Clustering

Jack Bennetto

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Objectives

Today's objectives:

- Explain the difference between **supervised** and **unsupervised** learning
- Implement a **k-means** algorithm for clustering
- Discuss how **curse of dimensionality** affects clustering
- Choose the best k using the **elbow method** or **silhouette scores**
- Implement and interpret **hierarchical clustering**

Agenda

Morning:

- Supervised/unsupervised learning
- Clustering
- k-means algorithm

Afternoon:

- Curse of dimensionality
- How to choose k
- Hierarchical and other clustering methods

Supervised learning

Most of what you've learned so far

- Linear & logistic regression with lasso or ridge regularization
- Decision trees, bagging, random forest, boosting
- SVM
- kNN

Label == target == endogenous variable == dependent variable == y

Unsupervised learning

No labels. No target.

Why use it?

Unsupervised learning

No labels. No target.

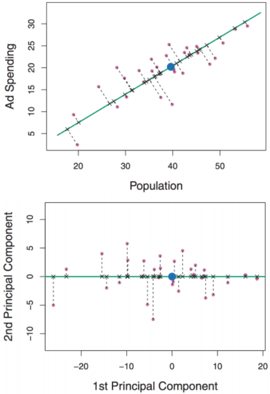
Used for:

- EDA
- Discovering latent variables
- Feature engineering
- Preprossessing

Unsupervised learning

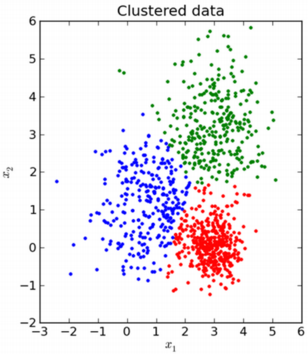
PCA

Low-dim representation of data that explains good fraction of variance



Clustering

Find homogenous subgroups among data



Clustering Problem

Divide data into **distinct subgroups** such that observations within each group are similar.

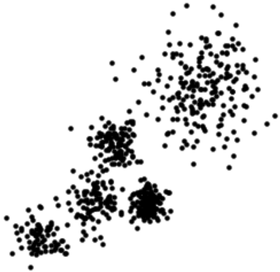
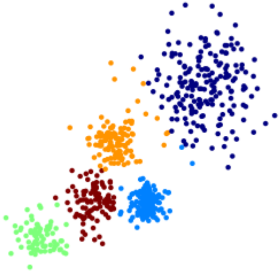
 

Figure 1:

Various Algorithms

There are several approaches to clustering, each with variations.

- k-means clustering
- Hierarchical clustering
- Density-based clustering (DBSCAN)
- Distribution-based clustering
- ...

How do we measure how good the clustering is?

Within-Cluster Sum of Squares

Measures the goodness of a clustering

$$W(C) = \sum_{k=1}^{K} \frac{1}{K} \sum_{C(i)=k} \sum_{C(j)=k} ||x_i - x_j||^2$$

where K is the number of clusters, $C(i)$ is the cluster label of point i, and x_i is the position of point i.

Do you need to normalize?

k-means Algorithm

The k-means algorithm

- Choose a number of clusters k
- Randomly assign each point to a cluster
- Repeat:
    - a. For each of k clusters, compute cluster *centroid* by taking mean vector of points in the cluster
    - b. Assign each data point to cluster for which centroid is closest (Euclidean)

. . . until clusters stop changing

k-means Algorithm

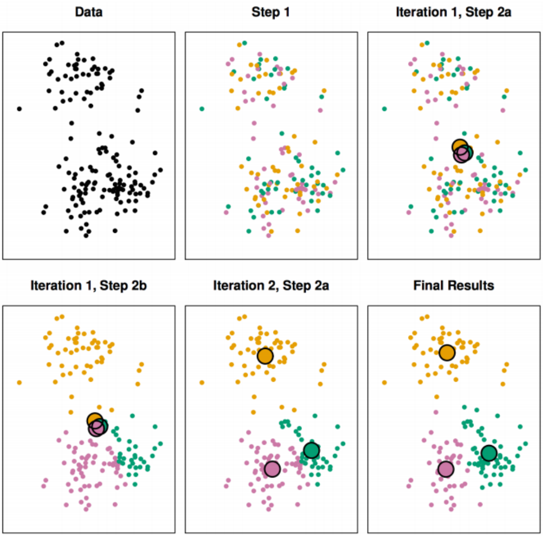


Figure 2:The k-means algorithm

k-means++

k-means finds a local minimum, and sometimes a bad one.

One alternative: use random points as cluster center.

k-means++ is the same algoritm but with a different start.

- Choose one point for first center.
- Repeat:
  - Calculate distance from each point to the nearest center d_i
  - Choose a point to be the next center, randomly, using a weighed probability d_i^2

... until k centers have been choosen.

The Curse of Dimensionality

Random variation in extra dimensions can many hide significant differences between clusters.

The more dimensions there are, the worse the problem.

More than 10 dimensions: consider PCA first.

How Many Clusters?

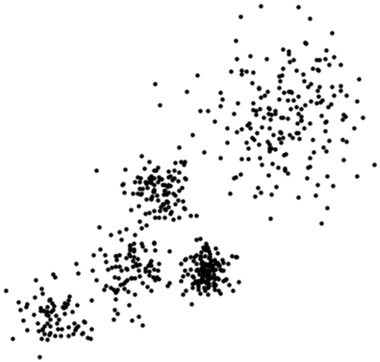


Figure 3:

How Many Clusters?

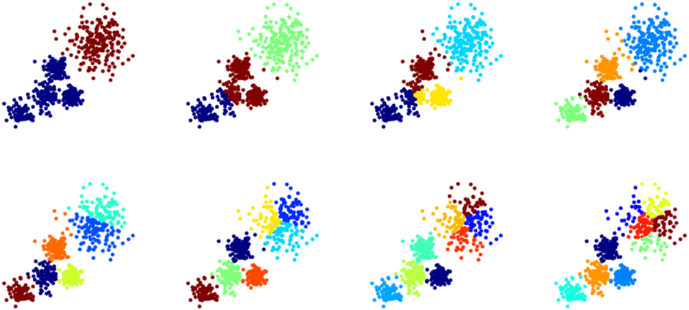


Figure 4:

Choosing K

Can we use within-cluster sum of squares (WCSS) to choose k?

Choosing K

More clusters $\implies$ lower WCSS

Several measures for the "best" K - no easy answer

- The Elbow Method
- Silhouette Score
- GAP Statistic

Choosing K – The Elbow Method

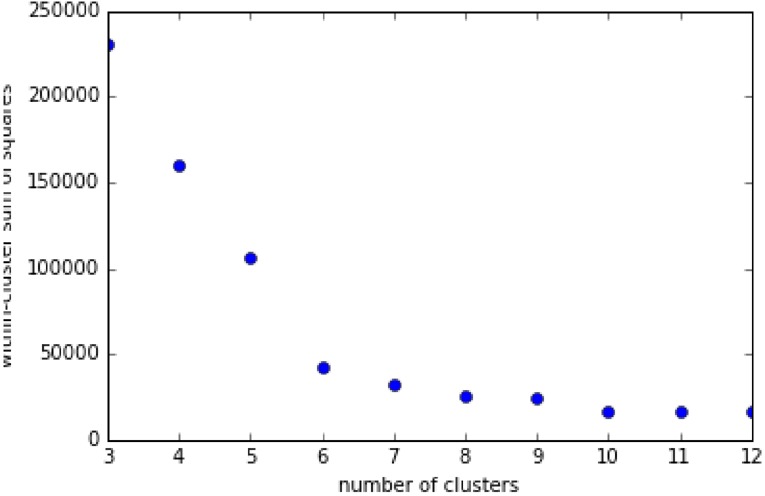


Figure 5:

Choosing K – Silhouette Score

For each point x_i:

- $a(i)$ average dissimilarity of x_i with points in the same cluster
- $b(i)$ average dissimilarity of x_i with points in the nearest cluster
  - "nearest" means cluster with the smallest $b(i)$

$$\text{silhouette}(i) = \frac{b(i) - a(i)}{max(a(i), b(i))}$$

What's the range of silhouette scores?

Choosing K – Silhouette Score

Silhouette score is between 1 and -1

- near 1: very small tight cluster.
- 0: at the edge of two clusters; could be in either.
- $<$ 0: oops.

The higher the the average silhouette score, the tigher and more separated the clusters.

Choosing K – Silhouette Score

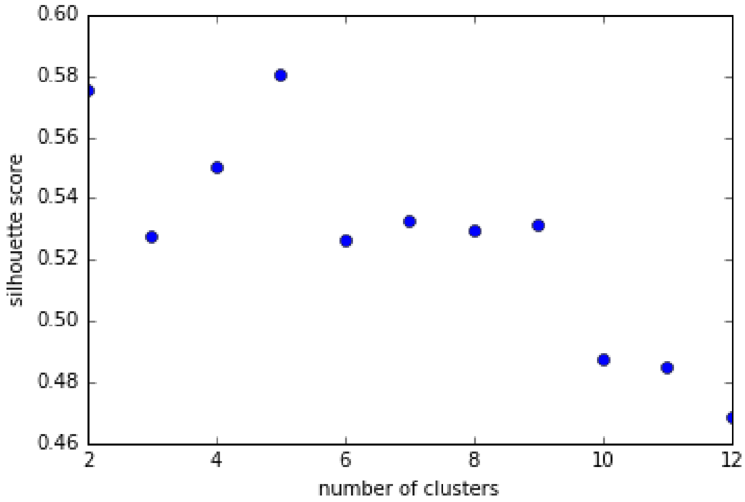


Figure 6:

Silhouette Graph

(see notebook)

Choosing K – GAP Statistic

For each K, compare W_K (within-cluster sum of squares) with that of randomly generated "reference distributions"

Generate B distributions

$$Gap(K) = \frac{1}{B} \sum_{b=1}^{B} \log W_{Kb} - \log W_K$$

Choose smallest K such that $Gap(K) \geq Gap(K+1) - s_{N+1}$

where s_K is the standard error of $Gap(K)$

Hierarchical Clustering

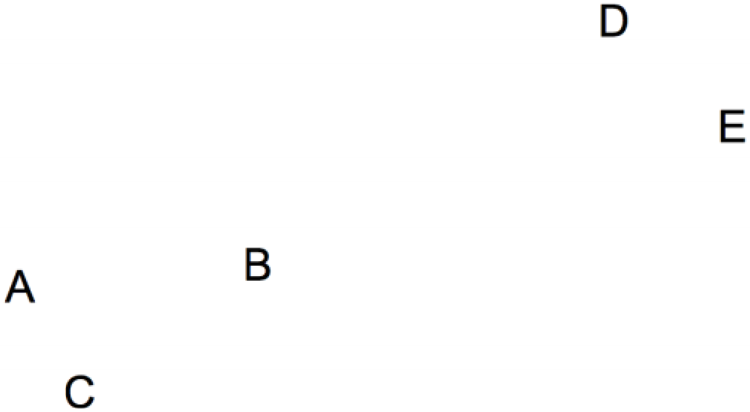
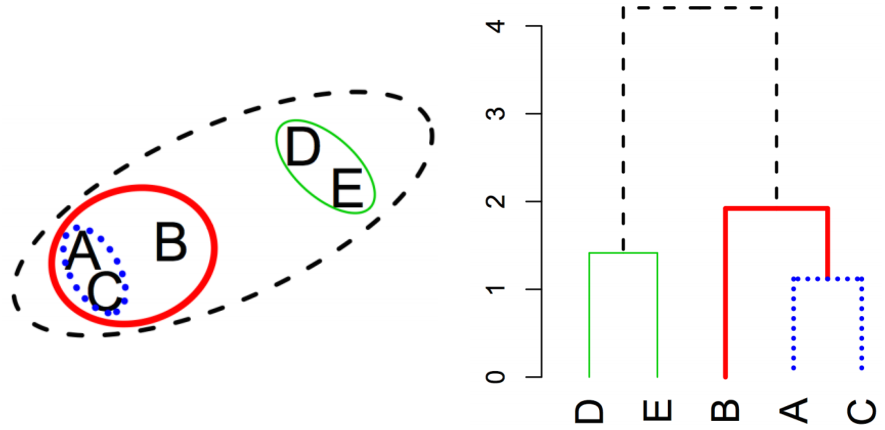


Figure 7:

Hierarchical Clustering



Hierarchical Clustering

Algorithm

- Assign each point to its own cluster
- Repeat:
- Compute distances between clusters
- Merge closest clusters

. . . until all are merged

How do we define dissimilarity between clusters?

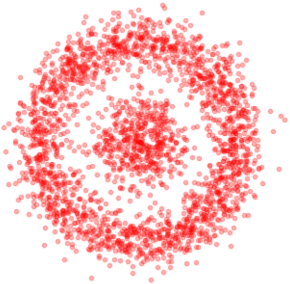
Hierarchical Clustering – Linkage

How do we define dissimilarity between clusters?

- **Complete:** Maximum pairwise dissimilarity between points in clusters – good
- **Average:** Average of pairwise dissimilarity between points in clusters – also good
- **Single:** Minimum pairwise dissimilarity between points in clusters – not as good; can lead to long narrow clusters
- **Centroid:** Dissimilarity between centroids – used in genomics; risk of inversions

Problems with k-means

k-means has limitations.



DBSCAN

Two parameters (number of clusters not specified)

- ϵ: distance between points for them to be connected
- minPts: number of connected points for a point to be a “core” point

A cluster is all connected core points, plus others within ϵ of one of those. Other points are noise.

Distribution-based clustering

Assume clusters follow some (generally gaussian) distribution

Find distributions with the **maximum likelihood** to produce this result

...except you don't know which point is part of which cluster, so you need to add some hidden variables and follow an **expectation-maximization** (EM) algorithm.