Clustering, K-Means, and K-Nearest Neighbors

CMSC 478

UMBC

Most slides courtesy Hamed Pirsiavash

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

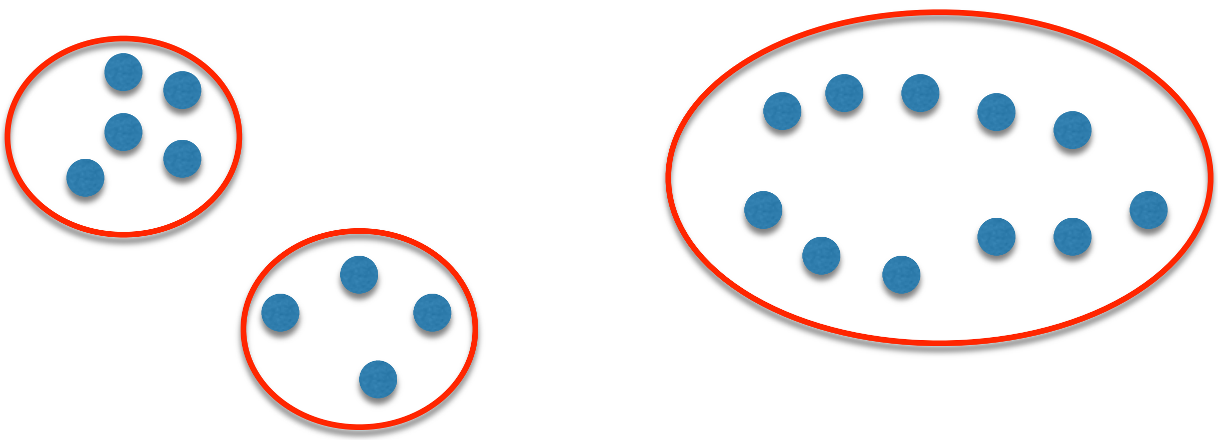
Hierarchical clustering

K-Nearest Neighbor

Clustering

Basic idea: group together similar instances

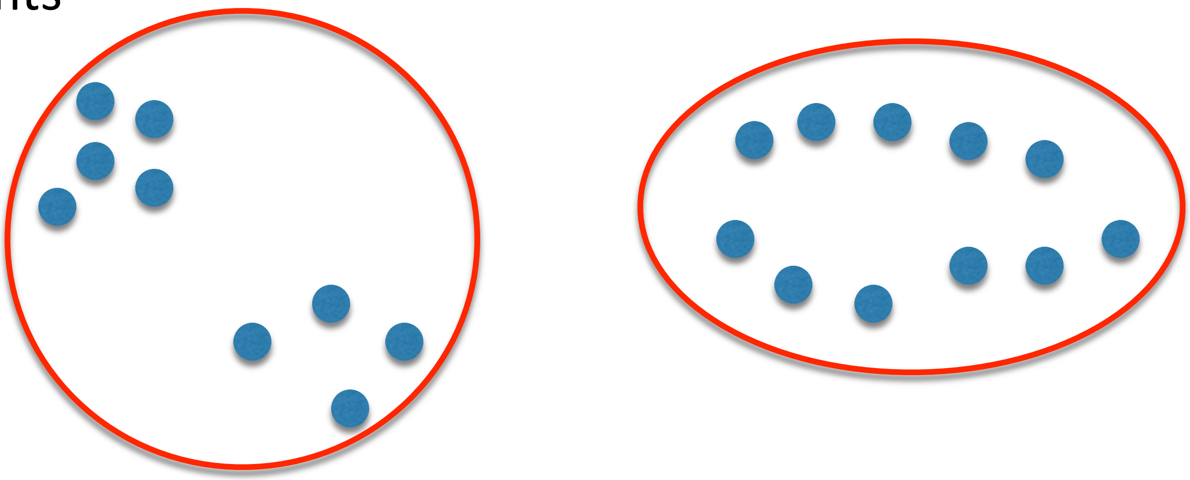
Example: 2D points



Clustering

Basic idea: group together similar instances

Example: 2D points



One option: small Euclidean distance (squared)

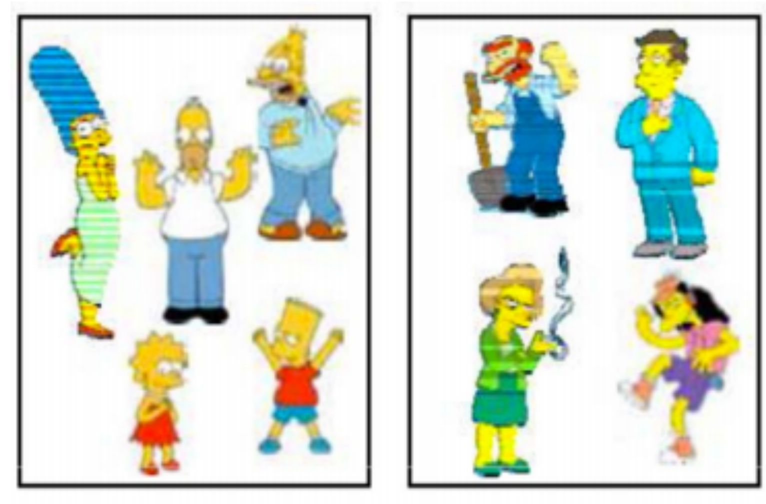
$$\text{dist}(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}||_2^2$$

Clustering results are crucially dependent on the measure of similarity (or distance) between points to be clustered

Clustering algorithms

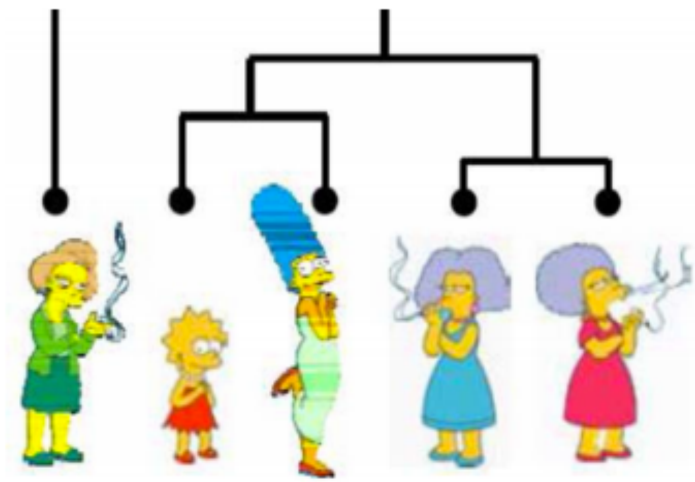
Simple clustering: organize elements into k groups

- K-means
- Mean shift
- Spectral clustering



Hierarchical clustering: organize elements into a hierarchy

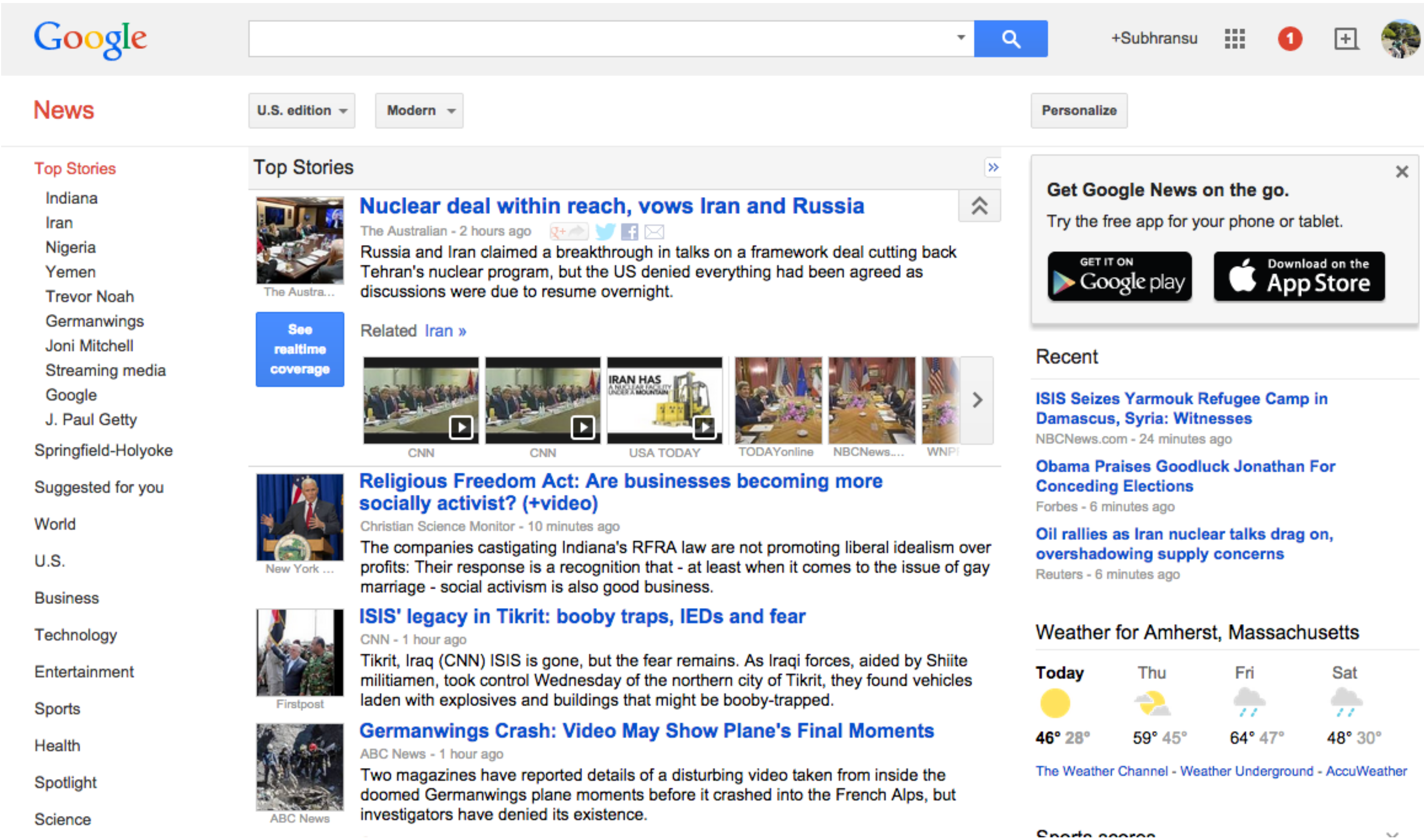
- Bottom up - agglomerative
- Top down - divisive



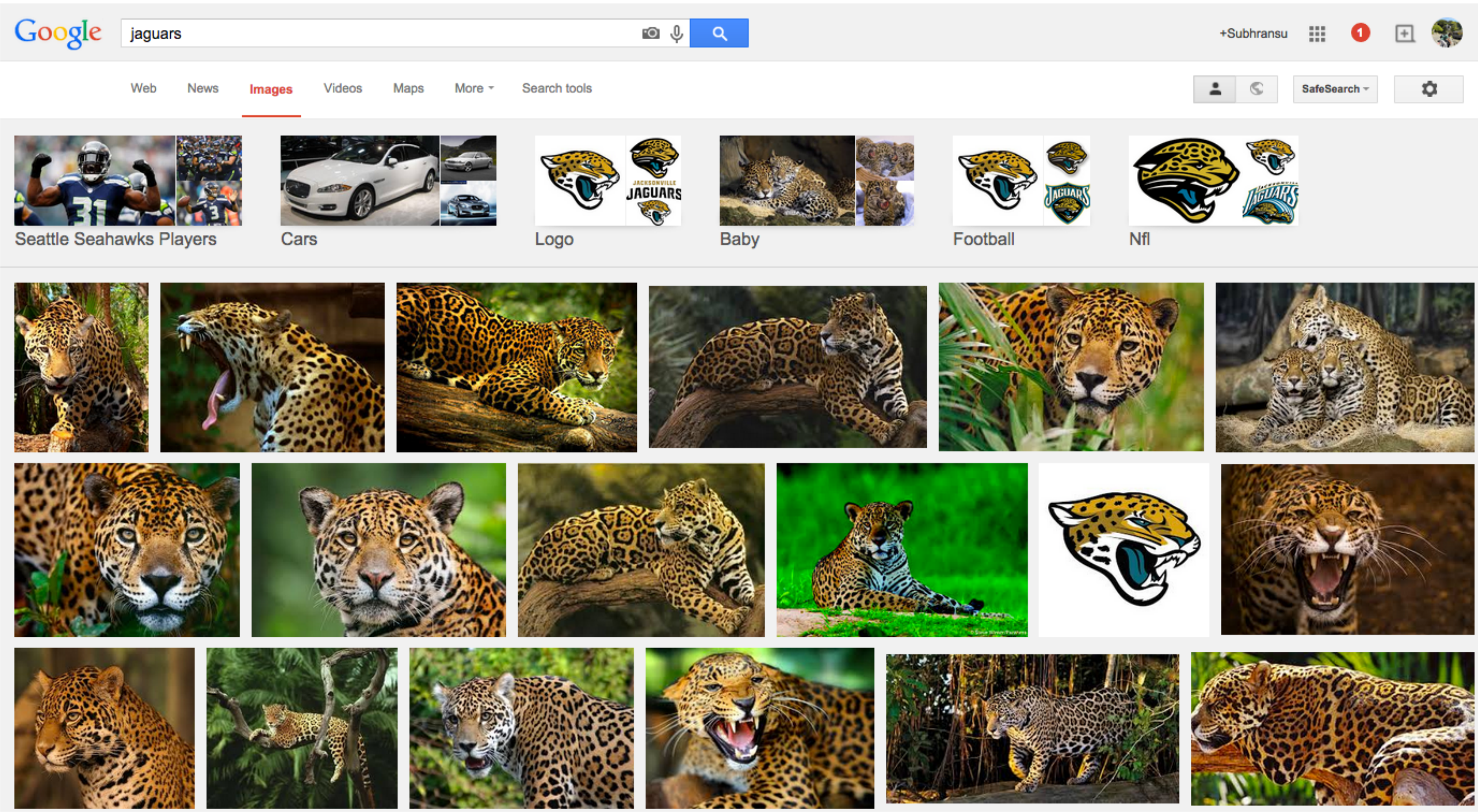
Clustering examples: Image Segmentation

image credit: Berkeley segmentation benchmark

Clustering examples: News Feed



Clustering examples: Image Search



Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

K-Nearest Neighbor

Clustering using k-means

Data: D-dimensional observations **($\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_n$)**

Goal: partition the **n** observations into **k (≤ n)** sets
S = {S_1, S_2, …, S_k} so as to minimize the within-cluster sum of squared distances

$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\mathbf{x} - \mu_i||^2$$

cluster center

Lloyd's algorithm for k-means

Initialize k centers by picking k points randomly among all the points

Repeat till convergence (or max iterations)

Assign each point to the nearest center (assignment step)

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\mathbf{x} - \mu_i||^2$$

Estimate the mean of each group (update step)

https://www.csee.umbc.edu/courses/graduate/678/spring18/kmeans/

Properties of the Lloyd's algorithm

Guaranteed to converge in a finite number of iterations

- objective decreases monotonically
- local minima if the partitions don't change.
- finitely many partitions → k-means algorithm must converge

Running time per iteration

- Assignment step: O(NKD)
- Computing cluster mean: O(ND)

Issues with the algorithm:

- Worst case running time is super-polynomial in input size
- No guarantees about global optimality
  - Optimal clustering even for 2 clusters is NP-hard [Aloise et al., 09]

k-means++ algorithm

A way to pick the good initial centers

Intuition: spread out the k initial cluster centers

The algorithm proceeds normally once the centers are initialized

[Arthur and Vassilvitskii'07] The approximation quality is O(log k) in expectation

k-means++ algorithm for initialization:

1. Chose one center uniformly at random among all the points
2. For each point **x**, compute D(**x**), the distance between x and the nearest center that has already been chosen
3. Chose one new data point at random as a new center, using a weighted probability distribution where a point **x** is chosen with a probability proportional to $D(\mathbf{x})^2$
4. Repeat Steps 2 and 3 until k centers have been chosen

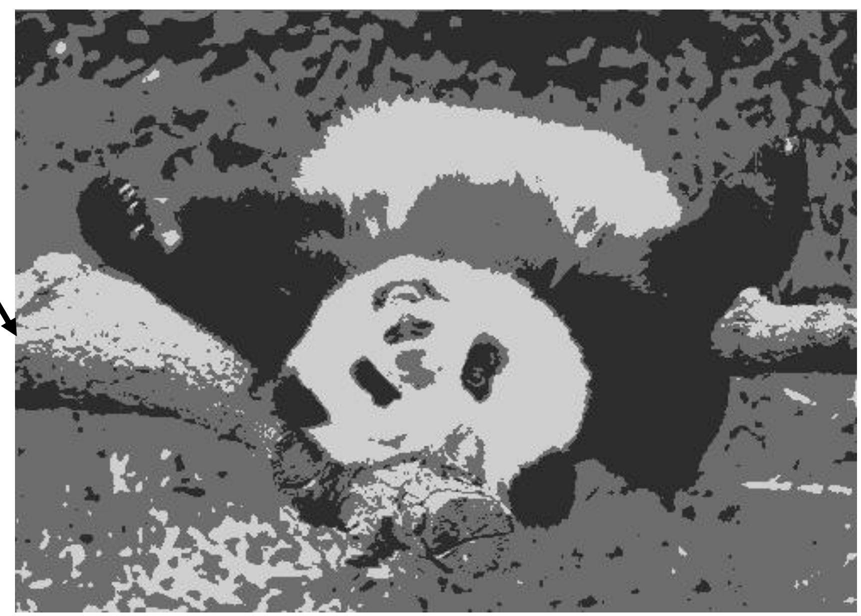
Fast kmeans

- Intuition: If a data point is close to center i and far from center j, and center j has not moved much since the last iteration, we don’t need to recalculate the distance for center j.
- Use triangle inequality to prune the number of distances that you should recalculate.

k-means for image segmentation

K=2

K=3



Grouping pixels based on intensity similarity

feature space: intensity value (1D)

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

K-Nearest Neighbor

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

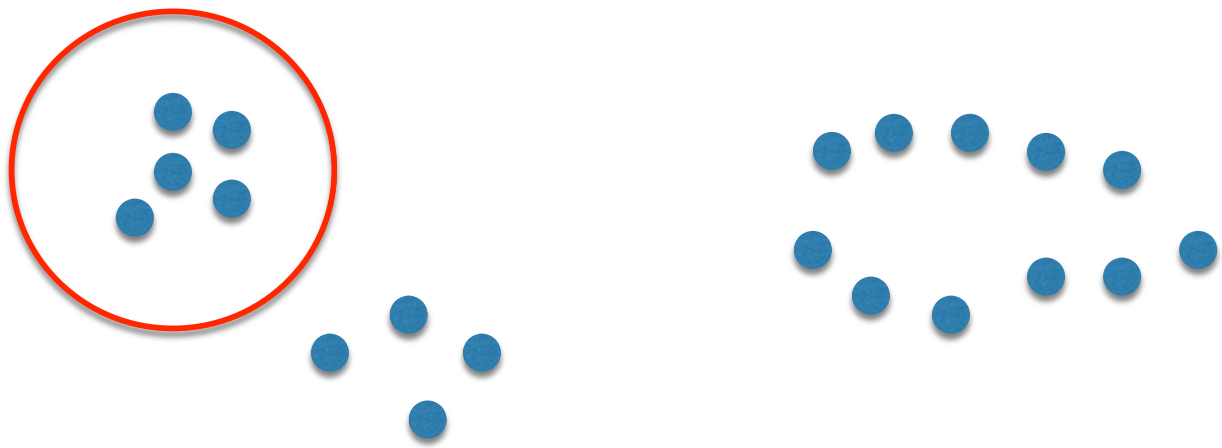
K-Nearest Neighbor

Clustering using density estimation

One issue with k-means is that it is sometimes hard to pick k

The mean shift algorithm seeks modes or local maxima of density in the feature space

Mean shift automatically determines the number of clusters



$$K(\mathbf{x}) = \frac{1}{Z} \sum_i \exp\left(-\frac{||\mathbf{x} - \mathbf{x}_i||^2}{h}\right)$$

Kernel density estimator

Small *h* implies more modes (bumpy distribution)

Mean shift algorithm

For each point x_i:

find m_i, the amount to shift each point x_i to its centroid

return $\{m_i\}$

Mean shift algorithm

For each point x_i:

set $m_i = x_i$

while not converged:

compute *weighted average of neighboring point*

return $\{m_i\}$

Mean shift algorithm

For each point x_i:

  set $m_i = x_i$

  while not converged:

    compute $$m_i = \frac{\sum_{x_j \in N(x_i)} x_j K(m_i, x_j)}{\sum_{x_j \in N(x_i)} K(m_i, x_j)}$$

return $\{m_i\}$

Neighbors of x_i

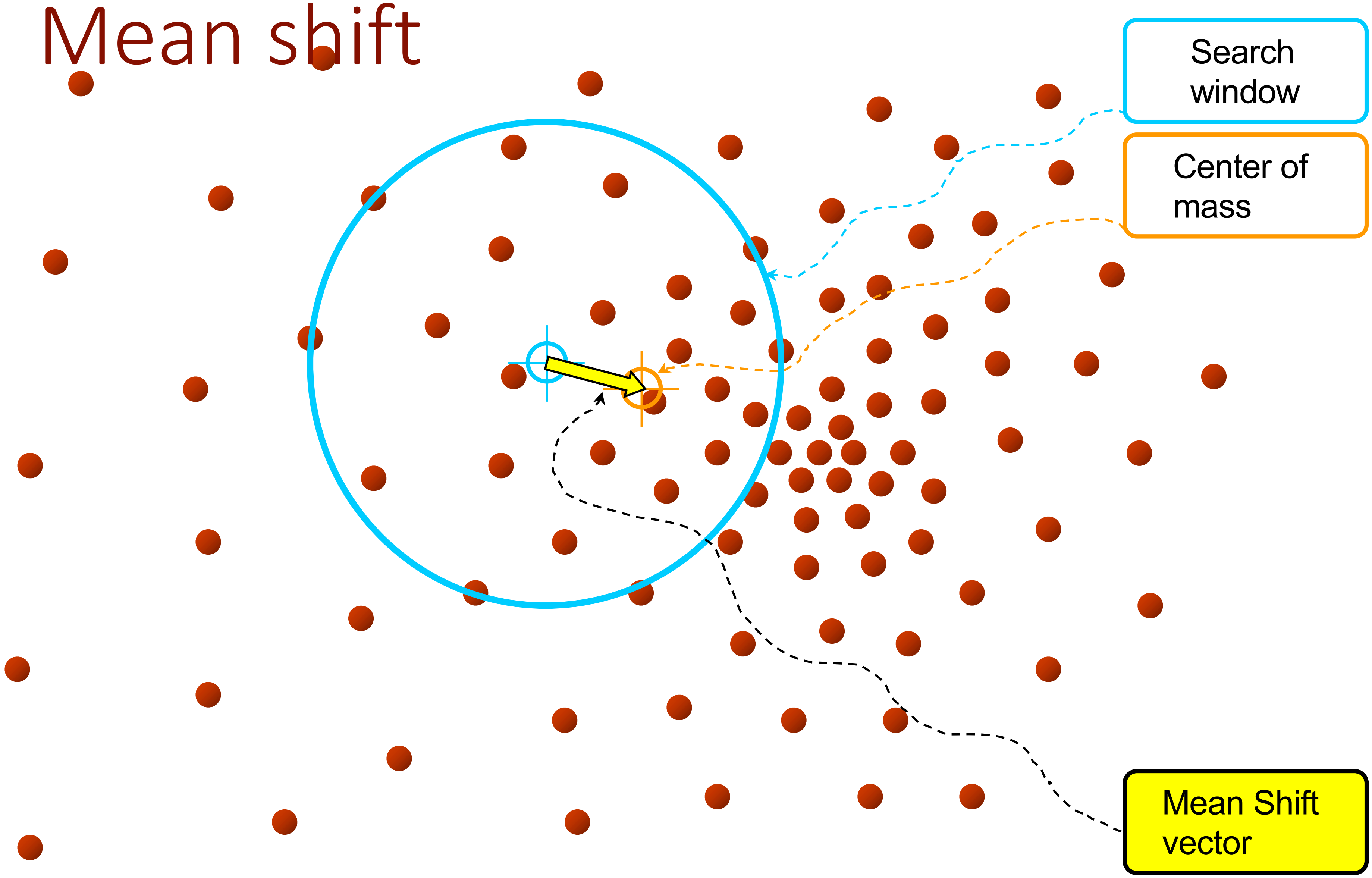
weighted average

self-clustering to based on kernel (similarity to other points)

Pros:
- Does not assume shape on clusters
- Generic technique
- Finds multiple modes
- Parallelizable

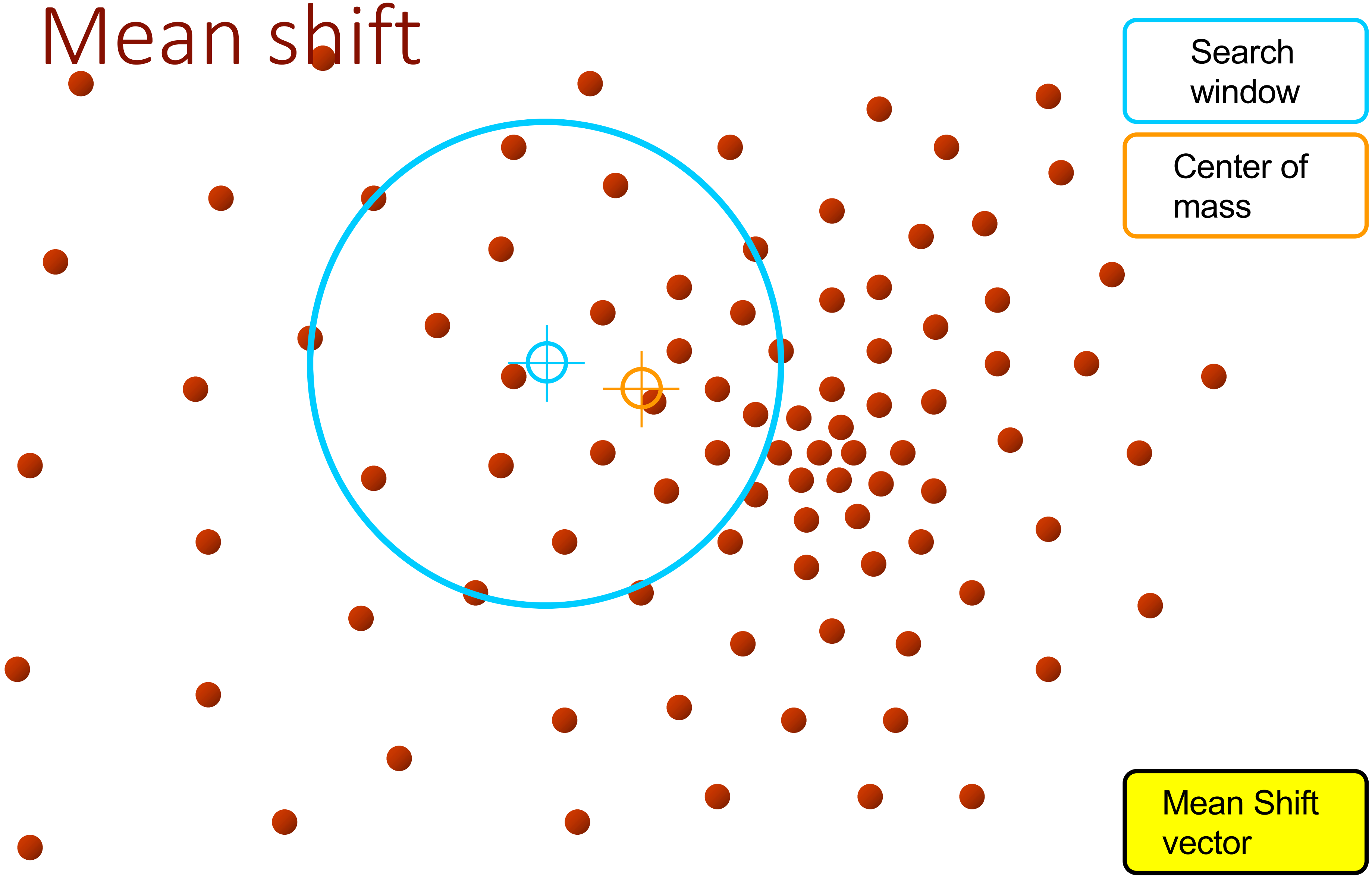
Cons:
- Slow: $O(DN^2)$ per iteration
- Does not work well for high-dimensional features

Mean shift



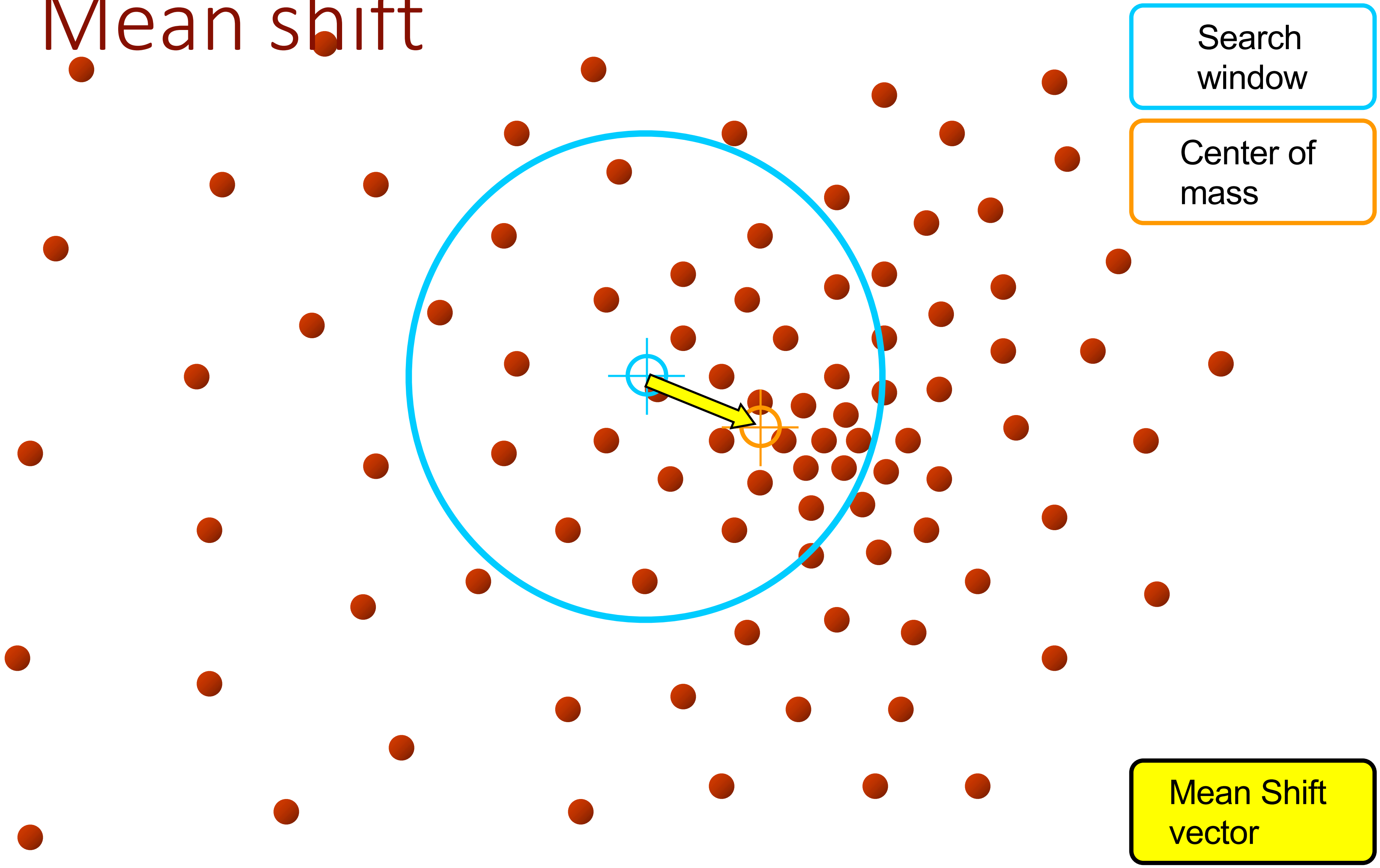
Slide by Y. Ukrainitz & B. Sar

Mean shift



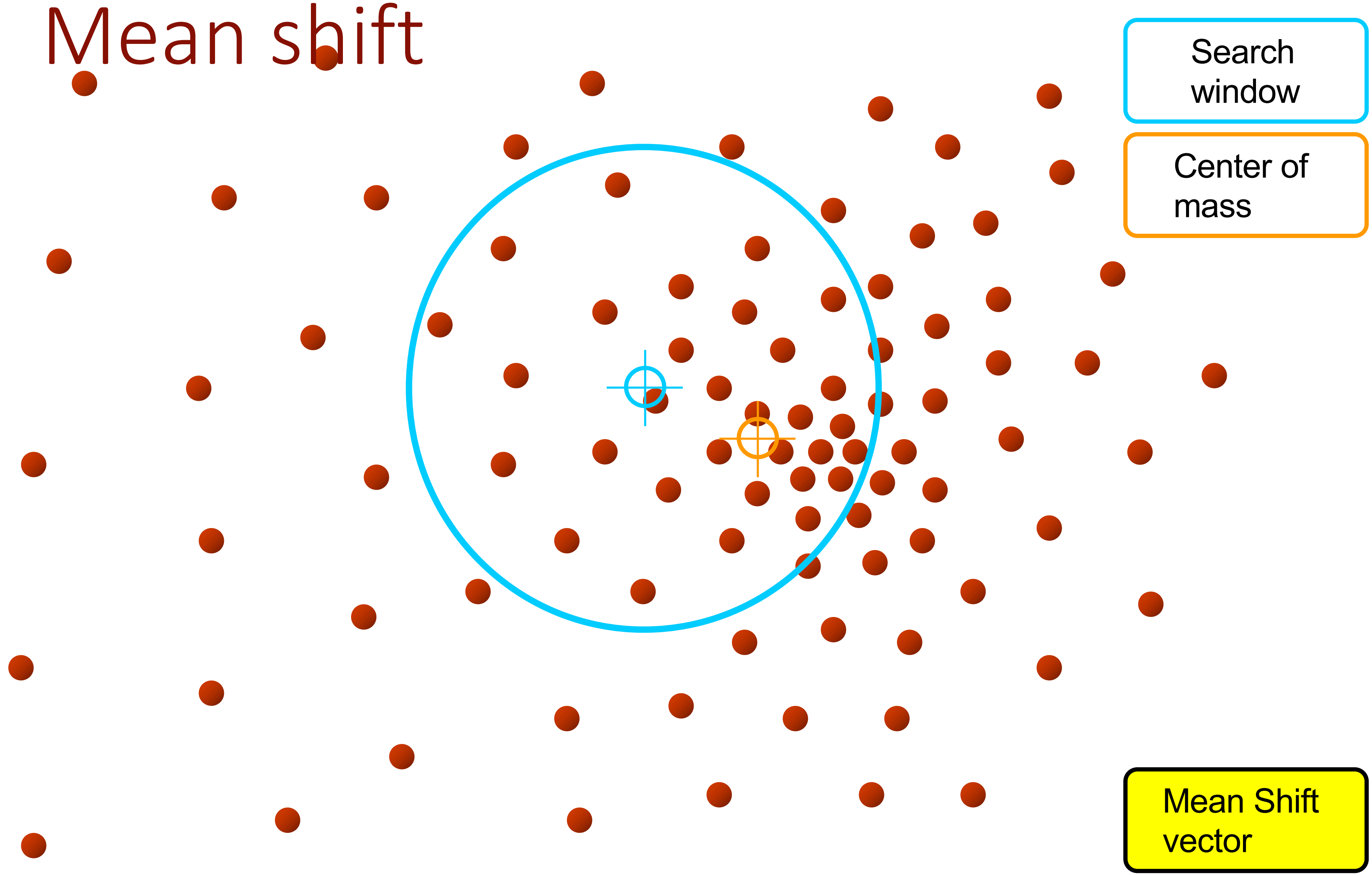
Slide by Y. Ukrainitz & B. Sar

Mean shift



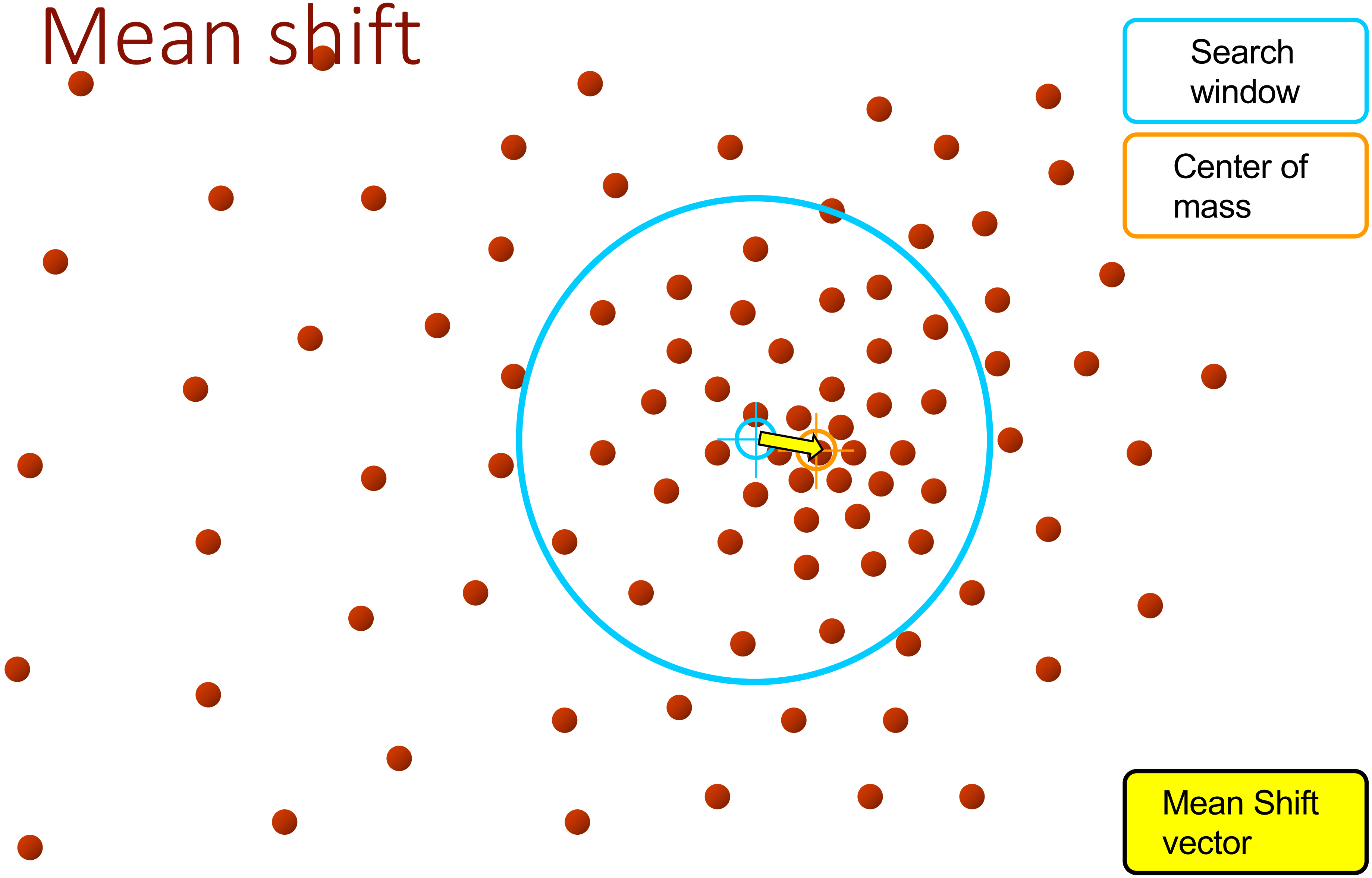
Slide by Y. Ukrainitz & B. Sar

Mean shift



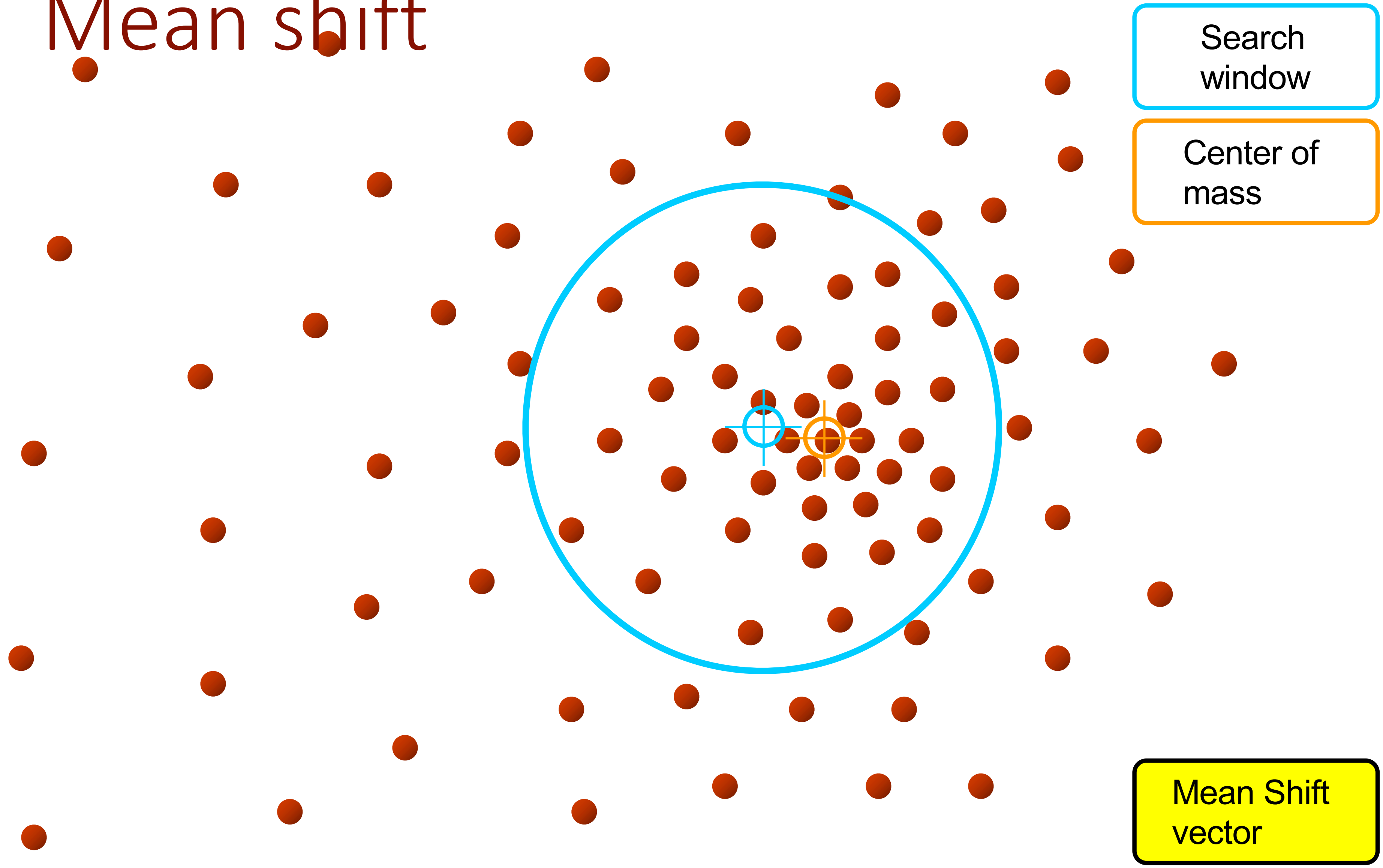
Slide by Y. Ukrainitz & B. Sare

Mean shift



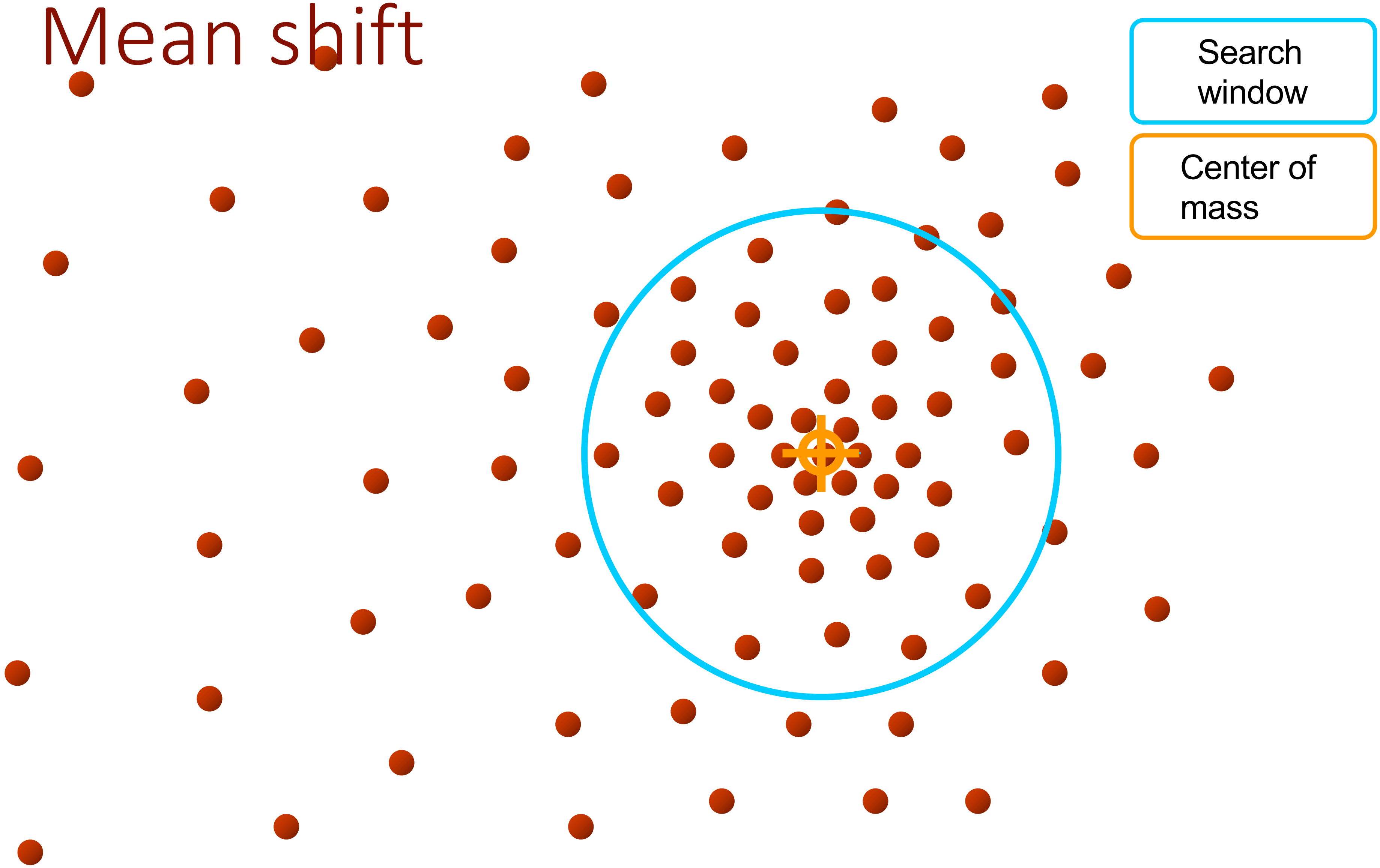
Slide by Y. Ukrainitz & B. Sar

Mean shift



Slide by Y. Ukrainitz & B. Sar

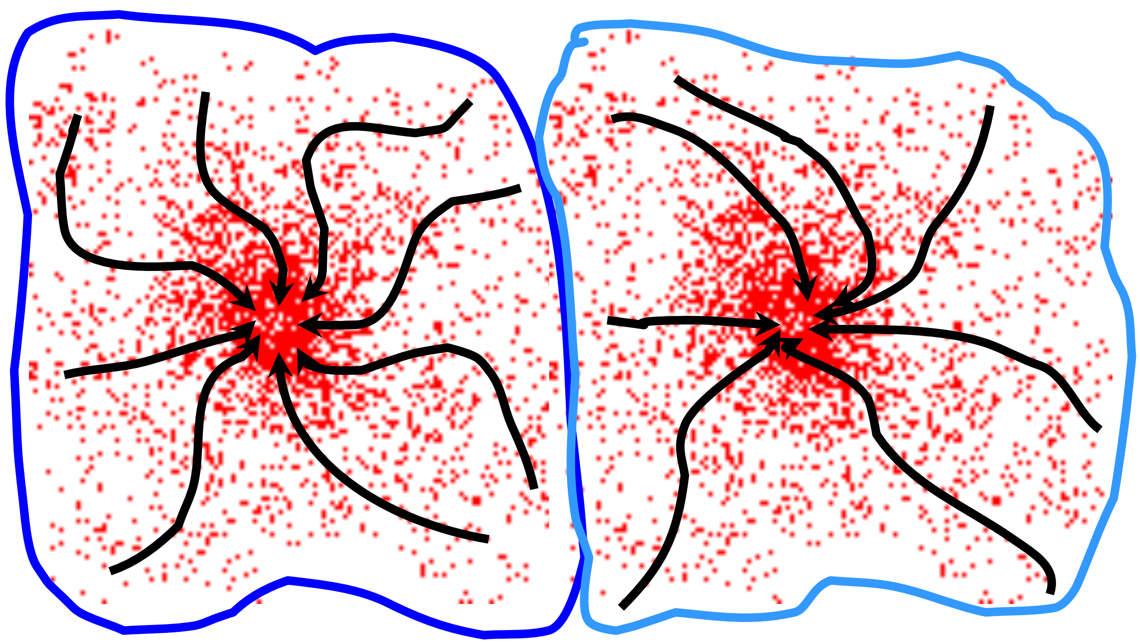
Mean shift



Slide by Y. Ukrainitz & B. Sar

Mean shift clustering

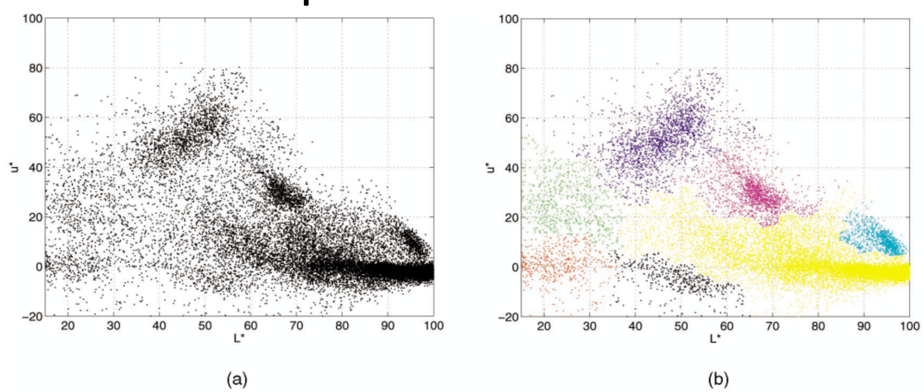
- Cluster all data points in the attraction basin of a mode
- Attraction basin is the region for which all trajectories lead to the same mode — correspond to clusters

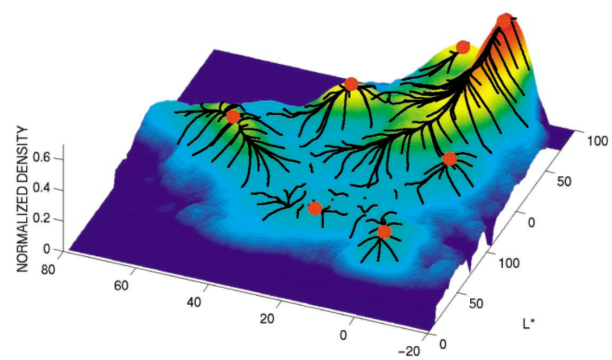


Slide by Y. Ukrainitz & B. Sar

Mean shift for image segmentation

- Feature: L*u*v* color values
- Initialize windows at individual feature points
- Perform mean shift for each window until convergence
- Merge windows that end up near the same "peak" or mode





Mean shift clustering results

http://www.caip.rutgers.edu/~comanici/MSPAMI/msPamiResults.html

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

K-Nearest Neighbor

Hierarchical clustering

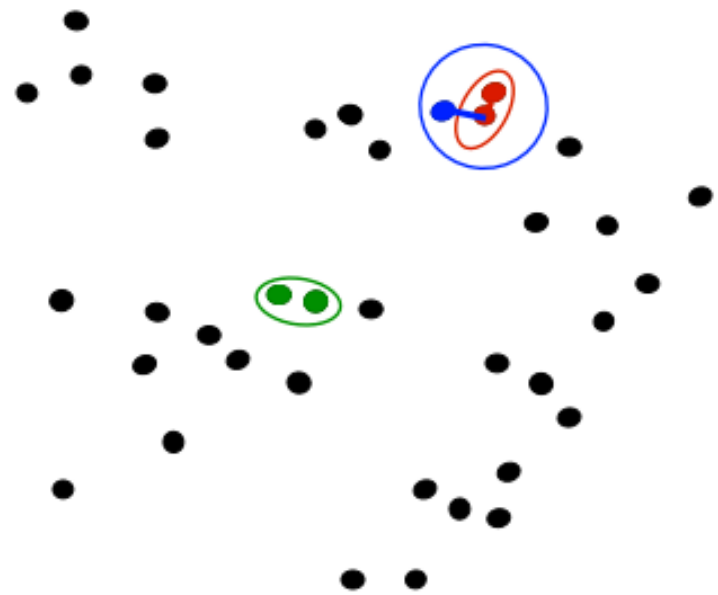
Agglomerative: a “bottom up” approach where elements start as individual clusters and clusters are merged as one moves up the hierarchy

Divisive: a “top down” approach where elements start as a single cluster and clusters are split as one moves down the hierarchy

Agglomerative clustering

Agglomerative clustering:

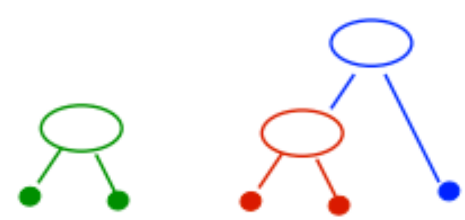
- First merge very similar instances
- Incrementally build larger clusters out of smaller clusters



Algorithm:

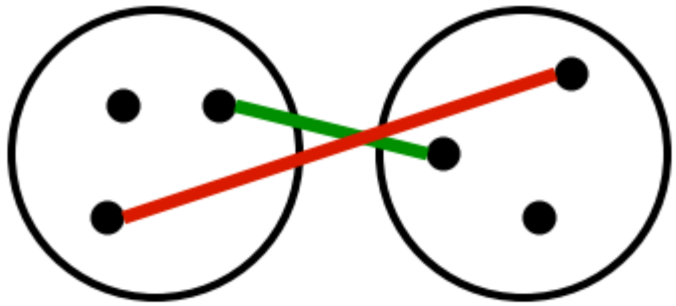
- Maintain a set of clusters
- Initially, each instance in its own cluster
- Repeat:
  - Pick the two “closest” clusters
  - Merge them into a new cluster
  - Stop when there’s only one cluster left

Produces not one clustering, but a family of clusterings represented by a dendrogram



Agglomerative clustering

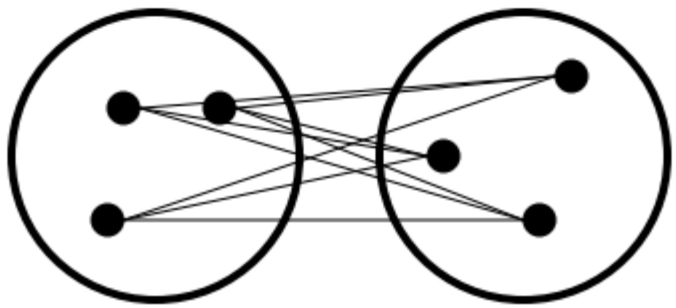
How should we define "closest" for clusters with multiple elements?



Closest pair: single-link clustering

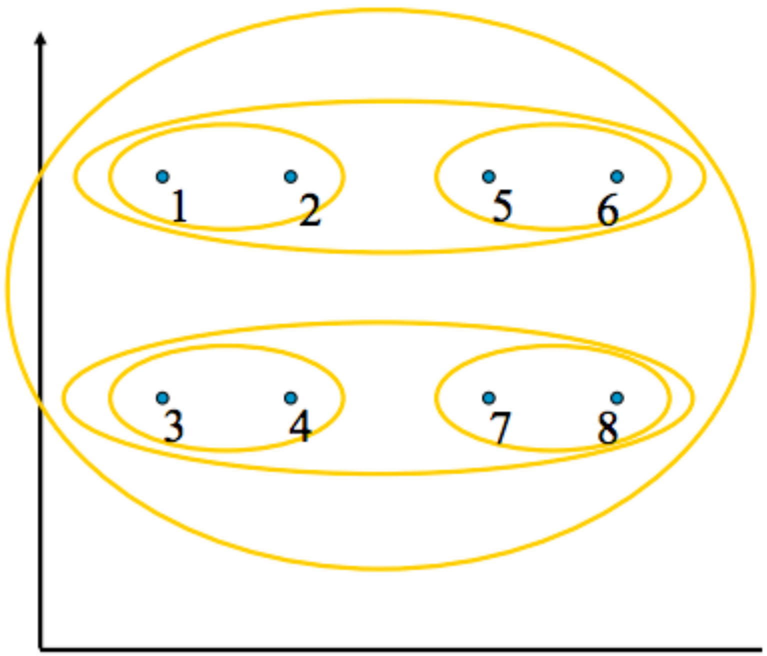
Farthest pair: complete-link clustering

Average of all pairs

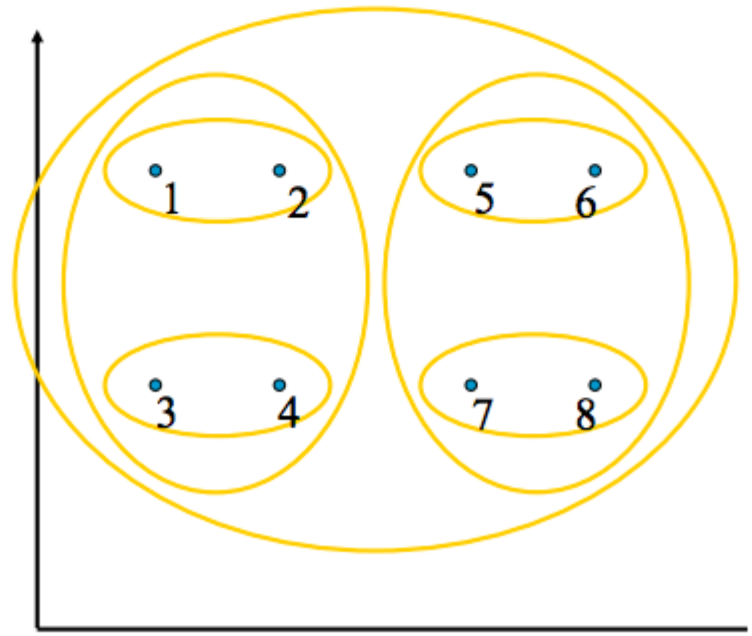


Agglomerative clustering

Closest pair
(single-link clustering)



Farthest pair
(complete-link clustering)



[Pictures from Thorsten Joachims]

Summary

- Clustering is an example of unsupervised learning
- Partitions or hierarchy
- Several partitioning algorithms:
  - k-means: simple, efficient and often works in practice
    - k-means++ for better initialization
  - mean shift: modes of density
    - slow but suited for problems with unknown number of clusters with varying shapes and sizes
  - spectral clustering: clustering as graph partitions
    - solve $(\mathbf{D} - \mathbf{W})x = \lambda \mathbf{D}x$ followed by k-means
- Hierarchical clustering methods:
  - Agglomerative or divisive
    - single-link, complete-link and average-link

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

K-Nearest Neighbor

Nearest neighbor classifier

Will Alice like the movie?

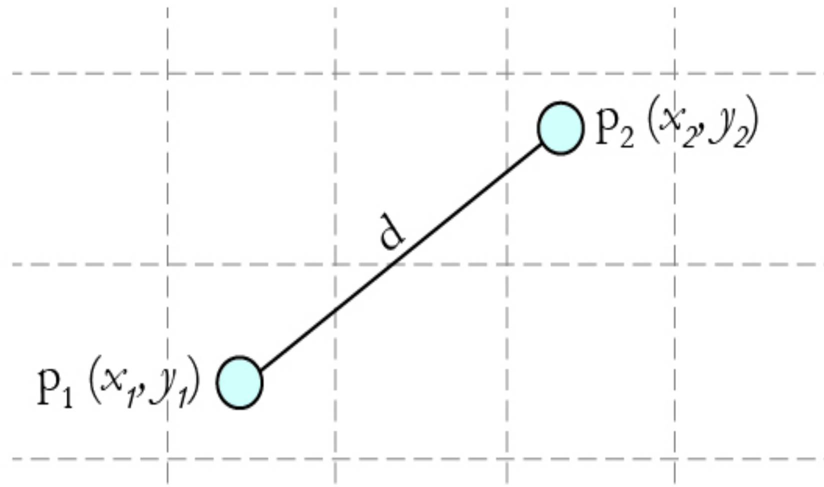
Alice and James are similar

James likes the movie →

Alice must/might also like the movie

Represent data as vectors of feature values

Find closest (Euclidean norm) points



Euclidean distance (d) $= \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

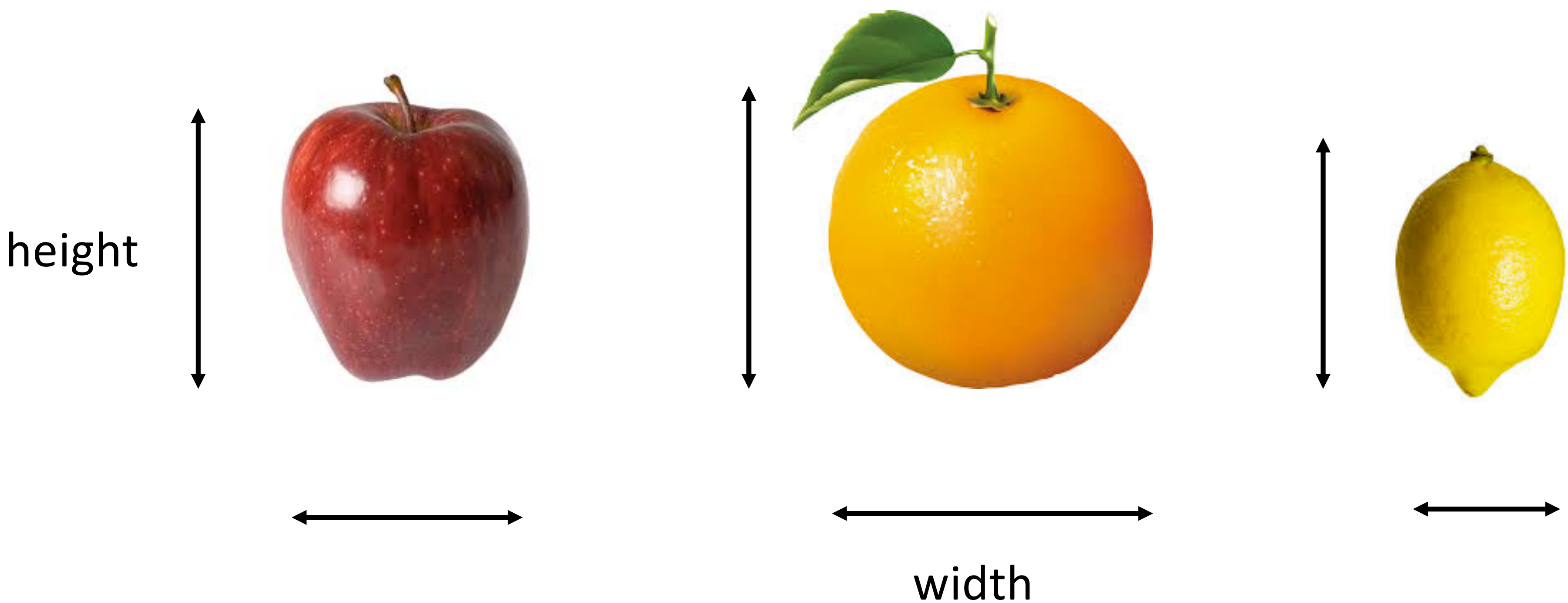
Nearest neighbor classifier

Training data is in the form of $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

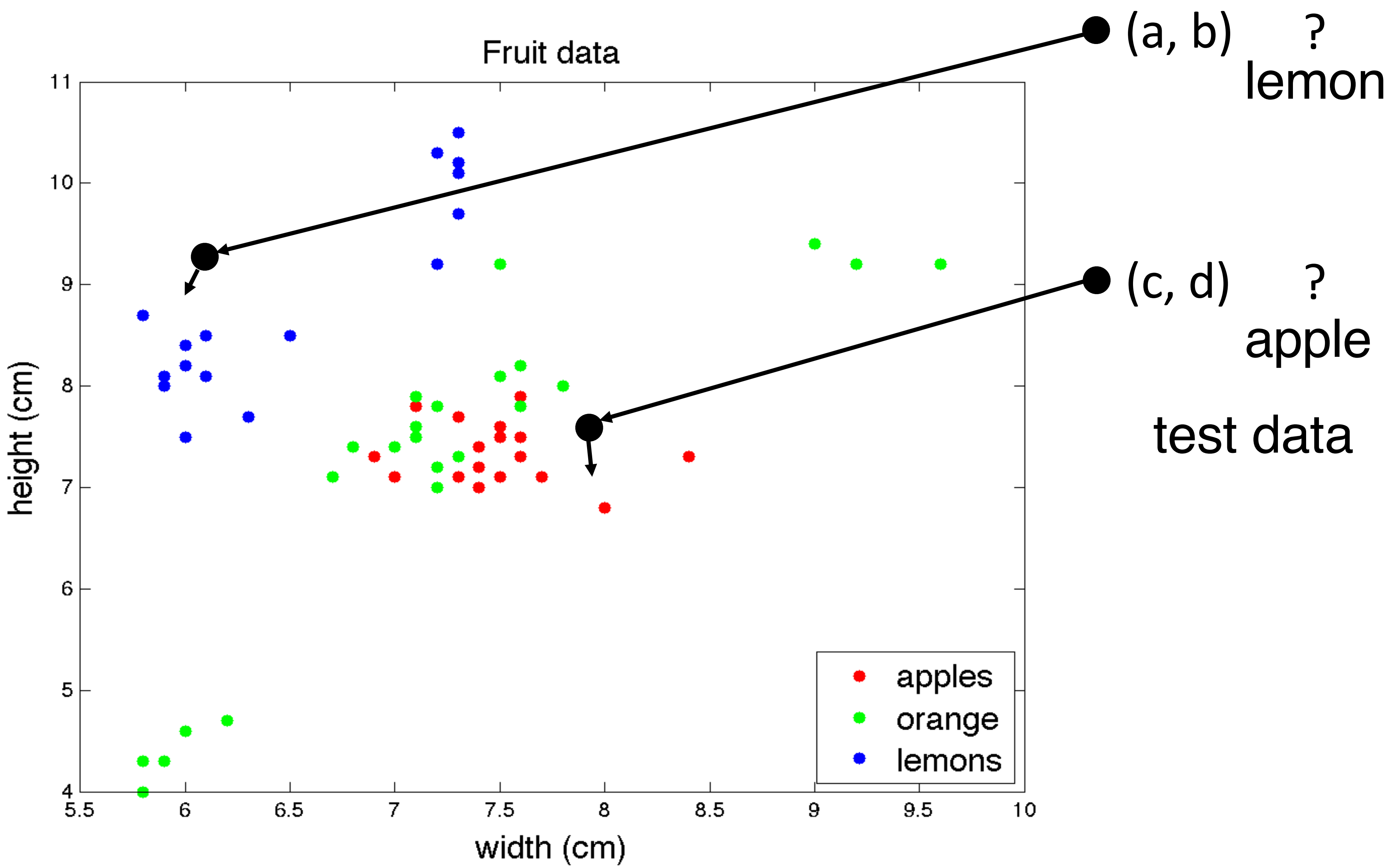
Fruit data:

label: {apples, oranges, lemons}

attributes: {width, height}

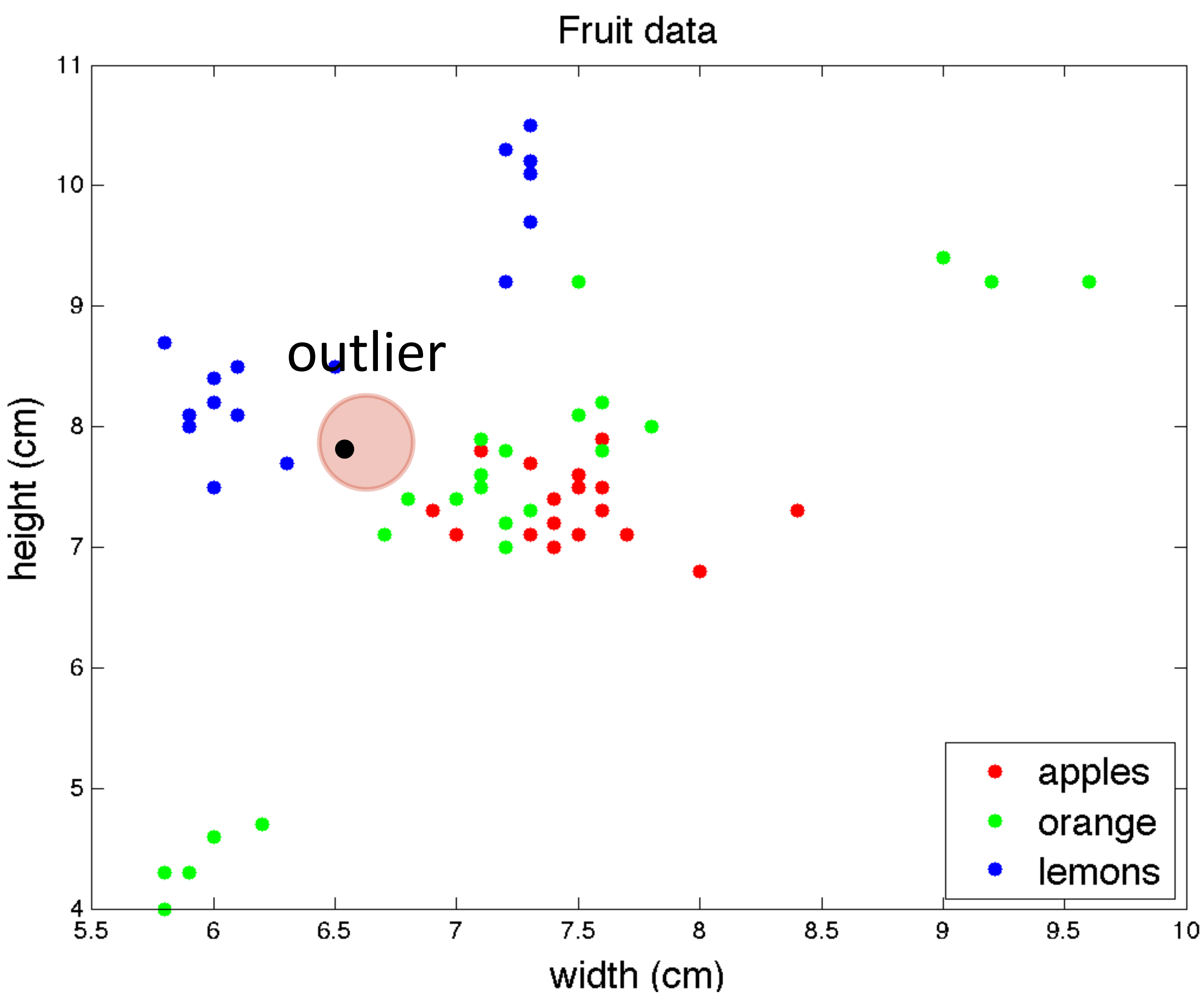


Nearest neighbor classifier



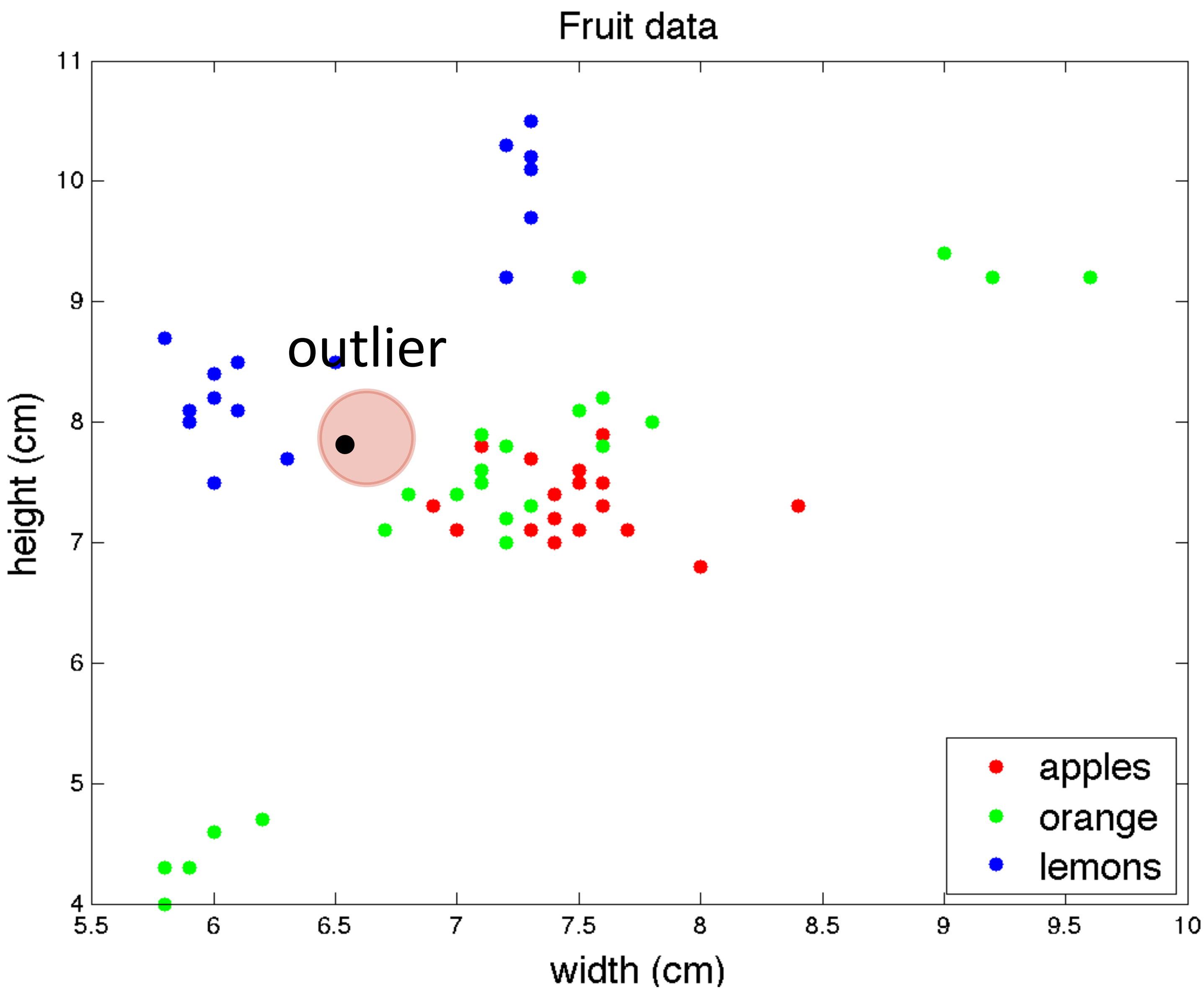
k-Nearest neighbor classifier

Take majority vote among the k nearest neighbors



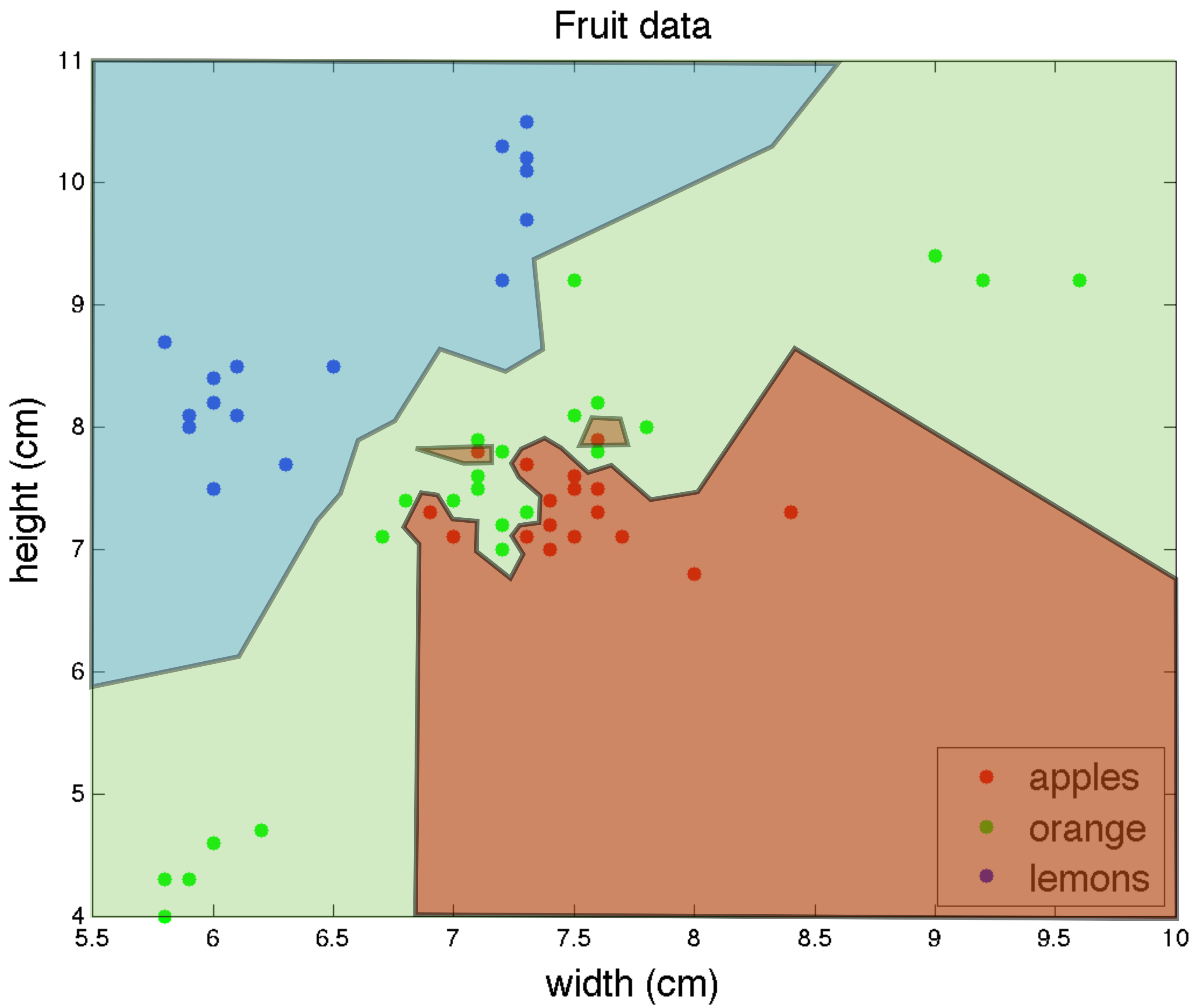
k-Nearest neighbor classifier

Take majority vote among the k nearest neighbors



What is the effect of k?

Decision boundaries: 1NN



Inductive bias of the kNN classifier

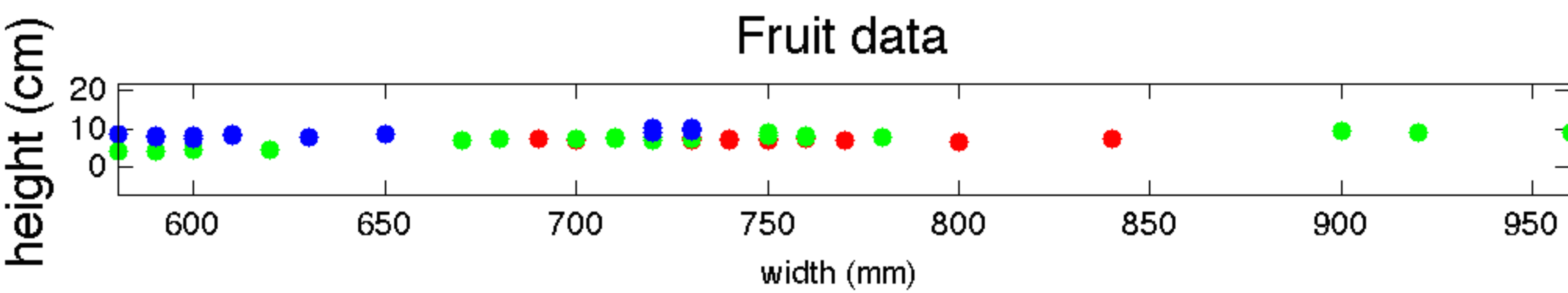
Choice of features

- We are assuming that all features are equally important
- What happens if we scale one of the features by a factor of 100?

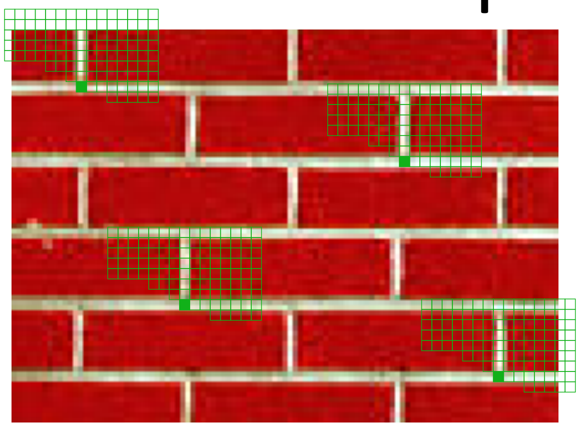
Choice of distance function

- Euclidean, cosine similarity (angle), Gaussian, etc …
- Should the coordinates be independent?

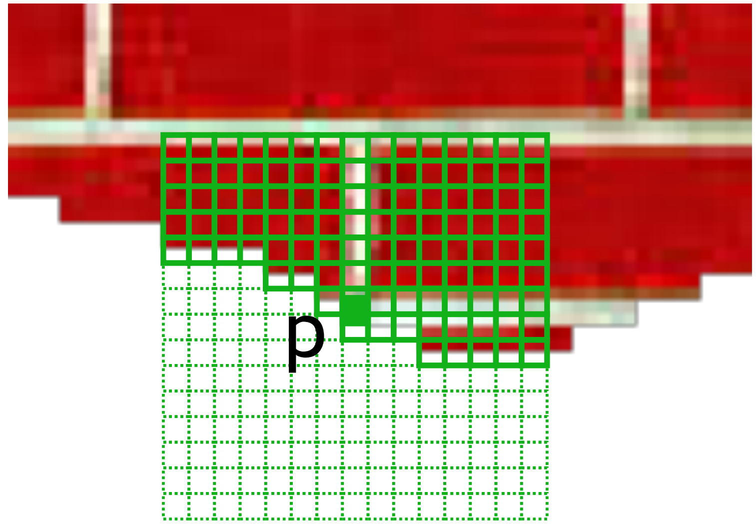
Choice of k



An example: Synthesizing one pixel



input image



synthesized image

What is $P(\mathbf{x}|\text{neighborhood of pixels around x})$

Find all the windows in the image that match the neighborhood

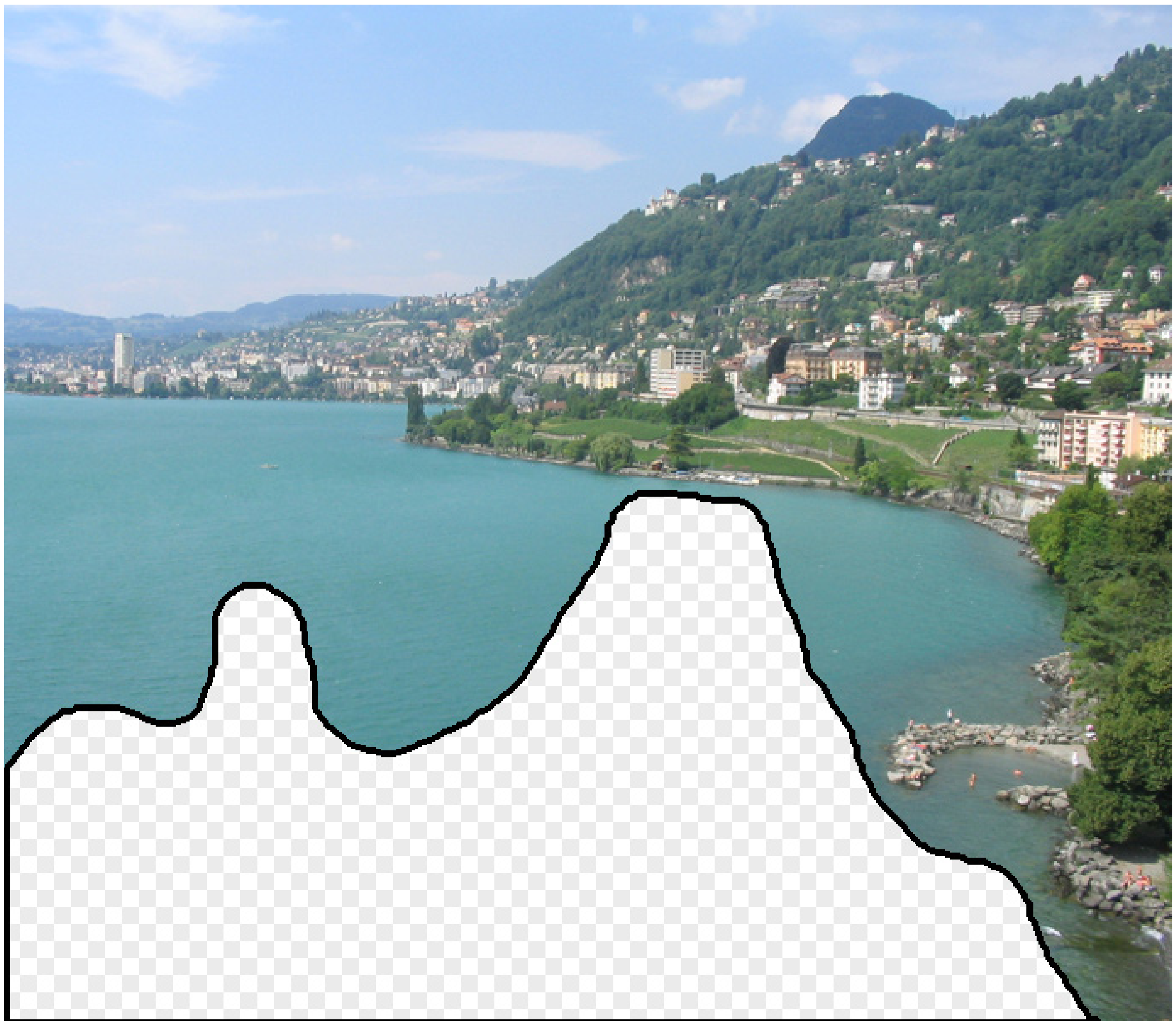
To synthesize **x**

- pick one matching window at random
- assign **x** to be the center pixel of that window

An **exact** match might not be present, so find the **best** matches using **Euclidean distance** and randomly choose between them, preferring better matches with higher probability

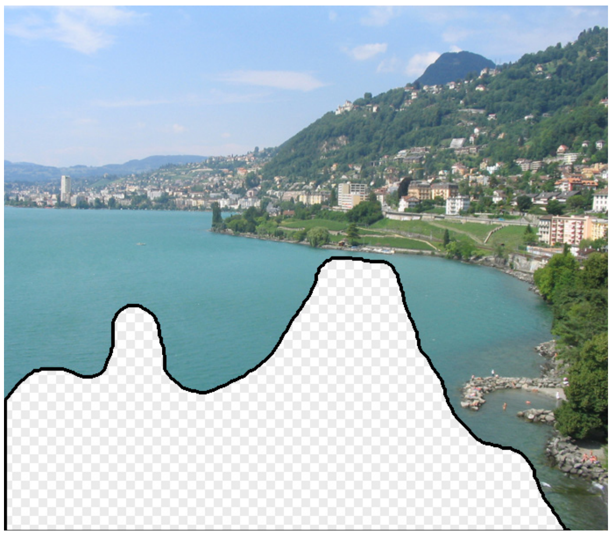
Slide from Alyosha Efros, ICCV 1999

kNN: Scene Completion

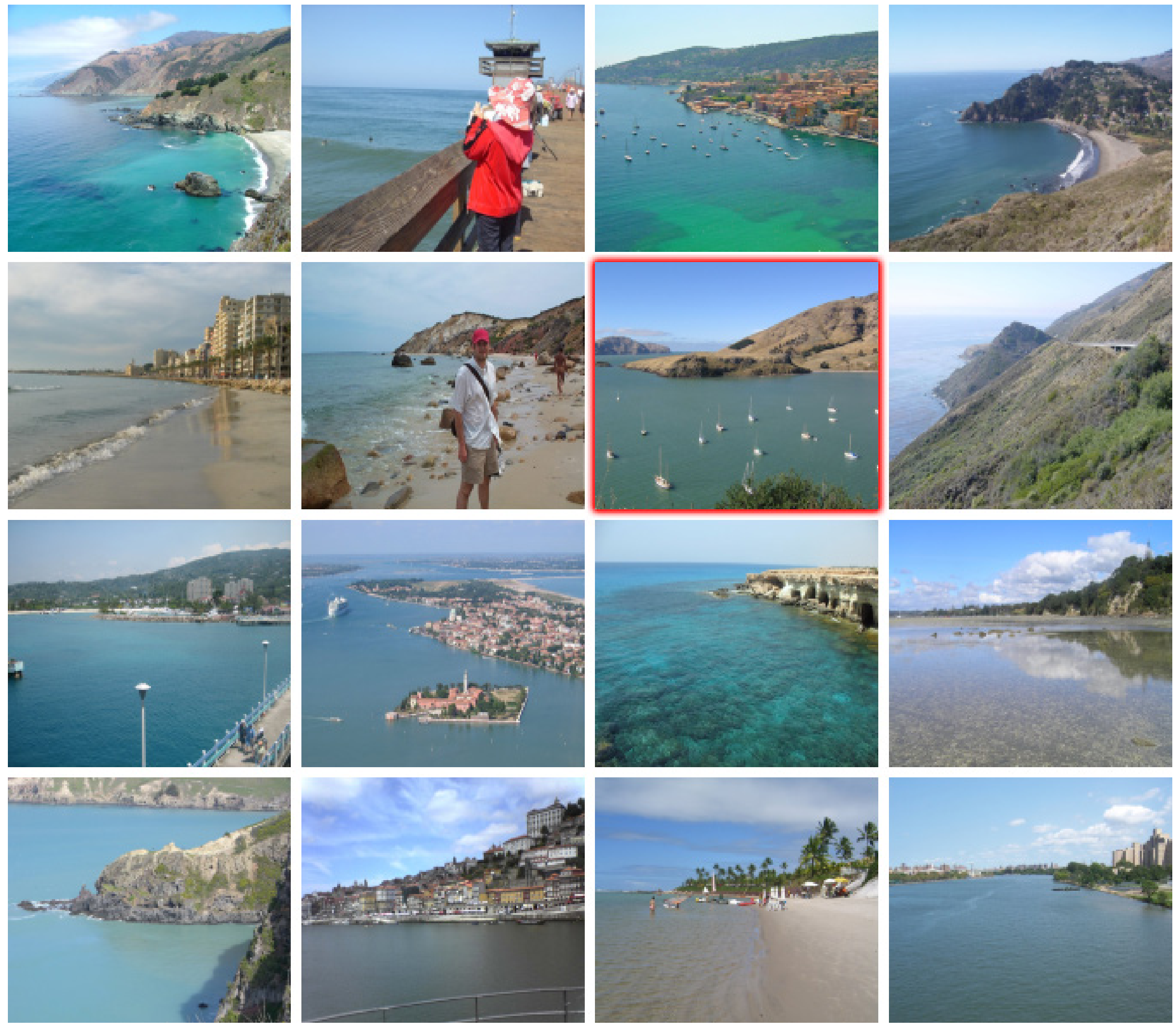


"Scene completion using millions of photographs", Hayes and Efros, TOG 2007

kNN: Scene Completion

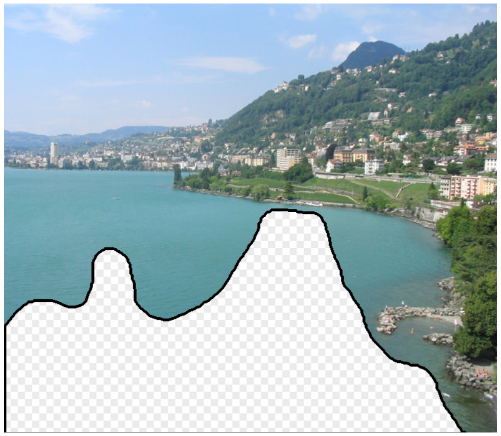


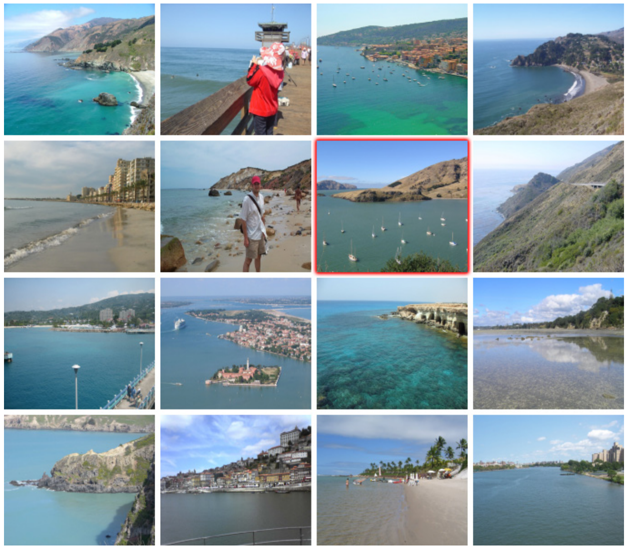
Nearest neighbors



"Scene completion using millions of photographs", Hayes and Efros, TOG 2007

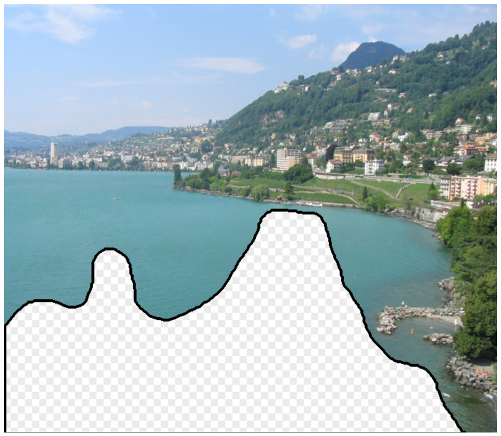
kNN: Scene Completion

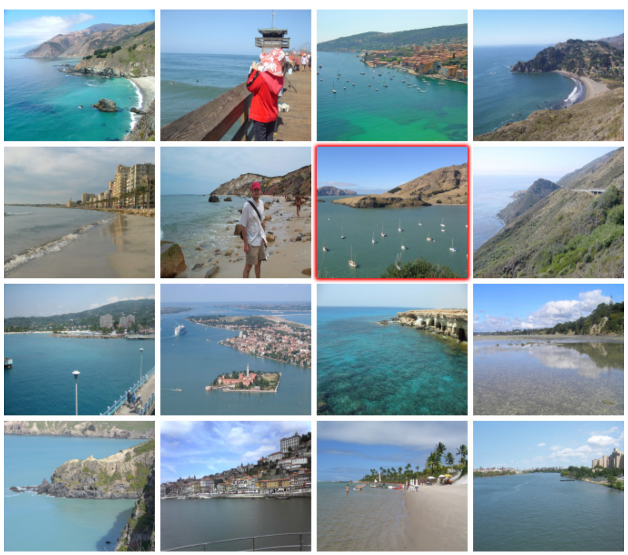




"Scene completion using millions of photographs", Hayes and Efros, TOG 2007

kNN: Scene Completion





“Scene completion using millions of photographs”, Hayes and Efros, TOG 2007

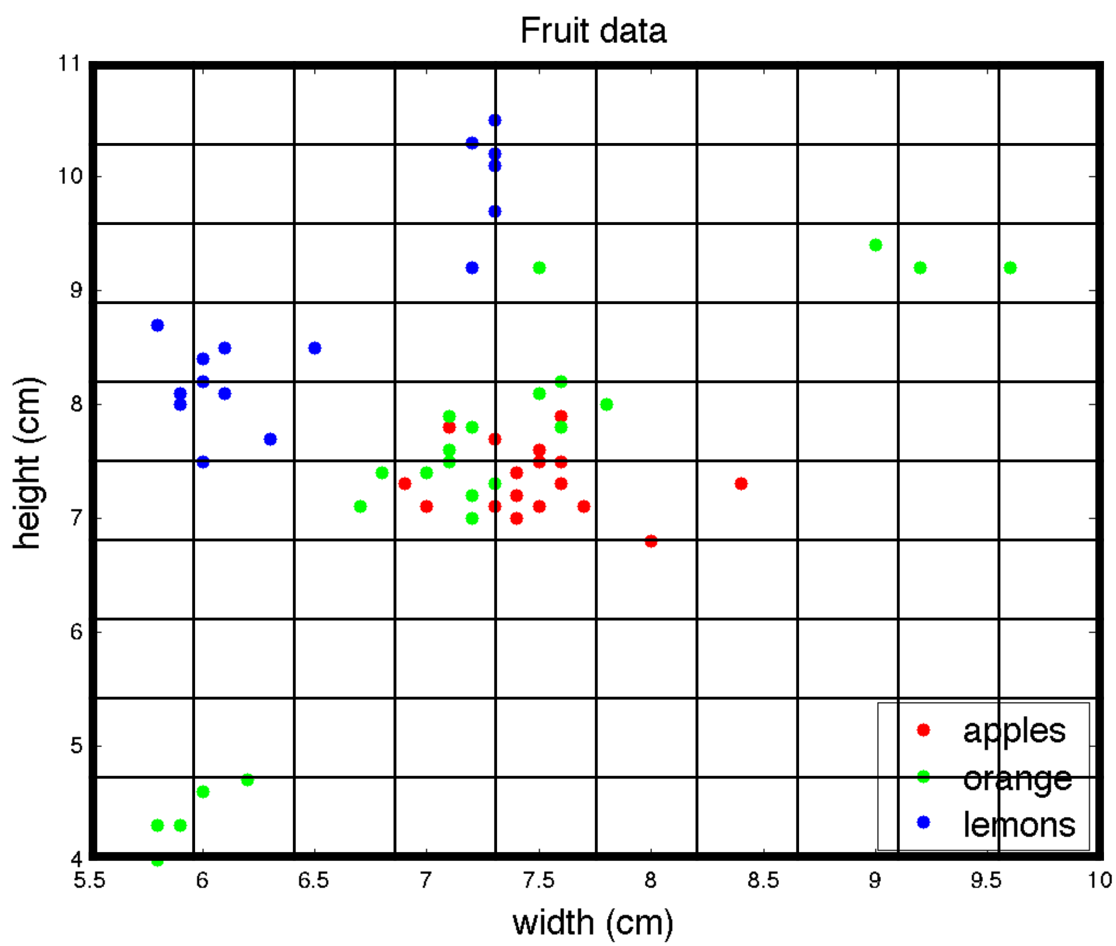
Practical issue when using kNN: speed

Time taken by kNN for N points of D dimensions

- time to compute distances: O(ND)
- time to find the k nearest neighbor
  - O(k N) : repeated minima
  - O(N log N) : sorting
  - O(N + k log N) : min heap
  - O(N + k log k) : fast median
- Total time is dominated by distance computation

We can be faster if we are willing to sacrifice exactness

Practical issue when using kNN: Curse of dimensionality



#bins = 10x10

d = 2

#bins = 10^d

d = 1000

Atoms in the universe: ~10^{80}

How many neighborhoods are there?

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

Hierarchical clustering

K-Nearest Neighbor

Slides credit

Slides are closely following and adapted from Hal Daume's book and Subranshu Maji's course.

The fruit classification dataset is from Iain Murray at University of Edinburgh

http://homepages.inf.ed.ac.uk/imurray2/teaching/oranges_and_lemons/.

The slides on texture synthesis are from Efros and Leung's ICCV 2009 presentation.

Many images are from the Berkeley segmentation benchmark

http://www.eecs.berkeley.edu/Research/Projects/CS/vision/bsds

Normalized cuts image segmentation:

http://www.timotheecour.com/research.html