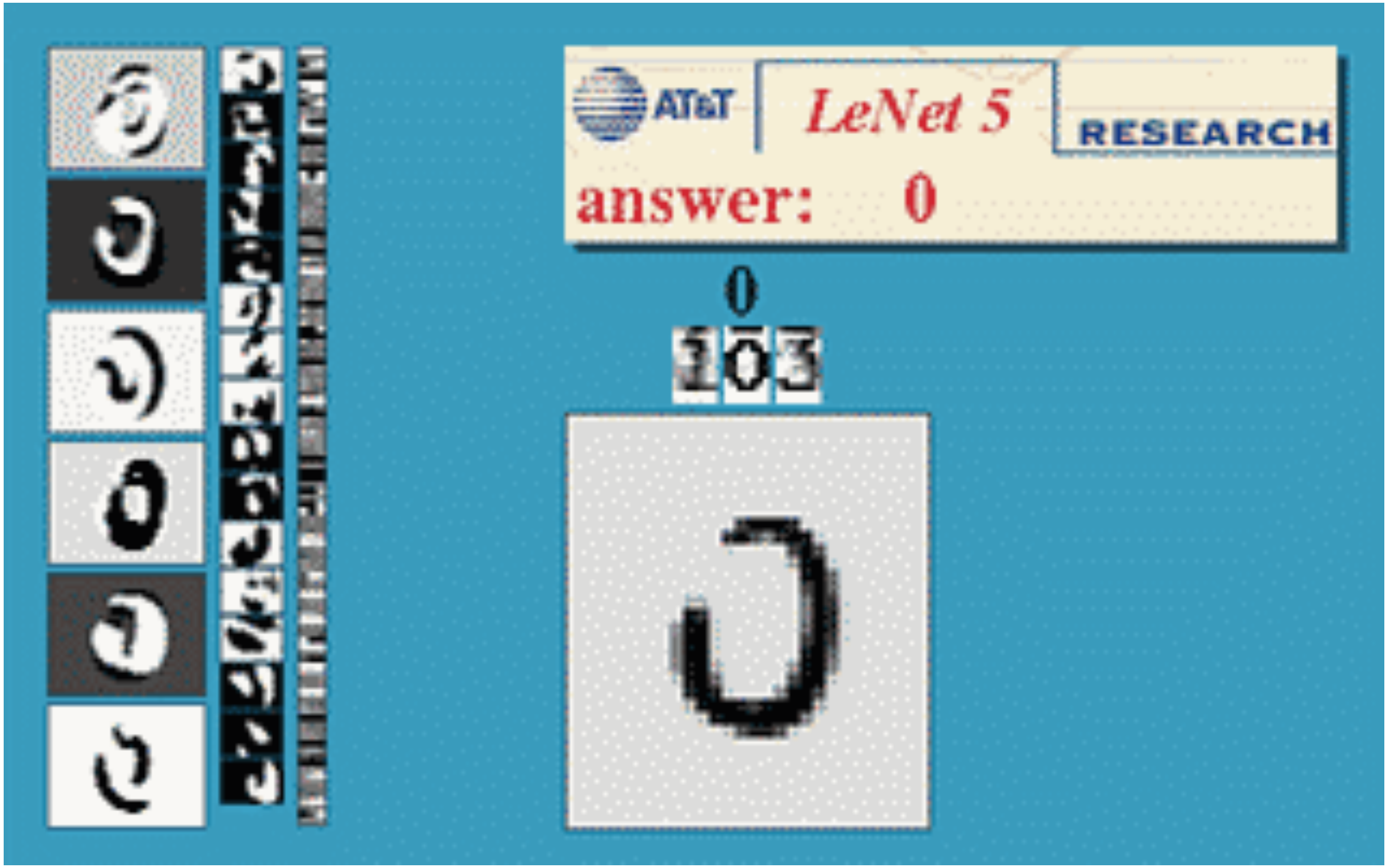
K-Means Clustering (and beyond)

Pascal Fua

(Taught by M. Salzmann)

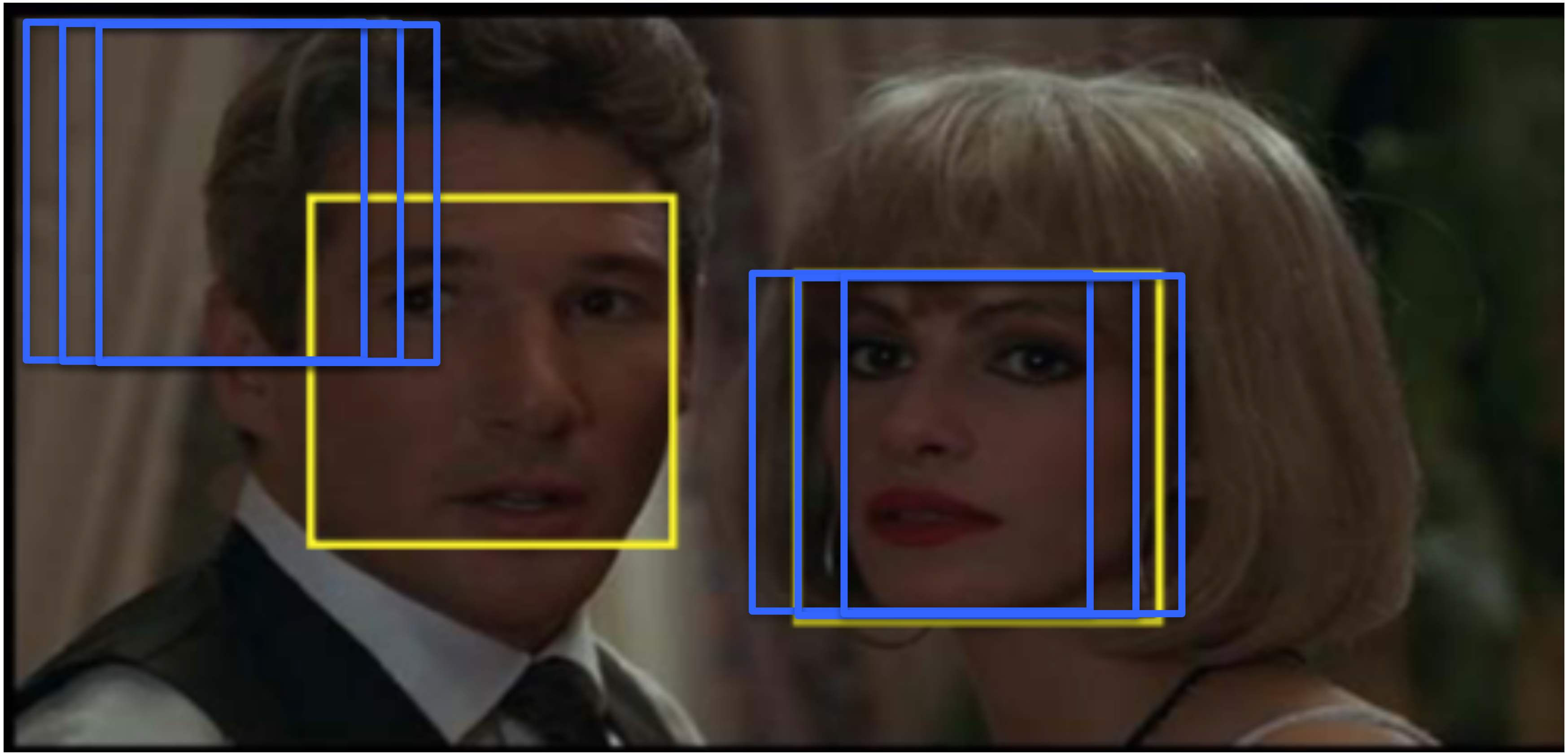
IC-CVLab

Reminder: Recognizing Hand-Written Digits



LeNet (1989-1999)

Reminder: Recognizing Faces



$$y \ : \mathbf{x} \in \mathbb{R}^{m \times n} \rightarrow \{\text{face, non-face}\} \quad ?$$

Reminder: Supervised Learning

Train using an annotated training set:

{(, face), (, face), (, face), … , (, not-face), (, not-face), (, not-face), …..}

{(, two), (, three), (, one), … , (, four), (, three), (, one), …..}

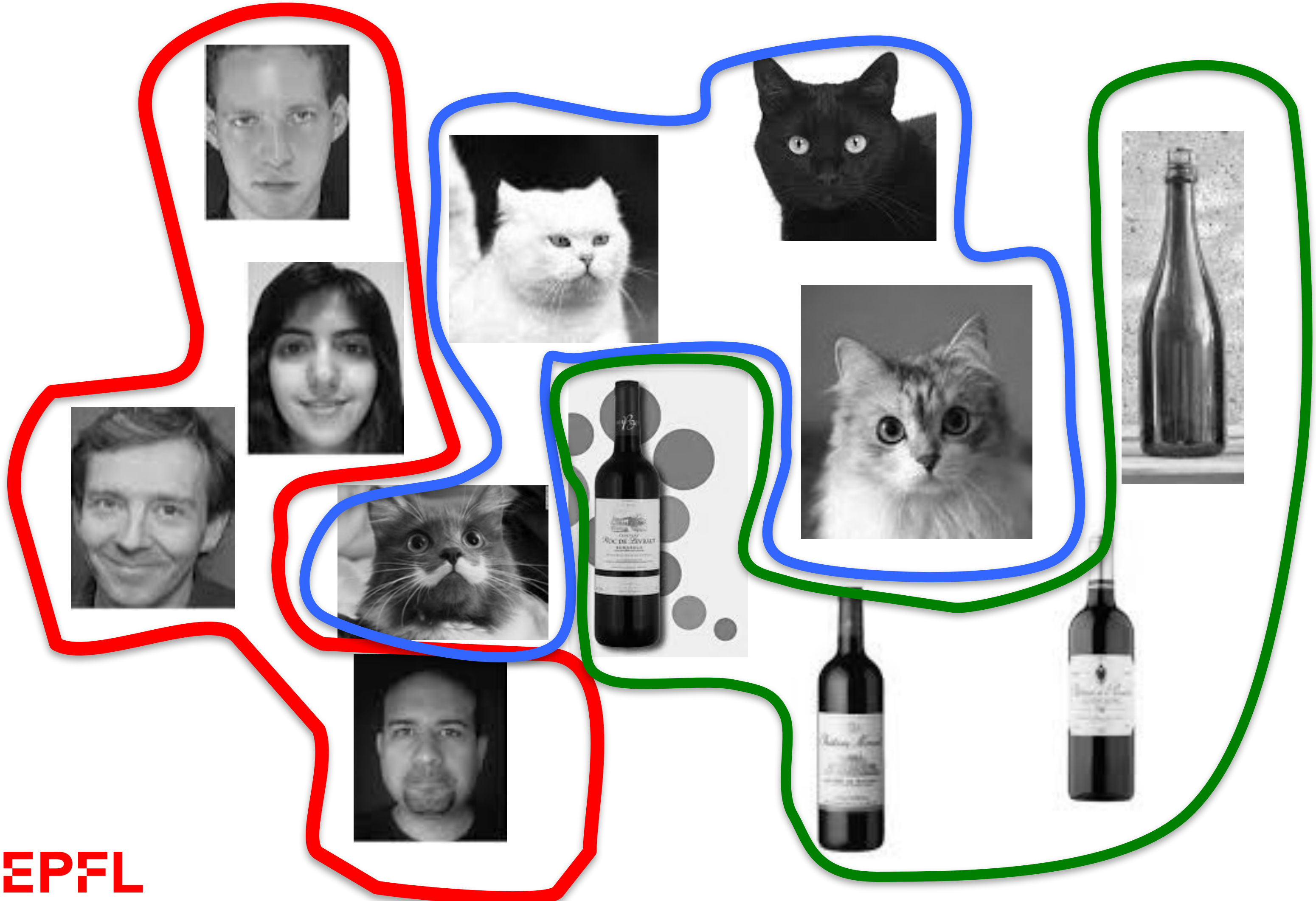
Test on previously unseen images:

—> Face or not?

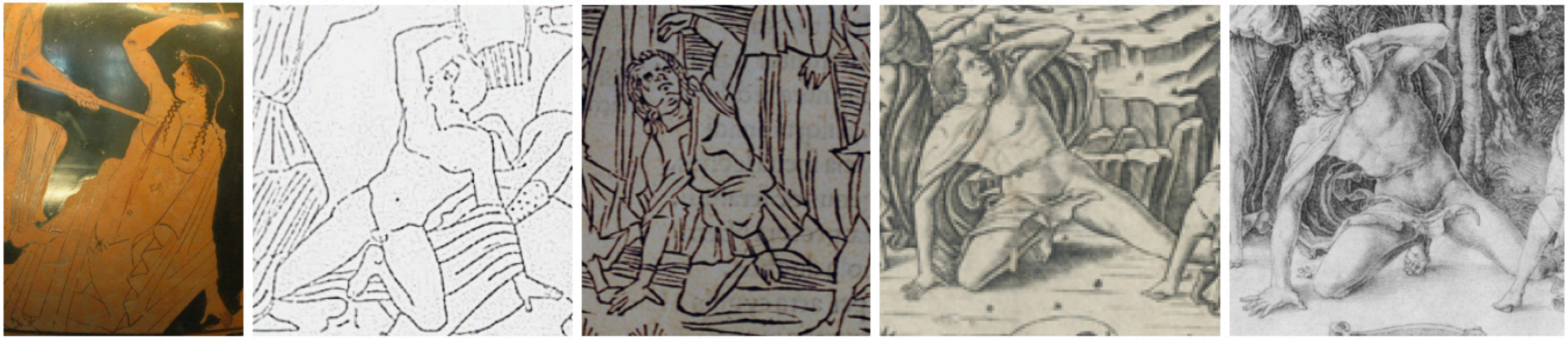
—> What digit?

Unsupervised Learning

The training set is not annotated and the system must also learn the classes.



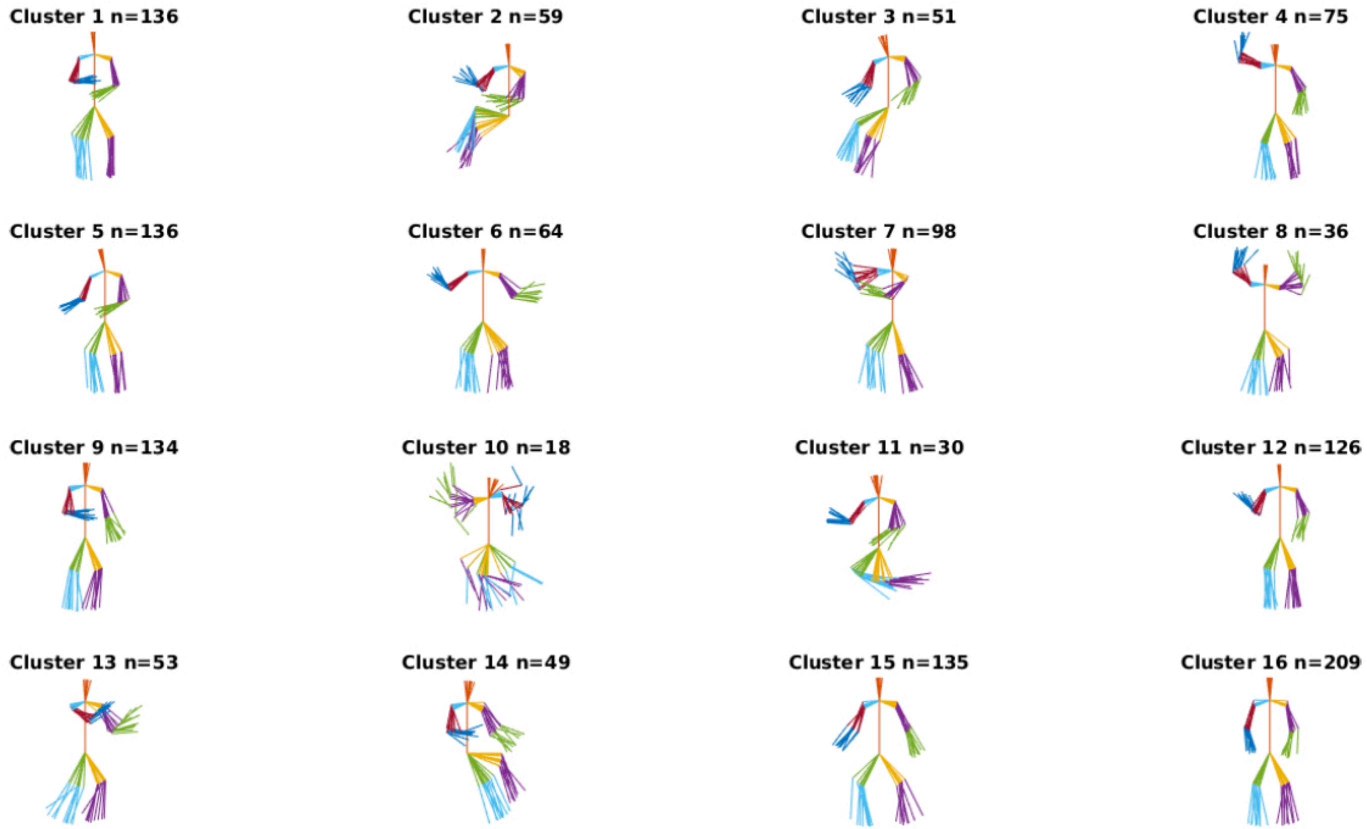
Digital Humanities Application



- Paintings by different artists representing the same scene depict the characters in the same pose.
- Can be used to search large databases of paintings.

Impett & Süsstrunk, ECCV'16

Digital Humanities Application



Cluster 1 n=136

Cluster 2 n=59

Cluster 3 n=51

Cluster 4 n=75

Cluster 5 n=136

Cluster 6 n=64

Cluster 7 n=98

Cluster 8 n=36

Cluster 9 n=134

Cluster 10 n=18

Cluster 11 n=30

Cluster 12 n=126

Cluster 13 n=53

Cluster 14 n=49

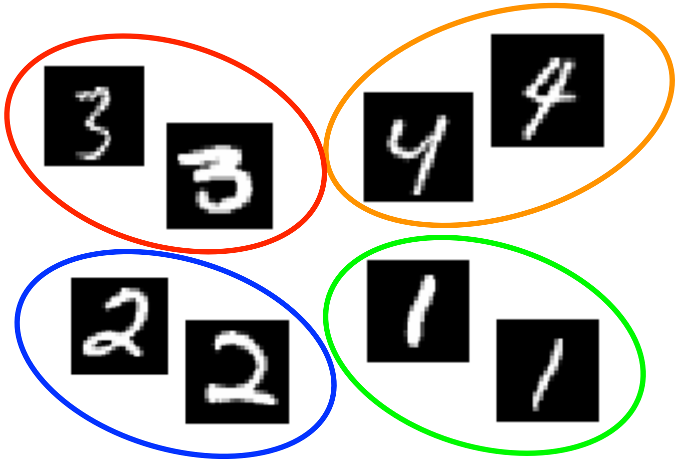
Cluster 15 n=135

Cluster 16 n=209

One can then think of analyzing this phenomenon by clustering the poses observed in a collection of paintings

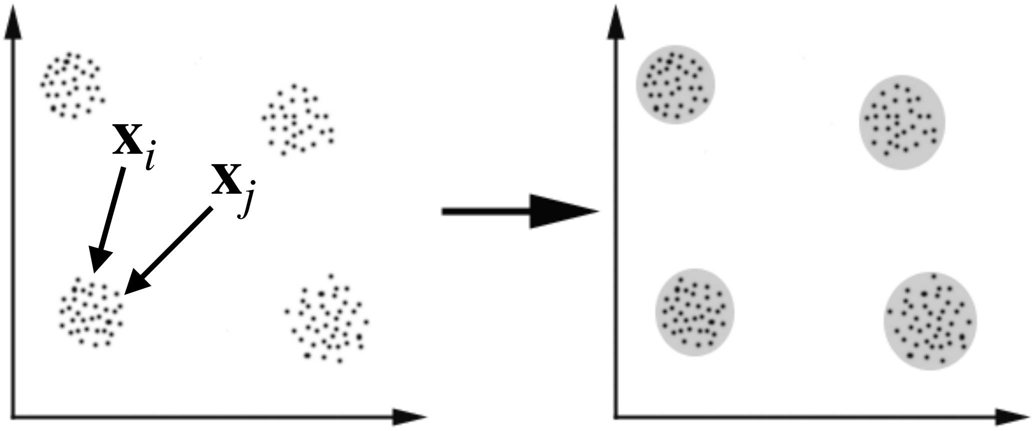
In the Simpler MNIST Context

Given input data **without** labels:



- Can we identify the groups, without performing any data transformation?
- Yes, and this operation is known as **clustering**.

K-Means Clustering

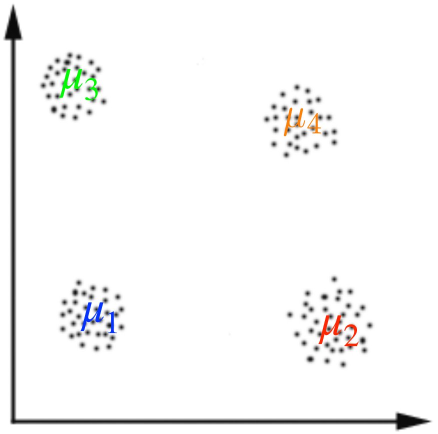


Given a set of input samples:

- Group the samples into K clusters.
- K is assumed to be known/given.
- In the toy example above, each data sample is a point in 2D.
- In our previous examples, each data sample was a human pose or an image.

$\mathbf{x}_i =$ or $\mathbf{x}_i =$

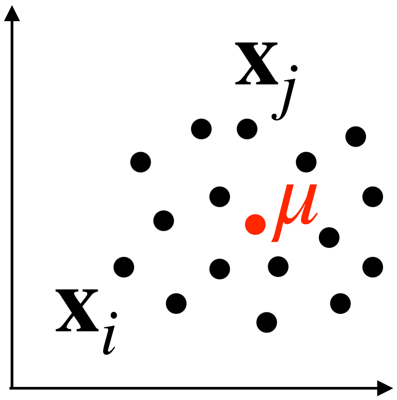
K-Means Clusters



- Cluster k is formed by the points $\{\mathbf{x}_{i_1^k}, \ldots, \mathbf{x}_{i_{n^k}^k}\}$.
- μ_k is the **center of gravity** of cluster k.

The mean of points $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, $\mathbf{x}_i \in \mathbb{R}^D$ is

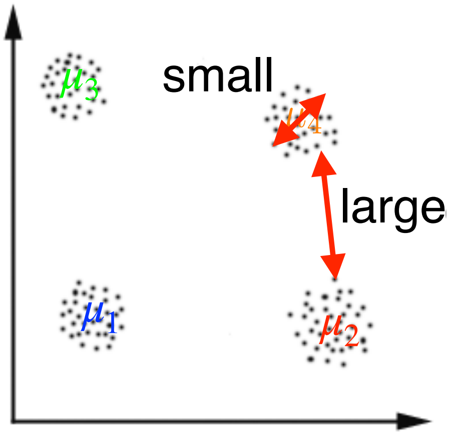
$$\mu = \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}_i \,, \mu \in \mathbb{R}^D$$



In 2D

- If the $\mathbf{x}_i$ were physical points of equal mass, μ would be their center of gravity.
- This applies in any dimension.

Formalization



- Cluster k is formed by the points $\{\mathbf{x}_{i_1^k}, \ldots, \mathbf{x}_{i_{n^k}^k}\}$.
- μ_k is the **center of gravity** of cluster k.

- The distances between the points within a cluster should be small.
- The distances across clusters should be large.
- This can be encoded via the distance to cluster centers $\{\mu_1, \ldots, \mu_K\}$:

$$\longrightarrow \text{Minimize } \sum_{k=1}^{K} \sum_{j=1}^{n^k} (\mathbf{x}_{i_j^k} - \mu_k)^2$$

where $\{\mathbf{x}_{i_1^k}, \ldots, \mathbf{x}_{i_{n^k}^k}\}$ are the n^k samples that belong to cluster k.

Difficult Minimization Problem

Minimize

$$\sum_{k=1}^{K} \sum_{j=1}^{n^k} (\mathbf{x}_{i_j^k} - \mu_k)^2$$

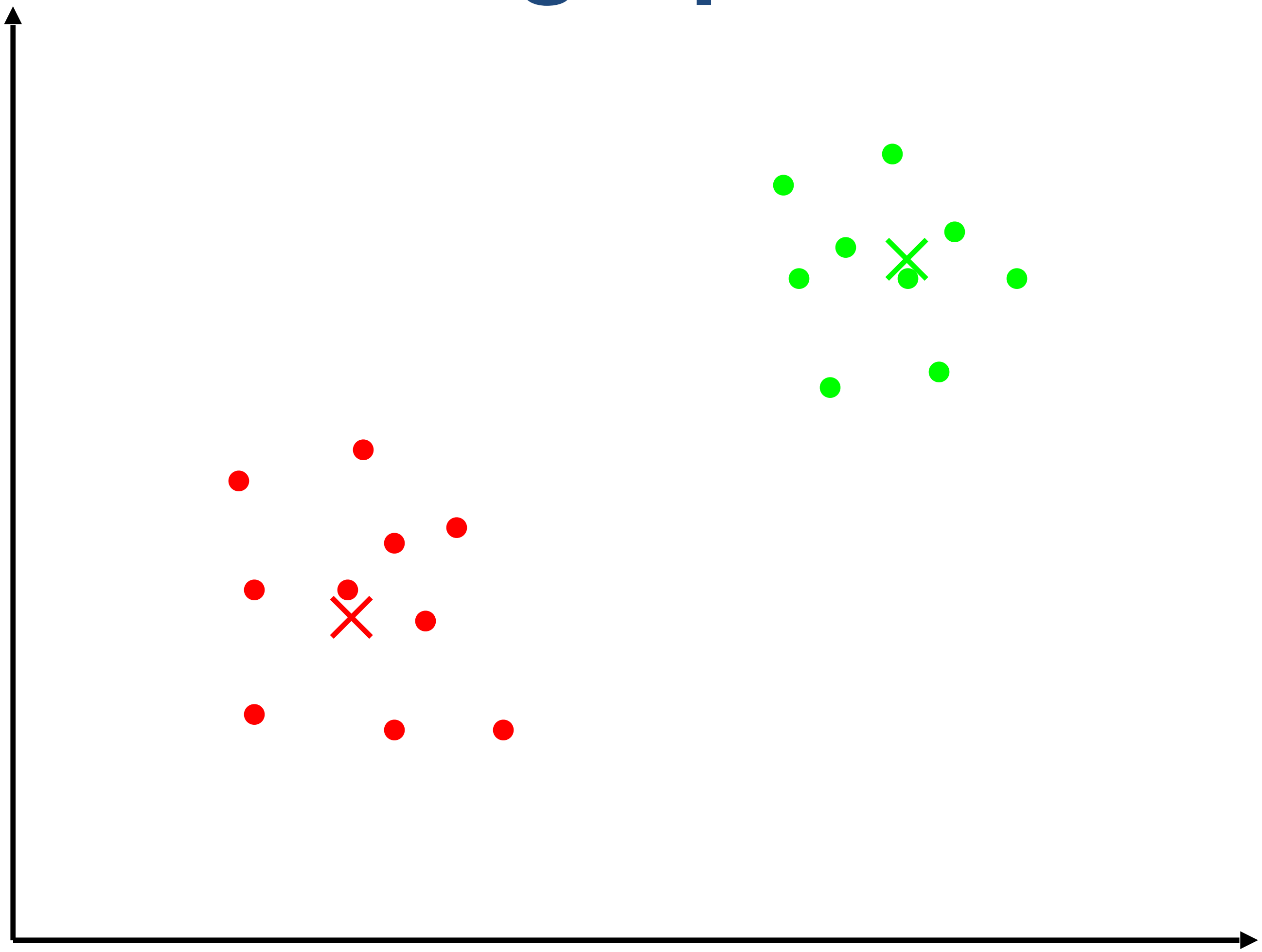
but:

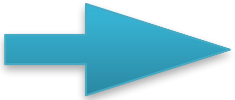
- We don’t know what points belong to what cluster.
- We don’t know the center of gravity of the clusters.

Simple Solution to the Problem

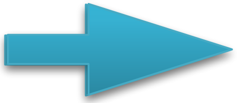
1. Initialize $\{\mu_1, \ldots, \mu_K\}$, randomly if need be.
2. Until convergence
   2.1. Assign each point $\mathbf{x}_i$ to the nearest center μ_k
   2.2. Update each center μ_k given the points assigned to it

Alternating Optimization

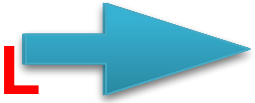




- Initialize

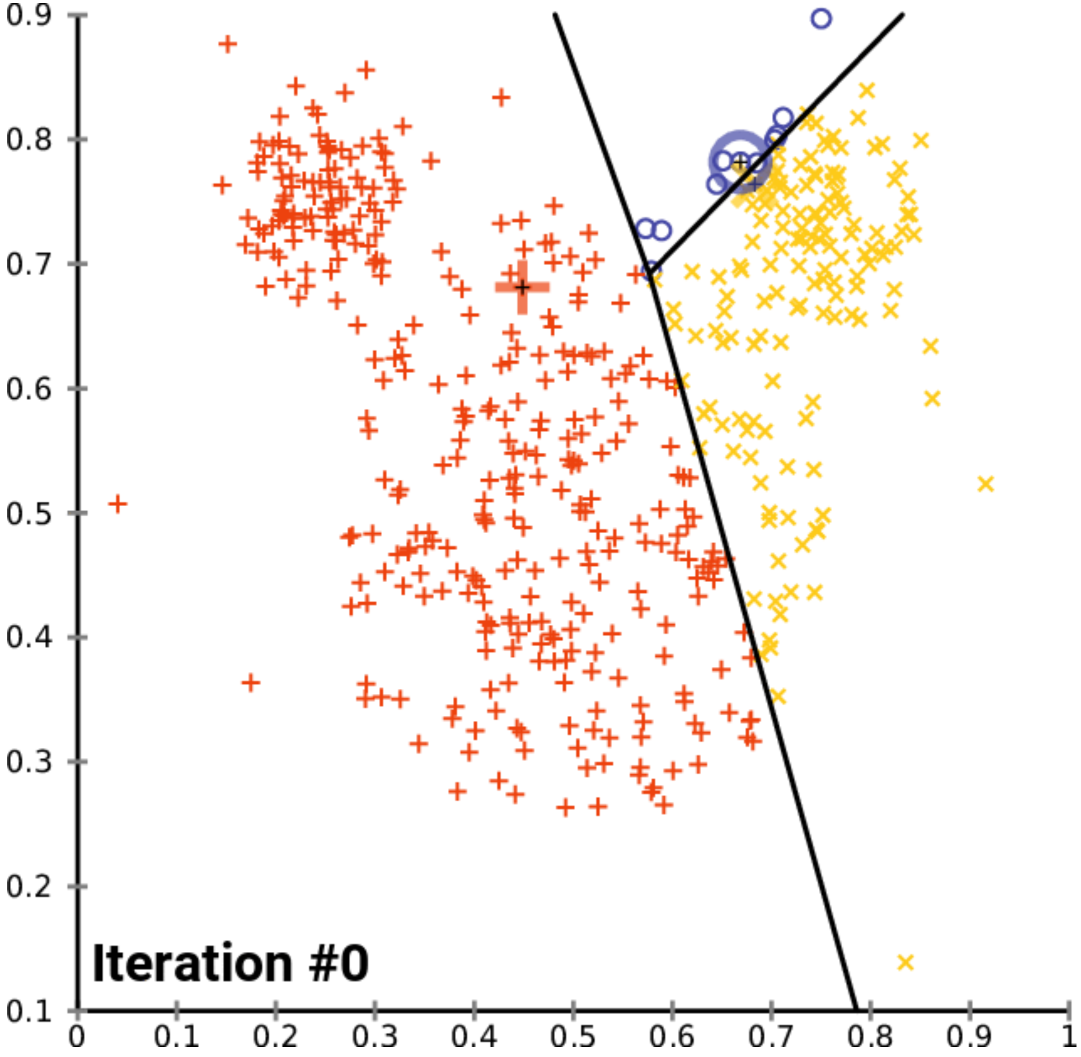


- Associate point to centers



- Recompute centers

Three Classes



K-means clustering: Demo

- https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

Algorithm: More details

- Step 2.1: Assign each point $\mathbf{x}_i$ to the nearest center μ_k.
  - For each point $\mathbf{x}_i$, compute the Euclidean distance to every center $\{\mu_1, \ldots, \mu_K\}$.
  - Find the smallest distance.
  - The point is said to be assigned to the corresponding cluster. Note that each point is assigned to a single cluster.

- Step 2.2: Update each μ_k given the points assigned to it.
  - Recompute each center μ_k as the mean of the points that were assigned to it.

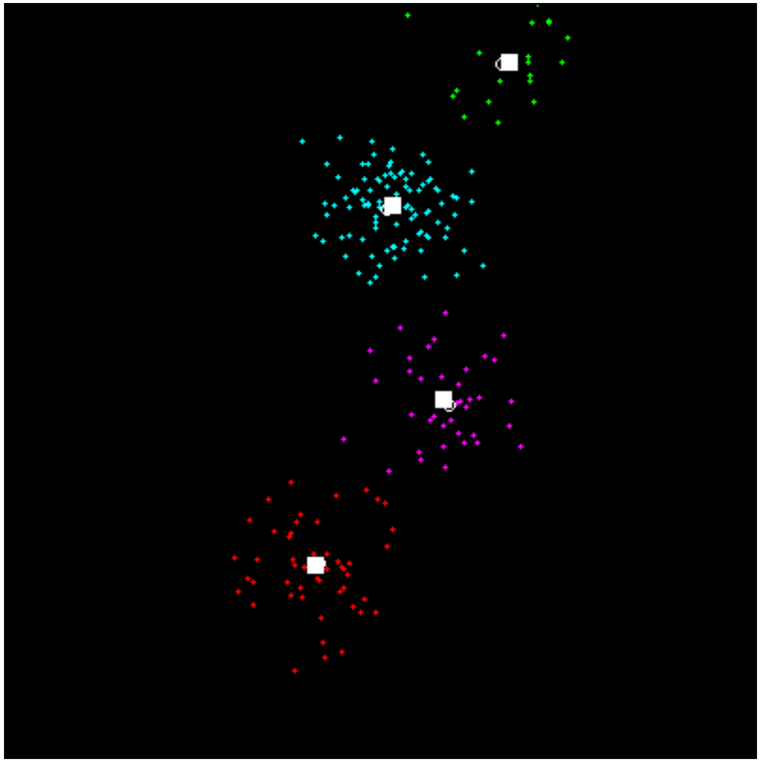
Algorithm: More details

- Stopping criterion:
  - The algorithm iteratively updates the cluster assignment for each point and the cluster centers. We need to eventually stop iterating.
  - This could be achieved by a fixed number of iterations. However, setting this number is arbitrary and a too small number can lead to bad results.
  - The algorithm is guaranteed to converge to a stable solution, where the cluster centers and the point assignments are fixed, that is, do not change as more iterations are performed.
  - The difference in assignments or center locations between two iterations can be used as criteria to stop the algorithm.

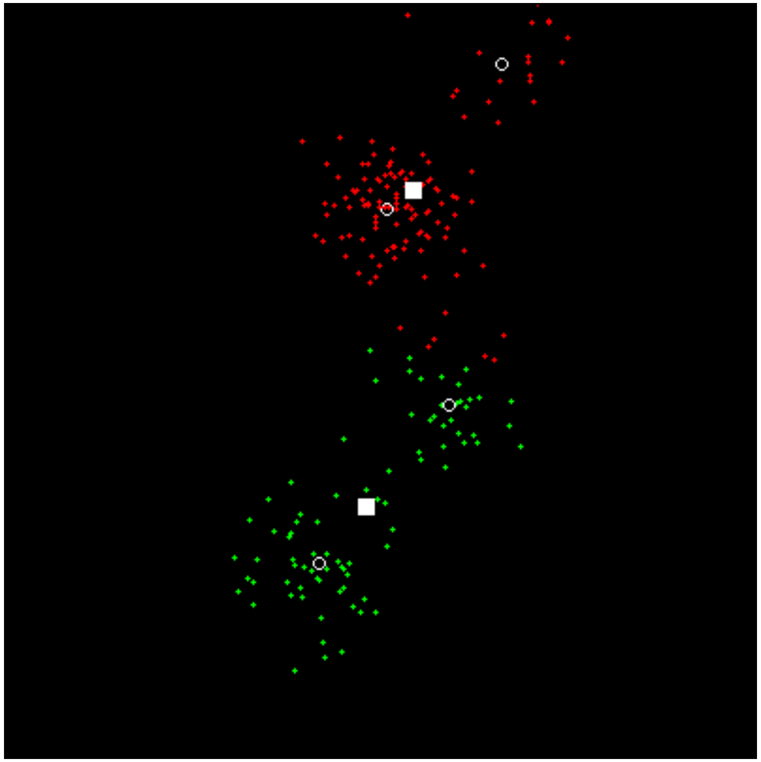
- Even though the algorithm always converges, it does not always converge to the best (desired) solution.

- The solution depends on the initialization.

Initial Conditions Matter



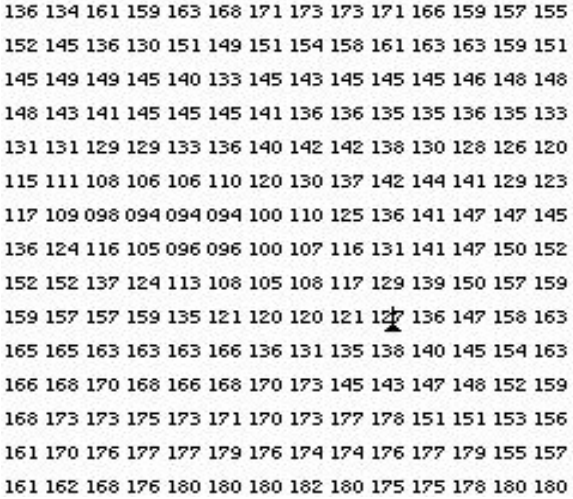
Initially, the points are assigned to the clusters at random—> Success.



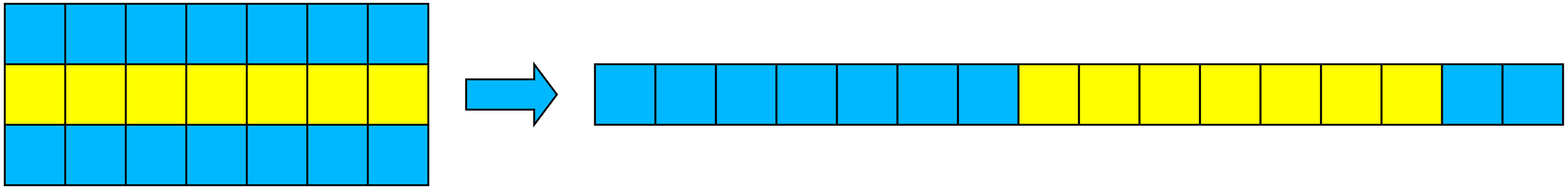
Initially, the points are assigned to the closest cluster —> Failure.

—> In practice try several different random initialization and keep the one that yields the best result in term of the sum of square distances.

Reminder: Black and White Images

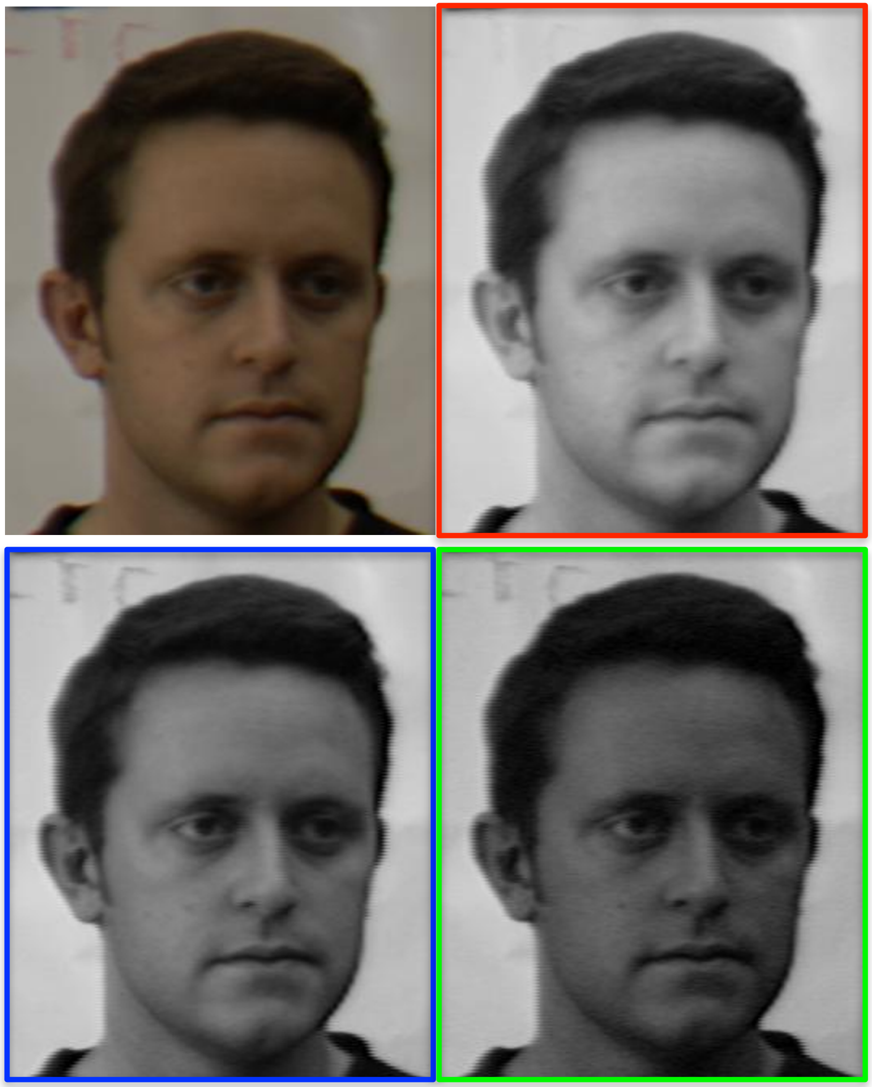


136	134	161	159	163	168	171	173	173	171	166	159	157	155
152	145	136	130	151	149	151	154	158	161	163	163	159	151
145	149	149	145	140	133	145	143	145	145	145	146	148	148
148	143	141	145	145	145	141	136	136	135	135	136	135	133
131	131	129	129	133	136	140	142	142	138	130	128	126	120
115	111	108	106	106	110	120	130	137	142	144	141	129	123
117	109	098	094	094	094	100	110	125	136	141	147	147	145
136	124	116	105	096	096	100	107	116	131	141	147	150	152
152	152	137	124	113	108	105	108	117	129	139	150	157	159
159	157	157	159	135	121	120	120	121	127	136	147	158	163
165	165	163	163	163	166	136	131	135	138	140	145	154	163
166	168	170	168	166	168	170	173	145	143	147	148	152	159
168	173	173	175	173	171	170	173	177	178	151	151	153	156
161	170	176	177	177	179	176	174	174	176	177	179	155	157
161	162	168	176	180	180	180	182	180	175	175	178	180	180



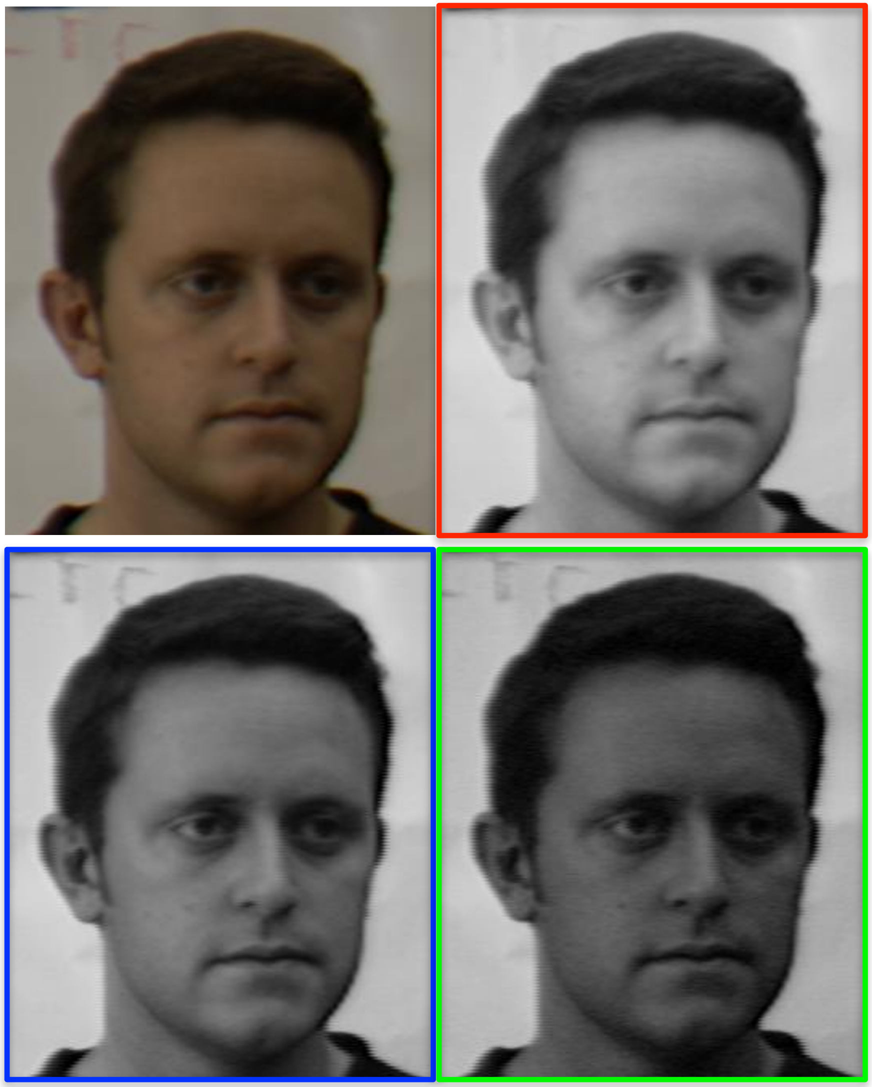
- A MxN image can also be represented as an MN vector.

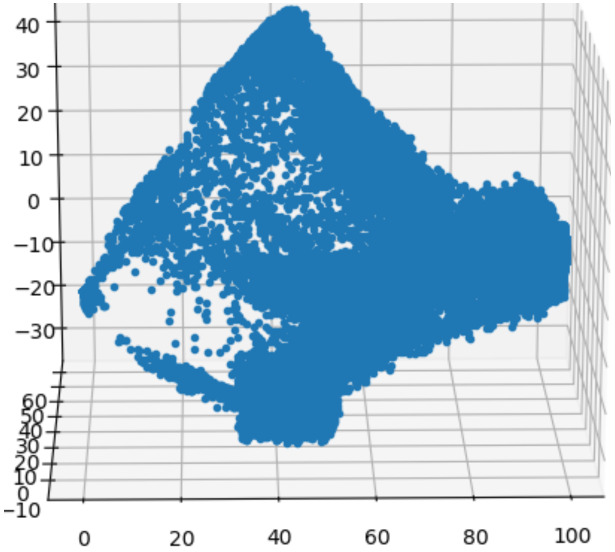
Color Images



A color image is often represented by three 8-bit images, one for red, one for green, and one for blue.

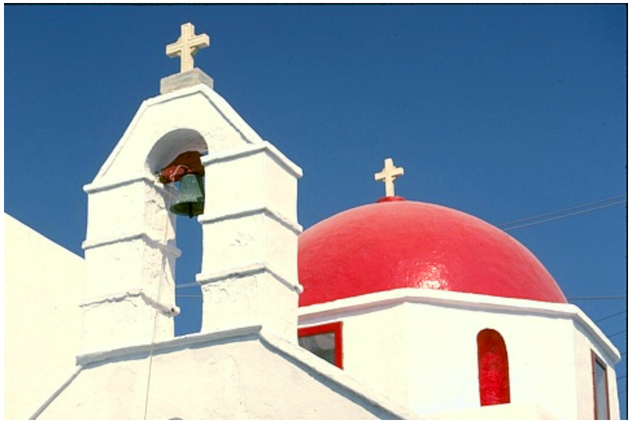
Color Image as 3D Point Cloud

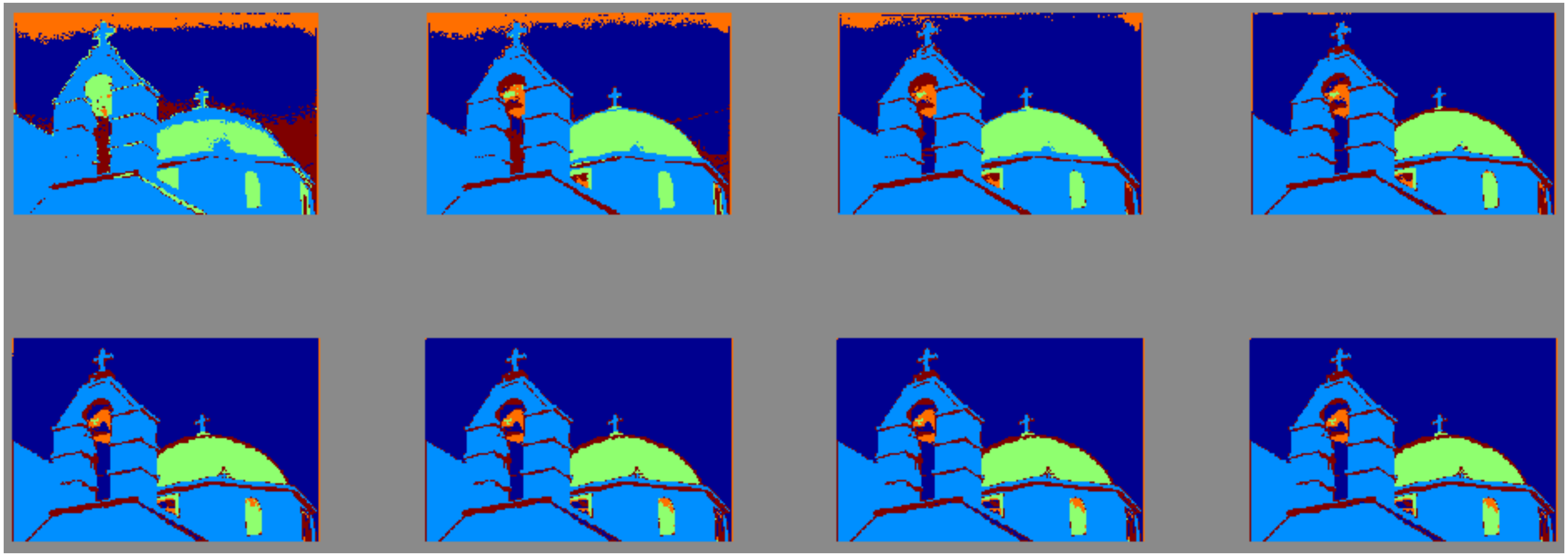




- Each pixel can be thought of as a 3D point.
- We can run k-means on the cloud of 3D points.

K-Means Clustering for Images



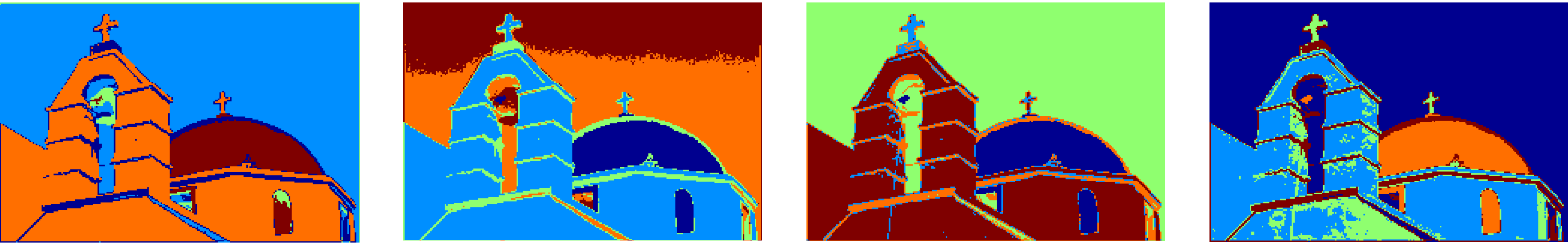


8 iterations for k=5

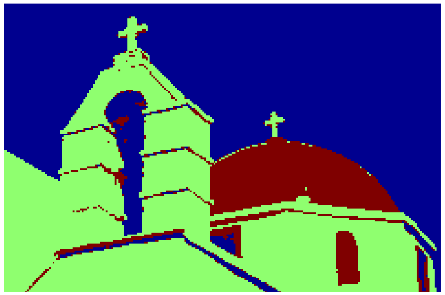
Bishop, Chapter 9.1

K-Means Clustering for Images

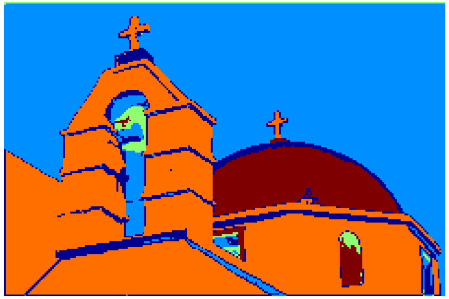
Different Initializations for k=5



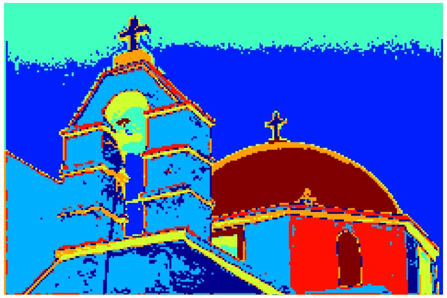
Different values of k



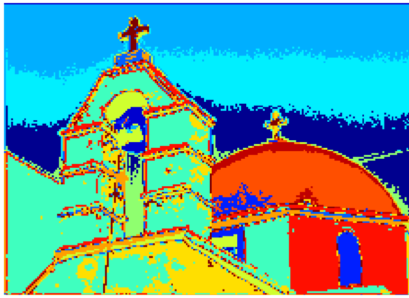
K=3



K=5



K=8

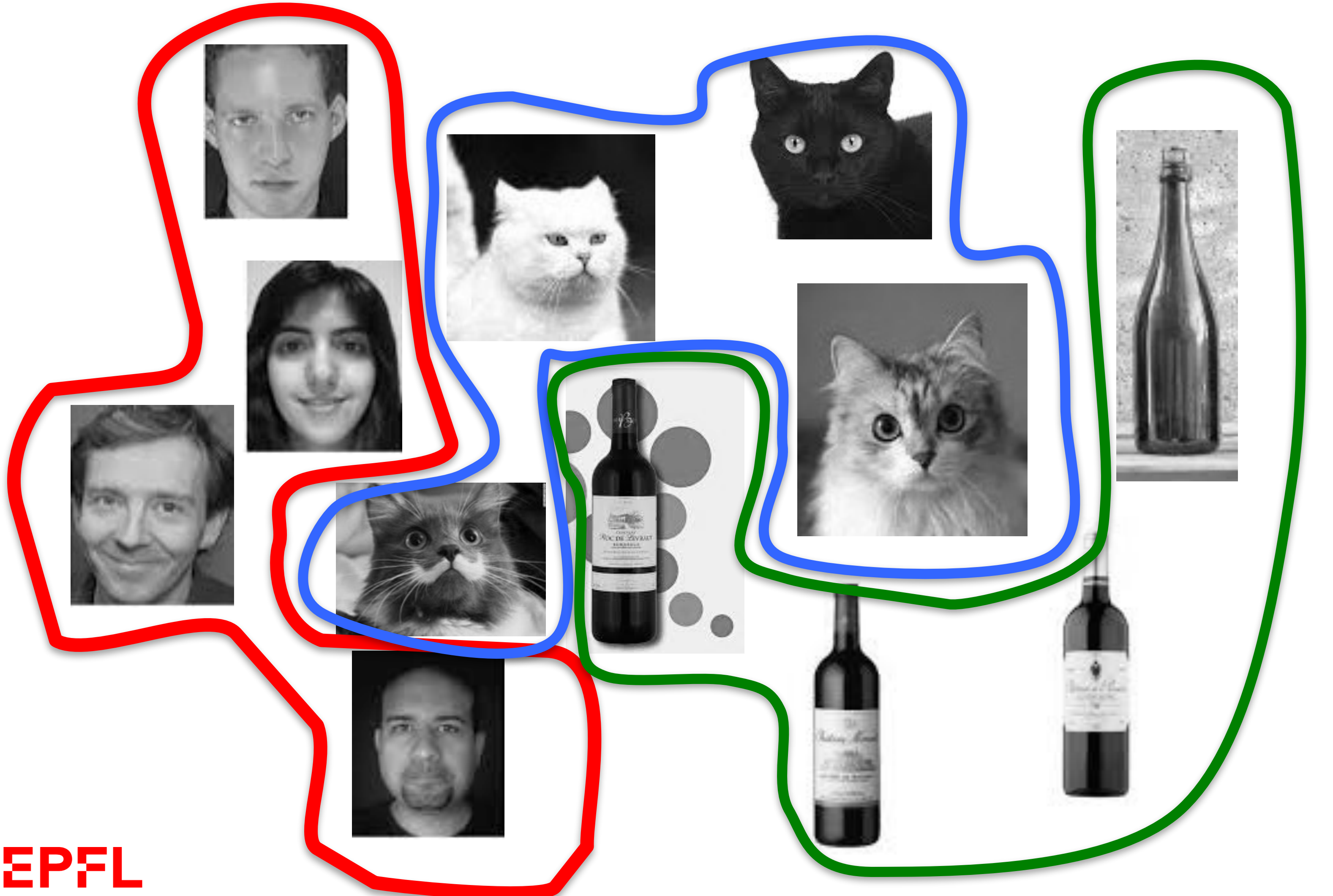


K=15

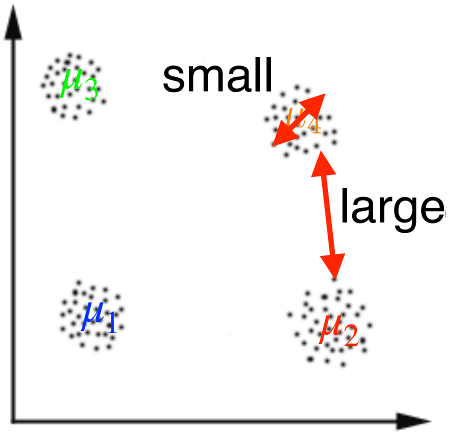
- Different results for different initializations.
- How do we choose k?

Reminder: Unsupervised Learning

The training set is not annotated and the system must also learn the classes.



Reminder: K-means Clustering



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Reminder: K-means Clustering

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Reminder: K-means clustering: Demo

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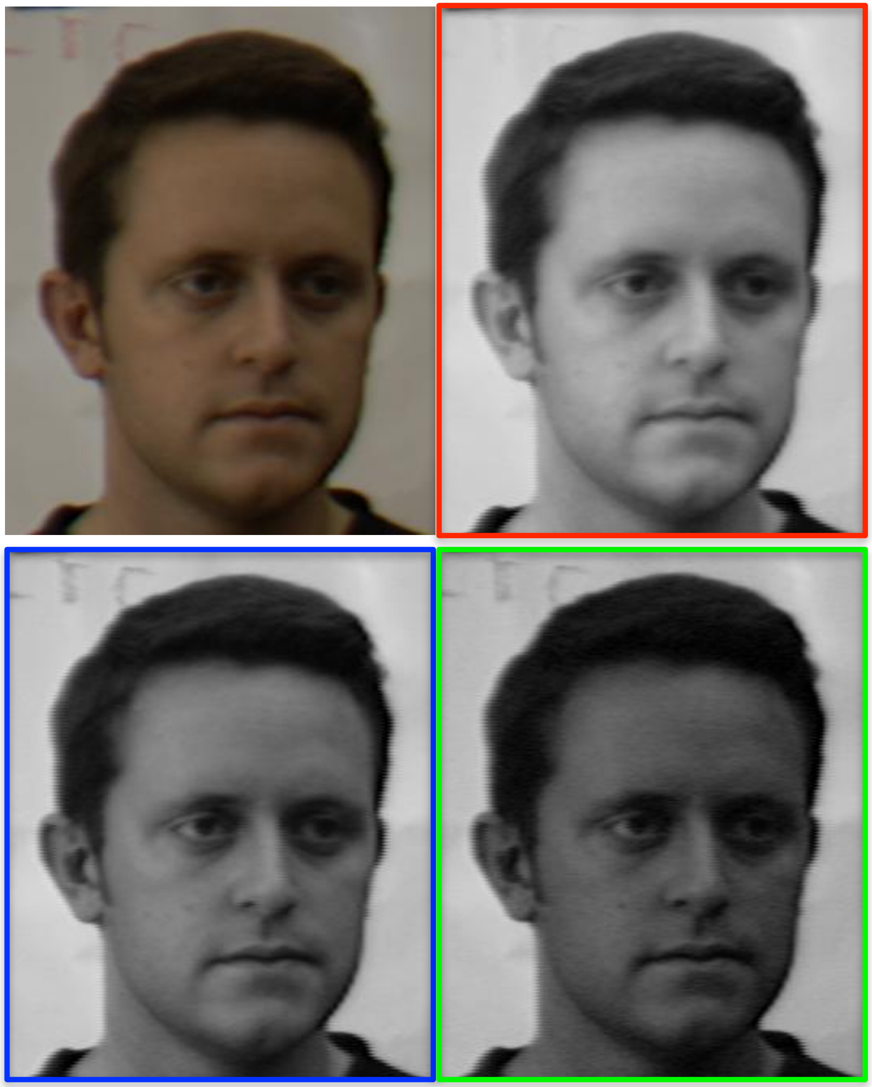
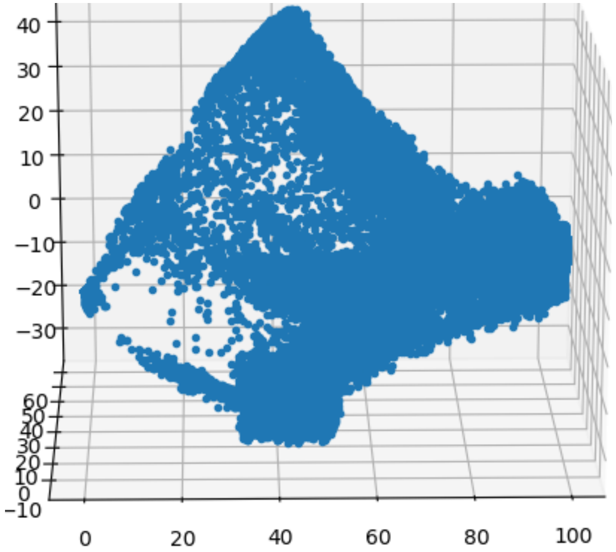
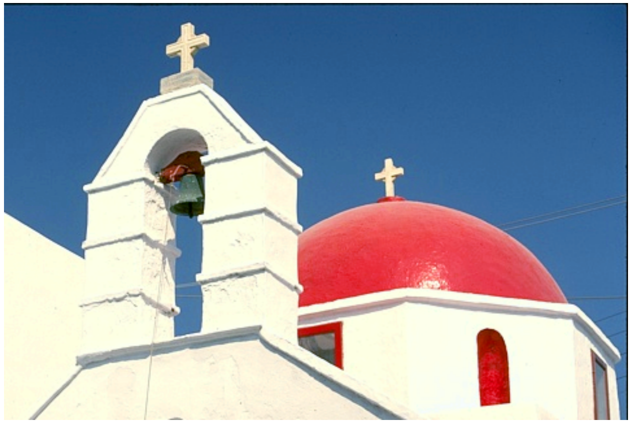
Reminder: Color Image as 3D Point Cloud

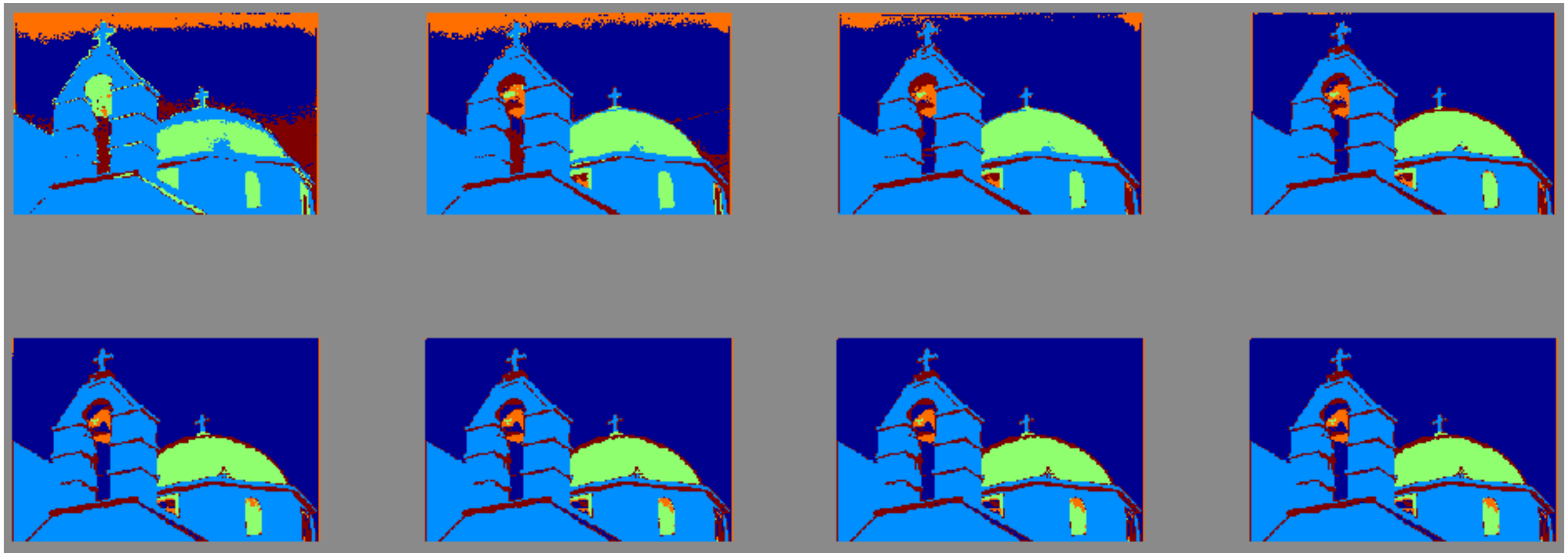




- Each pixel can be thought of as a 3D point.
- We can run k-means on the cloud of 3D points.

Reminder: K-Means Clustering for Images



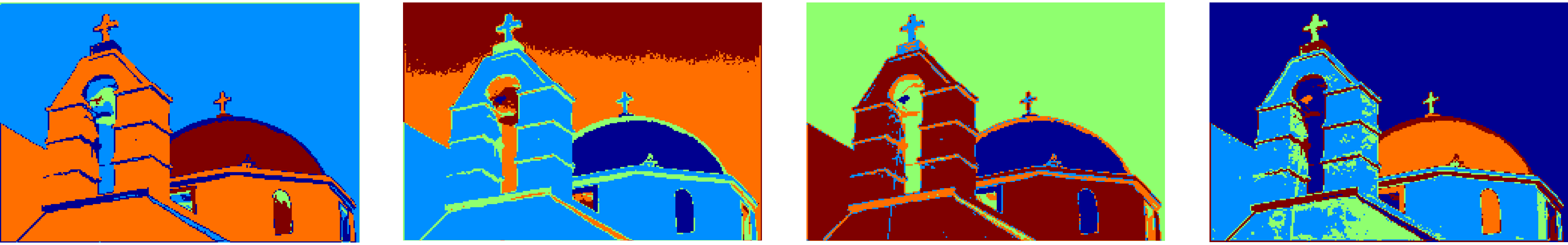


8 iterations for k=5

Bishop, Chapter 9.1

K-Means Clustering for Images

Different Initializations for k=5

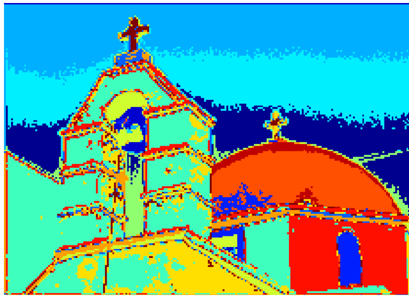


Different values of k

K=3

K=5

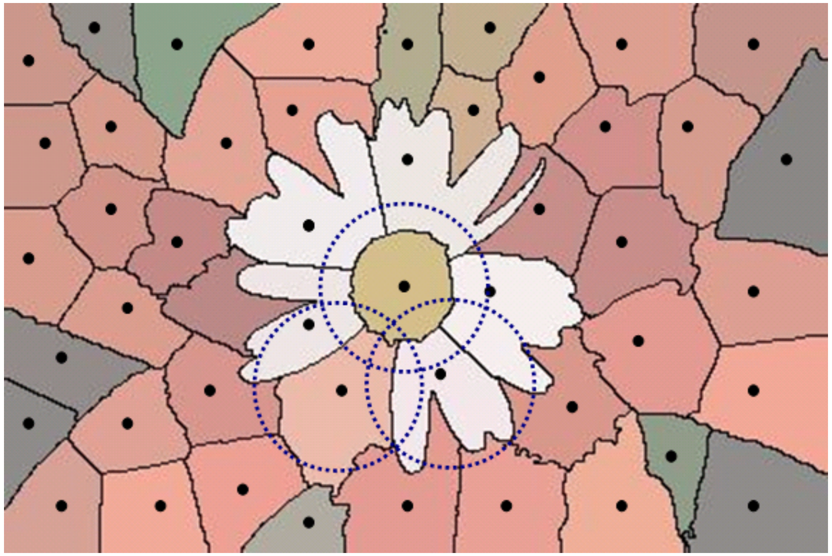
K=8



K=15

- Different results for different initializations.
- How do we choose k?

UV + Color (5D)



$$E(\mathcal{C}_1, \ldots, \mathcal{C}_k, \mathbf{c}_1, \ldots, \mathbf{c}_k) = \sum_j \sum_{i \in \mathcal{C}_j} d(\mathbf{x}_i, \mathbf{c}_j)^2$$

$$\mathbf{x} = \begin{bmatrix} u \\ v \\ L \\ a \\ b \end{bmatrix} \text{ or } \begin{bmatrix} u \\ v \\ I \\ 0 \\ 0 \end{bmatrix}$$

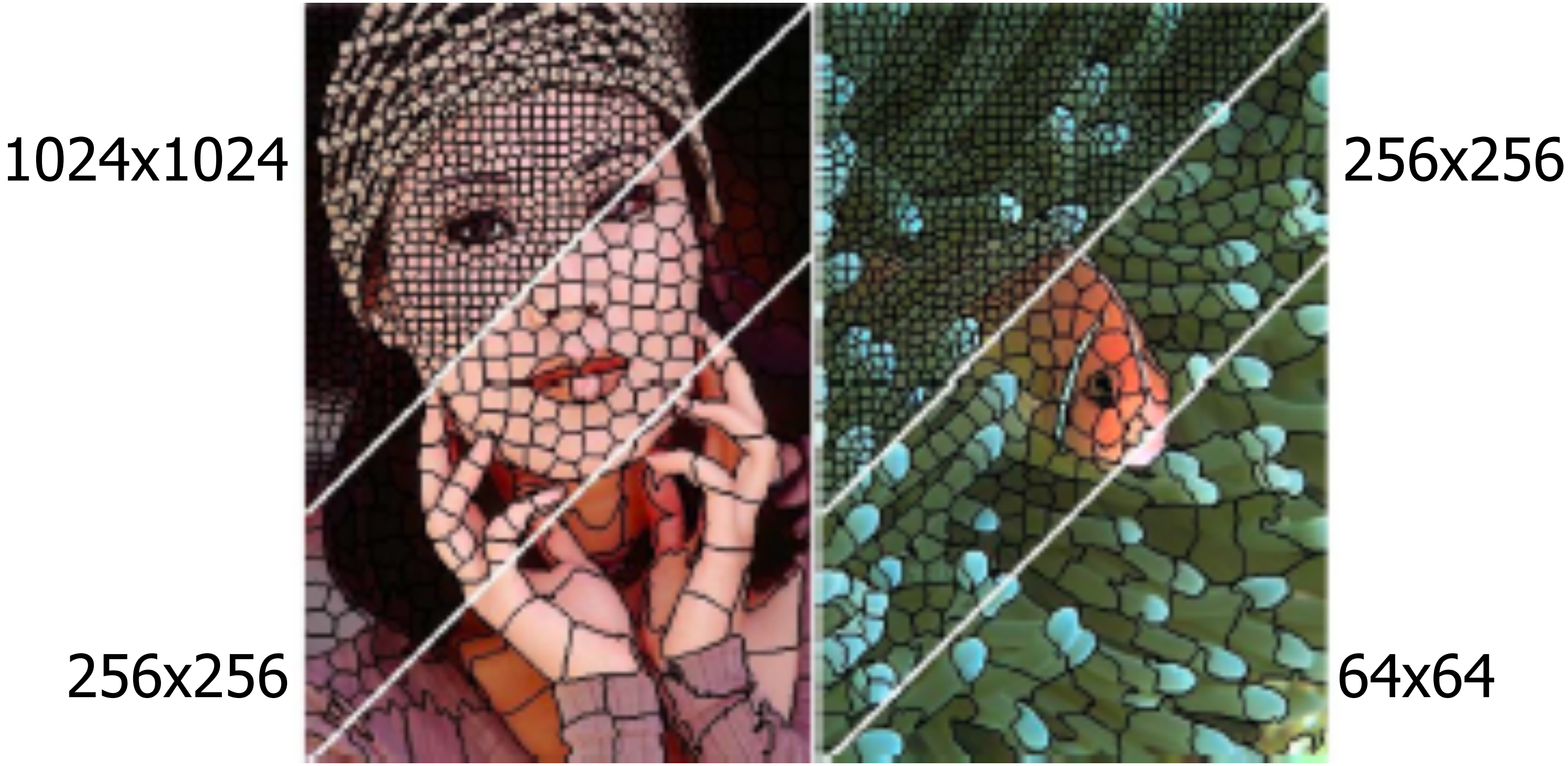
$$d(\mathbf{x}, \mathbf{c})^2 = \frac{(\mathbf{x}[0] - \mathbf{c}[0])^2 + (\mathbf{x}[1] - \mathbf{c}[1])^2}{h_s^2} + \frac{(\mathbf{x}[2] - \mathbf{c}[2])^2 + (\mathbf{x}[3] - \mathbf{c}[3])^2 + (\mathbf{x}[4] - \mathbf{c}[4])^2}{h_r^2}$$

Run K-Means algorithm with regularly spaced seeds on a grid and using a distance that is a weighted (h_s and h_r) sum of distances in image space and in gray level/color space.

—> Superpixels

Achanta et al. PAMI'12

SLIC Superpixels



- Superpixel segmentations with centers on a 64x64, 256x256, and 1024x1024 grid.
- Can be used to describe the image in terms of a set of small regions.

Heuristic for Choosing K

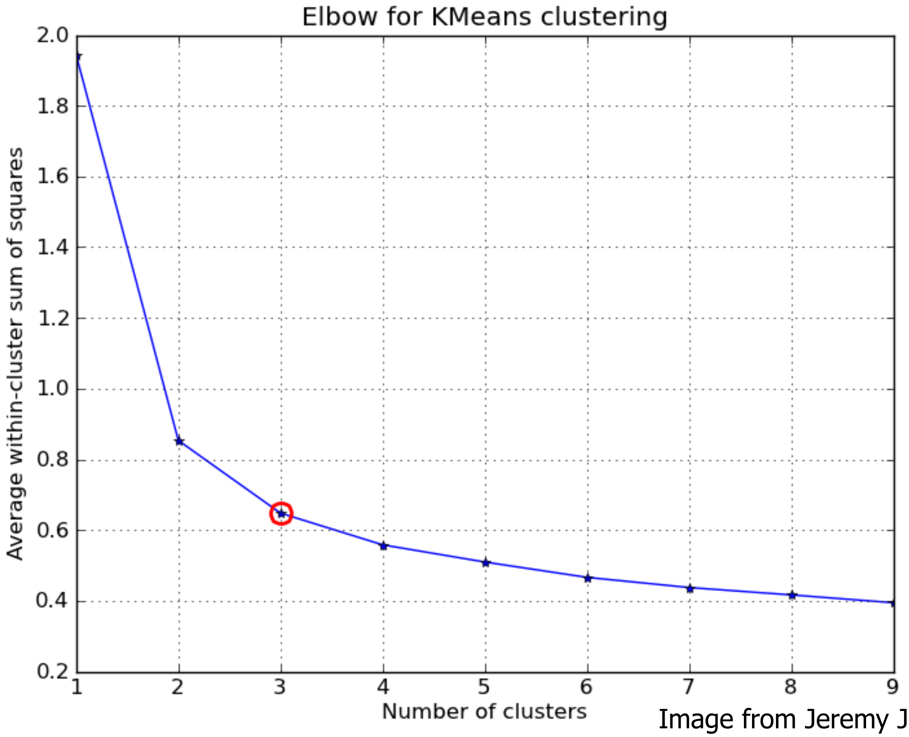


Image from Jeremy Jordan

- The average within-cluster distance typically decreases towards zero but using too many clusters make the results meaningless.
- The elbow of the curve is where the drop in within-cluster distances becomes less significant

Inhomogeneous Data

✓ The Euclidean distance is most appropriate for data with homogeneous dimensions:

- In the 2D toy data, both dimensions are of commensurate magnitude.
- In the color image, each dimension represents a color channel and varies in the range $[0,255]$.

x In practice, this is not always the case:

- Different data dimensions may have different magnitudes.
- They can encode different types of information.
- We have already seen this in the case of superpixels.

Example of Data with Heterogeneous Dims

- Wine dataset from the UCI ML repository:
  - 178 wines from 3 different producers.
  - Each wine is represented by 13 attributes, such as quantity of alcohol, malic acid concentration, and magnesium.

- Two samples from the dataset:

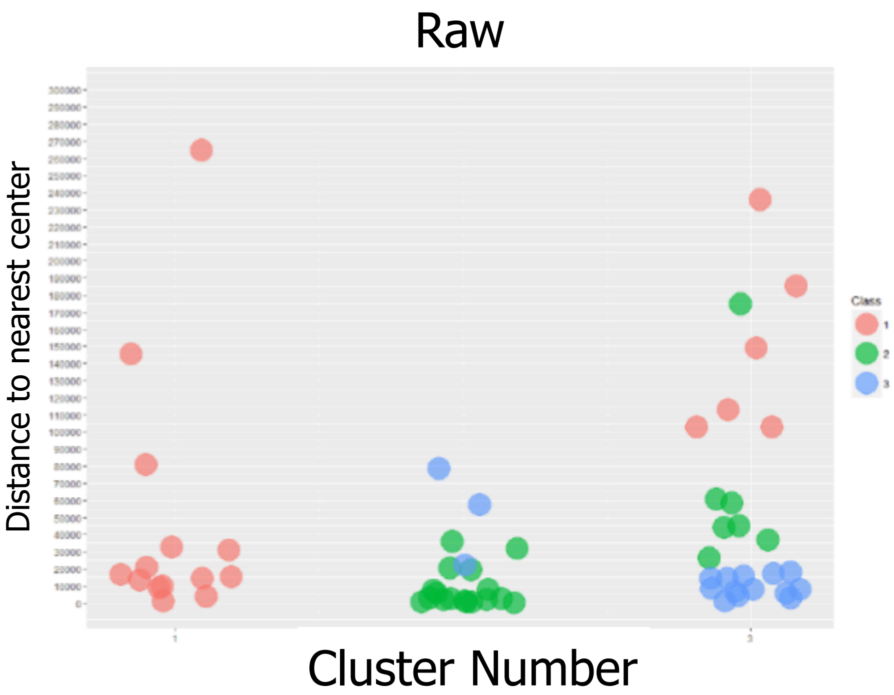
14.37	1.95	2.5	16.8	113	3.85	3.49	0.24	2.18	7.8	0.86	3.45	1480
13.24	2.59	2.87	21	118	2.8	2.69	0.39	1.82	4.32	1.04	2.93	735

- Large values will contribute a lot to the Euclidean distance and small ones much less.
- It does not mean that they are more or less meaningful for clustering!

Solutions

- Scale each dimension by subtracting the smallest value and scaling the result to be between 0 and 1.
- Use a different metric such as the Manhattan distance we saw earlier.
- ……

Wine Example



The color represents the true producer. Ideally all samples in one cluster should have the same color.

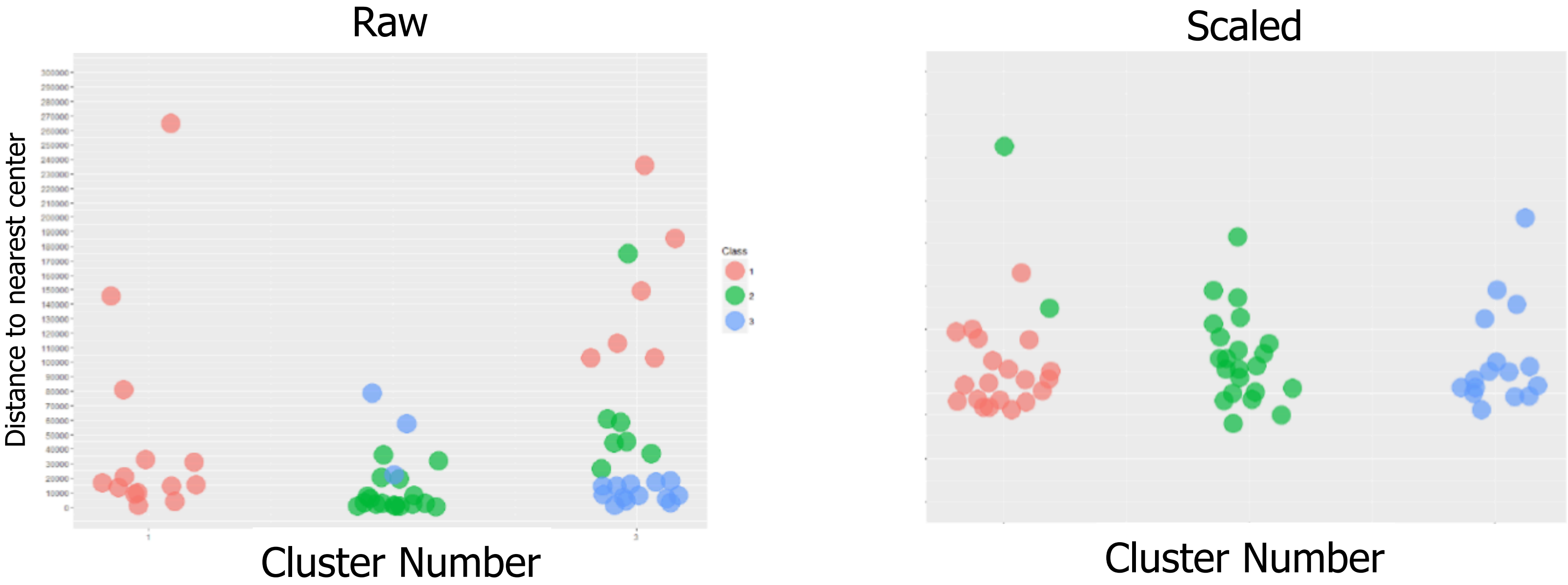
The vertical coordinate is the distance to the cluster center.

Accuracy is defined as the percentage of wines assigned to the correct cluster.

Euclidean distance with raw data: 73% accurate.

https://dinajankovich.com/2018/04/28/k-means-clustering-of-wine-data/

Wine Example

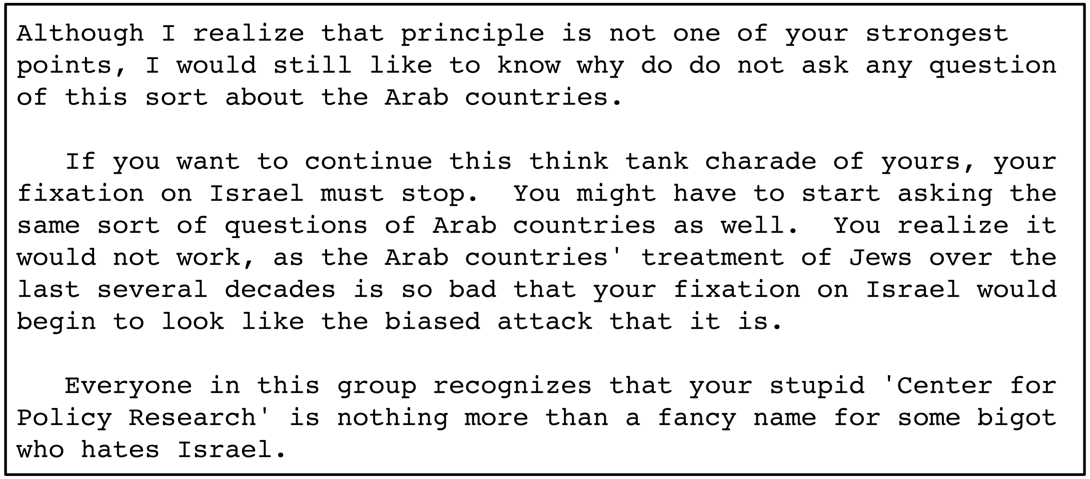


Euclidean distance with scaled data: 93.2% accurate.

Manhattan distance with scaled data: 94.5% accurate.

https://dinajankovich.com/2018/04/28/k-means-clustering-of-wine-data/

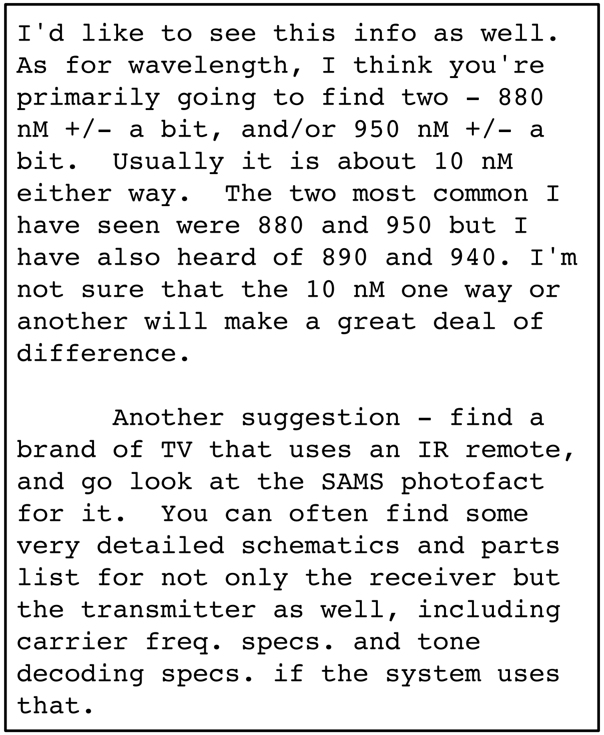
Even More Heterogeneous Data



Although I realize that principle is not one of your strongest points, I would still like to know why do do not ask any question of this sort about the Arab countries.

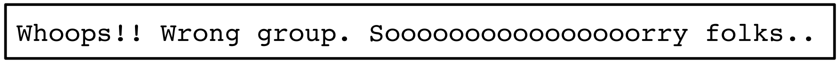
If you want to continue this think tank charade of yours, your fixation on Israel must stop. You might have to start asking the same sort of questions of Arab countries as well. You realize it would not work, as the Arab countries' treatment of Jews over the last several decades is so bad that your fixation on Israel would begin to look like the biased attack that it is.

Everyone in this group recognizes that your stupid 'Center for Policy Research' is nothing more than a fancy name for some bigot who hates Israel.



I'd like to see this info as well. As for wavelength, I think you're primarily going to find two - 880 nM +/- a bit, and/or 950 nM +/- a bit. Usually it is about 10 nM either way. The two most common I have seen were 880 and 950 but I have also heard of 890 and 940. I'm not sure that the 10 nM one way or another will make a great deal of difference.

Another suggestion - find a brand of TV that uses an IR remote, and go look at the SAMS photofact for it. You can often find some very detailed schematics and parts list for not only the receiver but the transmitter as well, including carrier freq. specs. and tone decoding specs. if the system uses that.



Whoops!! Wrong group. Soooooooooooooooorry folks..

- How can we compute a distance between these three pieces of text?
- One solution is to turn them into vectors.

—> We will revisit this issue when we talk about deep nets.

K-Means in Short

- A simple yet effective clustering algorithm.
- Sensitive to initialization.
- Works best on homogeneous data.

Clustering: Compactness

- K-means clustering exploits the notion of compactness of clusters

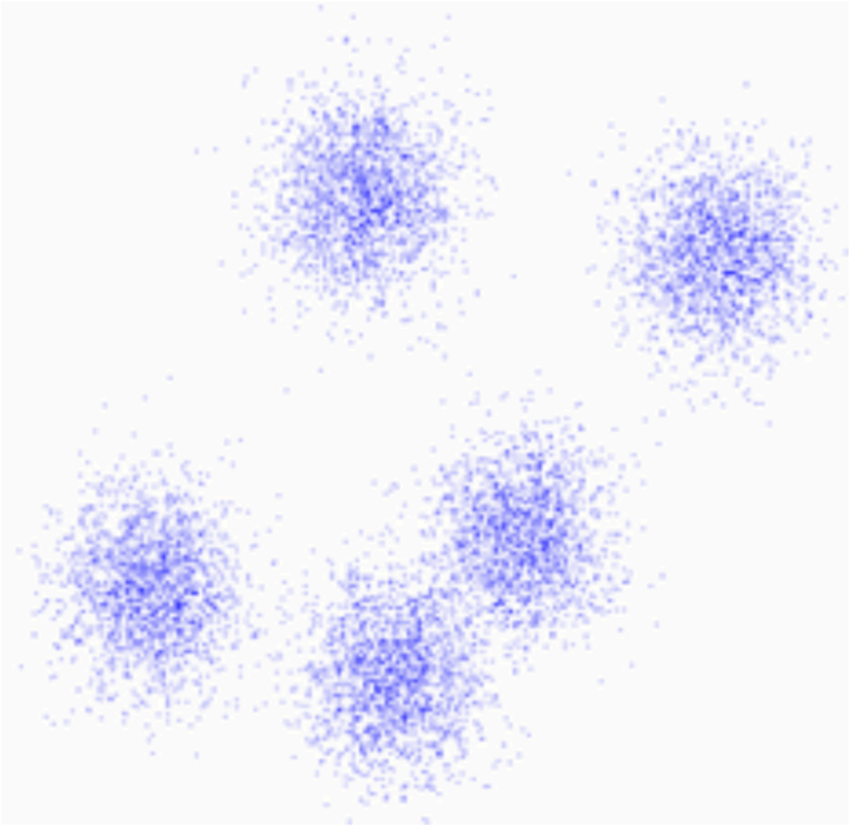
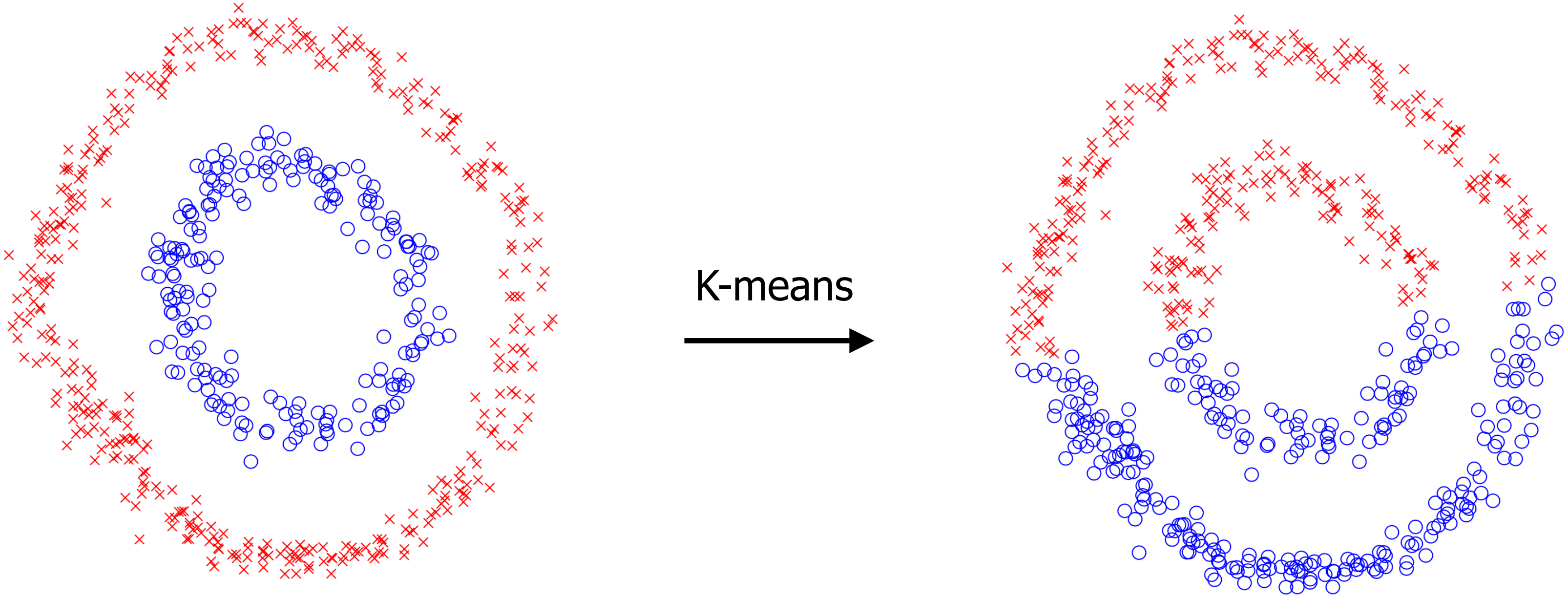


Figure from Eric Xing's slides

Clustering: Compactness

- What happens if the data is not compact
  - E.g., two concentric circles



- Yet, we still clearly identify the two “true” clusters

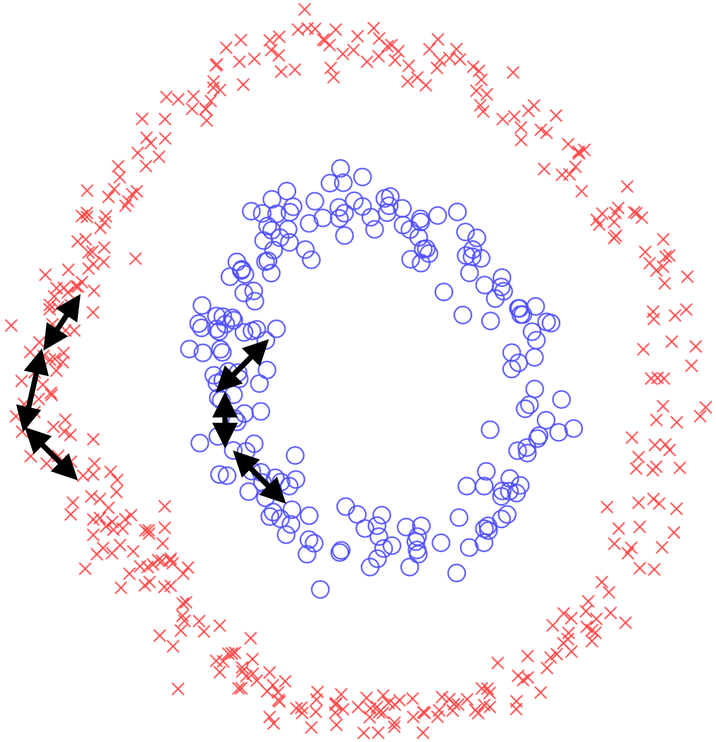
Figure from David Sontag’s slides

Back to the K-means clustering demo

- https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

Clustering: Connectivity

- The two clusters we observe arise from the connectivity of the points



Spectral clustering: Graph-based connectivity

- Group the points based on edges in a graph
  - Strong connections indicate points that should be clustered
  - Weaker ones suggest that the graph can be cut into pieces/ partitions

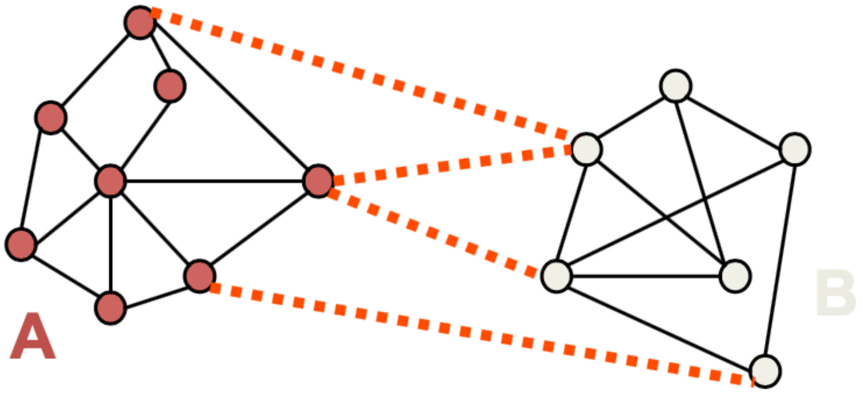


Figure from David Sontag's slides

How to create the graph?

- Compute a notion of similarity between the points
  - E.g., the similarity between point i and point j can be taken as

$$W_{ij} = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}\right)$$

where σ is a hyper-parameter

- This would lead to a fully connected graph (an edge with a weight W_{ij} for every pair of points)
  - The graph can also be restricted to the K-nearest neighbor of each point

From graph to similarity matrix

- A graph can be equivalently represented by a similarity (or affinity) matrix

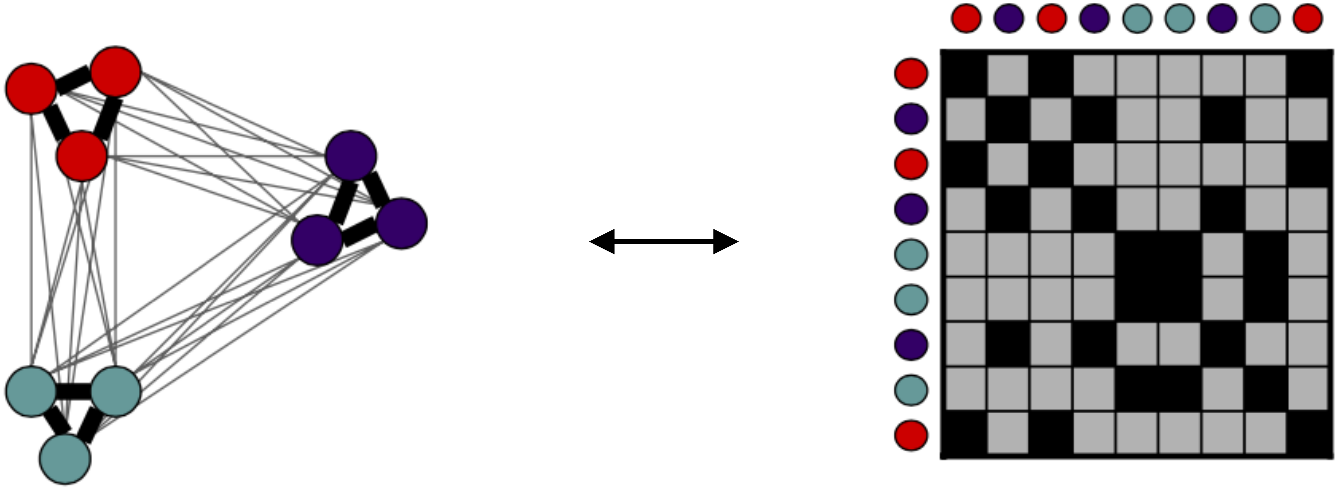
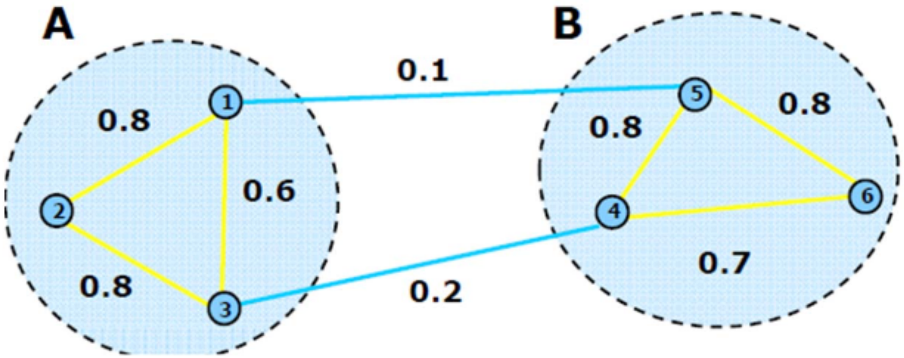


Figure from Eric Xing's slides

Graph cut

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



- A cost for cut is obtained by summing the weight of the edges that connect the two groups

$$cut(A,B) = \sum_{i\in A,\ j\in B} W_{ij}$$ (=0.3 in this example)

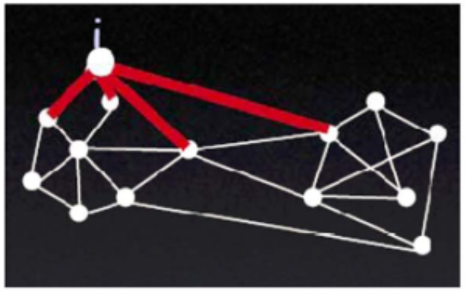
- Intuitively, for clustering, we would like to find the partition that minimizes such a cut

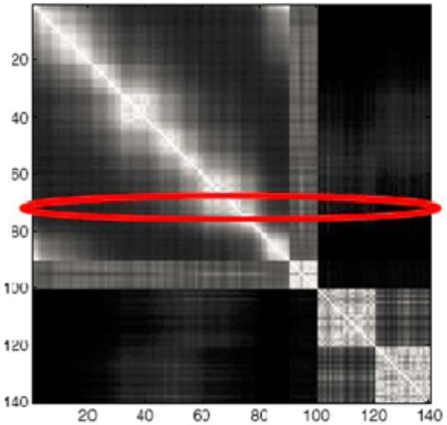
Figure from David Sontag’s slides

Graph terminology

- The degree of a node in the graph is given by

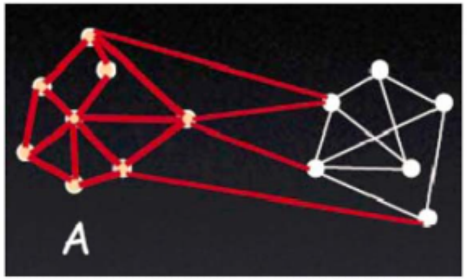
$$d_i = \sum_j W_{ij}$$

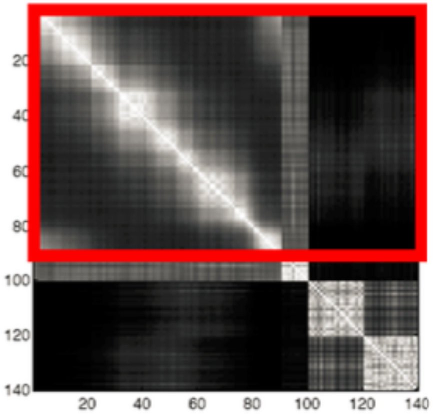




- The volume of a set (partition) is given by

$$vol(A) = \sum_{i \in A} d_i$$





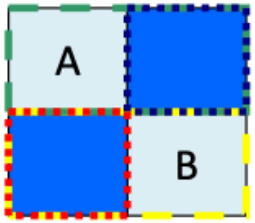
Figures from David Sontag's slides

Normalized cut

- Minimizing the cut might favor imbalanced partitions
  - E.g., a single point in A and all the others in B

- Instead, we can use a normalized cut

$$Ncut(A,B) = \frac{cut(A,B)}{Vol(A)} + \frac{cut(A,B)}{Vol(B)}$$



where $Vol(A)$ is the volume of partition A, defined in the previous slide

Figure from David Sontag's slides

Normalized cut: Relaxation

- Minimizing the normalized cut can be approximated as a generalized eigenvalue problem

$$(\mathbf{D} - \mathbf{W})\mathbf{y} = \lambda \mathbf{D}\mathbf{y}$$

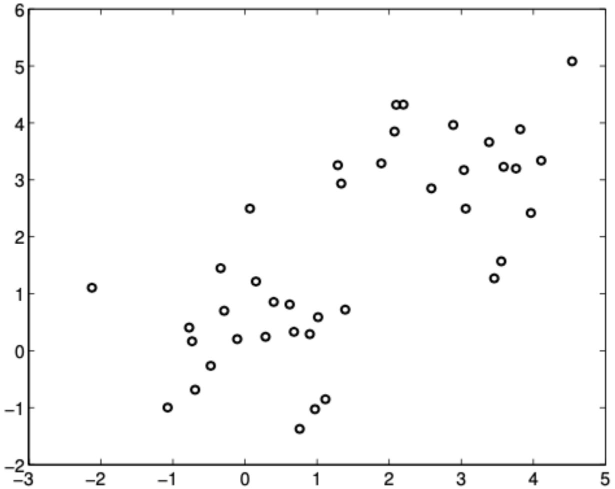
where $\mathbf{W} \in \mathbb{R}^{N \times N}$ is the similarity matrix between all pairs of points
$\mathbf{D} \in \mathbb{R}^{N \times N}$ is the diagonal degree matrix, with $\mathbf{D}_{ii} = d_i$

- Side note: $(\mathbf{D} - \mathbf{W})$ is referred to as the graph Laplacian

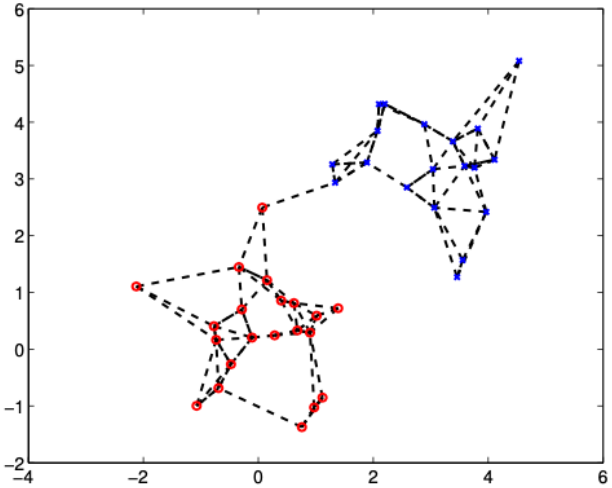
- The solution is then obtained by the eigenvector with the second smallest eigenvalue
  - Ideally, a positive value in this vector indicates that the corresponding point belongs to one partition, and a negative value to the other
  - Because of the relaxation, this is not so ideal; one then needs to threshold the values (e.g., by taking the median value as threshold for balanced data)

Normalized cut: Example

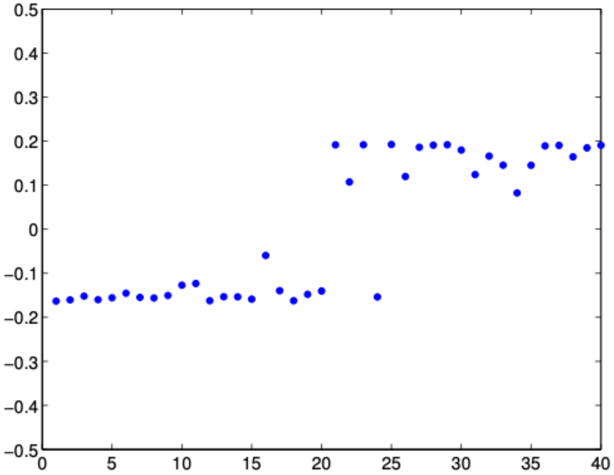
Input data



Graph and partition



2nd eigenvector



Figures from David Sontag's slides

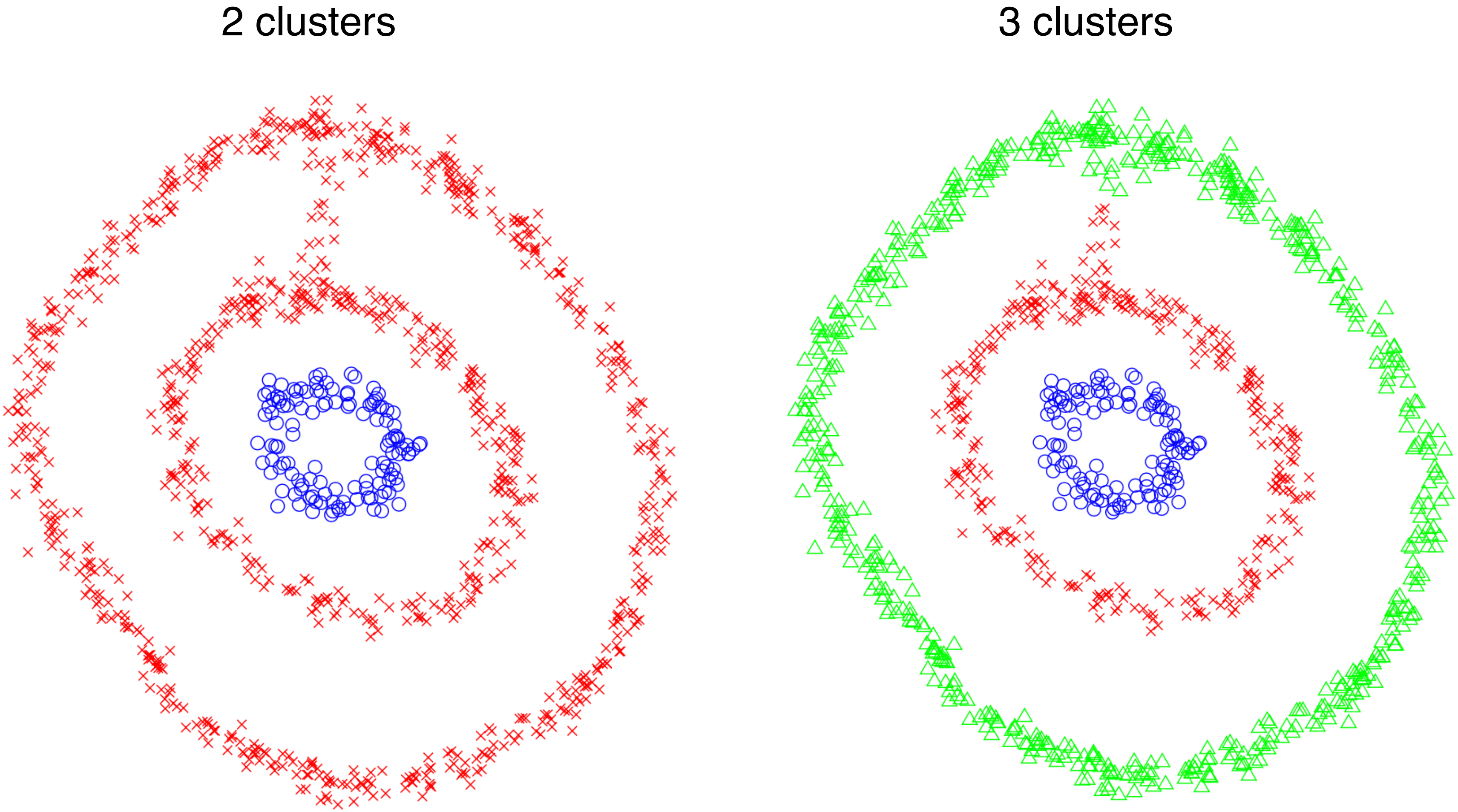
K-way partition

- To obtain more than 2 clusters, one can either

  1. Recursively apply the 2-way partitioning algorithm
     - Not efficient and unstable

  2. Use multiple (i.e., K) eigenvectors
     - Each point is represented as a K-dimensional vector
     - Apply K-means clustering to the resulting N vectors
     - Interpretation: Dimensionality reduction followed by K-means

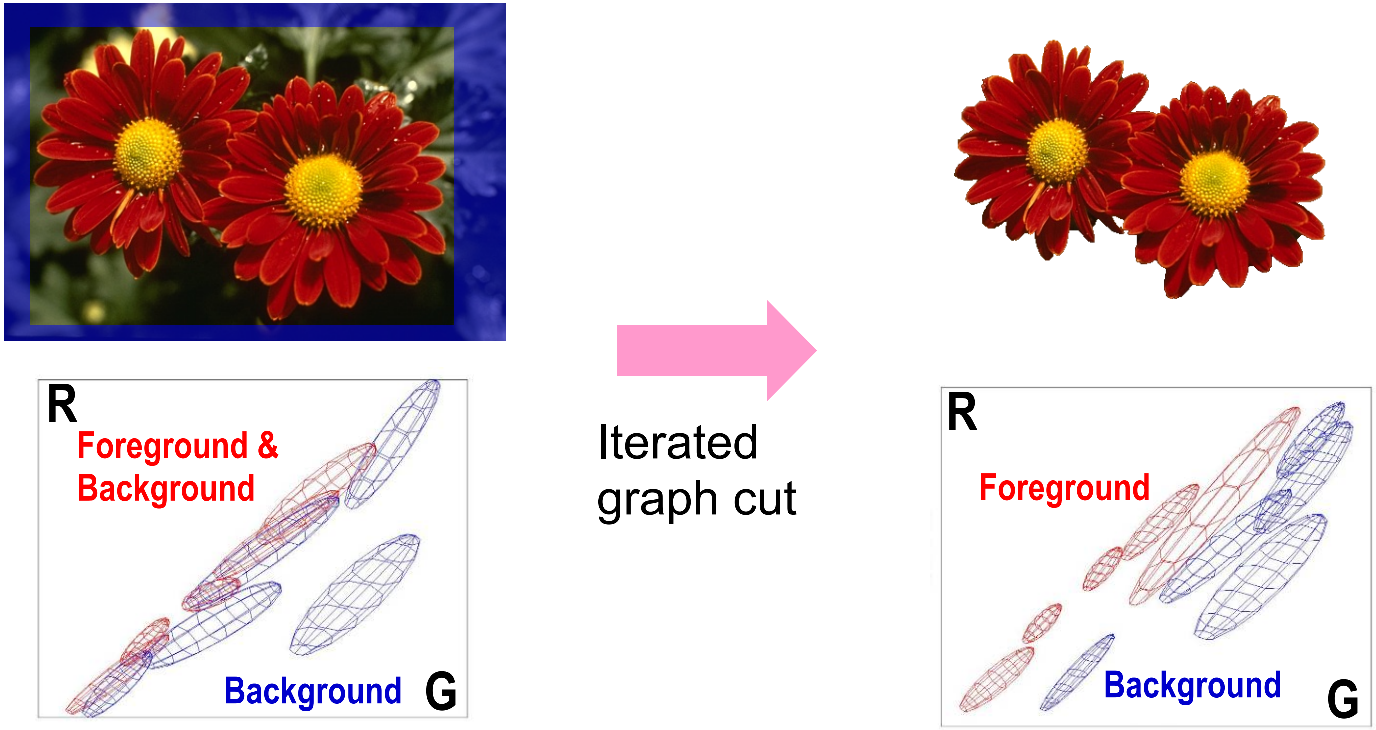
K-way partition: Example



2 clusters

3 clusters

Interactive Foreground Extraction



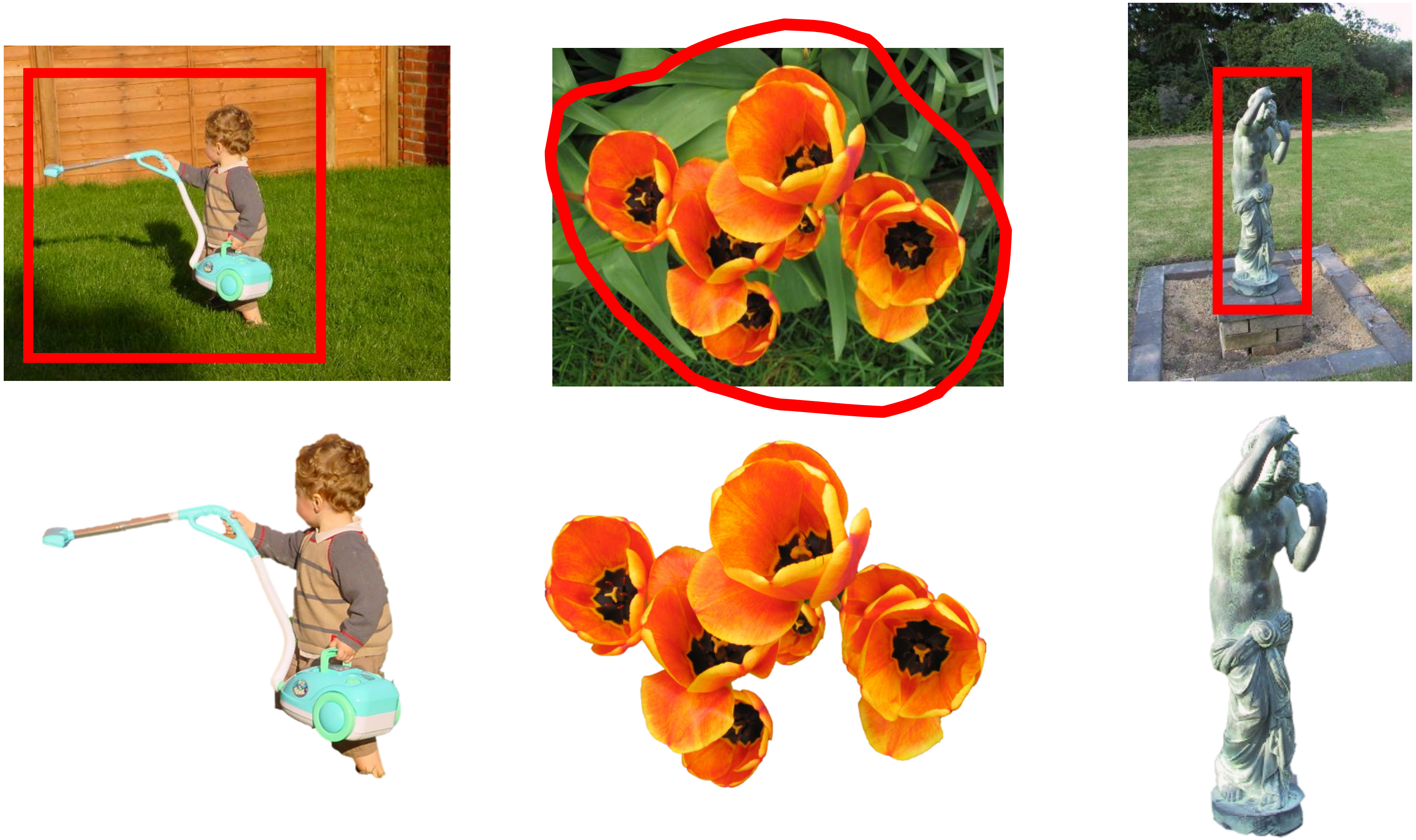
Iterated graph cut

- K-means to learn color distributions
- Graph cuts to infer the segmentation

Optional

GrabCut Rother & al. SIGGRAPH 04

Relatively Easy Examples



Optional

GrabCut Rother & al. SIGGRAPH 04

More Difficult Examples

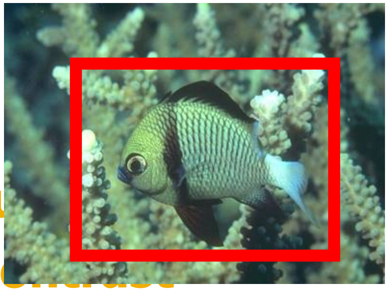
Fine structure

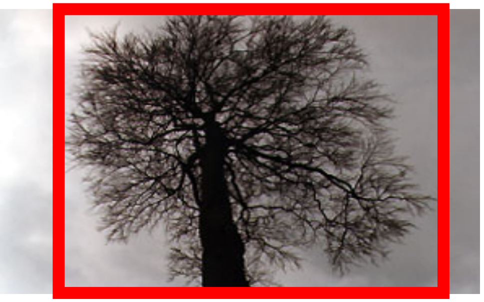
No telepathy

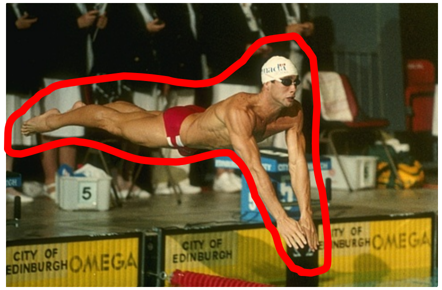
Initial Rectangle

Camou

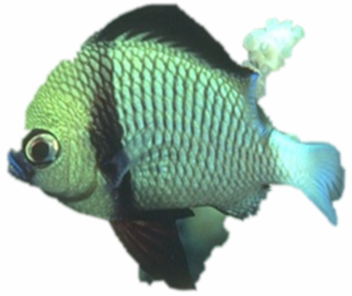
Low Contrast

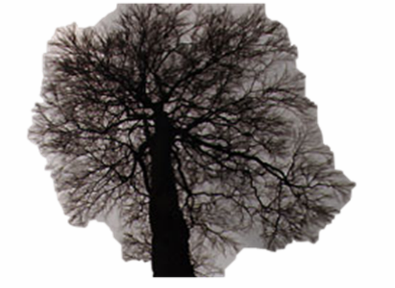


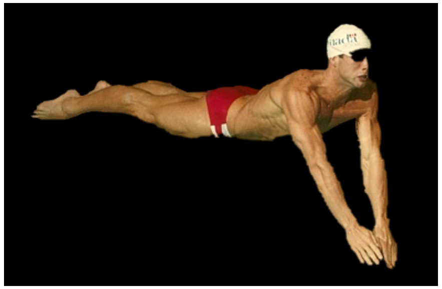




Initial Result







Optional

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Density-based clustering

- https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

Optional