Clustering, K-Means, and K-Nearest Neighbors

CMSC 678

UMBC

Most slides courtesy Hamed Pirsiavash

Recap from last time…

Geometric Rationale of LDiscA & PCA

Objective: to rigidly rotate the axes of the D-dimensional space to new positions (principal axes):

ordered such that principal axis 1 has the highest variance, axis 2 has the next highest variance, ... , and axis D has the lowest variance

covariance among each pair of the principal axes is zero (the principal axes are uncorrelated)

Courtesy Antano Žilinsko

L-Dimensional PCA

1. Compute mean μ, priors, and common covariance Σ

$$\Sigma = \frac{1}{N} \sum_{i:y_i=k} (x_i - \mu)(x_i - \mu)^T \qquad \mu = \frac{1}{N} \sum_i x_i$$

2. Sphere the data (zero-mean, unit covariance)
3. Compute the (top L) eigenvectors, from sphere-d data, via V

$$X^* = V D_B V^T$$

4. Project the data

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

Graph & spectral clustering

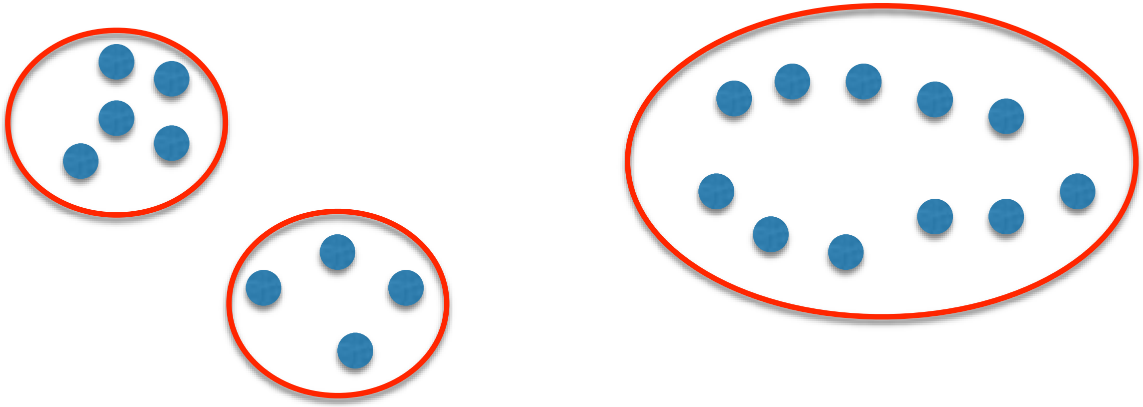
Hierarchical clustering

K-Nearest Neighbor

Clustering

Basic idea: group together similar instances

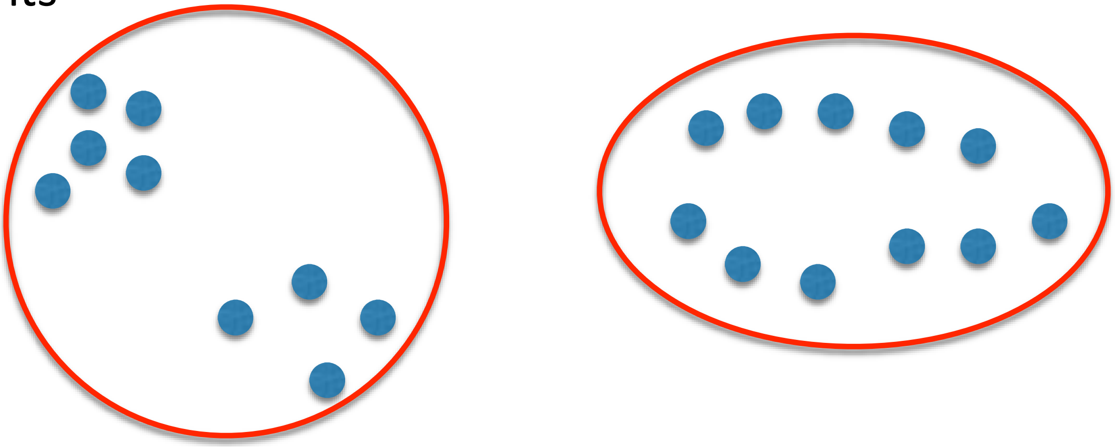
Example: 2D points



Clustering

Basic idea: group together similar instances

Example: 2D points



One option: small Euclidean distance (squared)

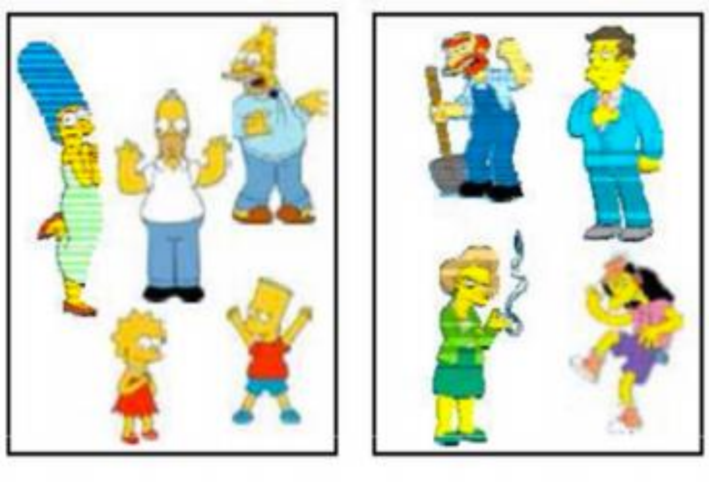
$$\mathrm{dist}(\mathbf{x},\mathbf{y}) = ||\mathbf{x}-\mathbf{y}||_2^2$$

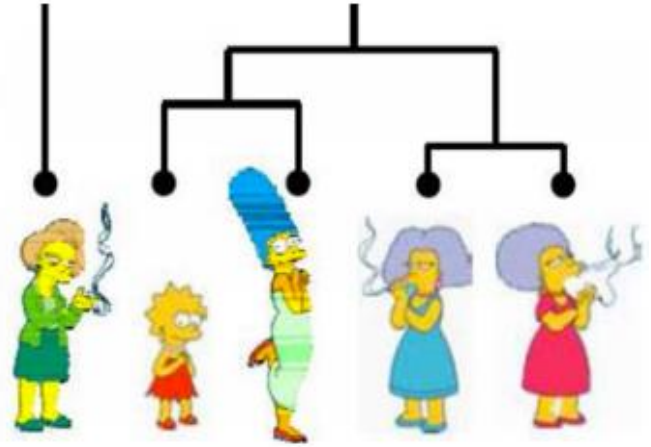
Clustering results are crucially dependent on the measure of similarity (or distance) between points to be clustered

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

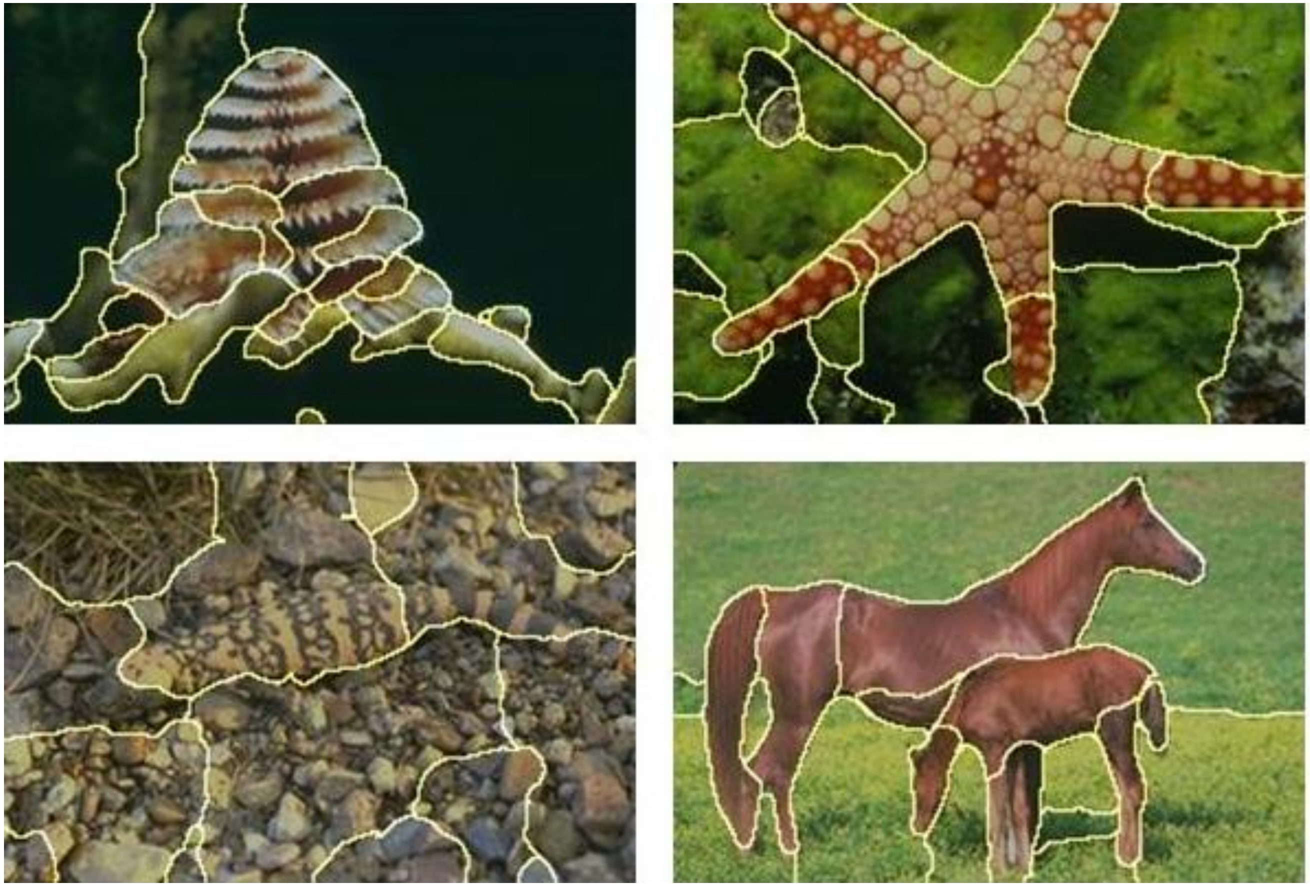
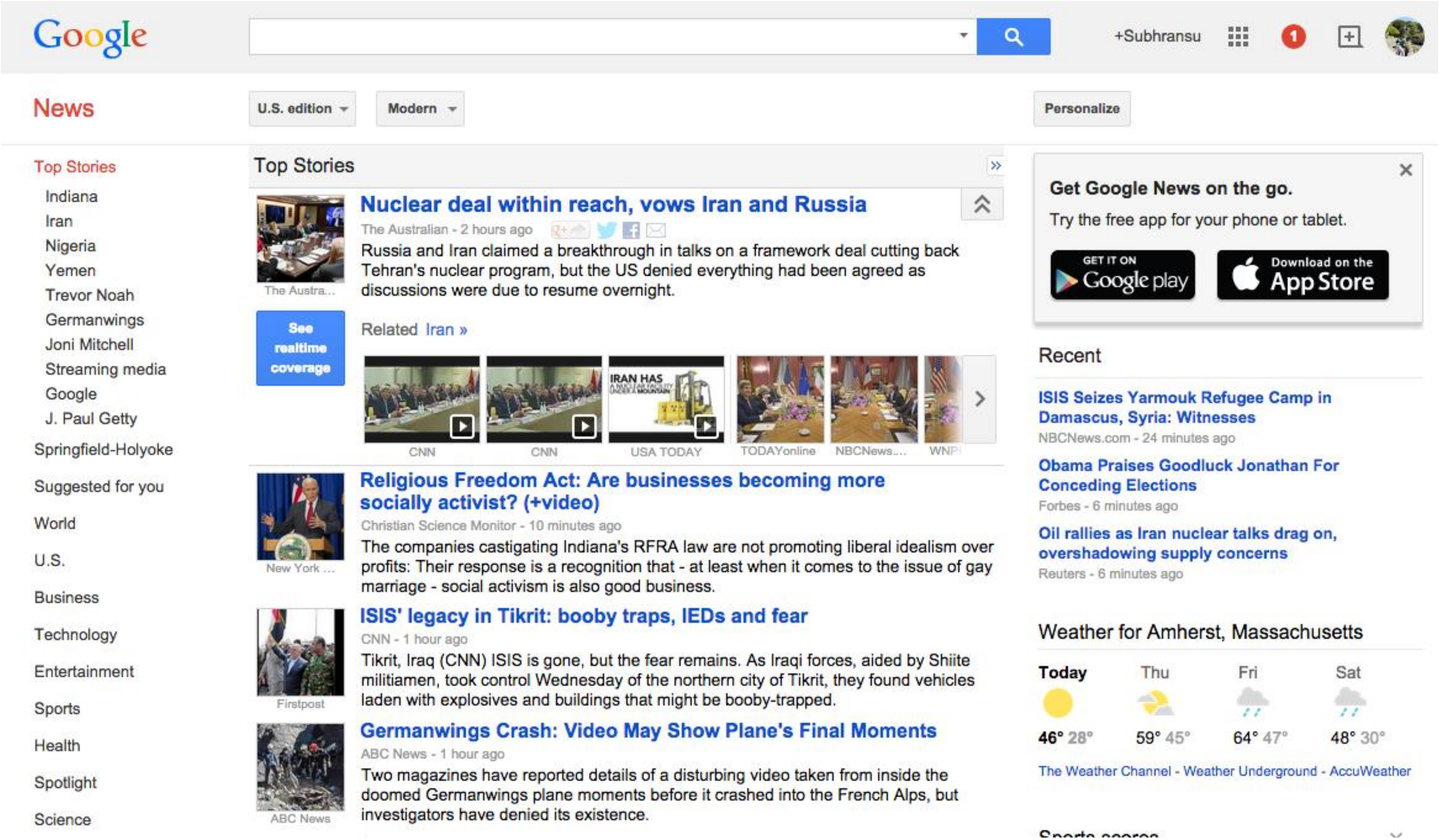


image credit: Berkeley segmentation benchmark

Clustering examples: News Feed



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+Subhransu

1

News

U.S. edition

Modern

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- Indiana
- Iran
- Nigeria
- Yemen
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- Germanwings
- Joni Mitchell
- Streaming media
- Google
- J. Paul Getty

Springfield-Holyoke

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World

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Nuclear deal within reach, vows Iran and Russia

The Australian - 2 hours ago

Russia and Iran claimed a breakthrough in talks on a framework deal cutting back Tehran's nuclear program, but the US denied everything had been agreed as discussions were due to resume overnight.

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WNP

Religious Freedom Act: Are businesses becoming more socially activist? (+video)

Christian Science Monitor - 10 minutes ago

The companies castigating Indiana's RFRA law are not promoting liberal idealism over profits: Their response is a recognition that - at least when it comes to the issue of gay marriage - social activism is also good business.

New York ...

ISIS' legacy in Tikrit: booby traps, IEDs and fear

CNN - 1 hour ago

Tikrit, Iraq (CNN) ISIS is gone, but the fear remains. As Iraqi forces, aided by Shiite militiamen, took control Wednesday of the northern city of Tikrit, they found vehicles laden with explosives and buildings that might be booby-trapped.

Firstpost

Germanwings Crash: Video May Show Plane's Final Moments

ABC News - 1 hour ago

Two magazines have reported details of a disturbing video taken from inside the doomed Germanwings plane moments before it crashed into the French Alps, but investigators have denied its existence.

ABC News

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Reuters - 6 minutes ago

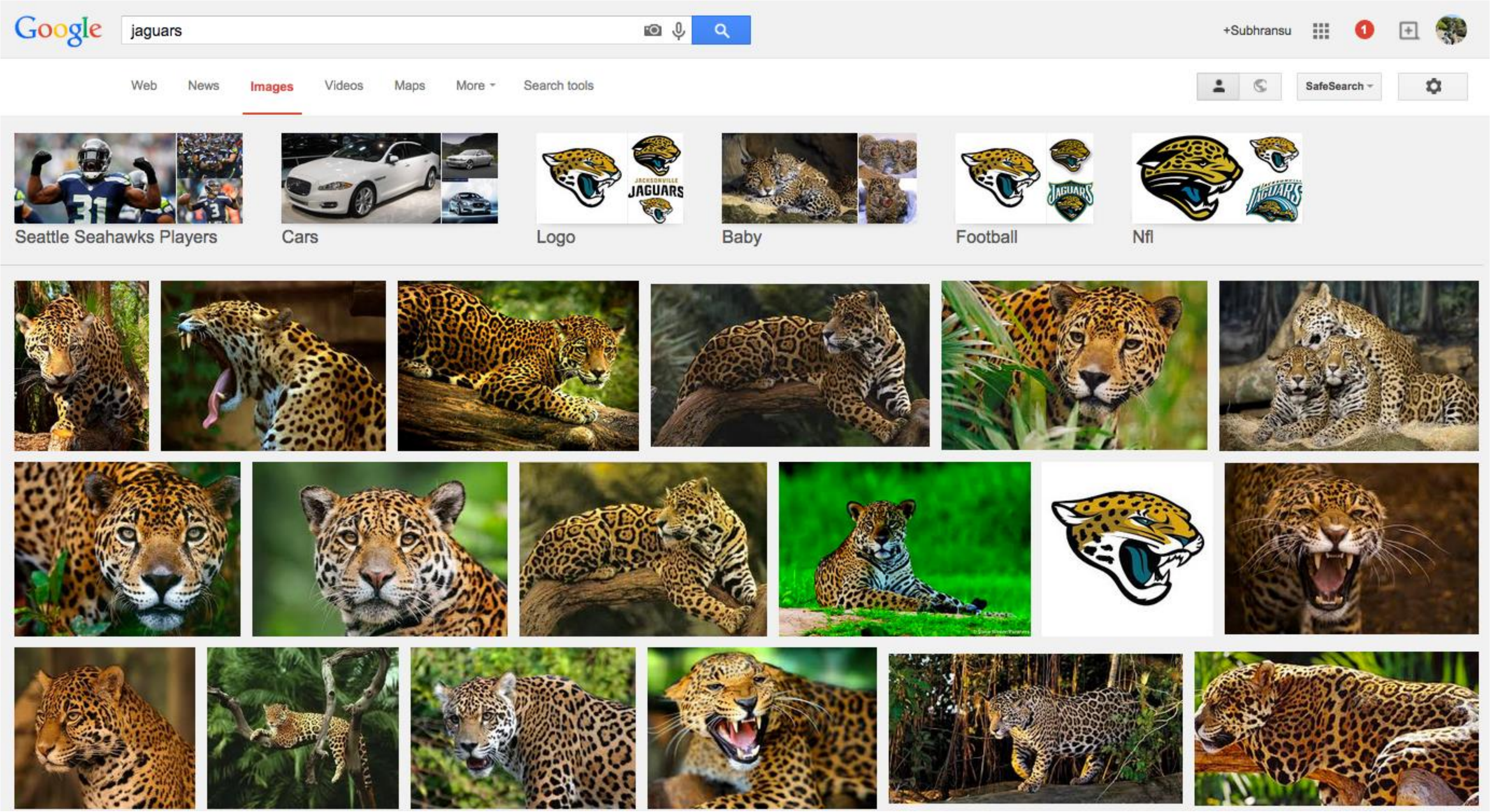
Weather for Amherst, Massachusetts

Today	Thu	Fri	Sat
46° 28°	59° 45°	64° 47°	48° 30°

The Weather Channel - Weather Underground - AccuWeather

Sports scores

Clustering examples: Image Search



jaguars

Outline

Clustering basics

K-means: basic algorithm & extensions

Cluster evaluation

Non-parametric mode finding: density estimation

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K-Nearest Neighbor

Clustering using k-means

Data: D-dimensional observations **(x_1, x_2, …, 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

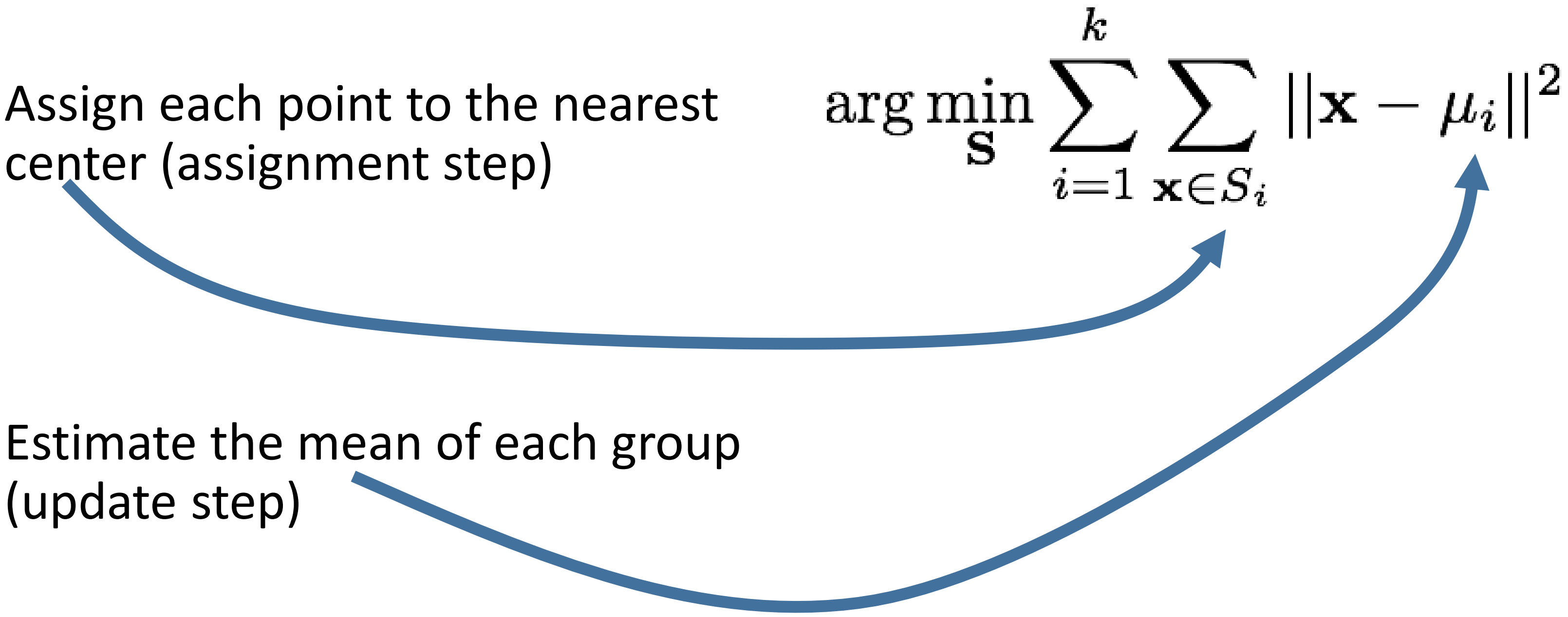
$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\mathbf{x} - \mu_i||^2$$

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

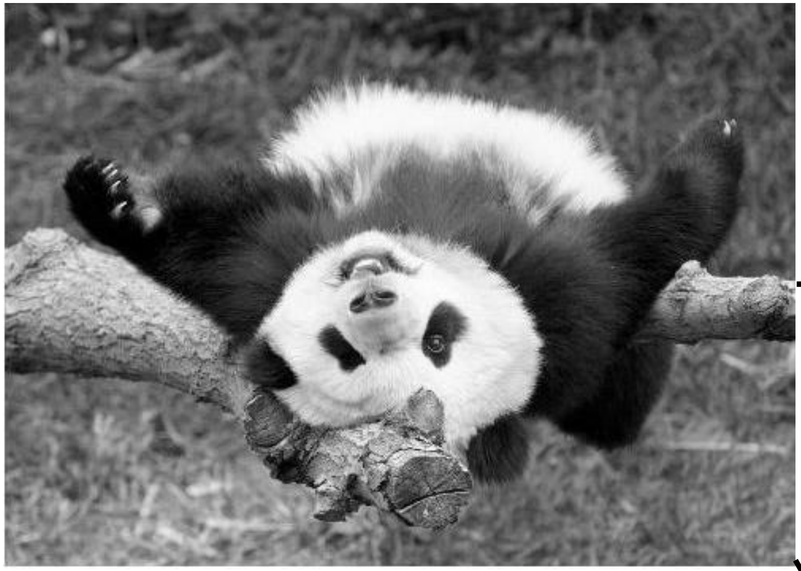
The algorithm proceeds normally once the centers are initialized

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

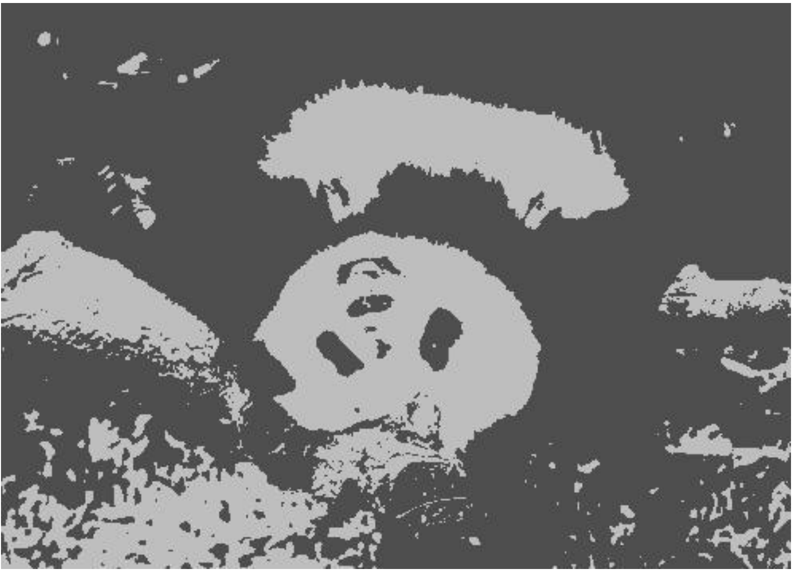
k-means++ algorithm for initialization:

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(**x**)^2
4. Repeat Steps 2 and 3 until k centers have been chosen

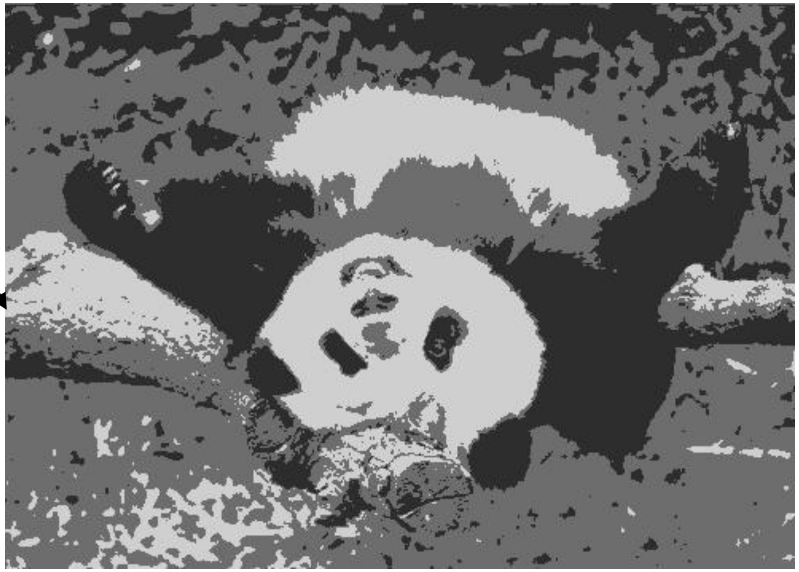
k-means for image segmentation



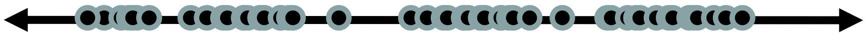
K=2



K=3



Grouping pixels based on intensity similarity



feature space: intensity value (1D)

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Clustering Evaluation

(Classification: accuracy, recall, precision, F-score)

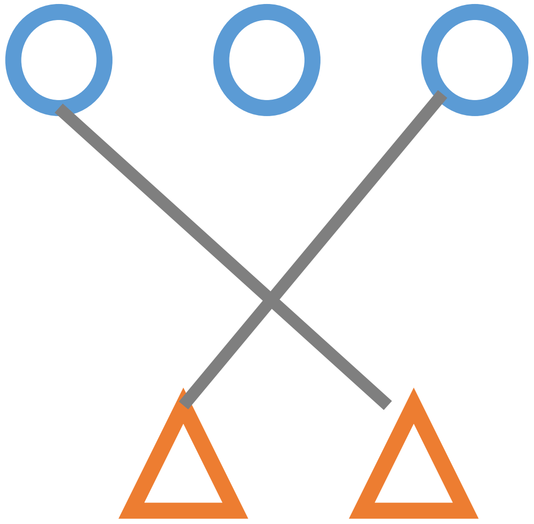
Greedy mapping: one-to-one

Optimistic mapping: many-to-one

Rigorous/information theoretic: V-measure

Clustering Evaluation: One-to-One

Each modeled cluster can *at most* only map to one gold tag type, and vice versa

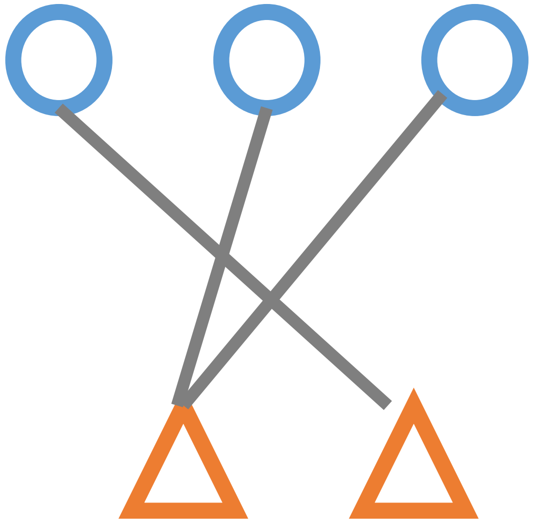


Greedily select the mapping to maximize accuracy

Clustering Evaluation: Many (classes)-to-One (cluster)

Each modeled cluster can map to at most one gold tag types, but multiple clusters can map to the same gold tag

For each cluster: select the majority tag



Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

$$H(X) = -\sum_i p(x_i) \log p(x_i)$$

entropy

Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

$$H(X) = -\sum_{i} p(x_i) \log p(x_i)$$

entropy

entropy(point mass) = 0

entropy(uniform) = log K

Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

k ➔ cluster
c ➔ gold class

Homogeneity: how well does each gold class map to a single cluster?

$$\text{homogeneity} = \begin{cases} 1, & H(K,C) = 0 \\ 1 - \frac{H(C|K)}{H(C)}, & \text{o/w} \end{cases}$$

relative entropy is maximized when a cluster provides no new info. on class grouping → not very homogeneous

> "In order to satisfy our homogeneity criteria, a clustering must assign only those datapoints that are members of a single class to a single cluster. That is, the class distribution within each cluster should be skewed to a single class, that is, zero entropy."

Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

k → cluster
c → gold class

Completeness: how well does each learned cluster cover a *single* gold class?

$$\text{completeness} = \begin{cases} 1, & H(K,C) = 0 \\ 1 - \frac{H(K|C)}{H(K)}, & \text{o/w} \end{cases}$$

relative entropy is maximized when each class is represented uniformly (relatively) → not very complete

> “In order to satisfy the completeness criteria, a clustering must assign all of those datapoints that are members of a single class to a single cluster. “

Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

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Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

$a_{ck} = \#\text{ elements of class c in cluster k}$

Homogeneity: how well does each gold class map to a single cluster?

Completeness: how well does each learned cluster cover a *single* gold class?

$$\text{homogeneity} = \begin{cases} 1, & H(K,C) = 0 \\ 1 - \frac{H(C|K)}{H(C)}, & \text{o/w} \end{cases}$$

$$H(C|K) = -\sum_{k}^{K} \sum_{c}^{C} \frac{a_{ck}}{N} \log \frac{a_{ck}}{\sum_{c'} a_{c'k}}$$

$$\text{completeness} = \begin{cases} 1, & H(K,C) = 0 \\ 1 - \frac{H(K|C)}{H(K)}, & \text{o/w} \end{cases}$$

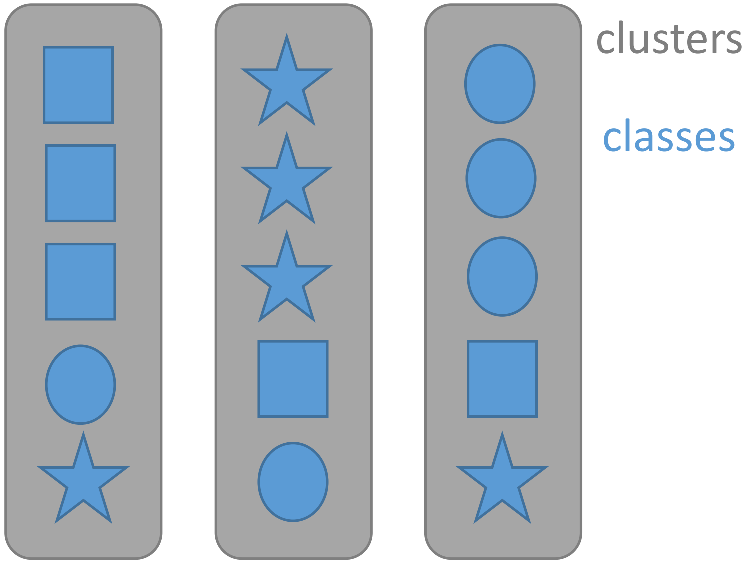
$$H(K|C) = -\sum_{c}^{C} \sum_{k}^{K} \frac{a_{ck}}{N} \log \frac{a_{ck}}{\sum_{k'} a_{ck'}}$$

Clustering Evaluation: V-Measure

Rosenberg and Hirschberg (2008): harmonic mean of *homogeneity* and *completeness*

Homogeneity: how well does each gold class map to a single cluster?

Completeness: how well does each learned cluster cover a *single* gold class?



$$H(C|K) = -\sum_{k}^{K}\sum_{c}^{C}\frac{a_{ck}}{N}\log\frac{a_{ck}}{\sum_{c'} a_{c'k}}$$

$$H(K|C) = -\sum_{c}^{C}\sum_{k}^{K}\frac{a_{ck}}{N}\log\frac{a_{ck}}{\sum_{k'} a_{ck'}}$$

a_{ck}	K=1	K=2	K=3
■	3	1	1
●	1	1	3
★	1	3	1

Homogeneity = Completeness = V-Measure=0.14

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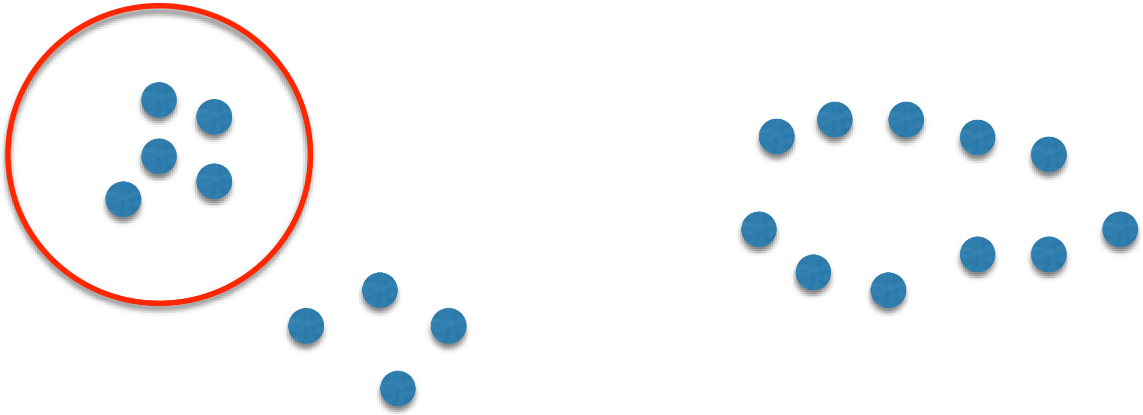
Clustering using density estimation

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 $m_i = \frac{\sum_{x_j \in N(x_i)} x_j K(m_i, x_j)}{\sum_{x_j \in N(x_i)} K\left(m_i, x_j\right)}$
return $\{m_i\}$
```

Neighbors of x_i

weighted average

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

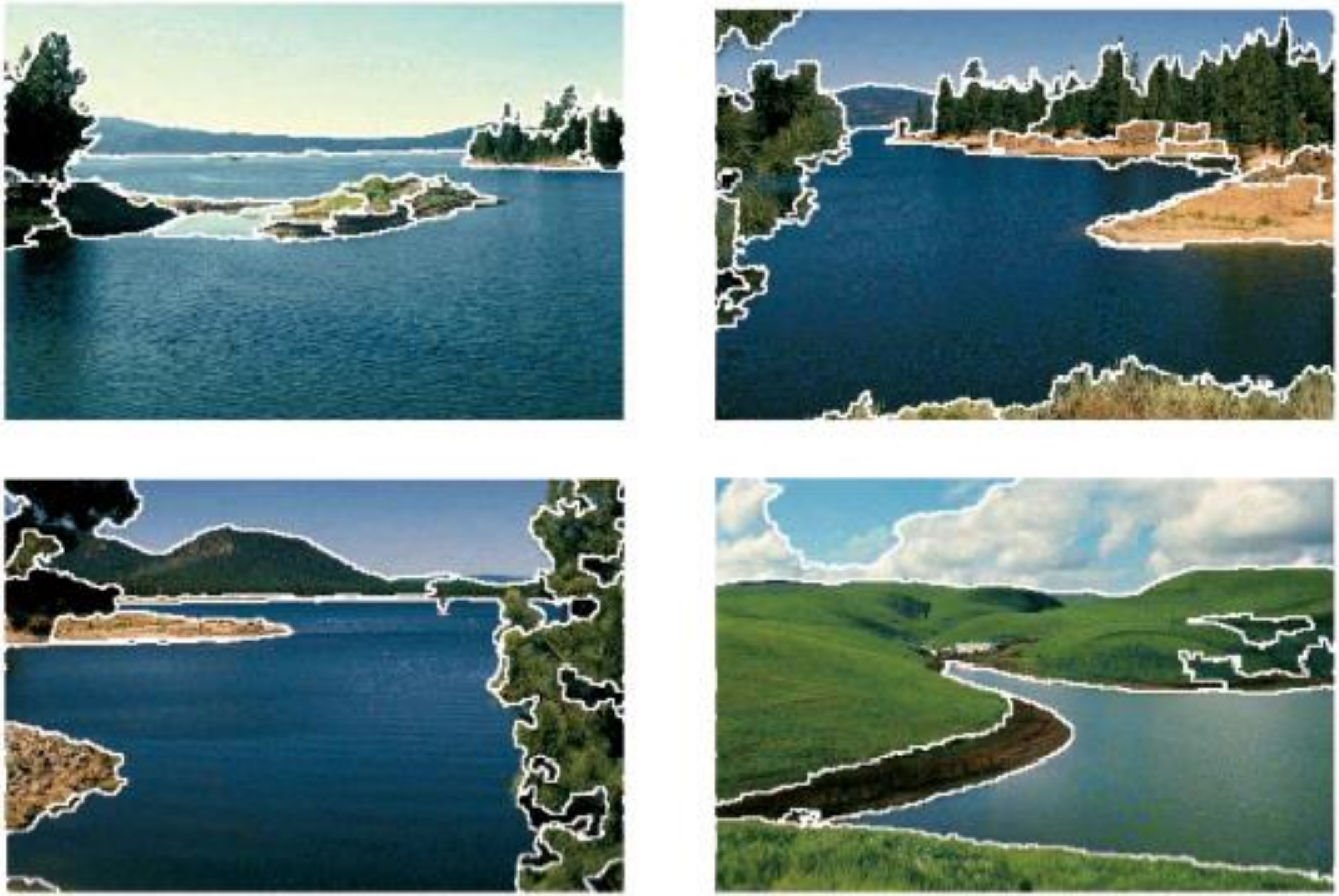
Pros:

- 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 clustering results



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

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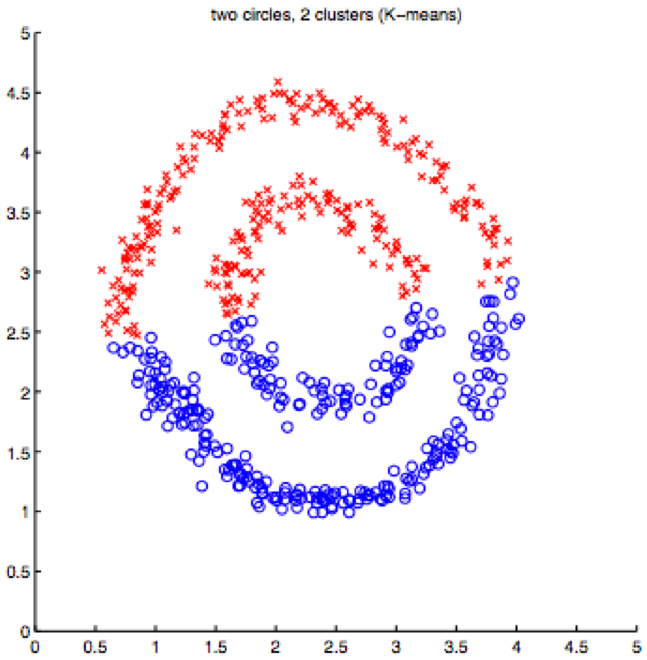
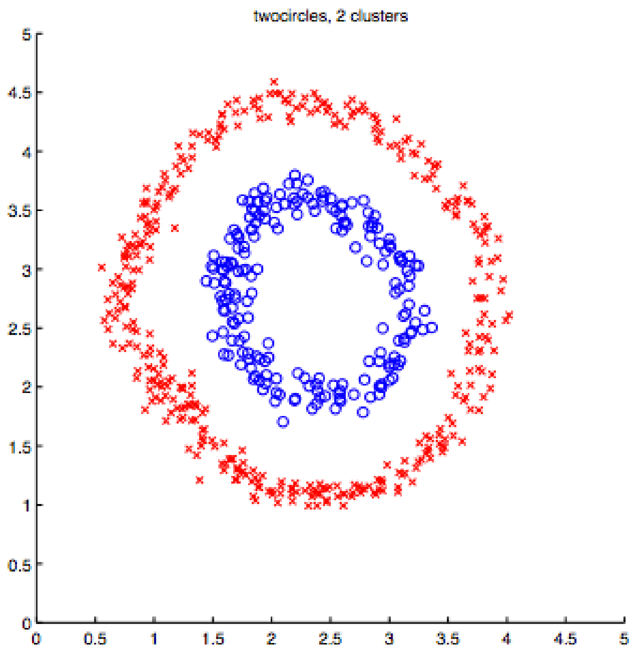
Spectral clustering

K-means



(i)

Spectral clustering

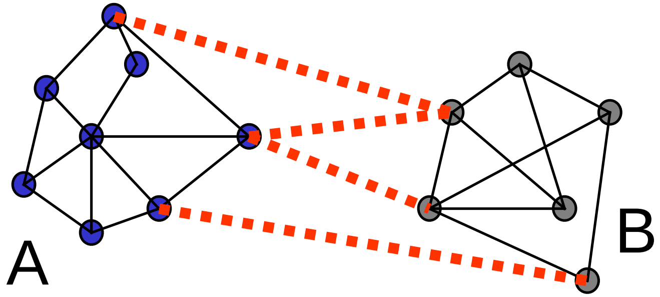


(e)

[Shi & Malik ‘00; Ng, Jordan, Weiss NIPS ‘01]

Spectral clustering

Group points based on the links in a graph



How do we create the graph?

Weights on the edges based on similarity between the points

A common choice is the Gaussian kernel

$$W(i,j) = \exp\left(-\frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}\right)$$

One could create

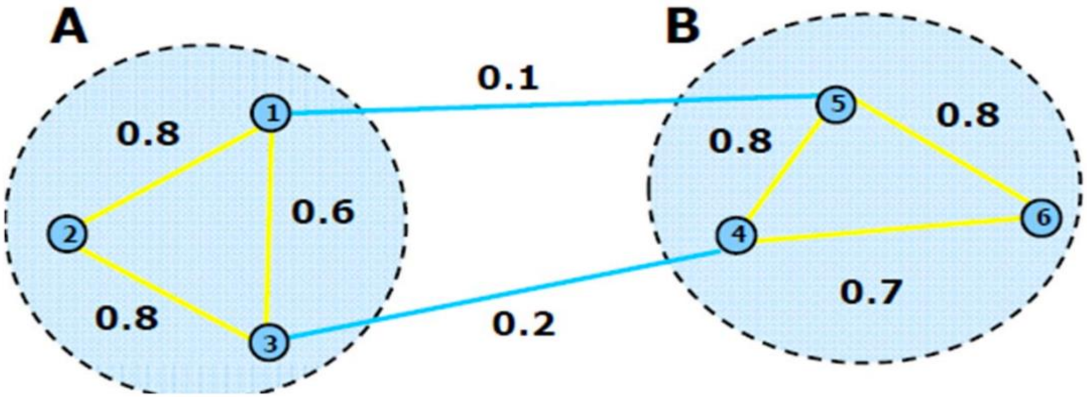
A fully connected graph

k-nearest graph (each node is connected only to its k-nearest neighbors)

Slide courtesy Alan Fern

Graph cut

Consider a partition of the graph into two parts A and B



Cut(A, B) is the weight of all edges that connect the two groups

$$\mathrm{Cut}(A,B) = \sum_{i \in A, j \in B} W(i,j) = 0.3$$

An intuitive goal is to find a partition that minimizes the cut
min-cuts in graphs can be computed in polynomial time

Problem with min-cut

The weight of a cut is proportional to number of edges in the cut; tends to produce small, isolated components.

We would like a balanced cut

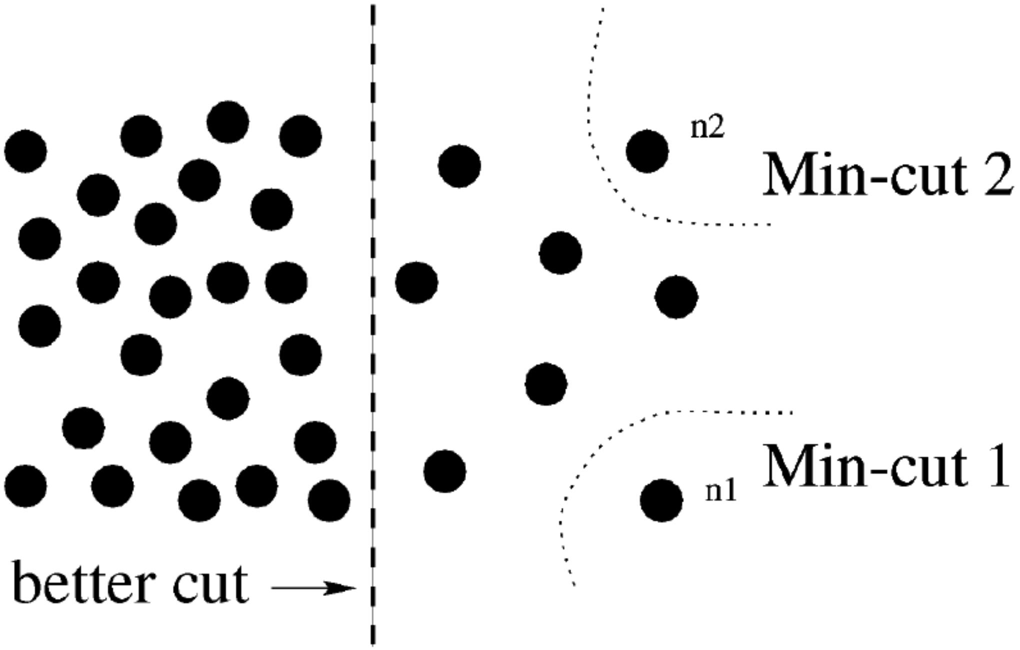
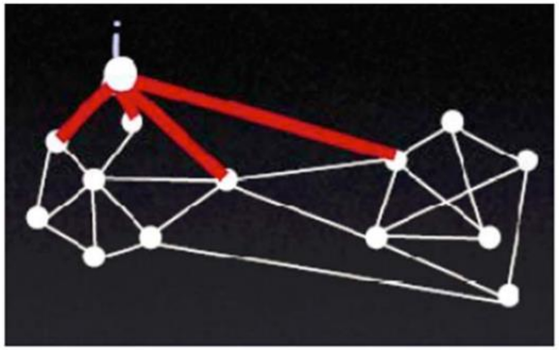
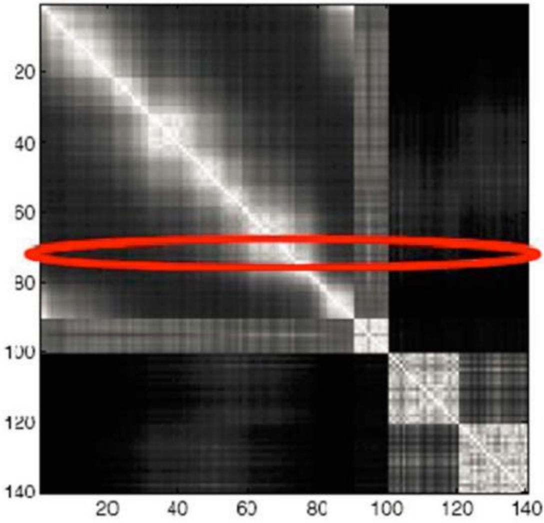


Fig. 1. A case where minimum cut gives a bad partition.

[Shi & Malik, 2000 PAMI]

Graphs as matrices





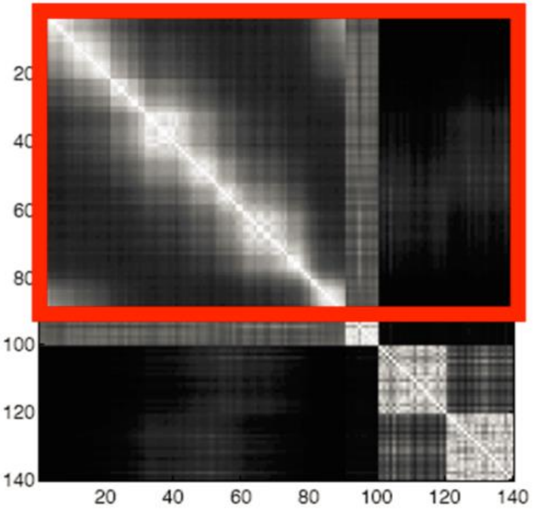
Let *W(i, j)* denote the matrix of the edge weights

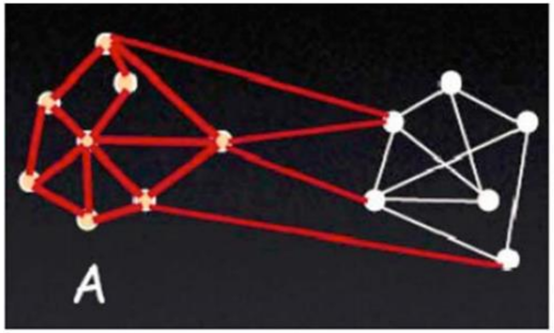
The degree of node in the graph is:

$$d(i) = \sum_j W(i,j)$$

The volume of a set A is defined as:

$$\mathrm{Vol}(A) = \sum_{i \in A} d(i)$$





Normalized cut

the connectivity between the groups relative to the volume of each group:

$$\mathrm{NCut}(A,B) = \frac{\mathrm{Cut}(A,B)}{\mathrm{Vol}(A)} + \frac{\mathrm{Cut}(A,B)}{\mathrm{Vol}(B)}$$

$$\mathrm{NCut}(A,B) = \mathrm{Cut}(A,B)\left(\frac{\mathrm{Vol}(A)+\mathrm{Vol}(B)}{\mathrm{Vol}(A)\mathrm{Vol}(B)}\right)$$

minimized when Vol(A) = Vol(B)

➔ a balanced cut

Minimizing normalized cut is NP-Hard even for planar graphs [Shi & Malik, 00]

Solving normalized cuts

W: the similarity matrix

D: a diagonal matrix with *D*(i,i) = d(i) — the degree of node i

y: a vector $\{1, -b\}^N$, y(i) = 1 ↔ i ∈ A

allow for differing penalty

The matrix *(D-W)* is called the Laplacian of the graph

$$\min_{\mathbf{x}} \mathrm{NCut}(\mathbf{x}) = \min_{\mathbf{y}} \frac{\mathbf{y}^T (D - W)\mathbf{y}}{\mathbf{y}^T D \mathbf{y}}$$

$$\text{subject to: } \mathbf{y}^T D \mathbf{1} = 0$$

$$\mathbf{y}(i) \in \{1, -b\}$$

Solving normalized cuts

Normalized cuts objective: $\min_{\mathbf{x}} \mathrm{NCut}(\mathbf{x}) = \min_{\mathbf{y}} \frac{\mathbf{y}^T (D - W)\mathbf{y}}{\mathbf{y}^T D \mathbf{y}}$

$$\text{subject to: } \mathbf{y}^T D \mathbf{1} = 0$$

$$\mathbf{y}(i) \in \{1, -b\}$$

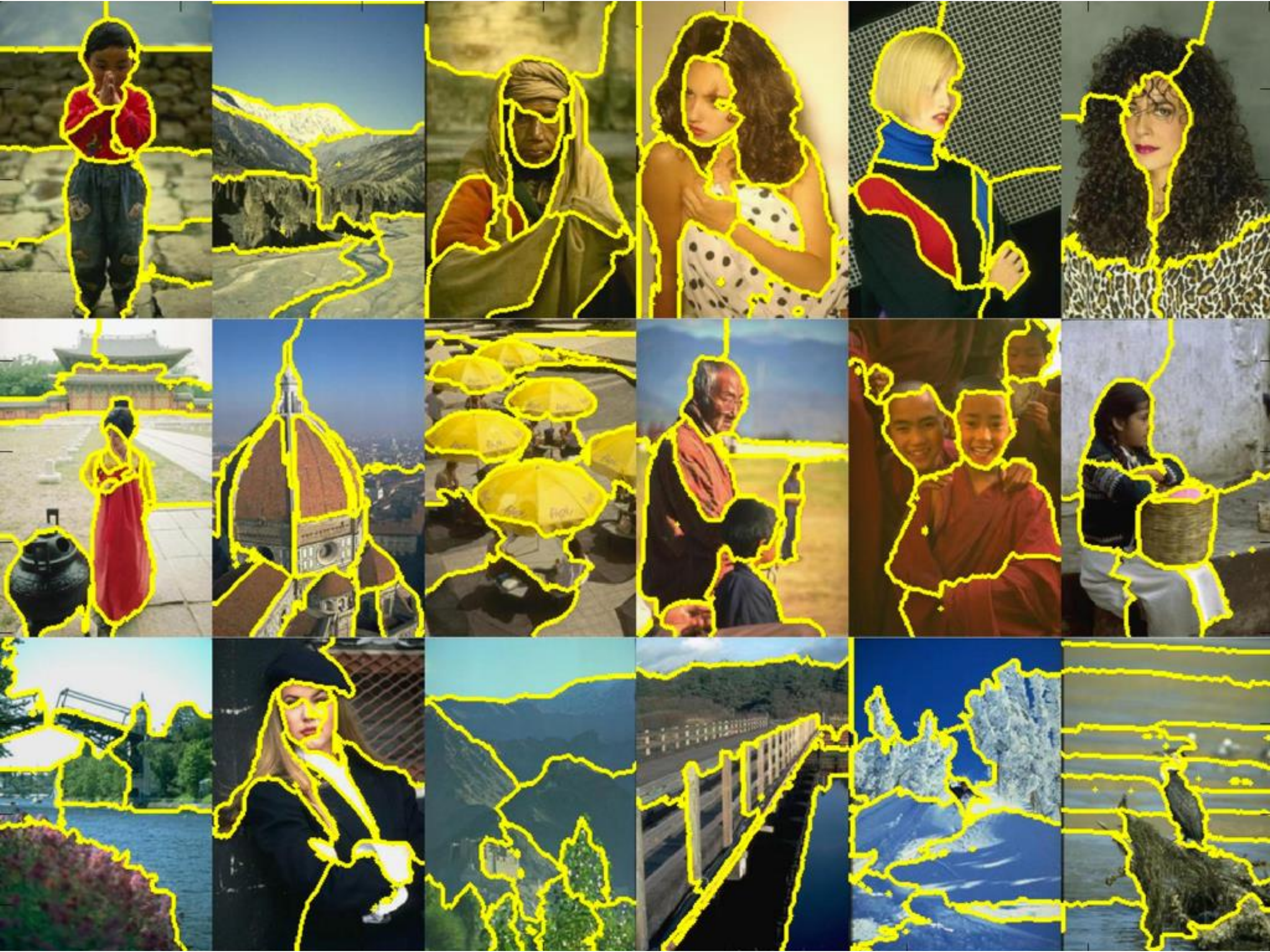
Relax the integer constraint on **y**:

$$\min_{\mathbf{y}} \mathbf{y}^T (D - W)\mathbf{y}; \text{ subject to: } \mathbf{y}^T D \mathbf{y} = 1, \mathbf{y}^T D \mathbf{1} = 0$$

Same as: $(D - W)\mathbf{1} = 0$ (Generalized eigenvalue problem)

$(D - W)\mathbf{y} = \lambda D \mathbf{y}$ → the first eigenvector is $\mathbf{y}_1 = \mathbf{1}$, with the corresponding eigenvalue of 0

The eigenvector corresponding to the second smallest eigenvalue is the solution to the relaxed problem



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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

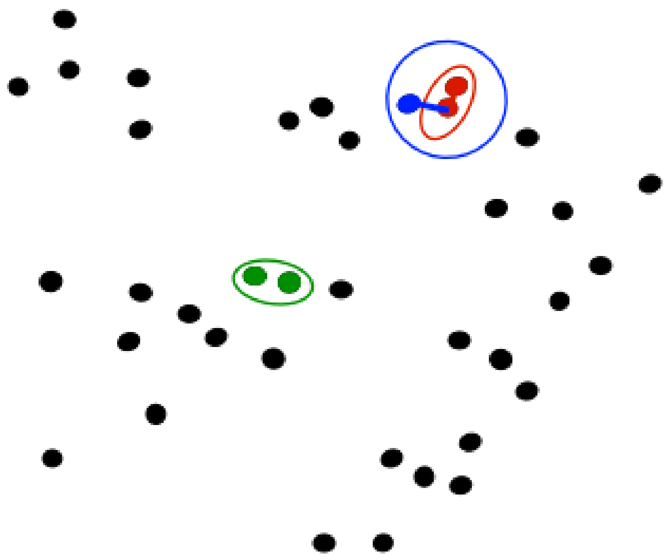
Agglomerative clustering:

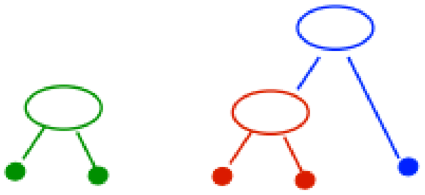
- First merge very similar instances
- Incrementally build larger clusters out of smaller clusters

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





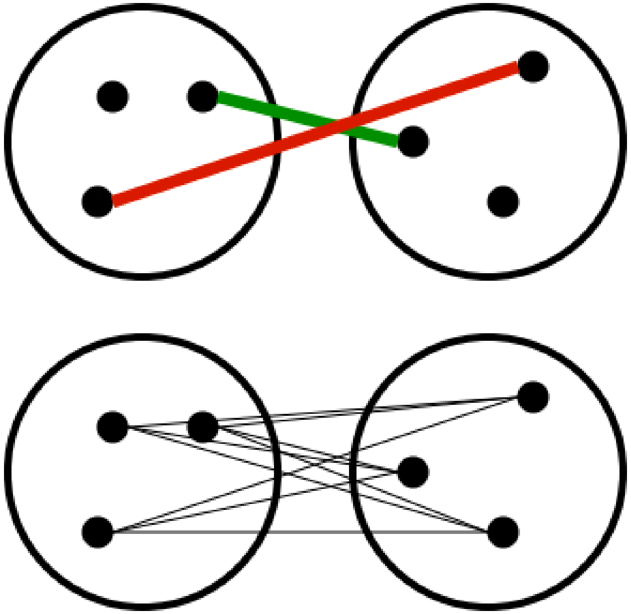
Agglomerative clustering

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

Closest pair: single-link clustering

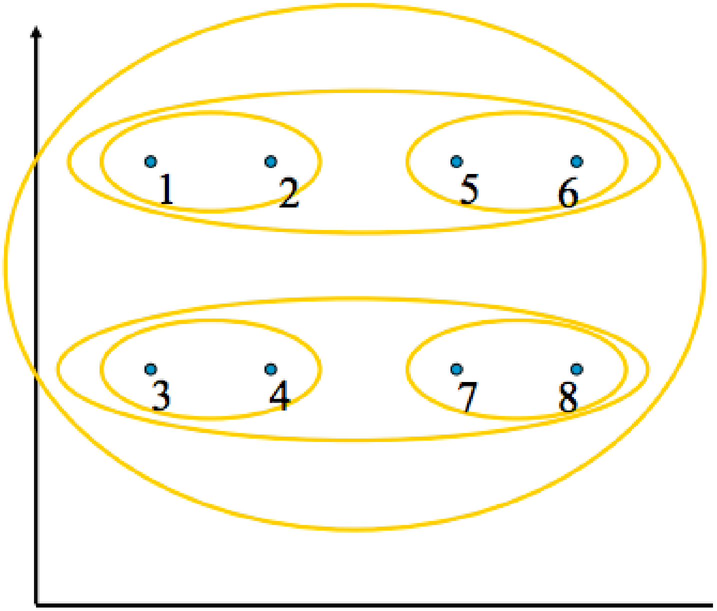
Farthest pair: complete-link clustering

Average of all pairs

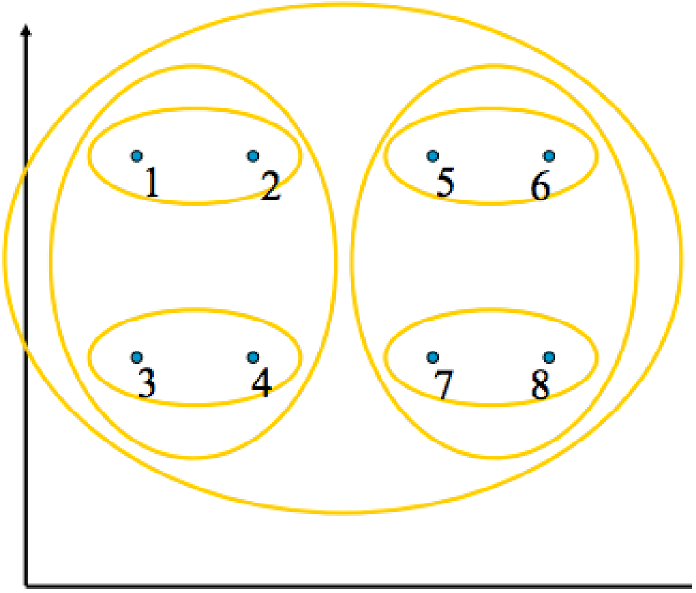


Agglomerative clustering

Closest pair
(single-link clustering)



Farthest pair
(complete-link clustering)



[Pictures from Thorsten Joachims]

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?

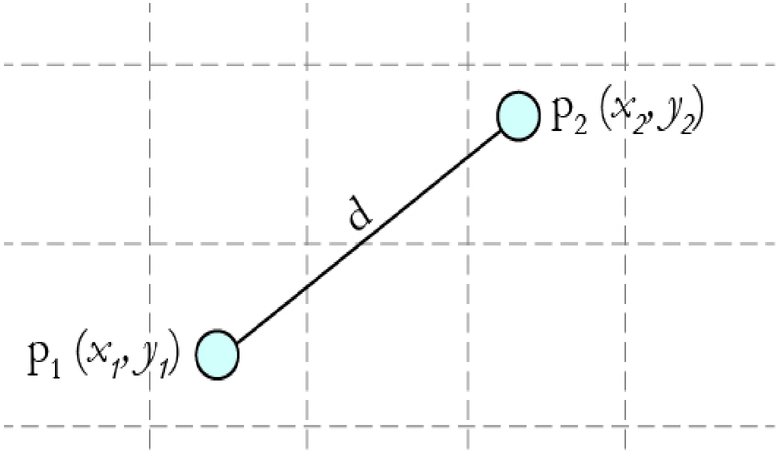
Alice and James are similar

James likes the movie →

Alice must/might also like the movie

Represent data as vectors of feature values

Find closest (Euclidean norm) points



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

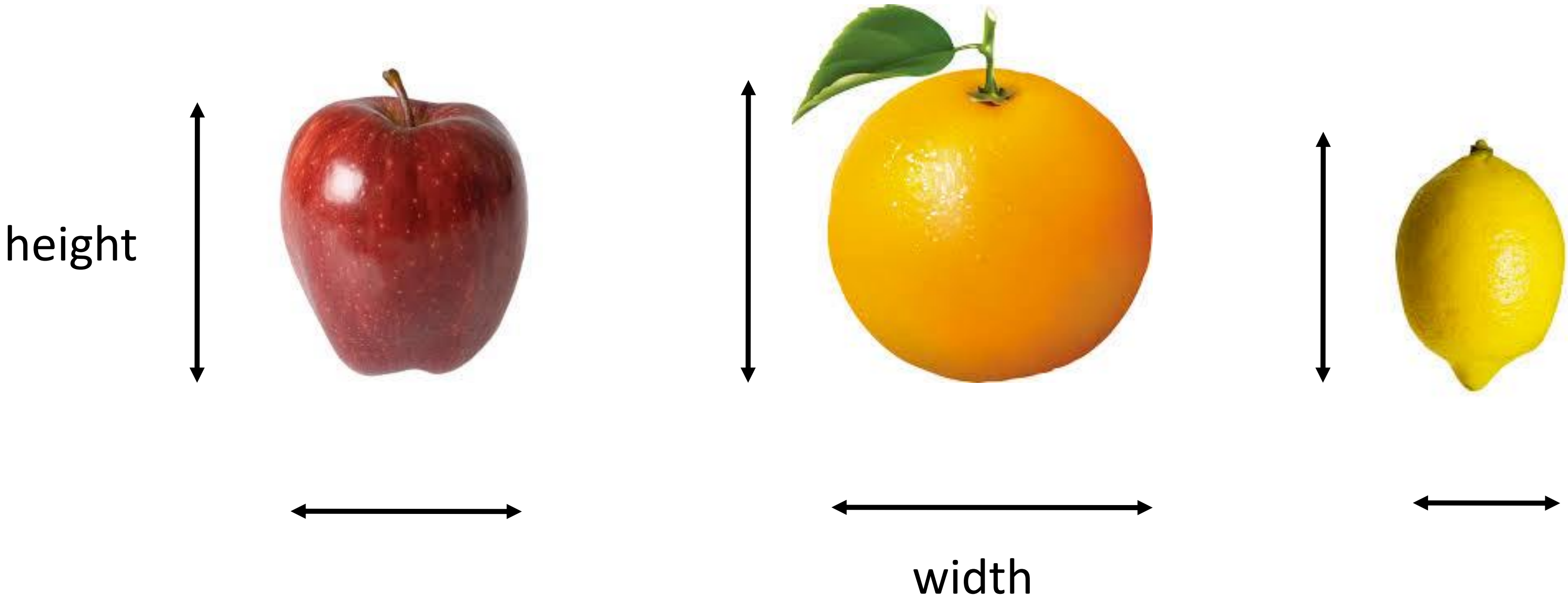
Nearest neighbor classifier

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

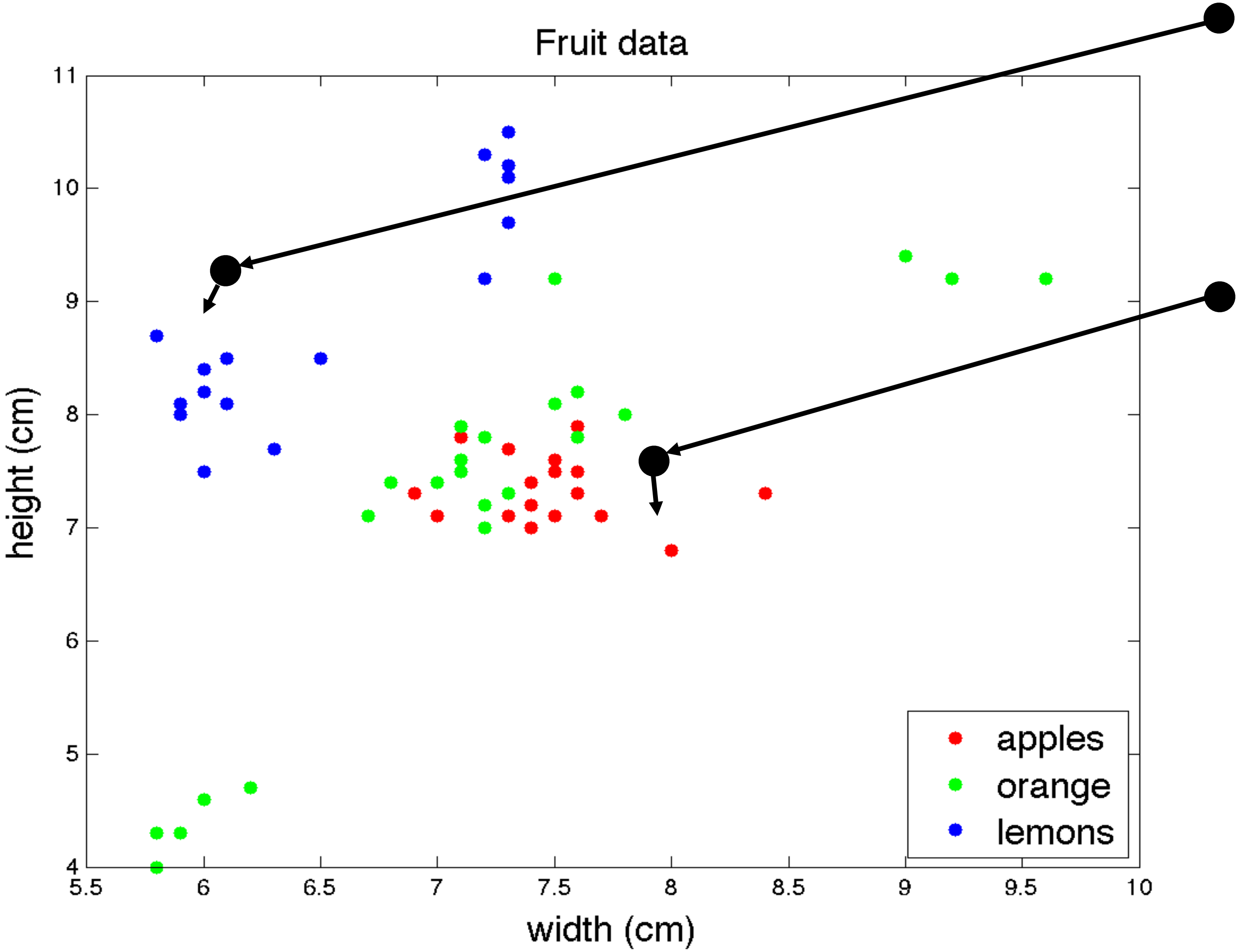
Fruit data:

label: {apples, oranges, lemons}

attributes: {width, height}



Nearest neighbor classifier



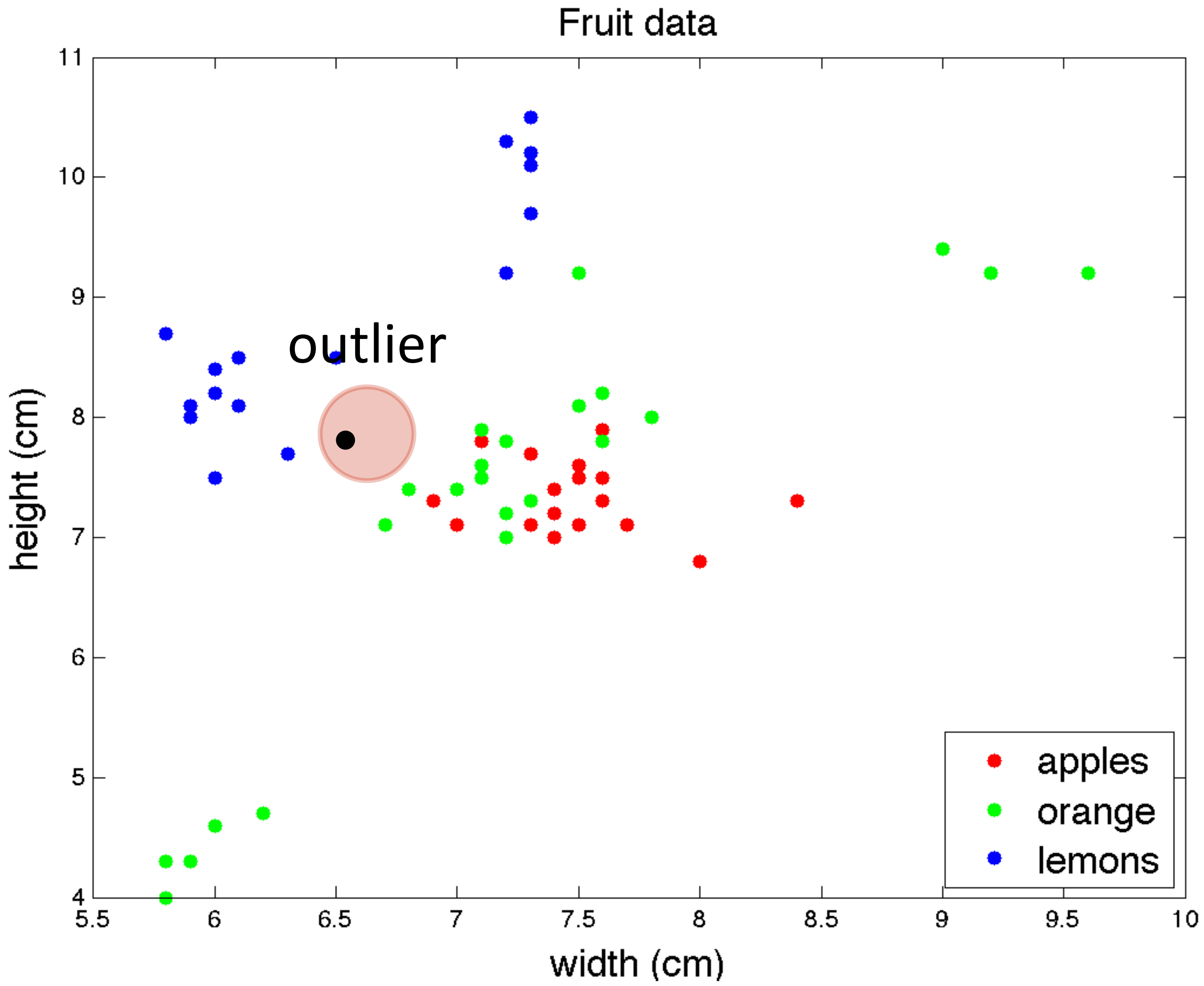
(a, b) ? lemon

(c, d) ? apple

test data

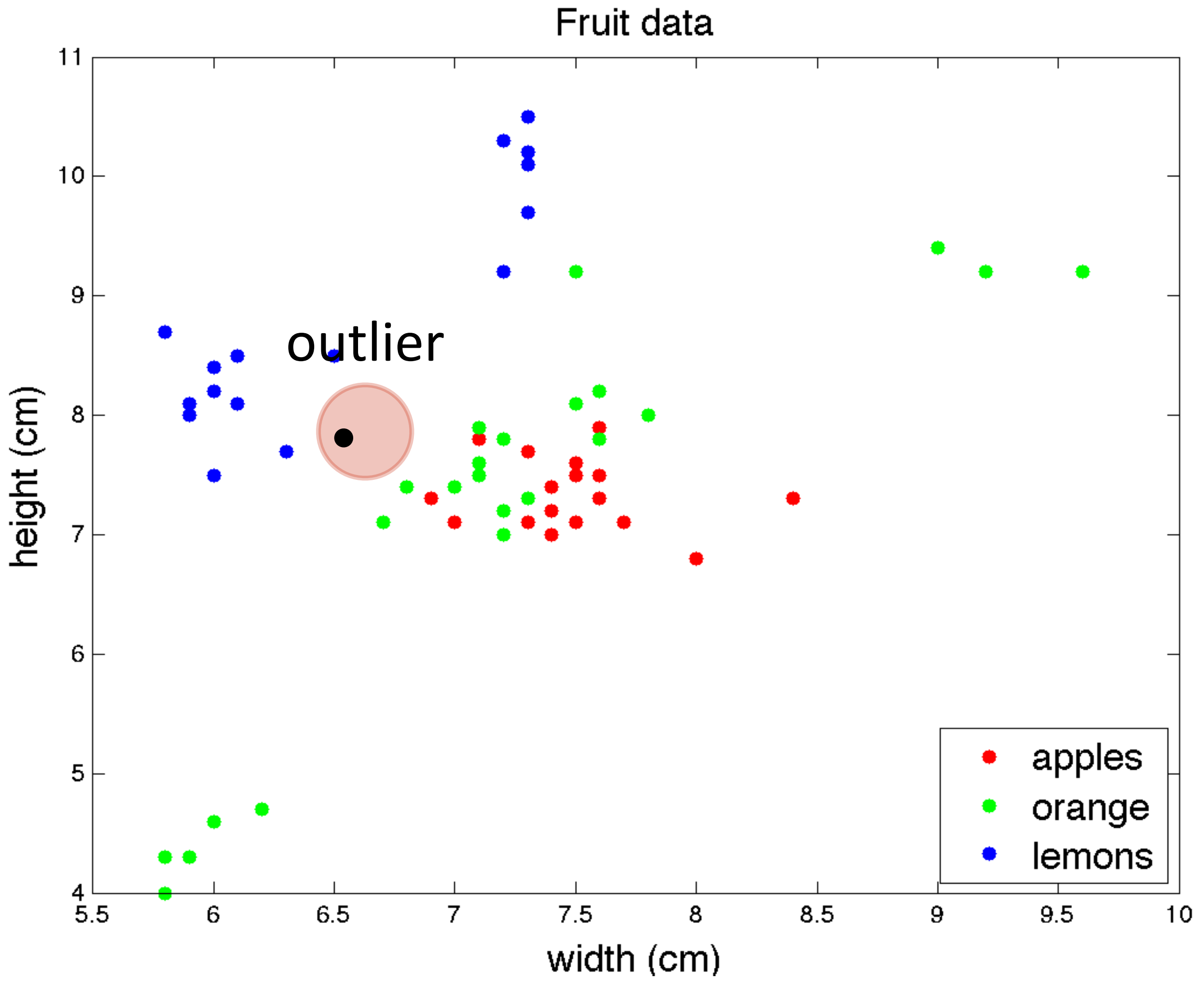
k-Nearest neighbor classifier

Take majority vote among the k nearest neighbors



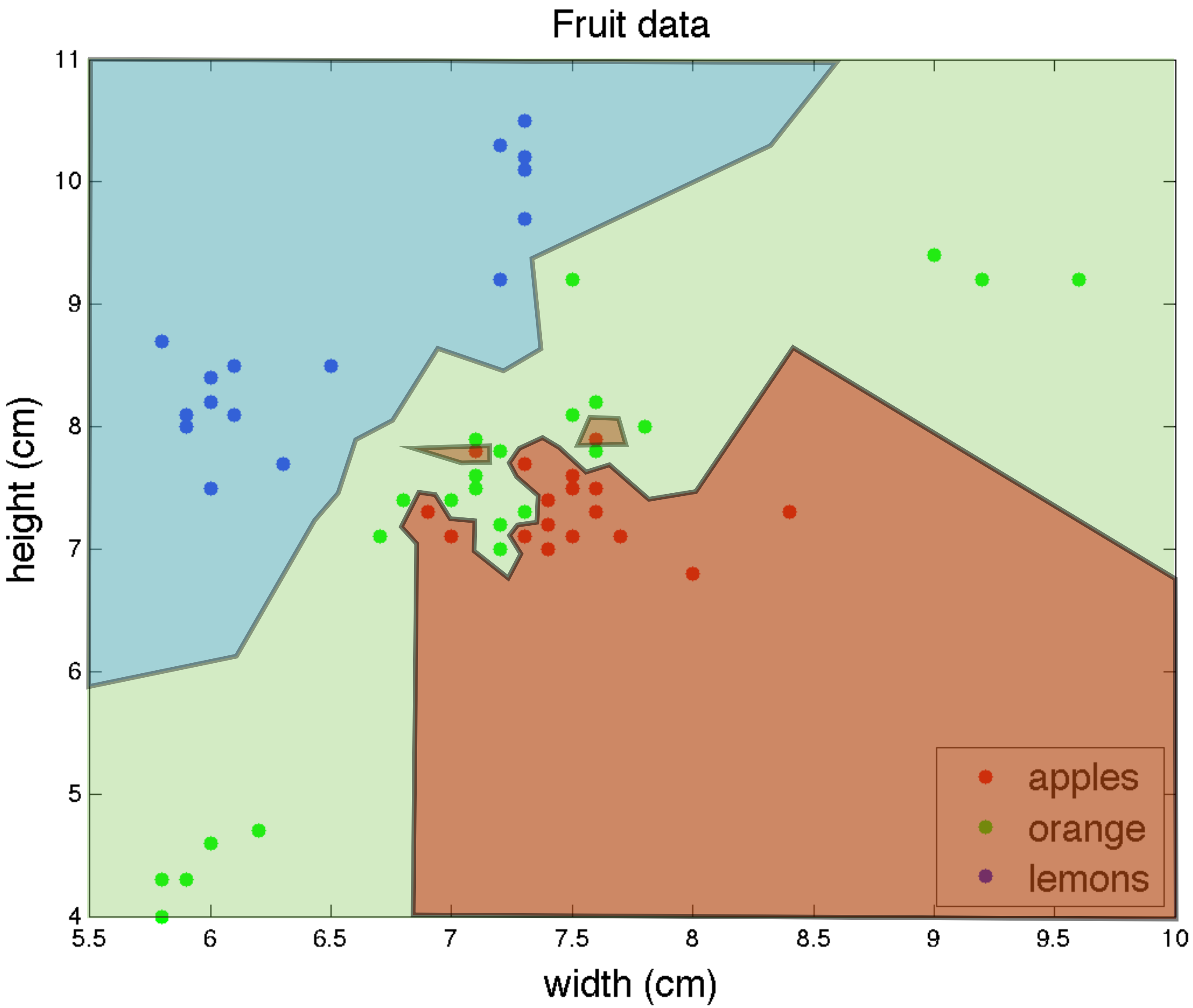
k-Nearest neighbor classifier

Take majority vote among the k nearest neighbors



What is the effect of k?

Decision boundaries: 1NN



Inductive bias of the kNN classifier

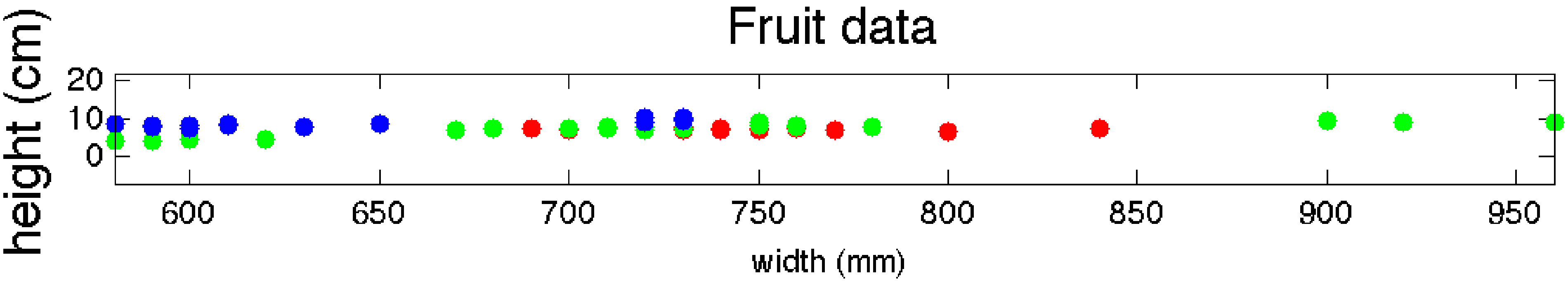
Choice of features

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

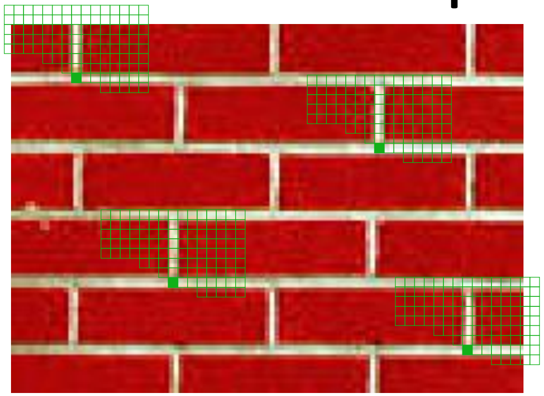
Choice of distance function

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

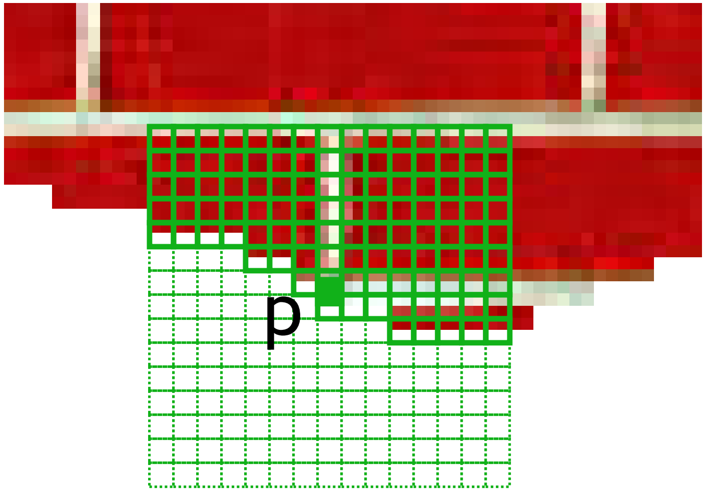
Choice of k



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

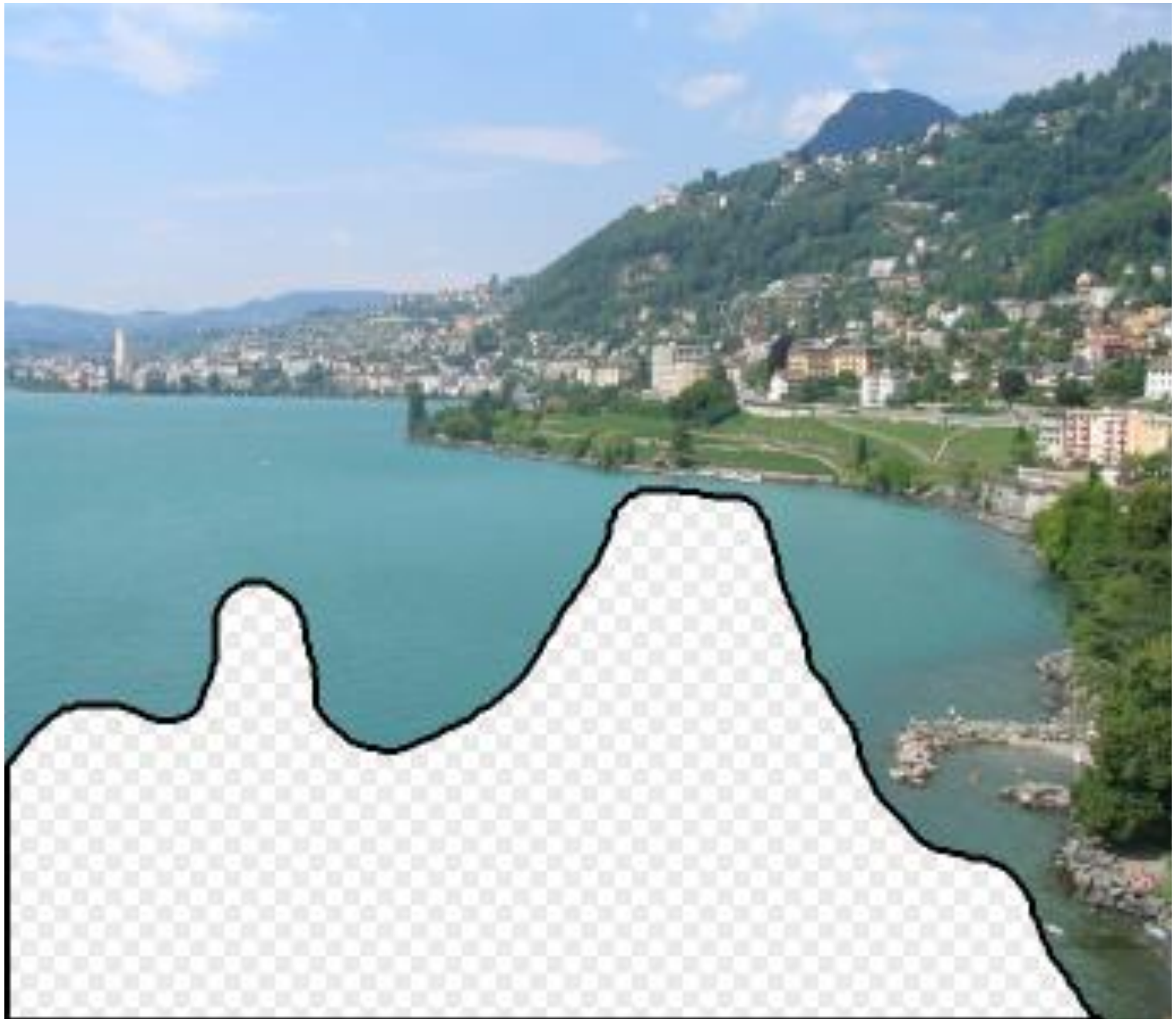
To synthesize **x**

- 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

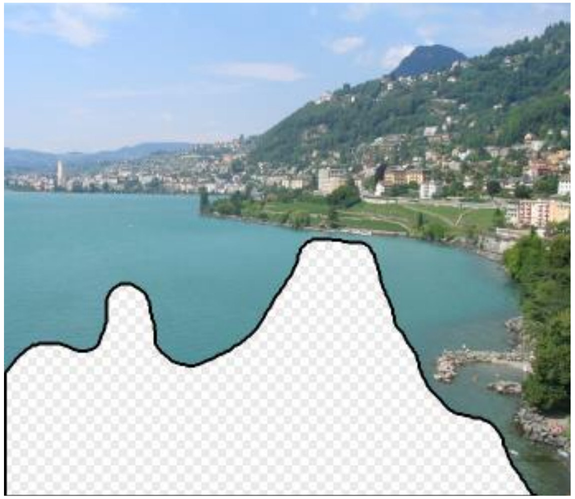
Slide from Alyosha Efros, ICCV 1999

kNN: Scene Completion

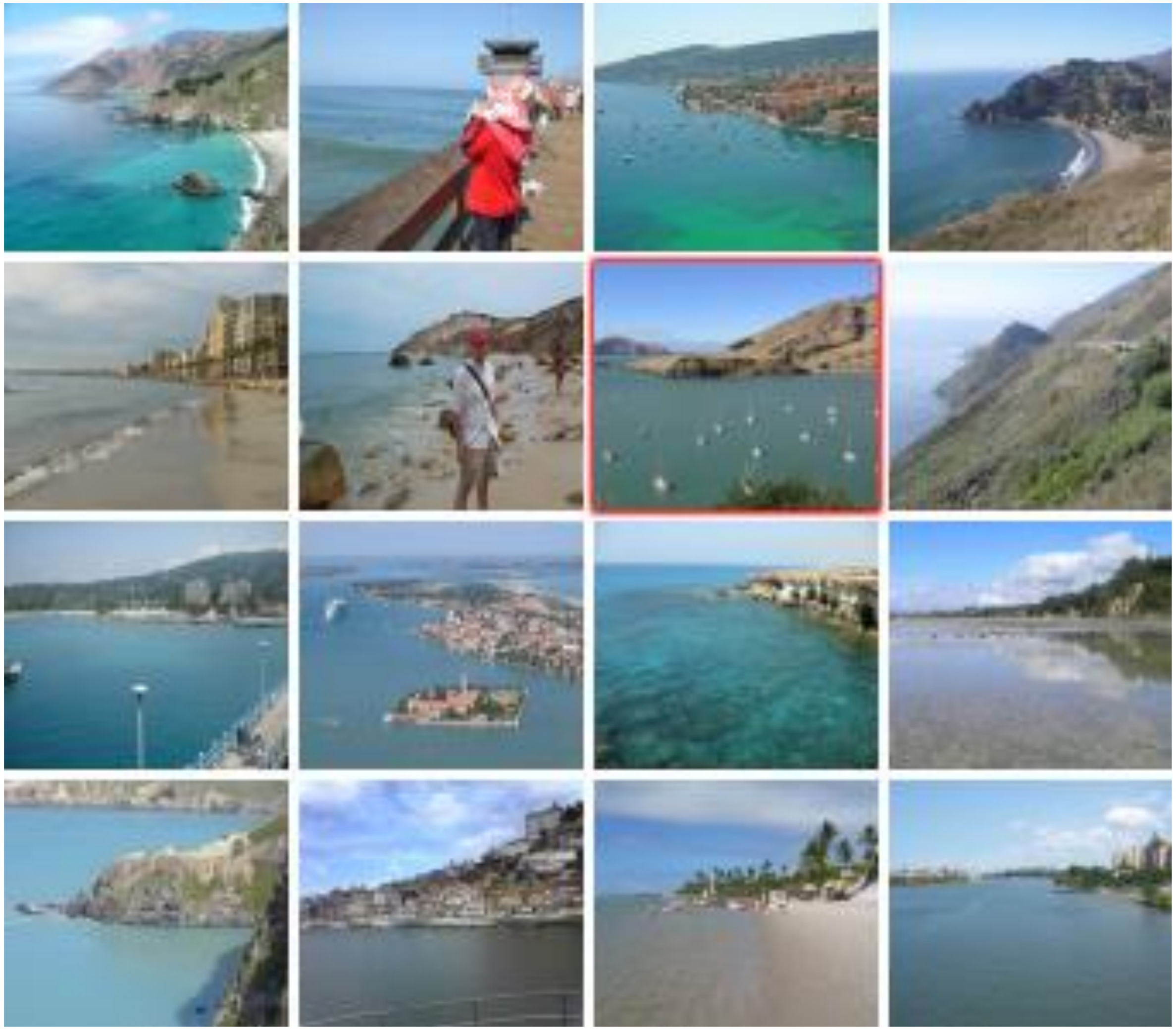


“Scene completion using millions of photographs”, Hayes and Efros, TOG 2007

kNN: Scene Completion

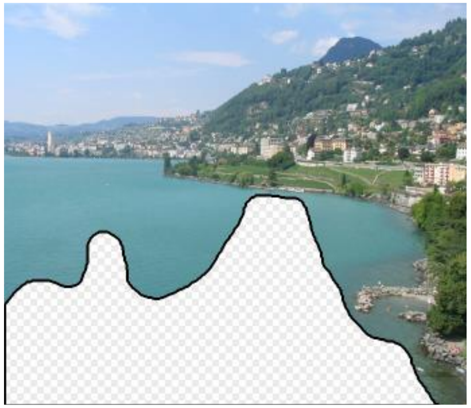


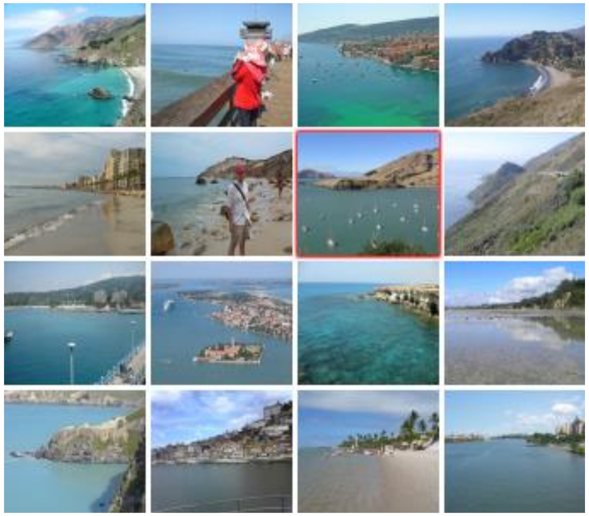
Nearest neighbors

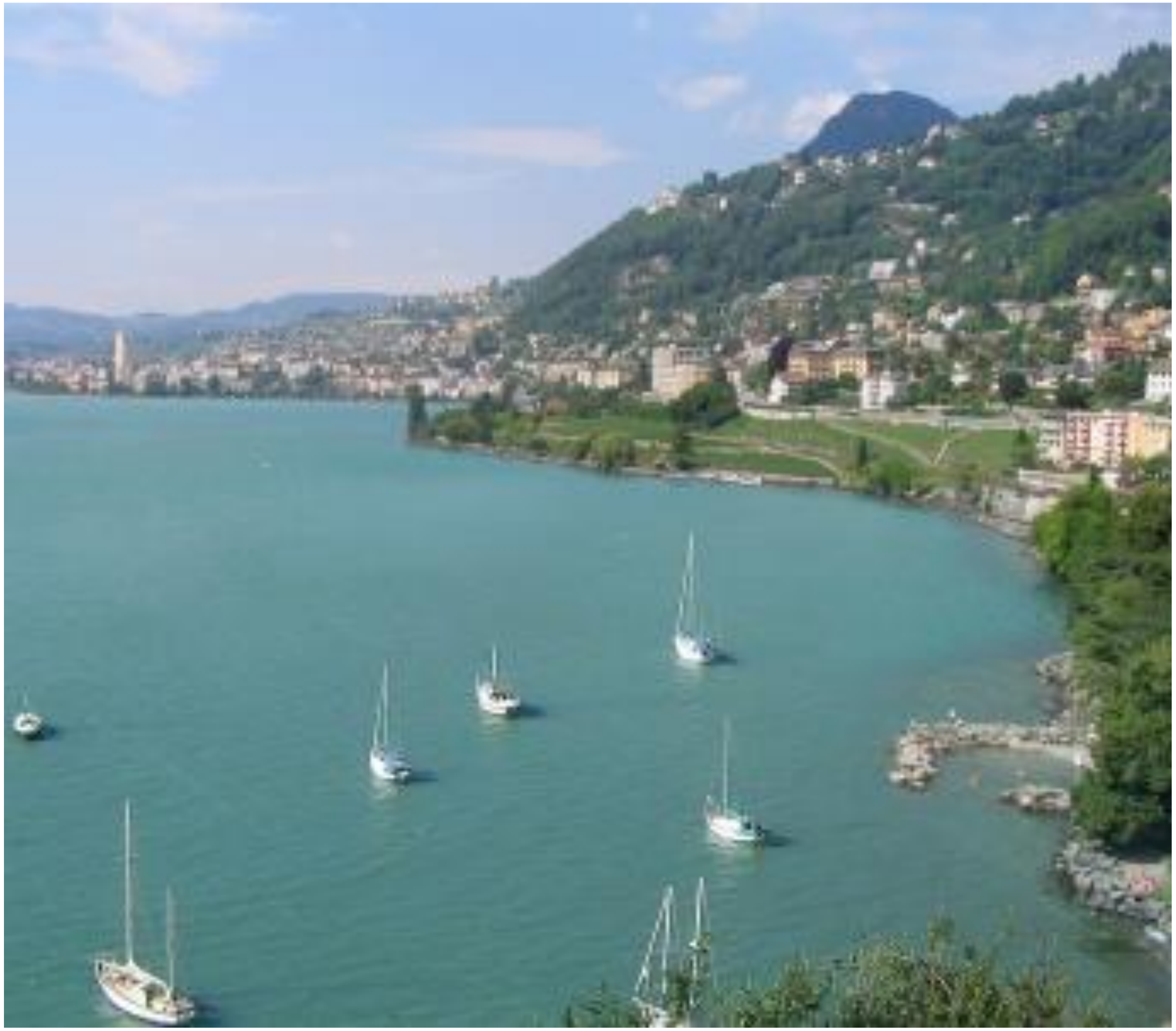


“Scene completion using millions of photographs”, Hayes and Efros, TOG 2007

kNN: Scene Completion

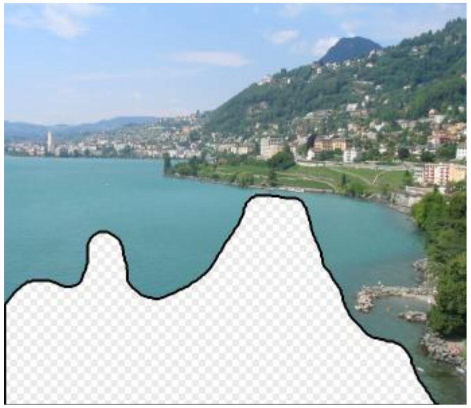


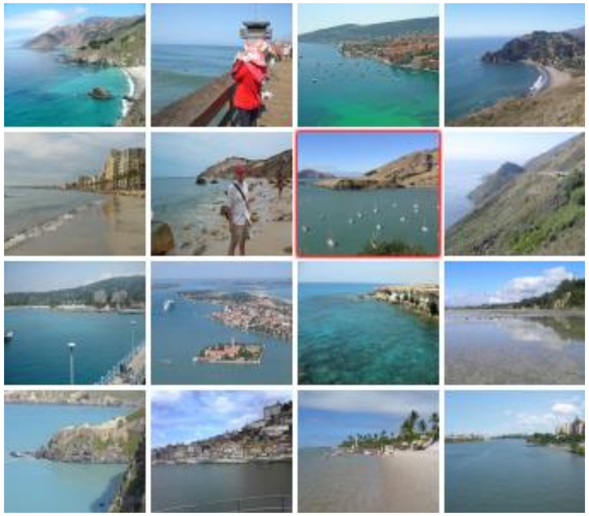


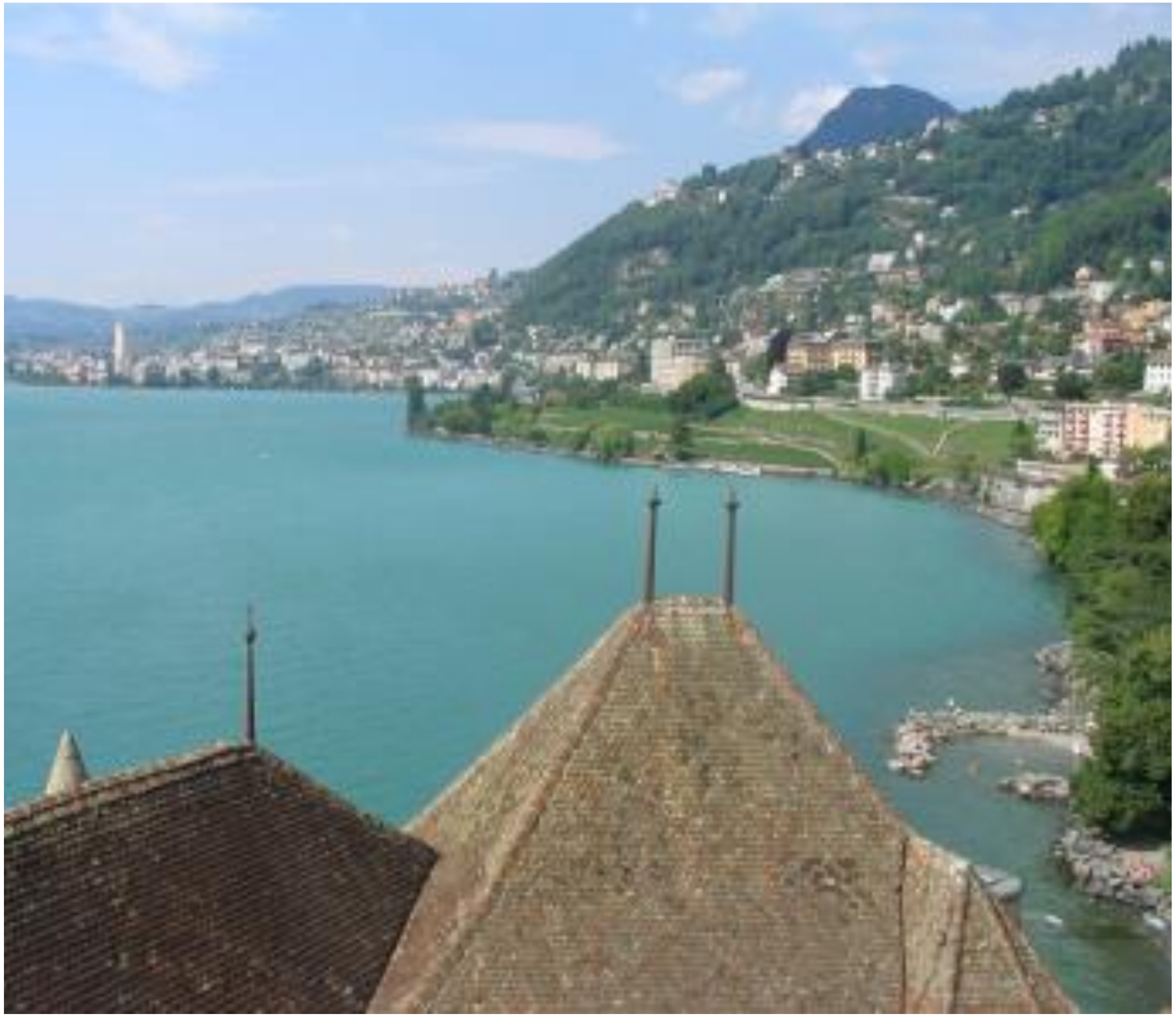


“Scene completion using millions of photographs”, Hayes and Efros, TOG 2007

kNN: Scene Completion





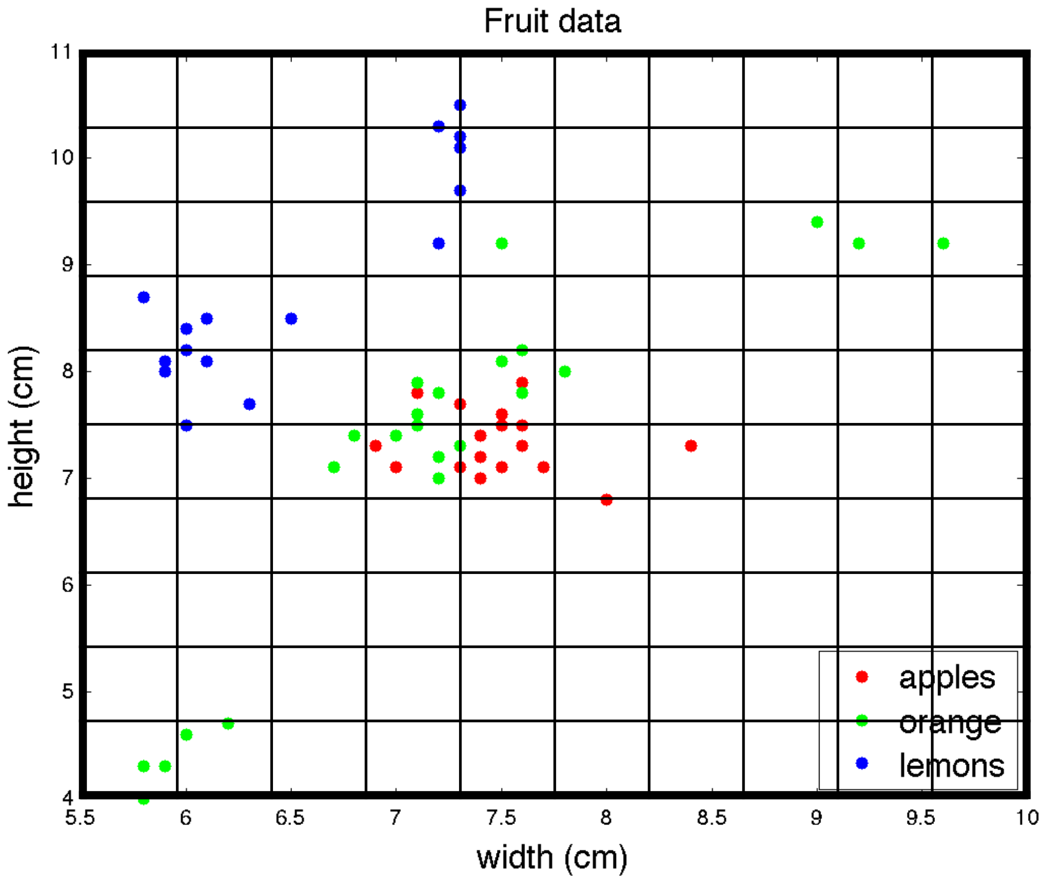


“Scene completion using millions of photographs”, Hayes and Efros, TOG 2007

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?

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