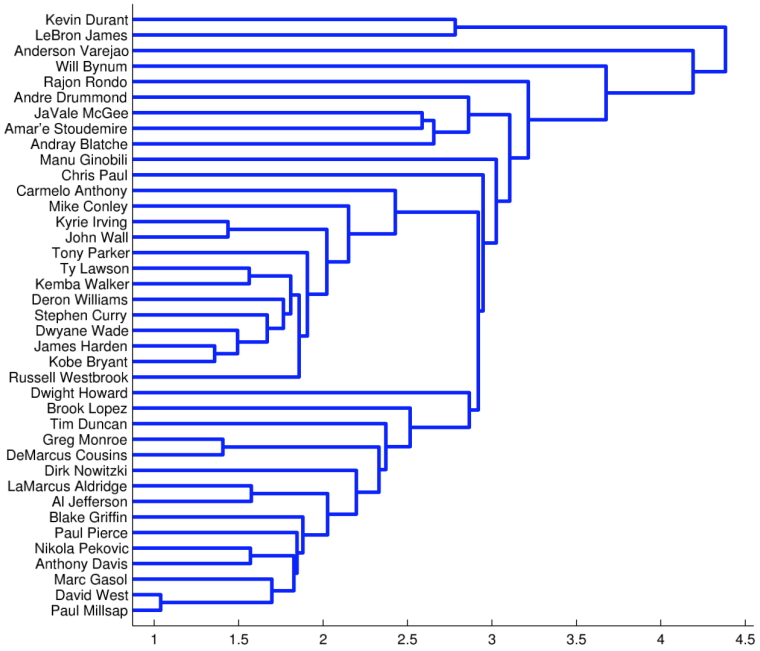
Features are per-game perf statistics (e.g., assists, rebounds) for NBA 2012-13 season. Pairwise distances, ordered to highlight structure:



(a) Pairwise Distances

Application of HAC: Basketball Players (2 of 2)

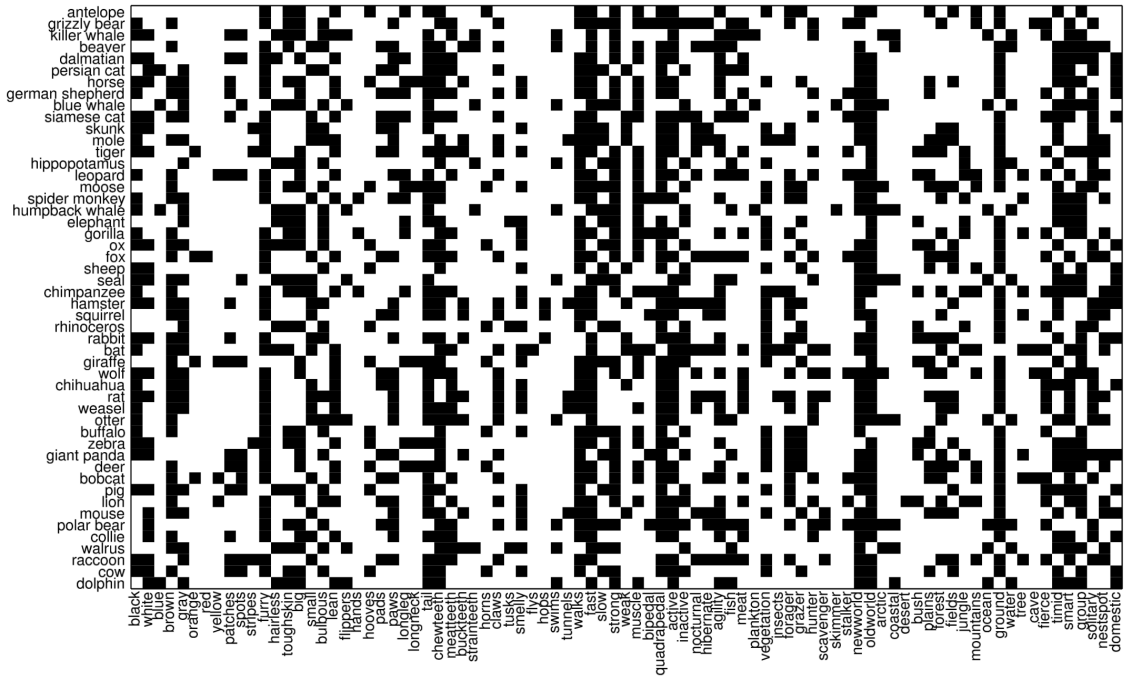
Dendrogram (from HAC using min distance):



(people who follow basketball can make sense of this!...)

Application of HAC: Animal Clustering (1 of 3)

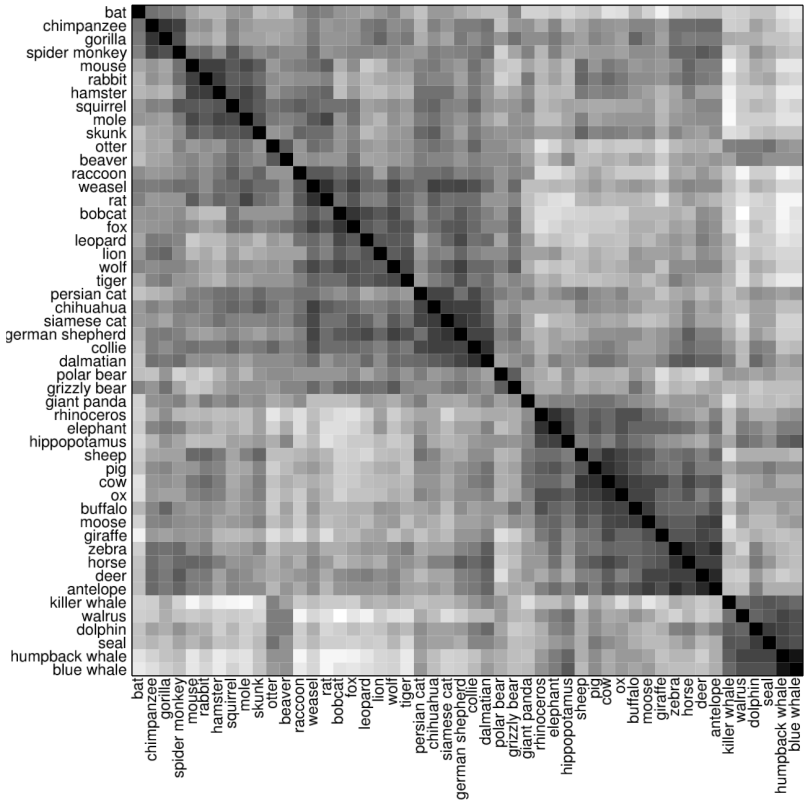
50 animals. 85 binary features. Features matrix:



(a) Animals and Features

Application of HAC: Animal Clustering (2 of 3)

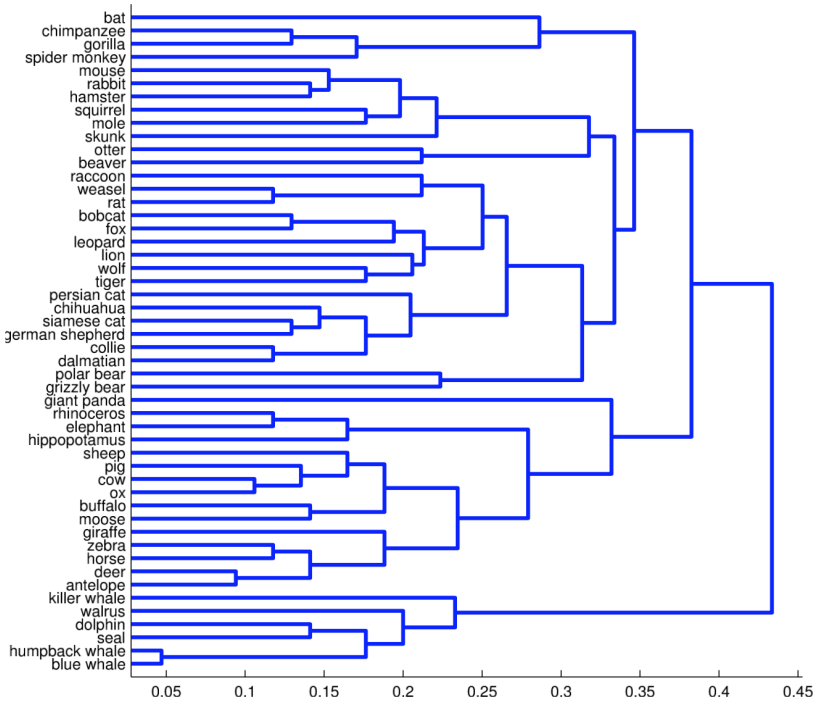
Distance matrix (using pairwise Hamming distances)



(b) Hamming Distances

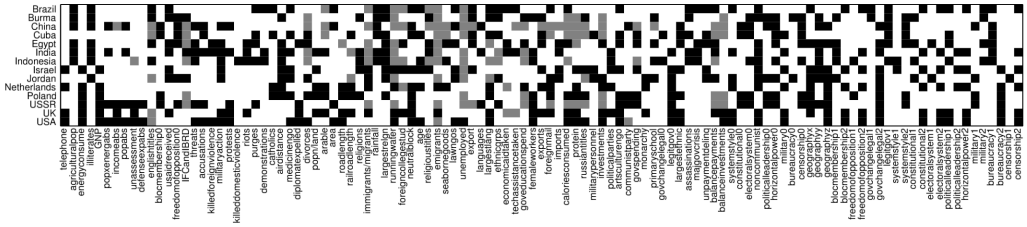
Application of HAC: Animal Clustering (3 of 3)

Dendrogram (from HAC using average distance):

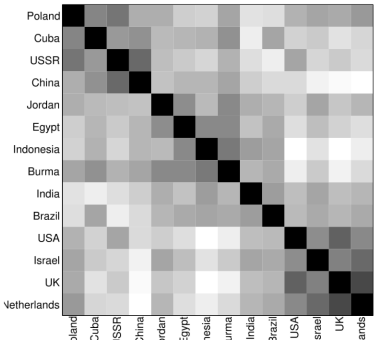


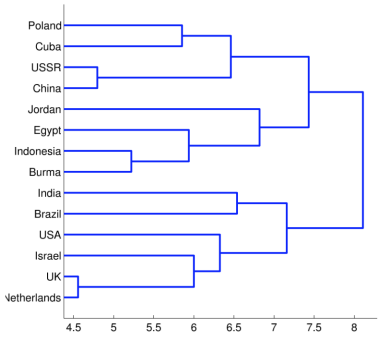
Application of HAC: Clustering World Nations

14 nations, binary features (eg., road length, monarchy, divorces). Collected in 1965. Feature matrix (use 1/2 if feature missing); distance matrix with ℓ_2 distance; and HAC with average distance.



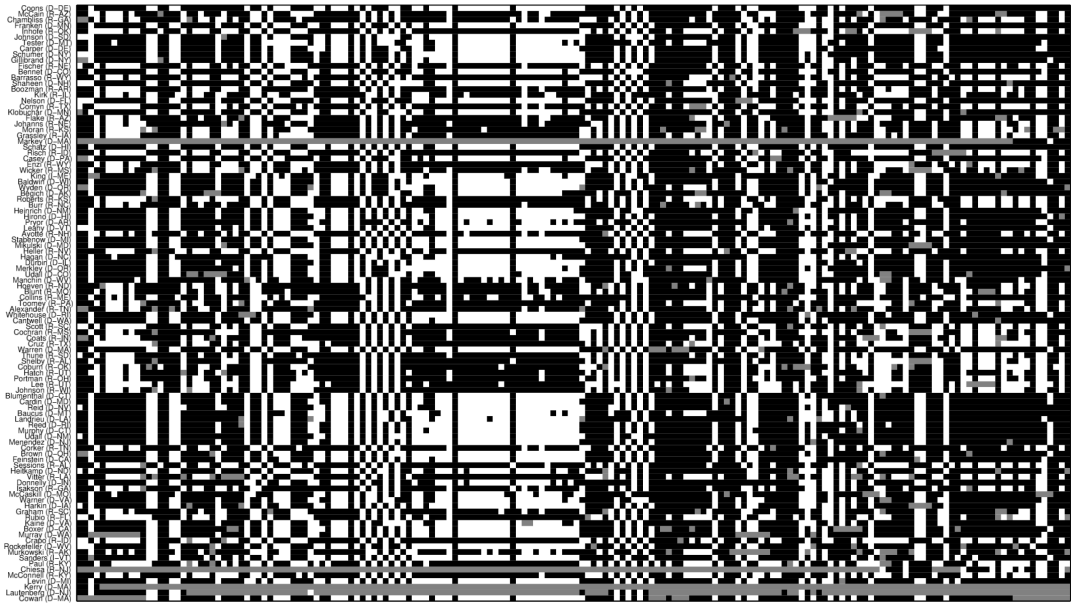
(a) Nations and Features





Application of HAC: Senator Vote Records (1 of 3)

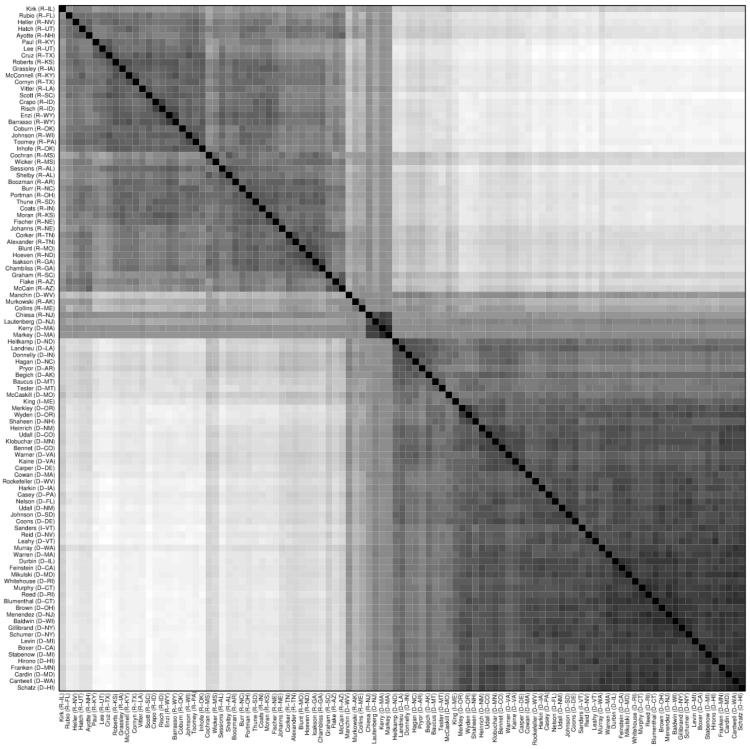
104 senators in 113th US congress. Binary features are votes on 172 bills. Features (if vote missing or abstention, replaced with 1/2)



(a) Senators and Votes

Application of HAC: Senator Vote Records (2 of 3)

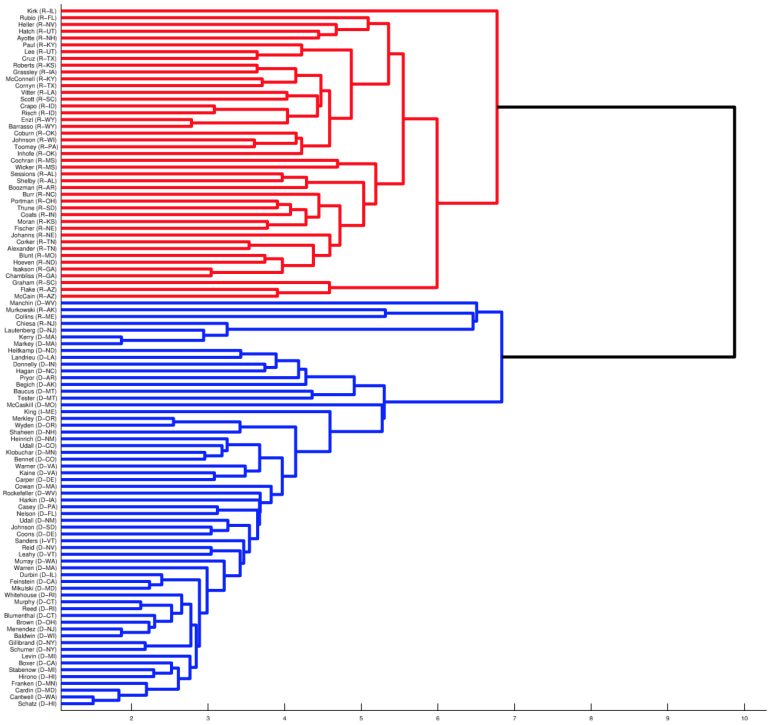
Distance matrix (ℓ_2 distances, darker smaller color, ordered)



(b) Euclidean Distances

Application of HAC: Senator Vote Records (3 of 3)

Dendrogram from HAC w/ average distance, and 2 colored clusters:



HAC: Discussion

- Average and centroid distances provide a compromise between min and max.
- Non-parametric. Can get arbitrary cluster shapes.
- Can over-fit in high dimensional spaces that have irrelevant features.

Computational complexity is $n(n-1)m$ to get pairwise distance between all examples, and then n^2T for T rounds since need to do pairwise checks. $T \ll m$, and thus $O(n^2m)$. (c.f., $O(nKmT)$ for K-means.)

Overfitting

Suppose the data looks like this:

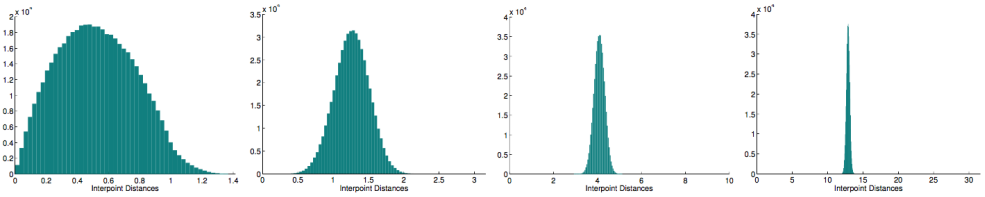
			ℓ		$m-\ell$
$\mathbf{x}_1$	1	1	1	1	random
$\mathbf{x}_2$	1	1	1	1	random
$\mathbf{x}_3$	0	0	0	0	random
$\mathbf{x}_4$	1	1	1	1	random
$\mathbf{x}_5$	0	0	0	0	random

Given $\mathbf{x}, \mathbf{x}'$ in the "1s" cluster and $\mathbf{z}$ in the "0s" cluster, the probability that $\mathbf{x}$ is closer to $\mathbf{x}'$ than to $\mathbf{z}$ goes to $1/2$ as $m \to \infty$, because the noise comes to dominate.

Note: K-means is OK here! $\boldsymbol{\mu}_1 = (1, 1, 1, 1, 0.5, 0.5, \ldots)$ and $\boldsymbol{\mu}_2 = (0, 0, 0, 0, 0.5, 0.5, \ldots)$, and it correctly clusters the data.

Curse of dimensionality

Histograms of inter-example distances for 1000 examples in unit hypercube.



(a) 2 Dimensions (b) 10 Dimensions (c) 100 Dimensions (d) 1000 Dimensions

As dimensions increase, we get concentration of the distances relative to min (0) and max ($\sqrt{m}$) distances (distances are sum of IID r.v.s) Because of this, HAC suffers the "curse of dimensionality." Becomes less useful as the dimensionality of the data grows.

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Clustering

- A very natural, unsupervised learning problem
- K-means and HAC are two simple, popular algorithms
- HAC is more flexible, but has poor performance in high dimensional problems
- Both are a bit ad hoc. We will turn to probabilistic methods to address this concern.