UNSUPERVISED LEARNING

David Kauchak
CS 158 – Fall 2025

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Administrative

Final project
- Project proposal feedback on Gradescope
- Progress report due Sunday

Midterm 2

No office hours next Mon/Tue

Class next Tuesday?

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Supervised learning

label

label$_1$

label$_3$

label$_4$

label$_5$

model/ predictor

Supervised learning: given labeled examples

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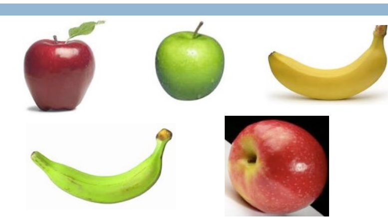
Unsupervised learning



Unsupervised learning: given data, i.e. examples, but no labels

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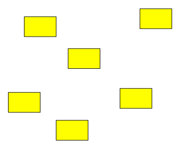
Unsupervised learning



Given some example without labels, do something!

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Unsupervised applications areas

learn clusters/groups without any label

customer segmentation (i.e. grouping)

image compression

bioinformatics: learn motifs

find important features

…

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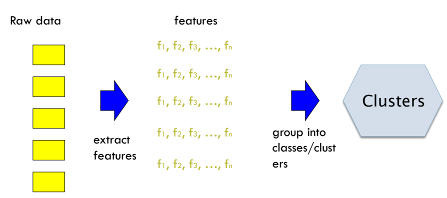
Unsupervised learning: clustering



No "supervision", we're only given data and want to find natural groupings

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Unsupervised learning: modeling

Most frequently, when people think of unsupervised learning they think of clustering

Another category: learning probabilities/parameters for models without supervision

- Learn a translation dictionary
- Learn a grammar for a language
- Learn the social graph

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Clustering

Clustering: the process of grouping a set of objects into classes of similar objects

Applications?

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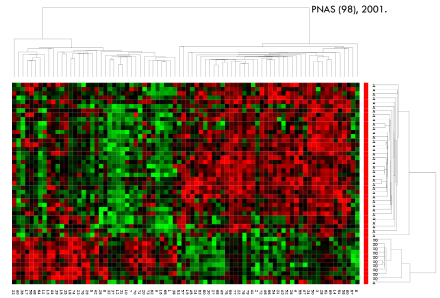
Gene expression data

Data from Garber et al. PNAS (98), 2001.



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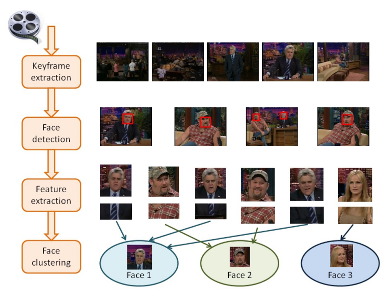
Face Clustering



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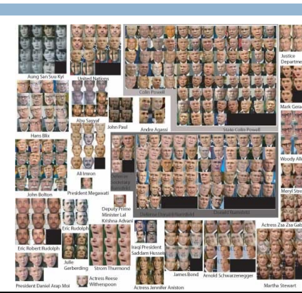
Face clustering



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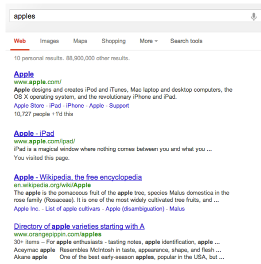
Search result clustering



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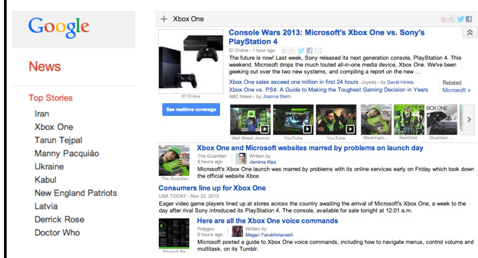
Google News



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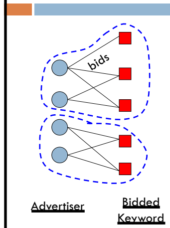
Clustering in search advertising



~10M nodes

Find clusters of advertisers and keywords
- Keyword suggestion
- Performance estimation

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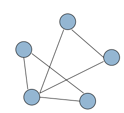
Clustering applications



Who-messages-who IM/text/twitter graph

~100M nodes

Find clusters of users
- Targeted advertising
- Exploratory analysis

Clusters of the Web Graph
- Distributed pagerank computation

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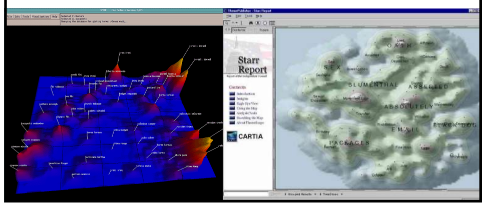
Data visualization

Wise et al, "Visualizing the non-visual" PNNL

ThemeScapes, Cartia

- [Mountain height = cluster size]



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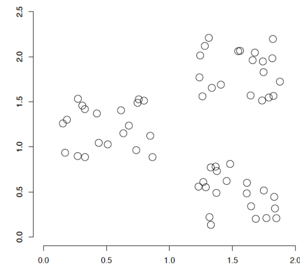
A data set with clear cluster structure



What are some of the issues for clustering?

What clustering algorithms have you seen/used?

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Issues for clustering

Representation for clustering
- How do we represent an example
  - features, etc.
- Similarity/distance between examples

Flat clustering or hierarchical

Number of clusters
- Fixed a priori
- Data driven?

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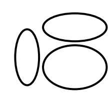
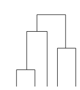
Clustering Algorithms

Flat algorithms
- Usually start with a random (partial) partitioning
- Refine it iteratively
  - K means clustering
  - Model based clustering
- Spectral clustering



Hierarchical algorithms
- Bottom-up, agglomerative
- Top-down, divisive



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Hard vs. soft clustering

Hard clustering: Each example belongs to exactly one cluster

Soft clustering: An example can belong to more than one cluster (probabilistic)

- Makes more sense for applications like creating browsable hierarchies
- You may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes

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K-means

Most well-known and popular clustering algorithm:

Start with some initial cluster centers

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

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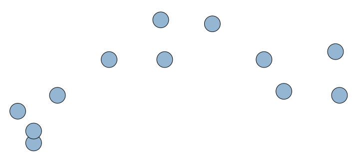
K-means: an example



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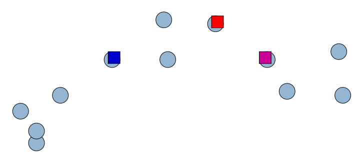
K-means: Initialize centers randomly



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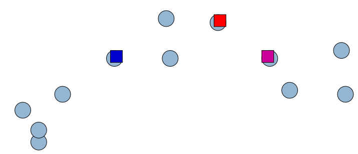
K-means: Initialize centers randomly



What points are closest?

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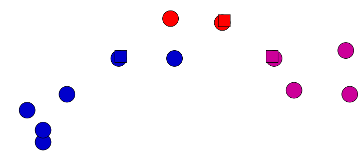
K-means: assign points to nearest center



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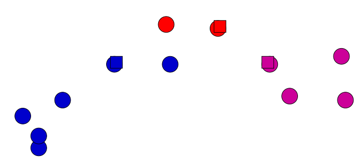
K-means: assign points to nearest center



Where are the new centers?

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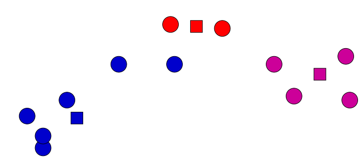
K-means: readjust centers



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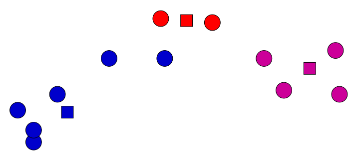
K-means: readjust centers



What points are closest?

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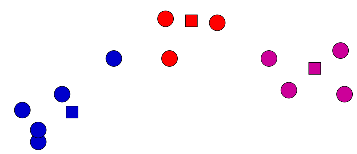
K-means: assign points to nearest center



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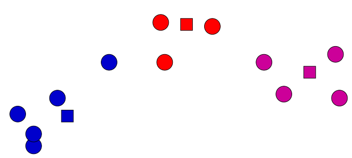
K-means: assign points to nearest center



Where are the new centers?

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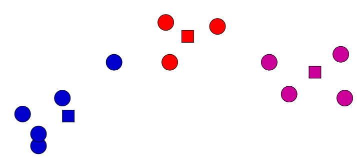
K-means: readjust centers



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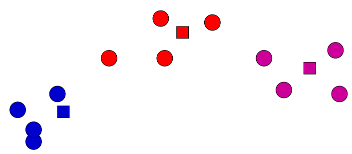
K-means: assign points to nearest center



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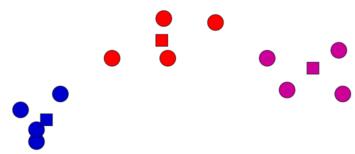
K-means: readjust centers



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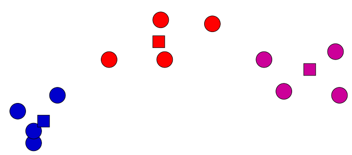
K-means: readjust centers



When do we stop?

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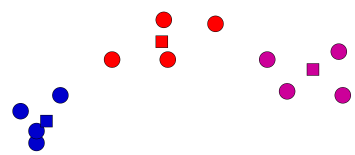
K-means: assign points to nearest center



No changes: Done

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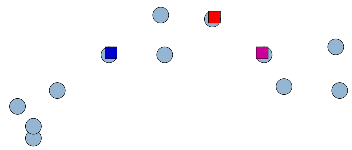
K-means

Iterate:

- **Assign/cluster each example to closest center**
- Recalculate centers as the mean of the points in a cluster



How do we do this?

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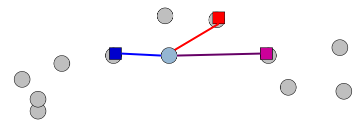
K-means

Iterate:

- **Assign/cluster each example to closest center**

  iterate over each point:
  - get distance to each cluster center
  - assign to closest center (hard cluster)
- Recalculate centers as the mean of the points in a cluster



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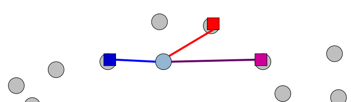
K-means

Iterate:

- **Assign/cluster each example to closest center**

  iterate over each point:
  - get **distance** to each cluster center
  - assign to closest center (hard cluster)
- Recalculate centers as the mean of the points in a cluster



What distance measure should we use?

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Distance measures

Euclidean:

$$d(x,y) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

good for spatial data

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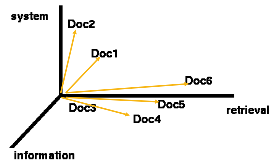
Clustering documents (e.g. wine data)

One feature for each word. The value is the number of times that word occurs.

Documents are points or vectors in this space



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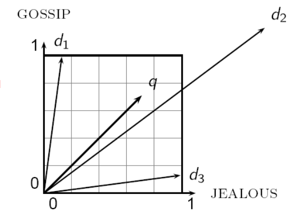
When Euclidean distance doesn't work

Which document is closest to q using Euclidian distance?

Which do you think should be closer?



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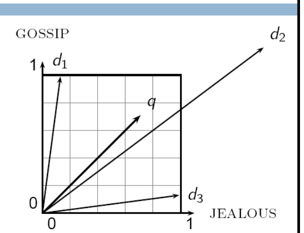
Issues with Euclidian distance

the Euclidean distance between q and d_2 is large

but, the distribution of terms in q and d_2 are very similar

This is not what we want!



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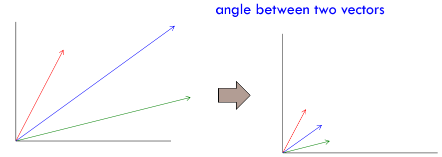
cosine similarity

$$sim(x,y) = \frac{x \bullet y}{|x||y|} = \frac{x}{|x|} \bullet \frac{y}{|y|} = \frac{\sum_{i=1}^{n} x_i y_i}{\sqrt{\sum_{i=1}^{n} x_i^2}\sqrt{\sum_{i=1}^{n} y_i^2}}$$

correlated with the angle between two vectors



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cosine distance

cosine similarity ranges from 0 and 1, with things that are similar 1 and dissimilar 0

cosine distance:

$$d(x, y) = 1 - sim(x, y)$$

- good for text data and many other "real world" data sets
- *computationally friendly* since we only need to consider features that have non-zero values for **both** examples

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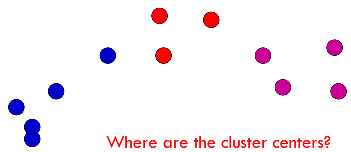
K-means

Iterate:
- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster



Where are the cluster centers?

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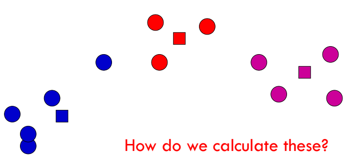
K-means

Iterate:
- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster



How do we calculate these?

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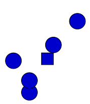
K-means

Iterate:
- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster



Mean of the points in the cluster:

$$\mu(\mathrm{C}) = \frac{1}{|C|} \sum_{x \in C} x$$

where:

$$x + y = \sum_{i=1}^{n} x_i + y_i \qquad \frac{x}{|C|} = \sum_{i=1}^{n} \frac{x_i}{|C|}$$

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K-means loss function

K-means tries to minimize what is called the "k-means" loss function:

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

the sum of the squared distances from each point to the associated cluster center

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Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Does each step of k-means move towards reducing this loss function (or at least not increasing it)?

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Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

This isn't quite a complete proof/argument, but:

1. Any other assignment would end up in a larger loss
2. The mean of a set of values minimizes the squared error

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Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Does this mean that k-means will always find the minimum loss/clustering?

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Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

NO! It will find a *minimum*.

Unfortunately, the k-means loss function is generally not convex and for most problems has many, many minima

We're only guaranteed to find one of them

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K-means variations/parameters

Start with some initial cluster centers

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

What are some other variations/parameters we haven't specified?

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K-means variations/parameters

Initial (seed) cluster centers

Convergence

- A fixed number of iterations
- partitions unchanged
- Cluster centers don't change

K!

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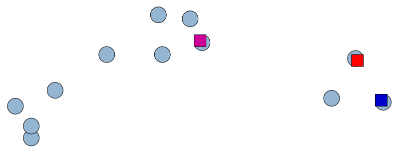
K-means: Initialize centers randomly



What would happen here?

Seed selection ideas?

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Seed choice

Results can vary drastically based on random seed selection

Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings

Common heuristics
- Random points (not examples) in the space
- Randomly pick examples
- Points least similar to any existing center (furthest centers heuristic)
- **Try out multiple starting points**
- Initialize with the results of another clustering method

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Furthest centers heuristic

μ_1 = pick random point

for i = 2 to K:

μ_i = point that is furthest from **any** previous centers

$$\mu_i = \underbrace{\arg\max_{x}}_{\text{point with the largest distance to any previous center}} \underbrace{\min_{\mu_j : 1 < j < i} d(x, \mu_j)}_{\text{smallest distance from x to any previous center}}$$

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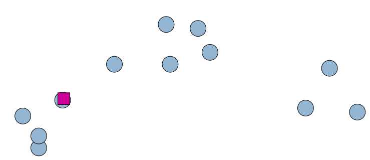
K-means: Initialize furthest from centers



Pick a random point for the first center

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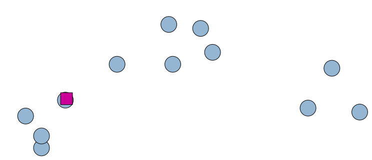
K-means: Initialize furthest from centers



What point will be chosen next?

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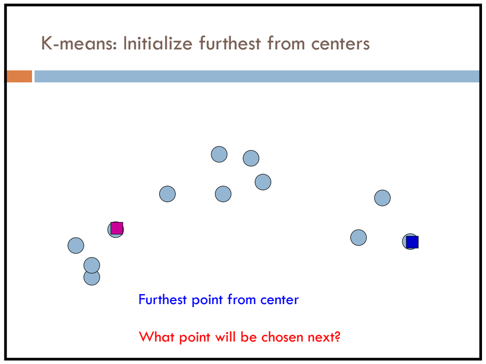
K-means: Initialize furthest from centers
Furthest point from center
What point will be chosen next?

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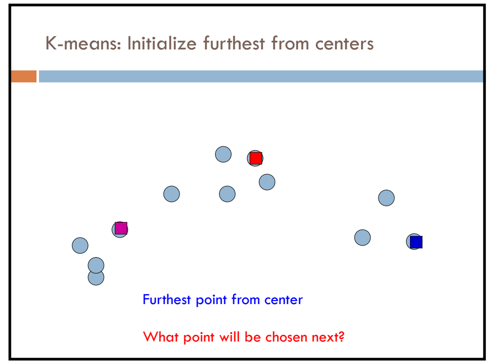
K-means: Initialize furthest from centers
Furthest point from center
What point will be chosen next?

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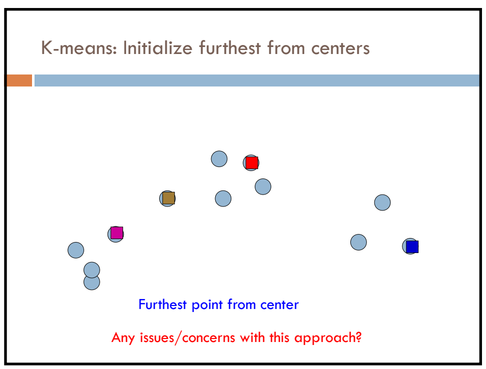
K-means: Initialize furthest from centers
Furthest point from center
Any issues/concerns with this approach?

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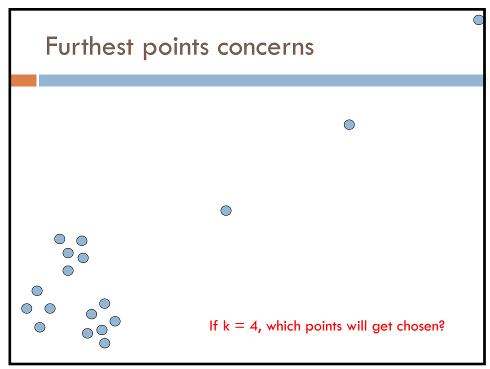
Furthest points concerns
If k = 4, which points will get chosen?

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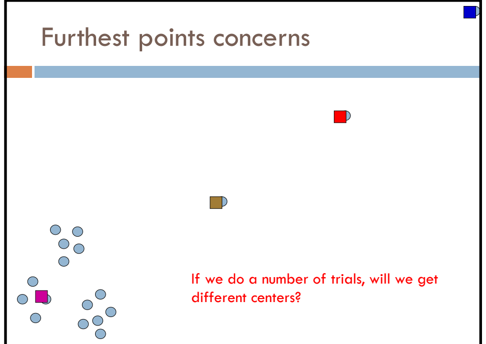
Furthest points concerns



If we do a number of trials, will we get different centers?

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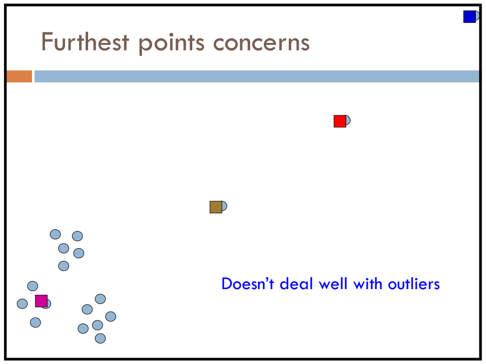
Furthest points concerns



Doesn't deal well with outliers

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K-means++

μ_1 = pick random point

for k = 2 to **K**:
  for i = 1 to **N**:
    $s_i = \min d(x_i, \mu_{1\ldots k-1})$ // smallest distance to any center

  μ_k = randomly pick point ***proportionate*** to *s*

How does this help?

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K-means++

μ_1 = pick random point

for k = 2 to **K**:
  for i = 1 to **N**:
    $s_i = \min d(x_i, \mu_{1\ldots k-1})$ // smallest distance to any center

  μ_k = randomly pick point ***proportionate*** to *s*

- Makes it possible to select other points
  - if #points >> #outliers, we will pick good points
- Makes it non-deterministic, which will help with random runs
- Nice theoretical guarantees!

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K-means variations/parameters

Initial (seed) cluster centers

Convergence
- A fixed number of iterations
- partitions unchanged
- Cluster centers don't change

K!

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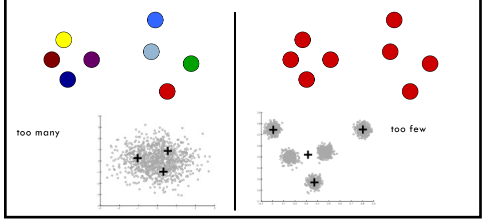
How Many Clusters?

Number of clusters *K* must be provided

How should we determine the number of clusters?

How did we deal with models becoming too complicated previously?



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Many approaches

Regularization!!!

Statistical test

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k-means loss revisited

K-means is trying to minimize:

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

What happens when k increases?

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k-means loss revisited

K-means is trying to minimize:

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Loss goes down!

Making the model more complicated allows us more flexibility, but can "overfit" to the data

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k-means loss revisited

K-means is trying to minimize:

$$loss_{kmeans} = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

2 regularization options

$$loss_{BIC} = loss_{kmeans} + K \log N$$ (where N = number of points)

$$loss_{AIC} = loss_{kmeans} + KN$$

What effect will this have?
Which will tend to produce smaller k?

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k-means loss revisited

2 regularization options

$$loss_{BIC} = loss_{kmeans} + K \log N$$ (where N = number of points)

$$loss_{AIC} = loss_{kmeans} + KN$$

AIC penalizes increases in K more harshly

Both require a change to the K-means algorithm

Tend to work reasonably well in practice if you don't know K

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