Course Update

Current Plan (updated)

- HW 8 (online)
- Mini-project proposal
- HW 9 (online)
- HW 10 (written/prog)
- Midterm 2
- Mini-project

Sun	Mon	Tue	Wed	Thu	Fri	Sat
2	3	4	5 HW8 Proj	6	7	8
9 HW8	10 HW9 HW10	11	12	13	14	15
16	17 HW9	18	19 Prop	20	21	22 HW10
23	24	25	26 MT2	27	28	29
30	1	2	3	4	5 Proj	6

10-315
Introduction to ML

Clustering:
K-means

Instructor: Pat Virtue

Plan

Last time

- Unsupervised Learning: Dimensionality Reduction

Today

- Recommender Systems
- Unsupervised Learning: Clustering
  - K-means

Next time

- Unsupervised Learning: Clustering
  - Gaussian mixture models and expectation maximization

Learning Paradigms

Paradigm	**Data**
Supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N \qquad \mathbf{x} \sim p^*(\cdot)$ and $y = c^*(\cdot)$
$\hookrightarrow$ Regression	$y^{(i)} \in \mathbb{R}$
$\hookrightarrow$ Classification	$y^{(i)} \in \{1, \ldots, K\}$
$\hookrightarrow$ Binary classification	$y^{(i)} \in \{+1, -1\}$
$\hookrightarrow$ Structured Prediction	$\mathbf{y}^{(i)}$ is a vector
Unsupervised	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N \qquad \mathbf{x} \sim p^*(\cdot)$
Semi-supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N_1} \cup \{\mathbf{x}^{(j)}\}_{j=1}^{N_2}$
Online	$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), (\mathbf{x}^{(3)}, y^{(3)}), \ldots\}$
Active Learning	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ and can query $y^{(i)} = c^*(\cdot)$ at a cost
Imitation Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}), (s^{(2)}, a^{(2)}), \ldots\}$
Reinforcement Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}, r^{(1)}), (s^{(2)}, a^{(2)}, r^{(2)}), \ldots\}$

Slide credit: CMU MLD, Matt Gormley

Clustering, Informal Goals

Goal: Automatically partition unlabeled data into groups of similar datapoints.

Question: When and why would we want to do this?

Useful for:

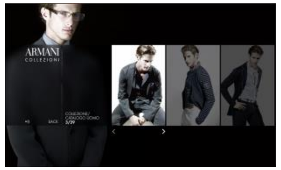
- Automatically organizing data.
- Understanding hidden structure in data.
- Preprocessing for further analysis.
    - Representing high-dimensional data in a low-dimensional space (e.g., for visualization purposes).

Slide credit: CMU MLD Nina Balcan

Applications (Clustering comes up everywhere…)

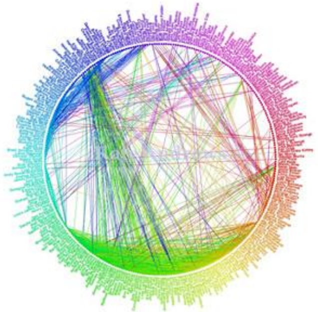
Cluster news articles or web pages or search results by topic.



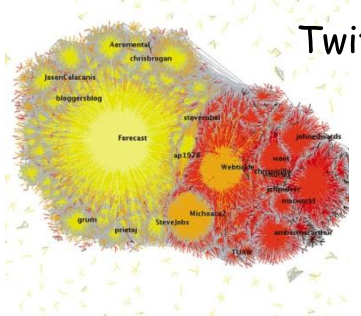



- Cluster protein sequences by function or genes according to expression profile.


- Cluster users of social networks by interest (community detection).



Facebook network

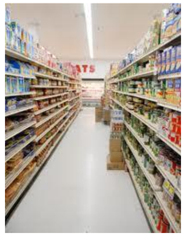


Twitter Network

Slide credit: CMU MLD Nina Balcan

Applications (Clustering comes up everywhere…)

Cluster customers according to purchase history.



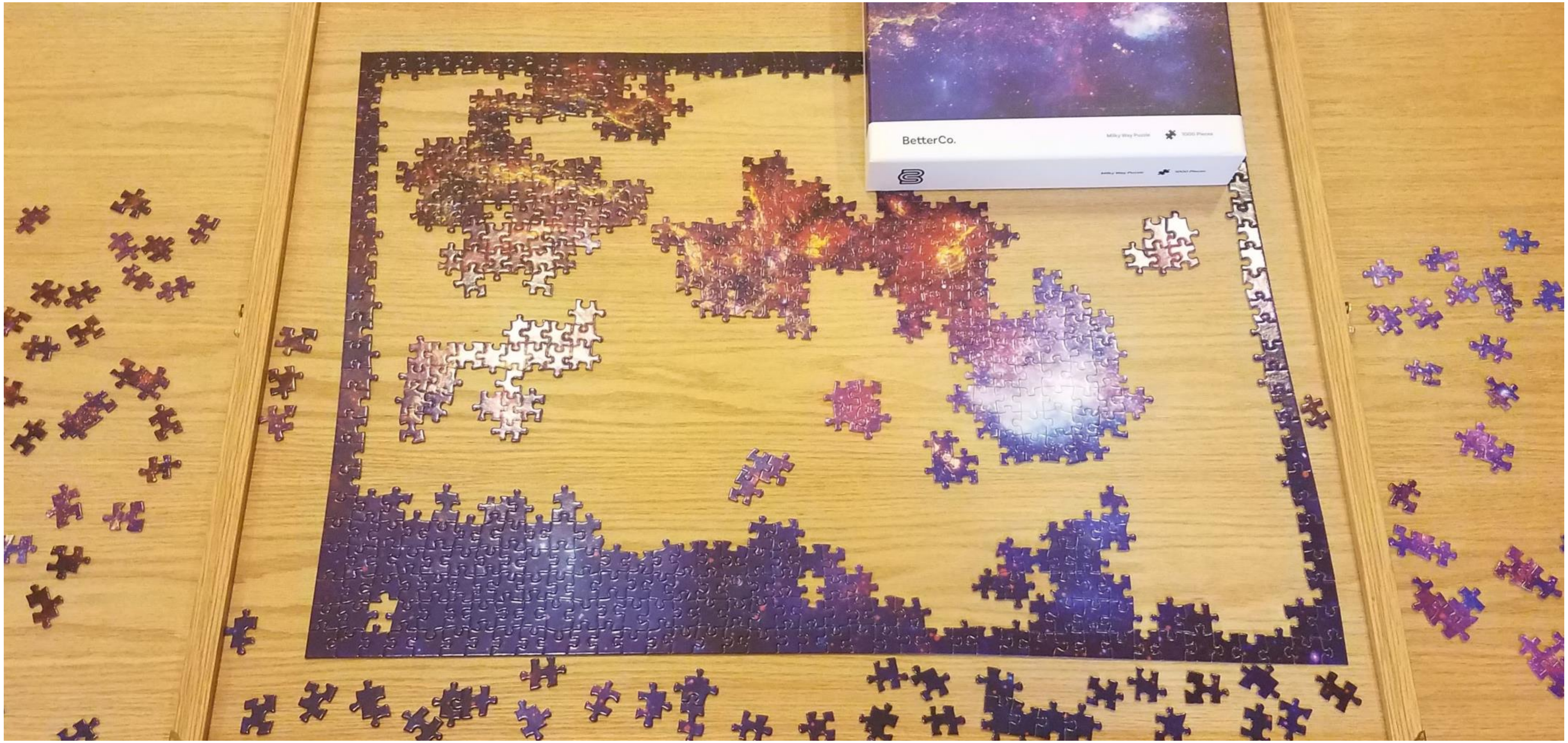
- Cluster galaxies or nearby stars (e.g. Sloan Digital Sky Survey)

- And many many more applications….

Slide credit: CMU MLD Nina Balcan

Clustering Applications

Jigsaw puzzles!



Semi-supervised Learning

Supervised: $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N}$

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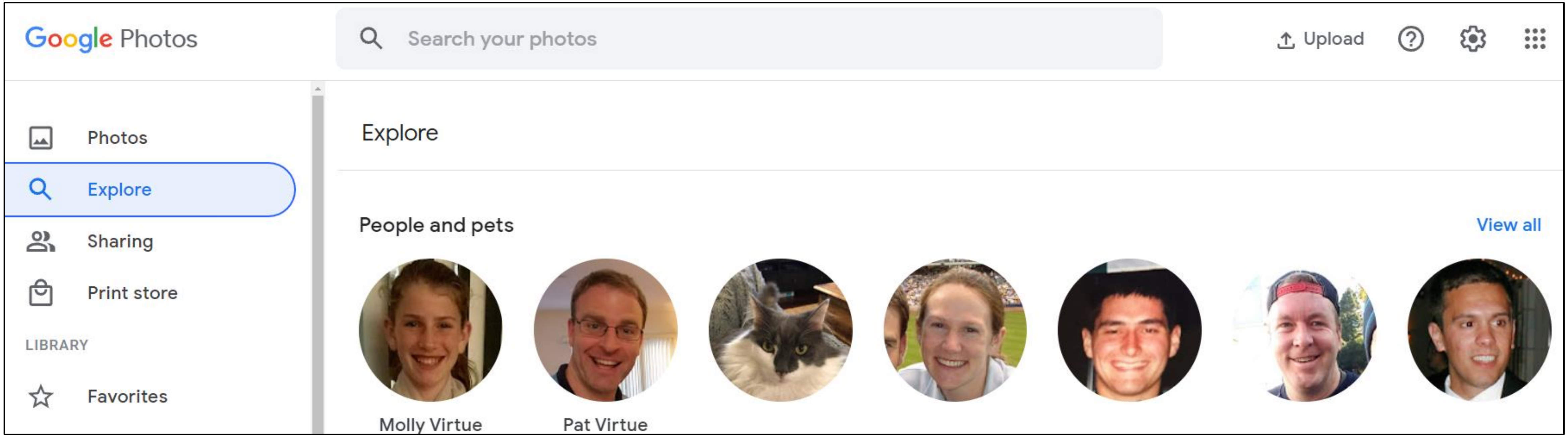

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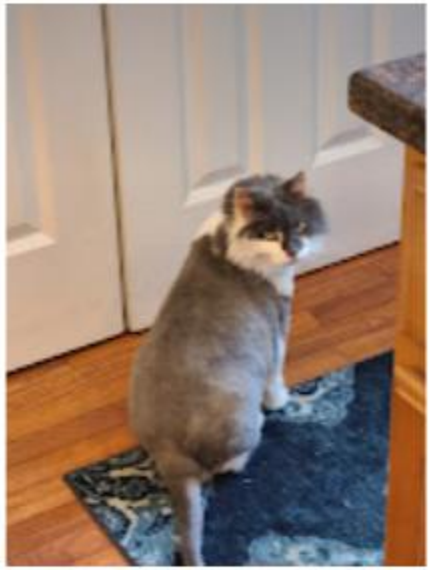
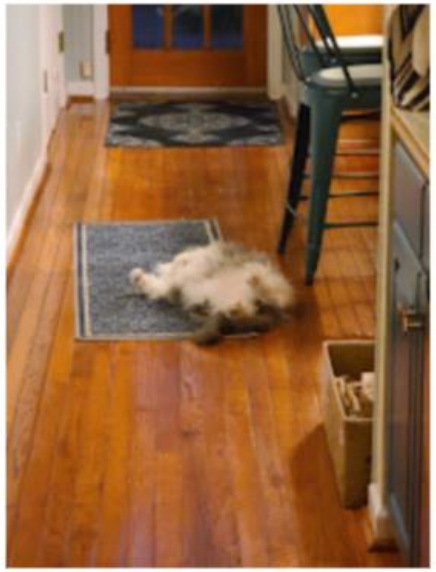
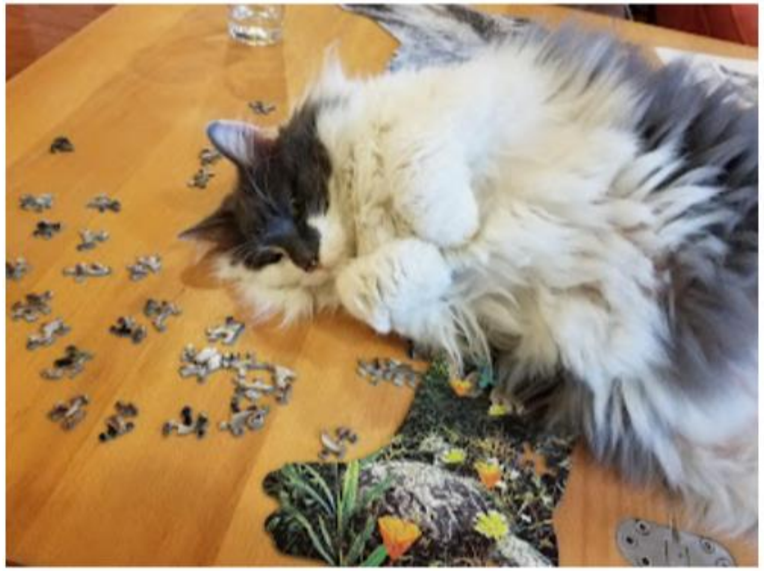


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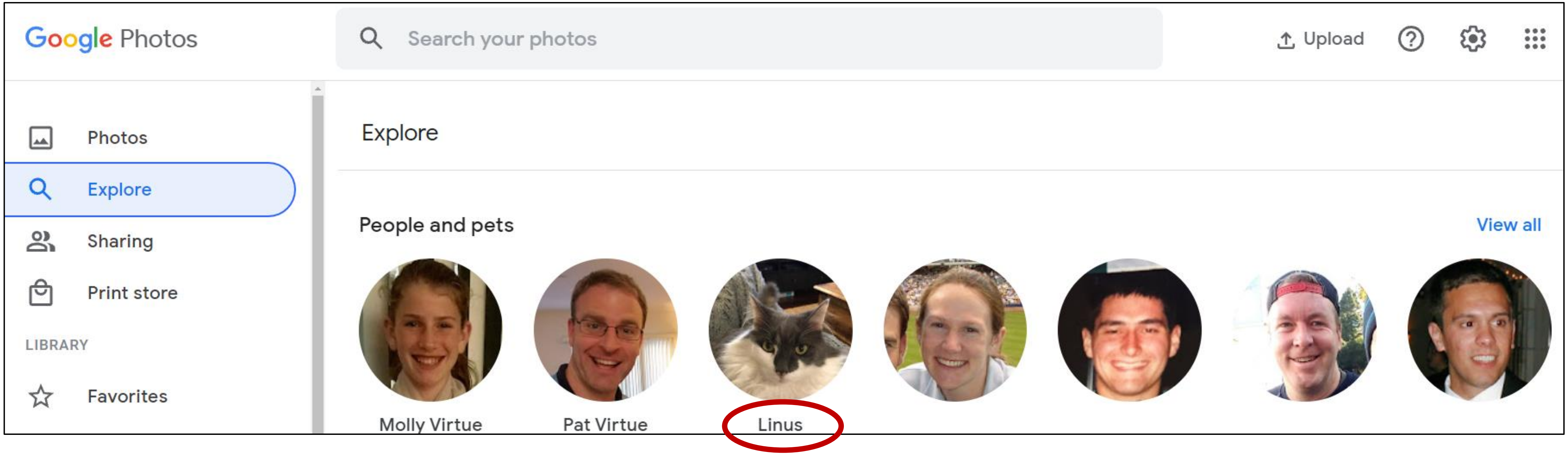

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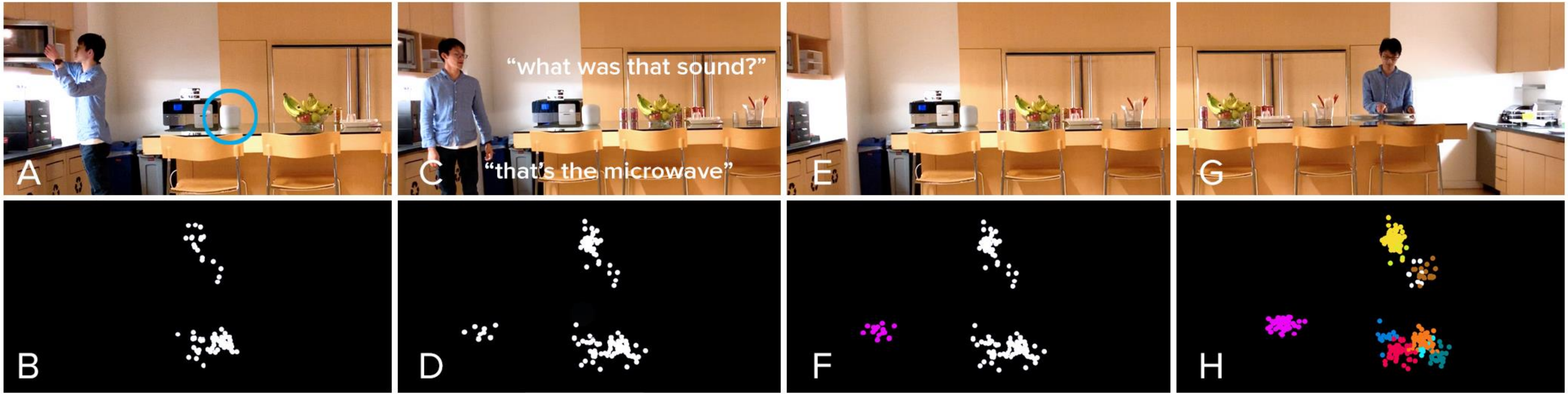
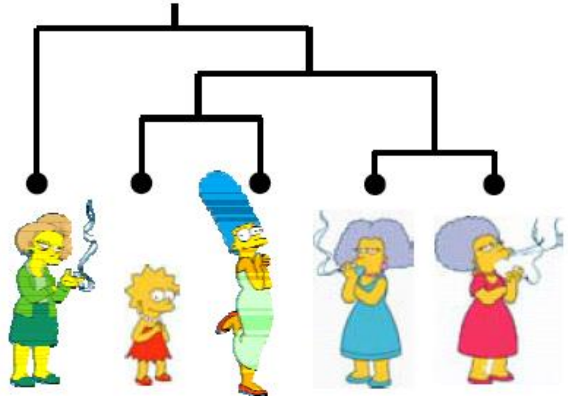


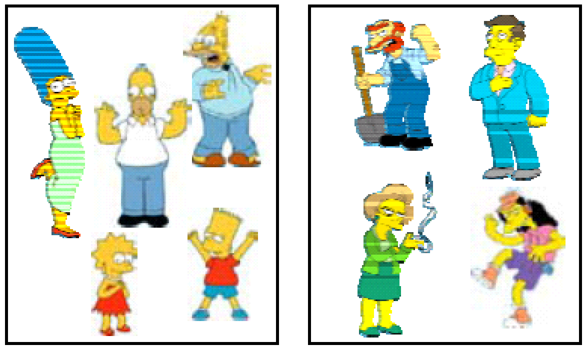
https://chrisharrison.net/index.php/Research/ListenLearner

Clustering Algorithms

- Hierarchical algorithms
  - Bottom-up: Agglomerative Clustering
  - Top-down: Divisive



- Partition algorithms
  - K means clustering
  - Mixture-Model based clustering



Slide credit: CMU MLD Aarti Singh and Eric Xing

Hierarchical Clustering

- Bottom-Up Agglomerative Clustering

  Starts with each object in a separate cluster, and repeat:

  – Joins the most similar pair of clusters,

  – Update the similarity of the new cluster to others

  until there is only one cluster.

  Greedy – less accurate but simple to implement

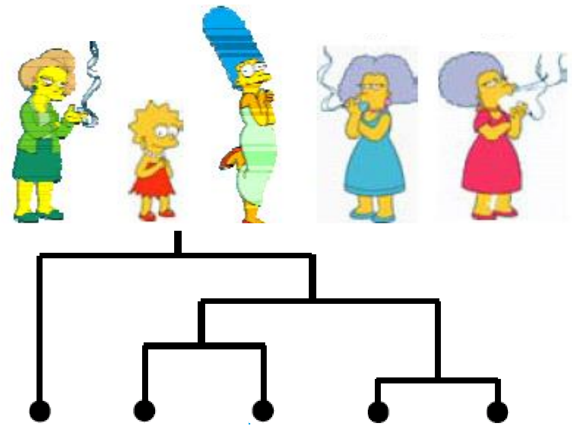
- Top-Down divisive

  Starts with all the data in a single cluster, and repeat:

  – Split each cluster into two using a partition algorithm

  Until each object is a separate cluster.

  More accurate but complex to implement



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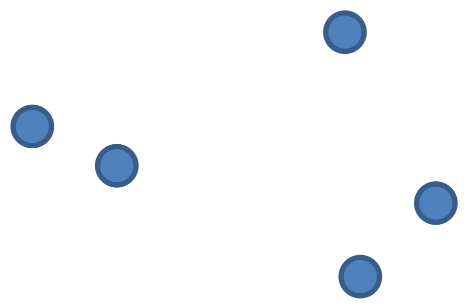

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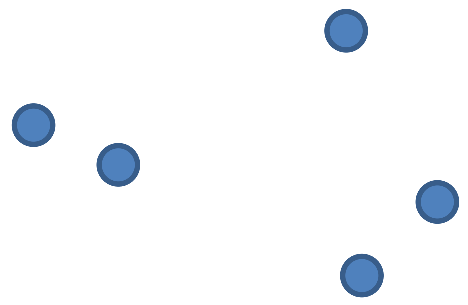


Partitioning Algorithms

- Partitioning method: Construct a partition of N objects into a set of K clusters
- Given: a set of objects and the number K
- Find: a partition of K clusters that optimizes the chosen partitioning criterion
  - Globally optimal: exhaustively enumerate all partitions
  - Effective heuristic method: K-means algorithm

Slide credit: CMU MLD Aarti Singh

K-Means

Algorithm

Input – Data, $\boldsymbol{x}^{(i)}$, Desired number of clusters, *K*

Initialize – the *K* cluster centers (randomly if necessary)

Iterate –

1. Assign points to the nearest cluster centers

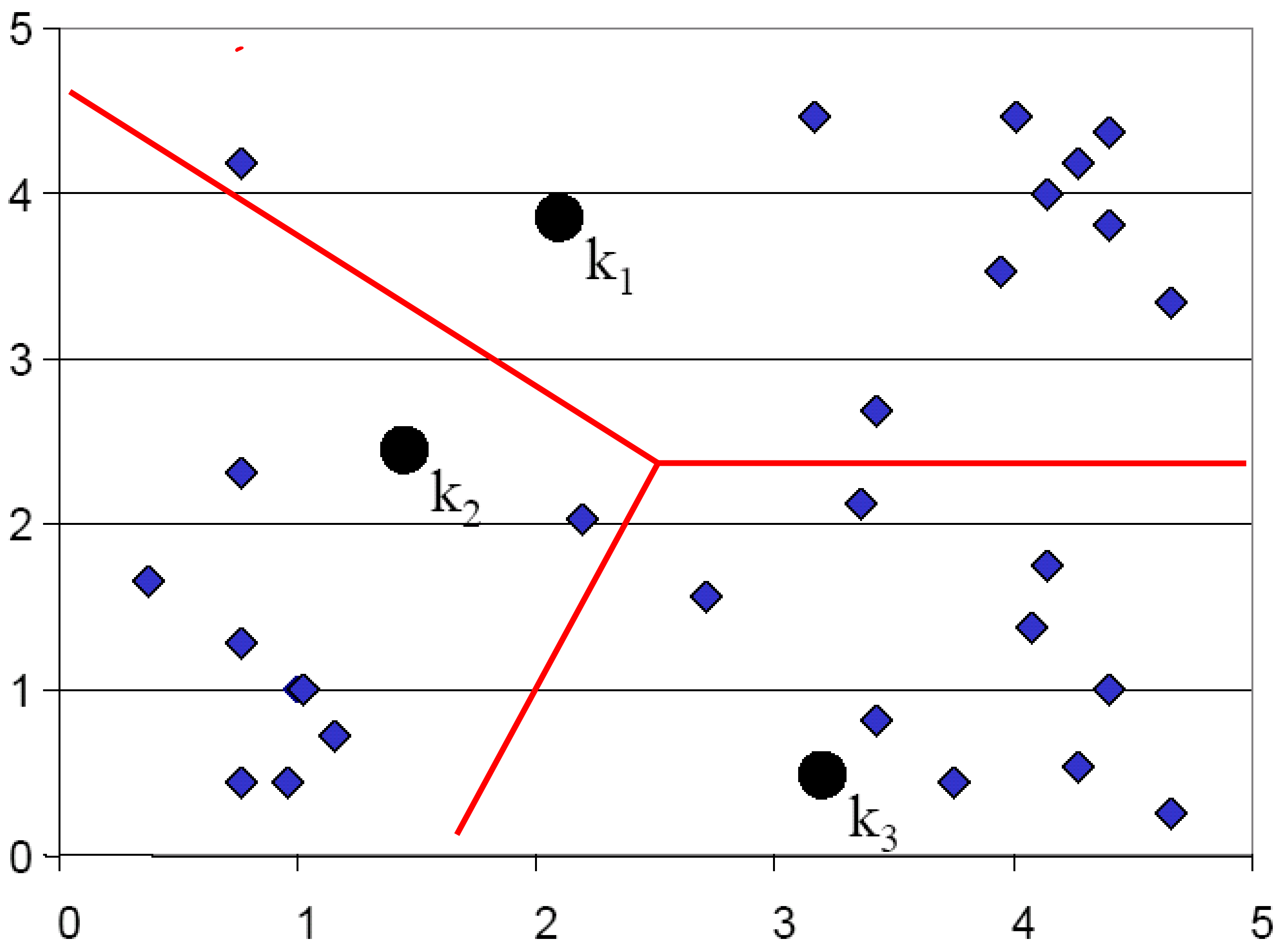
2. Re-estimate the *K* cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

Termination –

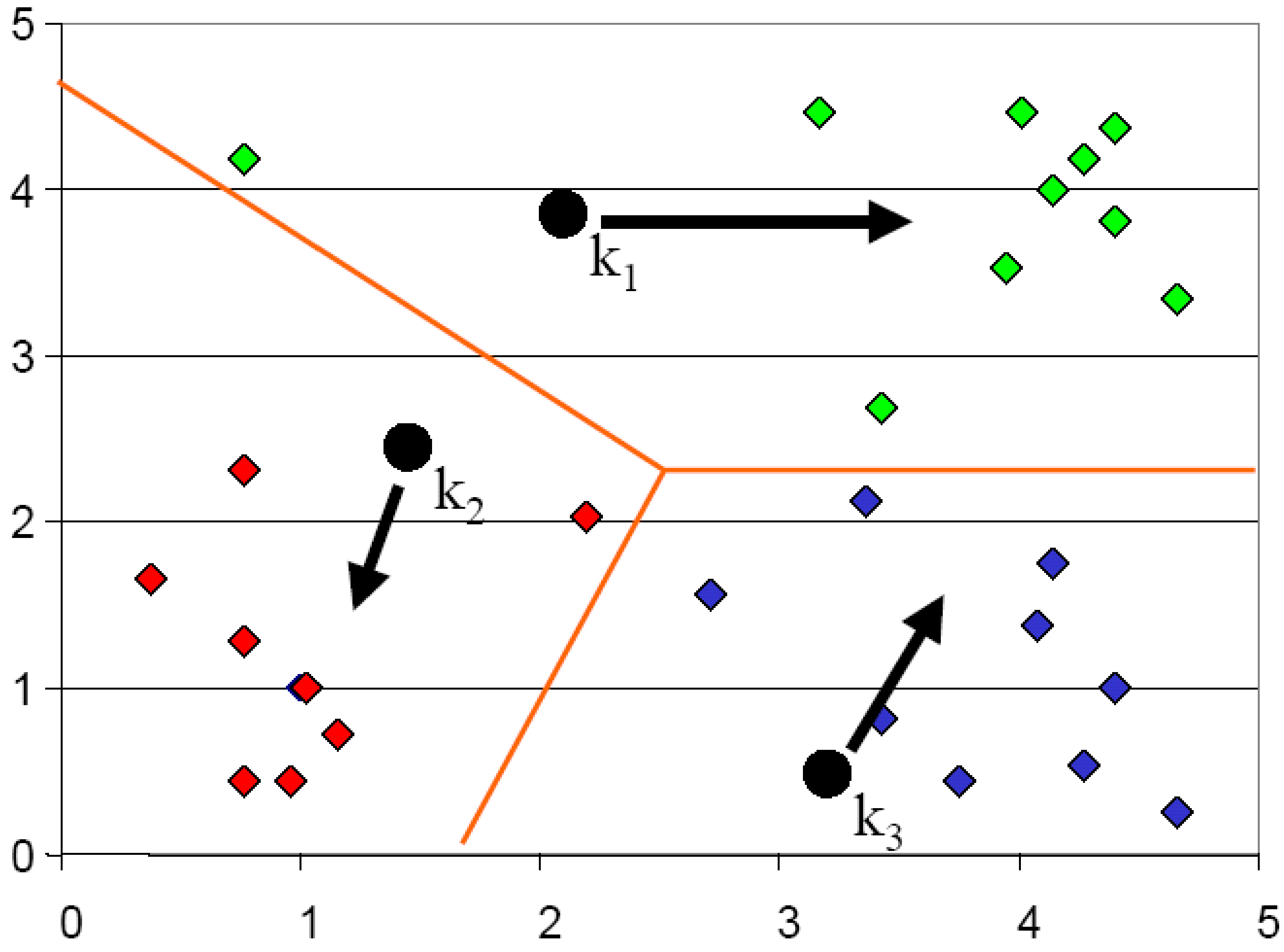
If none of the objects changed membership in the last iteration, exit. Otherwise go to 1.

Slide credit: CMU MLD Aarti Singh

K-means Clustering: Assign points



K-means Clustering: Update centers



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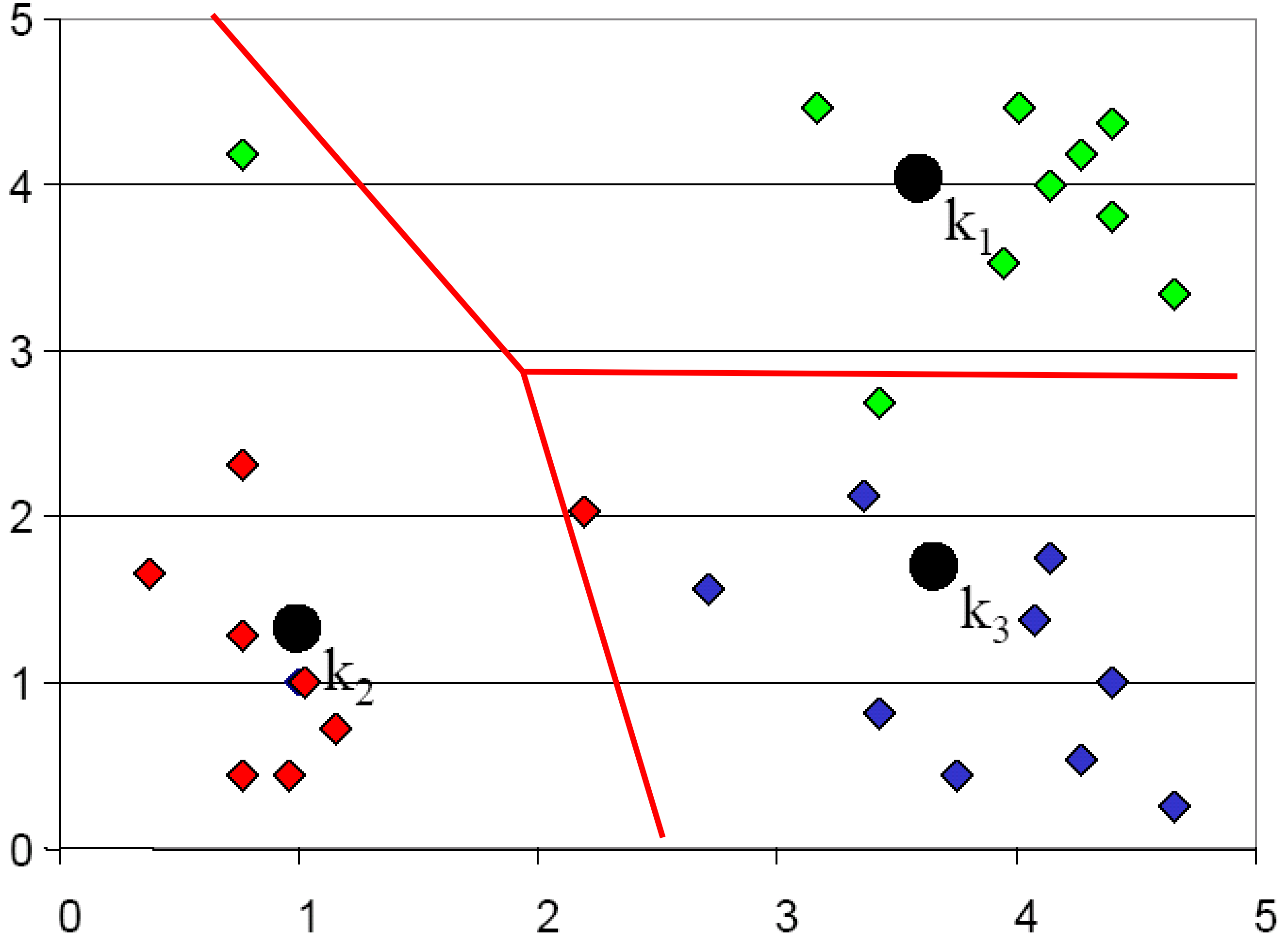

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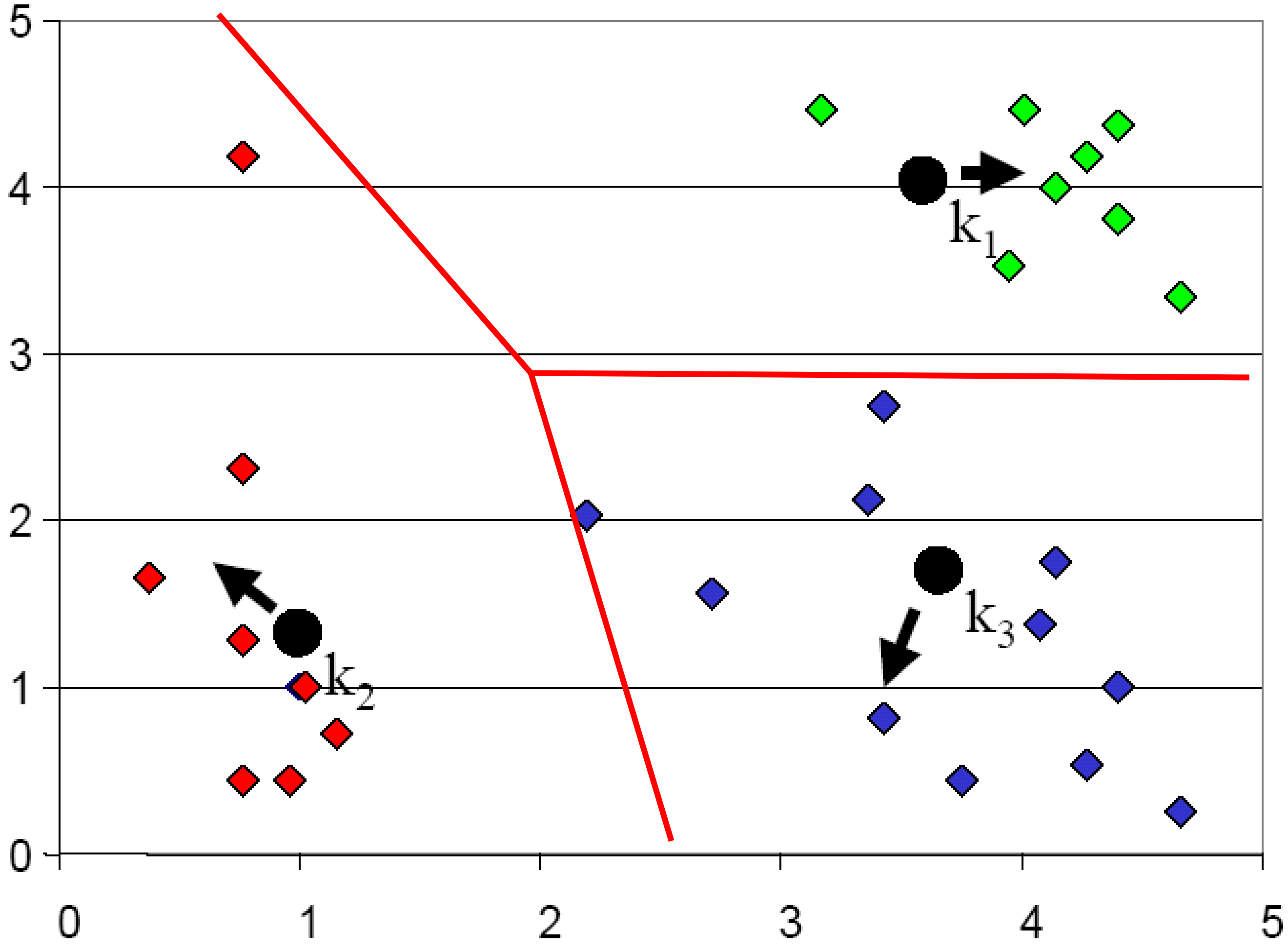

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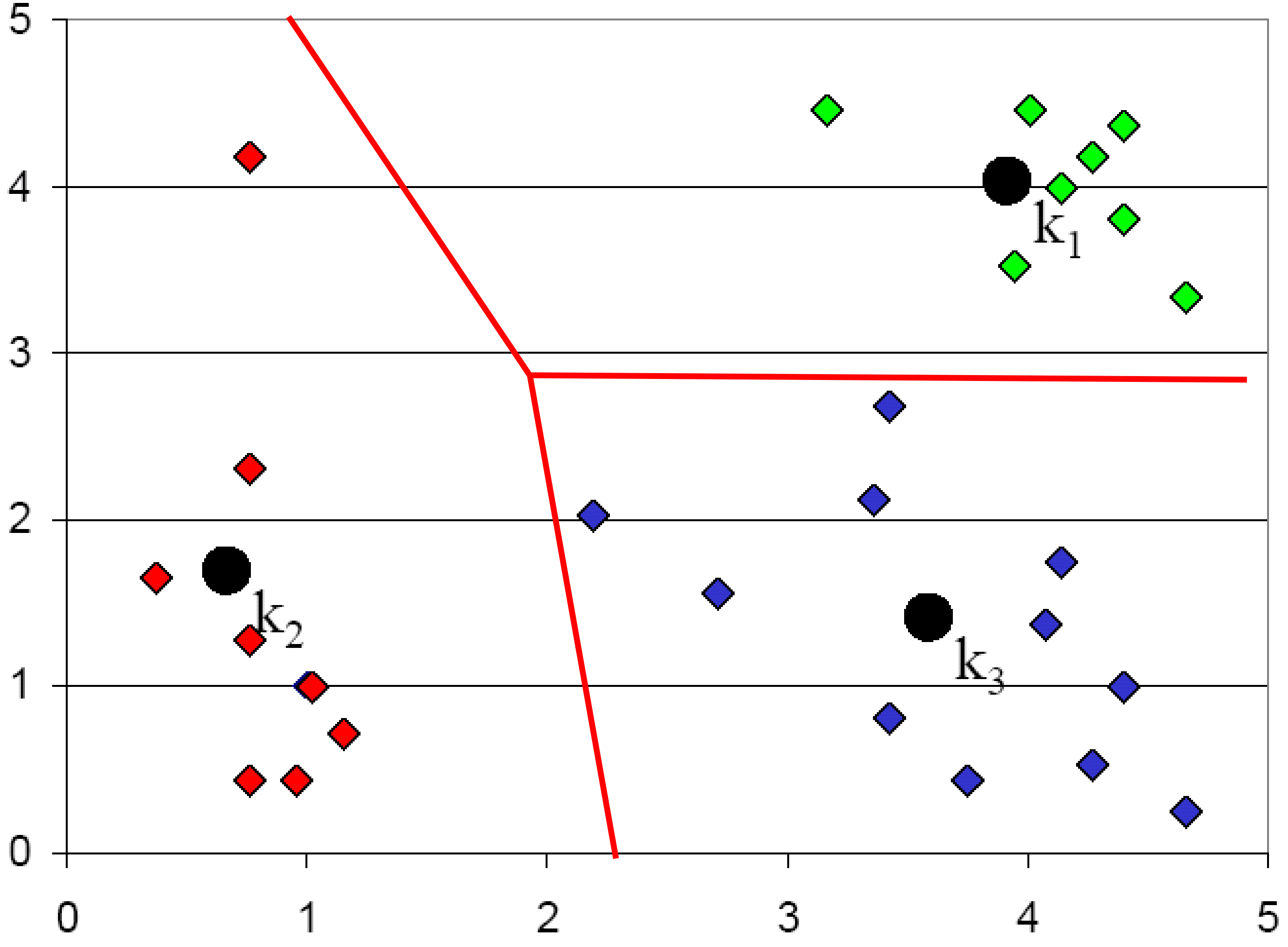

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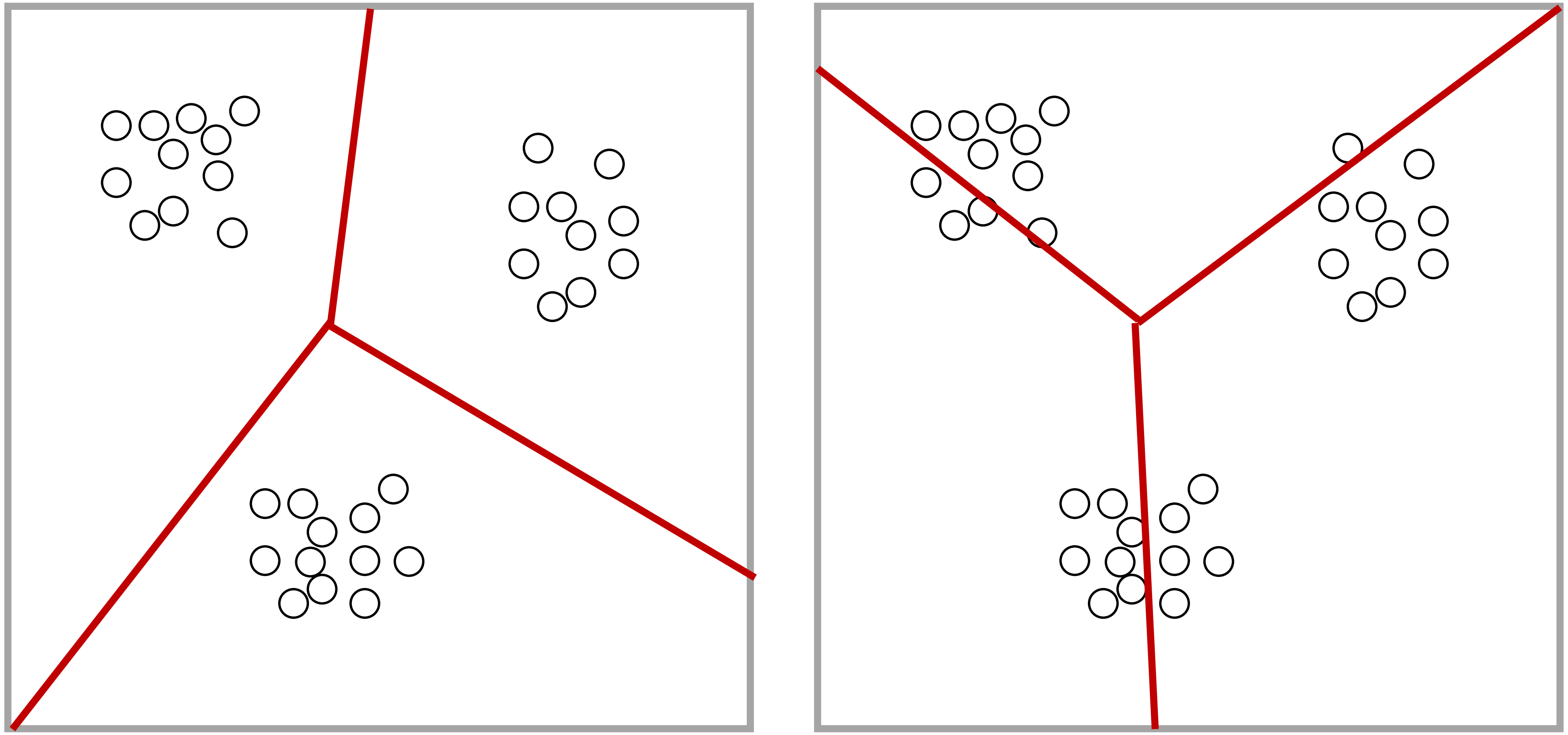
K-means Optimization

Optimization recipe

1. Formulate objective
2. Minimize objective

K-means Optimization

Question: Which of these partitions is "better"?



Slide credit: CMU MLD Matt Gormley

K-means Optimization

Input: K, $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}$, $\boldsymbol{x}^{(i)} \in \mathbb{R}^M$ Num clusters, unlabeled data

Output: $z^{(1)}, \ldots, z^{(N)}$, $z^{(i)} \in \{1 \ldots K\}$ Cluster assignments per point

Output: $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$, $\boldsymbol{\mu}_k \in \mathbb{R}^M$ Cluster centers

Slide credit: CMU MLD Matt Gormley

K-means Optimization

Computational complexity

$$\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{z} = \underset{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{z}}{\operatorname{argmin}} \sum_{i=1}^{N} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{z^{(i)}} \right\|_2^2$$

K-means Optimization

Alternating minimization

a) $$\boldsymbol{z} = \underset{\boldsymbol{z}}{\operatorname{argmin}} \sum_{i=1}^{N} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{z^{(i)}} \right\|_2^2$$

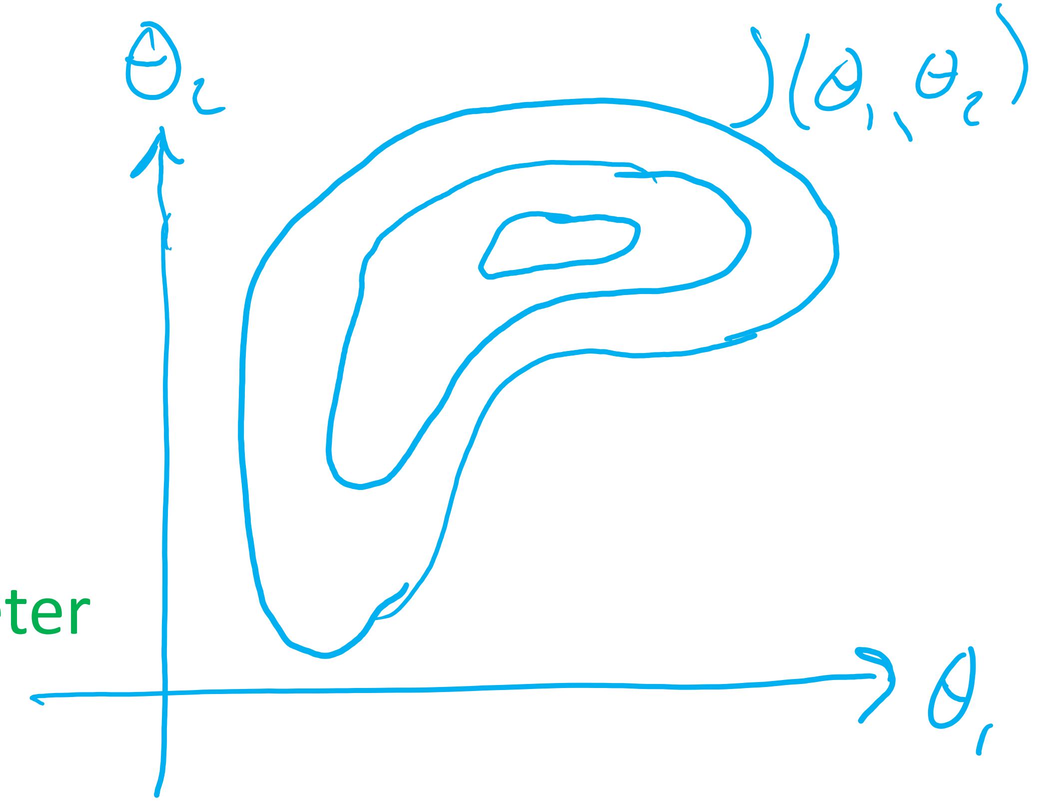
b) $$\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K = \underset{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K}{\operatorname{argmin}} \sum_{i=1}^{N} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{z^{(i)}} \right\|_2^2$$

Alternating minimization

Coordinate descent

Two different approaches

$$\min_{\theta_1,\theta_2} J(\theta_1, \theta_2)$$



1. Step based on derivative for one parameter
   a. $\theta_1 \leftarrow \theta_1 - \eta\, \partial J / \partial \theta_1$
   b. $\theta_2 \leftarrow \theta_2 - \eta\, \partial J / \partial \theta_2$

2. Find minimum for one parameter
   a. $\theta_1 \leftarrow \underset{\theta_1}{\operatorname{argmin}}\, J(\theta_1, \theta_2)$
   b. $\theta_2 \leftarrow \underset{\theta_2}{\operatorname{argmin}}\, J(\theta_1, \theta_2)$

Alternating minimization

Block coordinate descent

Two different approaches

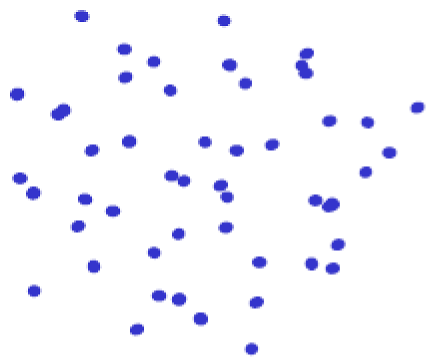
$$\min_{\boldsymbol{\alpha},\boldsymbol{\beta}} \; J(\boldsymbol{\alpha},\boldsymbol{\beta})$$

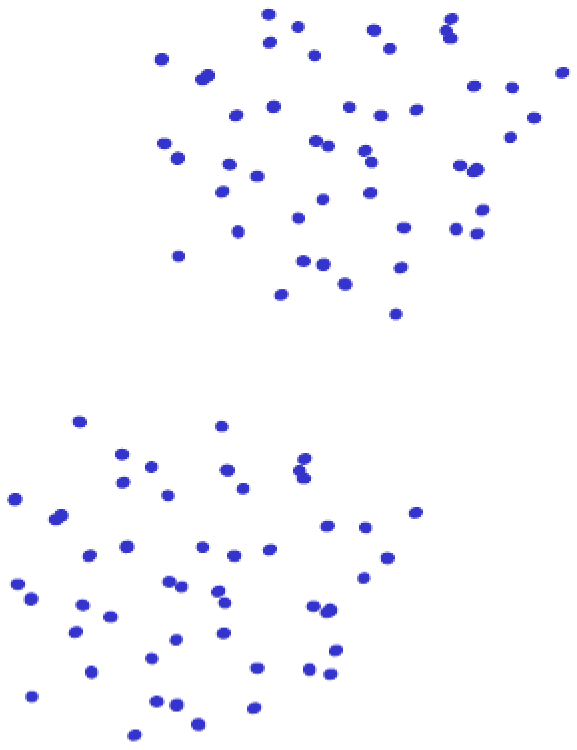
1. Step based on gradient for one set of parameters (step size η)
   a. $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \eta \nabla_{\boldsymbol{\alpha}} J$
   b. $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} - \eta \nabla_{\boldsymbol{\beta}} J$

2. Find minimum for one set of parameter (no hyperparameters!)
   a. $\boldsymbol{\alpha} \leftarrow \underset{\boldsymbol{\alpha}}{\operatorname{argmin}}\, \mathrm{J}(\boldsymbol{\alpha},\boldsymbol{\beta})$
   b. $\boldsymbol{\beta} \leftarrow \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\, \mathrm{J}(\boldsymbol{\alpha},\boldsymbol{\beta})$

Issues: Seed Choice

- Results are quite sensitive to seed selection.





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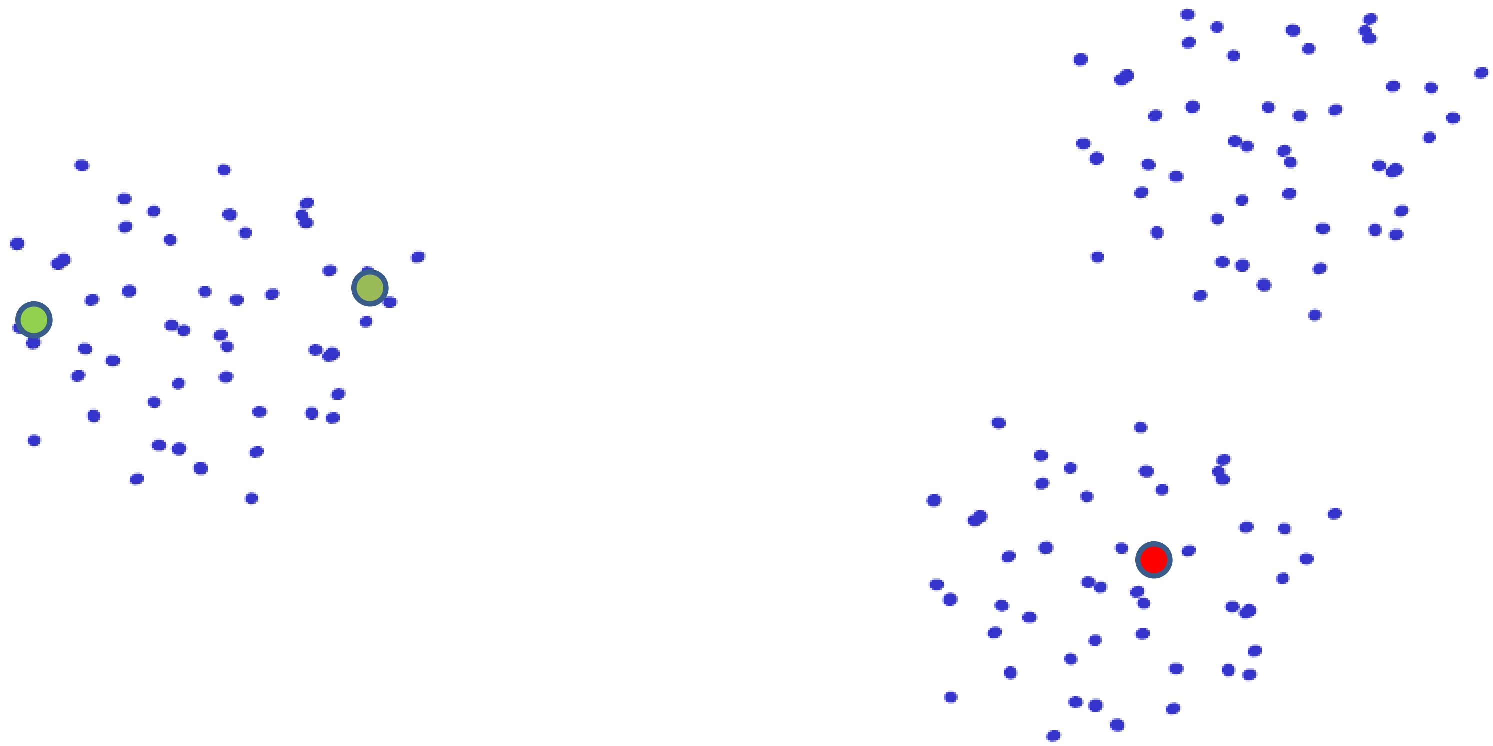

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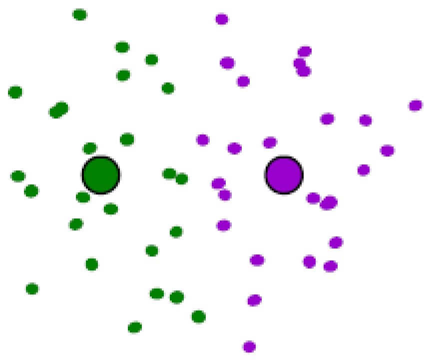

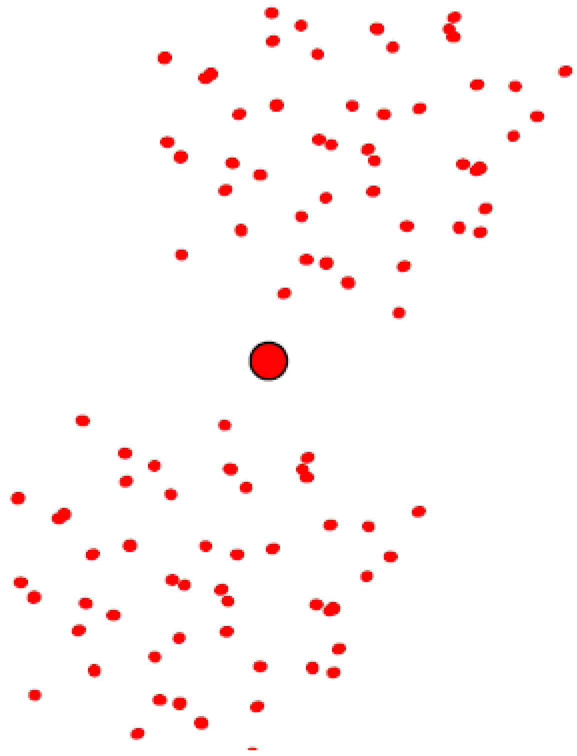

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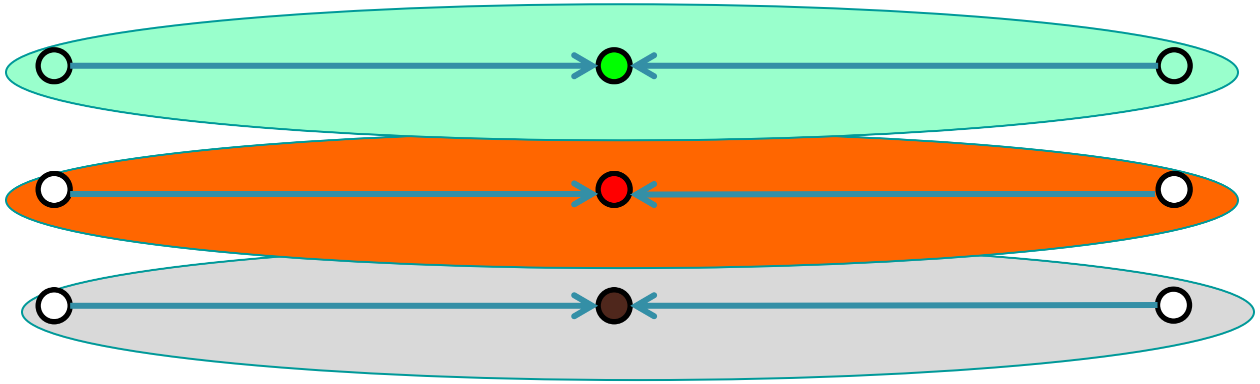


K-means always converges, but it may converge at a local optimum that is different from the global optimum, and in fact could be arbitrarily worse in terms of its objective.

Slide credit: CMU MLD Nina Balcan

Issues: Seed Choice

- Results can vary based on random seed selection.

- Some seeds can result in poor convergence rate, or convergence to sub-optimal clustering.
  - Try out multiple starting points (very important!!!)
  - k-means ++ algorithm of Arthur and Vassilvitskii

    key idea: choose centers that are far apart

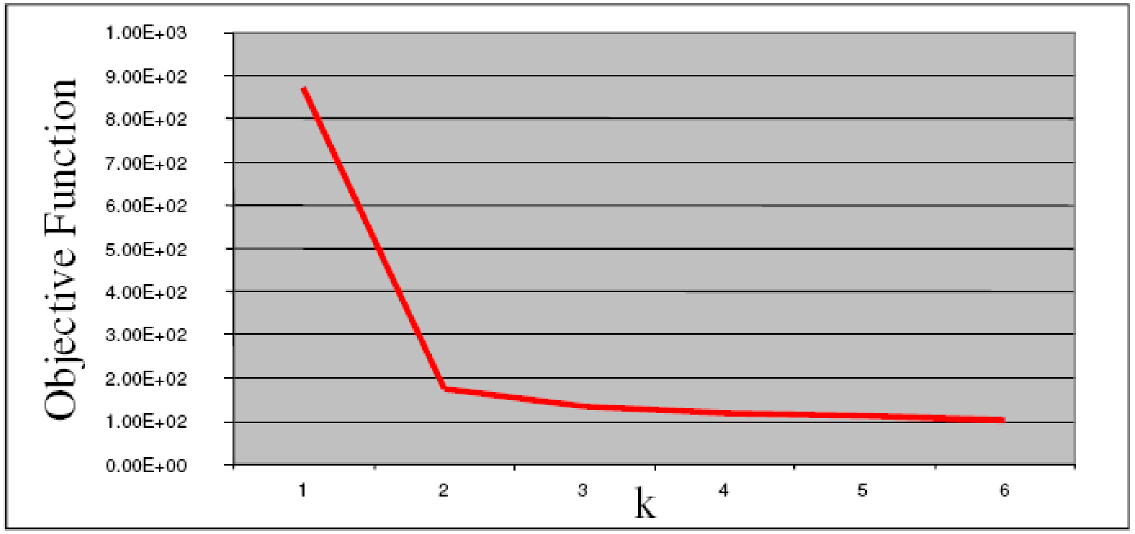
    (probability of picking a point as cluster center $\propto$ distance from nearest center picked so far)

Other Issues

- Number of clusters K
  - Objective function

$$\sum_{j=1}^{m} ||\mu_{C(j)} - x_j||^2$$

  - Look for “Knee” in objective function



  - Can you pick K by minimizing the objective over K?

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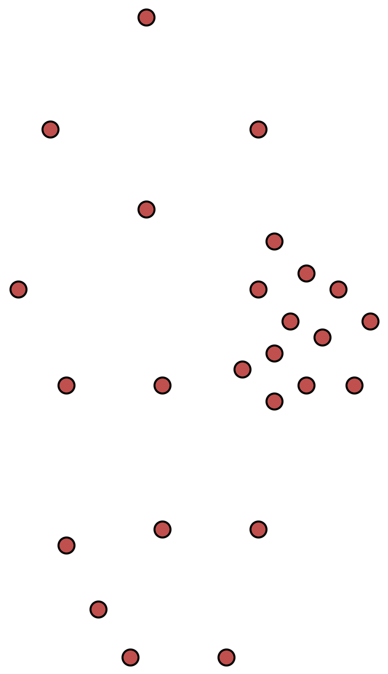
(One) bad case for K-means



- Clusters may overlap
- Some clusters may be “wider” than others
- Clusters may not be linearly separable