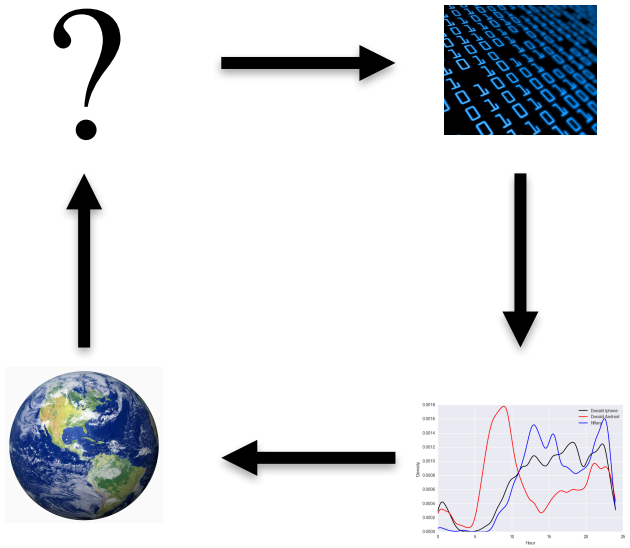
Data Science 100
Lec 25:
Clustering and K-means

DS100
Spring
2017

Slides by:
Bin Yu
binyu@stat.berkeley.edu
Joey Gonzalez
jegonzal@berkeley.edu
Thanks to Andrew Do for his assistance on data analysis



Cluster, defined by Oxford Dictionary

cluster | ˈkləstər |

noun

a group of similar things or people positioned or occurring closely together: ***clusters of*** *creamy-white flowers* | ***a cluster of*** *antique shops*.

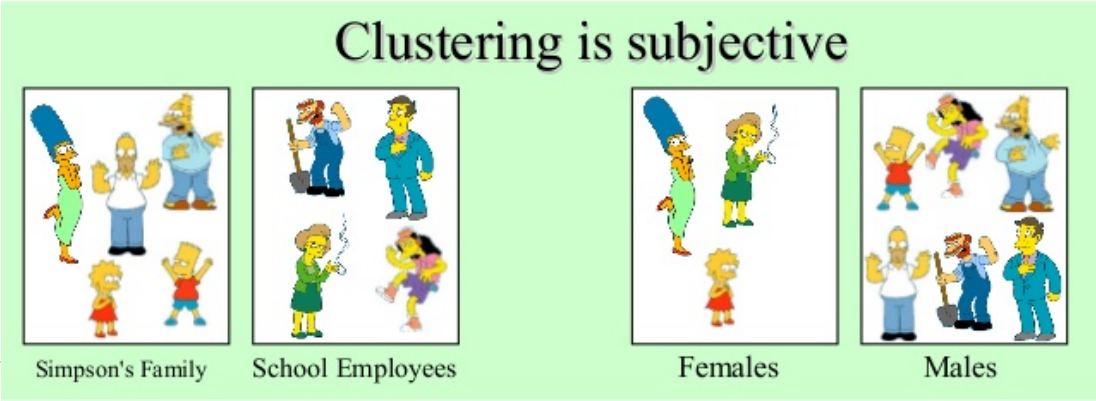
- Astronomy a group of stars or galaxies forming a relatively close association.
- Linguistics (also **consonant cluster**)a group of consonants pronounced in immediate succession, as *str* in *strong* .
- a natural subgroup of a population, used for statistical sampling or analysis.
- Chemistry a group of atoms of the same element, typically a metal, bonded closely together in a molecule.

Clustering, why bother?

Humans clustered similar things (objects and animals and people) way before statistics and machine learning…

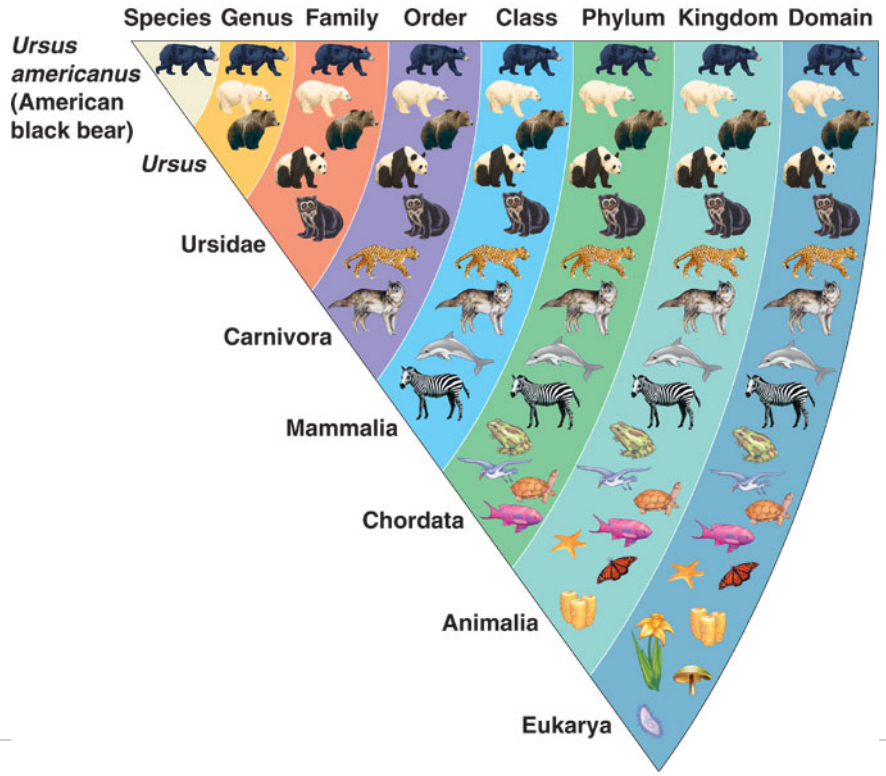
We even gave terms to the clusters: red, blue; big, small; good, bad…
Language is clustering of “reality” into words…

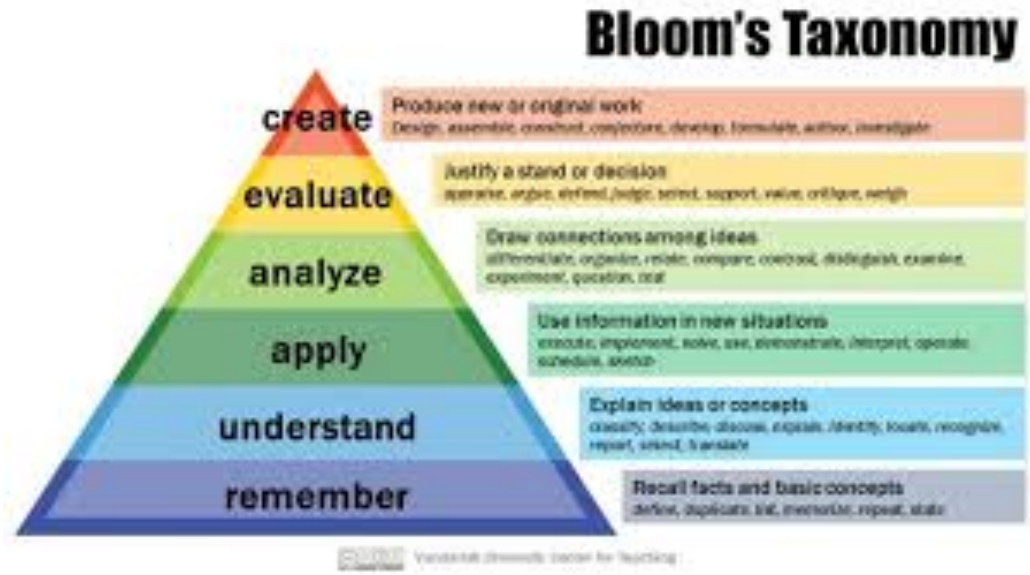
Clustering is old, vague, and subjective…



Taxonomy is clustering

Taxonomy (biology), a branch of science that encompasses
the description, identification, nomenclature, and classification of organisms
-- Wikipedia





Taxonomy
of Machine Learning/Statistics

Labeled Data

Indirect (reward)

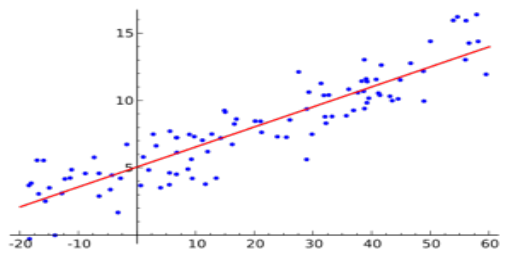
Unlabeled Data

Supervised Learning

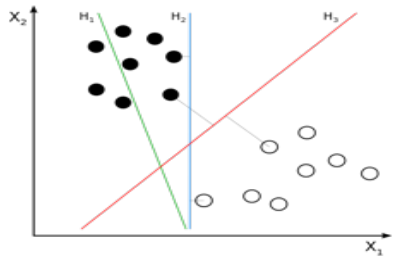
Reinforcement & Bandit Learning

Unsupervised Learning

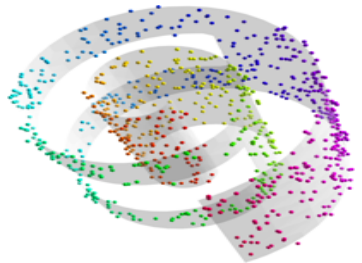
Regression



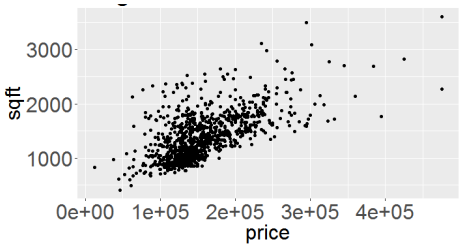
Classification



Dimensionality Reduction



Clustering



Clustering is a form of information reduction/organization

- To store in human finite memory (or computer's finite memory) and facilitate understanding

- To communicate between people (or processors) for more effective understanding between people and collective decisions

Effective decision-making is impossible based on raw big data

Understanding the Syria conflict

AGAINST ASSAD REGIME

TURKEY
GOALS: Depose the Assad regime in Syria. Curtail Syrian Kurdish groups affiliated with the PKK, a banned Kurdish group in Turkey.

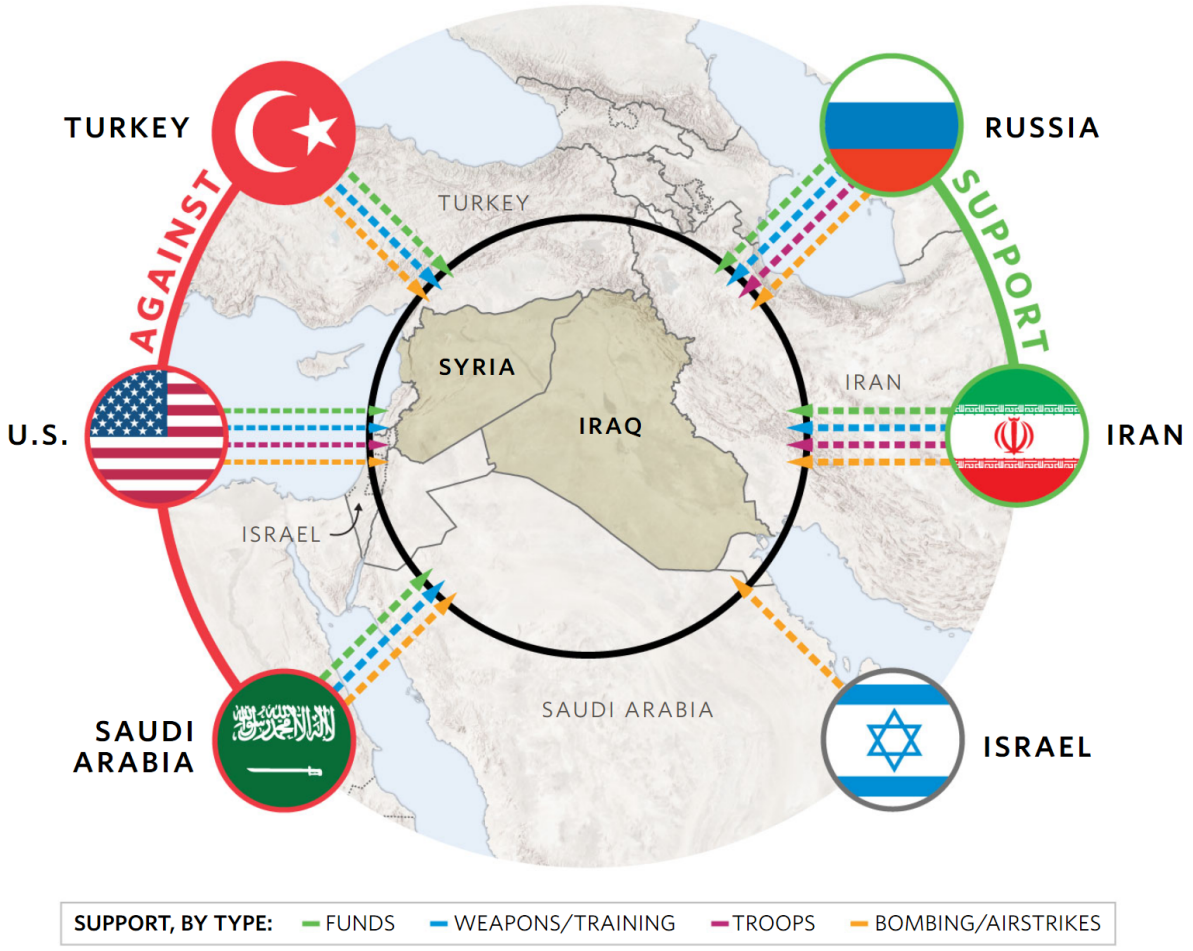
ACTIONS: Sends troops into Syria, backs Syrian rebel groups with weapons, funds and training.

U.S.
GOALS: With the help of Western and regional allies, degrade and ultimately defeat ISIS. Shore up the government in Iraq. Seek a political resolution to Syrian conflict, one that likely removes Assad.

ACTIONS: Strikes ISIS targets in both Syria and Iraq and assists Iraq, Kurdish and Syrian moderate forces with weapons, training and military advisers fighting ISIS.

SAUDI ARABIA
GOALS: Limit Iranian influence. Secure the ouster of the Assad regime. Combat ISIS.

ACTIONS: Provides financial backing to Syrian rebel groups fighting Assad. Limited participation in airstrikes against ISIS in Syria but not in Iraq.



SUPPORTS ASSAD REGIME

RUSSIA
GOALS: Prop up the Assad regime. Protect its naval facility in Syria, its only one in the Mediterranean. Constrain U.S. influence in the region and expand its own. Combat ISIS.

ACTIONS: Strikes moderate and Islamist Syrian rebels and, less frequently, ISIS. Provides weapons and advisers to the Syrian army. Shares intelligence with and sells weapons to Iraq.

IRAN
GOALS: Prop up the Assad regime. Secure the Shiite-dominated government in Iraq. Combat ISIS. Limit Saudi influence and bolster the rival Shiite axis.

ACTIONS: Provides weapons, military guidance and fighters to Iraq and Syria.

ON THE SIDELINES

ISRAEL
GOALS: Contain the rise of Iranian influence and the growth of Hezbollah's arsenal in Lebanon.

ACTIONS: Largely staying out of the Syrian conflict. Struck some Hezbollah targets in Syria with airstrikes. Provided limited medical help to some Syrian rebels.

Tangled Alliances Graphic In “Airstrike Raises Tension with Tehran” in WSJ, April 8, 2017

Very helpful **clustered** information in terms of countries and important dimensions to consider.

One criticism: country names could be placed better, not associated with the bars.

Syria conflict

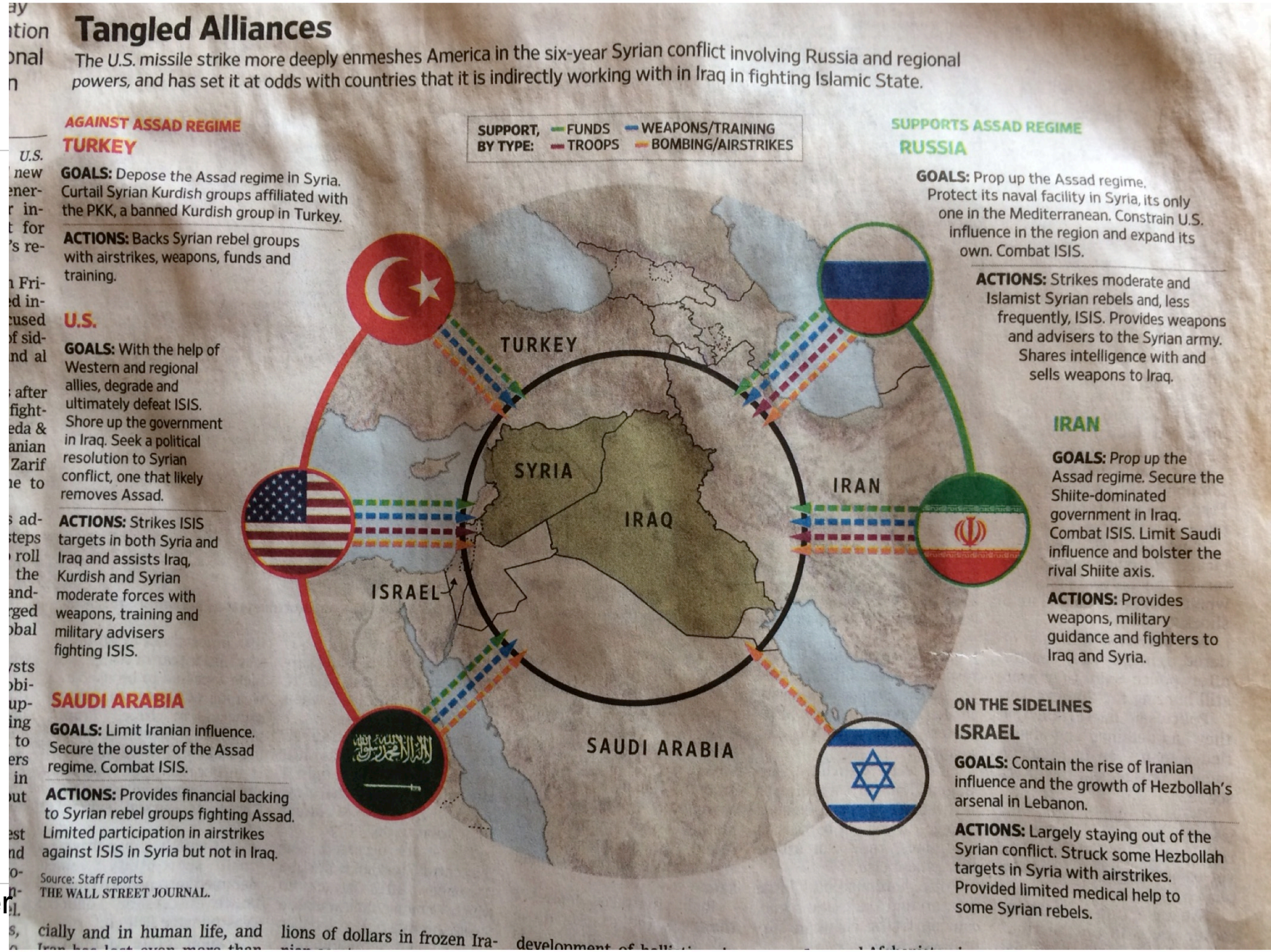
Tangled Alliances Graphic in

“Airstrike Raises Tensions with Tehran”

WSJ, April 8, 2017

Very helpful **clustered** information in terms of countries and important dimensions to consider.

One criticism: country names could be placed better, not associated with the bars- more pronounced in the paper version



QPRV in the context of Ames data

- Q (not unique: translating Q in English into a Q about data…)

To understand the data better and discover heterogeneity, which is ever present in data, especially in big data; to generate hypotheses to confirm with new data

- P: all houses in tax office from 2006-2010 in Ames
- R: yes, we did simple random sampling
- -
- V: do the clusters correspond to clusters in the population?

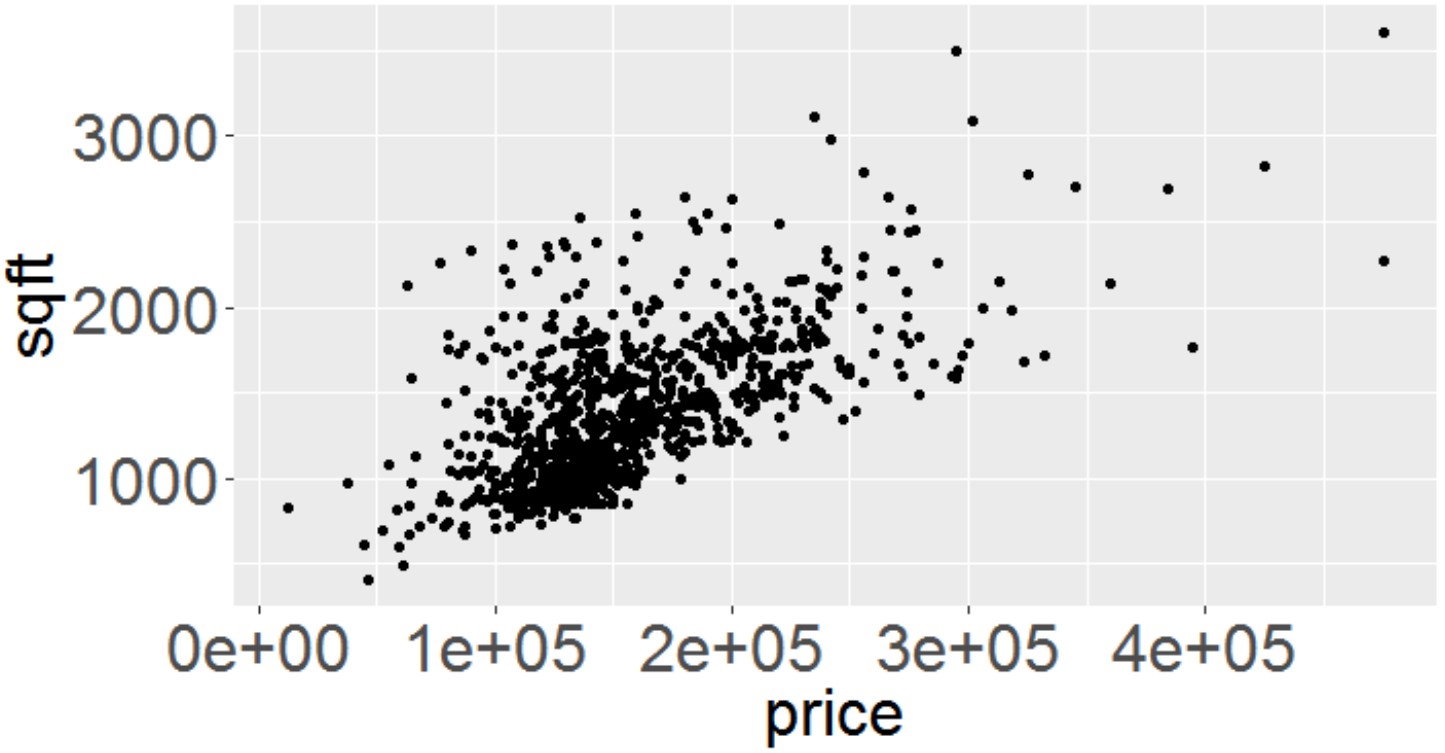
New name: PQRS (thanks to a discussion with Andrew)

- P: Population
- Q: Question
- R: Representativeness

…

- **S for Scrutinizing**

Raw and transformed (population) Ames data



How do we Compute a Clustering?

Many different clustering models and algorithms:

- Feature based Clustering: *Points in R^d*
  - **K-Means** (aka Lloyd-Max in signal processing)
    alternate minimization between finding centers and cluster memberships

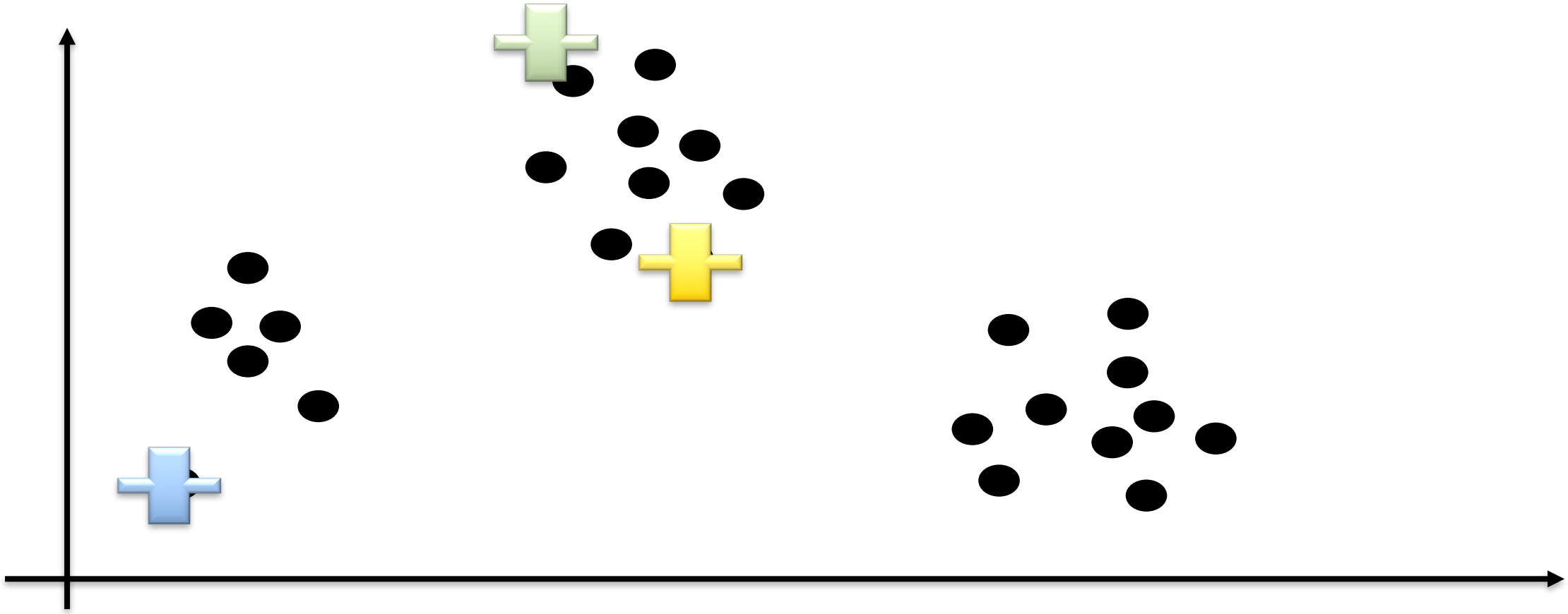
  - Expectation-Maximization (EM) (earliest example I know is from stat. genetics)

  - Spectral Methods: PCA (principal component analysis)+K-means on weighted or transformed data

- Hierarchical Clustering: feature based or not
  clustering in a greedy fashion, widely used in biology

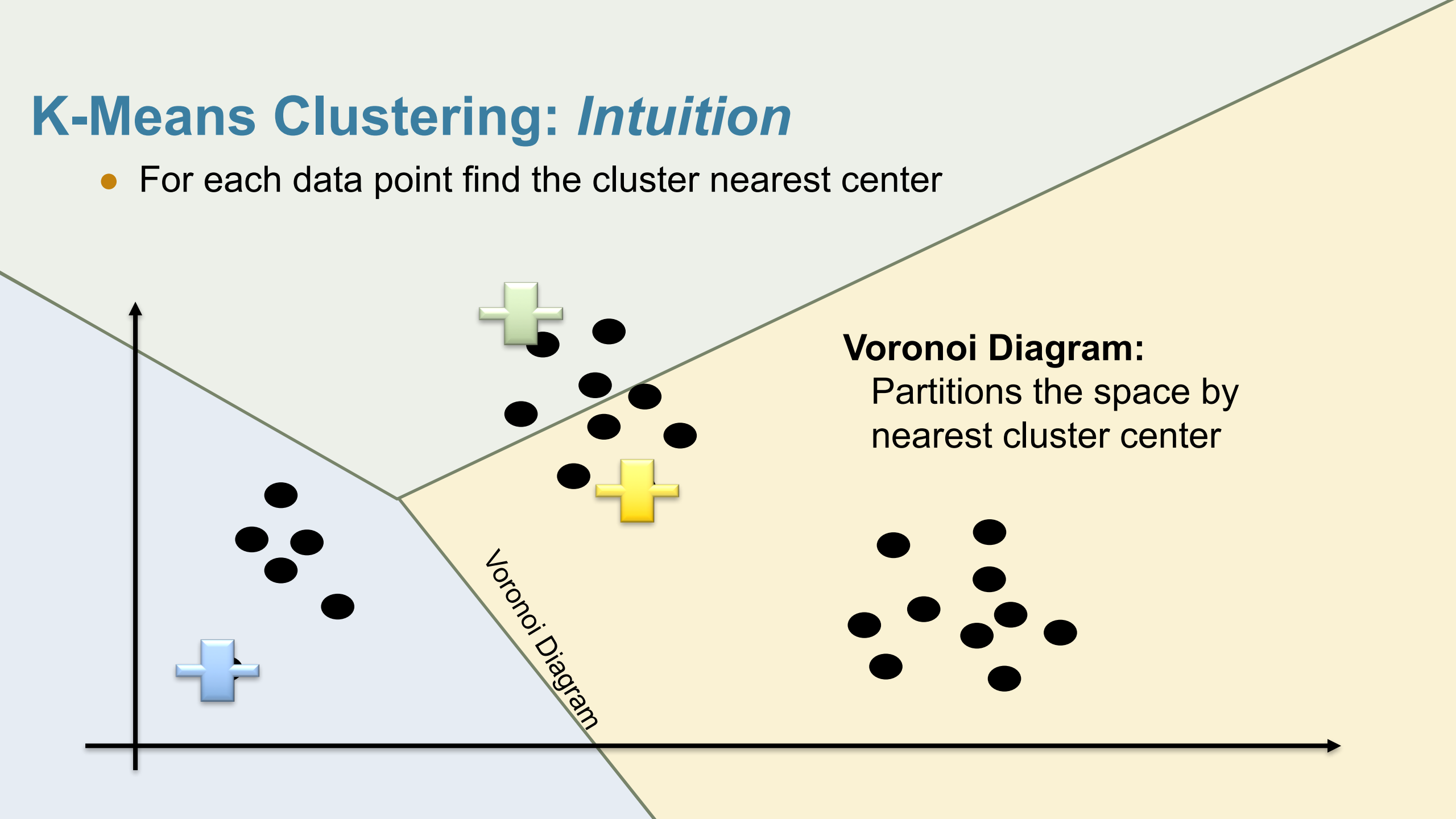
K-Means Clustering: *Intuition*

- Input K: The number of clusters to find
- Pick an initial set of points as cluster centers



K-Means Clustering: *Intuition*

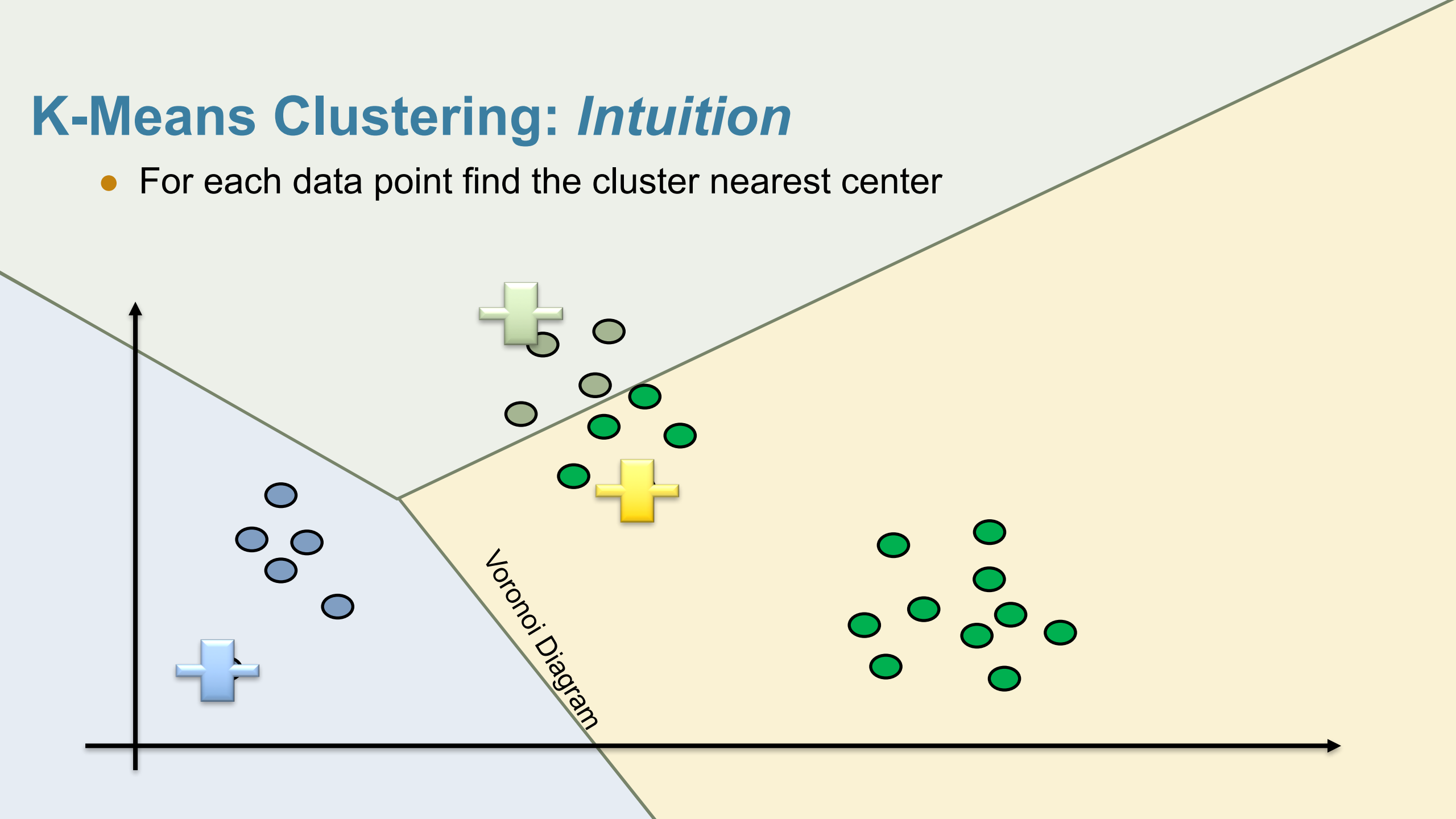
- For each data point find the cluster nearest center



Voronoi Diagram:
Partitions the space by nearest cluster center

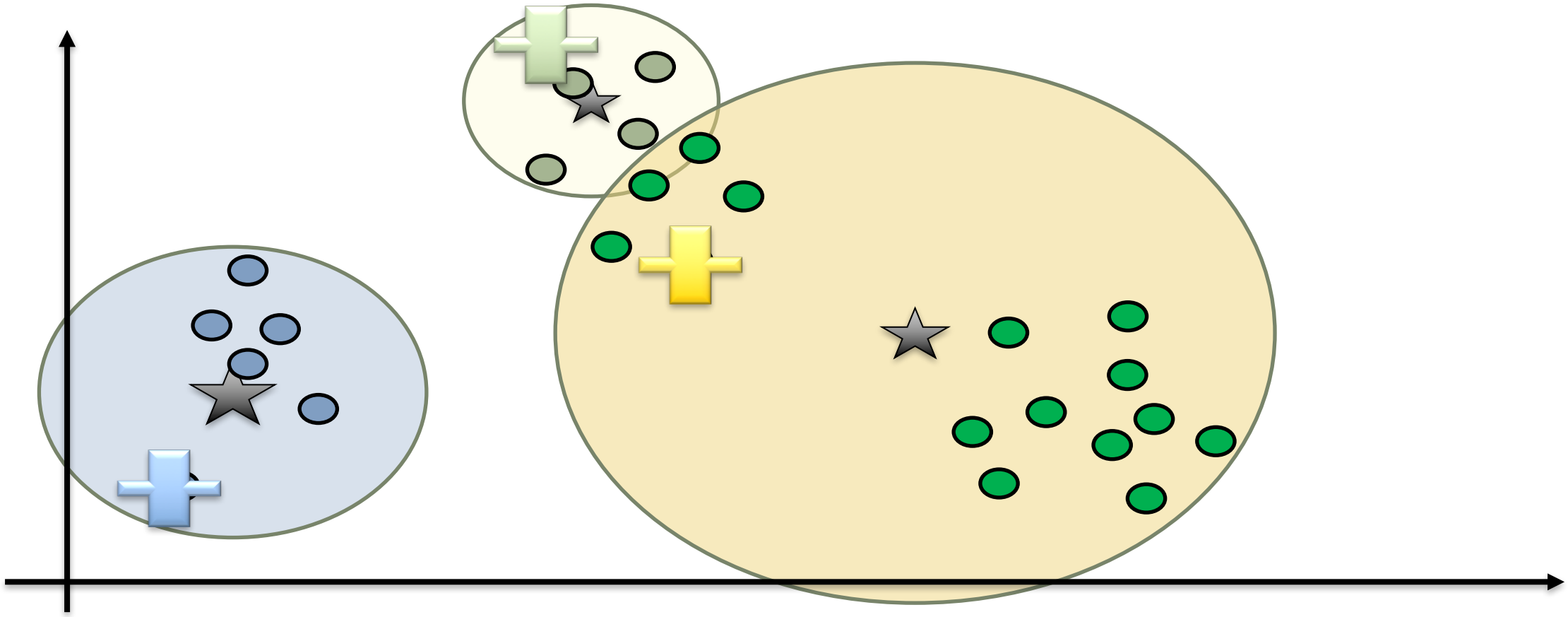
K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



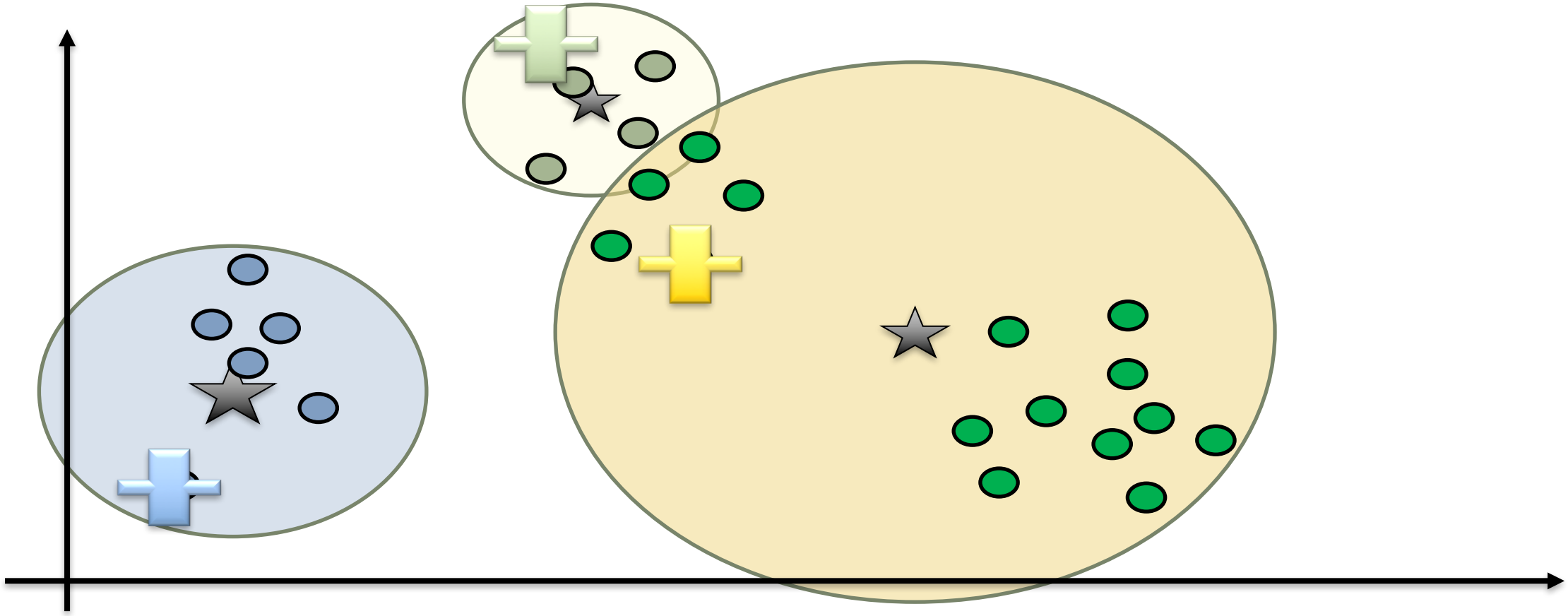
K-Means Clustering: *Intuition*

- Compute mean of points in each “cluster”



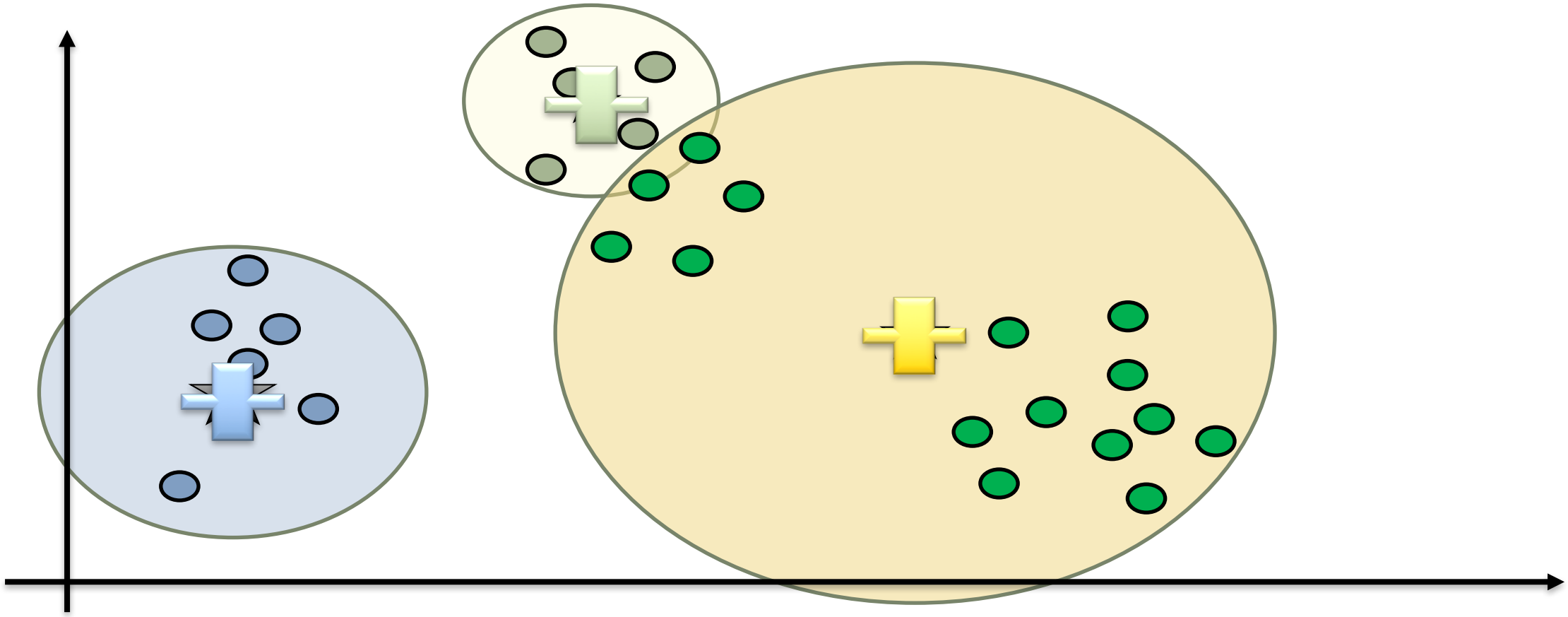
K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster



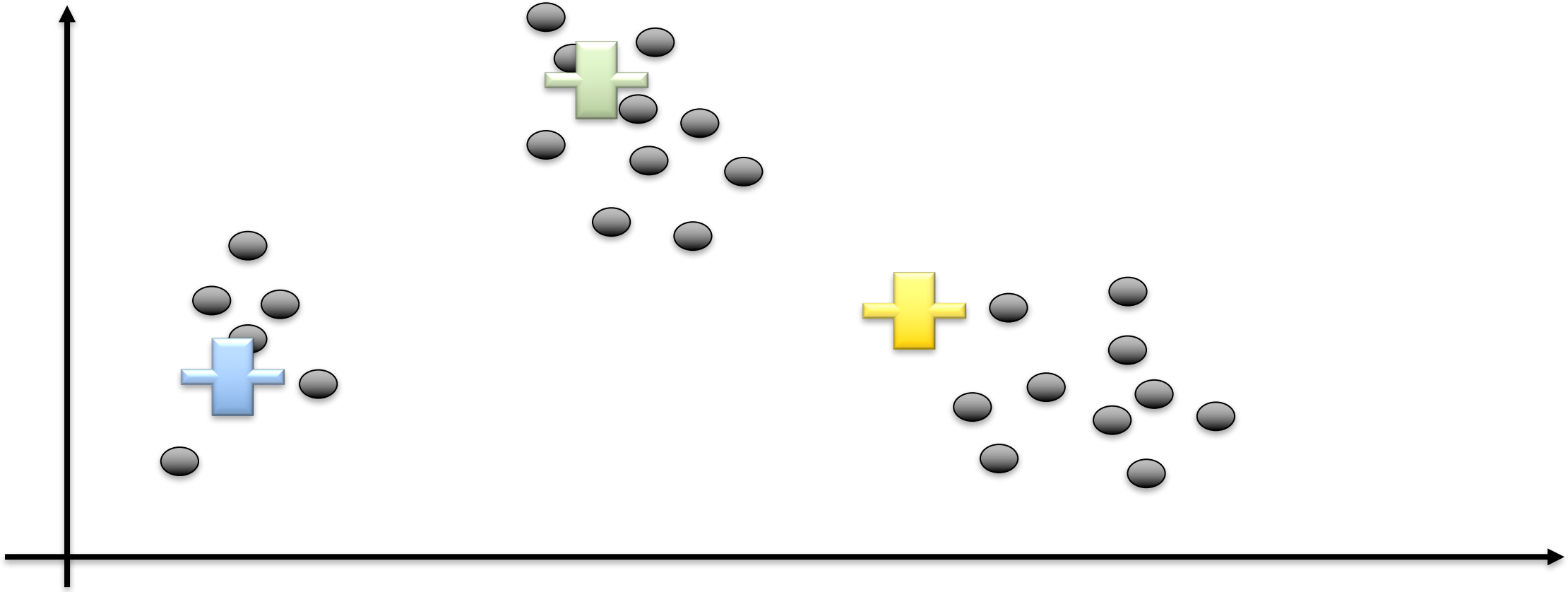
K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster



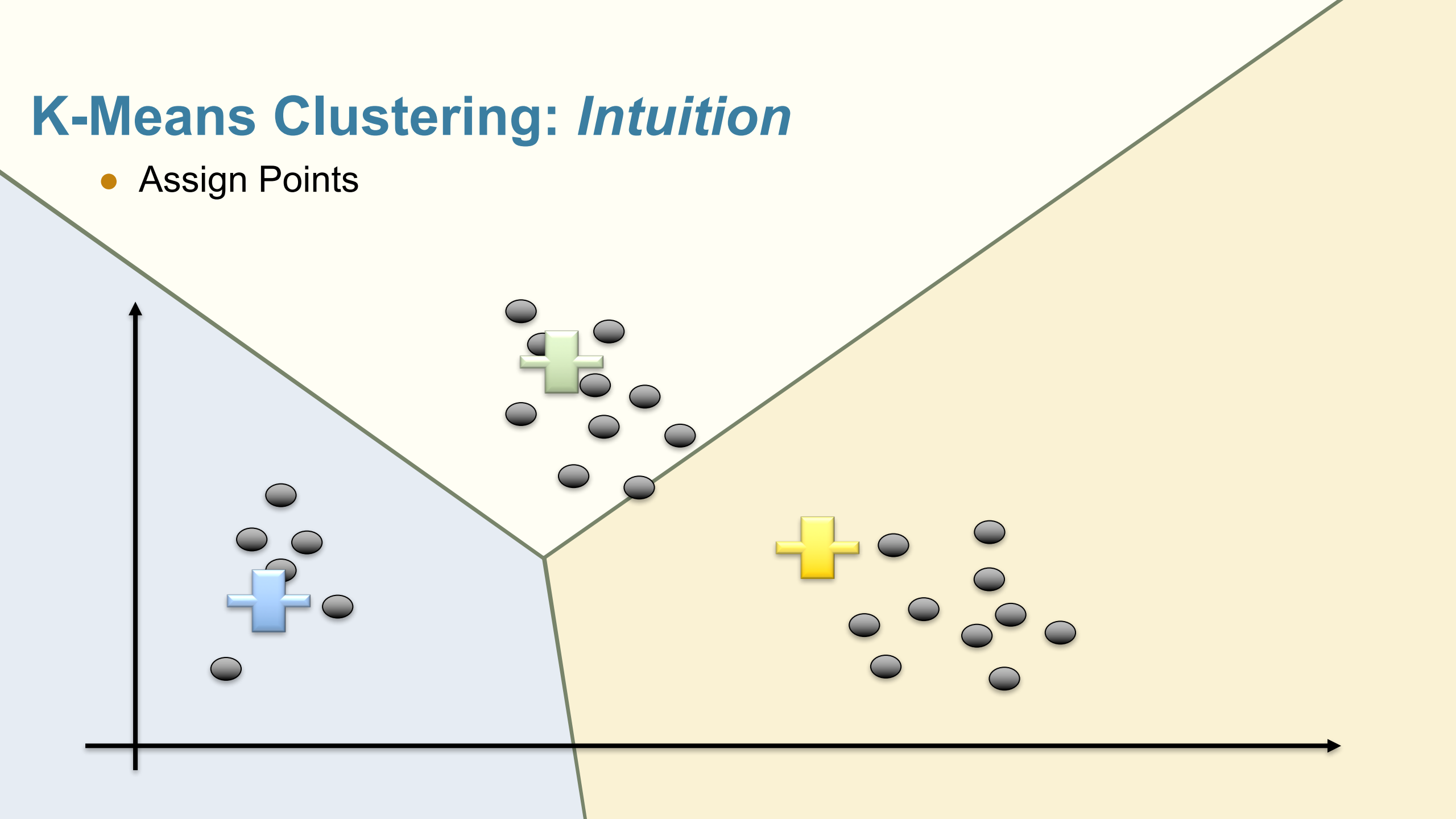
K-Means Clustering: *Intuition*

- Improved?
- Repeat



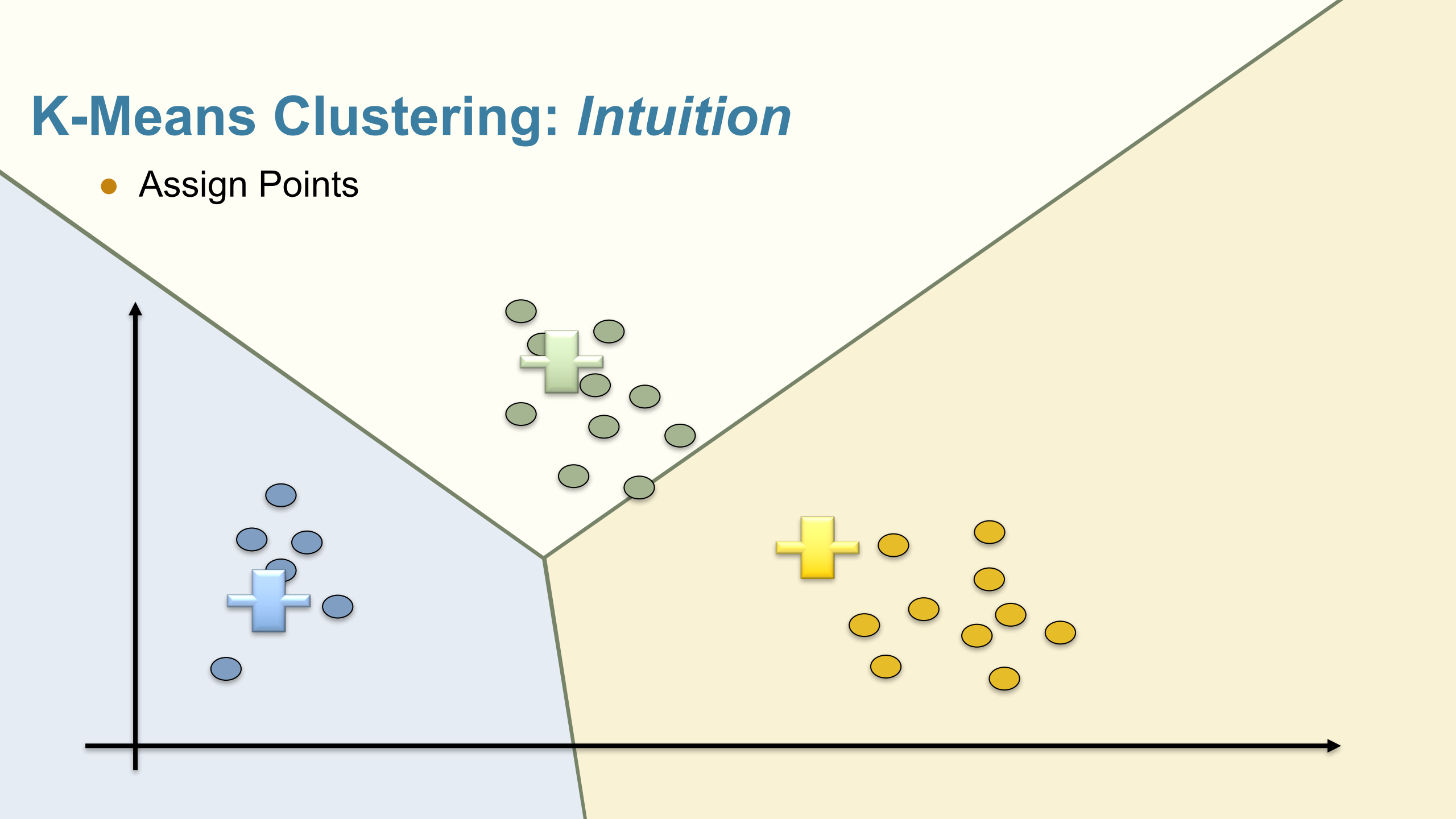
K-Means Clustering: *Intuition*

- Assign Points



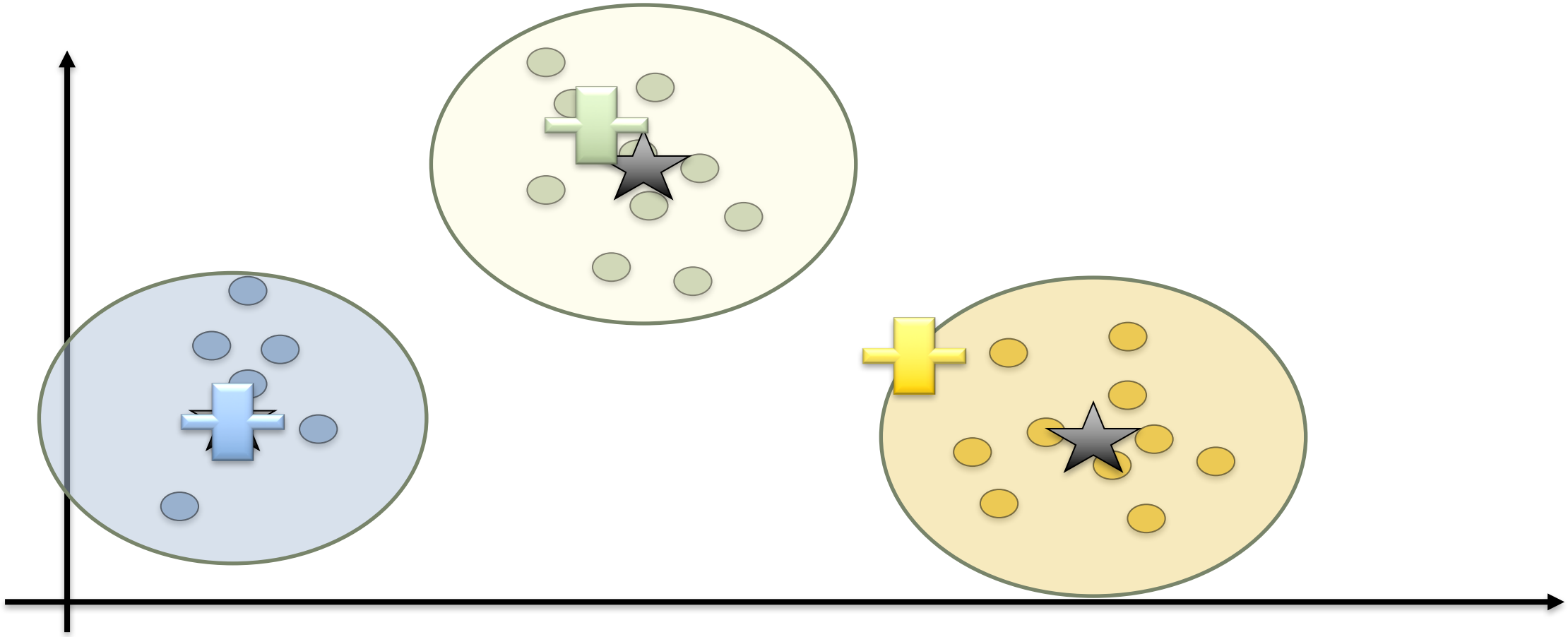
K-Means Clustering: *Intuition*

- Assign Points



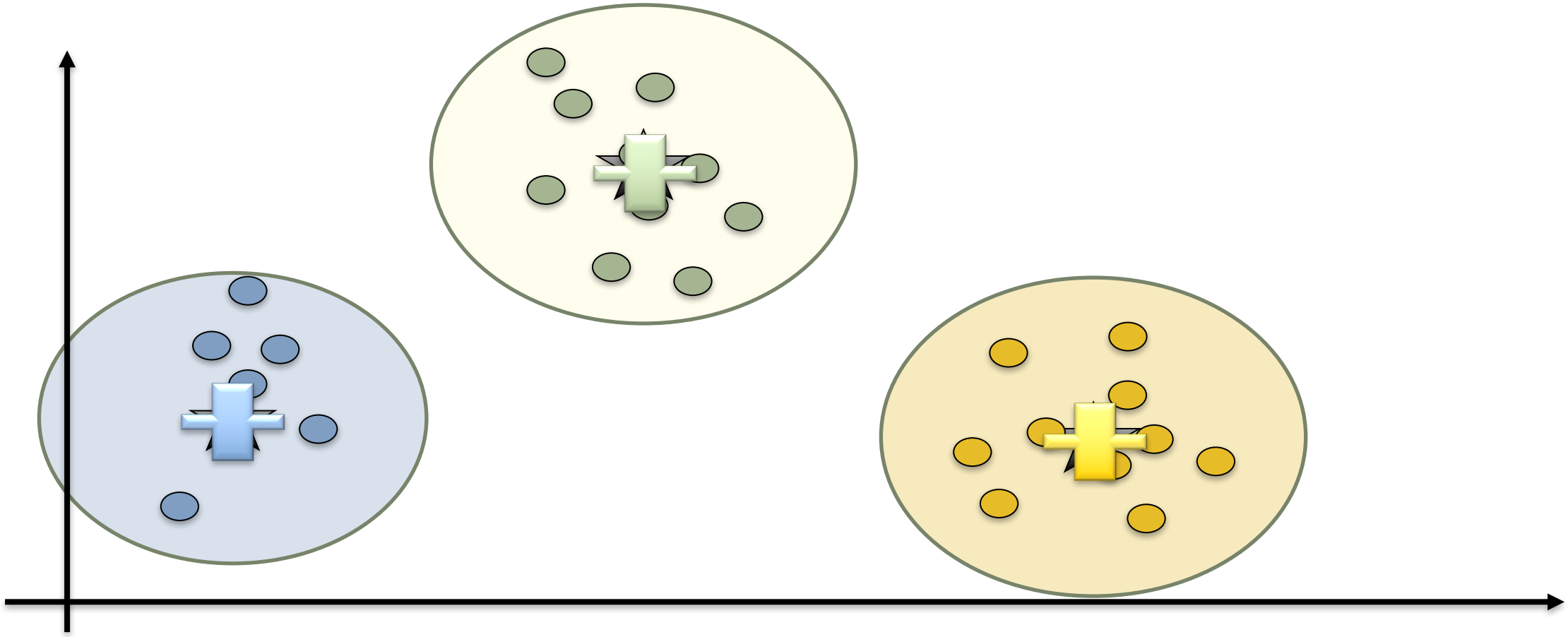
K-Means Clustering: *Intuition*

- Compute cluster means



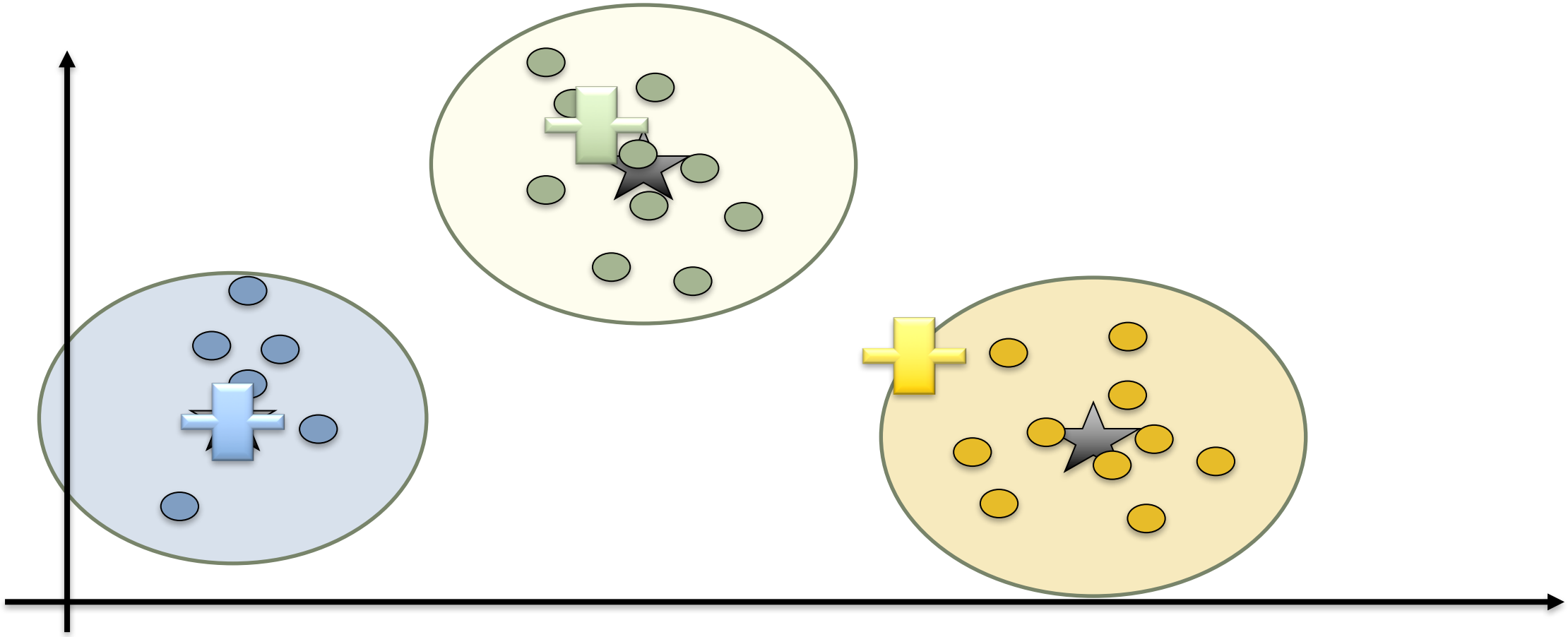
K-Means Clustering: *Intuition*

- Update cluster centers



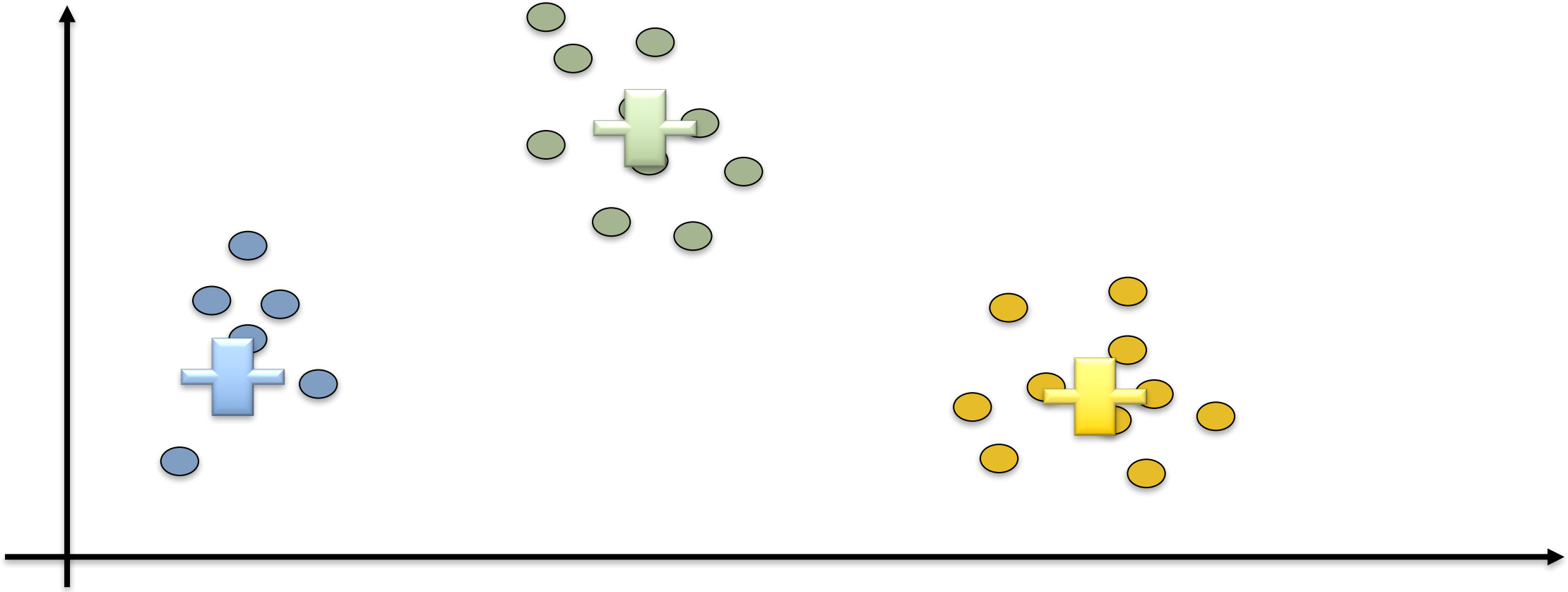
K-Means Clustering: *Intuition*

- Update cluster centers



K-Means Clustering: *Intuition*

- Repeat?
  - Yes to check that nothing changes → Converged!



K-Means Algorithm for a given k: Details

```
centers ← pick k initial Centers

while (centers are changing) {
   // Compute the assignments
   asg ← [(x, nearest(centers, x)) for x in data]
```

What do we mean by “nearest”?
A: Squared Euclidean distance

K-Means Algorithm: Details

```
centers ← pick k initial Centers

while (centers are changing) {
   // Compute the assignments
   asg ← [(x, nearest(centers, x)) for x in data]

   // Compute the new centers
   for j in range(K):
      centers[j] =
         mean([x for (x, c) in asg if c == j])
}
```

K-Means Algorithm: Details

```
centers ← pick k initial Centers

while (centers are changing) {
   // Compute the assignments
   asg ← [(x, nearest(centers, x)) for x in data]

   // Compute the new centers
   for j in range(k):
      centers[j] =
         mean([x for (x, c) in asg if c == j])
}
```

Guaranteed to converge!

… to what?

To a local optimum. ☹

Depends on Initial Centers

K-means global loss function for K clusters: n → K

Given n data points with feature vector x_i , we want

- a partition of the index set {1,…,n} into k subsets $I_1 = \{1, 3, 5\}, I_2, ..., I_K$
- and its associated cluster centers $c_1, c_2, \ldots, c_K$

K-means algorithm minimizes the following global loss function for a distance metric d (e.g. squared Euclidean distance) by alternating the minimizations over the partition and centers:

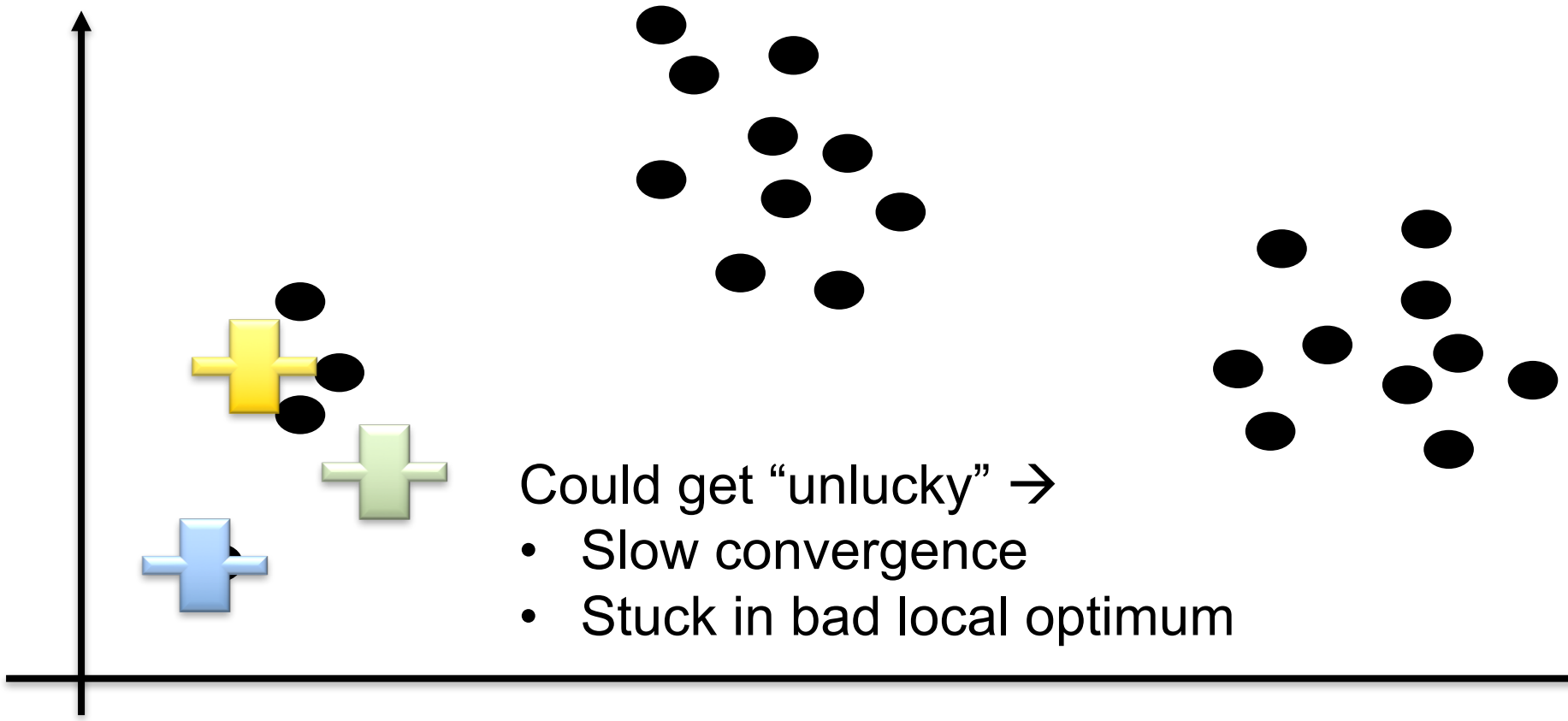
$$\sum_{j=1}^{K} \sum_{x_i : i \in I_j} d(x_i, c_j)$$

where the inner sum is over data points in a particular cluster j, and the outer sum is over the clusters

When d is absolute value loss, we have the group medians as the centers.

Picking the Initial Centers

- **Simple Strategy:** select *k* data points at random
  - What could go wrong?



Could get "unlucky" →

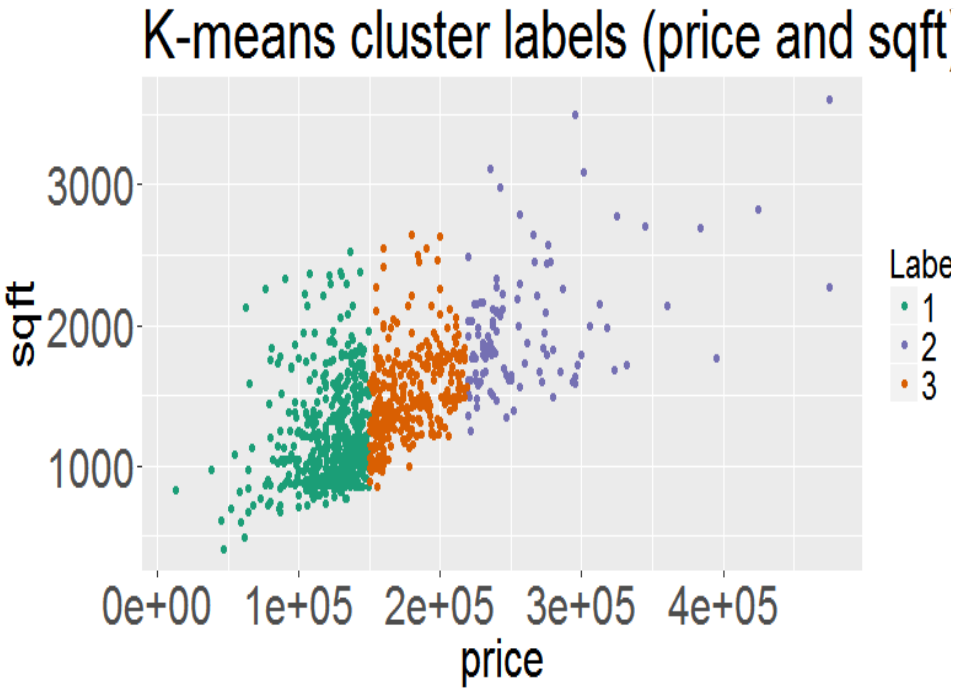
- Slow convergence
- Stuck in bad local optimum

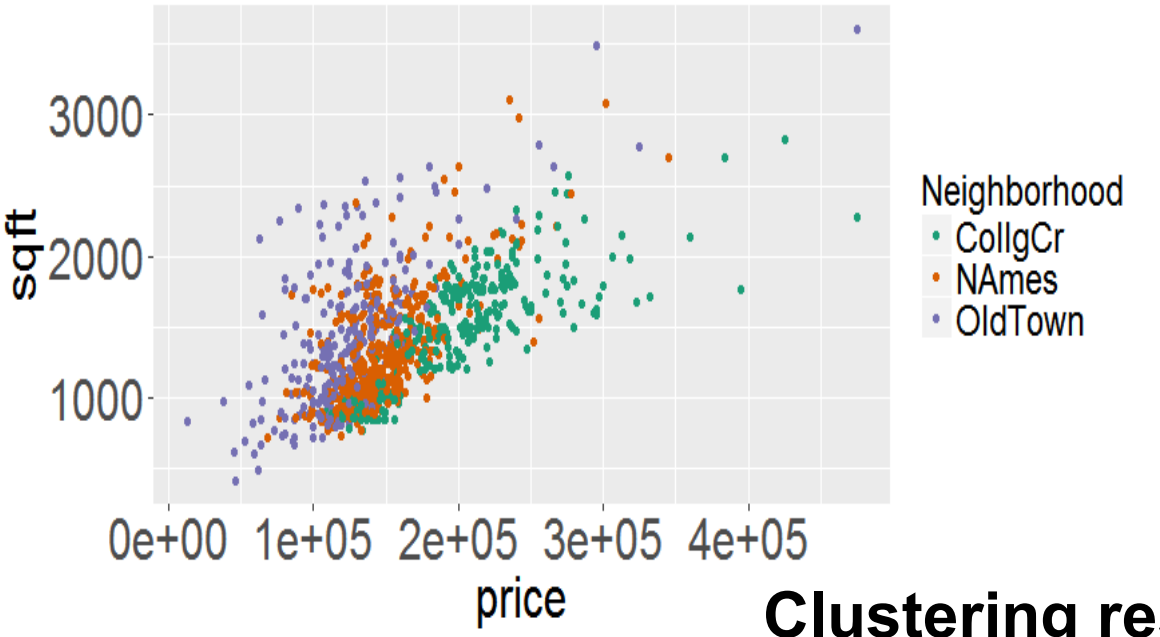
K-means with 3 clusters:
random picked data points as initial centers

Clustering results with NB labels

prop. In each row category

	1	2	3
NAmes	0.58	0.05	0.37
CollgCr	0.39	0.51	0.10
OldTown	0.28	0.04	0.68

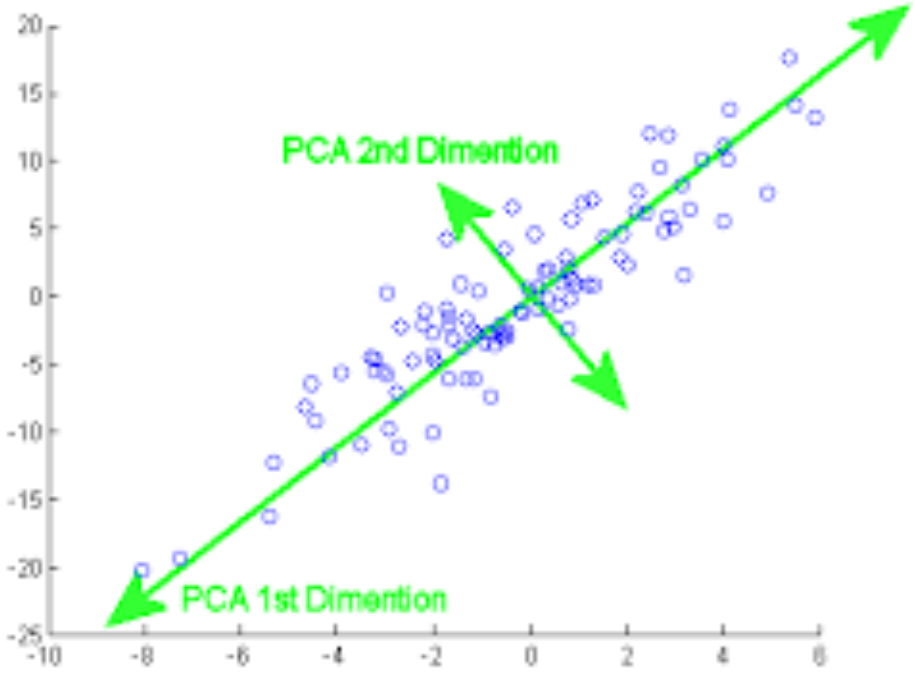




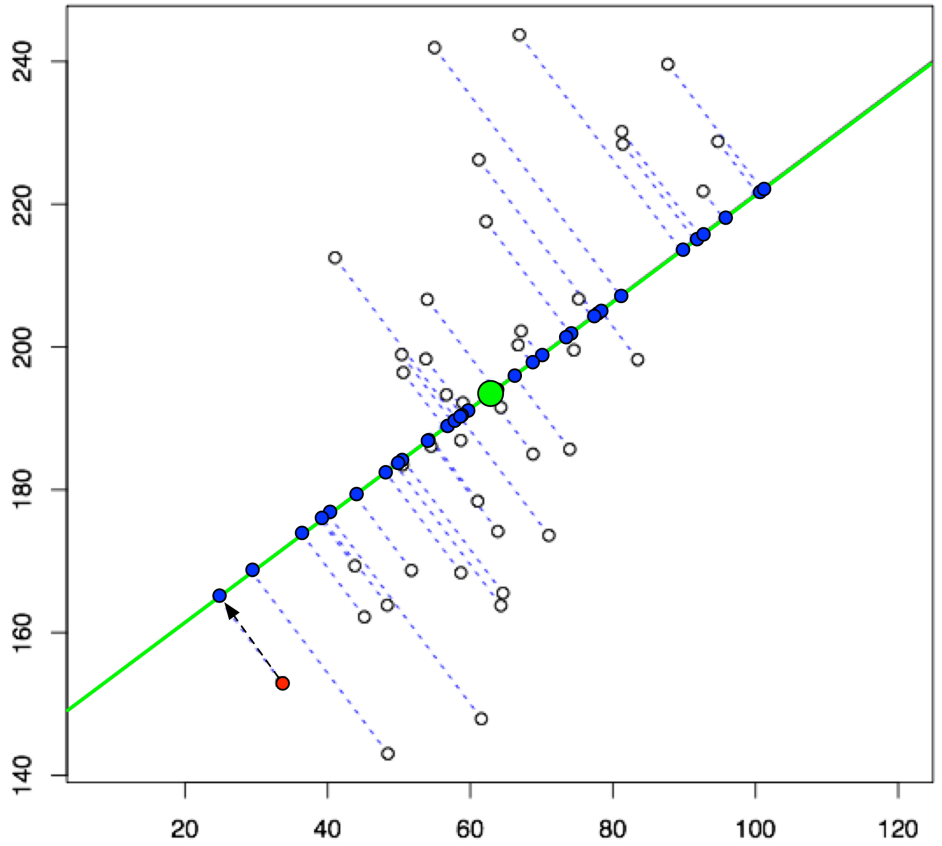
Clustering results are vetted or "scrutinized" by neighborhood labels

Principal Component Analysis (PCA)

PCA in a graph



Projecting to first PCA direction
to reduce data to 1-dim



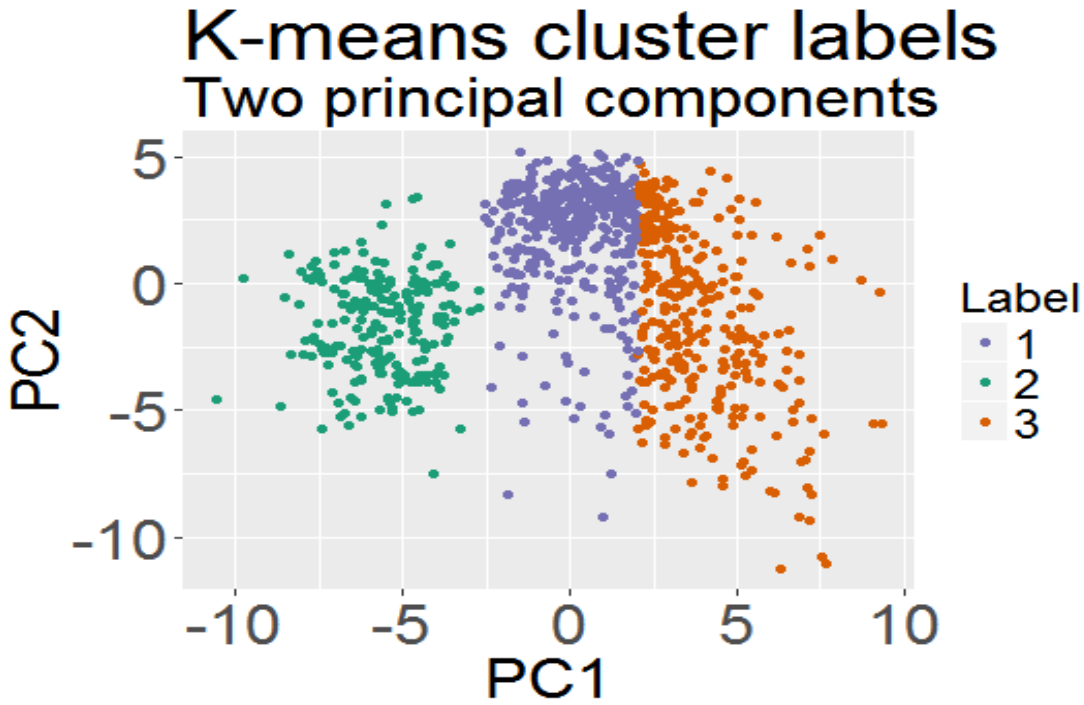
Data projected to first two PCAs give much better results

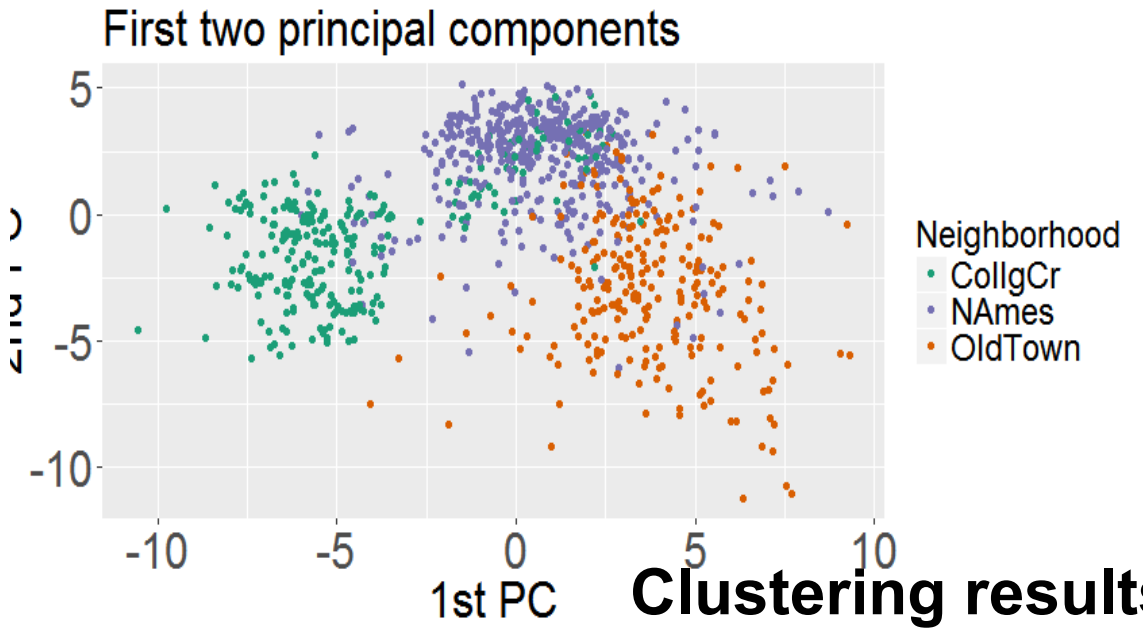
using all 81 features (untransformed)

Prop. In each row category

	1	2	3
NAmes	0.83	0.14	0.03
OldTown	0.05	0.95	0.00
CollgCr	0.17	0.02	0.81

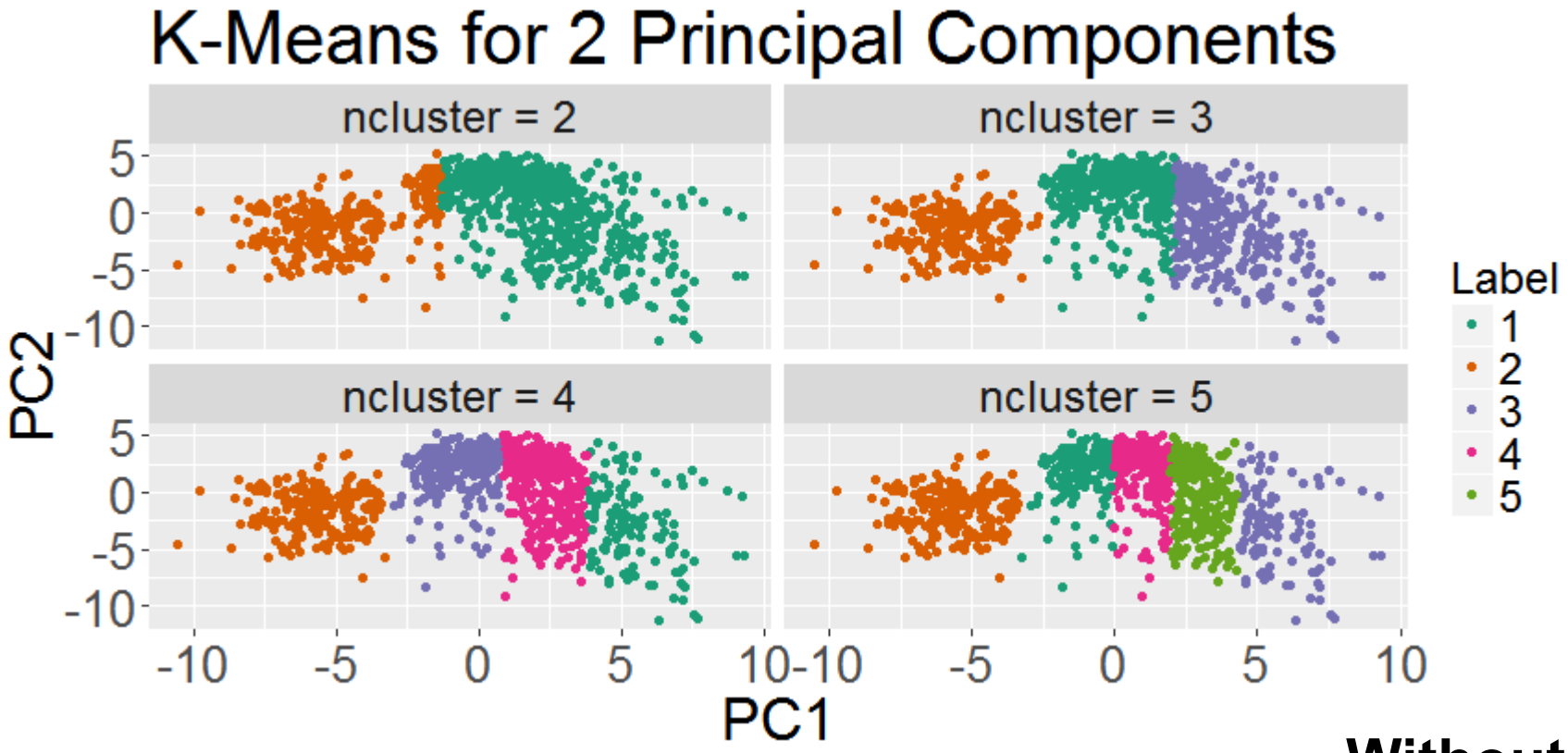
Clustering results with NB labels





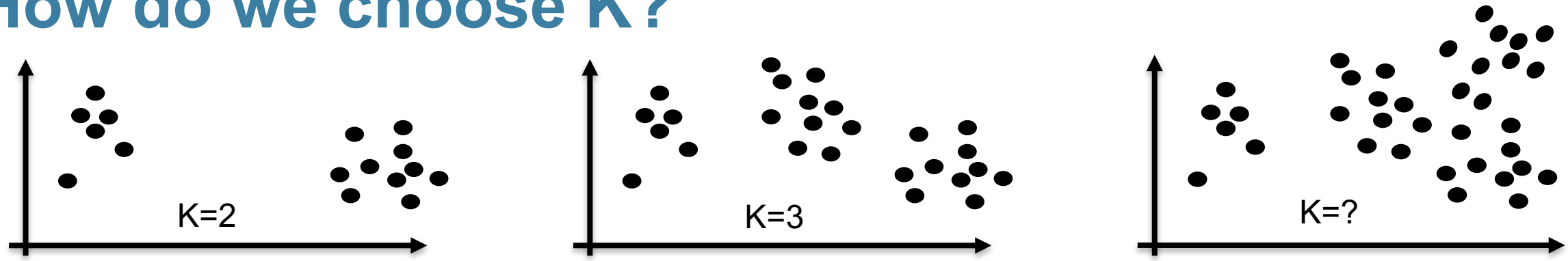
Clustering results are vetted or "scrutinized" by neighborhood labels

K-means results for K=2, 3, 4, 5: relying on first PC heavily

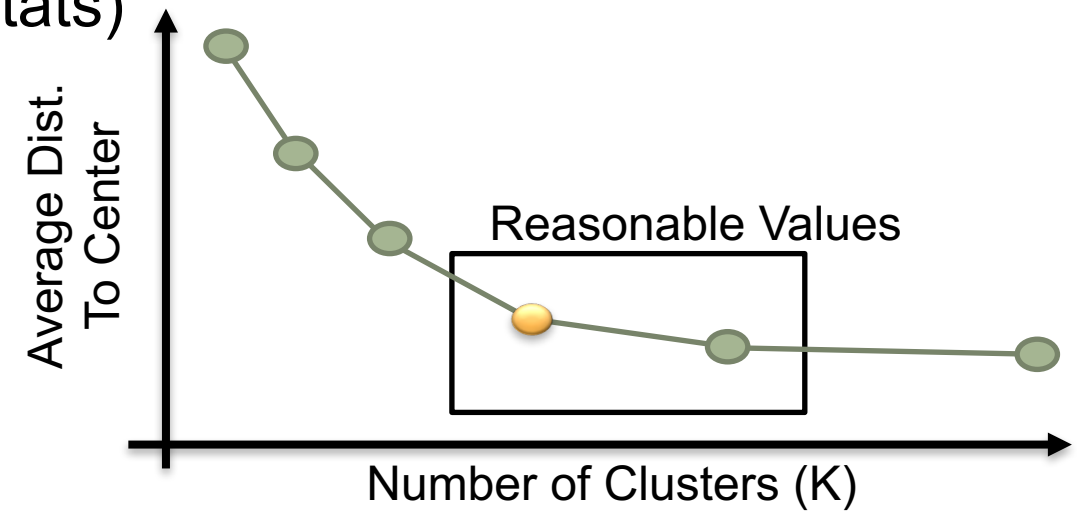


Without NB info, hard to know which K to use.

How do we choose K?



- Basic Elbow Method (you may try this out in your HW if you like)
- Try range of K values and plot average distance to centers
- Silhouette (graphical method, popular in stats)
- Cross-Validation (Better)
  - Repeatedly split the data into training and validation datasets
  - Cluster the training dataset
  - Measure avg. dist. To centers on validation data



Silhouette (Peter J. Rousseeuw, 1986): graphic method for K selection

Given k and k clusters, given any data point i , let a_i
be the average distance or dissimilarity of i with all other points in the same cluster.
For Euclidean k-means, use Euclidean distance for dissimilarity

a_i measures how well i fits into its cluster.
b_i is the smallest average distance of i to other clusters

$$s_i = \frac{b_i - a_i}{max(b_i, a_i)}$$ which is between -1 and 1.

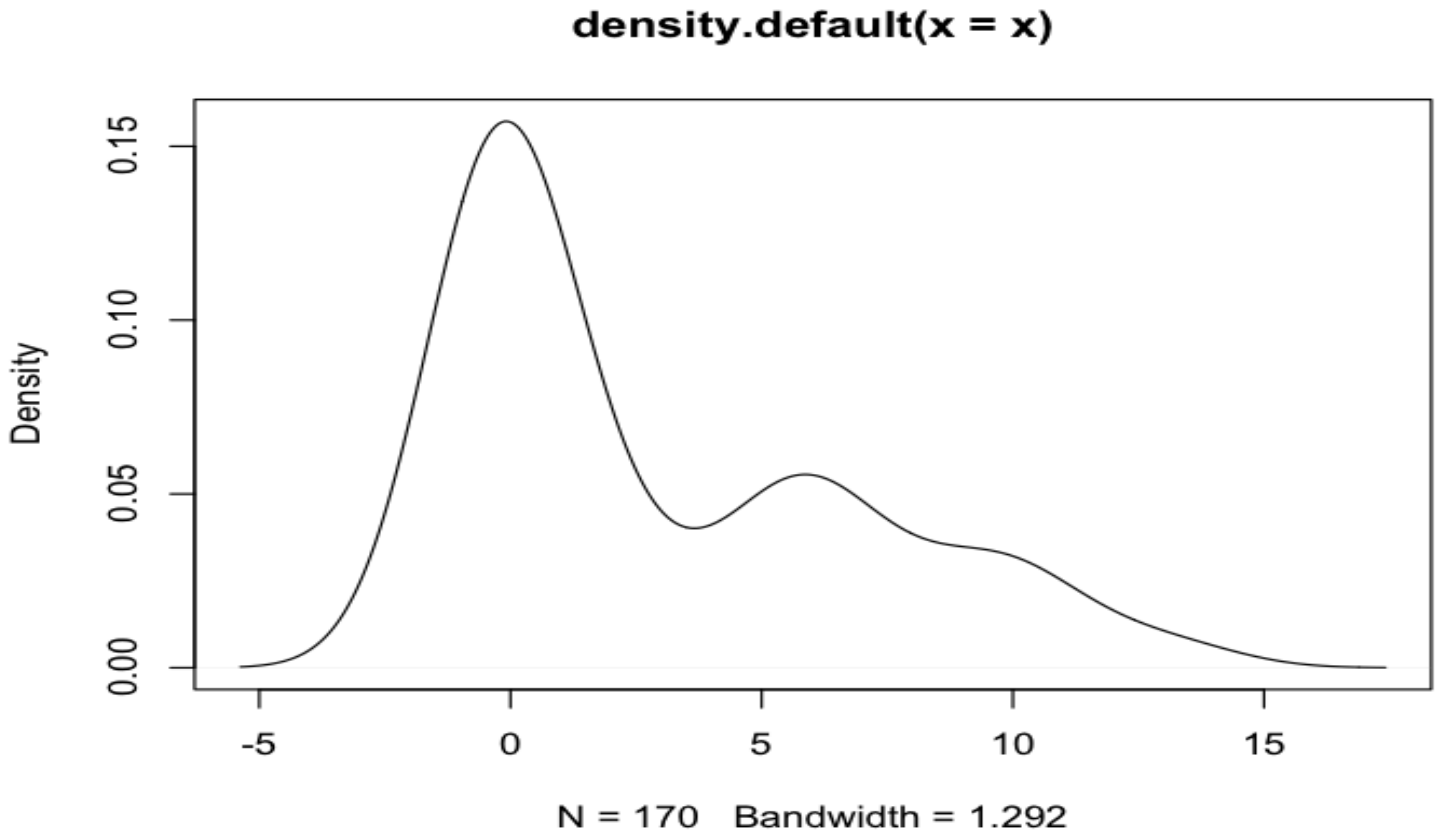
s_i is close to 1 if point i is in a tight cluster and far away from other clusters; close to -1, if it is in a loose cluster and close to other clusters.

Maximize $\frac{1}{n}\sum_{i=1}^{n} s_i$ over k.

Trying out Silhouette with simulated data

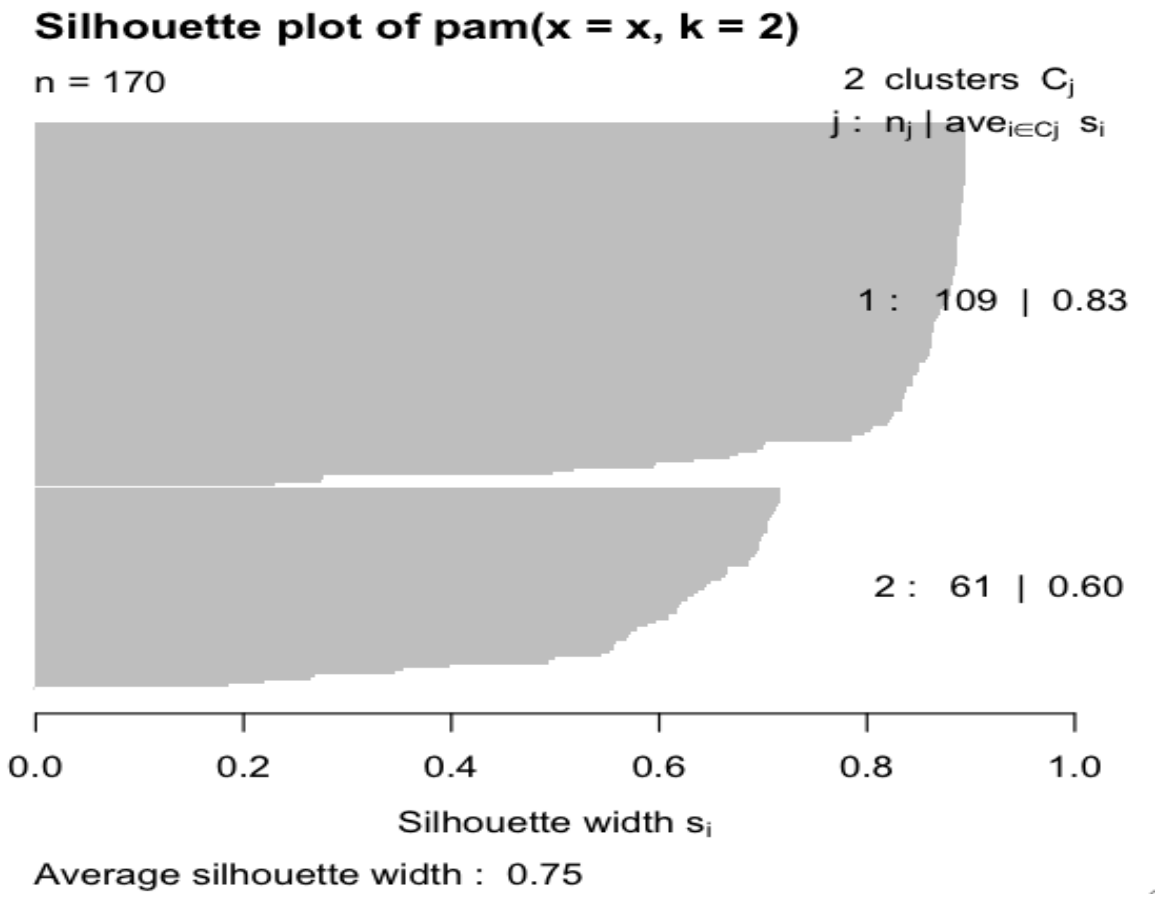
Example 1: simulated data from mixture of 3 Gaussians of n=170
N(0, 1), N(5, 4), and N(8, 9), with proportions 0.58, 0.17, and 0.23

The third Gaussian centered at 8 is not very visible.



Trying out Silhouette with 2-cluster data

Example 1: Silhouette for the results of two-clusters using pam, which is Euclidean K-means with the K-means centers as the data points closest to centers



Summary

- Clustering is an old activity and is used for information organization
- New name: PQRS
- One clustering method -- K-means algorithm: initial values, choice of K

  Euclidean distance in K-means corresponds to taking means – sensitive to outliers because of the squared Euclidean distance; using median corresponds to absolute loss function, robust.
- We do not always have labels to compare – other “S” investigation is needed to back up why the clustering results are meaningful in context
- PCA – dimensionality reduction (details to come)