

# **INTRO to DATA SCIENCE**

## **LECTURE 8: K-MEANS CLUSTERING**

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DAT10 SF // October 29, 2014

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**INTRO TO DATA SCIENCE, DIMENSIONALITY REDUCTION**

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# **DATA SCIENCE IN THE NEWS**

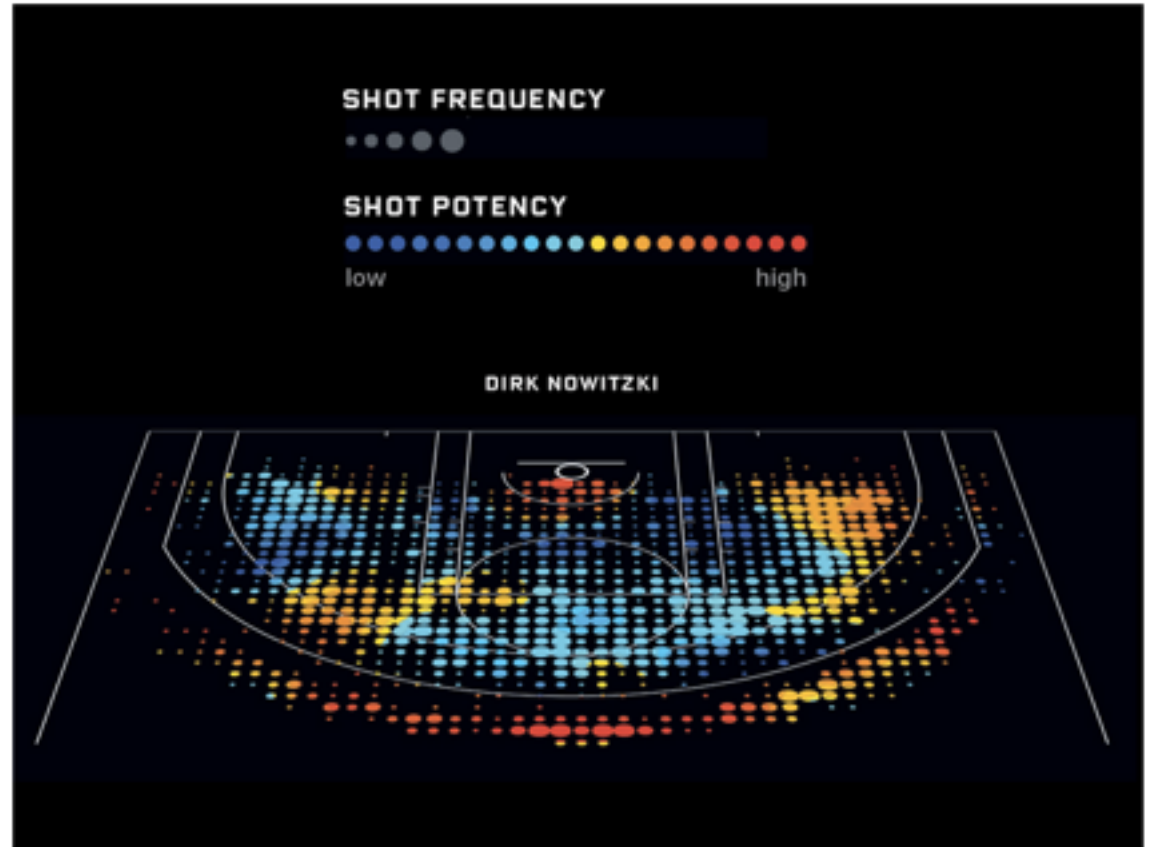
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## DATA SCIENCE IN THE NEWS

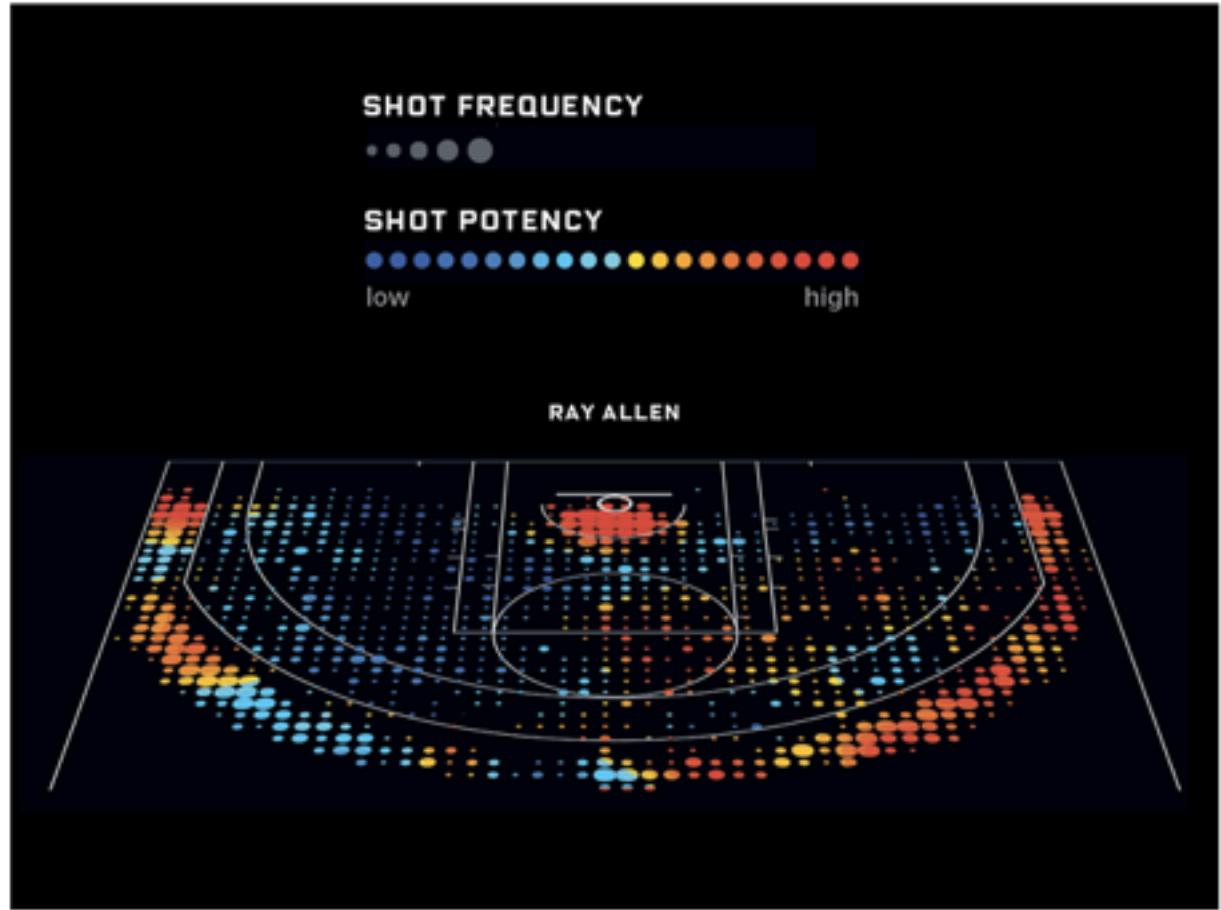
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### SHOTS FROM AROUND THE WORLD

By charting the location and frequency of every shot in the NBA, Kirk Goldsberry can create a map of the strengths and weaknesses of each player's offensive game. Here are the shot maps for two likely Hall of Famers, Ray Allen and Dirk Nowitzki.



## DATA SCIENCE IN THE NEWS



Even the most prolific three-point shooter of all time has relatively weak areas, like from the left wing.

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## DATA SCIENCE IN THE NEWS

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“It's not an exaggeration to say that 85 percent of the teams don't know what to do with this data,” Goldsberry says. “The idea that this is going to revolutionize the NBA—well, I'm not sure that's true unless teams awaken really quickly to things like machine learning and data visualization.”

## **LAST TIME:**

- RECAP: DIMENSIONALITY REDUCTION AND PCA**
- SINGULAR VALUE DECOMPOSITION**
- OTHER METHODS**

**QUESTIONS?**

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## **AGENDA**

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**I. CLUSTER ANALYSIS**

**II. K-MEANS CLUSTERING**

**III. CLUSTER VALIDATION**

**EXERCISES:**

**IV. K-MEANS CLUSTERING IN PYTHON**

# **I. CLUSTER ANALYSIS**



	Continuous	Categorical
Supervised	???	???
Unsupervised	???	???

	Continuous	Categorical
Supervised	regression	classification
Unsupervised	dimension reduction	clustering

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Q: What does categorical mean in this context?

Q: What is a cluster?

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The concept of similarity is central to the definition of a cluster, and therefore to cluster analysis.

In general, greater similarity between points leads to better clustering.

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Clustering provides a layer of abstraction from individual data points.

The goal is to extract and enhance the natural structure of the data (not to impose arbitrary structure!)

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The real purpose of clustering is data exploration, so a solution is anything that contributes to your understanding.

# **II. K-MEANS CLUSTERING**

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partition – performs complete clustering (each point belongs to exactly one cluster)

Q: How are these partitions determined?

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A: Each point is assigned to the cluster with the nearest centroid.

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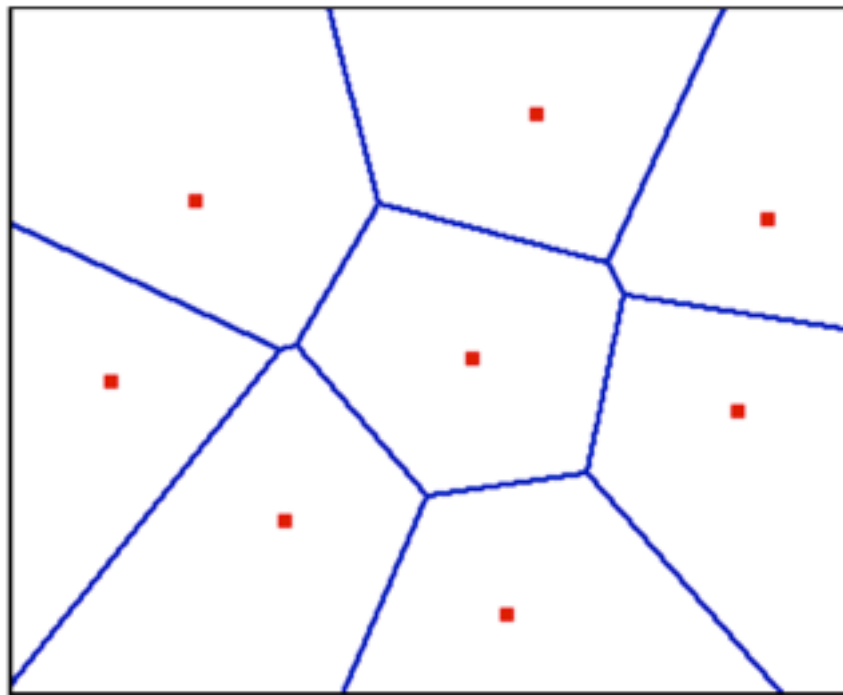
A: Each point is assigned to the cluster with the nearest centroid.

centroid – the mean of the data points in a cluster

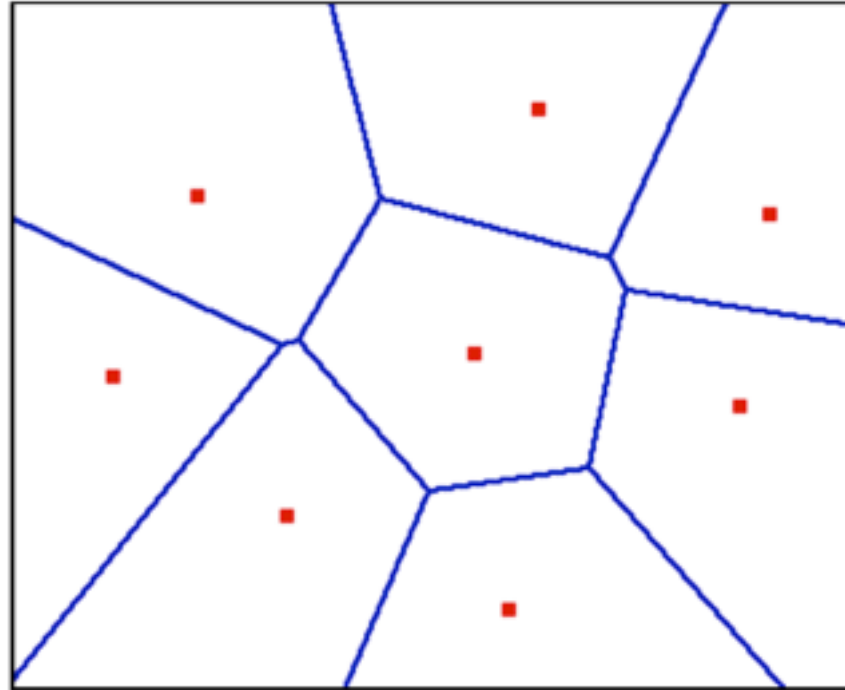
–> requires continuous (vector-like) features

–> highlights iterative nature of algorithm

Q: What do these partitions look like?







### NOTE

*These partitions are sometimes called Voronoi cells, and these maps Voronoi diagrams.*

One important point to keep in mind is that partitions are not scale-invariant!

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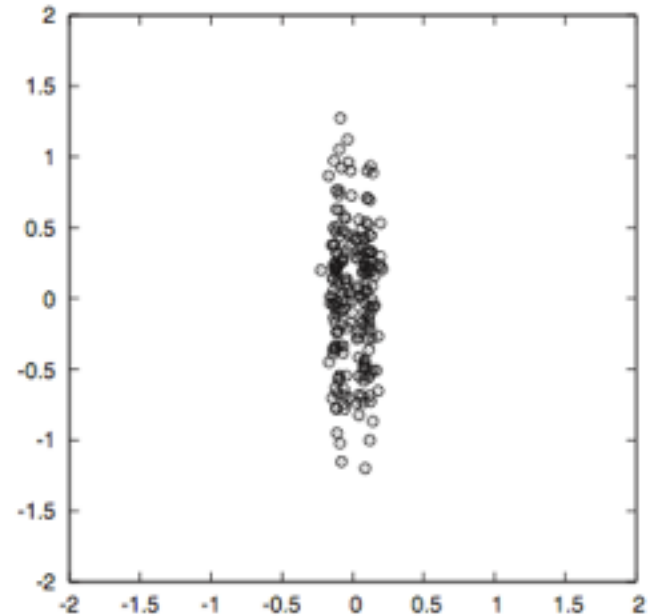
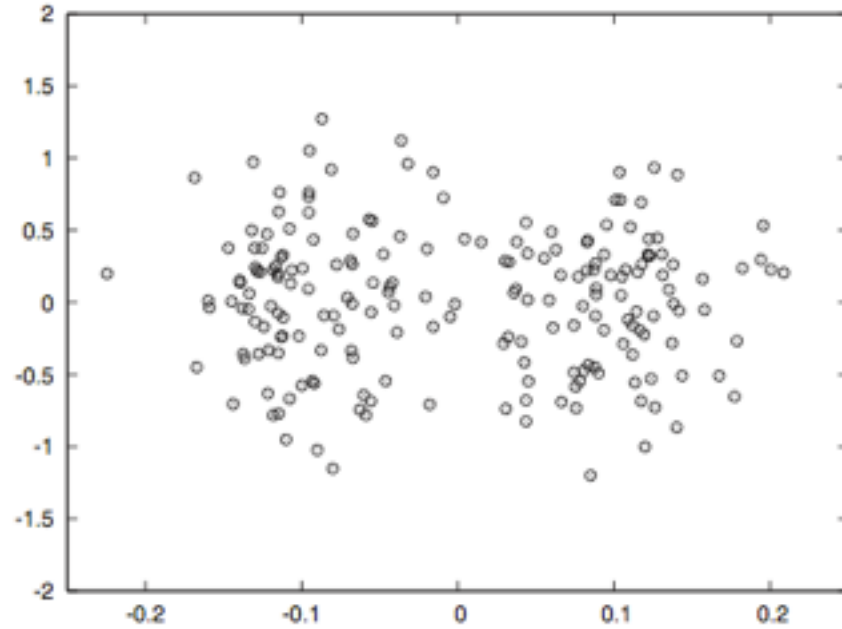
This means that the same data can yield very different clustering results depending on the scale and the units used.

Therefore it's important to think about your data representation before applying a clustering algorithm.

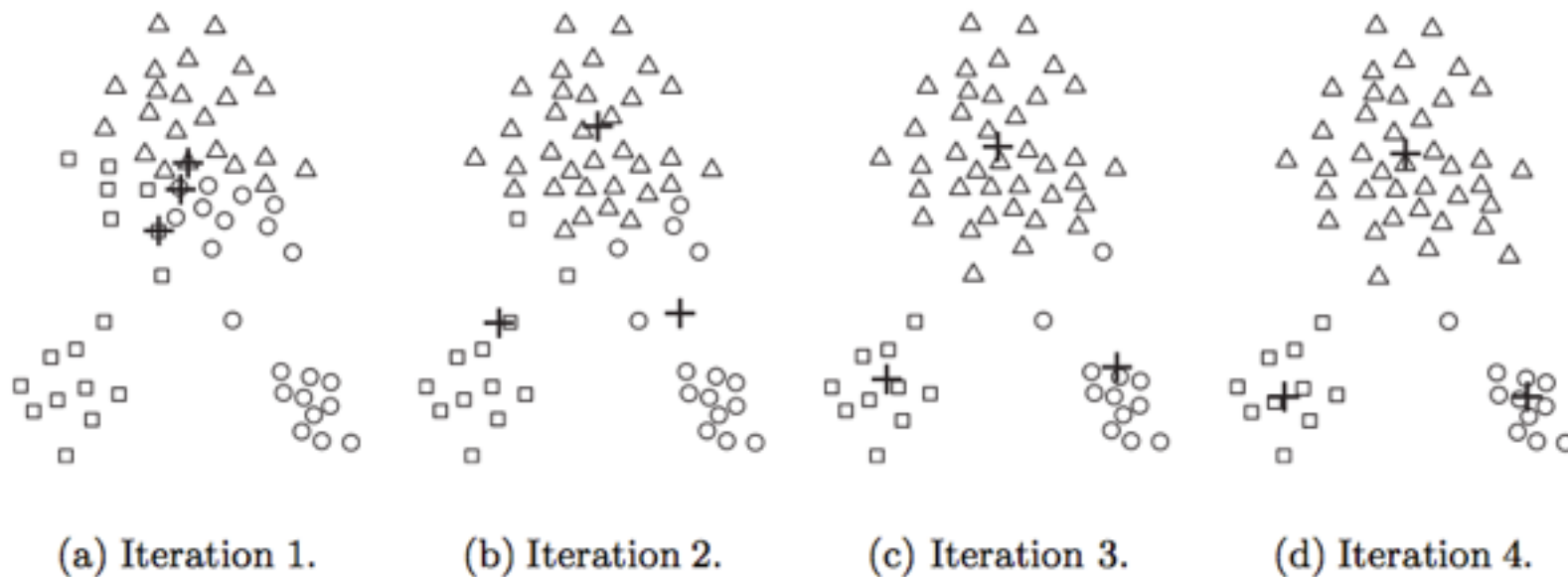
These graphs show two different representations of the same data:

## SCALE DEPENDENCE

These graphs show two different representations of the same data:



- 1) choose  $k$  initial centroids (note that  $k$  is an input)
- 2) for each point:
  - find distance to each centroid
  - assign point to nearest centroid
- 3) recalculate centroid positions
- 4) repeat steps 2–3 until stopping criteria met



**Figure 8.3.** Using the K-means algorithm to find three clusters in sample data.



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It has a hard time dealing with non-convex clusters, or data with widely varying shapes and densities.

Difficulties can sometimes be overcome by increasing the value of  $k$  and combining subclusters in a post-processing step.

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A: There are several options:

- randomly (but may yield divergent behavior)
- perform alternative clustering task, use resulting centroids as initial k-means centroids
- start with global centroid, choose point at max distance, repeat (but might select outlier)



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**NOTE**

*Technically, by defining a similarity measure we are mapping our observations into a metric space.*

A similarity measure must satisfy certain general conditions:

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$$d(x, y) \geq 0$$

$$d(x, y) = 0 \iff x = y$$

$$d(x, y) = d(y, x)$$

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**NOTE**

*Another useful property  
is smoothness.*

There are a number of different similarity measures to choose from, and in general the right choice depends on the problem.



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For data that takes values in  $R^n$ , the typical choice is the Euclidean distance:

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We can express different semantics about our data through the choice of metric.

Ex: One popular metric for text mining problems (or any problem with sparse binary data) is the Jaccard coefficient,

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$$J(A, B) = \frac{|A \cap B|}{|A \cup B|}$$

Applying this metric to a problem expresses the sparse nature of the data, and makes a variety of text mining techniques accessible.

The matrix whose entries  $D_{ij}$  contain the values  $d(x, y)$  for all  $x$  and  $y$  is called the distance matrix.

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For this reason, it's really the choice of metric that determines the definition of a cluster.

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A: By optimizing an objective function that tells us how “good” the clustering is.

The iterative part of the algorithm (recomputing centroids and reassigning points to clusters) explicitly tries to minimize this objective function.

Ex: Using the Euclidean distance measure, one typical objective function is the sum of squared errors from each point  $x$  to its centroid  $c_i$ :

$$SSE = \sum_{i=1}^K \sum_{x \in C_i} d(x, c_i)^2$$

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Given two clusterings, we will prefer the one with the lower SSE since this means the centroids have converged to better locations (a better local optimum).

We iterate until some stopping criteria are met; in general, suitable convergence is achieved in a small number of steps.

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## STEP 4 – CONVERGENCE

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Recall that, in general, different runs of the algorithm will converge to different local optima (centroid configurations).

# **III. CLUSTER VALIDATION**



In general, k-means will converge to a solution and return a partition of  $k$  clusters, even if no natural clusters exist in the data.

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We will look at two validation metrics useful for partitional clustering, cohesion and separation.

Cohesion measures clustering effectiveness within a cluster.

$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

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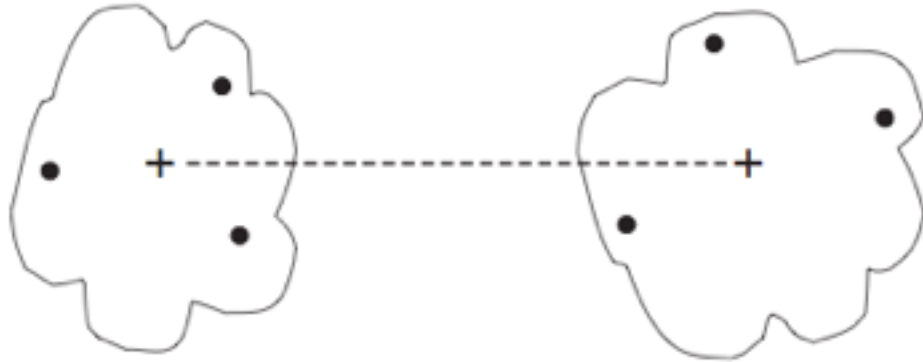
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Separation measures clustering effectiveness between clusters.

$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$



(a) Cohesion.



(b) Separation.

**Figure 8.28.** Prototype-based view of cluster cohesion and separation.

We can turn these values into overall measures of clustering validity by taking a weighted sum over clusters:

$$\hat{V}_{total} = \sum_1^K w_i \hat{V}(C_i)$$

Here  $V$  can be cohesion, separation, or some function of both.

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The weights can all be set to 1 (best for k-means), or proportional to the cluster masses (the number of points they contain).

Cluster validation measures can be used to identify clusters that should be split or merged, or to identify individual points with disproportionate effect on the overall clustering.



One useful measure than combines the ideas of cohesion and separation is the silhouette coefficient. For point  $x_i$ , this is given by:

$$SC_i = \frac{b_i - a_i}{\max(a_i, b_i)}$$

such that:

$a_i$  = average in-cluster distance to  $x_i$

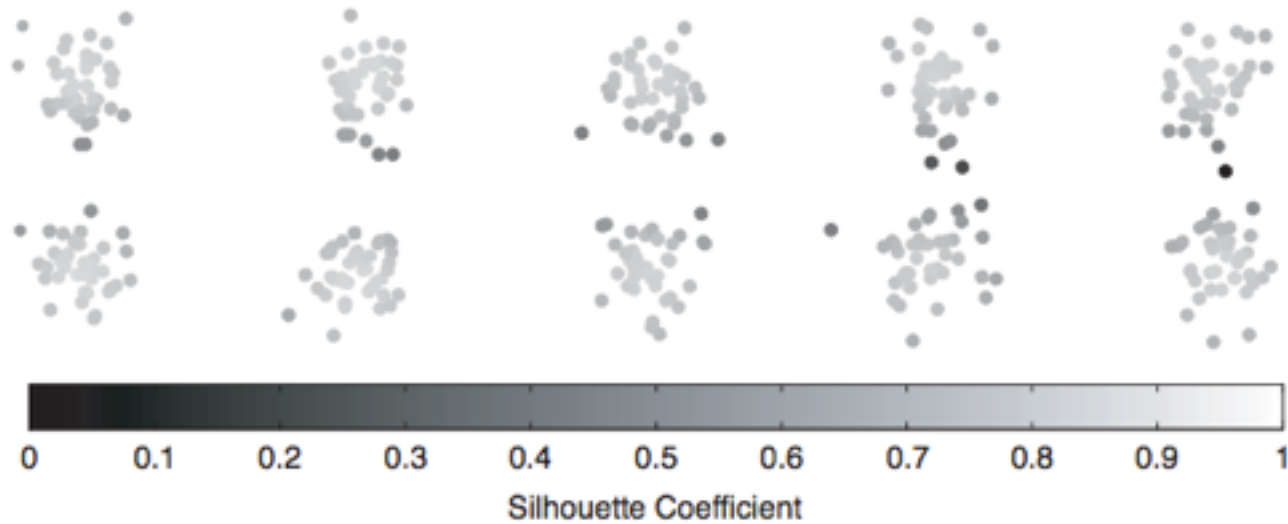
$b_{ij}$  = average between-cluster distance to  $x_i$

$b_i = \min_j(b_{ij})$

The silhouette coefficient can take values between  $-1$  and  $1$ .

In general, we want separation to be high and cohesion to be low. This corresponds to a value of SC close to  $+1$ .

A negative silhouette coefficient means the cluster radius is larger than the space between clusters, and thus clusters overlap.



**Figure 8.29.** Silhouette coefficients for points in ten clusters.

The silhouette coefficient for the cluster  $C_i$  is given by the average silhouette coefficient across all points in  $C_i$ :

$$SC(C_i) = \frac{1}{m_i} \sum_{x \in C_i} SC_i$$

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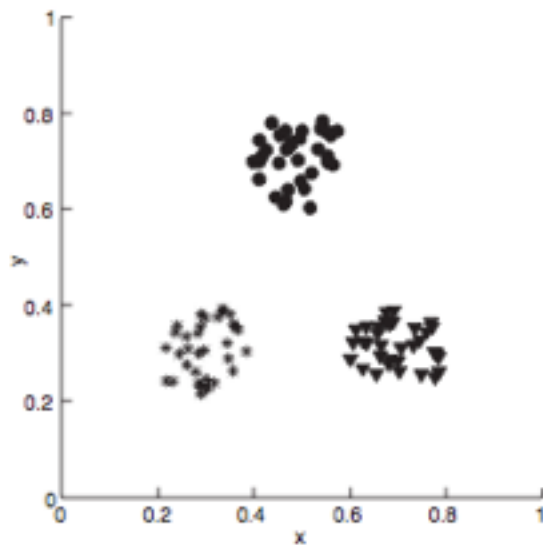
*This gives a summary measure of the overall clustering quality.*

An alternative validation scheme is given by comparing the similarity matrix with an idealized (0/1) similarity matrix that represents the same clustering configuration.

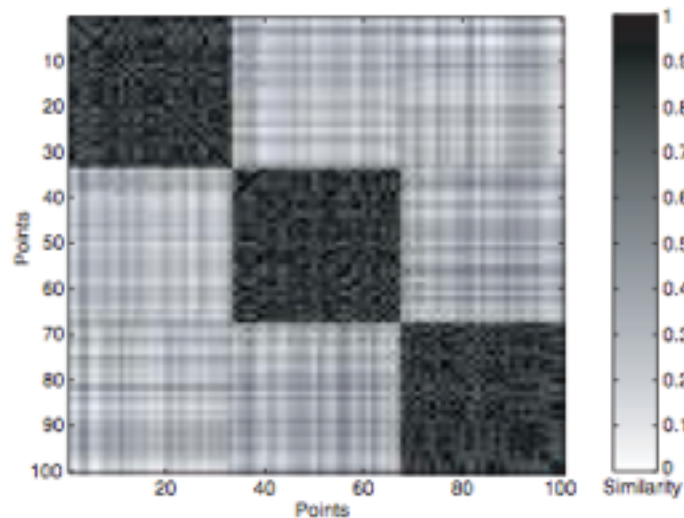
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This can be done either graphically or using correlations.





(a) Well-separated clusters.



(b) Similarity matrix sorted by K-means cluster labels.

One useful application of cluster validation is to determine the best number of clusters for your dataset.

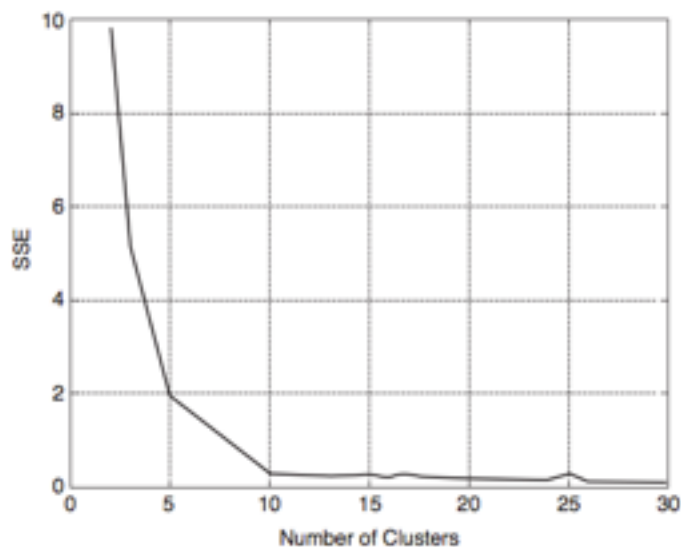
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Q: How would you do this?

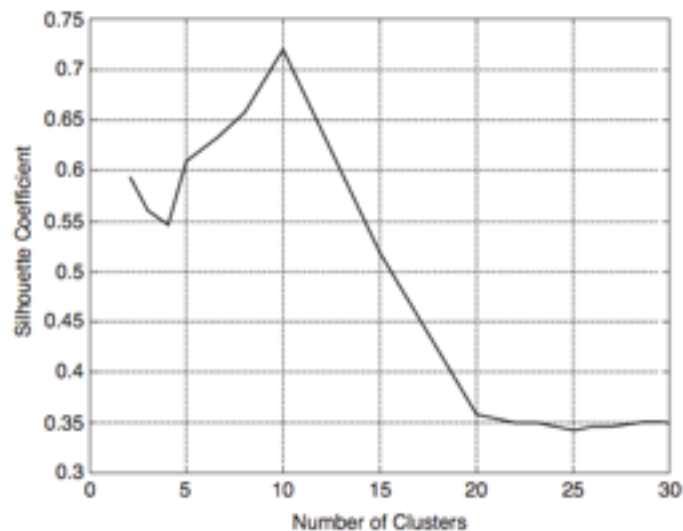
One useful application of cluster validation is to determine the best number of clusters for your dataset.

Q: How would you do this?

A: By computing the overall SSE or SC for different values of  $k$ .



**Figure 8.32.** SSE versus number of clusters for the data of Figure 8.29.



**Figure 8.33.** Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

Q: How can you determine your level of confidence in these validation metrics?

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A: Statistically; eg, by computing frequency distributions for these metrics (over several runs of the algorithm) and determining statistical significance.

Ultimately, cluster validation and clustering in general are suggestive techniques that rely on human interpretation to be meaningful.



# **EX: K-MEANS CLUSTERING**