Week 7 Video 2

Clustering

Validation and Selection of K

How do we choose?

- A value for k
- Which set of clusters to use, after 17 randomized restarts

First…

- Let's take the case where we have 17 randomized restarts, each involving the same number of clusters

Distortion
(Also called Mean Squared Deviation)

- Take each point P
- Find the centroid of P’s cluster C
- Find the distance D from C to P
- Square D to get D’

- Sum all D’ to get Distortion

Distance

- Usually Euclidean distance
- Distance from A to B in two dimensions

$$\sqrt{(Ax-Bx)^2+(Ay-By)^2}$$

Distance

- Euclidean distance can be computed for an arbitrary number of dimensions

$$\sqrt{\Sigma(Ai-Bi)^2}$$

Distortion

- Works for choosing between randomized restarts
- Does not work for choosing cluster size

Why not?

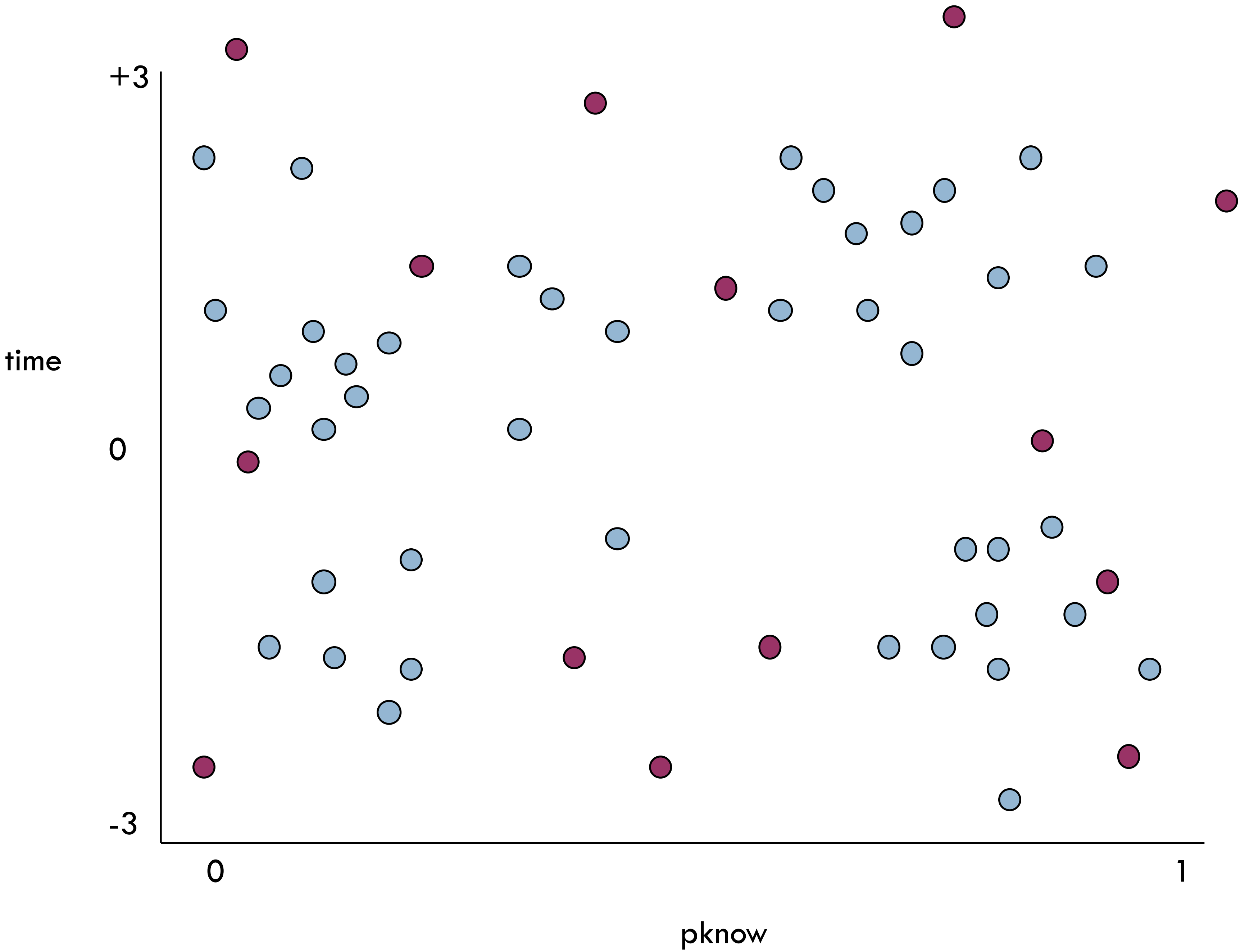
- More clusters almost always leads to smaller Distortion
  - Distance to nearest cluster center should almost always be smaller with more clusters
  - It only isn't when you have bad luck in your randomization

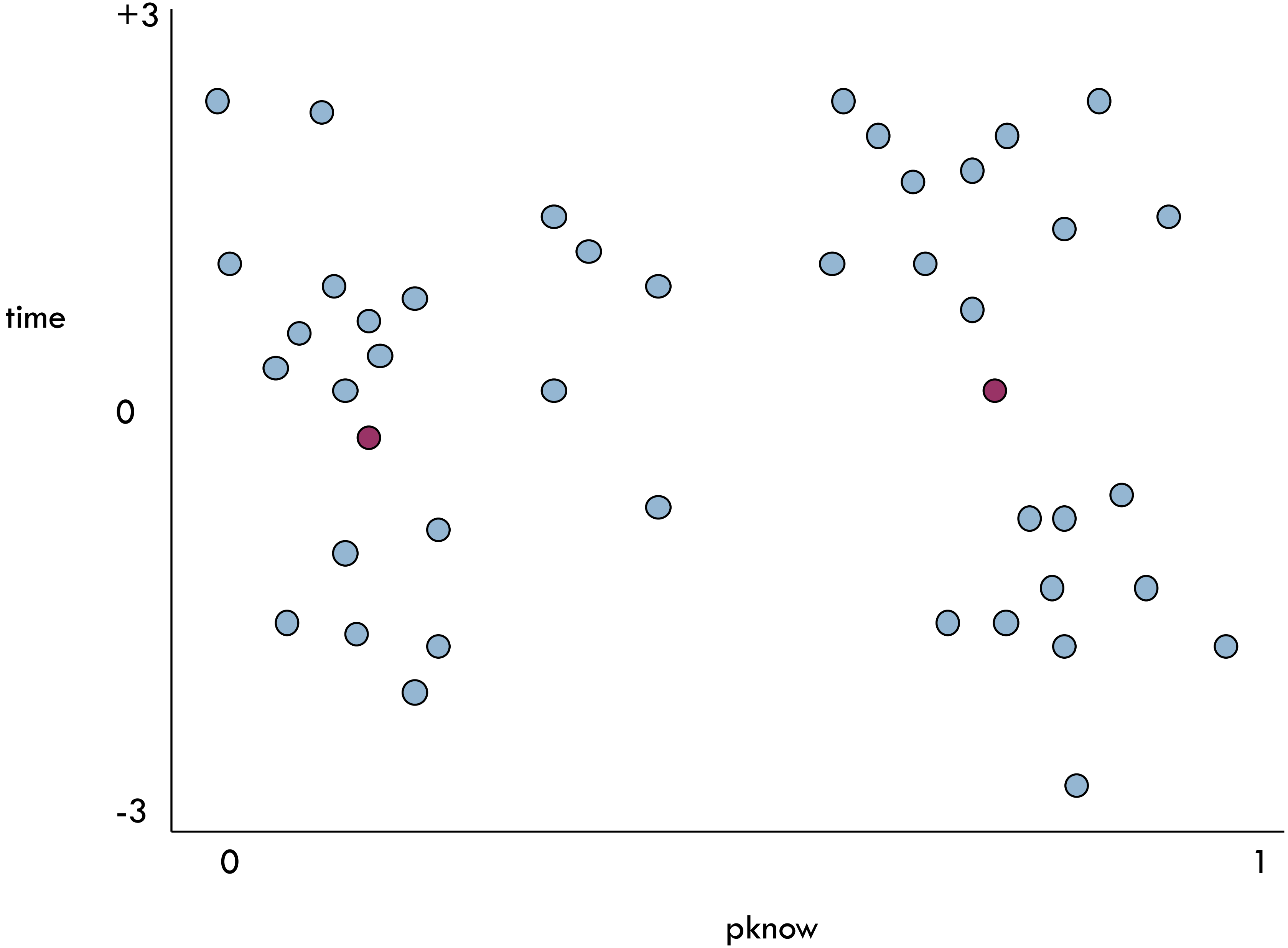
Cross-validation can't solve this problem

- A different problem than prediction modeling
  - You're not trying to predict specific values
  - You're determining whether ***any*** center is close to a given point
- More clusters cover the space more thoroughly
- So Distortion will often be smaller with more clusters, even if you cross-validate

An Example

- 14 centers, ill-chosen (you might get this by conducting cross-validation with too many centers)
- 2 centers, well-chosen (you might get this by conducting cross-validation with not enough centers)


+3
time
0
-3
0
1
pknow


+3
time
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An Example

- The ill-chosen 14 centers will achieve a better Distortion than the well-chosen 2 centers

Solution

- Penalize models with more clusters, according to how much extra fit would be expected from the additional clusters

- You can use the Bayesian Information Criterion or Akaike Information Criterion from week 2
  - Not just the same as cross-validation for this problem!

Using an Information Criterion

- Assess how much fit would be spuriously expected from a random N centroids (without allowing the centroids to move)
- Assess how much fit you actually had

- Find the difference

So how many clusters?

- Try several values of k
- Find “best-fitting” set of clusters for each value of k
- Choose k with best value of BiC (or AIC)

Silhouette Analysis (Rousseeuw, 1987; Kaufman & Rousseeuw, 1990)

- An increasingly popular method for determining how many clusters to use

Silhouette Analysis

- Silhouette plot shows how close each point in a cluster is to points in adjacent clusters

- Silhouette values scaled from -1 to 1
  - Close to +1: Data point is far from adjacent clusters
  - Close to 0: Data point is at boundary between clusters
  - Close to -1: Data point is closer to other cluster than its own cluster

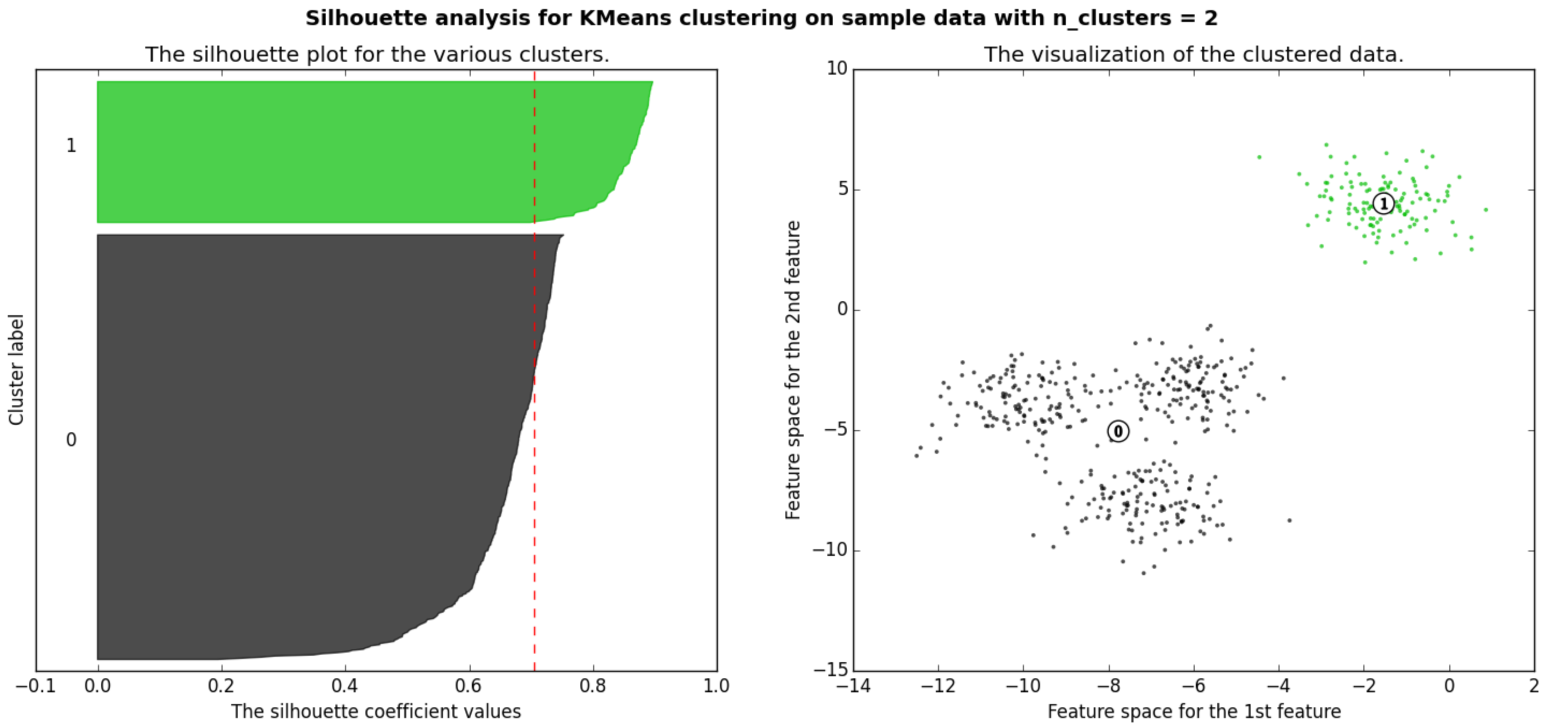
Silhouette Formula

- For each data point i
- A(i) = average distance of i from all other data points in same cluster C
- C* = cluster with lowest average distance of i from all other data points in cluster c*
- B(i) = average dissimilarity of i from all other data points in cluster C*
- $S(i) = \frac{B(i) - A(i)}{\max\{A(i), B(i)\}}$

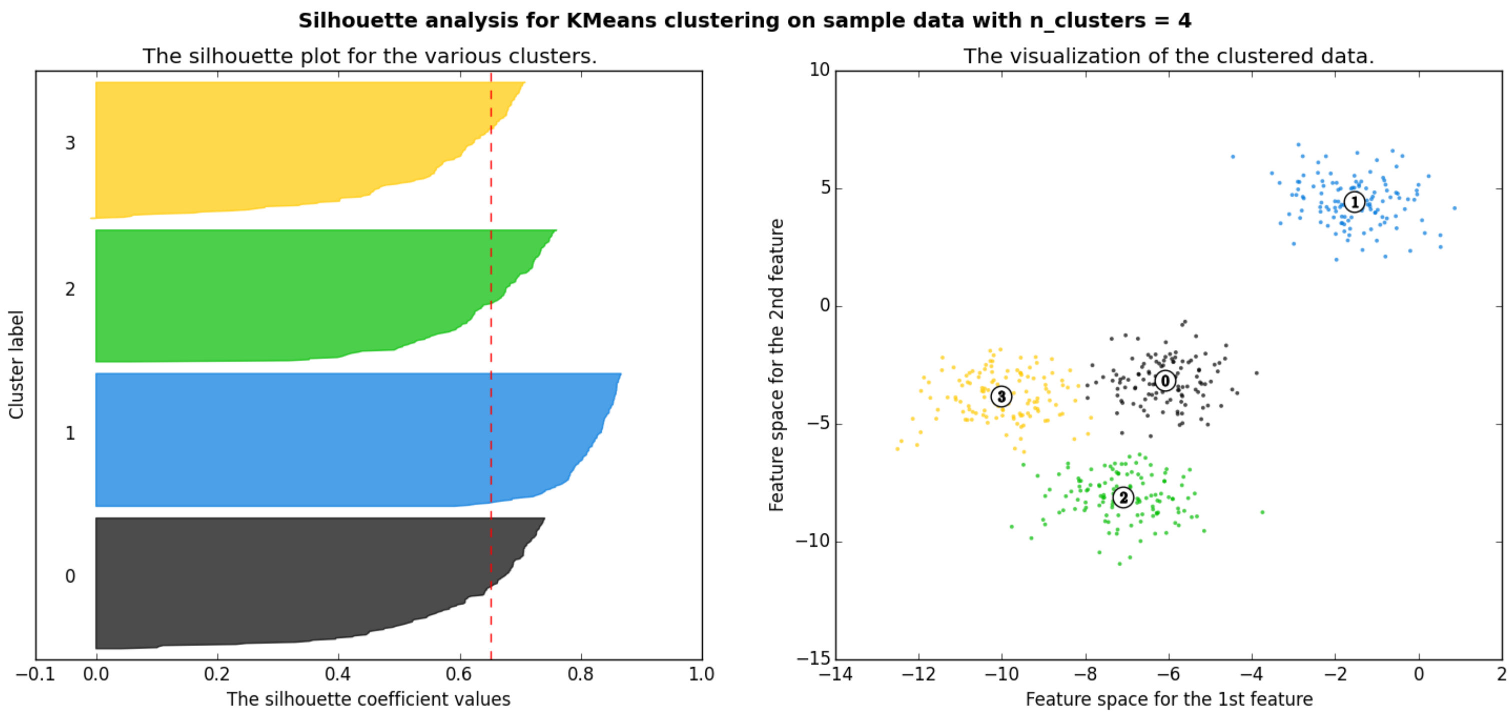
Example from

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

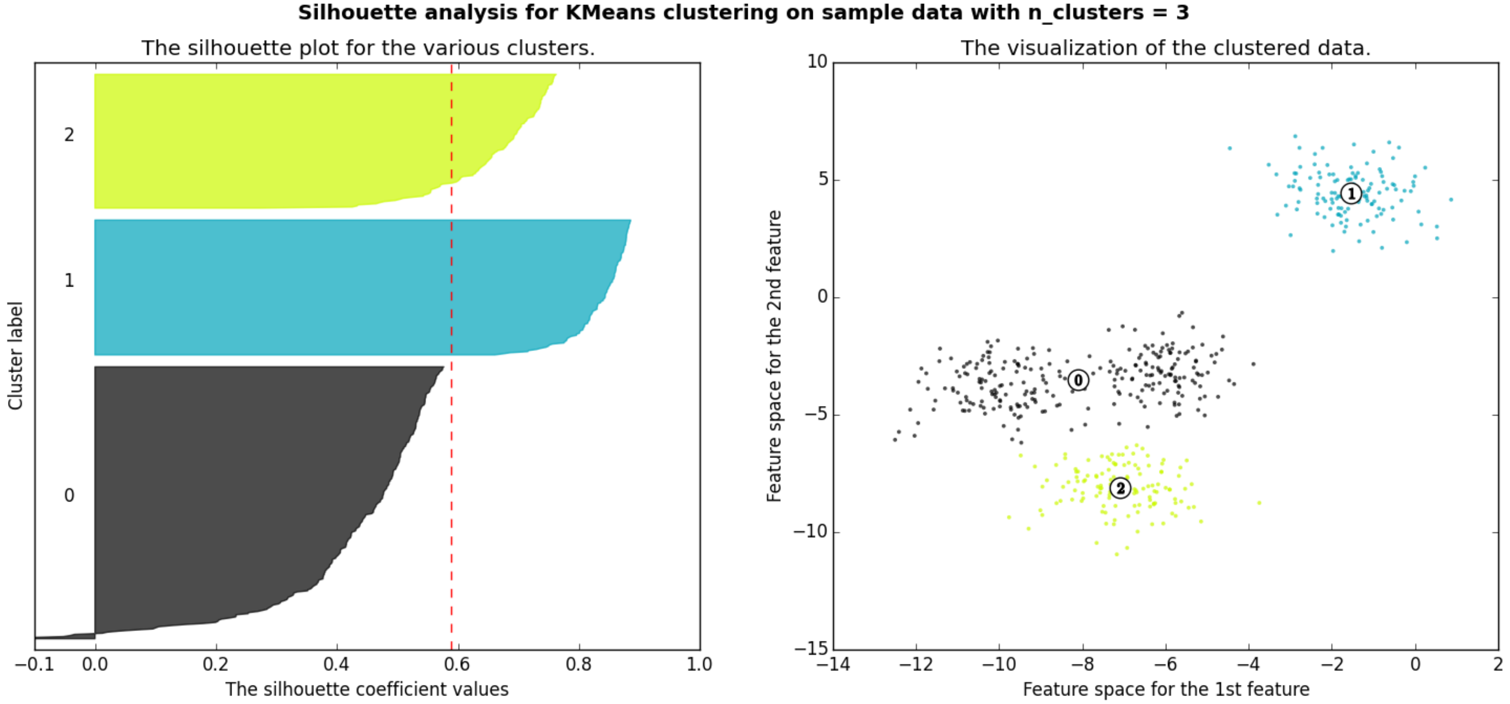
Good clusters



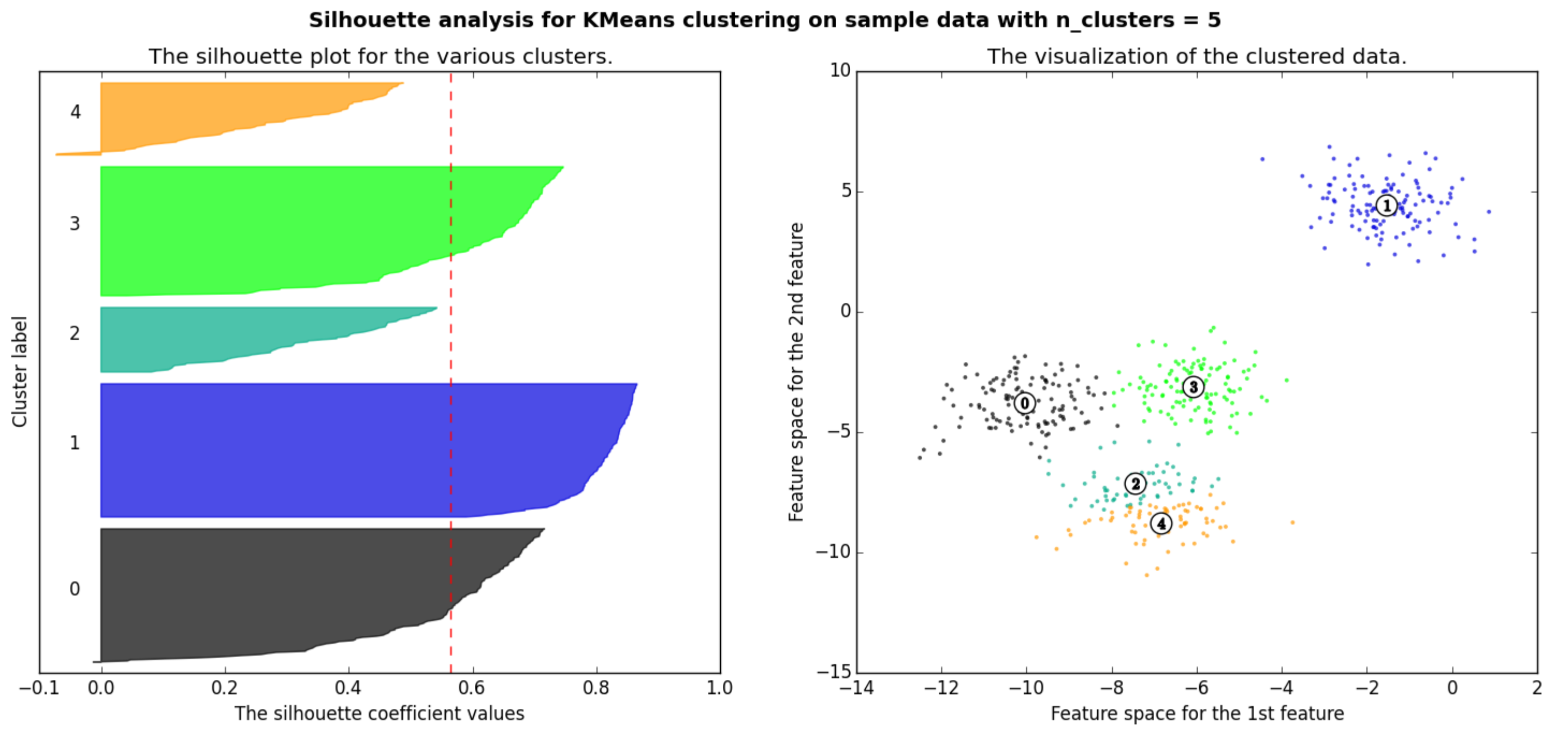
Good clusters



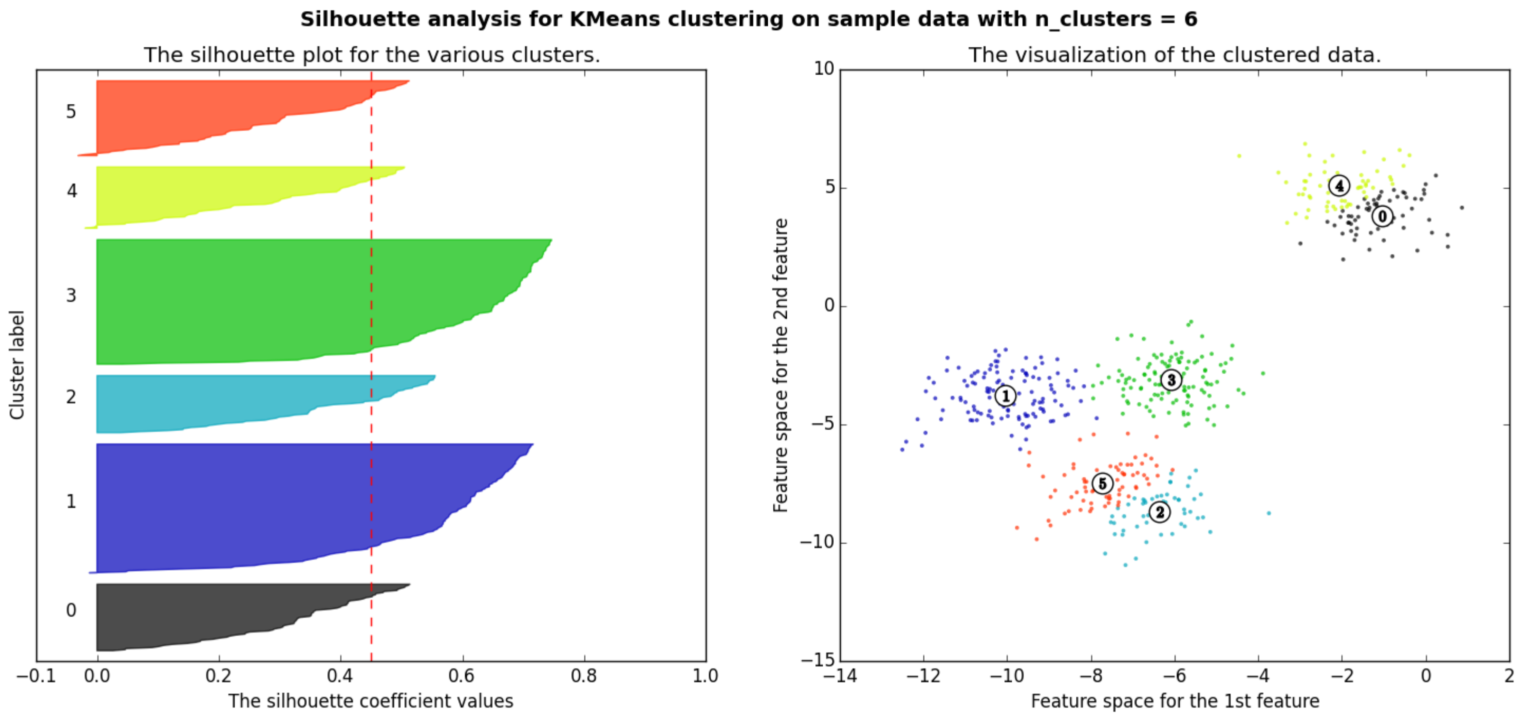
Bad clusters



Bad clusters



Bad clusters



So in this example

- 2 and 4 clusters are reasonable choices
- 3, 5, and 6 clusters are not good choices

Eigengap

- In spectral clustering (which we haven't talked about yet)
- There is also the option of choosing the number of clusters that maximizes the eigengap (difference between consecutive eigenvalues)

Alternate approach

- One question you should ask when choosing the number of clusters is – why am I conducting cluster analysis?

- If your goal is to just discover qualitatively interesting patterns in the data, you may want to do something simpler than using an information criterion
  - Add clusters until you don't get interesting new clusters anymore

Next lecture

- Clustering – Advanced clustering algorithms