Un-Supervised Learning

Clustering Techniques

Topics to be covered…

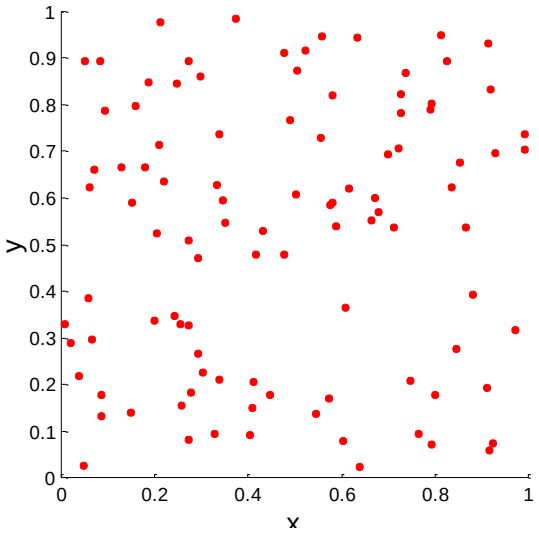
- Introduction to clustering
- Similarity and dissimilarity measures
- Clustering techniques
  - Hierarchical algorithms
  - Partitioning algorithms (Kmedoids, Clara Calarans)
  - Density-based algorithm (DBScan, Optics , Denclue).
    - **Mean Shift**
  - **Model Based algorithms (GMM)**
  - Spectral Clustering

Cluster Validity

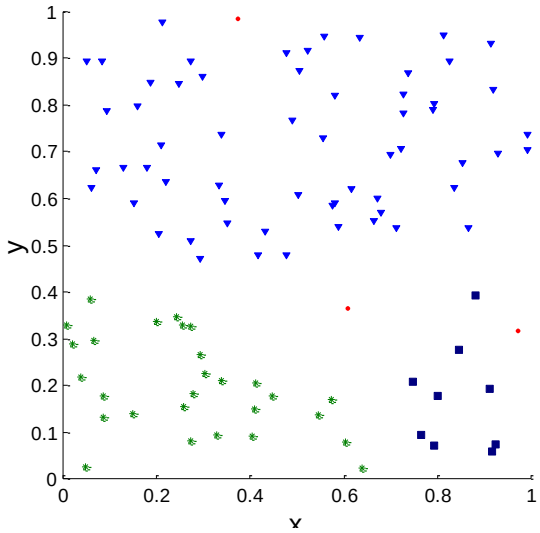
- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?
- But "clusters are in the eye of the beholder"!
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Clusters found in Random Data

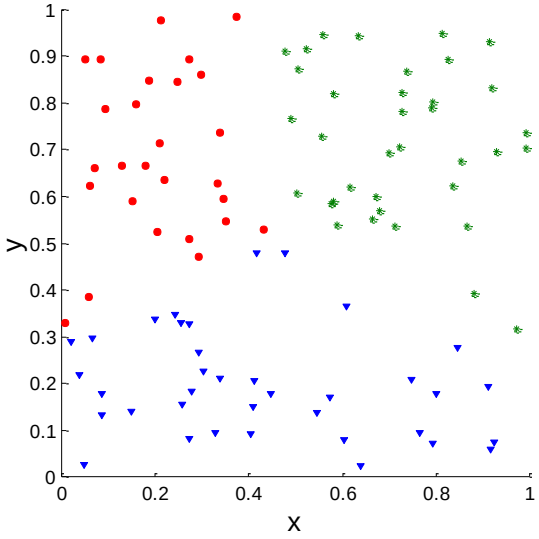
Random Points



DBSCAN



K-means



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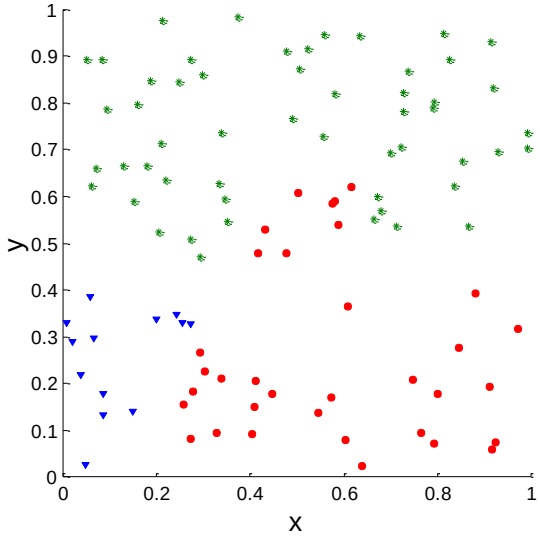


Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
   - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

Measures of Cluster Validity

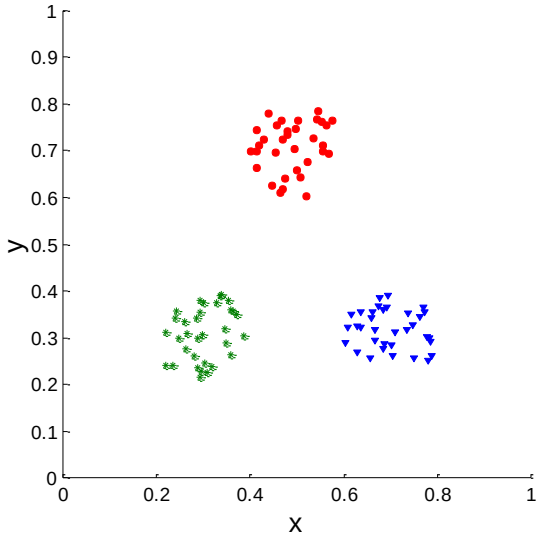
- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Entropy
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    - Sum of Squared Error (SSE)
  - Relative Index: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy
- Sometimes these are referred to as criteria instead of indices
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

Measuring Cluster Validity Via Correlation

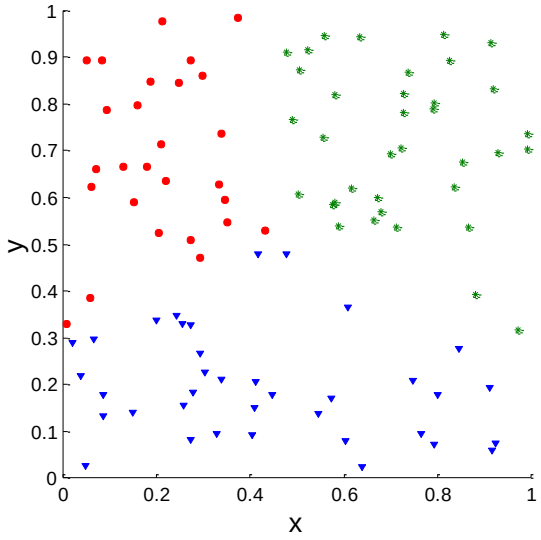
- Two matrices
  - Proximity Matrix
  - “Incidence” Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between the two matrices
  - Since the matrices are symmetric, only the correlation between n(n-1) / 2 entries needs to be calculated.
- High correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity-based clusters.

Measuring Cluster Validity Via Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



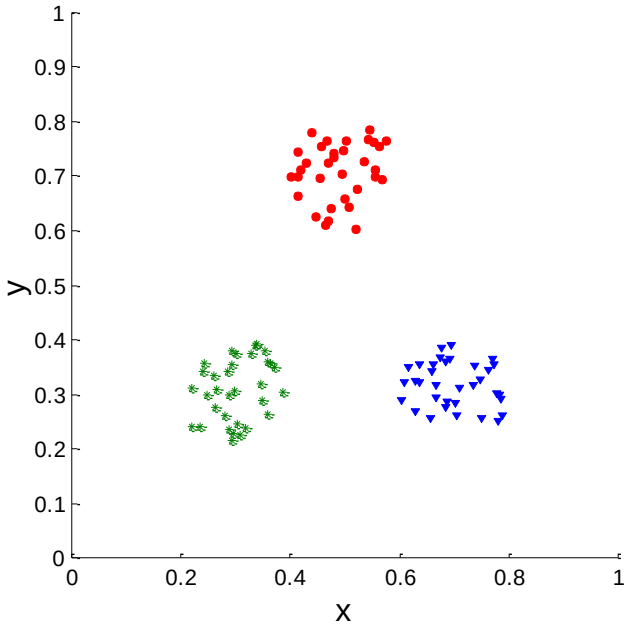
Corr = -0.9235

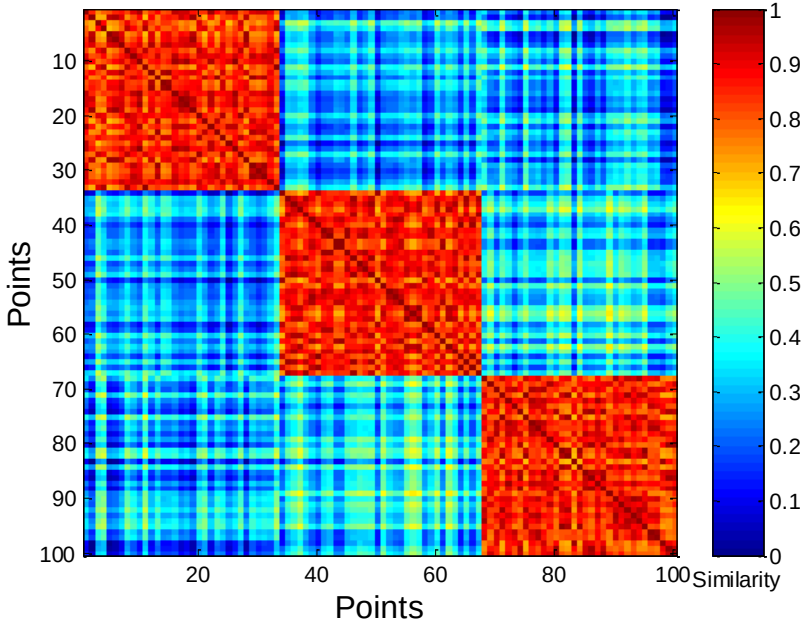


Corr = -0.5810

Using Similarity Matrix for Cluster Validation

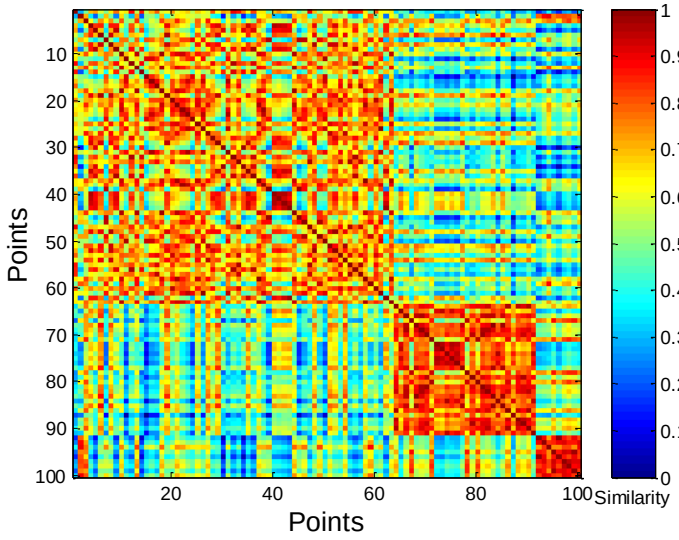
- Order the similarity matrix with respect to cluster labels and inspect visually.

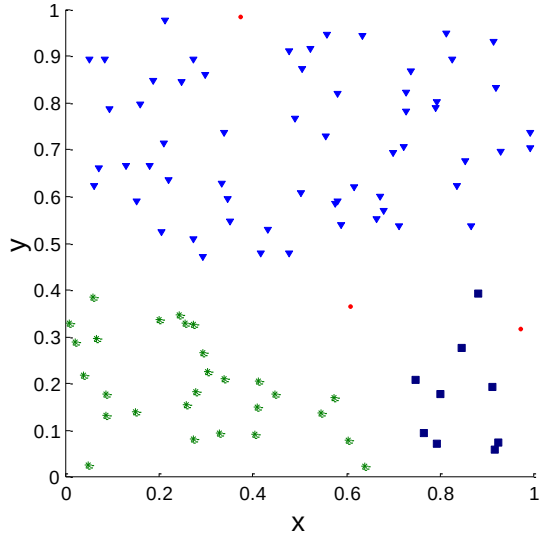




Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

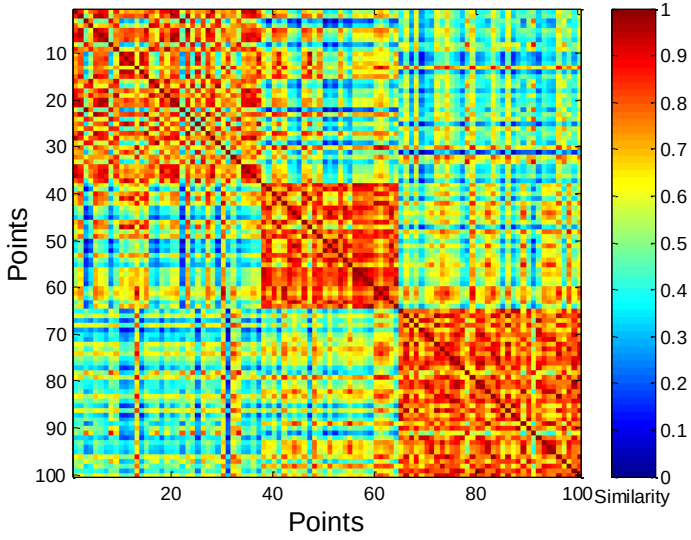


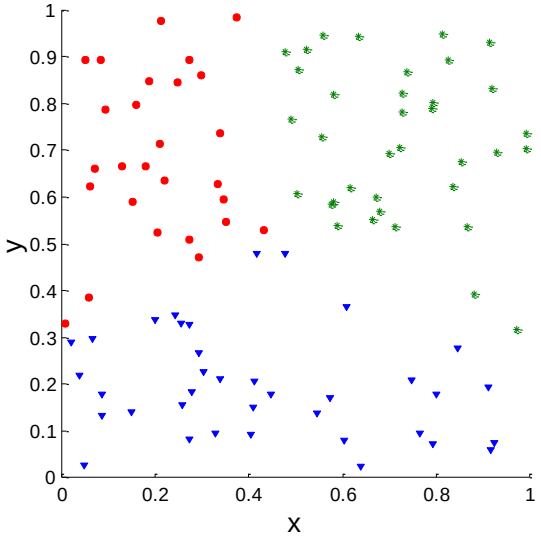


DBSCAN

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





K-means

Using Similarity Matrix for Cluster Validation

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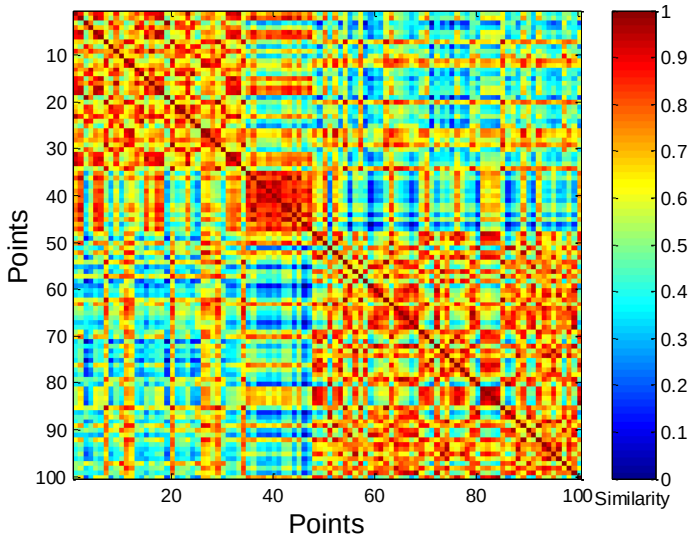
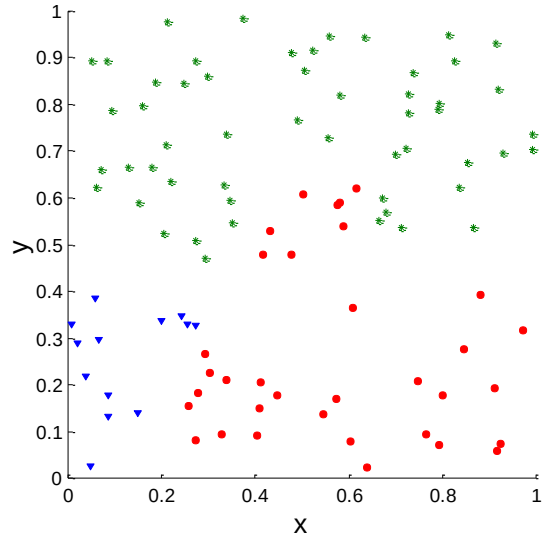
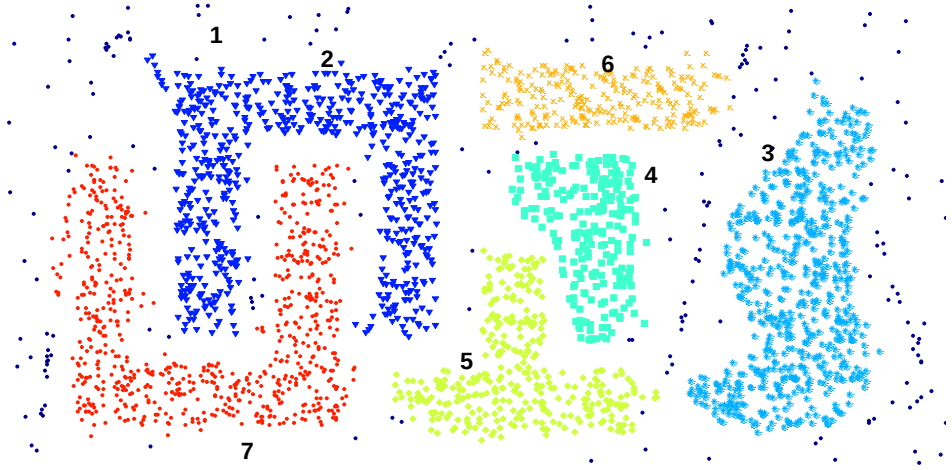
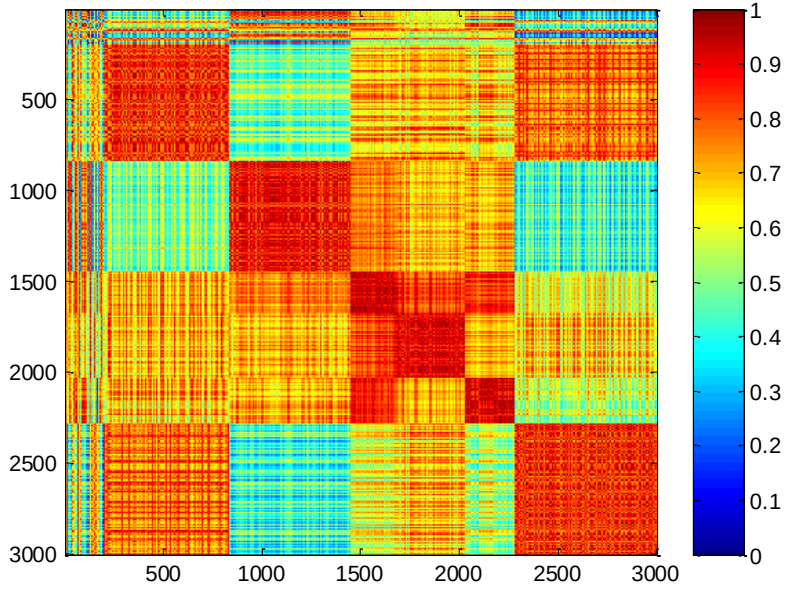




Complete Link

Using Similarity Matrix for Cluster Validation

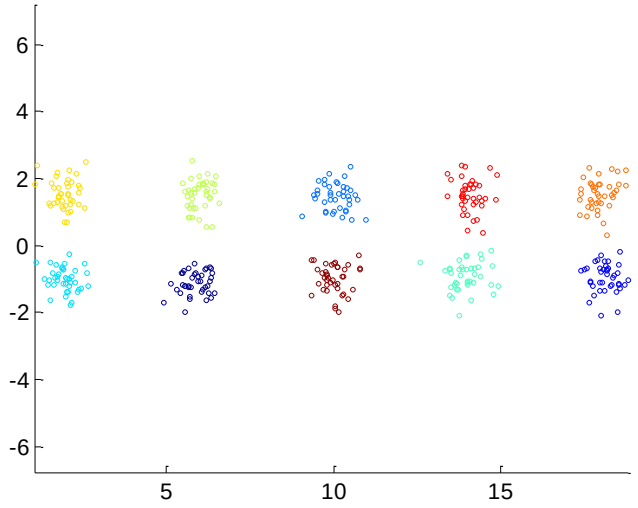


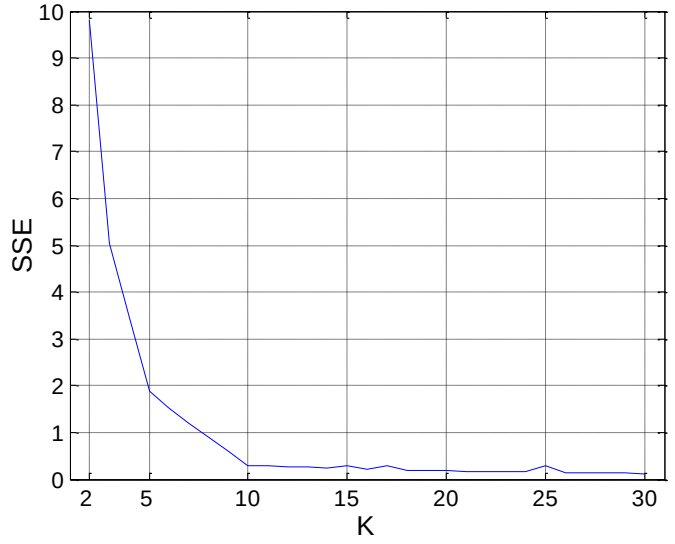


DBSCAN

Internal Measures: SSE

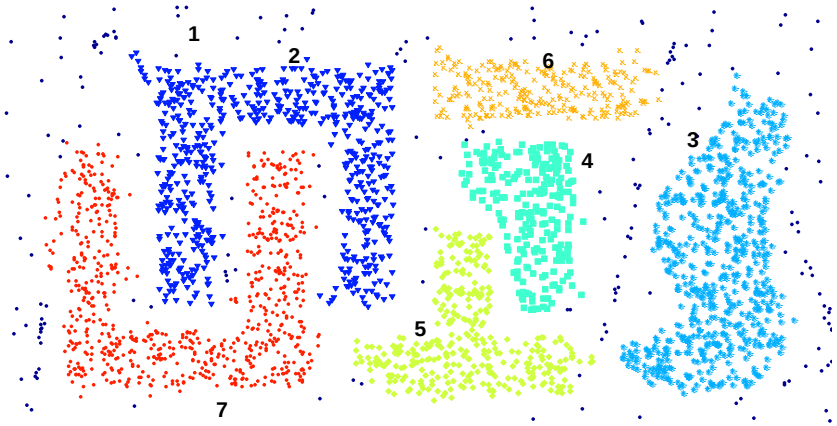
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters

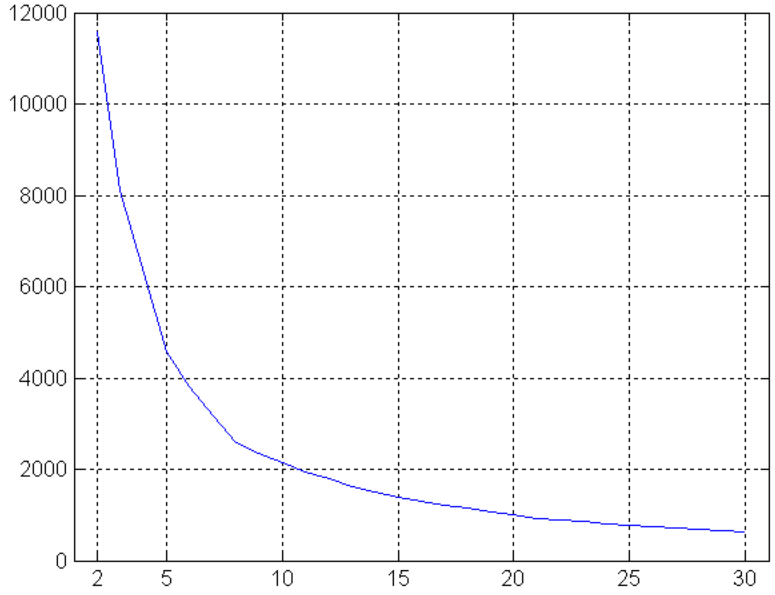




Internal Measures: SSE

- SSE curve for a more complicated data set





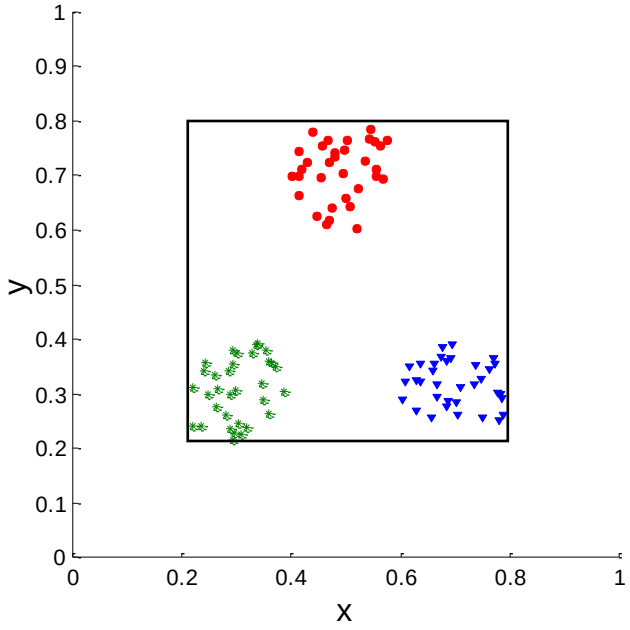
SSE of clusters found using K-means

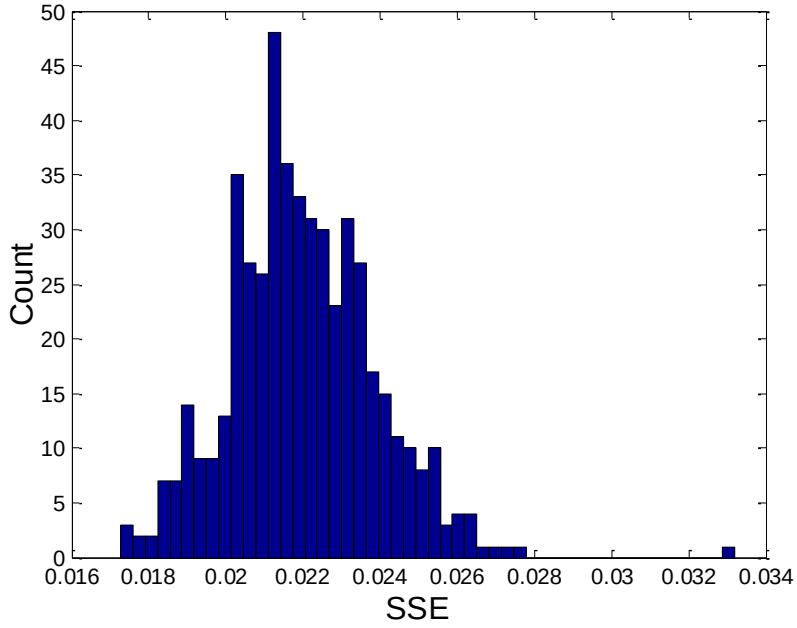
Framework for Cluster Validity

- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more “atypical” a clustering result is, the more likely it represents valid structure in the data
  - Can compare the values of an index that result from random data or clusterings to those of a clustering result.
    - If the value of the index is unlikely, then the cluster results are valid
  - These approaches are more complicated and harder to understand.
- For comparing the results of two different sets of cluster analyses, a framework is less necessary.
  - However, there is the question of whether the difference between two index values is significant

Statistical Framework for SSE

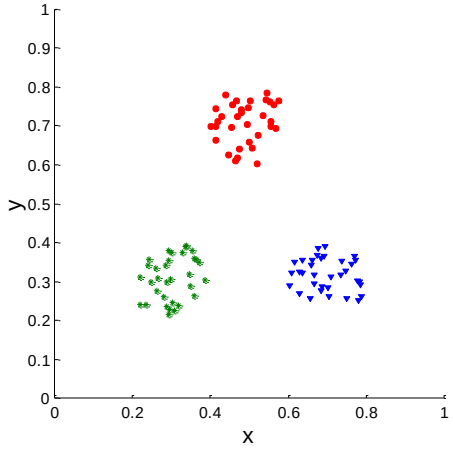
- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values

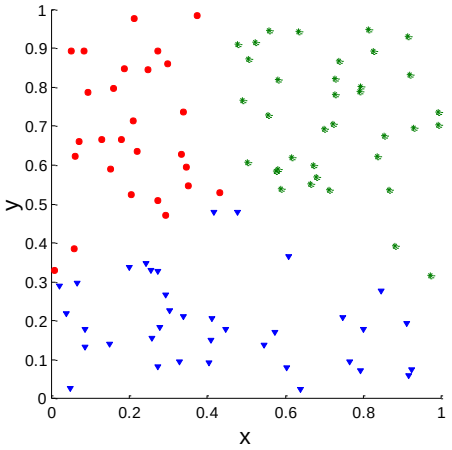


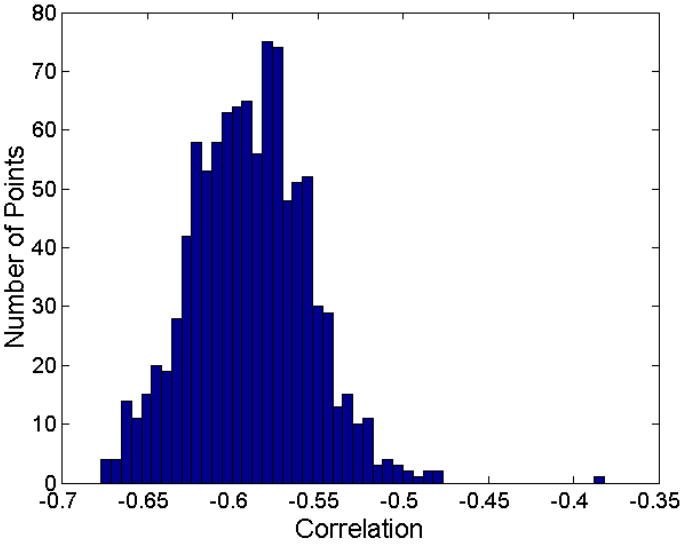


Statistical Framework for Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.







Corr = -0.9235

Corr = -0.5810

Internal Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: SSE
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$\boldsymbol{WSS} = \sum_{\boldsymbol{i}} \sum_{\boldsymbol{x} \in \boldsymbol{C}_i} (\boldsymbol{x} - \boldsymbol{m}_{\boldsymbol{i}})^2$$

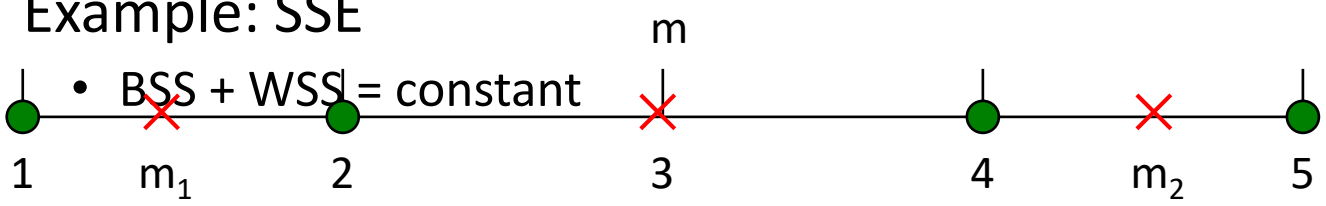
  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_i |C_i|(m - m_i)^2$$

    - Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

$$WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

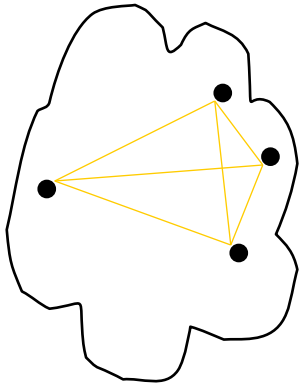
$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

$$BSS = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

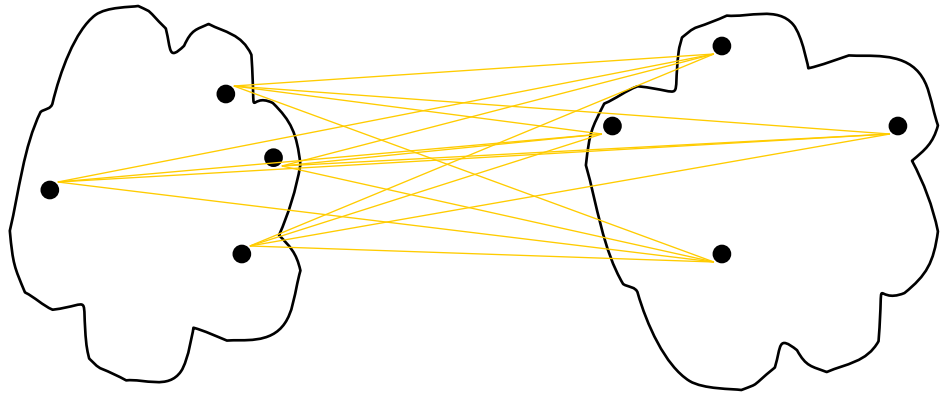
$$Total = 1 + 9 = 10$$

Internal Measures: Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion



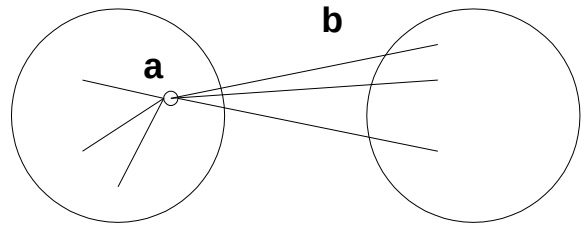
separation

Internal Measures: Silhouette Coefficient

- Silhouette Coefficient combine ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings
- For an individual point, *i*
  - Calculate ***a*** = average distance of *i* to the points in its cluster
  - Calculate ***b*** = min (average distance of *i* to points in another cluster)
  - The silhouette coefficient for a point is then given by

    $s = 1 - a/b$ if $a < b$, (or $s = b/a - 1$ if $a \geq b$, not the usual case)

  - Typically between 0 and 1.
  - The closer to 1 the better.



- Can calculate the Average Silhouette width for a cluster or a clustering

External Measures of Cluster Validity: Entropy and Purity

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Final Comment on Cluster Validity

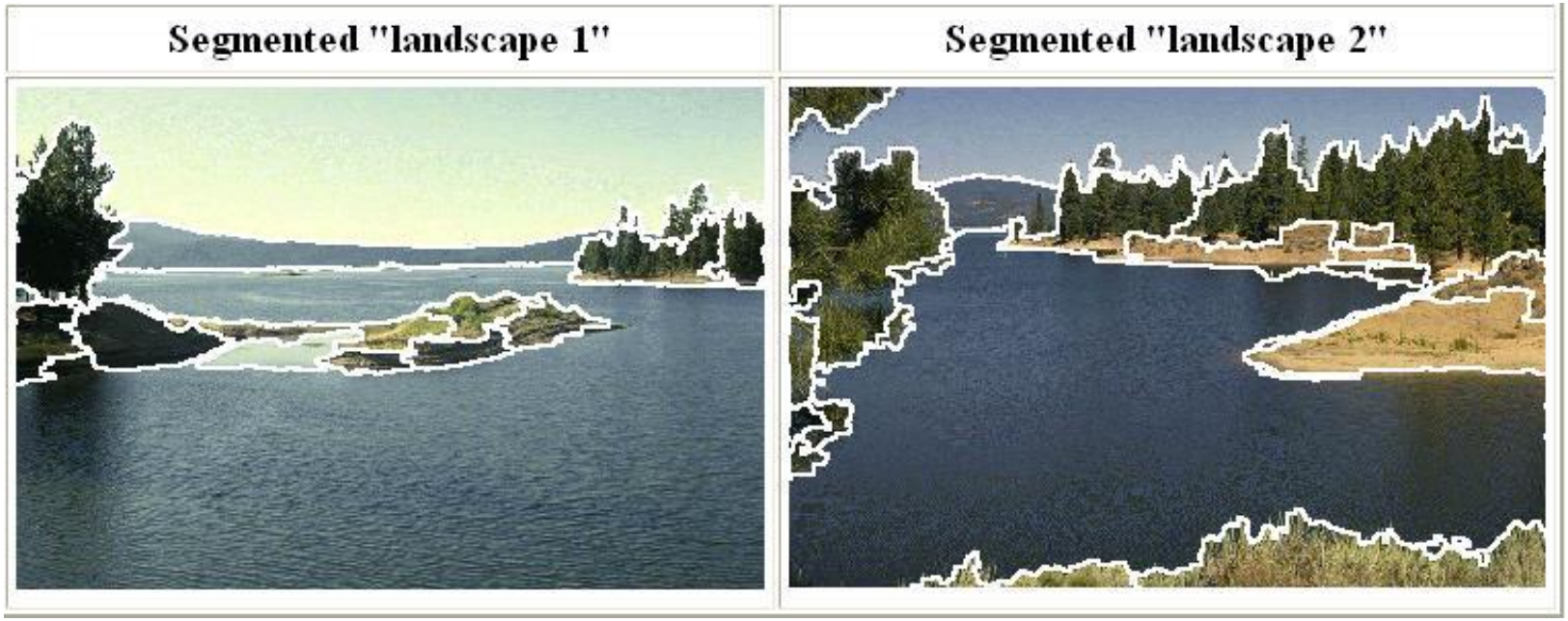
"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes

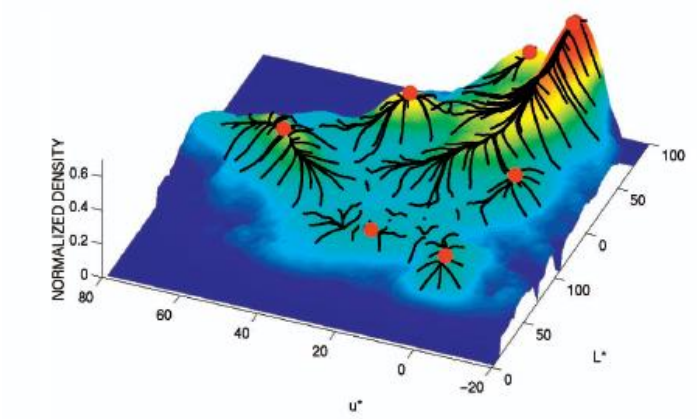
Mean shift segmentation

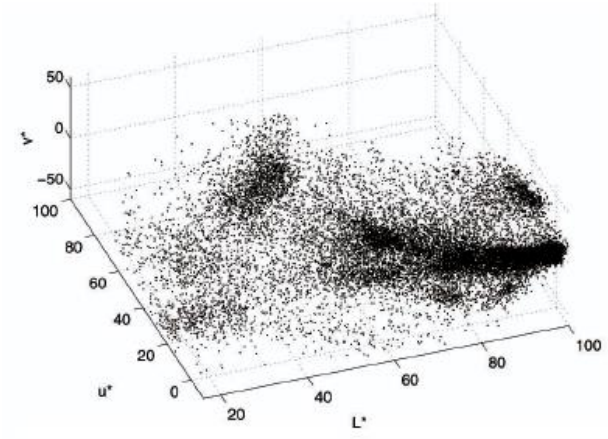
- Versatile technique for clustering-based segmentation

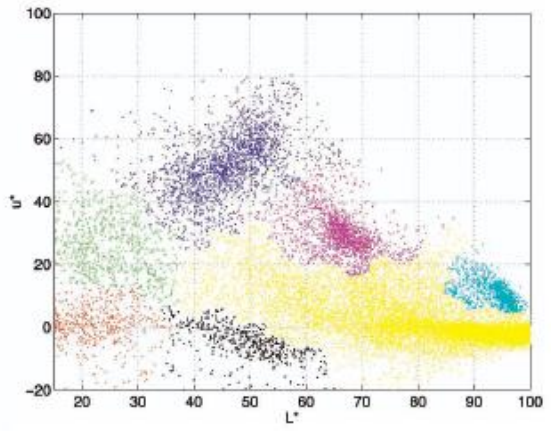


Mean shift algorithm

- Try to find *modes* of this non-parametric density







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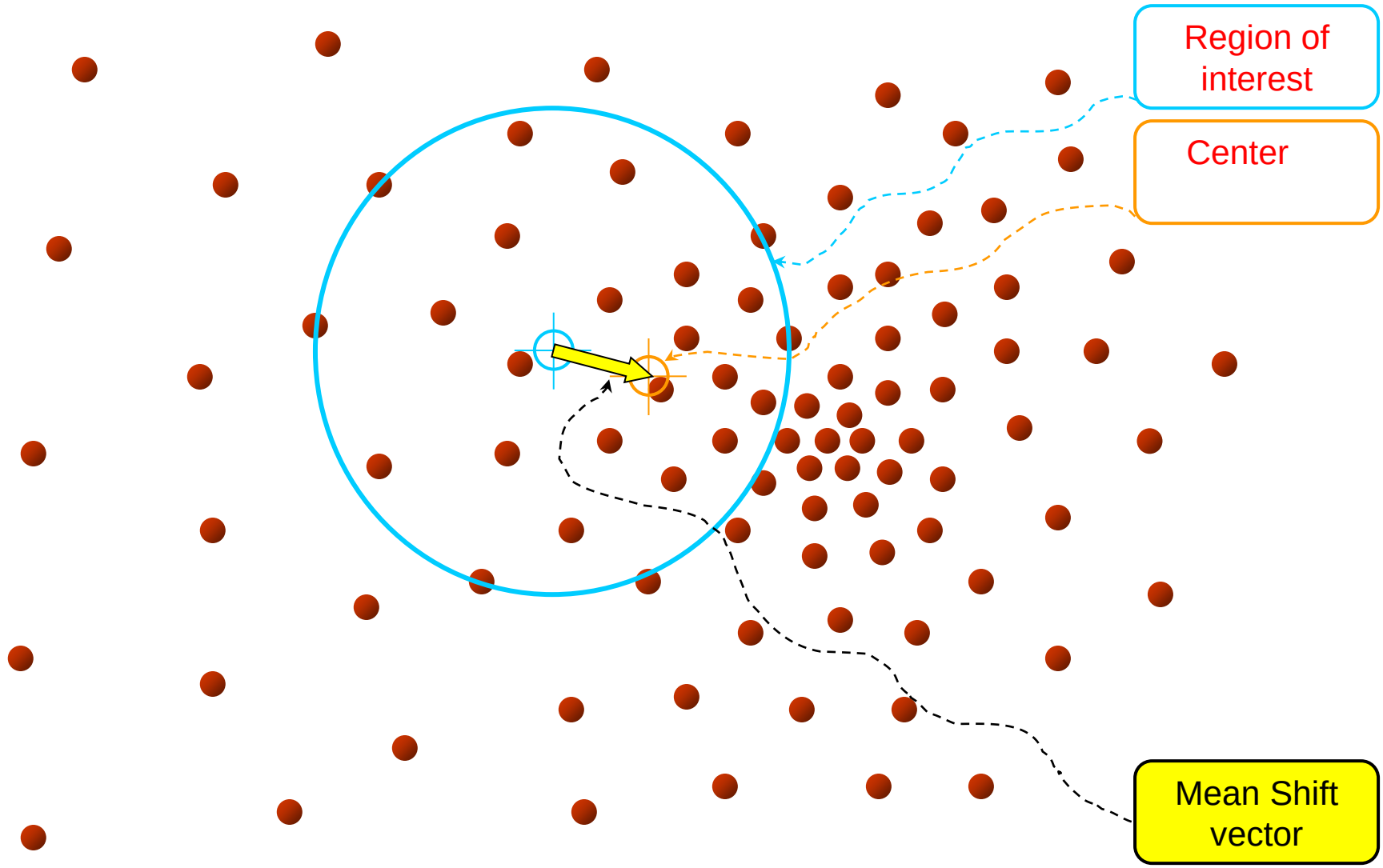

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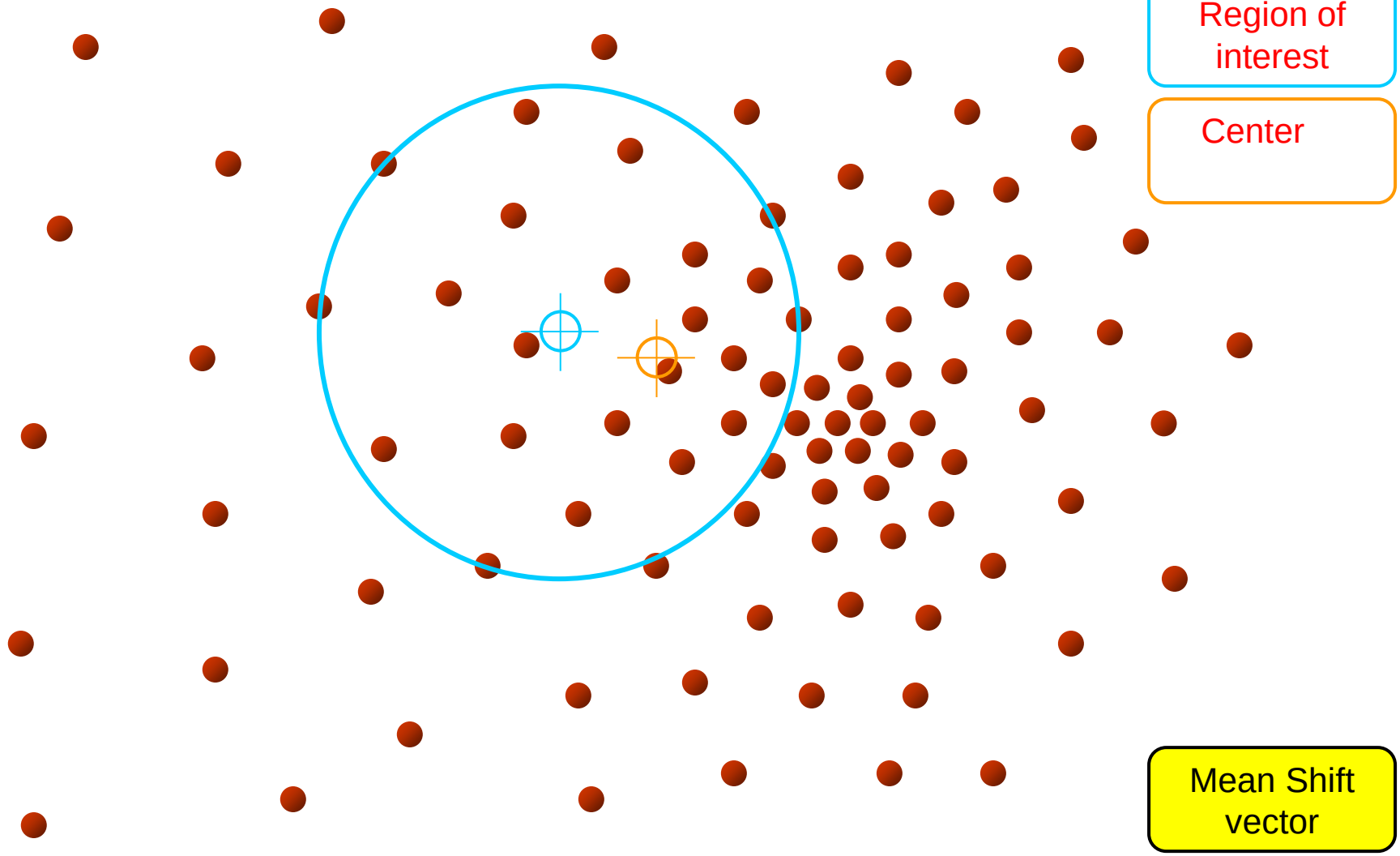

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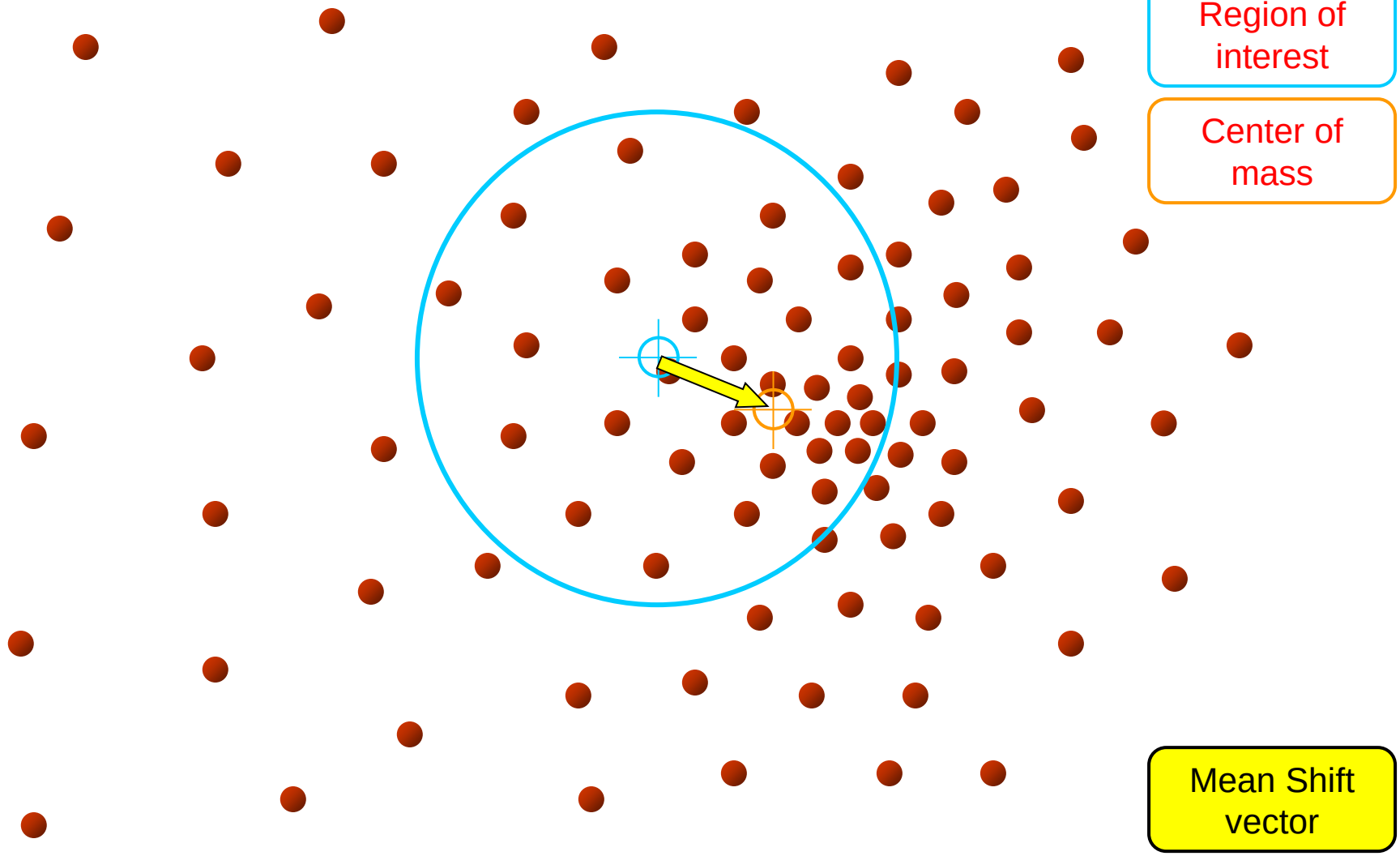

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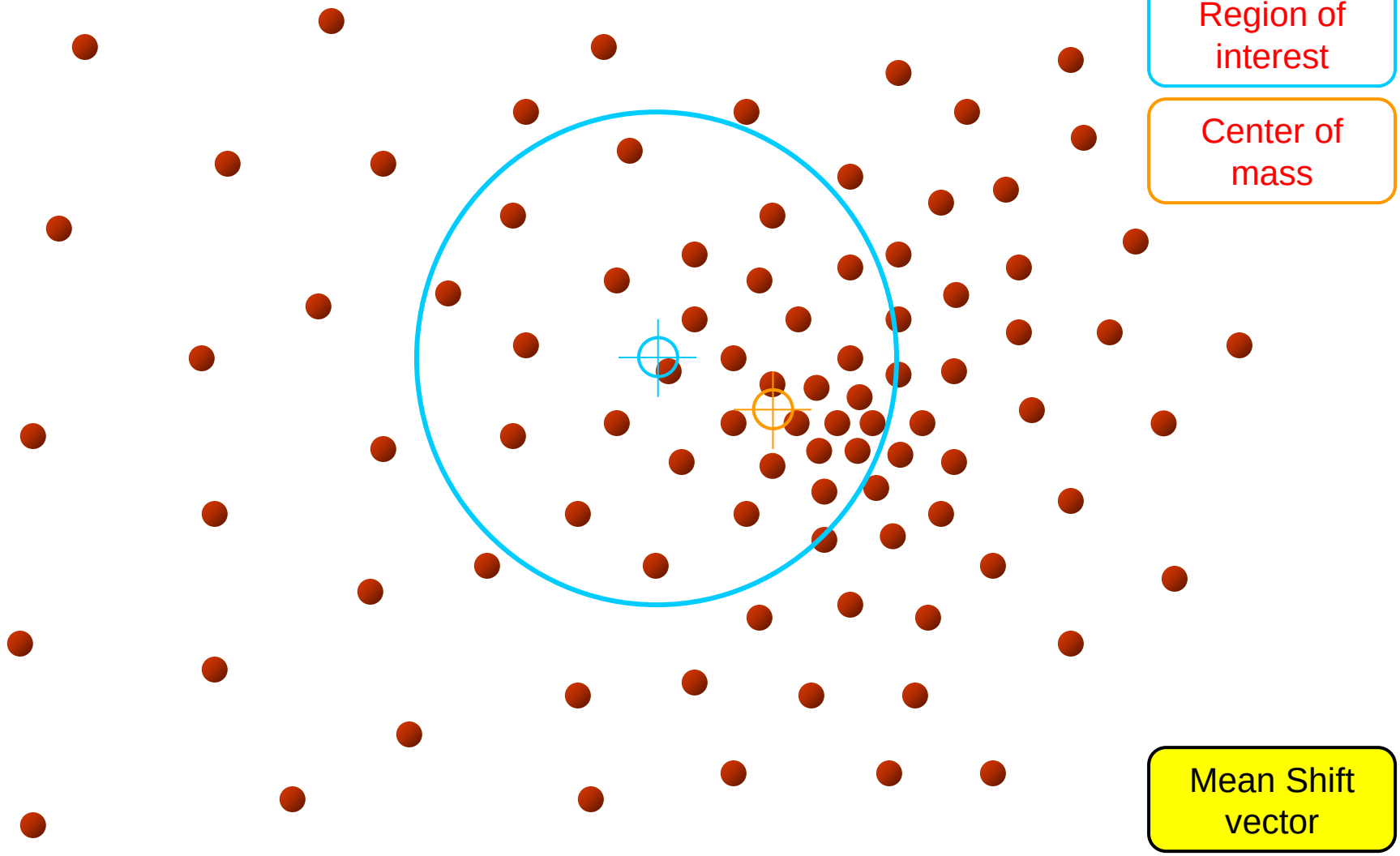
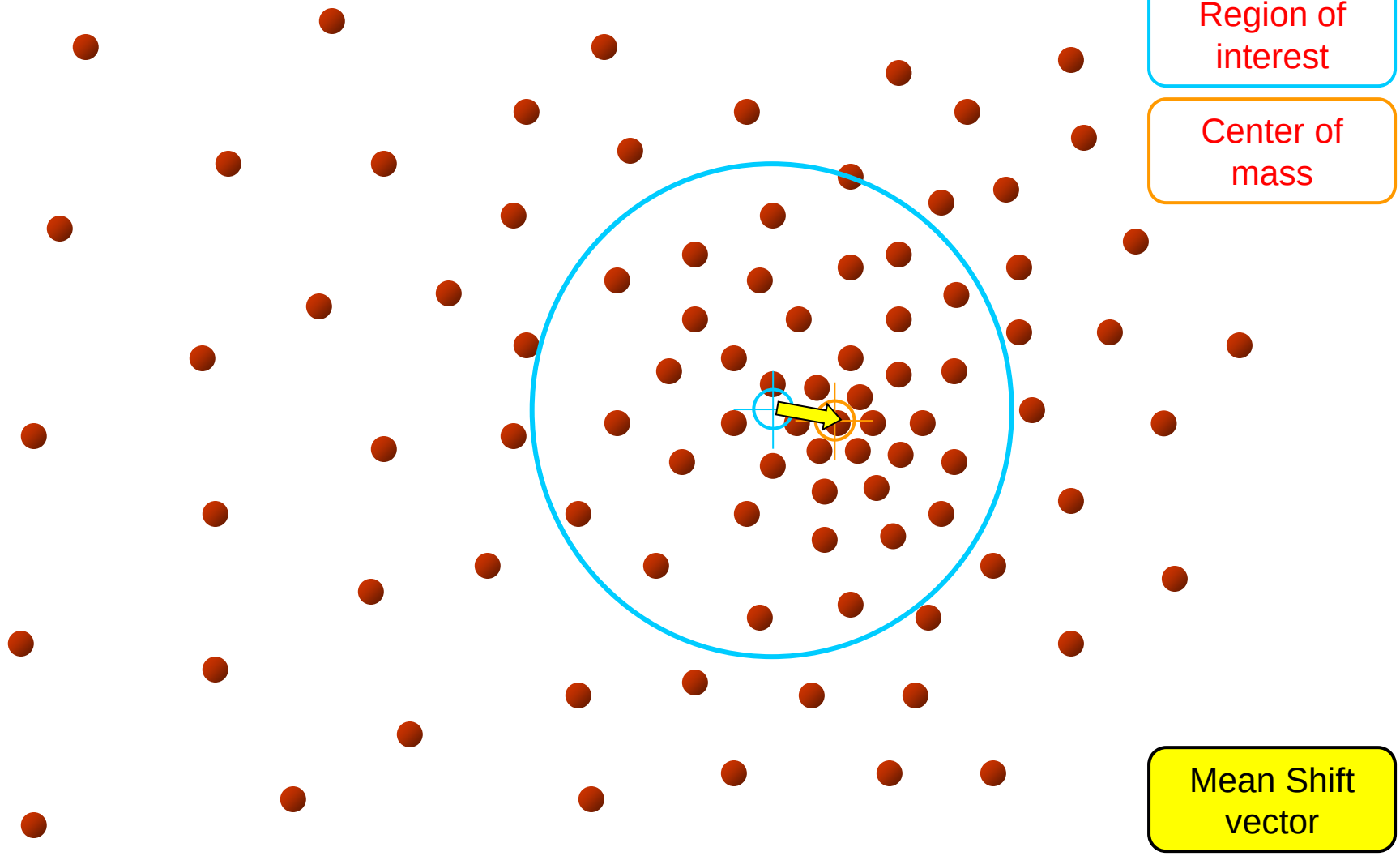
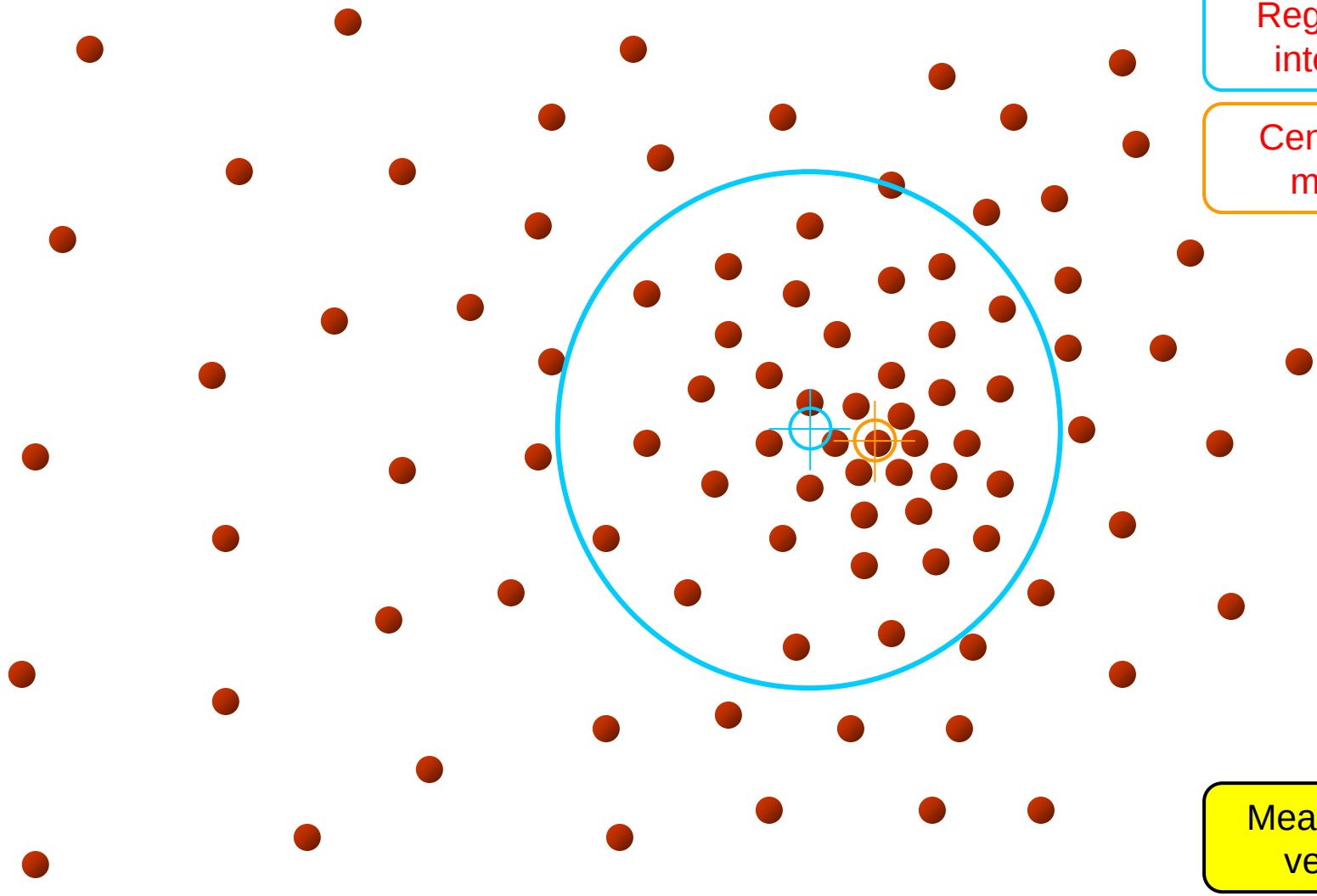


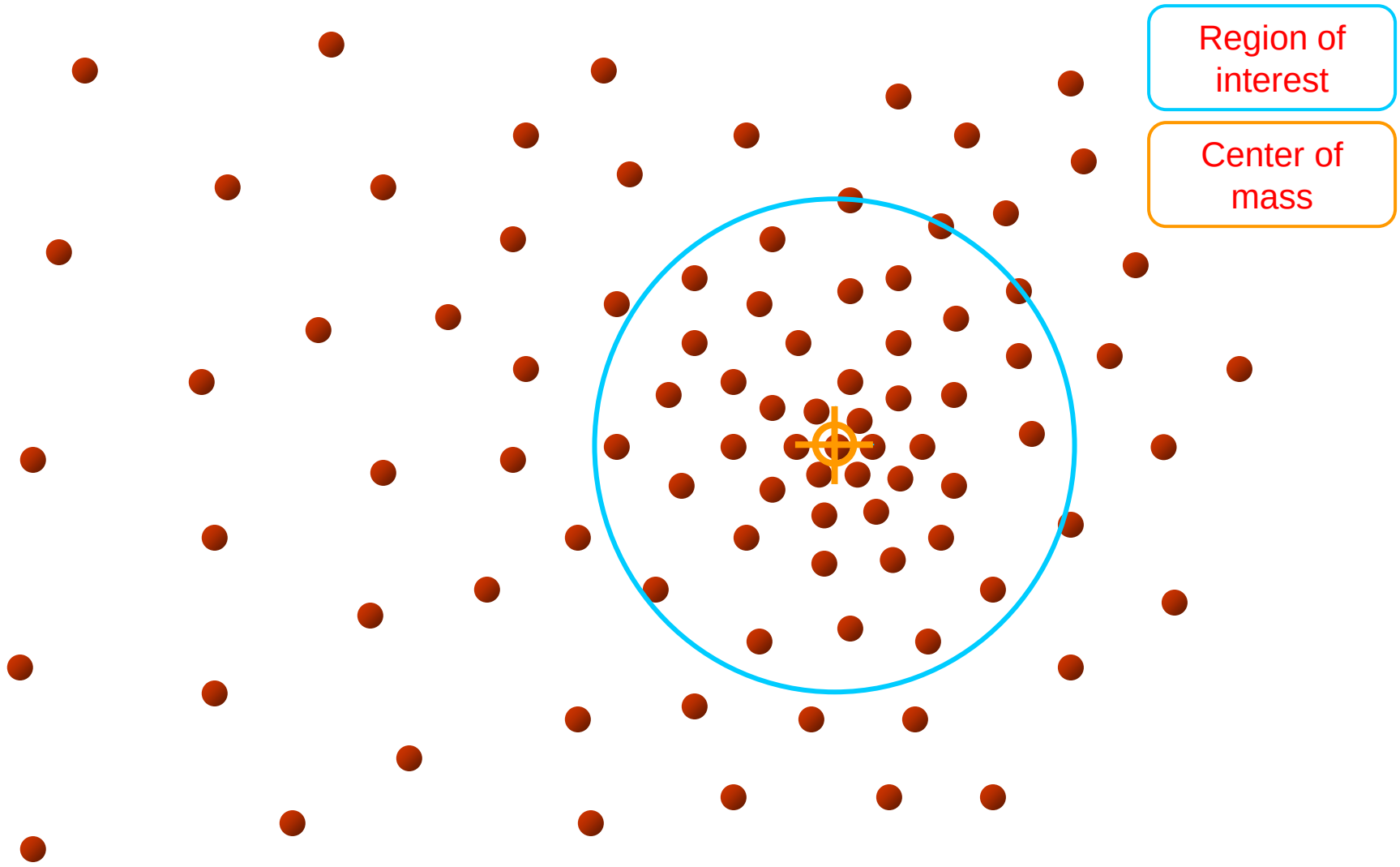
Mean shift



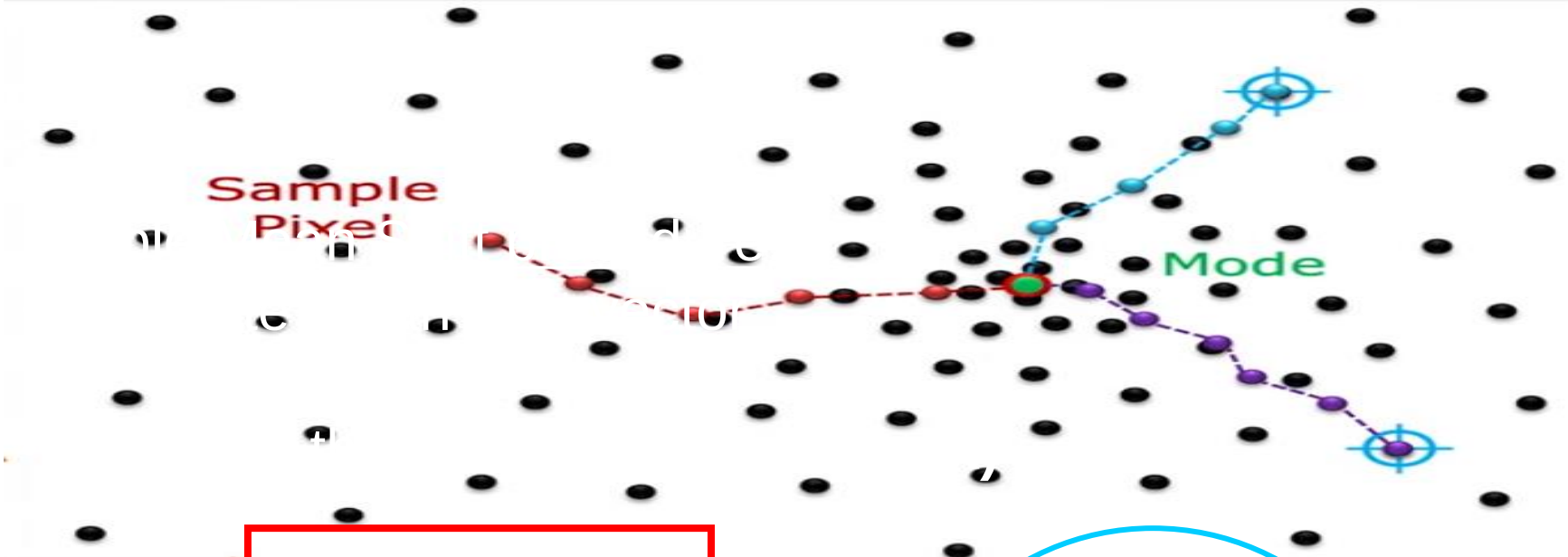
Mean shift



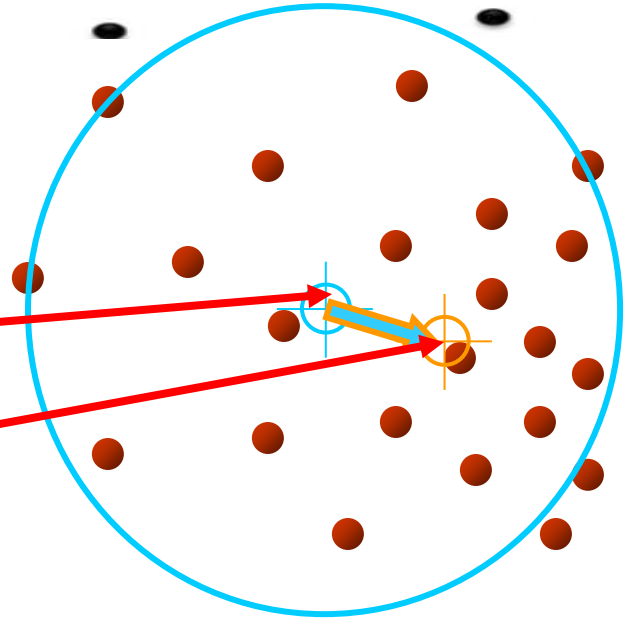
Mean shift



Computing the mean shift



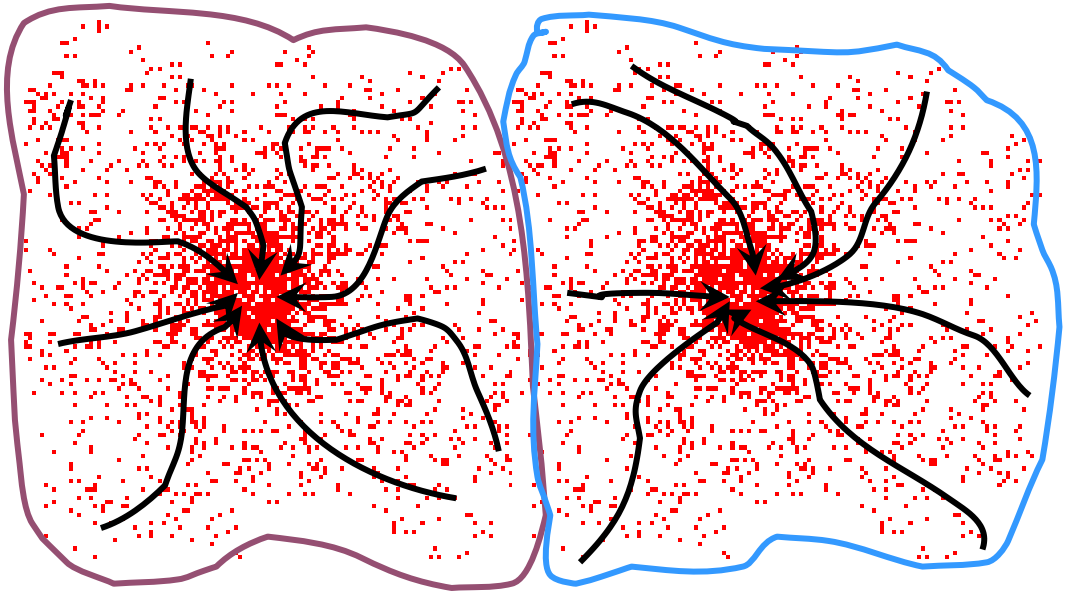
$$\mathbf{m}(\mathbf{x}) = \left[\frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\frac{\|\mathbf{x} - \mathbf{x}_i\|^2}{h} \right)}{\sum_{i=1}^{n} g\left(\frac{\|\mathbf{x} - \mathbf{x}_i\|^2}{h} \right)} - \mathbf{x} \right]$$



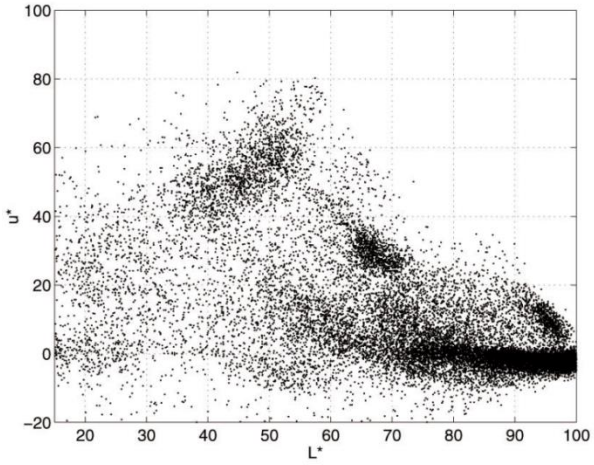
$$\mathbf{g}(\mathbf{x}) = -k'(\mathbf{x})$$

Attraction basin

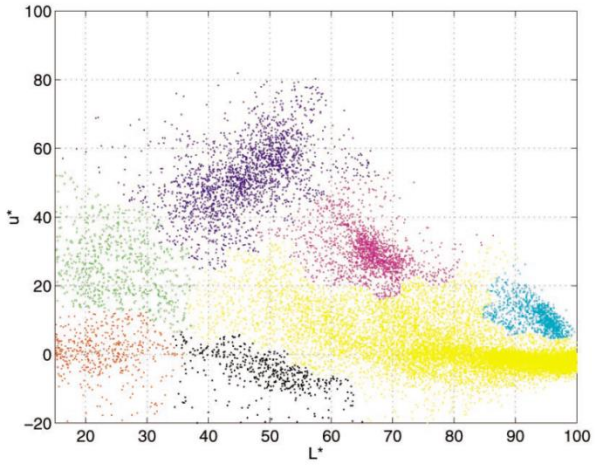
- Attraction basin: the region for which all trajectories lead to the same mode
- Cluster: all data points in the attraction basin of a mode



Attraction basin



(a)



(b)

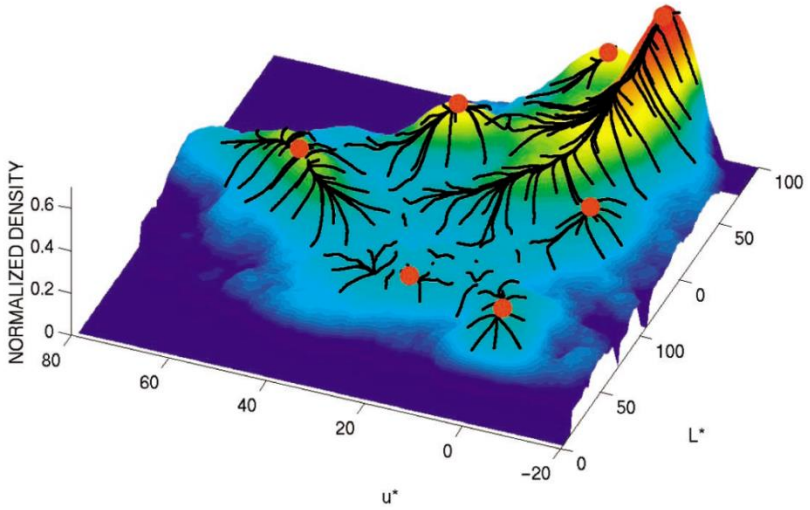
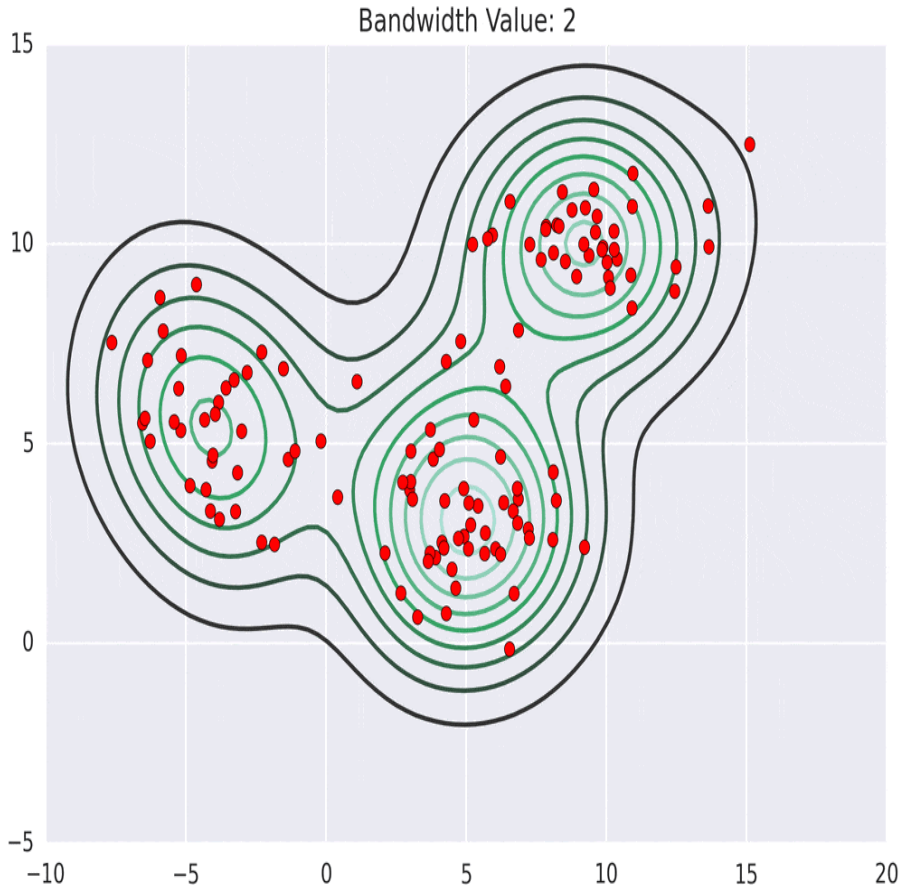
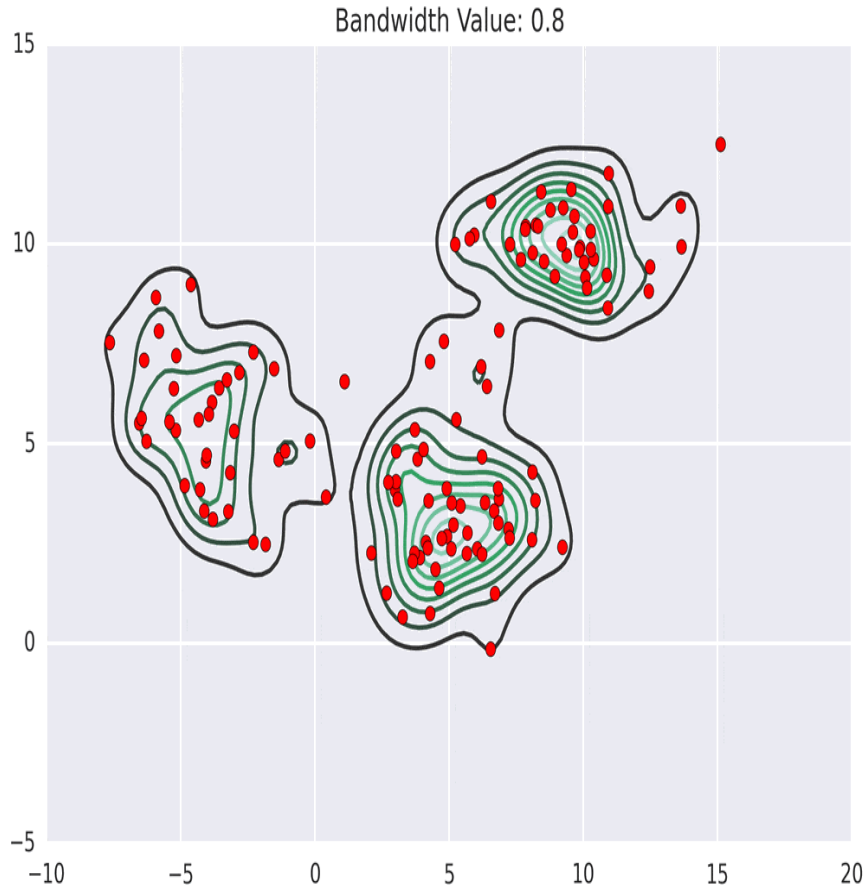


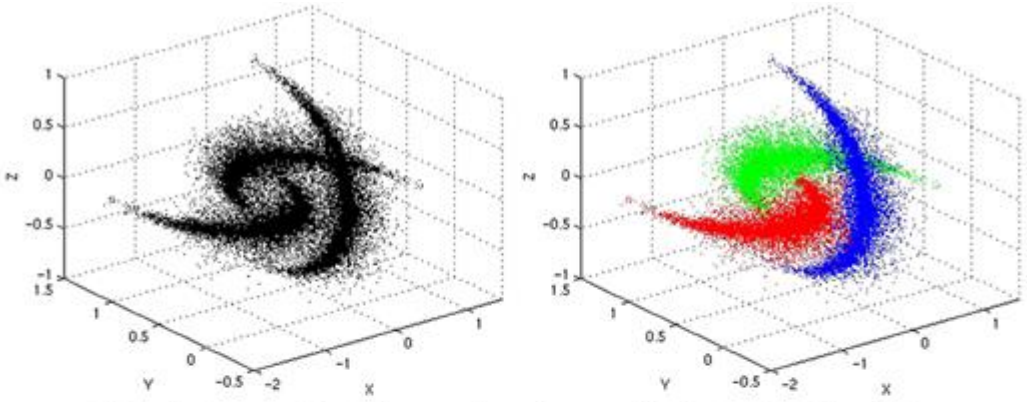
Illustration of Mean Shift



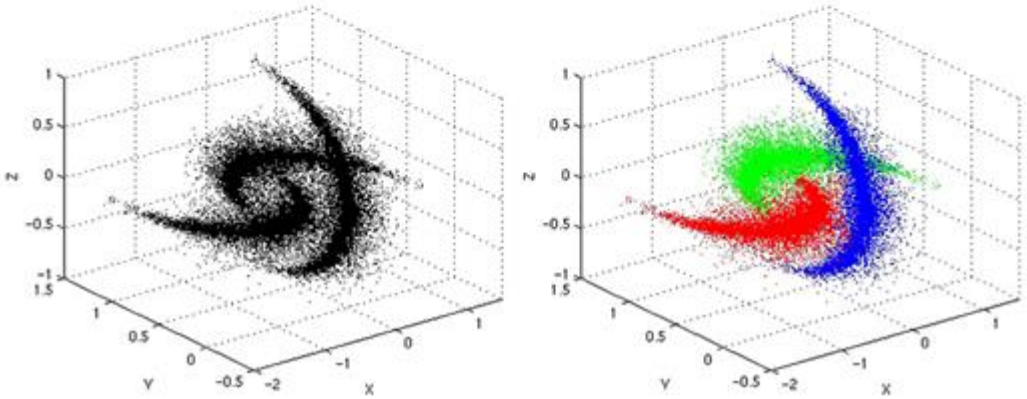


The Effect of the Bandwidth Parameter

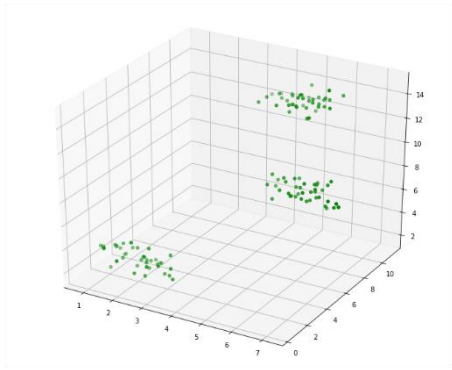
Samples

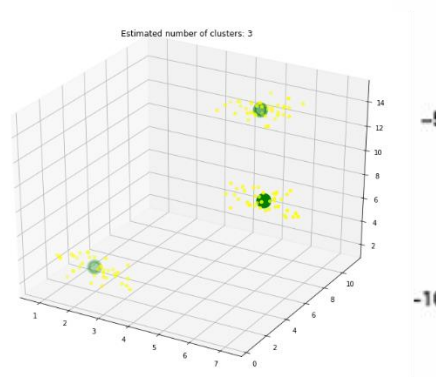


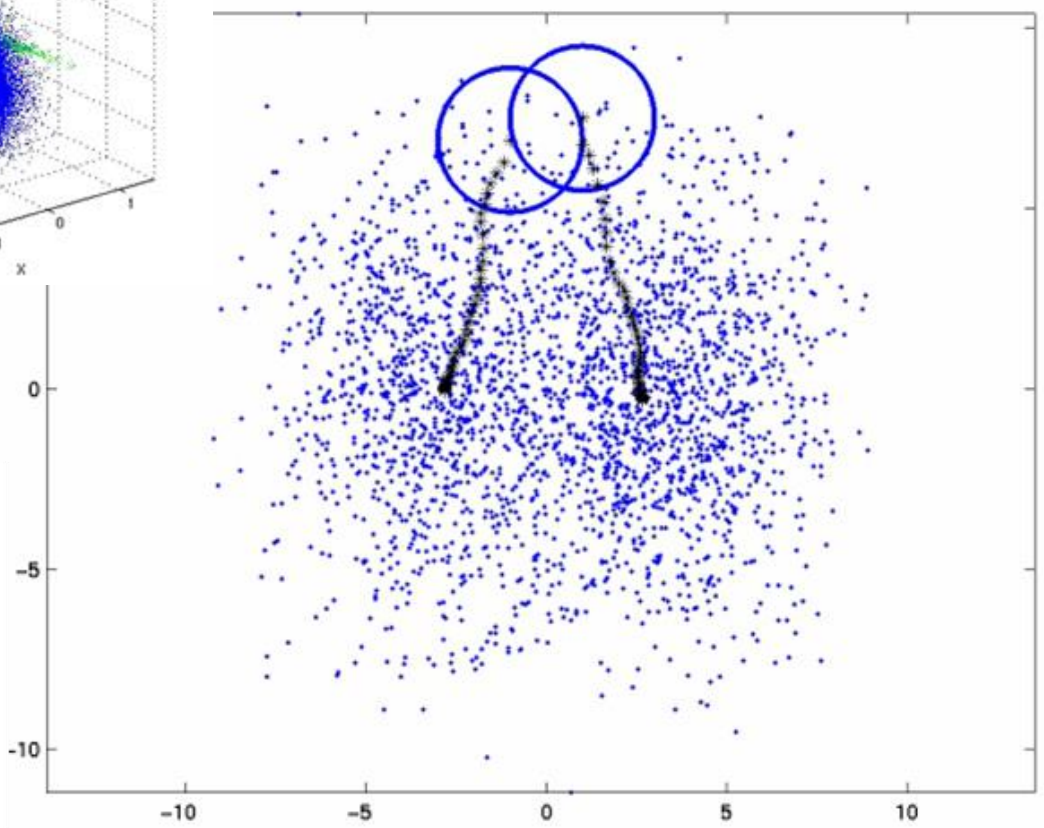
(a) Synthetic example of three non-linearly separable clusters (32640 points).



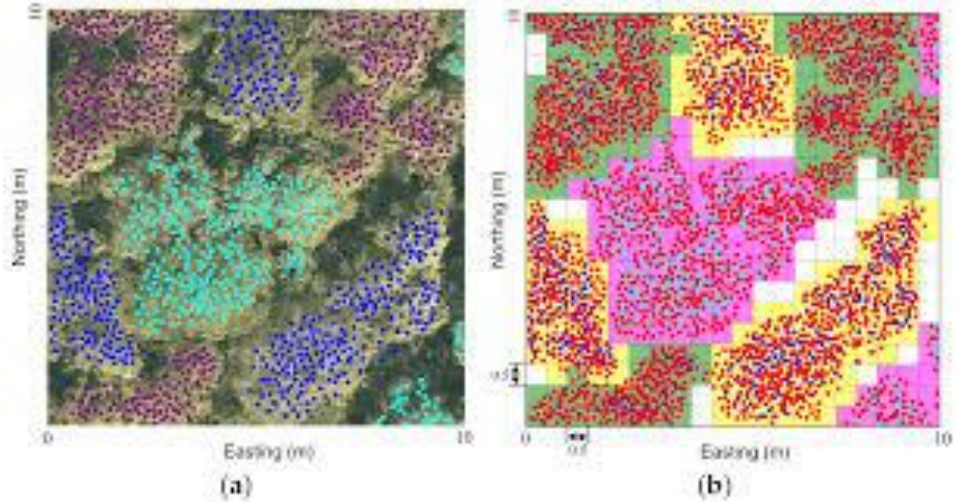
Real Example 0f 14826
in the LUV Color Space



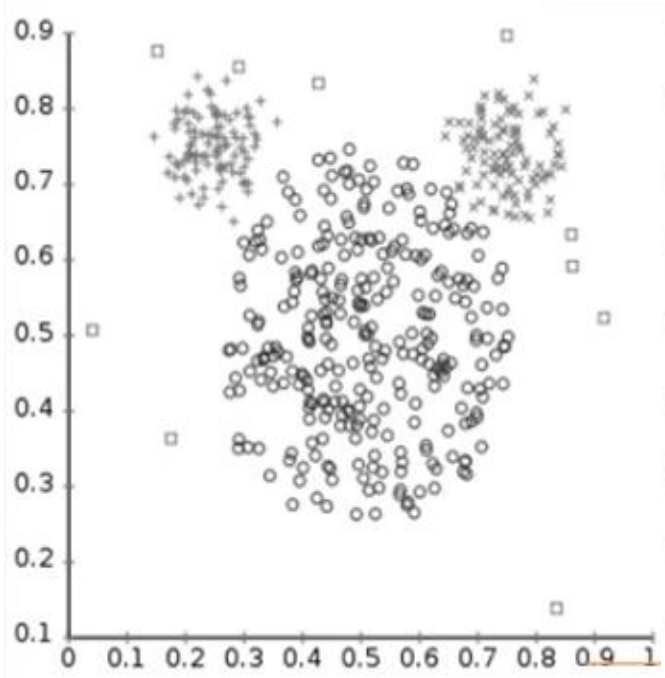




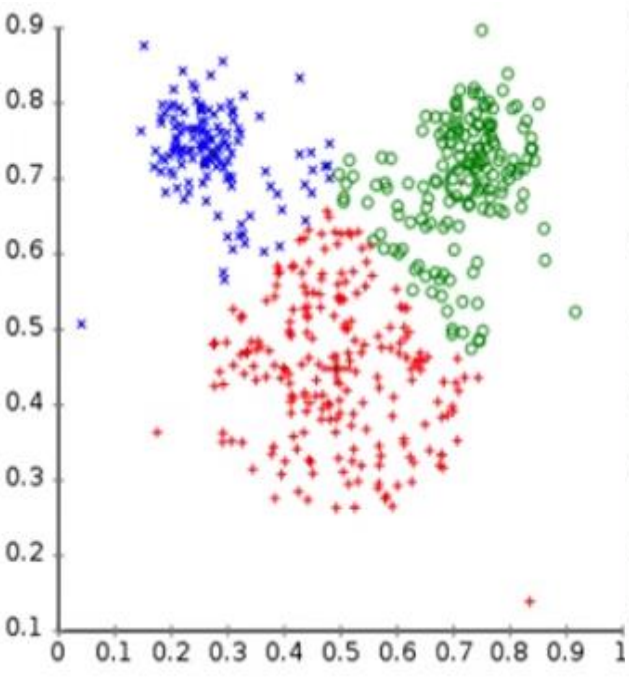
Some Results



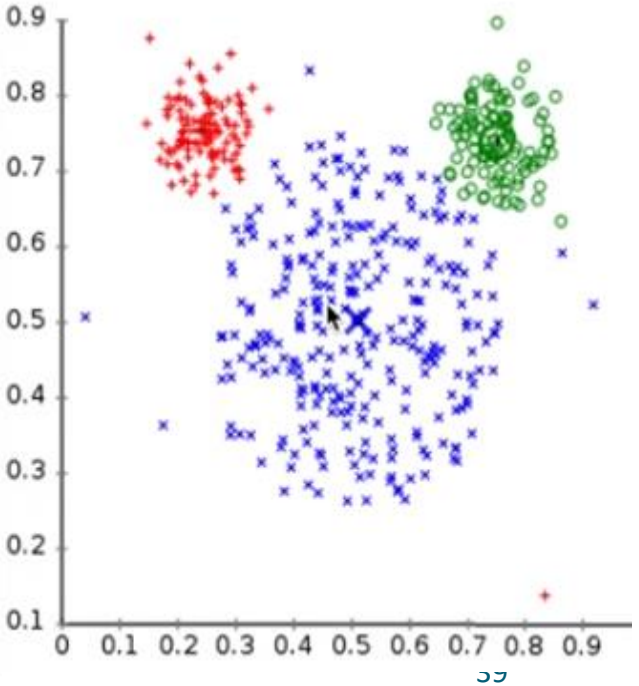
Original Data



K-means k=3



Mean Shift

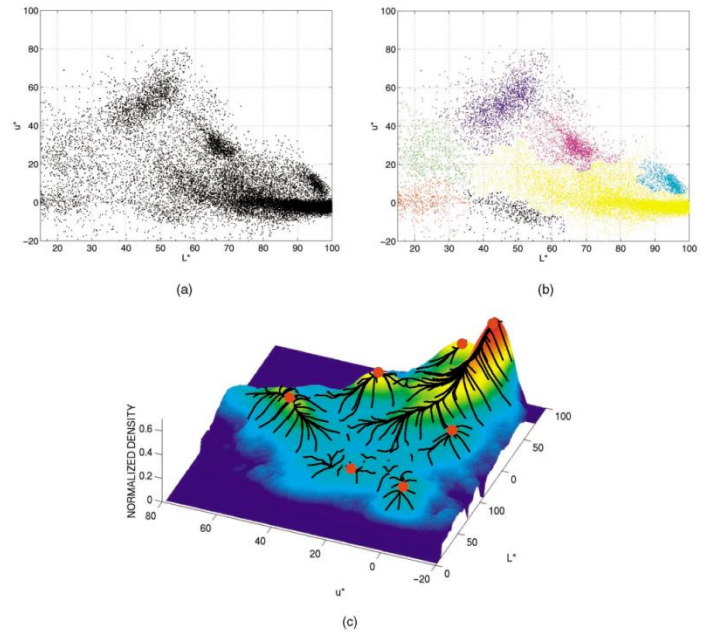


Mean shift clustering

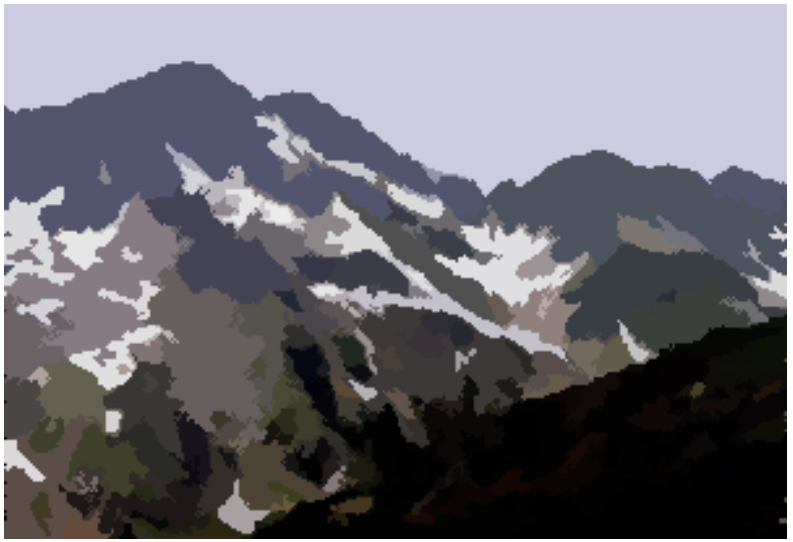
- The mean shift algorithm seeks *modes* of the given set of points
  1. Choose kernel and bandwidth
  2. For each point:
     a) Center a window on that point
     b) Compute the mean of the data in the search window
     c) Center the search window at the new mean location
     d) Repeat (b,c) until convergence
  3. Assign points that lead to nearby modes to the same cluster

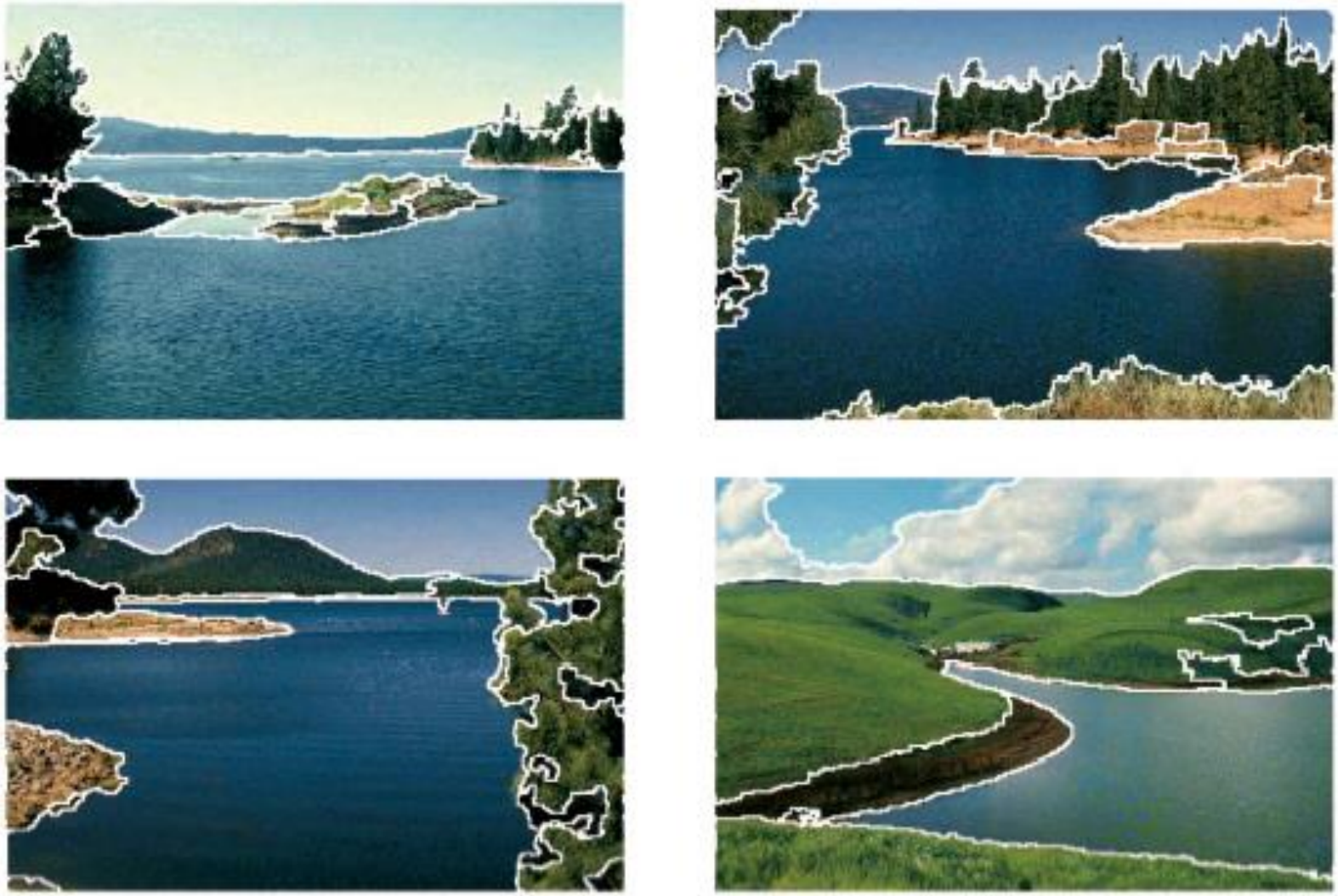
Segmentation by mean shift

- Compute features for each pixel (color, gradients, texture, etc)
- Set kernel size for features K_f and position K_s
- Initialize windows at individual pixel locations
- Perform mean shift for each window until convergence
- Merge windows that are within width of K_f and K_s



Mean shift segmentation





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

Some Results

Input Image

K-means k=16

Mean Shift

5-D space , 3 for RGB and 2 for X,Y

Mean shift pros and cons

- Pros
  - Good general-practice segmentation
  - Flexible in number and shape of regions
  - Robust to outliers
- Cons
  - Have to choose kernel size in advance
  - Not suitable for high-dimensional features
- When to use it
  - Oversegmentatoin
  - Multiple segmentations
  - Tracking, clustering, filtering applications

Topics to be covered…

- Introduction to clustering
- Similarity and dissimilarity measures
- Clustering techniques
  - Hierarchical algorithms
  - Partitioning algorithms (Kmedoids, Clara Calarans)
  - Density-based algorithm (DBScan, Optics , Denclue).
  - **Model Based algorithms (GMM)**
  - **Spectral Clustering**

Mixture Gaussian Models and the EM Algorithm

Model-based clustering

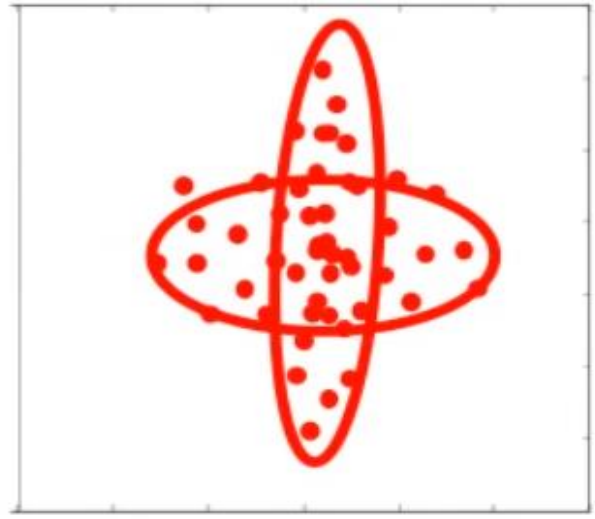
- In order to understand our data, we will assume that there is a generative process (a model) that creates/describes the data, and we will try to find the model that best fits the data.
  - Models of different complexity can be defined, but we will assume that our model is a distribution from which data points are sampled
  - Example: the data is the height of all people in Greece

- In most cases, a single distribution is not good enough to describe all data points: different parts of the data follow a different distribution
  - Example: the data is the height of all people in Greece and China
  - We need a mixture model
  - Different distributions correspond to different clusters in the data.

Mixture Gaussian

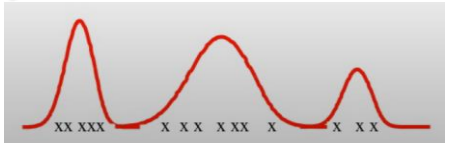
- K-means algorithm
  - Assigned each example to exactly one cluster
  - What if clusters are overlapping?
    - Hard to tell which cluster is right
    - Maybe we should try to remain uncertain
  - Used Euclidean distance
  - What if cluster has a non-circular shape?

- Gaussian mixture models
  - Clusters modeled as Gaussians
    - Not just by their mean
  - EM algorithm: assign data to cluster with some *probability*
  - Gives probability model of x! ("generative")



Mixture of Gaussians

- Start with parameters describing each cluster
- Mean μ_c, variance σ_c, "size" π_c
- Probability distribution: $p(x) = \sum_c \pi_c \mathcal{N}(x\ ;\ \mu_c, \sigma_c)$



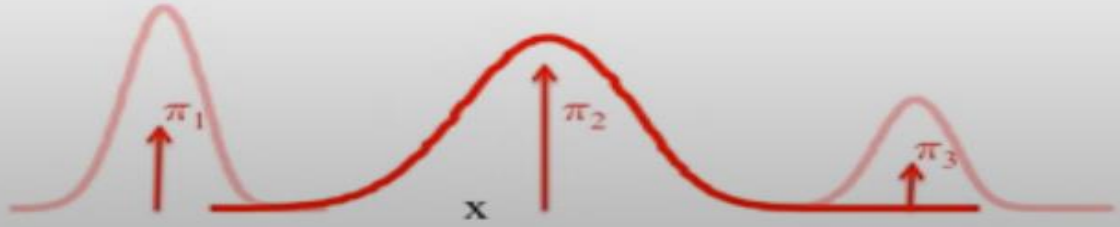
- Equivalent "latent variable" form:

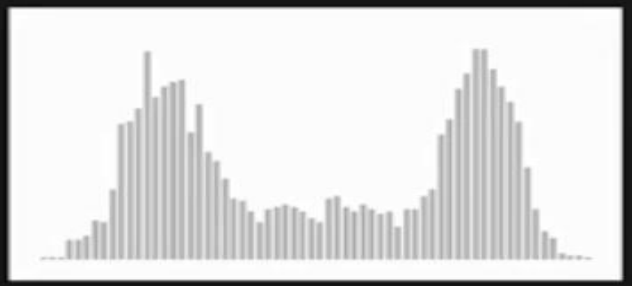
$p(z = c) = \pi_c$ Select a mixture component with probability π

$p(x|z = c) = \mathcal{N}(x\ ;\ \mu_c, \sigma_c)$ Sample from that component's Gaussian

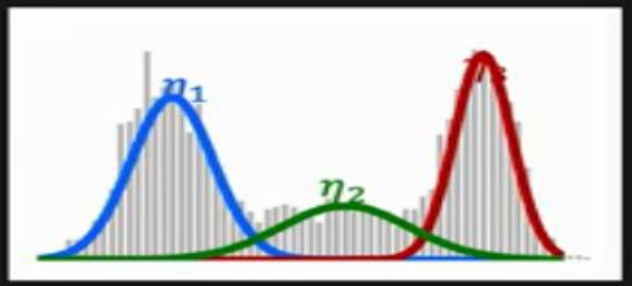
"Latent assignment" z:
we observe x, but z is hidden

p(x) = marginal over x

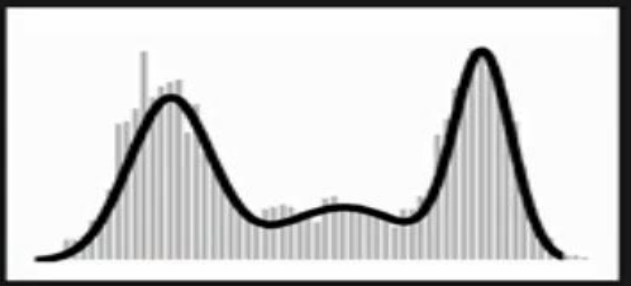




Probability Distribution
$P(x)$ (x: pixel intensity)



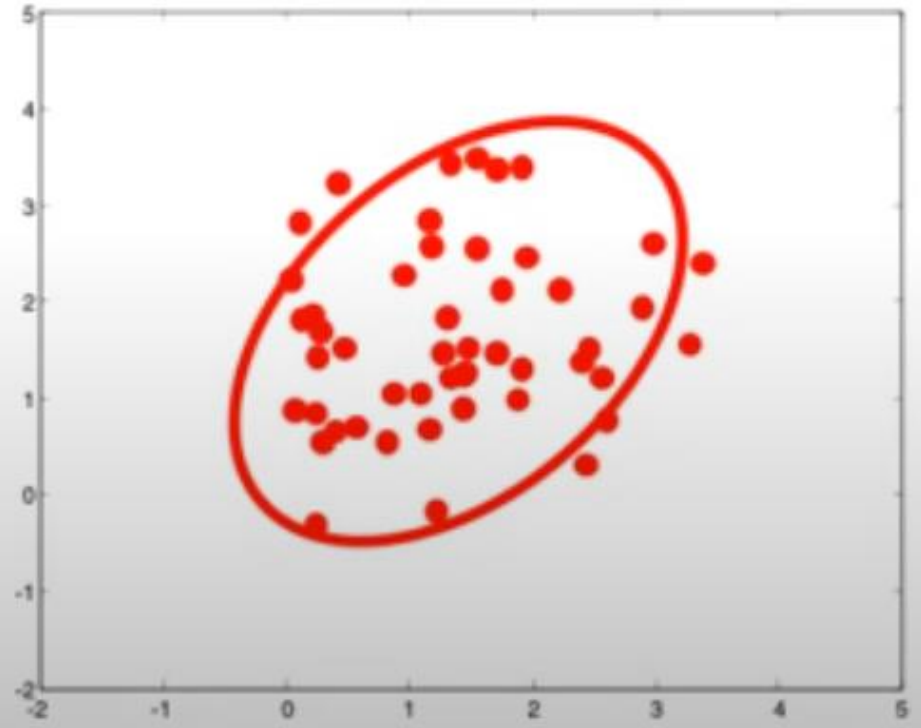
Mixture of Gaussians
$\omega_k \eta_k(x, \mu_k, \sigma_k)$



Gaussian Mixture Model
$P(x) = \sum_{k=1}^{K} \omega_k \eta_k(x, \mu_k, \sigma_k)$

Mixture of Gaussians Multivariate Model

$$\mathcal{N}(\underline{x}\,;\ \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}}|\Sigma|^{-1/2}\exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu})^T\Sigma^{-1}(\underline{x}-\underline{\mu})\right\}$$



Maximum Likelihood estimates

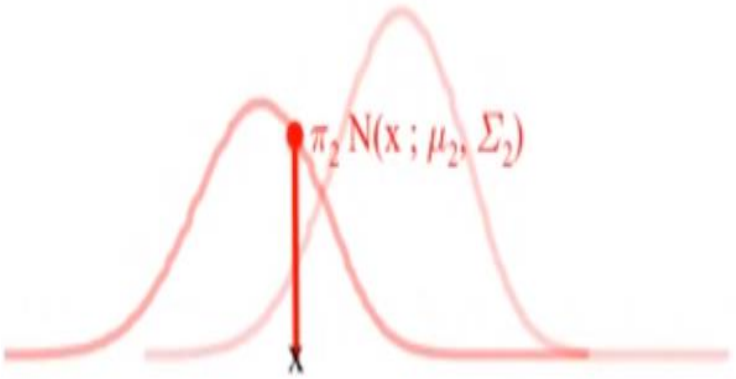
$$\hat{\mu} = \frac{1}{m}\sum_i x^{(i)}$$

$$\hat{\Sigma} = \frac{1}{m}\sum_i (x^{(i)}-\hat{\mu})^T(x^{(i)}-\hat{\mu})$$

We'll model each cluster using one of these Gaussian "bells"…

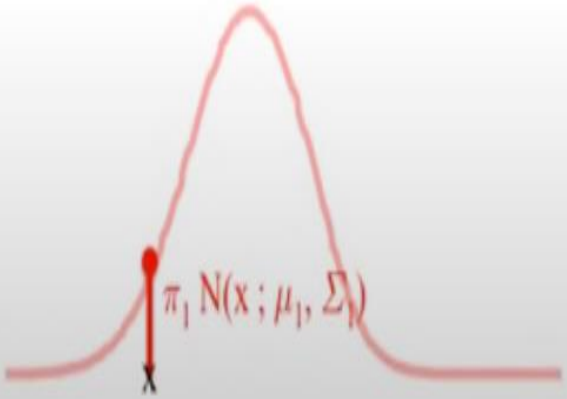
E-Step

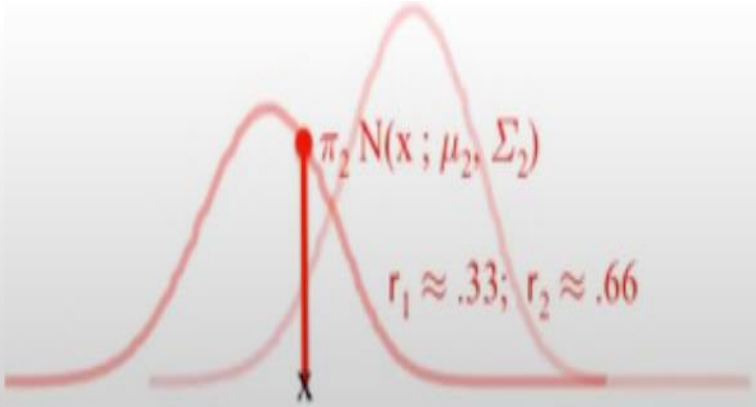
- Start with clusters: Mean μ_c, Covariance Σ_c, "size" π_c



- E-step ("Expectation")
  - For each datum (example) x_i,
  - Compute "r_{ic}", the probability that it belongs to cluster c
    - Compute its probability under model c
    - Normalize to sum to one (over clusters c)

$$r_{ic} = \frac{\pi_c \mathcal{N}(x_i ; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'} \mathcal{N}(x_i ; \mu_{c'}, \Sigma_{c'})}$$





M-Step

- Start with assignment probabilities r_{ic}
- Update parameters: mean μ_c, Covariance Σ_c, "size" π_c

- M-step ("Maximization")
  - For each cluster (Gaussian) z = c,
  - Update its parameters using the (weighted) data points

$$m_c = \sum_i r_{ic}$$ Total responsibility allocated to cluster c

$$\pi_c = \frac{m_c}{m}$$ Fraction of total assigned to cluster c

$$\mu_c = \frac{1}{m_c} \sum_i r_{ic} x^{(i)}$$ Weighted mean of assigned data

$$\Sigma_c = \frac{1}{m_c} \sum_i r_{ic} (x^{(i)} - \mu_c)^T (x^{(i)} - \mu_c)$$ Weighted covariance of assigned data (use new weighted means here)

EM-Algorithm

- Each step increases the log-likelihood of our model

$$\log p(X) = \sum_i \log \left[\sum_c \pi_c \, \mathcal{N}(x_i \; ; \; \mu_c, \Sigma_c) \right]$$

(we won't derive this here, though)

- Iterate until convergence
  - Convergence guaranteed – another ascent method
  - Local optima: initialization often important
- What should we do
  - If we want to choose a single cluster for an "answer"?
  - With new data we didn't see during training?
- Choosing the number of clusters
  - Can use penalized likelihood of training data (like k-means
  - True probability model: can use log-likelihood of test data, log p(x')

Gaussian Distribution

- Example: the data is the height of all people in Greece
  - Experience has shown that this data follows a Gaussian (Normal) distribution
  - Reminder: Normal distribution:

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

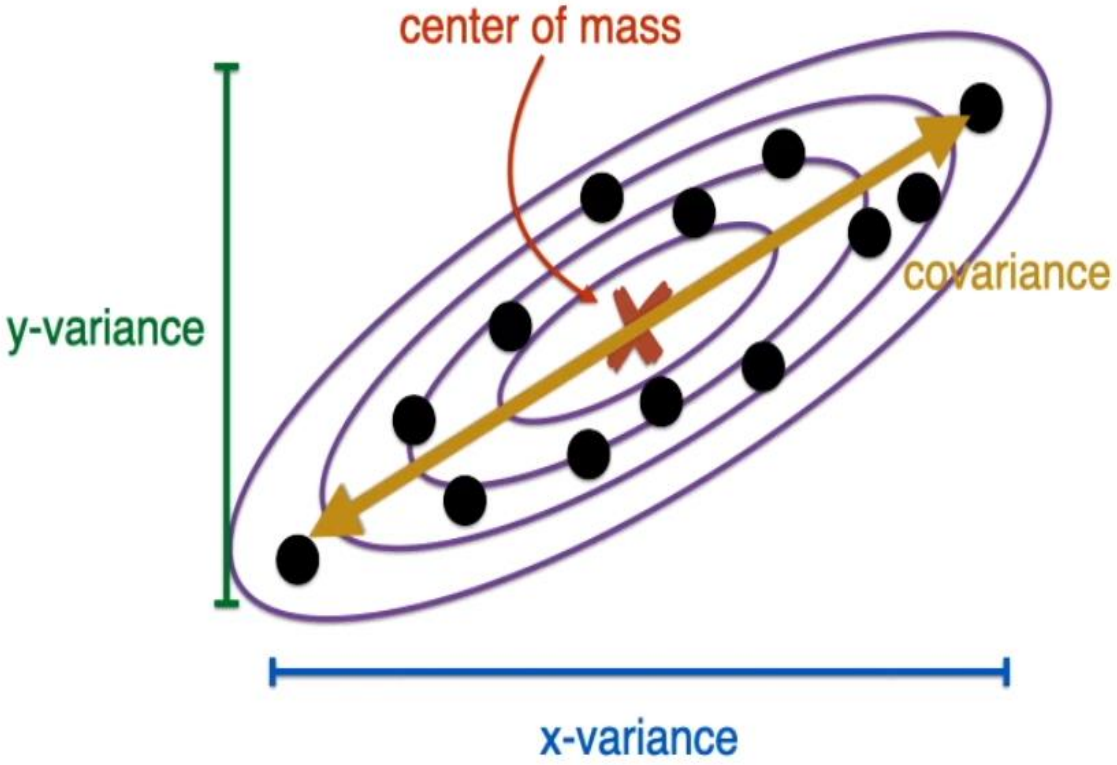
  - μ = mean, σ = standard deviation

Gaussian Model

- What is a model?
  - A Gaussian distribution is fully defined by the mean μ and the standard deviation σ
  - We define our model as the pair of parameters $\theta = (\mu, \sigma)$

- This is a general principle: a model is defined as a vector of parameters θ

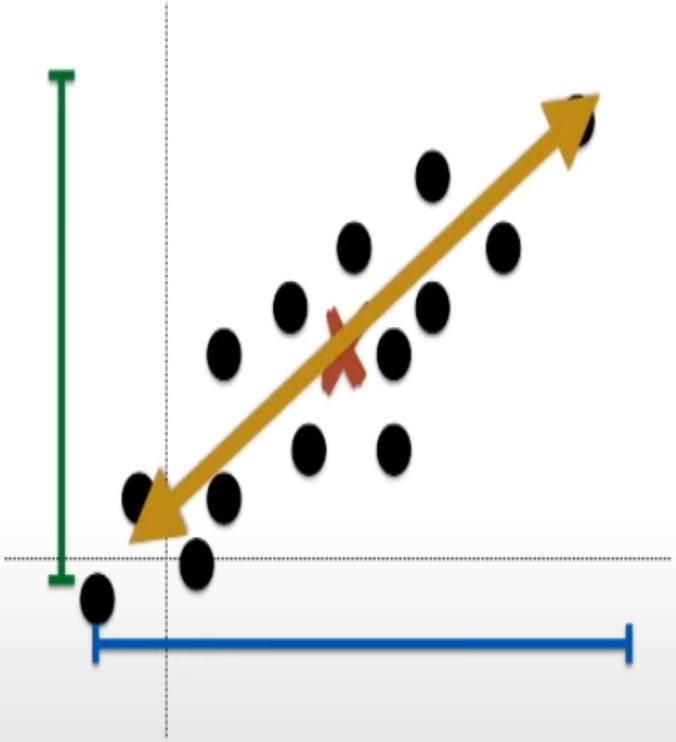
The covariance matrix



$$\mu = Average$$

$$\Sigma = \begin{pmatrix} Var(x) & Cov(x,y) \\ Cov(x,y) & Var(y) \end{pmatrix}$$

Formulas



Points

$$(x_1, y_1)$$
$$(x_2, y_2)$$
$$\vdots$$
$$(x_n, y_n)$$

Mean

$$(\mu_x, \mu_y) = (\frac{1}{n}\sum_{i=1}^{n} x_i, \frac{1}{n}\sum_{i=1}^{n} y_i)$$

x-Variance

$$var(x) = \frac{1}{n}\sum_{i=1}^{n} (x_i - \mu_x)^2$$

y-Variance

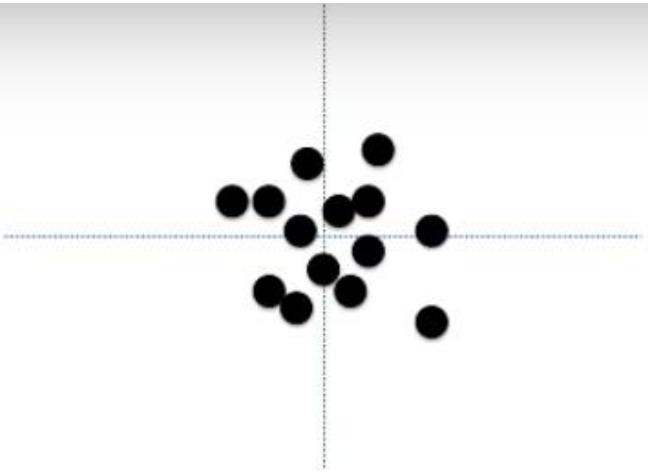
$$var(y) = \frac{1}{n}\sum_{i=1}^{n} (y_i - \mu_y)^2$$

Covariance

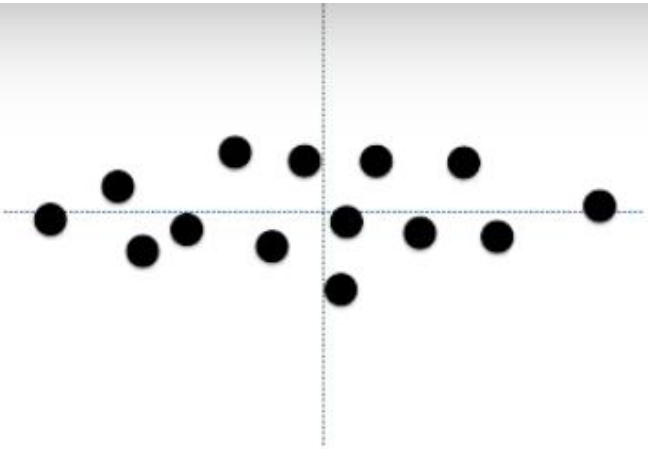
$$cov(x, y) = \frac{1}{n}\sum_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y)$$

Covariance matrix

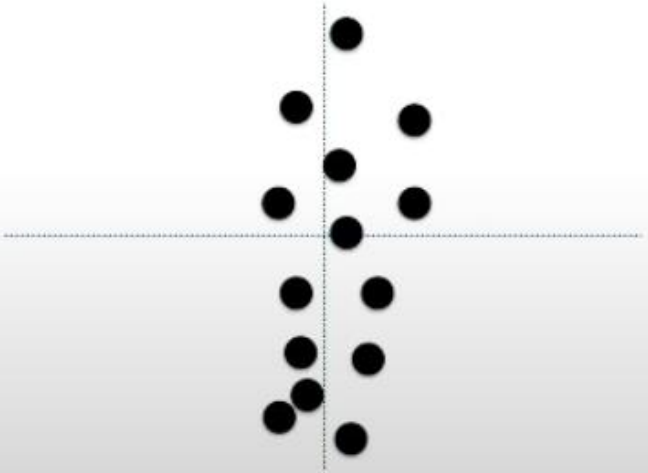
$$\Sigma = \begin{pmatrix} var(x) & cov(x, y) \\ cov(x, y) & var(y) \end{pmatrix}$$



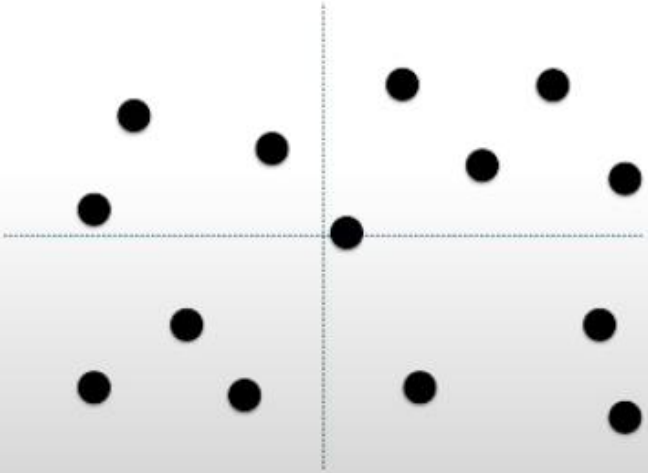
Small x-variance
Small y-variance



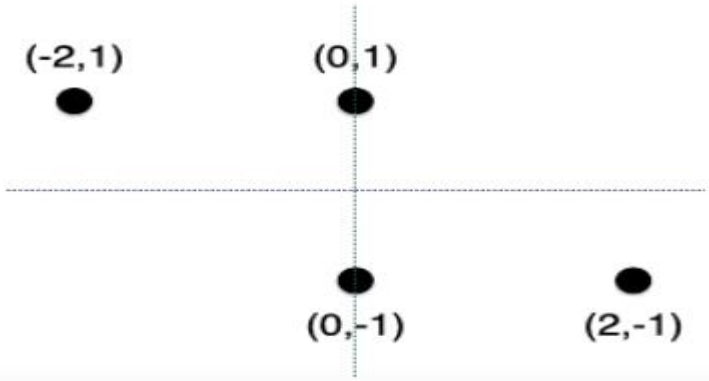
Large x-variance
Small y-variance



Small x-variance
Large y-variance

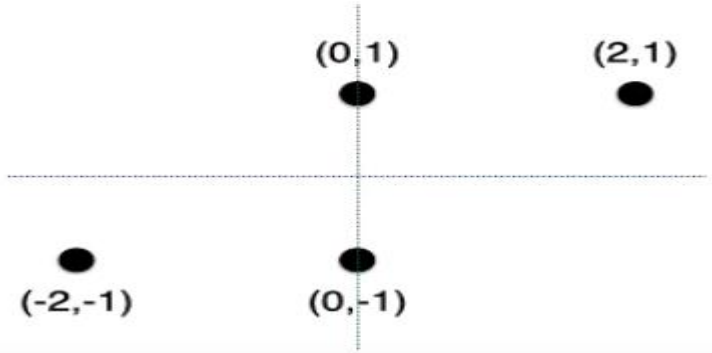


Large x-variance
Large y-variance



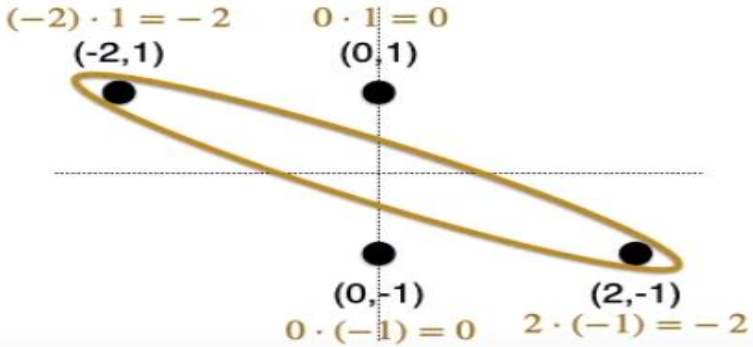
$$var(x) = \frac{1}{4}((-2)^2 + 0^2 + 0^2 + 2^2) = 2$$

$$var(y) = \frac{1}{4}(1^2 + 1^2 + (-1)^2 + (-1)^2) = 1$$



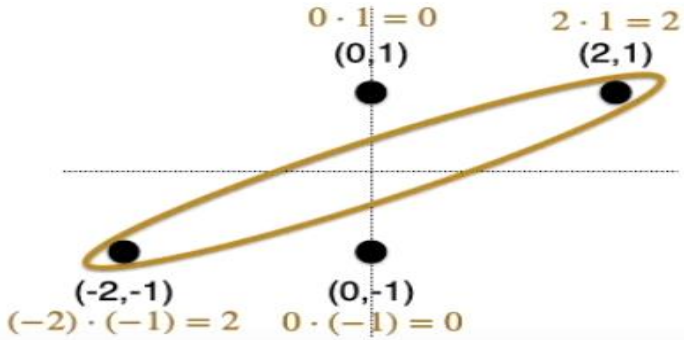
$$var(x) = \frac{1}{4}((-2)^2 + 0^2 + 0^2 + 2^2) = 2$$

$$var(y) = \frac{1}{4}((-1)^2 + (-1)^2 + 1^2 + 1^2) = 1$$



$$cov(x, y) = \frac{1}{4}(-2 + 0 + 0 - 2)$$

$$cov(x, y) = -1$$

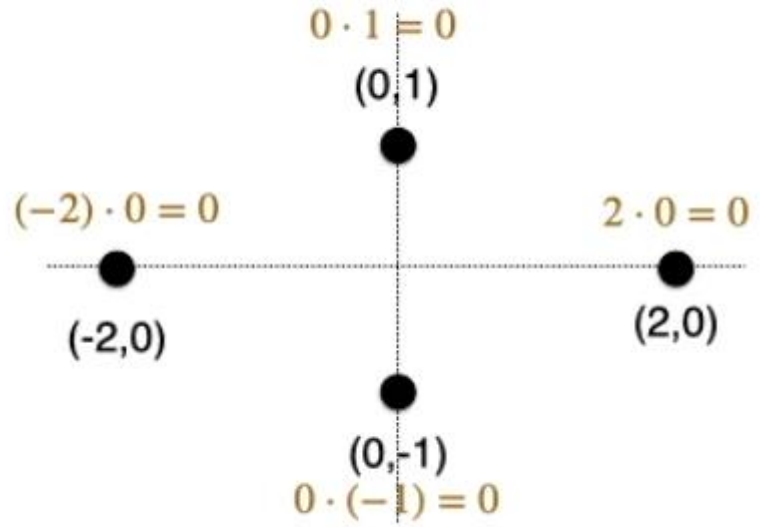


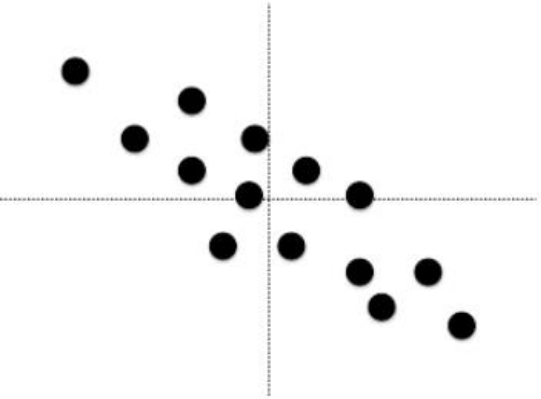
$$cov(x, y) = \frac{1}{4}(2 + 0 + 0 + 2)$$

$$cov(x, y) = 1$$

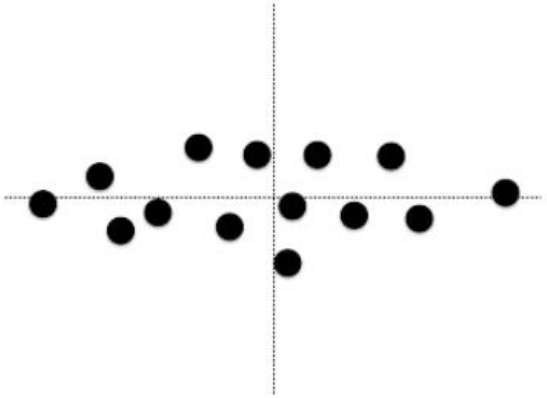
$$cov(x, y) = \frac{1}{4}(0 + 0 + 0 + 0)$$

$$cov(x, y) = 0$$

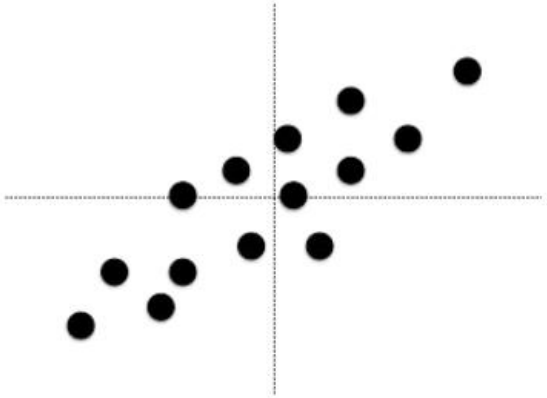




Negative covariance

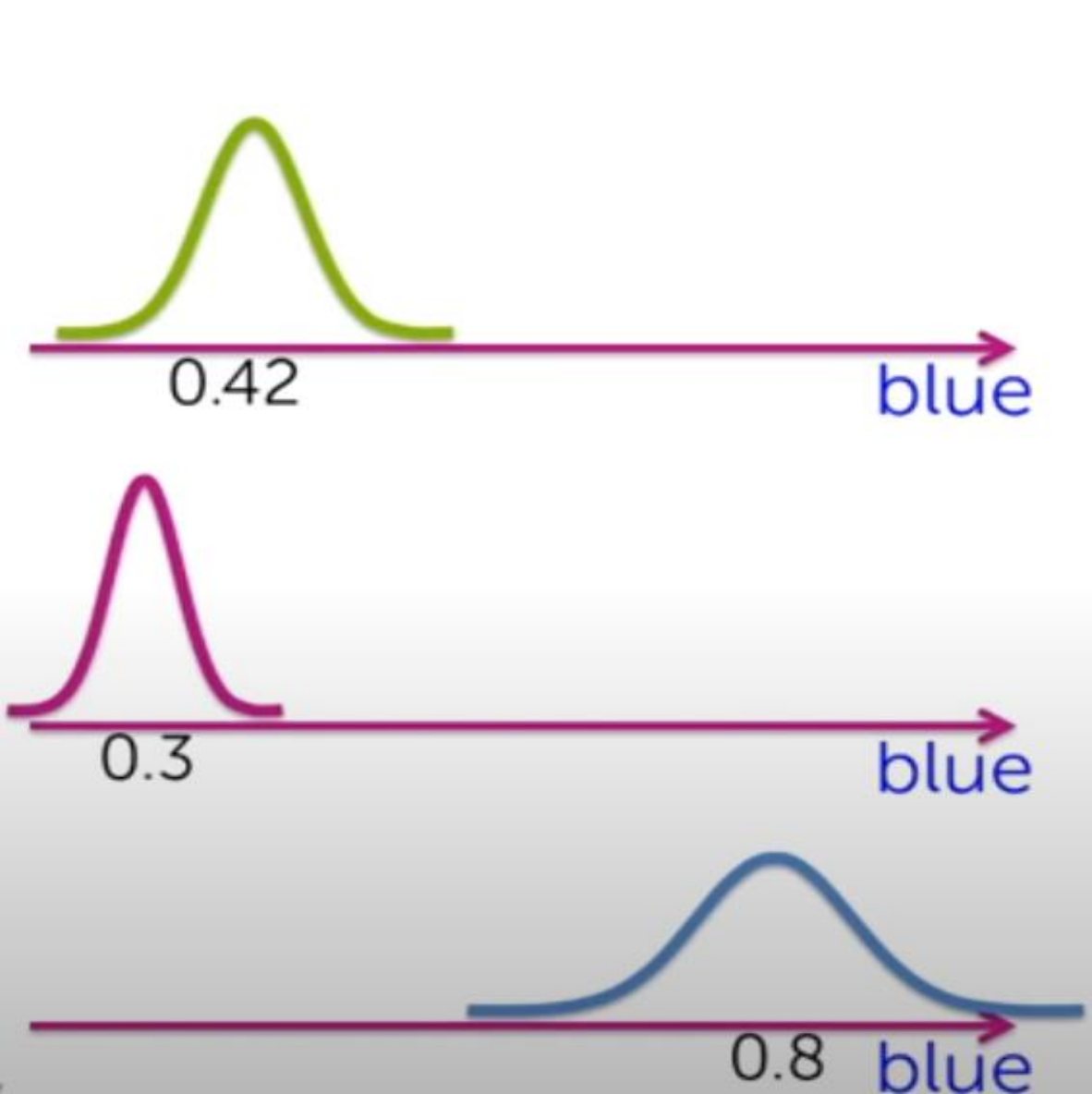


Zero covariance
(or very small)

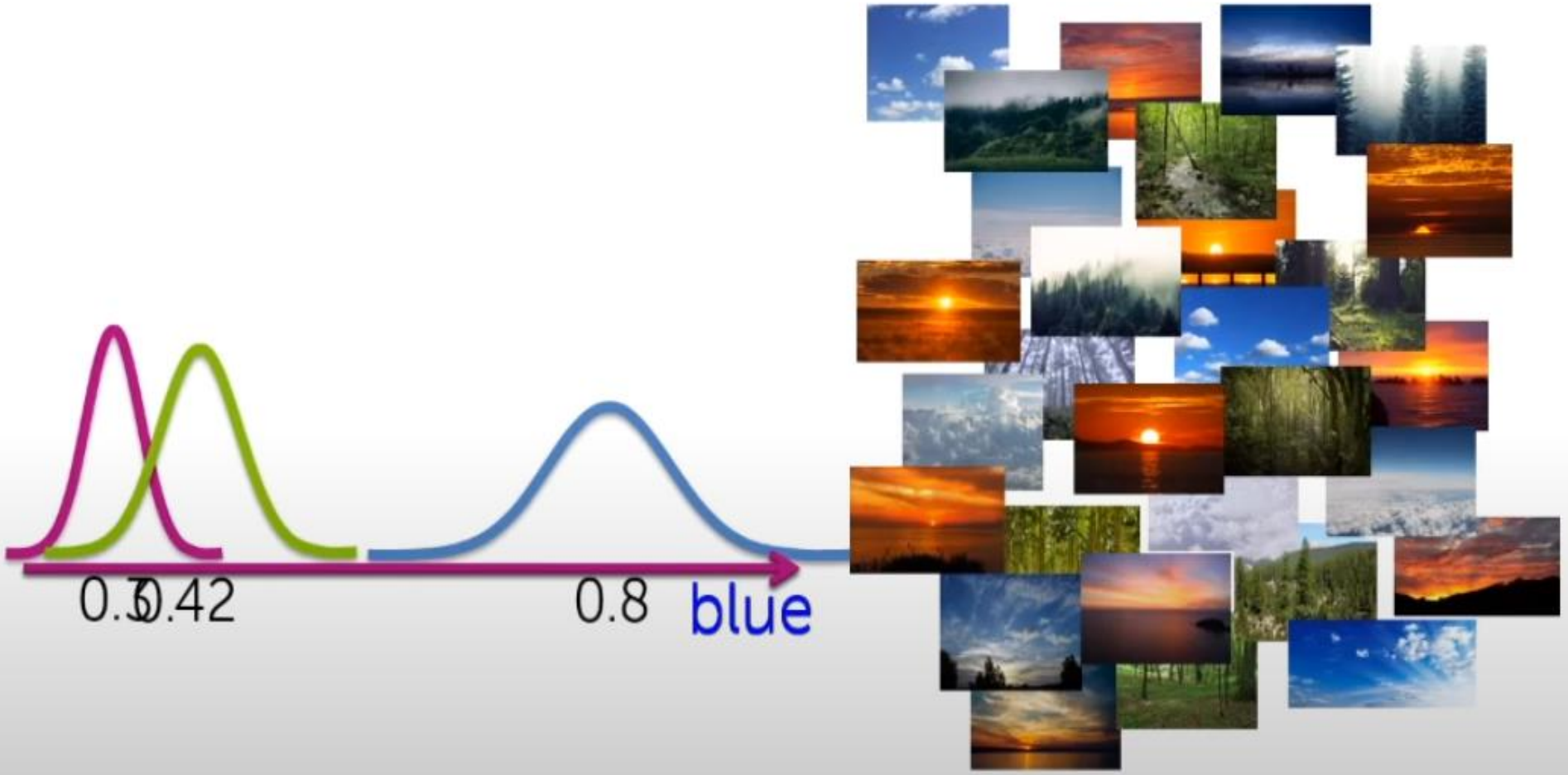


Positive covariance

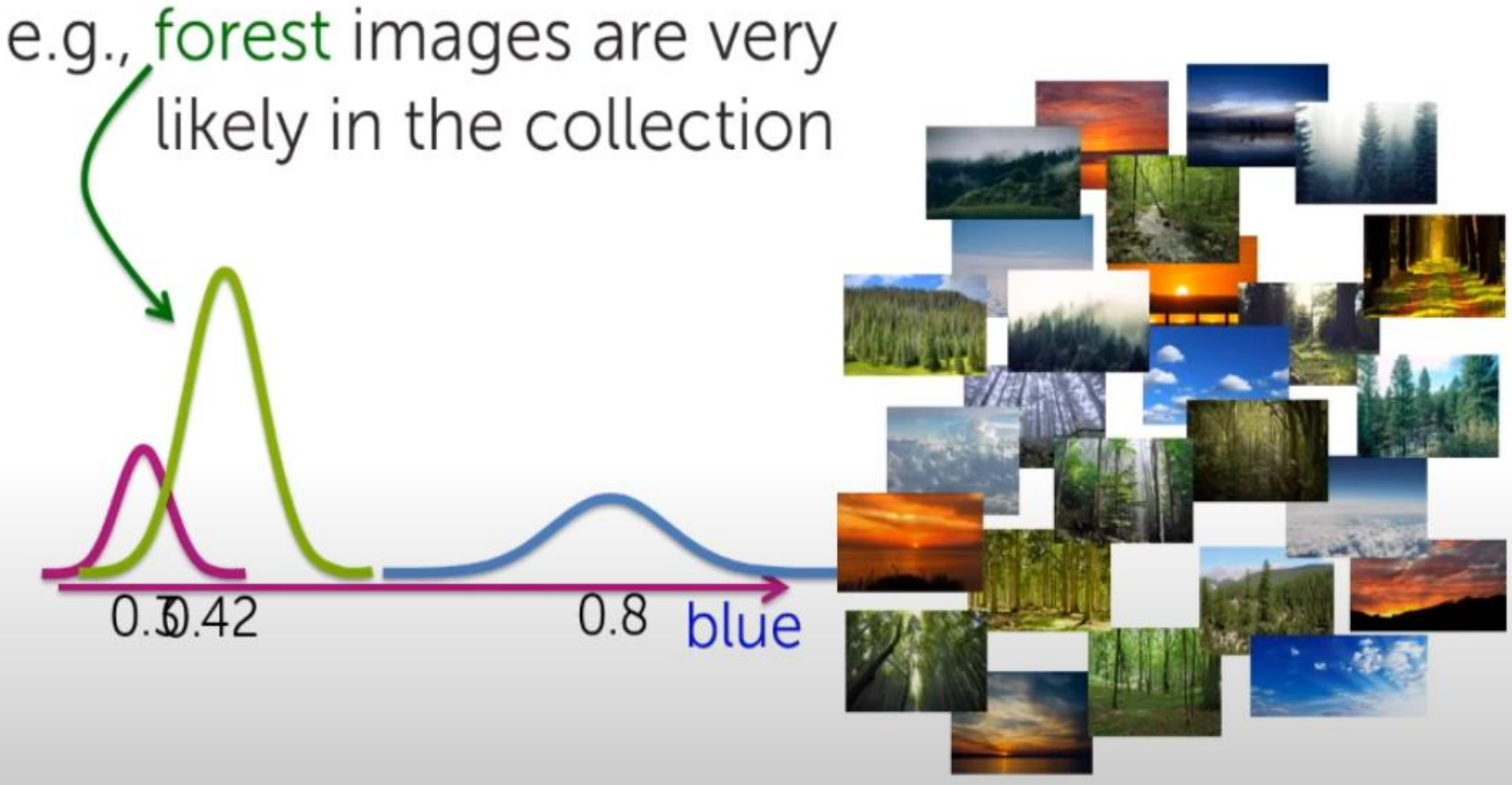
Model as Gaussian per Category/Cluster



Model as Jumble of Unlabeled data



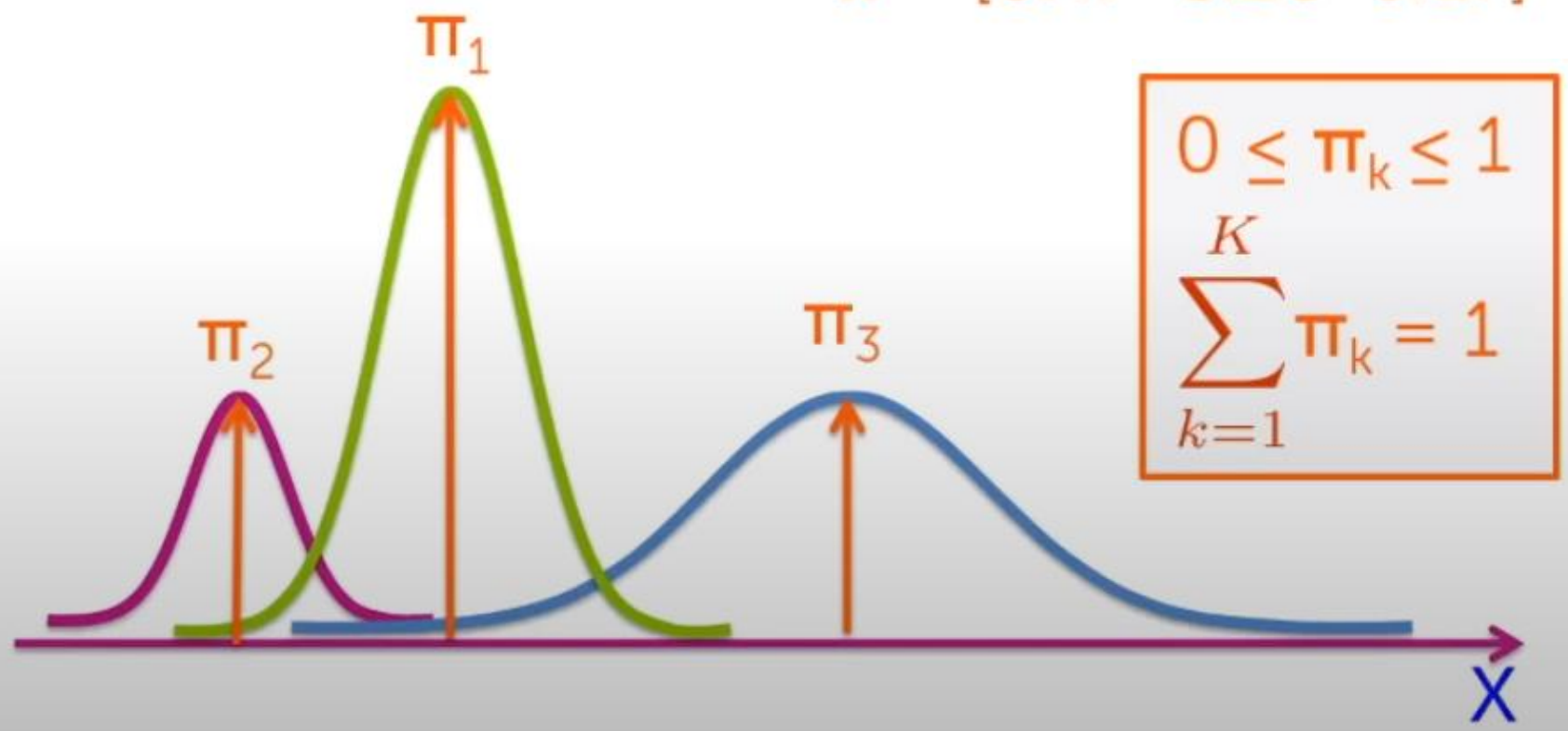
Unbalanced representative of categories



Combination of weighted Gaussians

Associate a weight π_k with each Gaussian component

$$\boldsymbol{\pi} = [\pi_1 \quad \pi_2 \quad \pi_3] = [0.47 \quad 0.26 \quad 0.27]$$

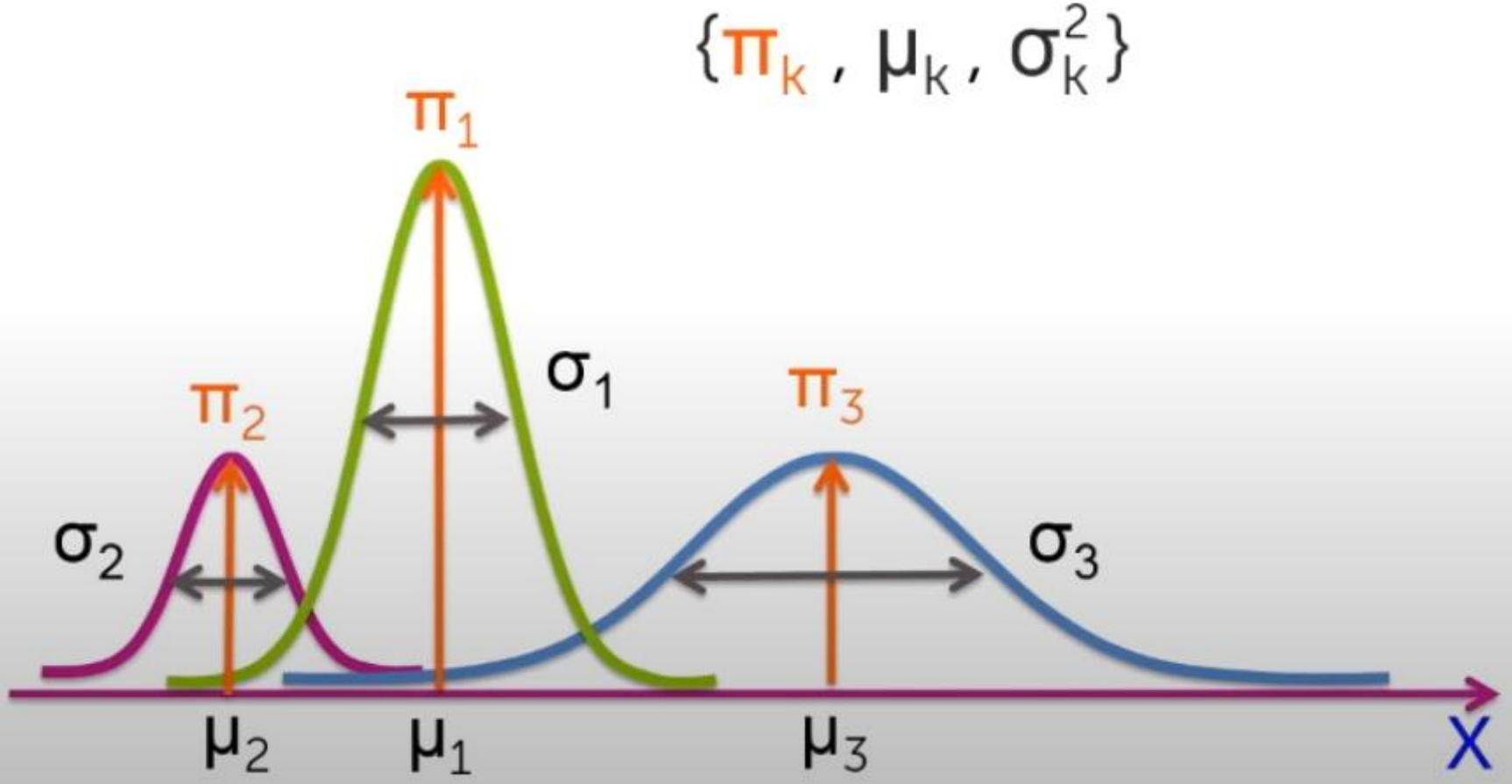


$$0 \leq \pi_k \leq 1$$

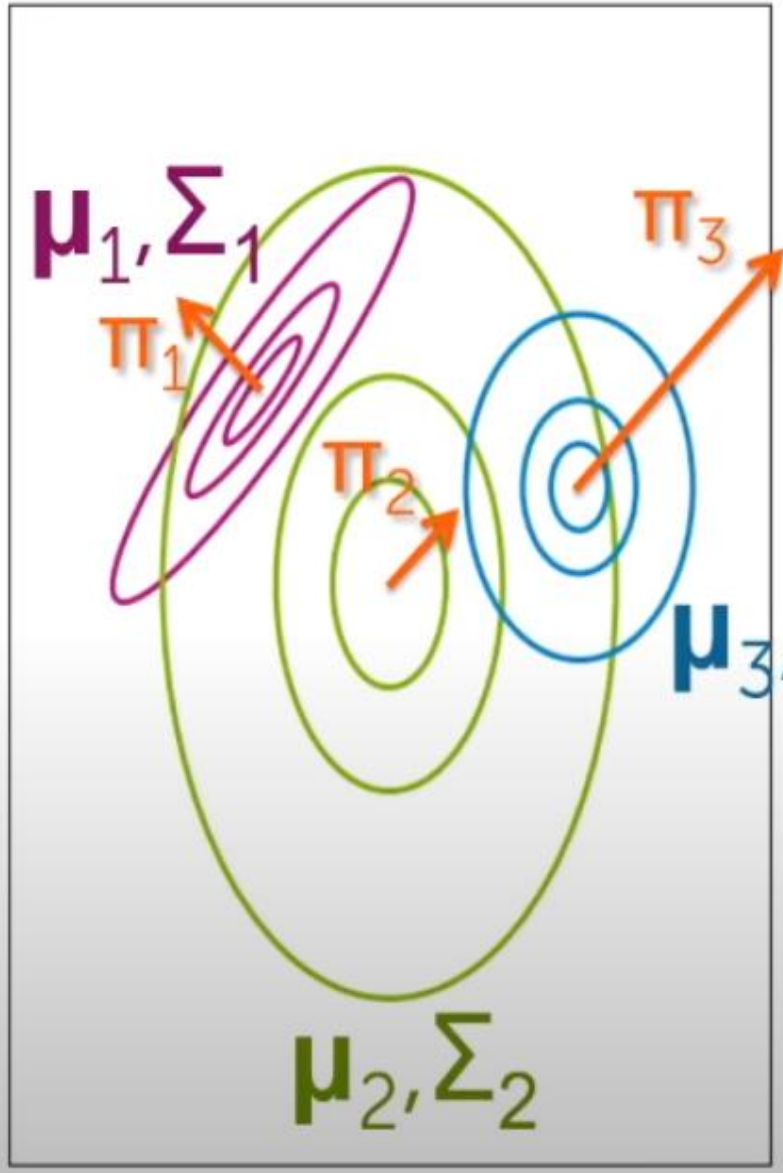
$$\sum_{k=1}^{K} \pi_k = 1$$

1-D Mixture of Gaussians

Each mixture component represents a unique cluster specified by:



Mixture of Gaussians



Each mixture component represents a unique cluster specified by:

$$\{\pi_k, \mu_k, \Sigma_k\}$$

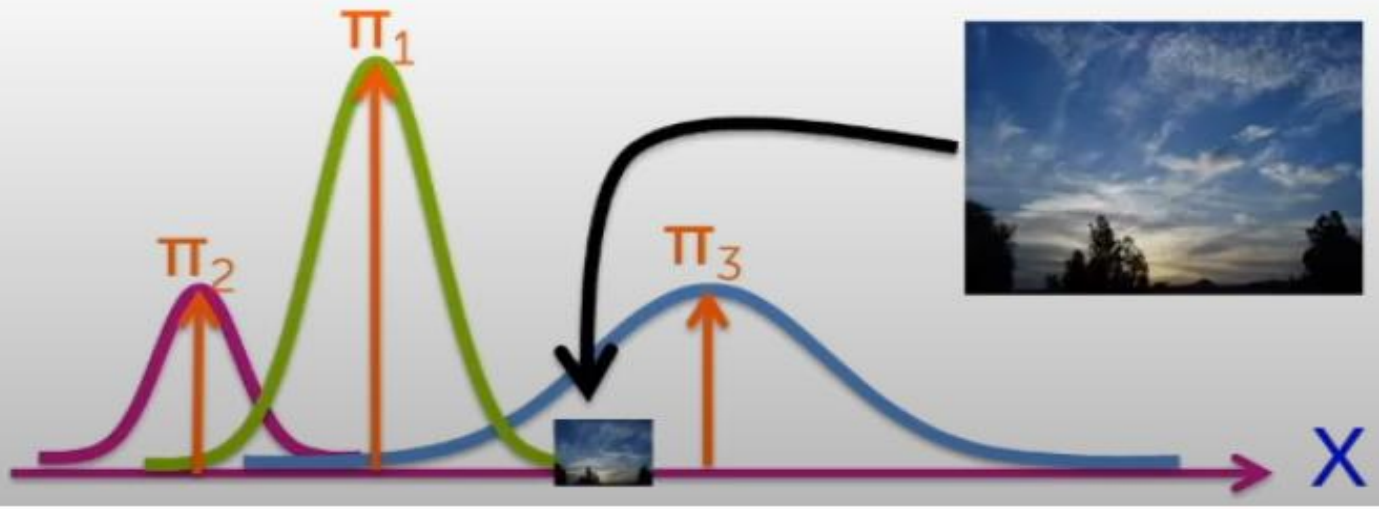
According to the model

Without observing the image content, what's the probability it's from cluster k? (e.g., prob. of seeing "clouds"

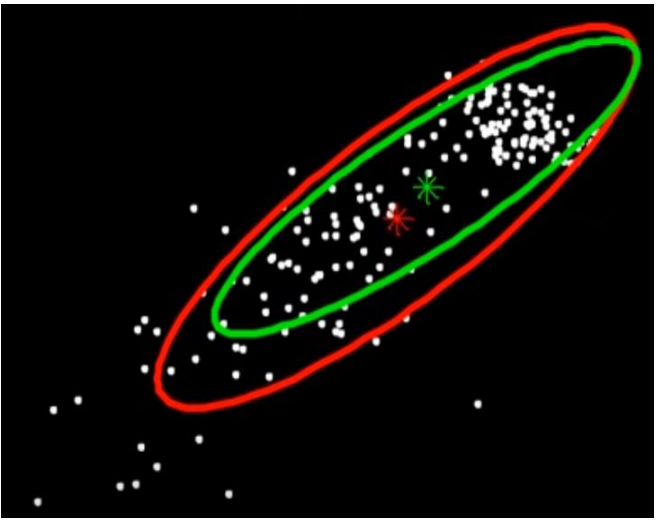
$$p(z_i = k) = \pi_k$$

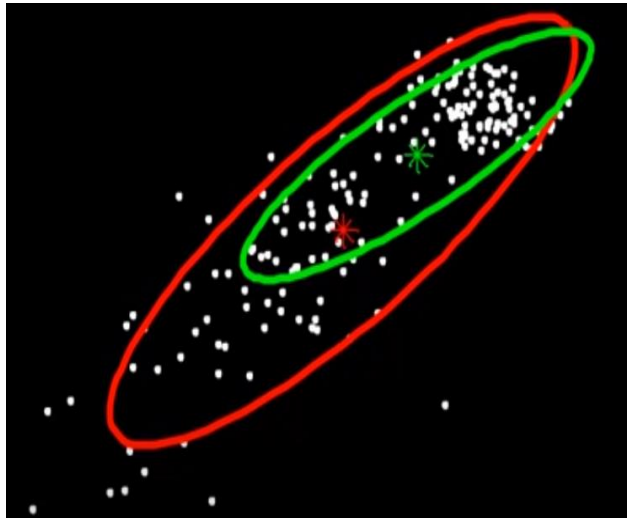
Given observation $\mathbf{x}_i$ is from cluster k, what's the likelihood of seeing $\mathbf{x}_i$? (e.g., just look at distribution for "clouds"

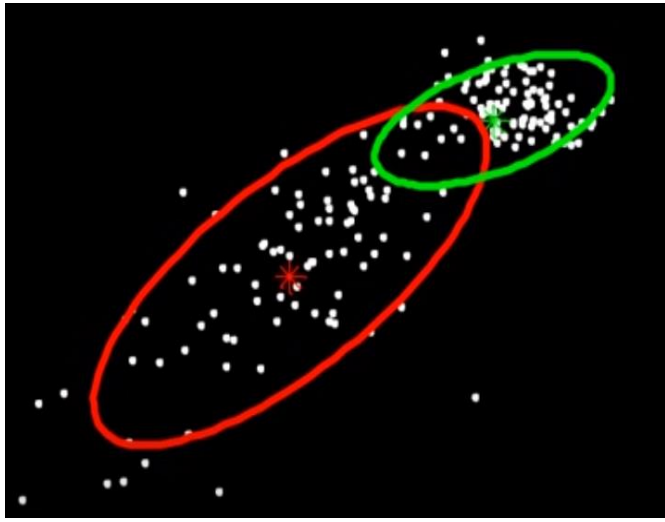
$$p(x_i \mid z_i = k, \mu_k, \Sigma_k) = N(x_i | \mu_k, \Sigma_k)$$

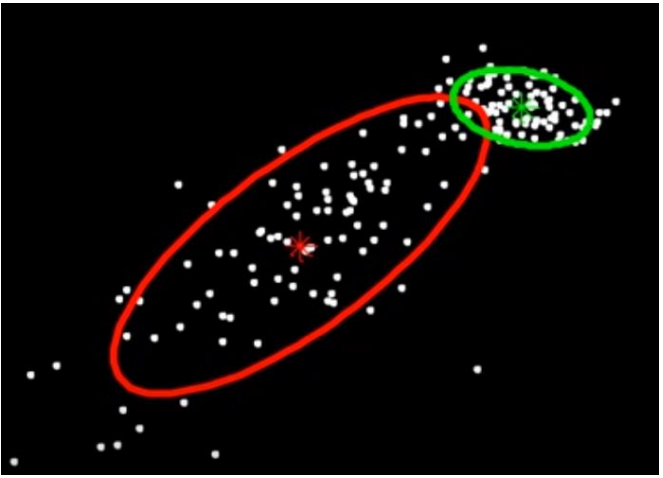


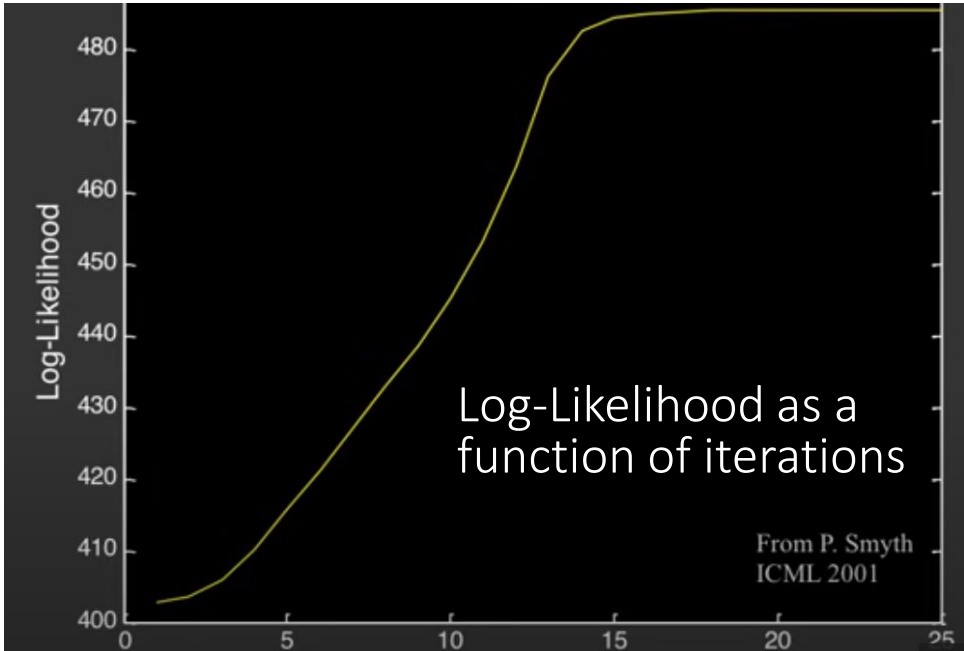
Demonstration of GMM and The EM Method











Fitting the model

- We want to find the normal distribution that best fits our data
  - Find the best values for μ and σ
  - But what does best fit mean?

Maximum Likelihood Estimation (MLE)

- Suppose that we have a vector $X = (x_1, \dots, x_n)$ of values
- And we want to fit a Gaussian $N(\mu, \sigma)$ model to the data
- Probability of observing point x_i:

$$P(x_i) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- Probability of observing all points (assume independence)

$$P(X) = \prod_{i=1}^{n} P(x_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- We want to find the parameters $\theta = (\mu, \sigma)$ that maximize the probability $P(X|\theta)$

Maximum Likelihood Estimation (MLE)

- The probability $P(X|\theta)$ as a function of θ is called the Likelihood function

$$L(\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- It is usually easier to work with the Log-Likelihood function

$$LL(\theta) = -\sum_{i=1}^{n} \frac{(x_i-\mu)^2}{2\sigma^2} - \frac{1}{2} n \log 2\pi - n \log \sigma$$

- Maximum Likelihood Estimation
  - Find parameters μ, σ that maximize $LL(\theta)$

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i = \mu_X$$

Sample Mean

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n} (x_i-\mu)^2 = \sigma_X^2$$

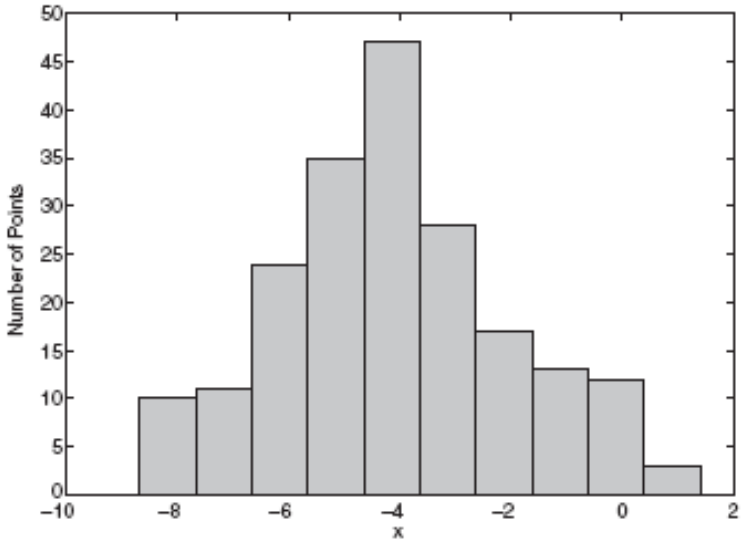
Sample Variance

MLE

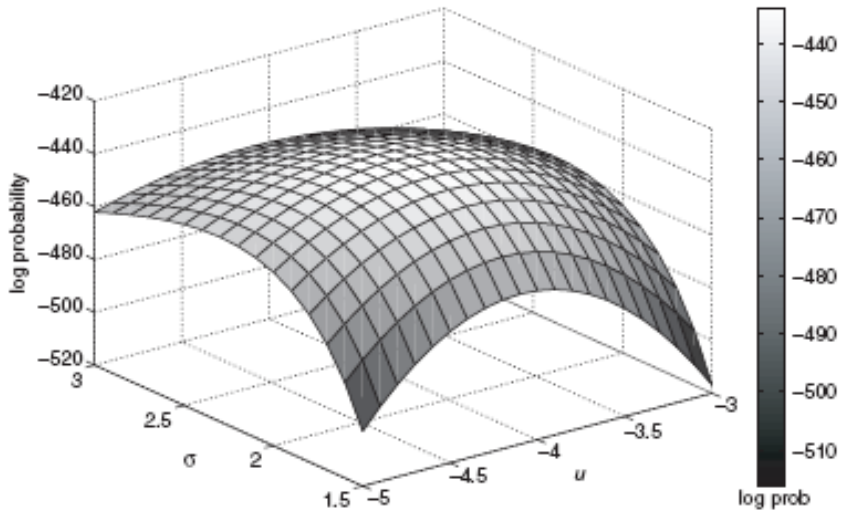
- Note: these are also the most likely parameters given the data

$$P(\theta|X) = \frac{P(X|\theta)P(\theta)}{P(X)}$$

- If we have no prior information about θ, or X, then maximizing $P(X|\theta)$ is the same as maximizing $P(\theta|X)$



(a) Histogram of 200 points from a Gaussian distribution.

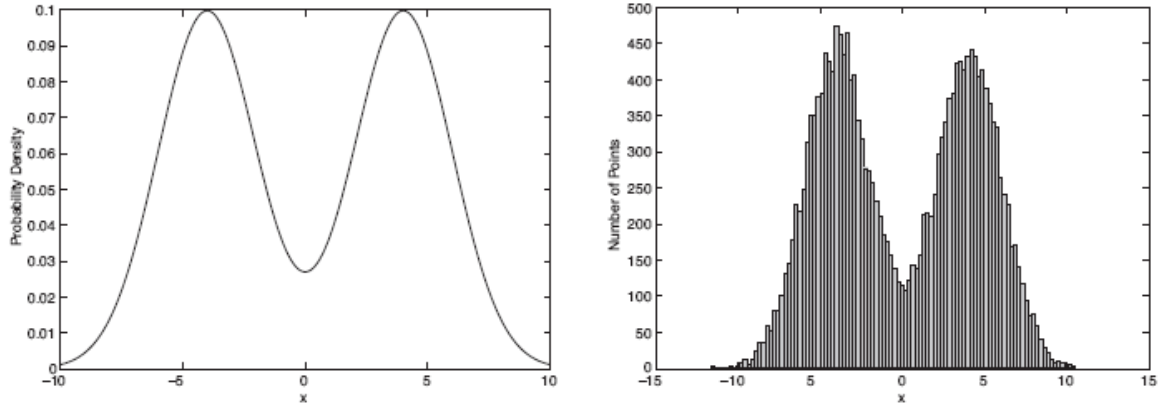


(b) Log likelihood plot of the 200 points for different values of the mean and standard deviation.

Figure 9.3. 200 points from a Gaussian distribution and their log probability for different parameter values.

Mixture of Gaussians

- Suppose that you have the heights of people from Greece and China and the distribution looks like the figure below (dramatization)



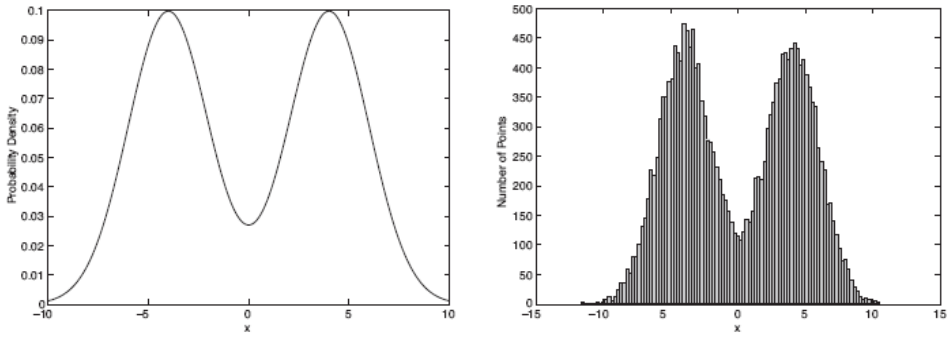
(a) Probability density function for the mixture model.

(b) 20,000 points generated from the mixture model.

Figure 9.2. Mixture model consisting of two normal distributions with means of -4 and 4, respectively. Both distributions have a standard deviation of 2.

Mixture of Gaussians

- In this case the data is the result of the mixture of two Gaussians
  - One for Greek people, and one for Chinese people
  - Identifying for each value which Gaussian is most likely to have generated it will give us a clustering.



(a) Probability density function for the mixture model.

(b) 20,000 points generated from the mixture model.

Figure 9.2. Mixture model consisting of two normal distributions with means of -4 and 4, respectively. Both distributions have a standard deviation of 2.

Mixture model

- A value x_i is generated according to the following process:
  - First select the nationality
    - With probability π_G select Greek, with probability π_C select China ($\pi_G + \pi_C = 1$)

      We can also think of this as a Hidden Variable Z
  - Given the nationality, generate the point from the corresponding Gaussian
    - $P(x_i|\theta_G) \sim N(\mu_G, \sigma_G)$ if Greece
    - $P(x_i|\theta_G) \sim N(\mu_G, \sigma_G)$ if China

Mixture Model

- Our model has the following parameters

$$\Theta = (\pi_G, \pi_C, \mu_G, \mu_C, \sigma_G, \sigma_C)$$

Mixture probabilities | Distribution Parameters

- For value x_i, we have:

$$P(x_i|\Theta) = \pi_G P(x_i|\theta_G) + \pi_C P(x_i|\theta_C)$$

- For all values $X = (x_1, \ldots, x_n)$

$$P(X|\Theta) = \prod_{i=1}^{n} P(x_i|\Theta)$$

- We want to estimate the parameters that maximize the Likelihood of the data

Mixture Models

- Once we have the parameters $\Theta = (\pi_G, \pi_C, \mu_G, \mu_C, \sigma_G, \sigma_C)$ we can estimate the membership probabilities $P(G|x_i)$ and $P(C|x_i)$ for each point x_i:
  - This is the probability that point x_i belongs to the Greek or the Chinese population (cluster)

$$P(G|x_i) = \frac{P(x_i|G)P(G)}{P(x_i|G)P(G) + P(x_i|C)P(C)}$$
$$= \frac{P(x_i|G)\pi_G}{P(x_i|G)\pi_G + P(x_i|C)\pi_C}$$

EM (Expectation Maximization) Algorithm

- Initialize the values of the parameters in Θ to some random values
- Repeat until convergence
  - E-Step: Given the parameters Θ estimate the membership probabilities $P(G|x_i)$ and $P(C|x_i)$
  - M-Step: Compute the parameter values that (in expectation) maximize the data likelihood

$$\pi_G = \frac{1}{n}\sum_{i=1}^{n} P(G|x_i) \qquad \pi_C = \frac{1}{n}\sum_{i=1}^{n} P(C|x_i)$$

Fraction of population in G,C

$$\mu_C = \sum_{i=1}^{n} \frac{P(C|x_i)}{n * \pi_C} x_i \qquad \mu_G = \sum_{i=1}^{n} \frac{P(G|x_i)}{n * \pi_G} x_i$$

MLE Estimates if π's were fixed

$$\sigma_C^2 = \sum_{i=1}^{n} \frac{P(C|x_i)}{n * \pi_C} (x_i - \mu_C)^2 \qquad \sigma_G^2 = \sum_{i=1}^{n} \frac{P(G|x_i)}{n * \pi_G} (x_i - \mu_G)^2$$

Relationship to K-means

- E-Step: Assignment of points to clusters
  - K-means: hard assignment, EM: soft assignment
- M-Step: Computation of centroids
  - K-means assumes common fixed variance (spherical clusters)
  - EM: can change the variance for different clusters or different dimensions (elipsoid clusters)
- If the variance is fixed then both minimize the same error function

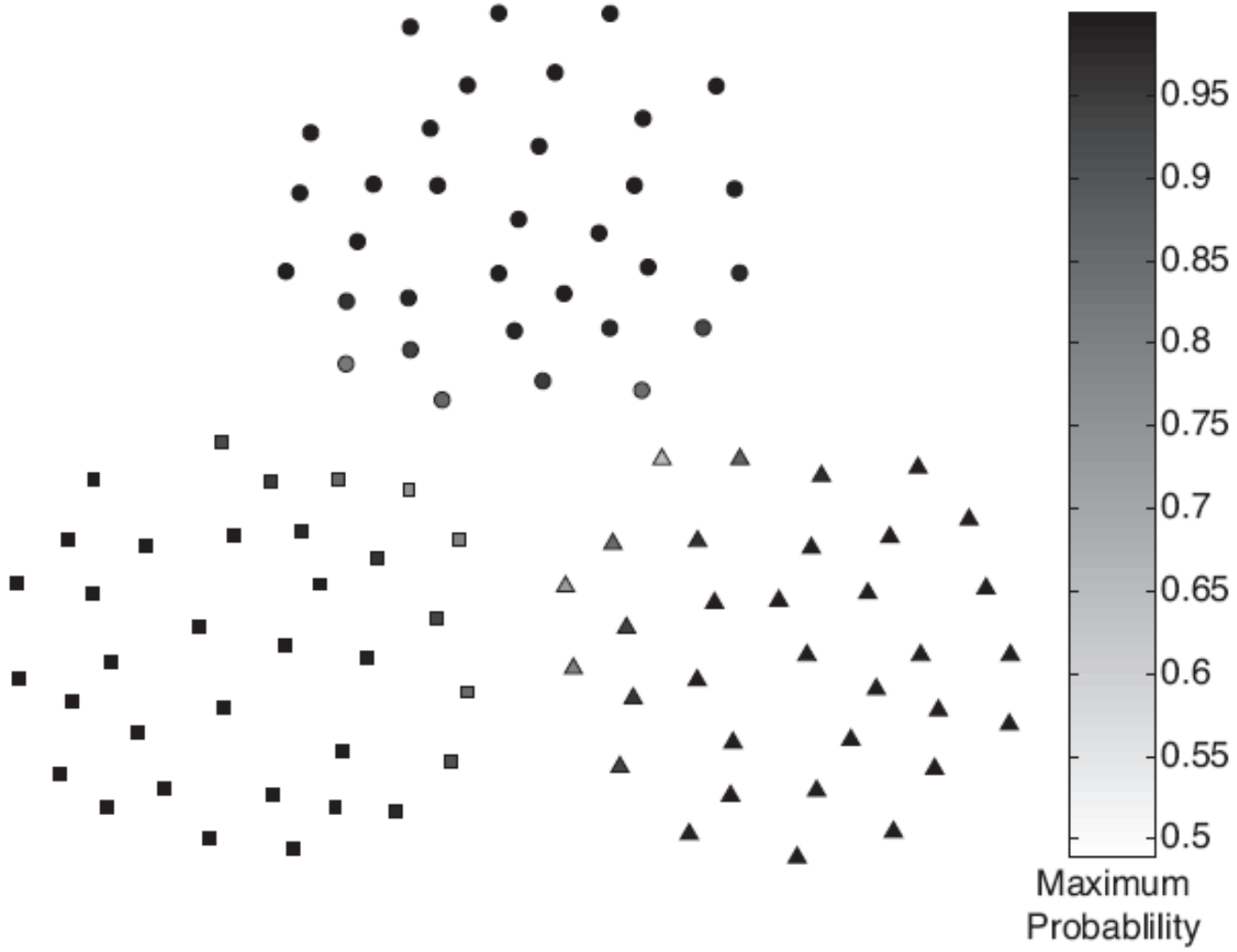


Figure 9.4. EM clustering of a two-dimensional point set with three clusters.

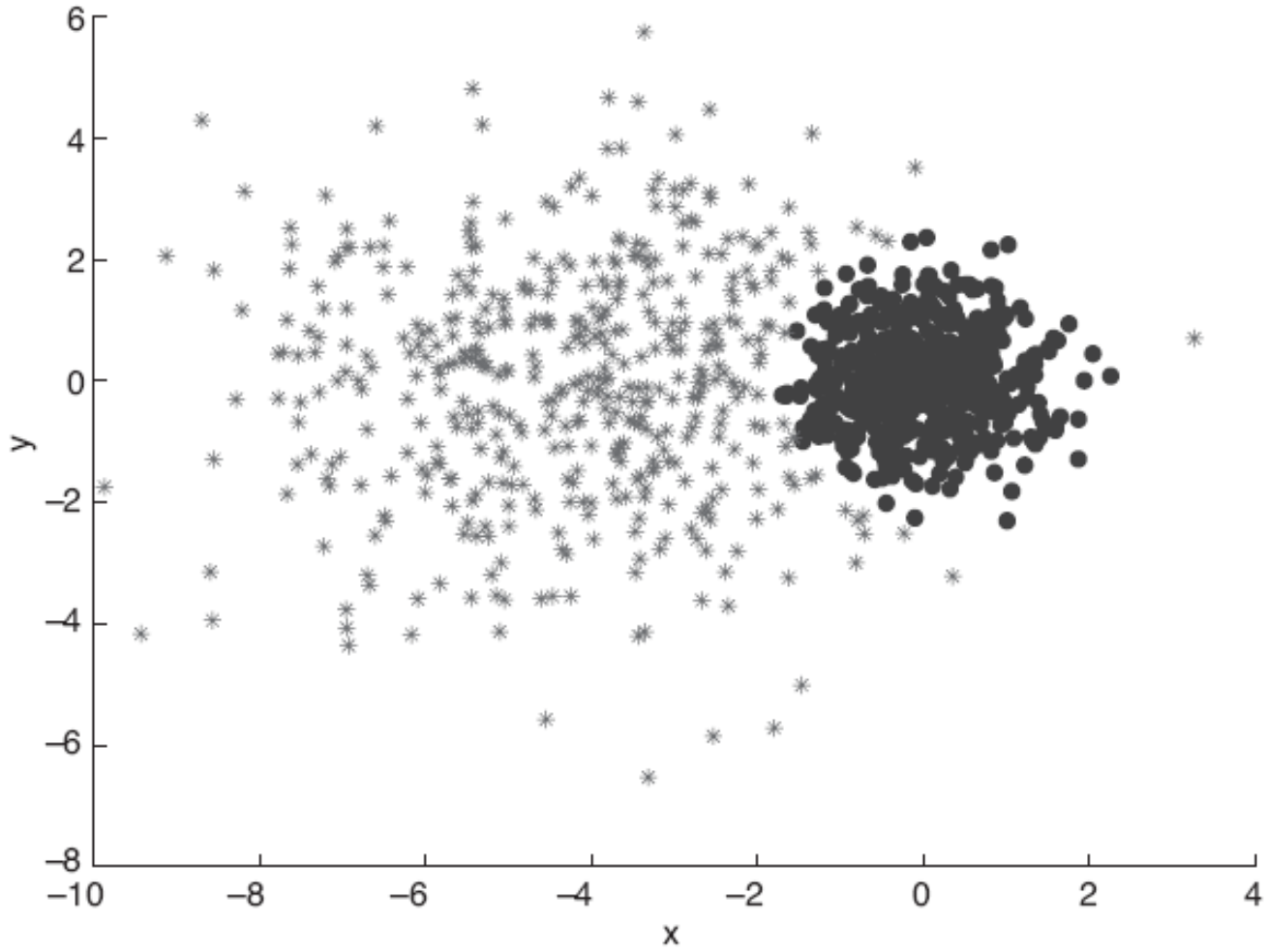
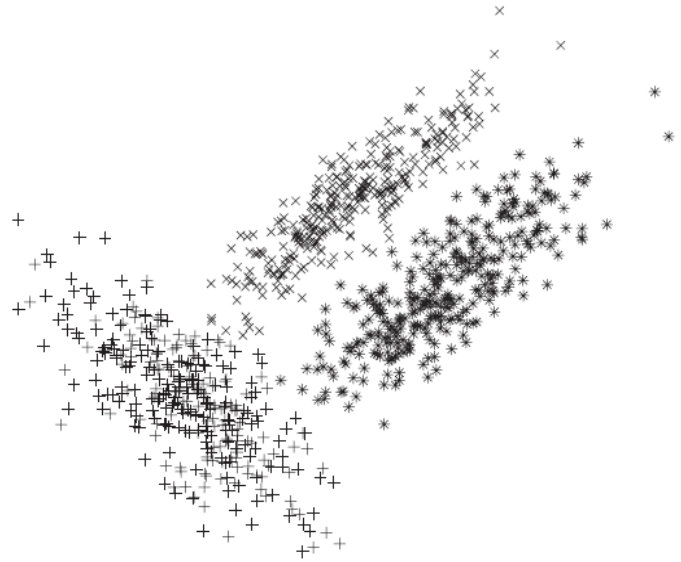
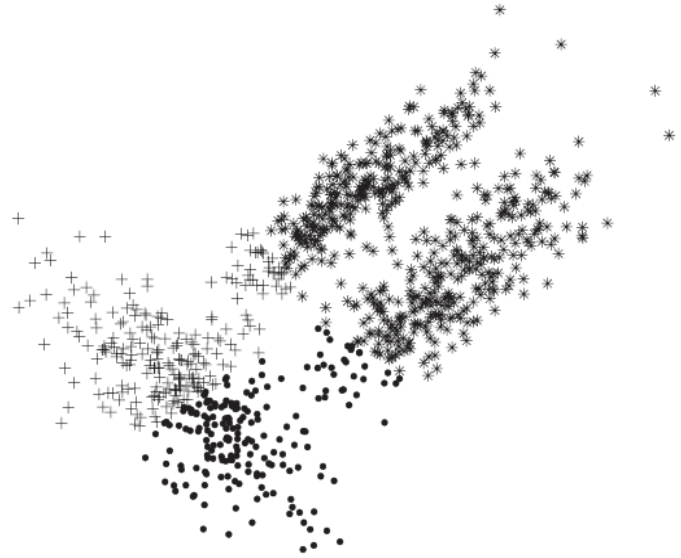


Figure 9.5. EM clustering of a two-dimensional point set with two clusters of differing density.



(a) Clusters produced by mixture model clustering.



(b) Clusters produced by K-means clustering.

Figure 9.6. Mixture model and K-means clustering of a set of two-dimensional points.