IERG4300 Web-Scale Information Analytics

Clustering

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Acknowledgements

- The slides used in this chapter are adapted from:
  - CS246 Mining Massive Data-sets, by Jure Leskovec, Stanford University.
  - Statistical Data Mining Tutorials – Tutorial Slides by Andrew W. Moore, CMU, http://www.autonlab.org/tutorials/list.html
  - Ch 1 and 9 of Pattern Recognition and Machine Learning (PRML) by Christopher M. Bishop, Publisher: Springer Science and Business.
    - http://www.cse.psu.edu/~rcollins/CSE586Spring2010/papers/prmlMixturesEM.pdf

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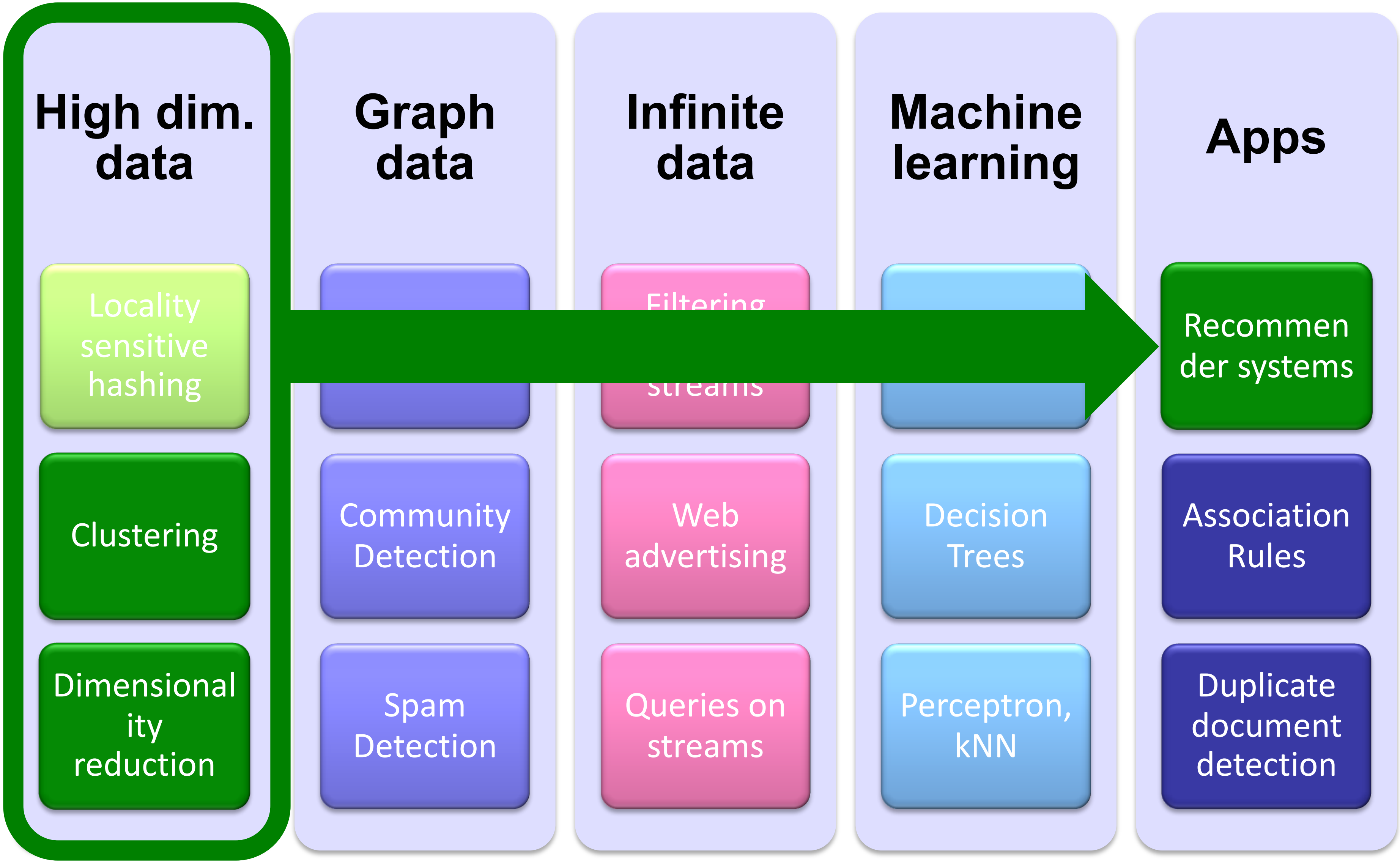
High Dimensional Data



High dim. data

Locality sensitive hashing

Clustering

Dimensionality reduction

Graph data

Community Detection

Spam Detection

Infinite data

Filtering

streams

Web advertising

Queries on streams

Machine learning

Decision Trees

Perceptron, kNN

Apps

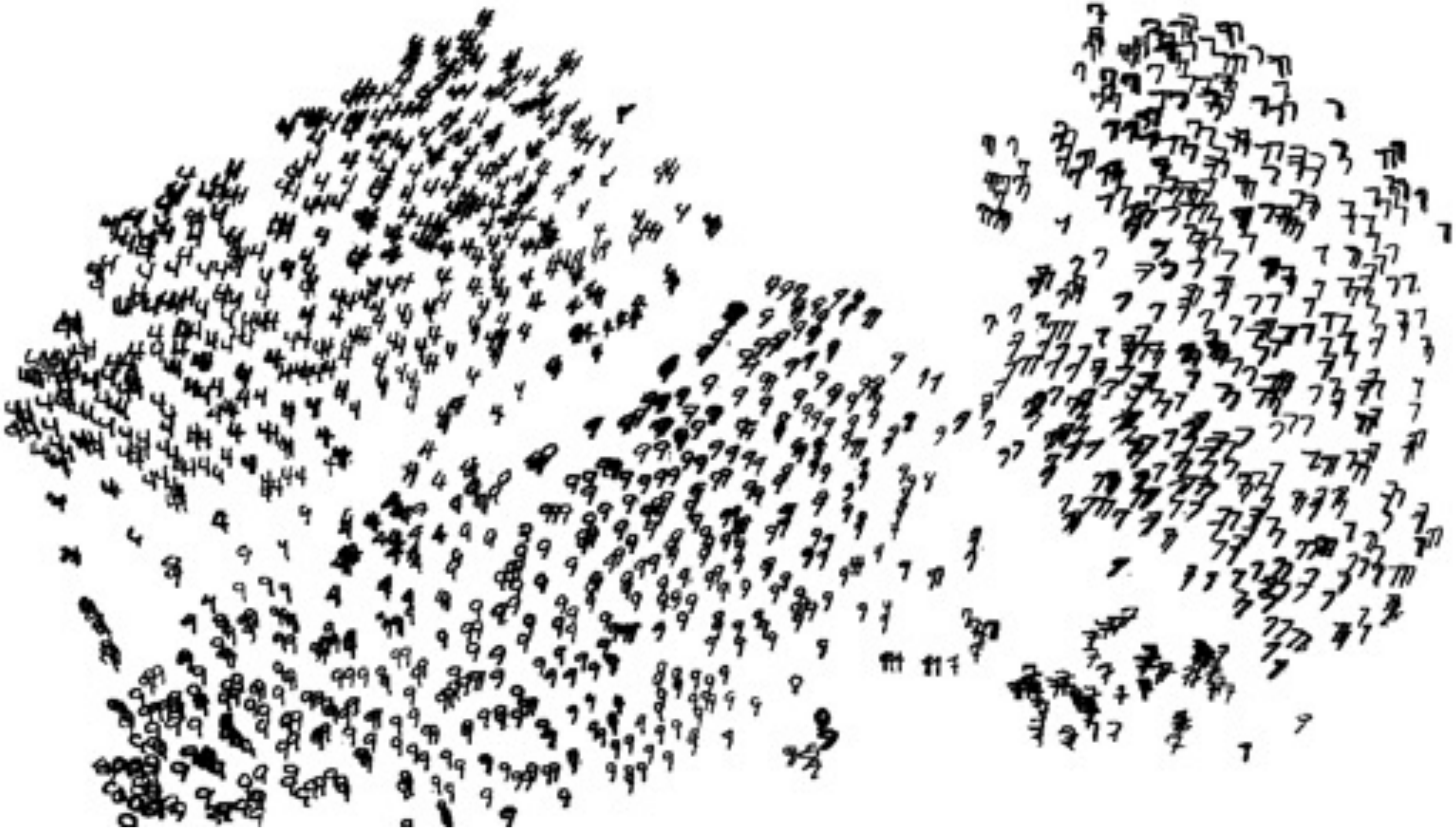
Recommender systems

Association Rules

Duplicate document detection

High Dimensional Data

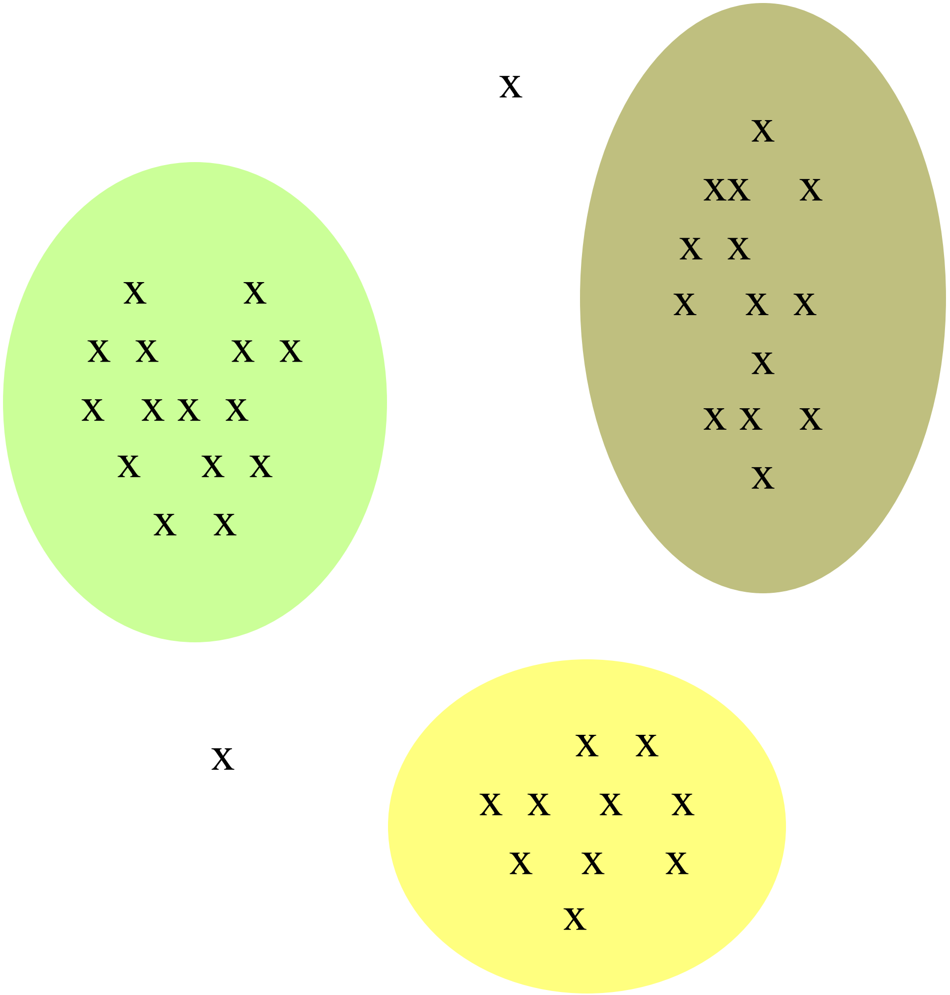
- Given a cloud of data points we want to understand their structure



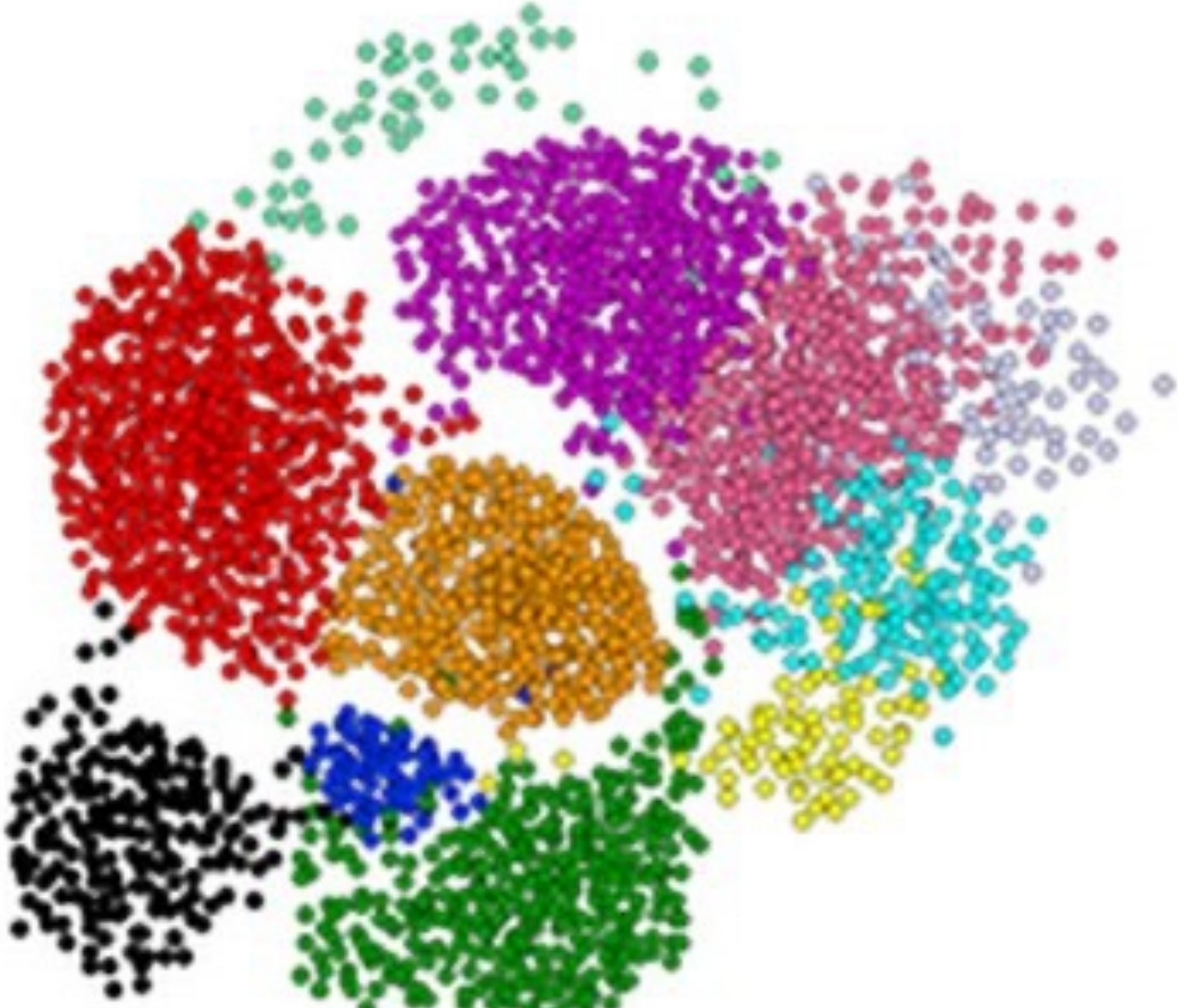
The Problem of Clustering

- Given a **set of points**, with a notion of **distance** between points, **group the points** into some number of ***clusters***, so that
  - Members of a cluster are close/similar to each other
  - Members of different clusters are dissimilar
- **Usually:**
  - Points are in a high-dimensional space
  - Similarity is defined using a distance measure
    - Euclidean, Cosine, Jaccard, edit distance, …

Example: Clusters



Clustering is a hard problem!



Why is it hard?

- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy
- And in most cases, looks are *not* deceiving
- Many applications involve not 2, but 10 or 10,000 dimensions
- **High-dimensional spaces look different**

Curse of Dimensionality

- **High-dimensional spaces look different:** The so-called "Curse of Dimensionality"
  - Need many more data points scattered in the High Dimensional (HD) space in order to form clusters (instead of being isolated dots in the mostly empty space) !
  - Almost all pairs of points are at about the same distance in HD space

=> The notion of neighborhood becomes not very useful as the distance between a data point and is its nearest neighbor approaches the distance to its farthest neighbor.

=> "neighborhood is not that local !

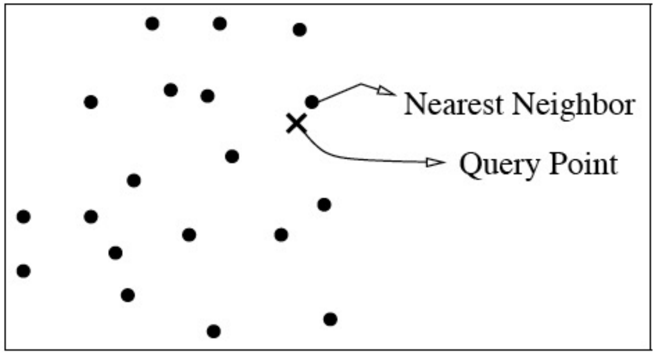


Fig. 1. Query point and its nearest neighbor.

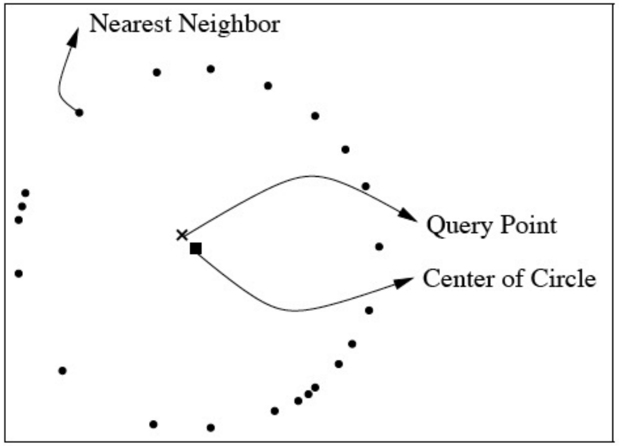


Fig. 2. Another query point and its nearest neighbor.

Source: K.Beyer et al, "When is "Nearest Neighbor" Meaningful ?", ICDT 99.

Curse of Dimensionality (cont'd)

Consider a sphere of radius r=1 in a D-dimensional space

Fraction of the volume of the sphere that lies between radius r=1-ε and r=1 is given by:

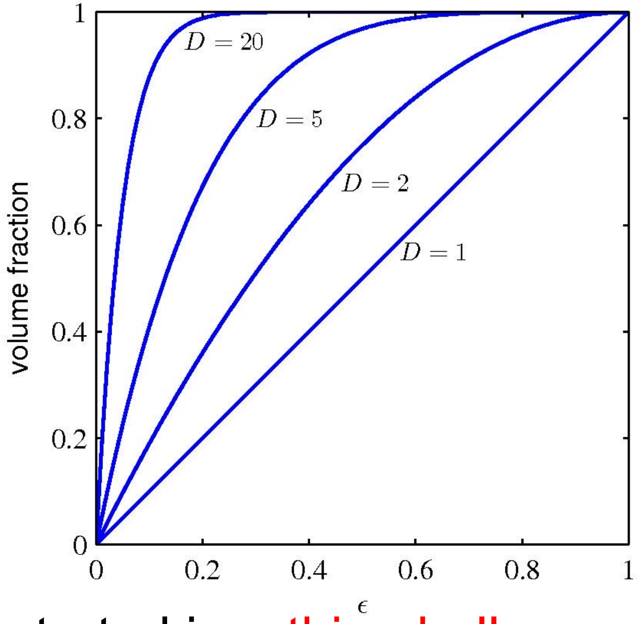
$$\frac{V_D(1)-V_D(1-\varepsilon)}{V_D(1)} = 1-(1-\varepsilon)^D$$

where

$$V_D(r) = \text{Vol. of a D-dim sphere of radius } r$$

$$= K_D r^D$$

for some constant K_D.



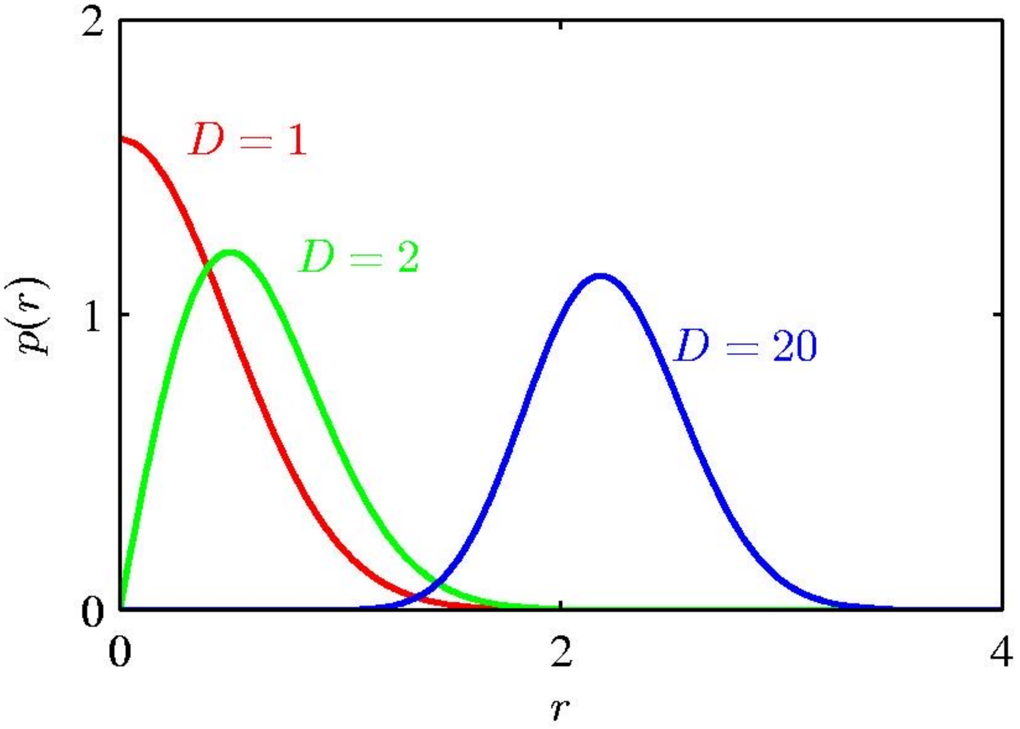
=> As D >> 1, most of the vol. of the sphere is concentrated in a thin-shell near the surface of the sphere…………………(**)

Assume data points are randomly scattered in the D-dim space under uniform density (i.e. const. # of data points per unit volume)

For an arbitrary data point P (whose position is taken as the origin), (**) implies that most of the neighboring points of P are of more or less the same distance from it (and NOT quite local to P) when D >> 1

Curse of Dimensionality (cont'd)

Gaussian Densities in
higher dimensions



Clustering Problem: SkyCat

- **A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands)**

- **Problem: Cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.**

- Sloan Digital Sky Survey is a newer, better version of this

Example: Clustering CD’s

- **Intuitively: Music divides into categories, and customers prefer a few categories**
  - But what are categories really?
- Represent a CD by a set of customers who bought it
- Similar CDs have similar sets of customers, and vice-versa

Example: Clustering CDs

Space of all CDs:

- Think of a space with one dim. for each customer
  - Values in a dimension may be 0 or 1 only
  - A CD is a point in this space is (x_1, x_2,…, x_k), where x_i = 1 iff the i th customer bought the CD
    - Compare with boolean matrix: rows = customers; cols. = CDs
- For Amazon, the dimension is tens of millions
- **Task:** Find clusters of similar CDs
- **An alternative:** Use Minhash/LSH to get Jaccard distance between “close” CDs
- Use that as input to clustering

Example: Clustering Documents

Finding topics:

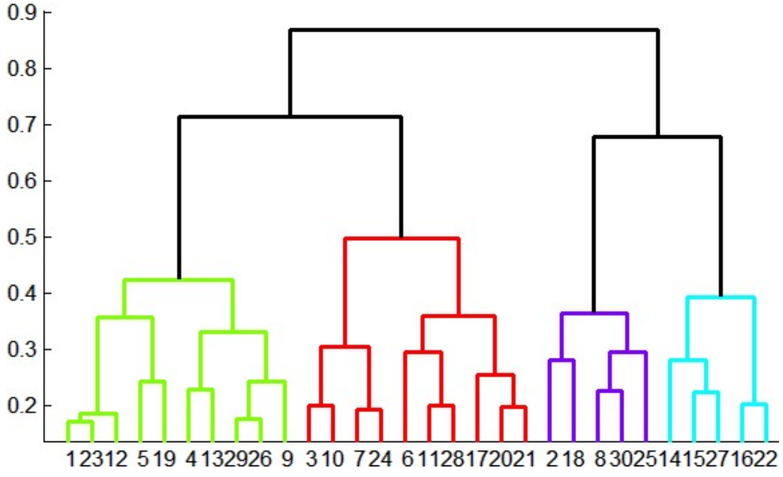
- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i th word (in some order) appears in the document
  - It actually doesn't matter if k is infinite; i.e., we don't limit the set of words

- **Documents with similar sets of words may be about the same topic**

Cosine, Jaccard, and Euclidean

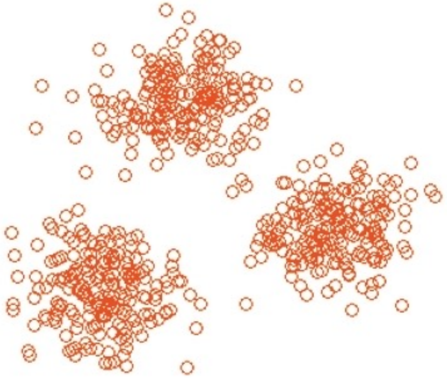
- **As with CDs we have a choice when we think of documents as sets of words or shingles:**
  - **Sets as vectors:** measure similarity by the cosine distance
  - **Sets as sets:** measure similarity by the Jaccard distance
  - **Sets as points:** measure similarity by Euclidean distance

Overview: Methods of Clustering

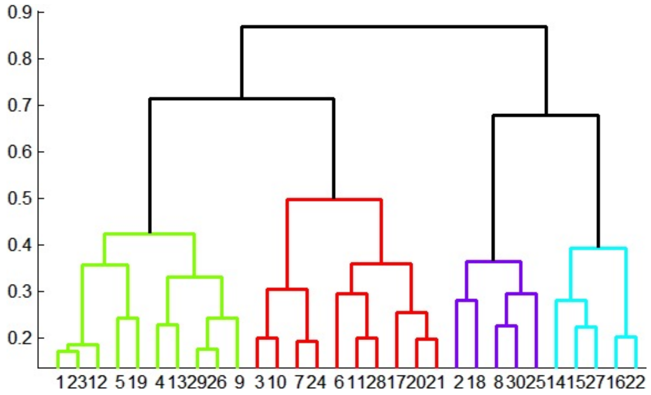


- **Hierarchical:**
  - **Agglomerative** (bottom up):
    - Initially, each point is a cluster
    - Repeatedly combine the two "nearest" clusters into one
  - **Divisive** (top down):
    - Start with one cluster and recursively split it

- **Point assignment:**
  - Maintain a set of clusters
  - Points belong to "nearest" cluster



Hierarchical Clustering



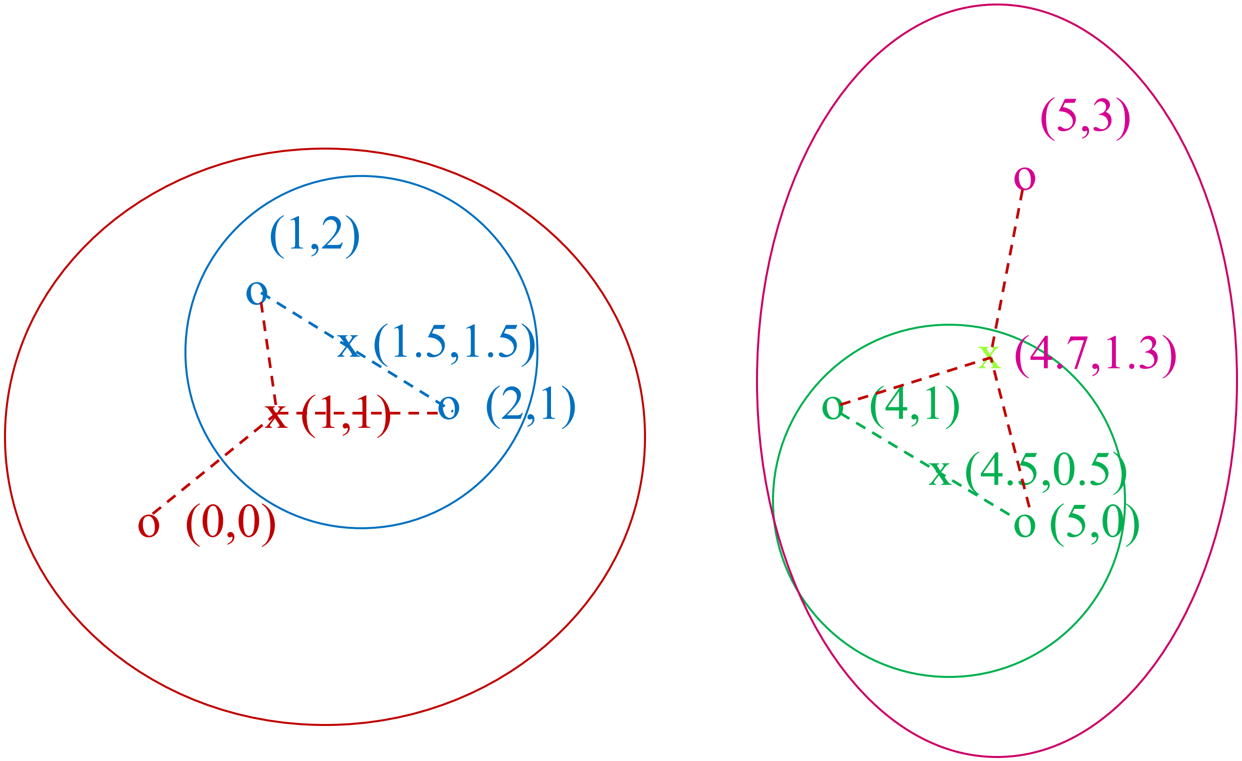
- **Key operation:**
  Repeatedly combine two nearest clusters

- **Three important questions:**
  - **1)** How do you represent a cluster of more than one point?
  - **2)** How do you determine the “nearness” of clusters?
  - **3)** When to stop combining clusters?

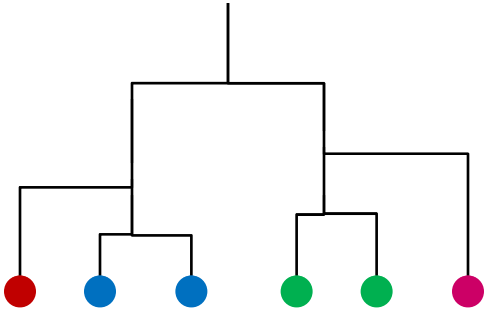
Hierarchical Clustering

- **Key operation: Repeatedly combine two nearest clusters**
- **(1) How to represent a cluster of many points?**
  - **Key problem:** As you build clusters, how do you represent the location of each cluster, to tell which pair of clusters is closest?
- **Euclidean case:** each cluster has a ***centroid*** = average of its (data)points
- **(2) How to determine "nearness" of clusters?**
  - Measure cluster distances by distances of centroids

Example: Hierarchical clustering



Data:
o … data point
x … centroid



Dendrogram

And in the Non-Euclidean Case?

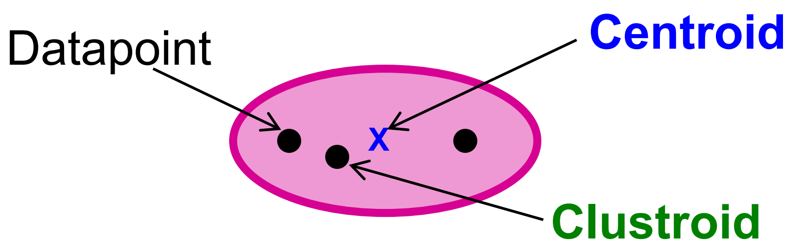
What about the Non-Euclidean case?

- The only "locations" we can talk about are the points themselves
  - i.e., there is no "average" of two points

- **Approach 1:**
  - **(1) How to represent a cluster of many points?**
    clustroid = (data)point "***closest*** " to other points
  - **(2) How do you determine the "nearness" of clusters?** Treat clustroid as if it were centroid, when computing intercluster distances

“Closest” Point?

- **(1) How to represent a cluster of many points?**
  clustroid = point “***closest*** ” to other points
- **Possible meanings of “closest”:**
  - Smallest maximum distance to other points
  - Smallest average distance to other points
  - Smallest sum of squares of distances to other points
    - For distance metric ***d*** clustroid ***c*** of cluster ***C*** is: $\min_{c} \sum_{x \in C} d(x,c)^2$



Cluster on
3 datapoints

Centroid is the avg. of all (data)points in the cluster. This means centroid is an “artificial” point.
Clustroid is an **existing** (data)point that is “closest” to all other points in the cluster.

Defining "Nearness" of Clusters

- **(2) How do you determine the "nearness" of clusters?**
  - **Approach 2:**
    Intercluster distance = minimum of the distances between any two points, one from each cluster
  - **Approach 3:**
    Pick a notion of "**cohesion**" of clusters, *e.g.*, maximum distance from the clustroid
    - Merge clusters whose *union* is most cohesive

Cohesion

- **Approach 3.1:** Use the **diameter** of the merged cluster = maximum distance between points in the cluster
- **Approach 3.2:** Use the **average distance** between points in the cluster
- **Approach 3.3:** Use a **density-based approach**
  - Take the diameter or avg. distance, e.g., and divide by the number of points in the cluster
  - Perhaps raise the number of points to a power first, e.g., square-root

Implementation

- **Naïve implementation of hierarchical clustering:**
  - At each step, compute pairwise distances between all pairs of clusters, then merge
  - O(N^3)

- Careful implementation using priority queue can reduce time to O(N^2 log N)
  - **Still too expensive for really big datasets that do not fit in memory**

k-means clustering

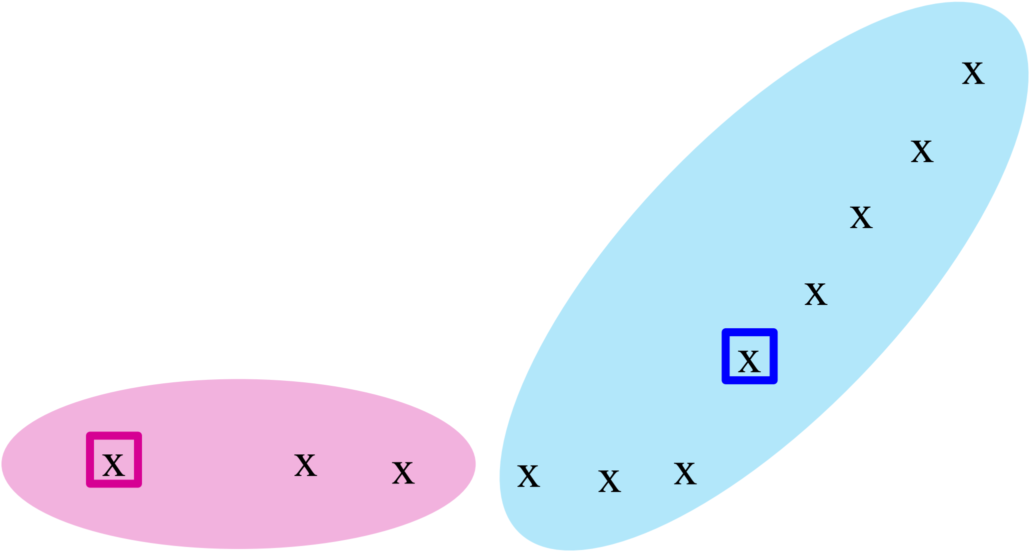
k–means Algorithm(s)

- Assumes Euclidean space/distance
- Start by picking ***k***, the number of clusters
- Initialize clusters by picking one point per cluster
  - **Example:** Pick one point at random, then ***k*-1** other points, each as far away as possible from the previous points

Populating Clusters

- **1)** For each point, place it in the cluster whose current centroid it is nearest
- **2)** After all points are assigned, update the locations of centroids of the ***k*** clusters
- **3)** Reassign all points to their closest centroid
  - Sometimes moves points between clusters
- **Repeat 2 and 3 until convergence**
  - **Convergence:** Points don’t move between clusters and centroids stabilize

Example: Assigning Clusters

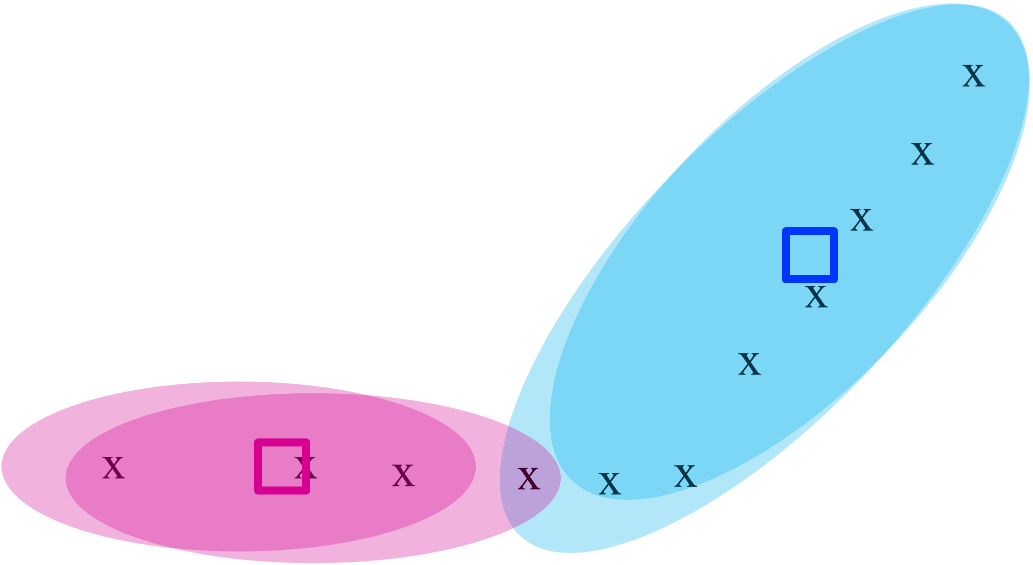


x … data point

□ … centroid

Clusters after round 1

Example: Assigning Clusters

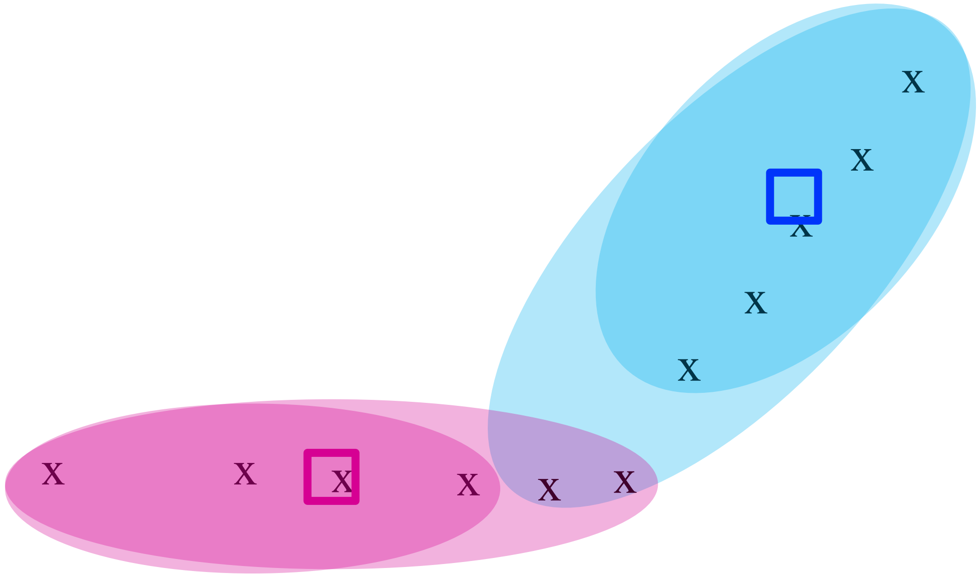


x … data point

□ … centroid

Clusters after round 2

Example: Assigning Clusters



x … data point

□ … centroid

Clusters at the end

K-means

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

Mean of the points in the cluster:

$$\mu(\mathrm{C}) = \frac{1}{|C|} \sum_{x \in C} x$$

K-means loss function

K-means tries to minimize what is called the “k-means” loss function:

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

that is, the sum of the squared distances from each point to the associated cluster center

Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Does each step of k-means move towards reducing this loss function (or at least not increasing)?

Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Sketch of proof/ argument:

1. Any other assignment would end up in a larger loss

1. The mean of a set of values minimizes the squared error

Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

---

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

Does this mean that k-means will always find the minimum loss/clustering?

Minimizing k-means loss

Iterate:

1. Assign/cluster each example to closest center
2. Recalculate centers as the mean of the points in a cluster

---

$$loss = \sum_{i=1}^{n} d(x_i, \mu_k)^2 \quad \text{where } \mu_k \text{ is cluster center for } x_i$$

NO! It will find *a minimum*.

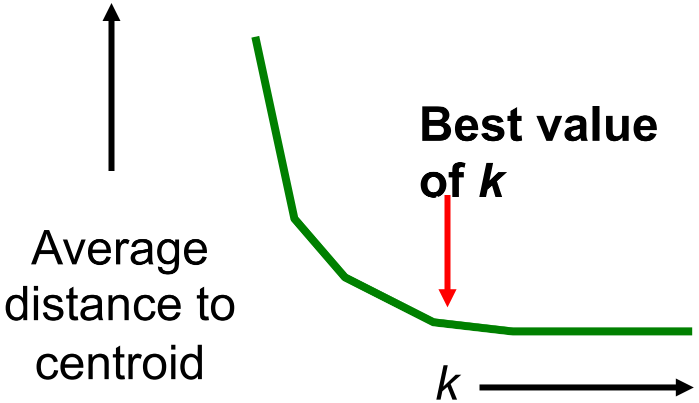
Unfortunately, the k-means loss function is generally not convex and for most problems has many, many minima

We're only guaranteed to find one of them
=> It's therefore important to try different random seeds

Getting the *k* right

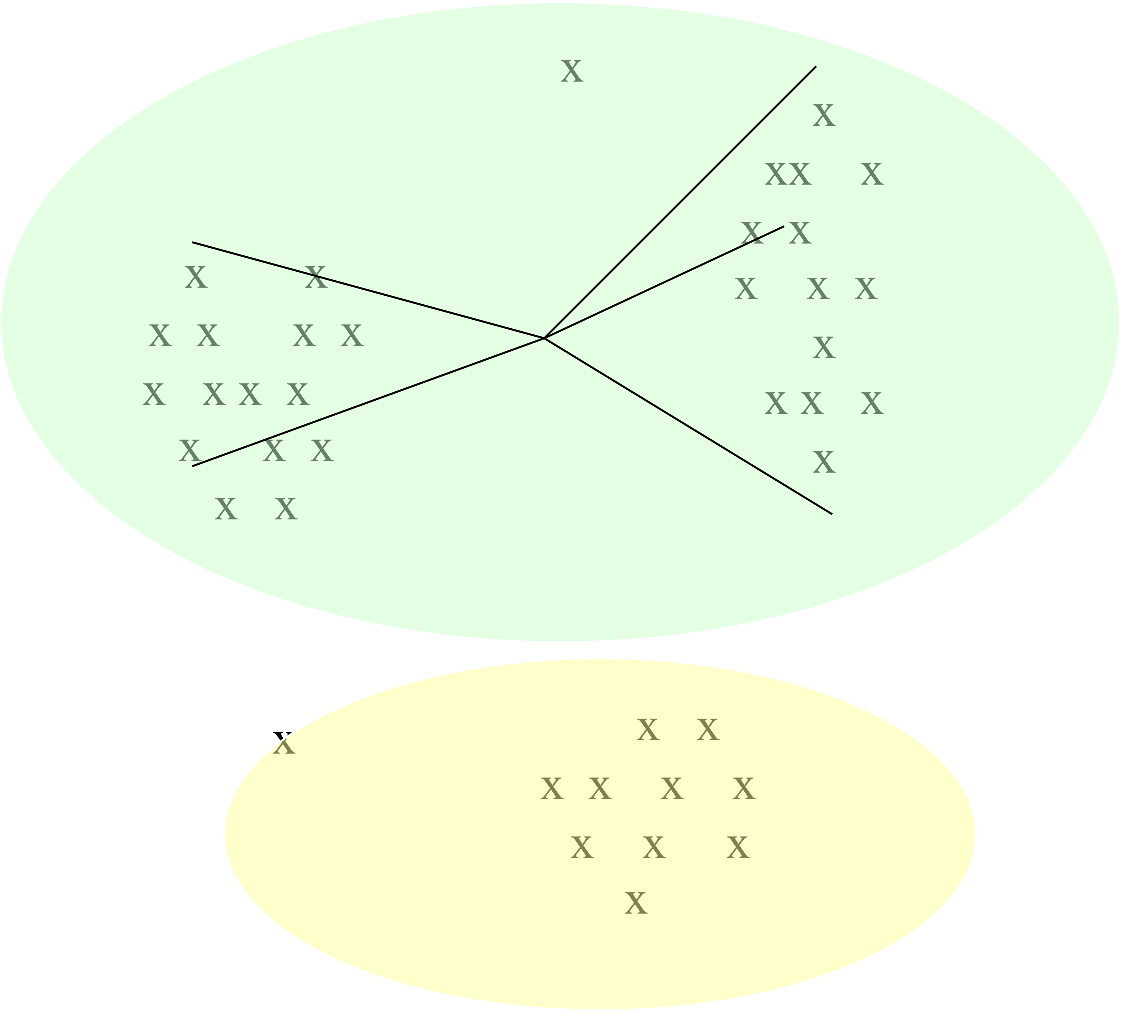
How to select *k*?

- Try different *k*, looking at the change in the average distance to centroid, as *k* increases.
- Average falls rapidly until right *k*, then changes little



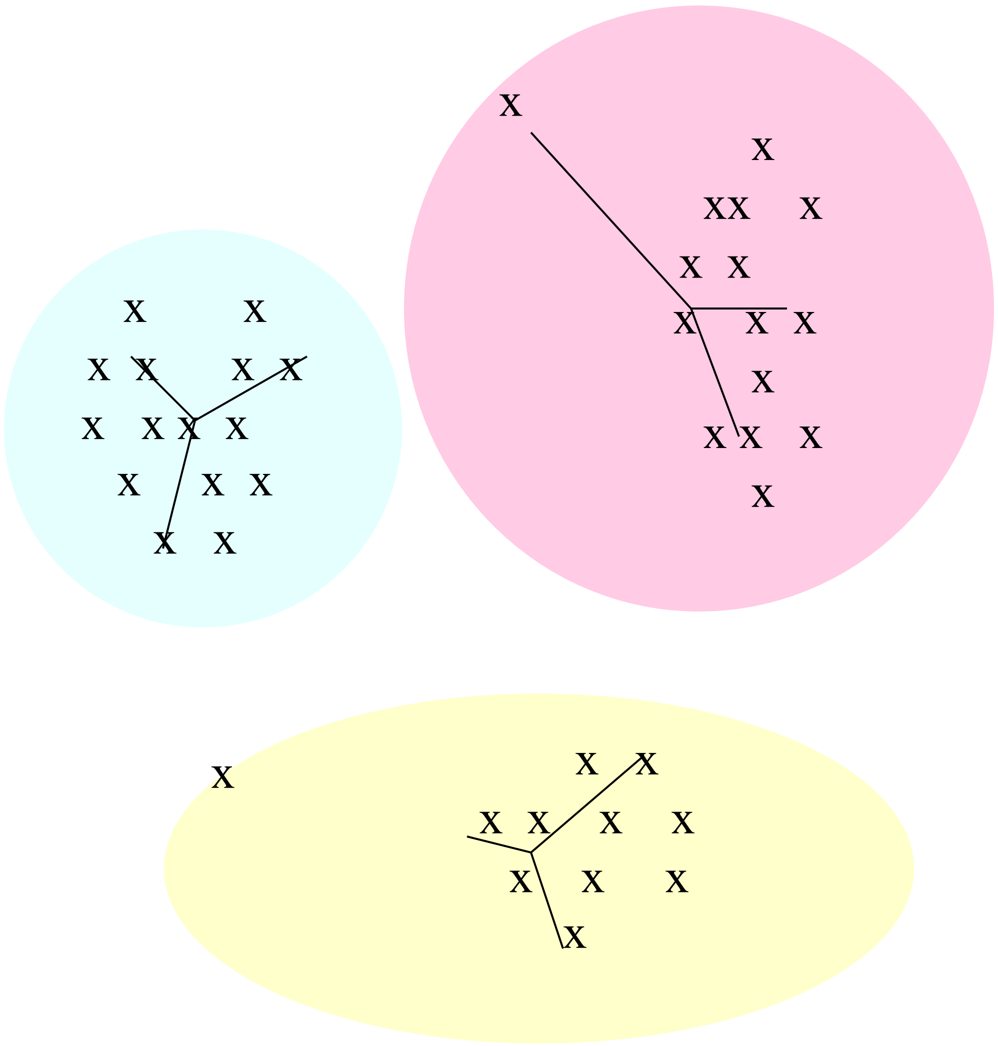
Example: Picking *k*

Too few;
many long
distances
to centroid.



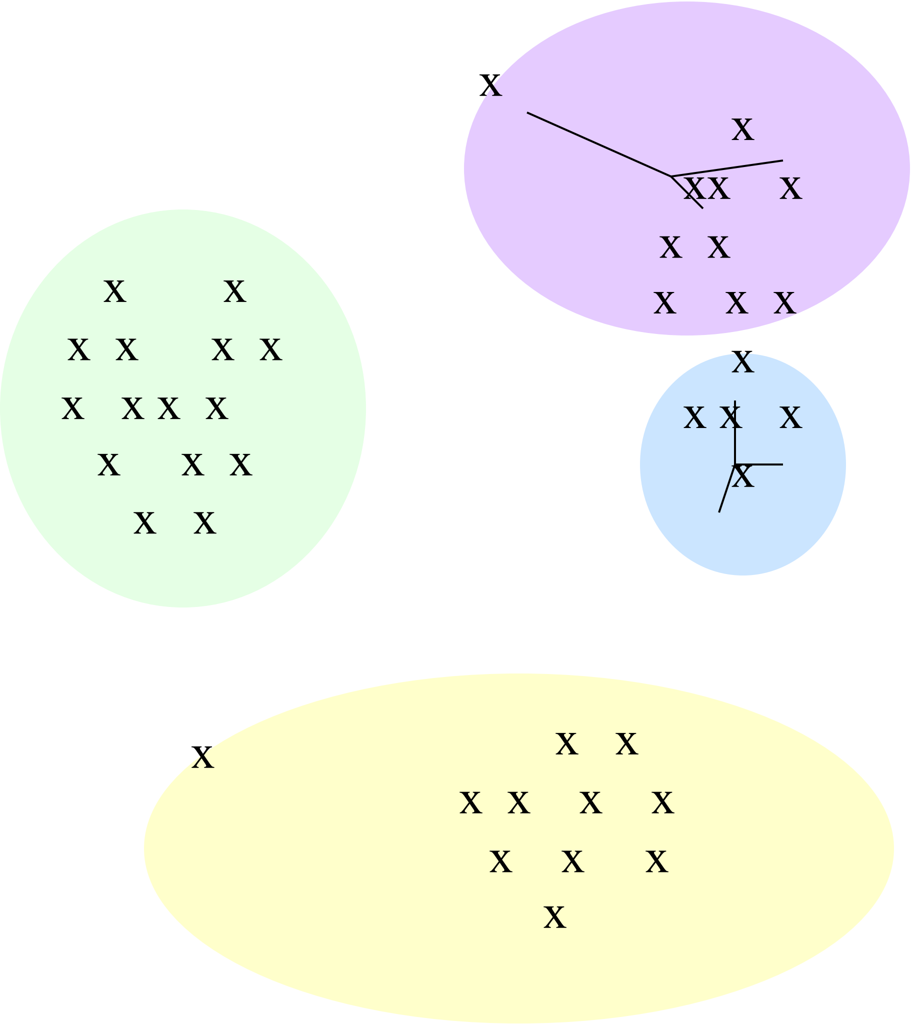
Example: Picking *k*

Just right;
distances
rather short.



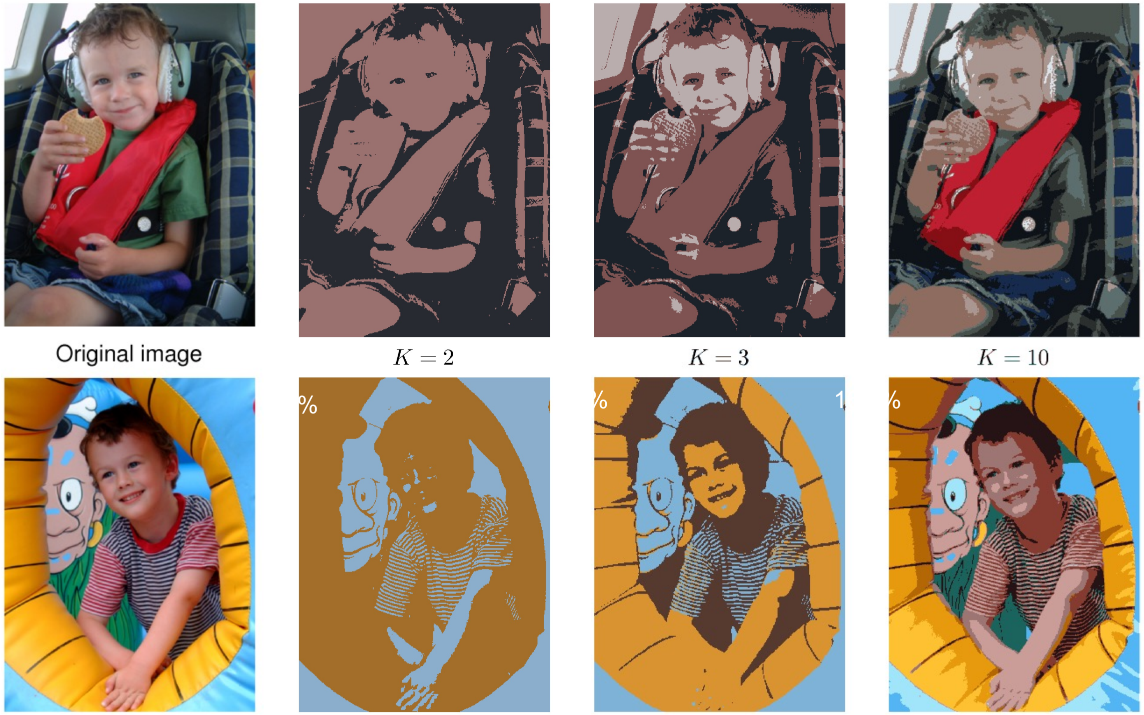
Example: Picking *k*

Too many;
little improvement in average distance.



Examples of k-means clustering

- Clustering RGB vectors of pixels in images
- Compression of image file: N x 24 bits
  - Store RGB values of cluster centers: K x 24 bits
  - Store cluster index of each pixel: N x log K bits



K-Means time complexity

Variables: *K* clusters, *n* data points,
m features/dimensions, *I* iterations

What is the runtime complexity?

- Computing distance between two points (e.g. Euclidean)
- Reassigning clusters
- Computing new centers
- Iterate…

K-Means time complexity

Variables: *K* clusters, *n* data points,
m features/dimensions, *I* iterations

What is the runtime complexity?

- Computing distance between two points is O*(m)* where *m* is the dimension of the vectors/number of features.
- Reassigning clusters: O*(Kn)* distance computations, or O*(Knm)*
- Computing centroids: Each points gets added once to some centroid: O*(nm)*
- Assume these two steps are each done once for *I* iterations: O*(IKnm)*

In practice, K-means converges quickly and is fairly fast

Limitations of K-means

- Need to determine "K" via domain knowledge or heuristics (as stated before)
- Only converge to local optimal
  - Need to try multiple starting points
  - Nice and Practical Research results on "Careful Randomized Seeding" in available, e.g. :
    - K-means++ and
    - K-means // (aka K-means parallel)

    Refer to the "More on K-means" supplementary lecture notes in course website.
- "Hard" assignment of each data point to a single cluster:
  - Each data point can only be assigned to 1 cluster (class)
  - What about points that lie in between groups ? e.g. Jazz + Classical
- Overall results can be affected by a few Outliners

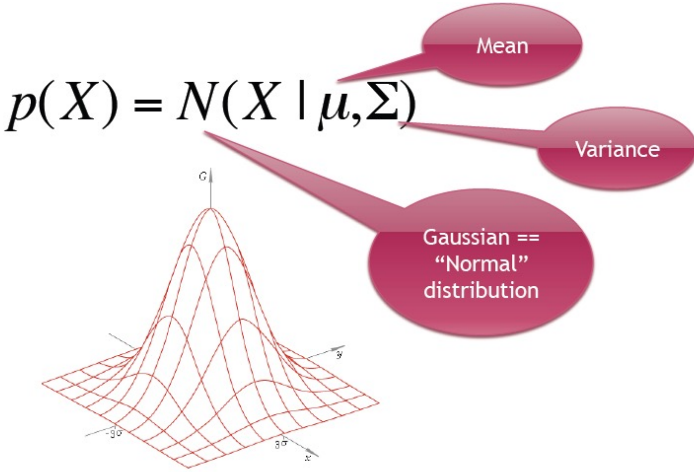
Can we do better ?

The famous “GMM” – The Gaussian Mixture Model

Key Idea:

Assume Gaussian distribution of data points

within each cluster



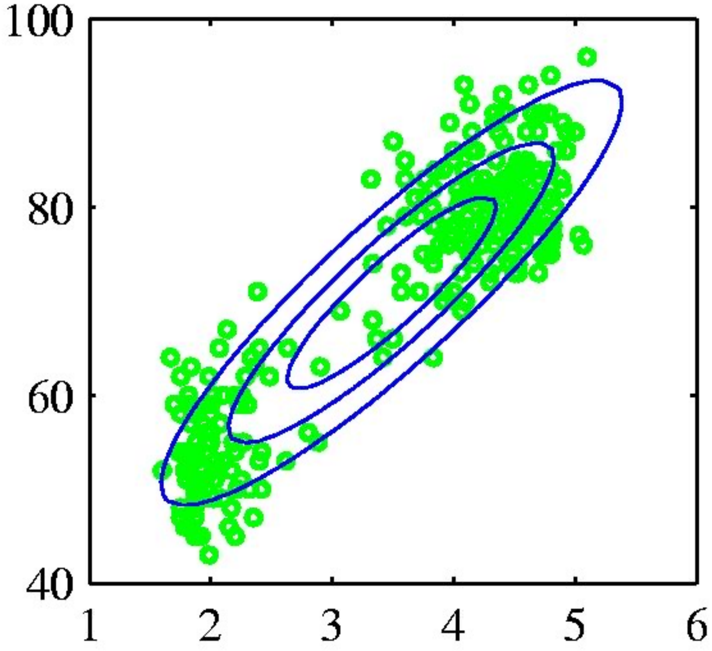
$$p(X) = N(X \mid \mu, \Sigma)$$

Mean

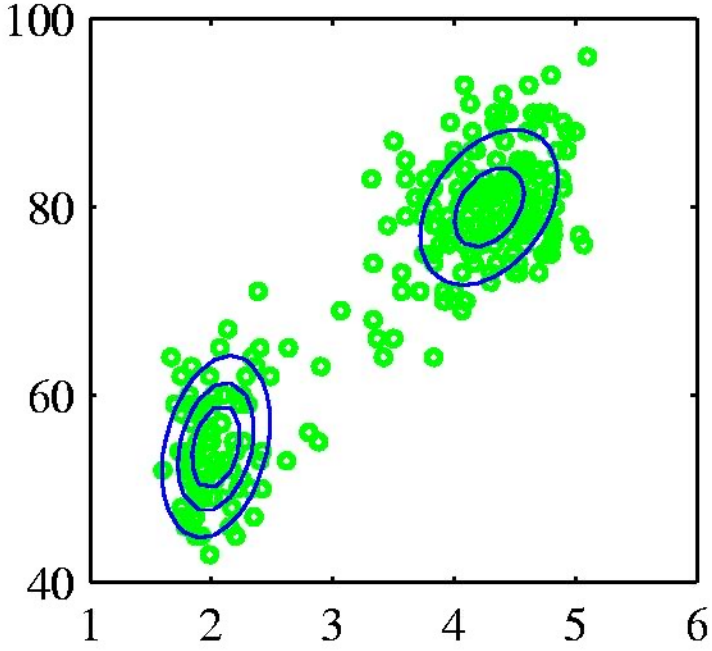
Variance

Gaussian == “Normal” distribution

- A sample data set



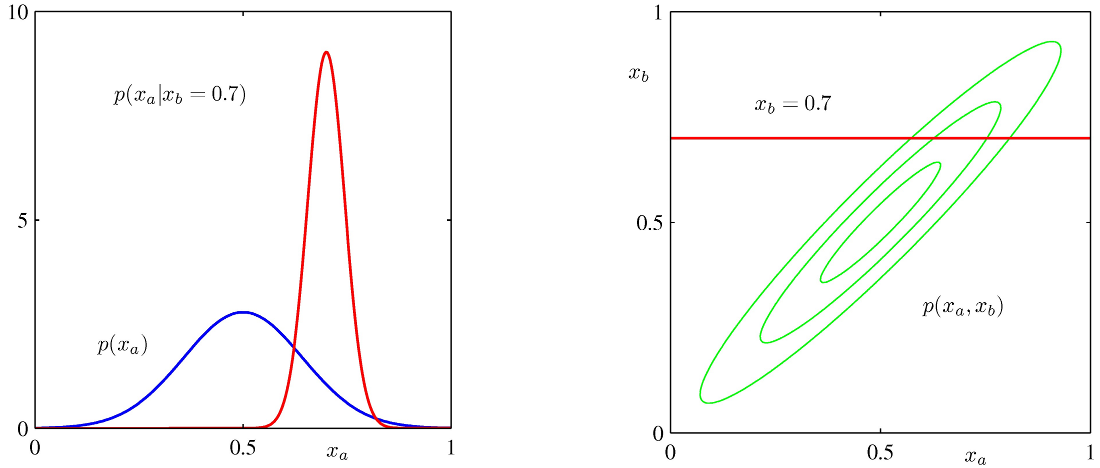
Single Gaussian



Mixture of two Gaussians

Clustering with Gaussian mixture density

- Each cluster represented by Gaussian density
  - Center, as in K-means
  - Covariance matrix: cluster spread around center



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

Data dimension d

Determinant of covariance matrix Σ

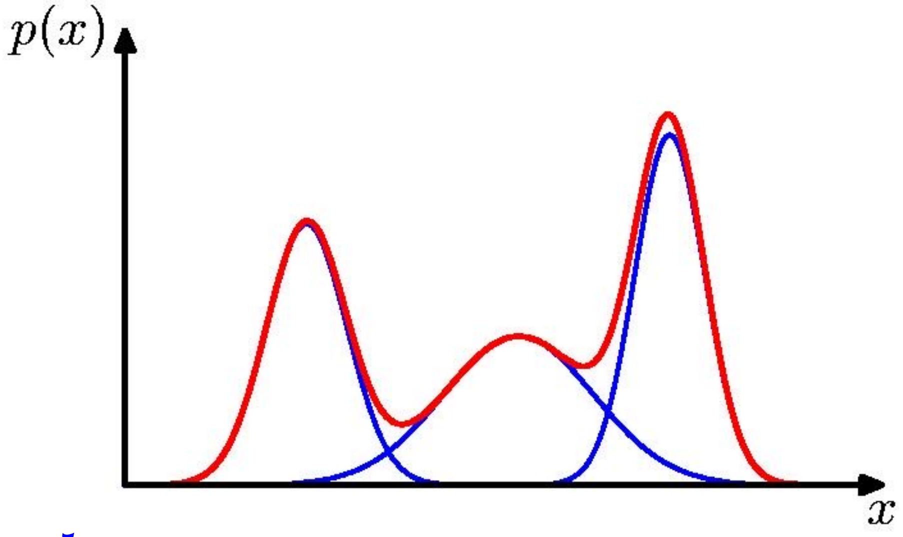
Quadratic function of point x and mean μ

The Gaussian Mixture Model (GMM) (cont’d)

Combine simple models into a complex model:

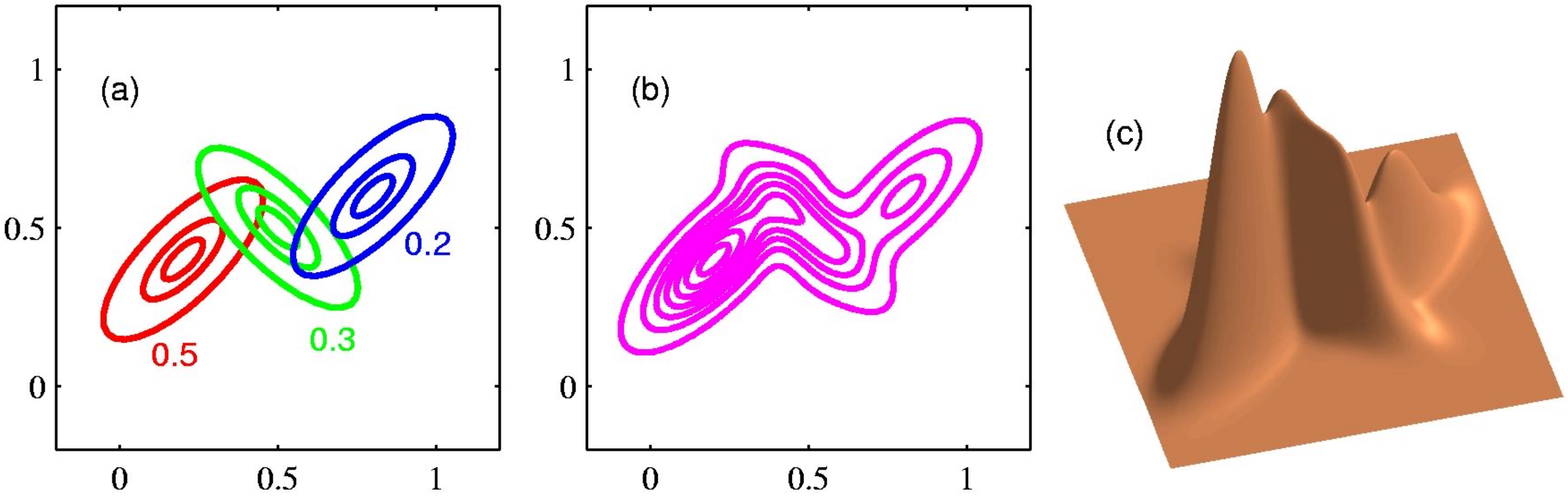
$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \underbrace{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

Mixing coefficient: can be seen as the “contribution” from Gaussian component k

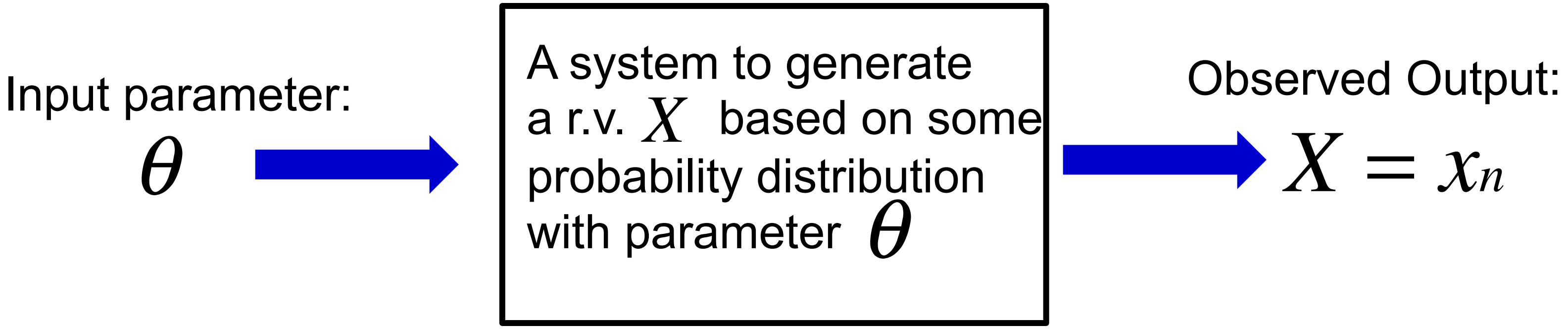


$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

The Gaussian Mixture Model (GMM) (cont'd)



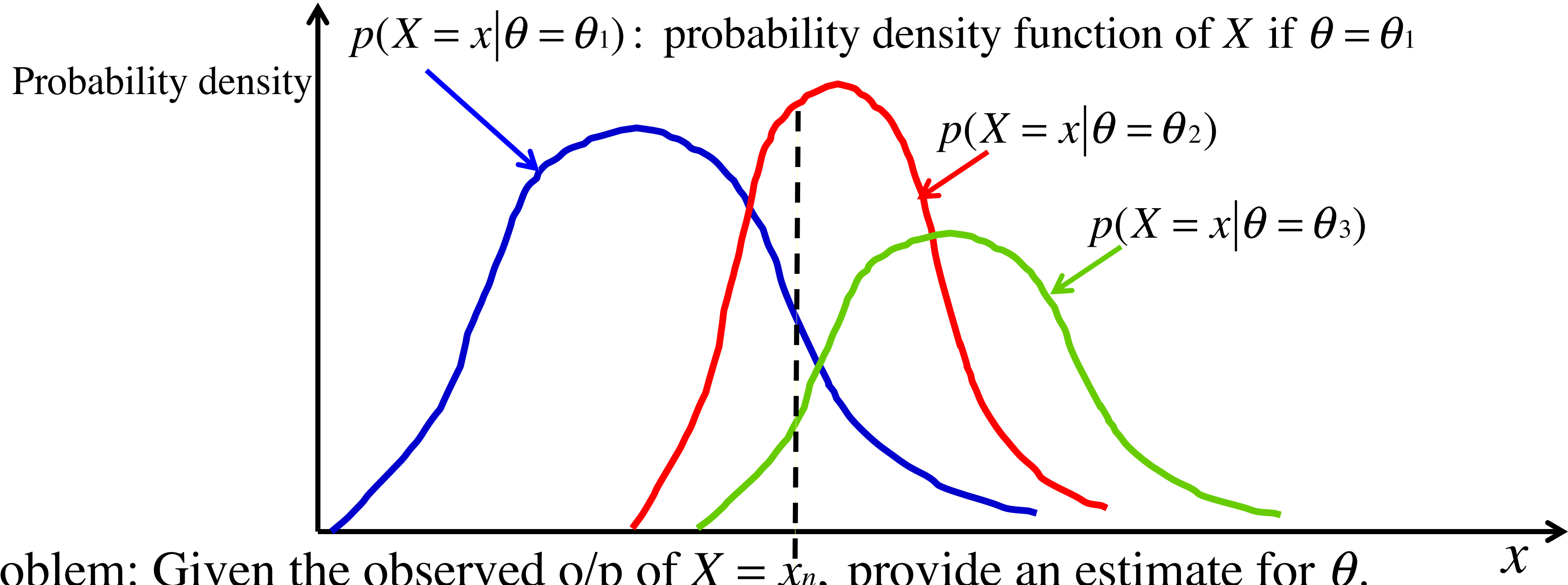
The Maximum Likelihood Estimator (MLE)



Input parameter: θ

A system to generate a r.v. X based on some probability distribution with parameter θ

Observed Output: $X = x_n$

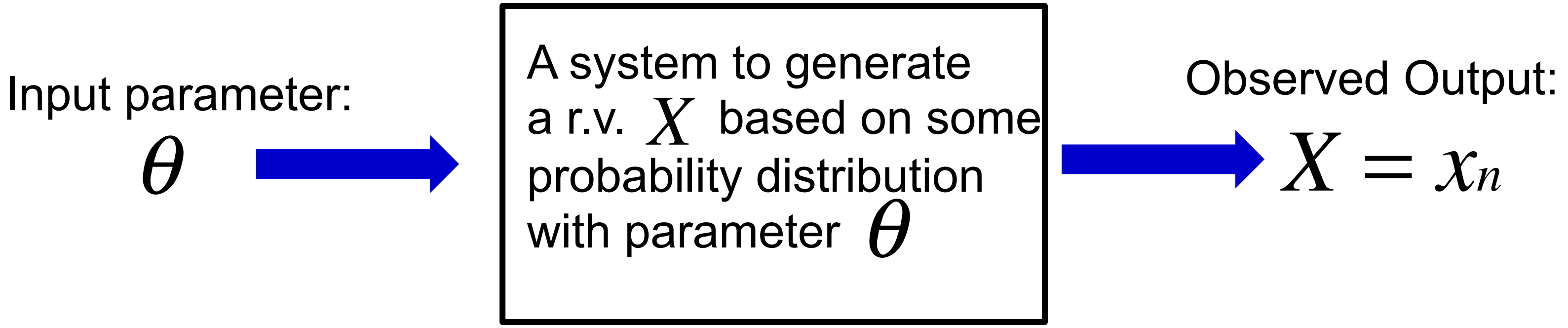


Problem: Given the observed o/p of $X = x_n$, provide an estimate for θ.

$$\theta^*_{MLE} = \text{Max. Likelihood Estimator (MLE) of } \theta = \arg\{\max_{\theta i}[p(X = x_n|\theta = \theta_i)]\}$$

and in the above example, $\theta^*_{MLE} = \theta_2$

An Alternative Estimator: The Maximum A Posteriori (MAP) Estimator


Input parameter:
θ
A system to generate a r.v. X based on some probability distribution with parameter θ
Observed Output:
$X = x_n$

$$\theta^*_{MAP} = \text{Max. a posteriori estimator (MAP) of } \theta = \arg\{\max_{\theta i}[p(\theta = \theta_i | X = x_n)]\}$$

$$= \arg\{\max_{\theta i}[\frac{p(X = x_n \text{ and } \theta = \theta_i)}{p(X = x_n)}]\} = \arg\{\max_{\theta i}[\frac{p(X = x_n | \theta = \theta_i) p(\theta = \theta_i)}{p(X = x_n)}]\}$$

$$= \arg\{\max_{\theta i}[p(X = x_n | \theta = \theta_i) p(\theta = \theta_i)]\}$$

The "true" probability distribution, $p(\theta)$, of the parameter, i.e. θ, to be estimated is the so-called prior distribution.

If no prior knowledge about the distribution of θ is available,

we can assume $p(\theta) \sim$ uniform distribution, i.e. $p(\theta = \theta_i) =$ some constant.

In this case, we have $\theta^*_{MAP} = \theta^*_{MLE}$

The Gaussian Mixture Model (GMM) (cont'd)

- Given the set of N data points represented by a matrix $\mathbf{X}$, we find the model parameters π , μ and Σ (which are vectors and a matrices) which maximize the probability of the occurrence of the observed data, via the Maximum (log) Likelihood Estimation (MLE) approach

$$p(X|\pi,\mu,\Sigma)=\prod_{n=1}^{N}p(x_n)=\prod_{n=1}^{N}\sum_{k=1}^{K}\pi_k\mathcal{N}(x_n|\mu_k,\Sigma_k)$$

$$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N} \underbrace{\ln\left\{\sum_{k=1}^{K}\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}}_{\text{Log of a sum; no closed form maximum}}$$

- Solution: use standard, iterative, numeric optimization methods or the *Expectation Maximization (EM)* algorithm (see next slides and Chapter 9 of PRML of C.M.Bishop).

How to Maximizing Log Likelihood for GMM

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

Maximum of log likelihood:

derivatives of $\ln p(\mathbf{X}|\pi, \mu, \Sigma)$ w.r.t parameters to 0.

$$\gamma(z_{k,n}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \qquad N_k = \sum_{n=1}^{N} \gamma(z_{k,n})$$

$\gamma(z_{k,n})$ is called a “responsibility”: how much is this Gaussian k responsible for this point X_n?

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{k,n}) \mathbf{x}_n \qquad \pi_k^{\text{new}} = \frac{N_k}{N}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{k,n}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\mathrm{T}}$$

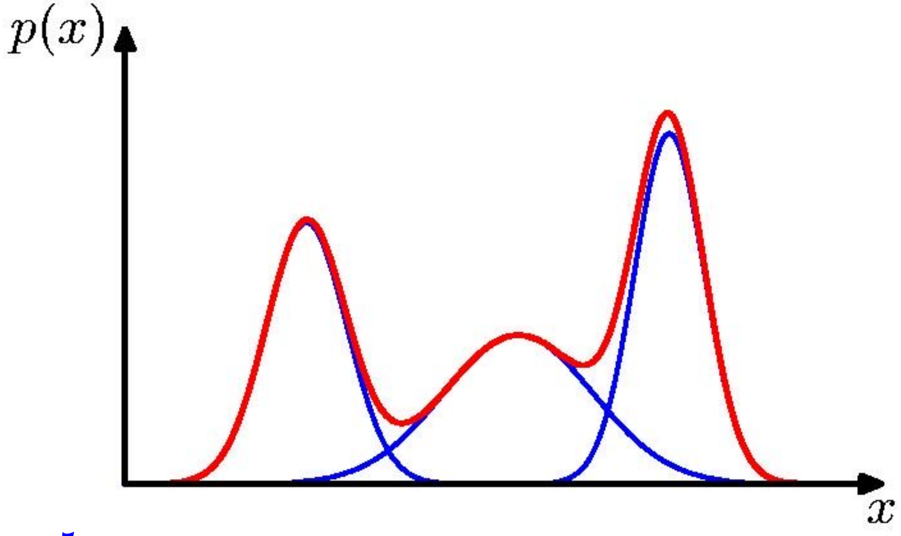
The Gaussian Mixture Model (GMM) (cont’d)

Combine simple models into a complex model:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \underset{\uparrow}{\pi_k} \underbrace{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

Mixing coefficient: can be seen as the “contribution” from Gaussian component k

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$



Derivation of MLE for GMM

Maximum of log likelihood:
derivatives of $\ln p(\mathbf{X}|\pi, \mu, \Sigma)$ w.r.t parameters to 0.

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k) \right\}$$

For the μ_k-:

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

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_k \pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}}_{\gamma(z_{k,n})} \Sigma_k^{-1}(\mathbf{x}_n - \mu_k)$$

$$\mu_k = \frac{1}{\sum_n \gamma(z_{k,n})} \sum_n \gamma(z_{k,n}) \mathbf{x}_n$$

$\gamma(z_{k,n}) \equiv \text{Prob}(z_{k,n} = 1 \mid x_n)$ where $z_{k,n} = 1$ iff the n^{th} data point x_n is generated by cluster k

$N_k \equiv \sum_n \gamma(z_{k,n}) =$ effective number of data points in the k^{th}cluster.

Derivation of MLE for GMM (cont'd)

For Σ_k:

$$\Sigma_k = \frac{1}{\sum_n \gamma(z_{kn})} \sum_n \gamma(z_{kn})(\mathbf{x}_n - \mu_k)(\mathbf{x}_n - \mu_k)^T$$

For the π_k:

- Take into account constraint $\sum_k \pi_k = 1$
- Lagrange multiplier

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) + \lambda(\sum_k \pi_k - 1)$$

$$0 = \sum_n \frac{\mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_k \pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)} + \lambda$$

Multiply by π_k and summing over k, we get $\lambda = -N \Rightarrow \pi_k = \frac{\sum_n \gamma(z_{kn})}{N}$

The Gaussian Mixture Model (GMM)

- Given the set of N data points represented by a matrix $\mathbf{X}$, we find the model parameters π , μ and Σ (which are vectors and a matrices) which maximize the probability of the occurrence of the observed data, via the Maximum (log) Likelihood Estimation (MLE) approach

$$p(X|\pi,\mu,\Sigma) = \prod_{n=1}^{N} p(x_n) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k,\Sigma_k)$$

$$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N} \underbrace{\ln\left\{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}}_{\text{Log of a sum; no closed form maximum}}$$

- Solution: use standard, iterative, numeric optimization methods or the *Expectation Maximization (EM)* algorithm (see next slides and Chapter 9 of PRML of C.M.Bishop).

Summary: How to Maximizing Log Likelihood for GMM

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

Maximum of log likelihood:

derivatives of $\ln p(\mathbf{X}|\pi, \mu, \Sigma)$ w.r.t parameters to 0.

$$\gamma(z_{k,n}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \qquad N_k = \sum_{n=1}^{N} \gamma(z_{k,n})$$

$\gamma(z_{k,n})$ is called a "responsibility": how much is this Gaussian k responsible for this point X_n?

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{k,n}) \mathbf{x}_n \qquad \pi_k^{\text{new}} = \frac{N_k}{N}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{k,n}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$$

Derivation of MLE for the Mixture of Gaussian model (cont’d)

- No closed form solutions: $\gamma(z_{k,n})$ depends on parameters
- But these equations suggest simple iterative scheme for finding maximum likelihood:
  Alternate between estimating the current $\gamma(z_{k,n})$ and updating the parameters $\{\mu_k, \Sigma_k, \pi_k\}$.

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

1. Initialize the parameters: means μ_k , covariances Σ_k and mixing coeff. π_k of the K Gaussian components.
2. E Step: Assign each point x_n an assignment score $\gamma(z_{k,n})$ for each cluster k
3. M Step: Given scores, adjust μ_k, Σ_k , π_k for each cluster k
4. Evaluate Likelihood value. If likelihood value or parameters converge, stop ; Otherwise Goto Step 2. (the E Step)

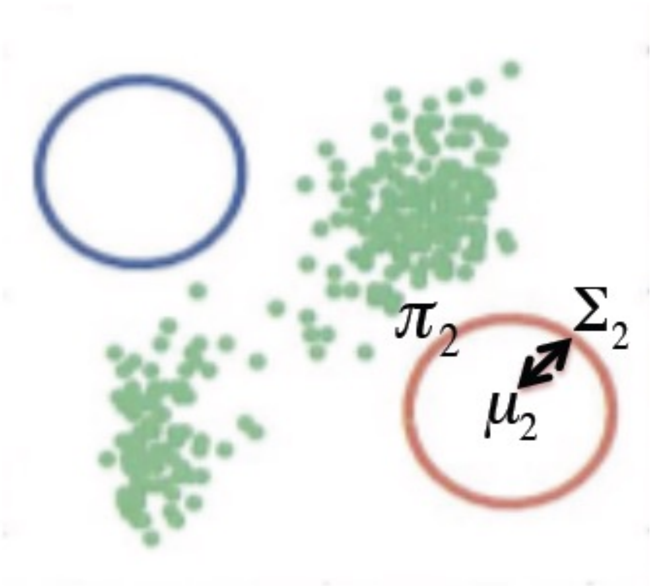
where

$z_{k,n}$ is the 0-1 indicator r.v. showing whether x_n belongs to cluster k

$\gamma(z_{k,n})$ is an estimate of the posterior probability that data point x_n is “contributed” by cluster k , i.e. the conditional probability that x_n belongs to cluster k given the value of x_n and parameters μ_k , Σ_k , π_k

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

1. Initialize μ_k , Σ_k π_k , one for each Gaussian k



- Tip! Use K-means result to initialize:

$$\mu_k \leftarrow \mu_k$$

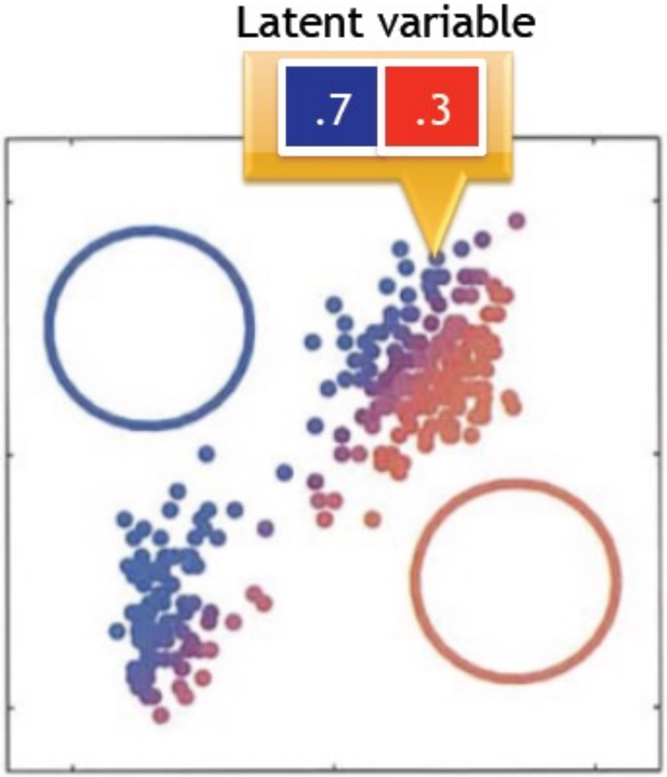
$$\Sigma_k \leftarrow \mathrm{cov}(cluster(K))$$

$$\pi_k \leftarrow \frac{\text{Number of points in k}}{\text{Total number of points}}$$

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

2. **E Step:** For each point X_n, determine its assignment score to each Gaussian k:

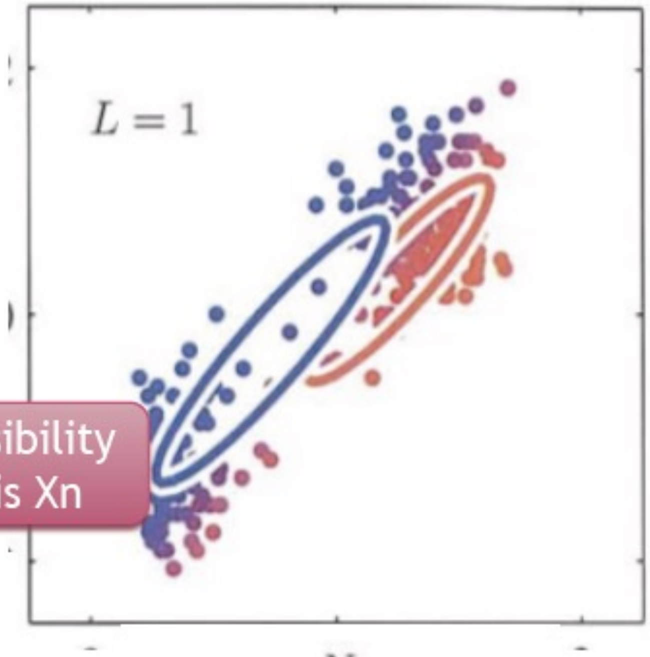
$$\gamma(z_{k,n}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$



$\gamma(z_{k,n})$ is called a “responsibility”: how much is this Gaussian k responsible for this point X_n?

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

3. **M Step:** For each Gaussian k, update parameters using new $\gamma(z_{k,n})$



Responsibility for this Xn

Mean of Gaussian k

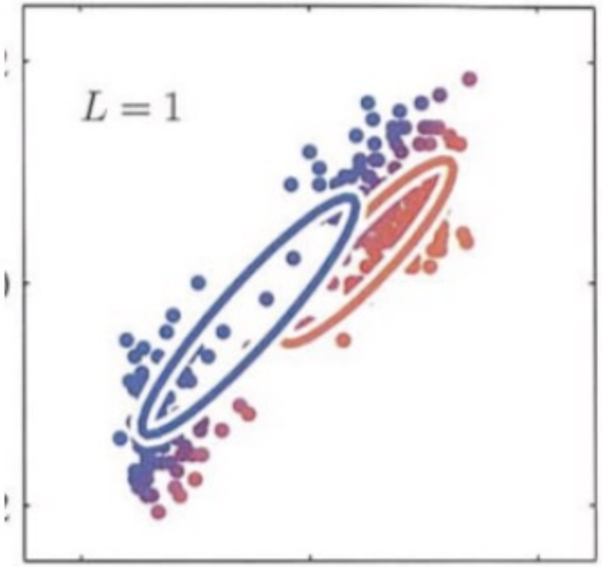
$$\mu_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{k,n})\,\mathbf{x}_n$$

$$N_k = \sum_{n=1}^{N}\gamma(z_{k,n})$$

Find the mean that “fits” the assignment scores best

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

3. **M Step:** For each Gaussian k, update parameters using new $\gamma(z_{k,n})$



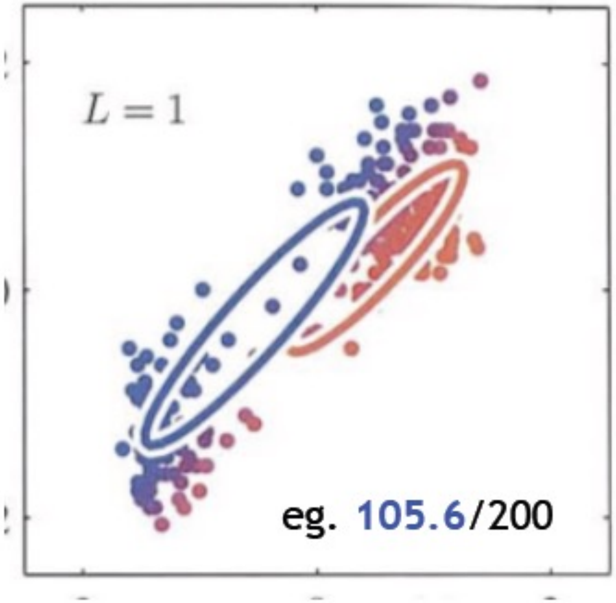
Covariance matrix of Gaussian k

$$\Sigma_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{k,n})\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$$

Just calculated this!

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

3. **M Step:** For each Gaussian k, update parameters using new $\gamma(z_{k,n})$



eg. 105.6/200

Mixing Coefficient for Gaussian k

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

Total # of points

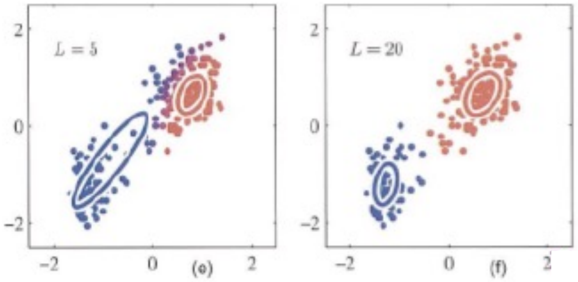
$$N_k = \sum_{n=1}^{N} \gamma(z_{k,n})$$

Expectation Maximization (EM) approach for the Gaussian Mixture Model (GMM)

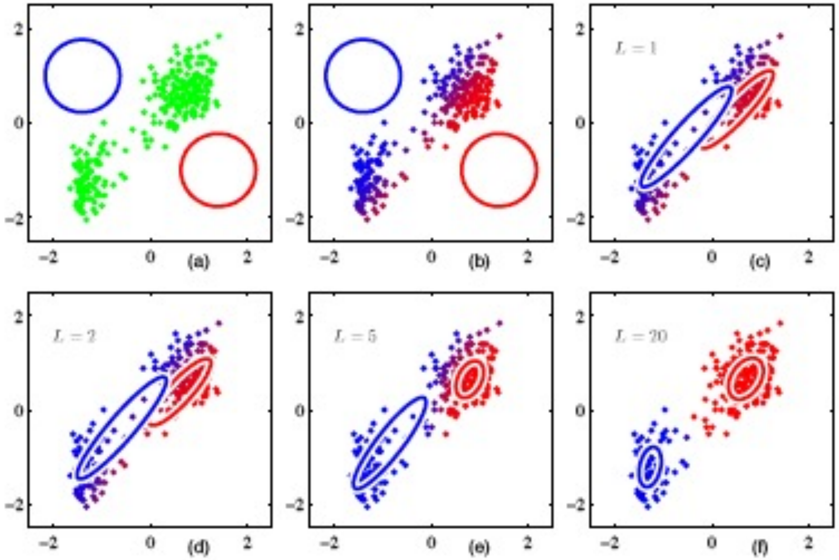
4. Evaluate log **likelihood**. If likelihood or parameters converge, stop. Else go to Step 2 (**E step**).

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \underline{\pi_k} \mathcal{N}(\mathbf{x}_n | \underline{\boldsymbol{\mu}_k}, \underline{\boldsymbol{\Sigma}_k}) \right\}$$

Likelihood is the probability for the observed data-set X to occur (i.e to be generated) given the current values of the parameters.



The EM approach for GMM (cont'd)



- More iterations needed to converge than K-means algorithm, and each cycle requires more computation
- Common, initialise parameters based K-means run.

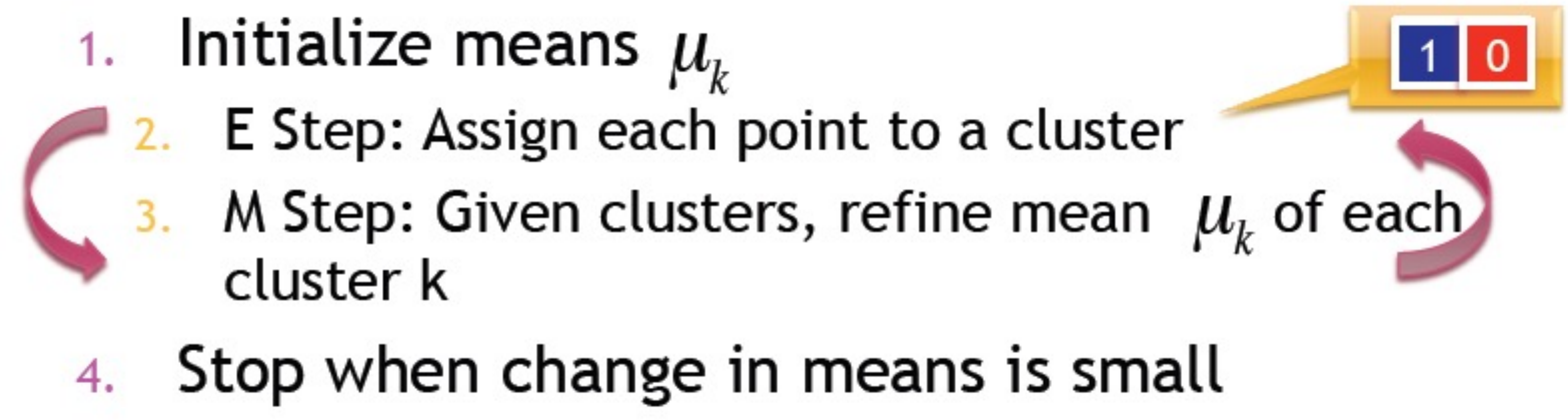
Recap: EM for GMM

The EM Algorithm

1. Initialize the parameters: means μ_k , covariances Σ_k and mixing coeff. π_k of the K Gaussian components.
2. E Step: Assign each point x_n an assignment score $\gamma(z_{k,n})$ for each cluster k
3. M Step: Given scores, adjust μ_k, Σ_k, π_k for each cluster k
4. Evaluate Likelihood value. If likelihood value or parameters converage, stop ; Otherwise Goto Step 2. (the E Step)

$\gamma(z_{k,n})$ is an estimate of the posterior probability that data point x_n is "contributed" by (or belongs to) cluster k, i.e. the conditional probability given the parameters μ_k, Σ_k, π_k and the observation x_n

Comparing to the K-means algorithm



1. Initialize means μ_k
   2. E Step: Assign each point to a cluster
   3. M Step: Given clusters, refine mean μ_k of each cluster k
4. Stop when change in means is small

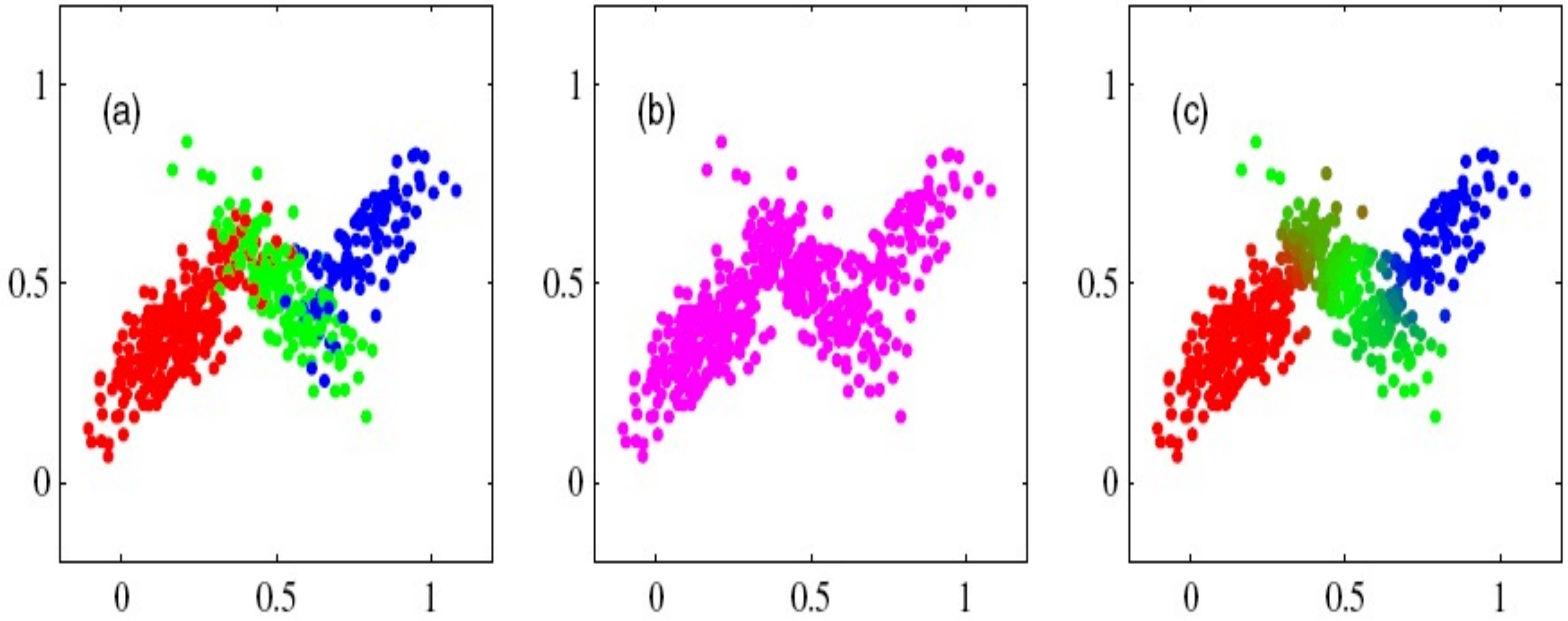
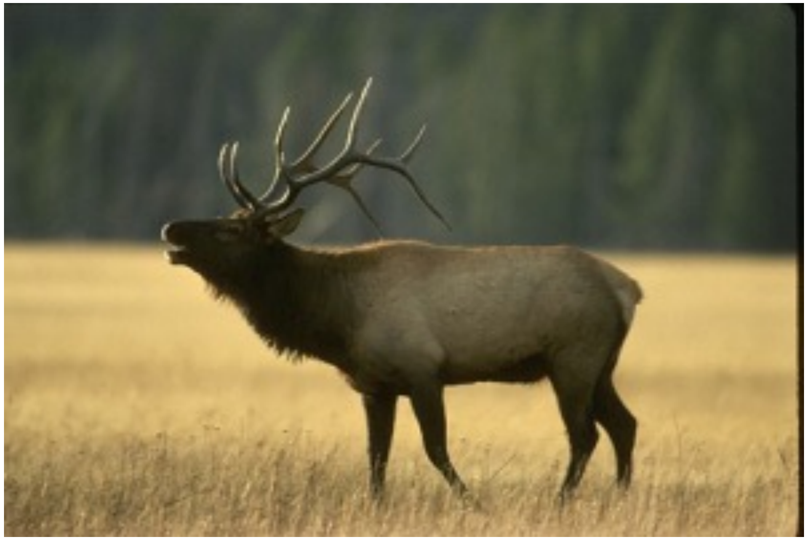


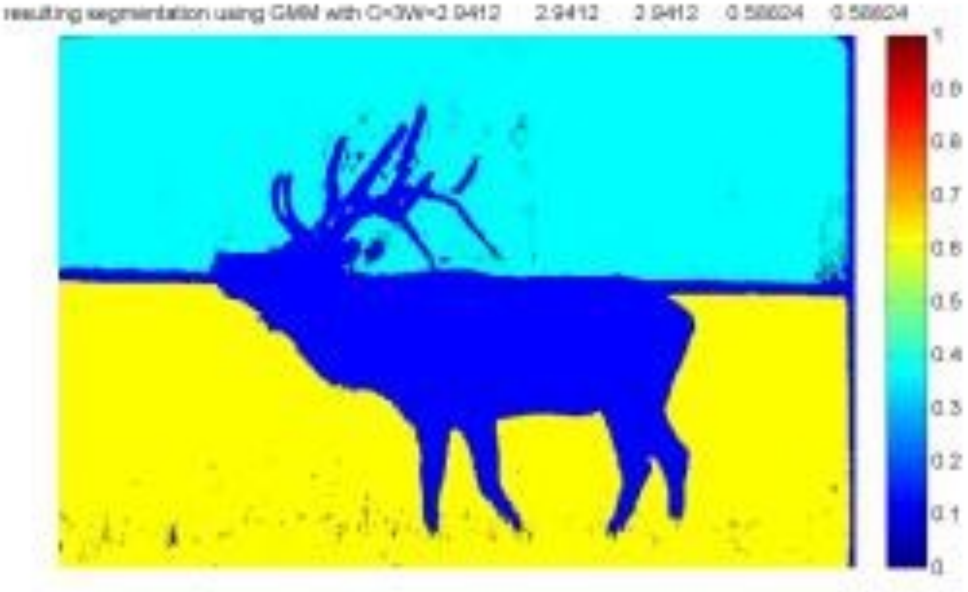
Figure 9.5 Example of 500 points drawn from the mixture of 3 Gaussians shown in Figure 2.23. (a) Samples from the joint distribution $p(\mathrm{z})p(\mathrm{x}|\mathrm{z})$ in which the three states of z, corresponding to the three components of the mixture, are depicted in red, green, and blue, and (b) the corresponding samples from the marginal distribution $p(\mathrm{x})$, which is obtained by simply ignoring the values of z and just plotting the x values. The data set in (a) is said to be *complete*, whereas that in (b) is *incomplete*. (c) The same samples in which the colours represent the value of the responsibilities $\gamma(z_{nk})$ associated with data point x_n, obtained by plotting the corresponding point using proportions of red, blue, and green ink given by $\gamma(z_{nk})$ for $k = 1, 2, 3$, respectively

Application: Using GMM for Image Segmentation

Source:
https://kittipatkampa.wordpress.com/2011/02/17/image-segmentation-using-gaussian-mixture-models/



Original Image



Segmentation results using GMM with 3 components

Input Features:

x-y pixel locations & pixel lightness/color in L*a*b color space

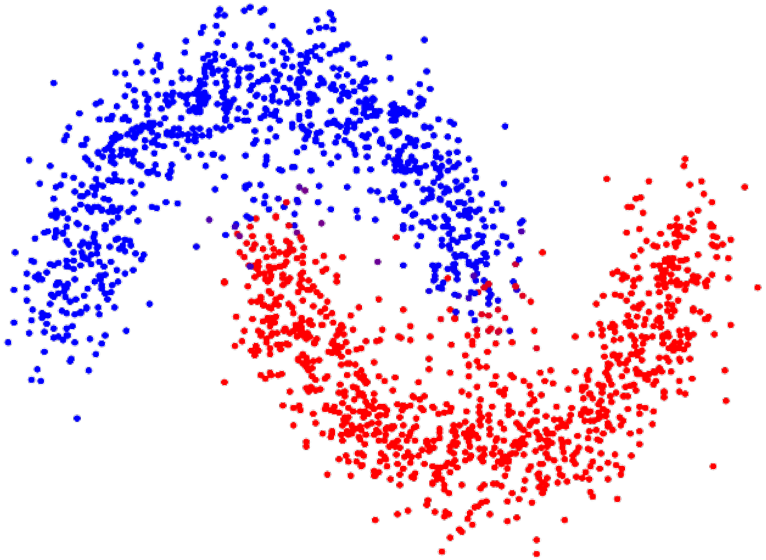
Output Results:

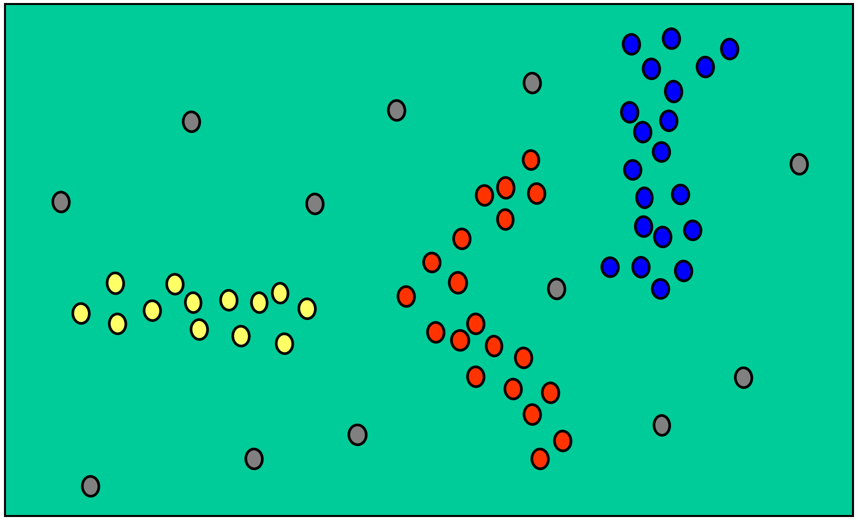
Each color represents a class ; The brightness represents the posterior probability – darker pixels represent high uncertainty of the posterior distribution.

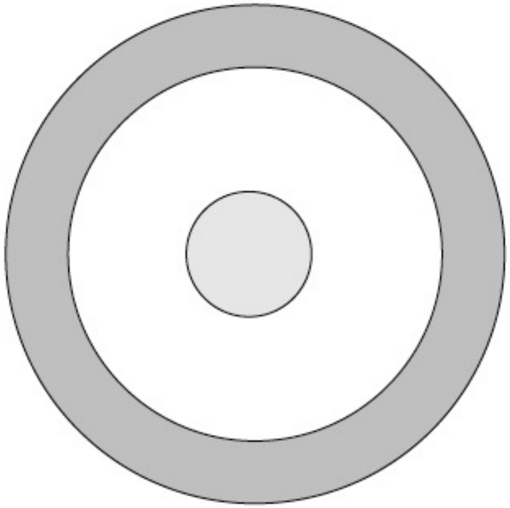
From K-means to GMM

- K-means is a 0-1 classifier, which assigns every data point to one and only one cluster
  - As shown previously, K-means can also be formulated as EM
- Mixture of Gaussians is a Probability Model to describe/characterize a given set of data
  - GMM can be used as a "Soft" classifier
  - For every point we can quantify the **likelihood** that it belongs to a particular cluster
  - Once you have established the model for a given data set, you can use it for other applications, e.g. Prediction, Density Estimator, statistical inference etc.
- The EM-approach can be generalized to other non-Gaussian distributions.
- K-means, GMM and the general EM-approach are all widely used in practice for large-scale problems.

K-means and GMM CANNOT deal with Clusters of Random Shapes !!



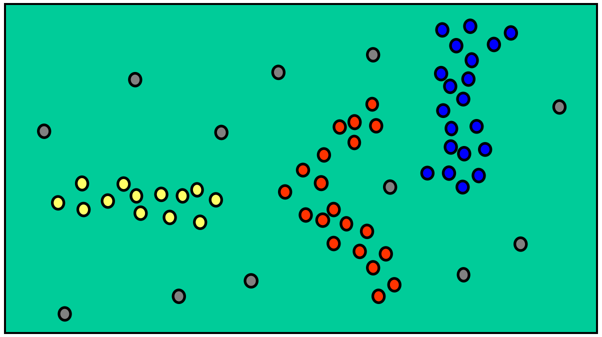




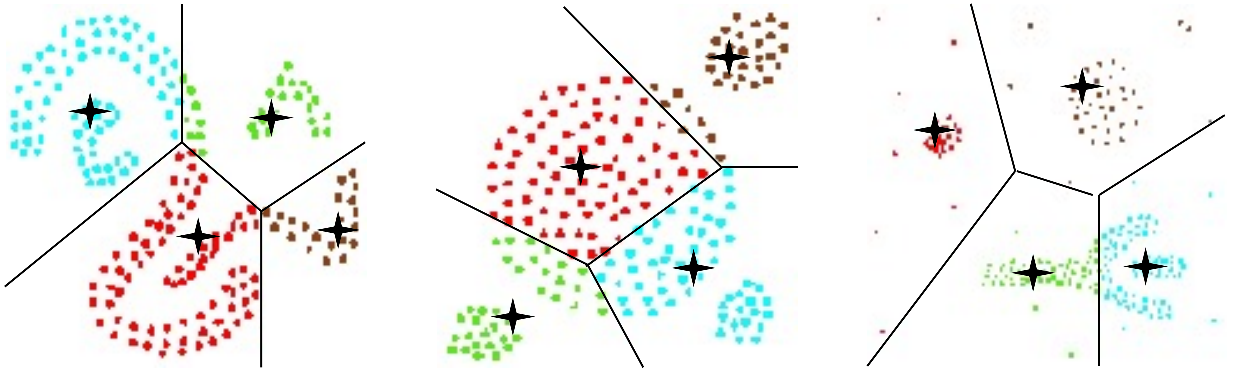
Density-based Clustering

- *Basic Idea*:

  Clusters are dense regions in the data space, separated by regions of lower object density



Why Density-Based Clustering?



Results of a *k*-medoid algorithm for *k*=4

Density-based Clustering

- Density-based Clustering locates regions of high density that are separated from one another by regions of low density.
- Density = number of points within a specified radius (ε) (in d-dimensional space)
- Why Density-Based Clustering methods?
  - Discover clusters of arbitrary shape.
  - Clusters – Dense regions of objects separated by regions of low density
- DBSCAN – the first density based clustering
  - To be covered in ESTR4300 ! All are welcome

Backup Slides

DBSCAN: Density Based Spatial Clustering of Applications with Noise

- Proposed by Ester, Kriegel, Sander, and Xu (KDD1996) – 2014 SIGKDD Test of Time Award
- Relies on a density-based notion of cluster: A cluster is defined as a maximal set of density-connected points.
- Discovers clusters of arbitrary shape in spatial databases with noise

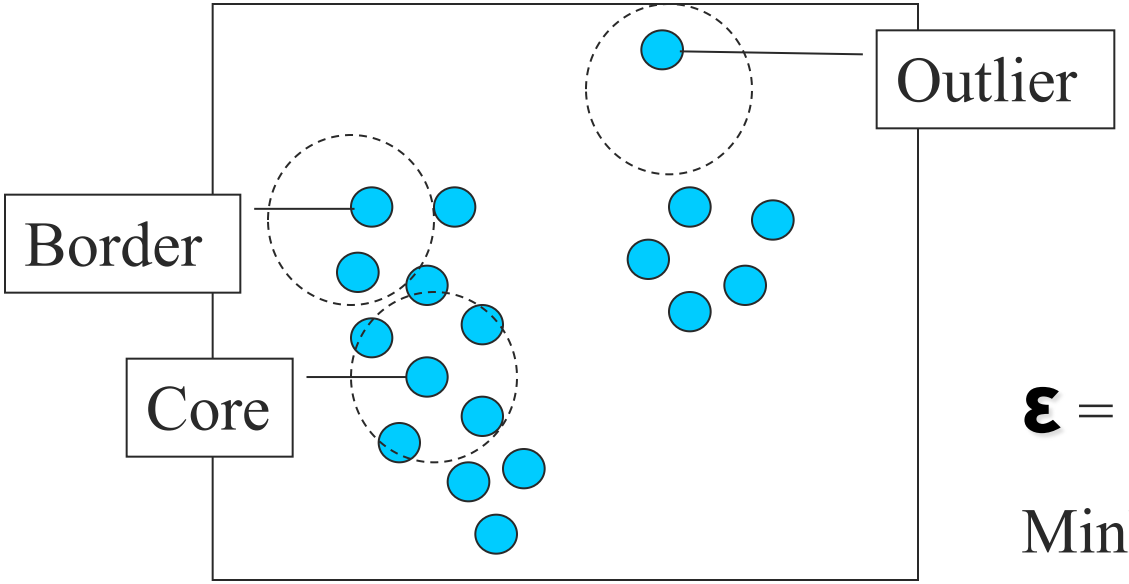
DBSCAN Terminology

- A point is a core point if it has more than a specified number of points (MinPts) within a radius of **ε**
  - These are points that are at the interior of a cluster

- A border point has fewer than MinPts within **ε**, but is in the neighborhood of a core point

- A noise point is any point that is not a core point or a border point.

Border & Core



ε = 1 unit

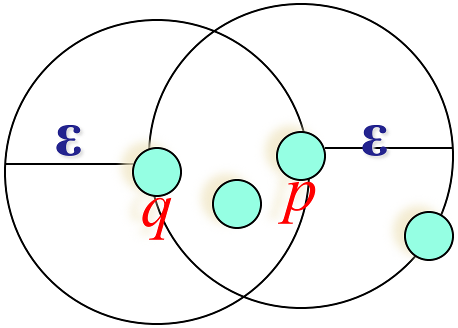
MinPts = 5

Key Idea for Cluster Formation under DBSCAN

- Any two core points are close enough– within a distance ε of one another – are put in the same cluster
- Any border point that is close enough to a core point is put in the same cluster as the core point
- Noise points are discarded

Concepts: ε-Neighborhood

- **ε-Neighborhood** - Points within a radius of ε from a point. (epsilon-neighborhood)
- "High density" - ε-Neighborhood of a point contains at least **MinPts** of points



ε-Neighborhood of *p*

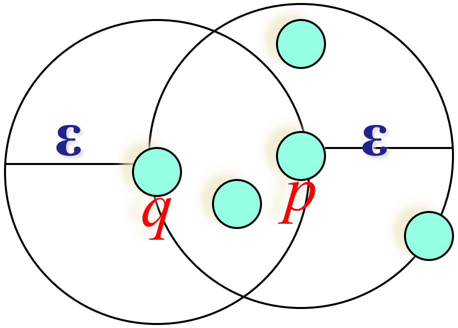
ε-Neighborhood of *q*

Density of *p* is "high" (w.r.t. MinPts = 4)

Density of *q* is "low" (w.r.t. MinPts = 4)

Concepts: Reachability

- **Directly Density-Reachable**
  - A point q is directly density-reachable from a point p if q is within the ε-Neighborhood of p and p is a core point.

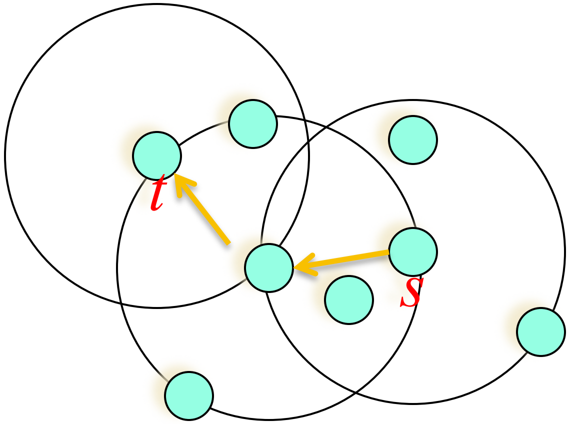


- q is directly density-reachable from p
- p is not directly density-reachable from q !

=> Asymmetric in general

Concepts: Reachability

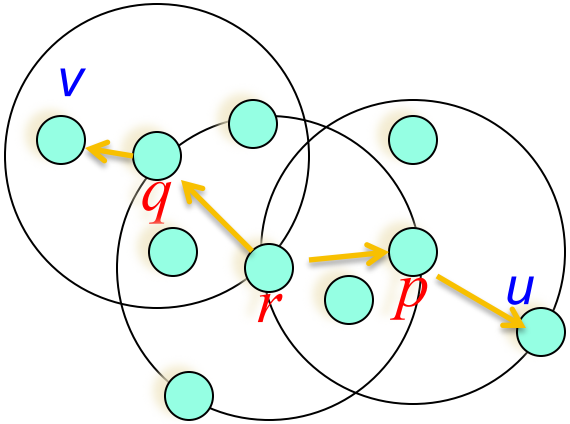
- **Density-Reachable:**
  - A point q is density-reachable from p w.r.t ε and *MinPts* if there is a chain of points $p_1,\ldots,p_n$, with $p_1=p$, $p_n=q$ such that p_{i+1} is directly density-reachable from p_i w.r.t ε and *MinPts* for all $1 <= i <= n$



- *t* is density-reachable from *s*
- *BUT s* is not density-reachable from *t* !
- Transitive closure of Direct Density-Reachability ; Asymmetric in general !

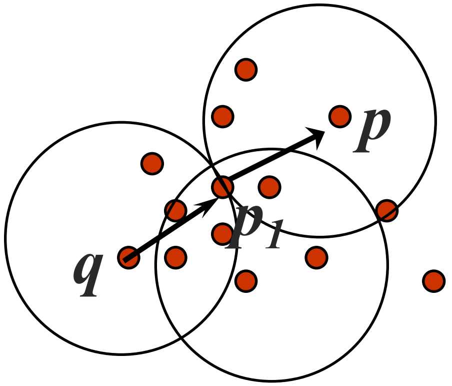
Concepts: Connectivity

- **Density-connectivity**
  - Point *p* is density-connected to Point *q* w.r.t ε and *MinPts* if there is a point *r* such that both *p* and *q* are density-reachable from *r* w.r.t ε and *MinPts*

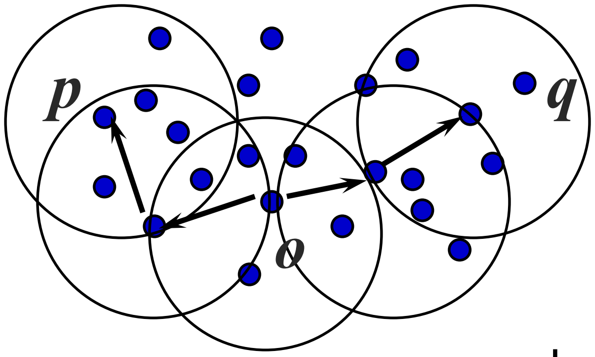


- *p* and *q* are density-connected to each other by *r*
- *v* and *u* are density-connected to each other by *r*
- Density-connectivity is symmetric

Density-reachable vs. Density-Connected



p is Density-reachable from q



p and q are Density-connected via o

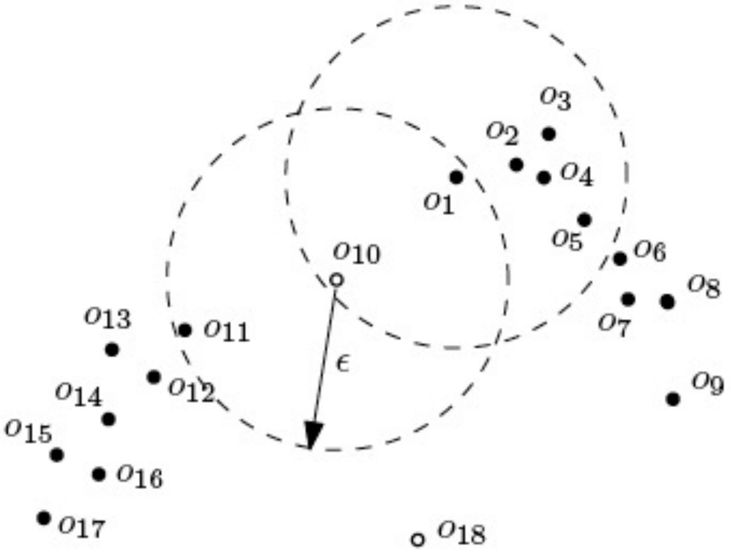
Formal Description of a Cluster

- Given a data set D, parameter ε and a threshold of MinPts.
- A cluster C is a subset of points satisfying two criteria:
  - *Connected:* For all p,q in C: p and q are density-connected.
  - *Maximal:* For all p,q: if p in C and q is density-reachable from p, then q in C (=> p is a core point)

  => Each cluster has at least 1 Core point

  => Each cluster contains at least MinPts points
- Note: a Cluster contains both Core and Border points
- **Noise:** points which are not directly density-reachable from at least one core point.
- The set of Clusters defined as above is ALWAYS Unique !...except…=> border point may belong to multiple cluster

Cluster Examples



C1 = {o1, o2,…o10}
C2 = {o10, o11,…,o17}
o18 is a noise point

Figure 2: An example dataset (the two circles have radius ϵ; $MinPts = 4$)

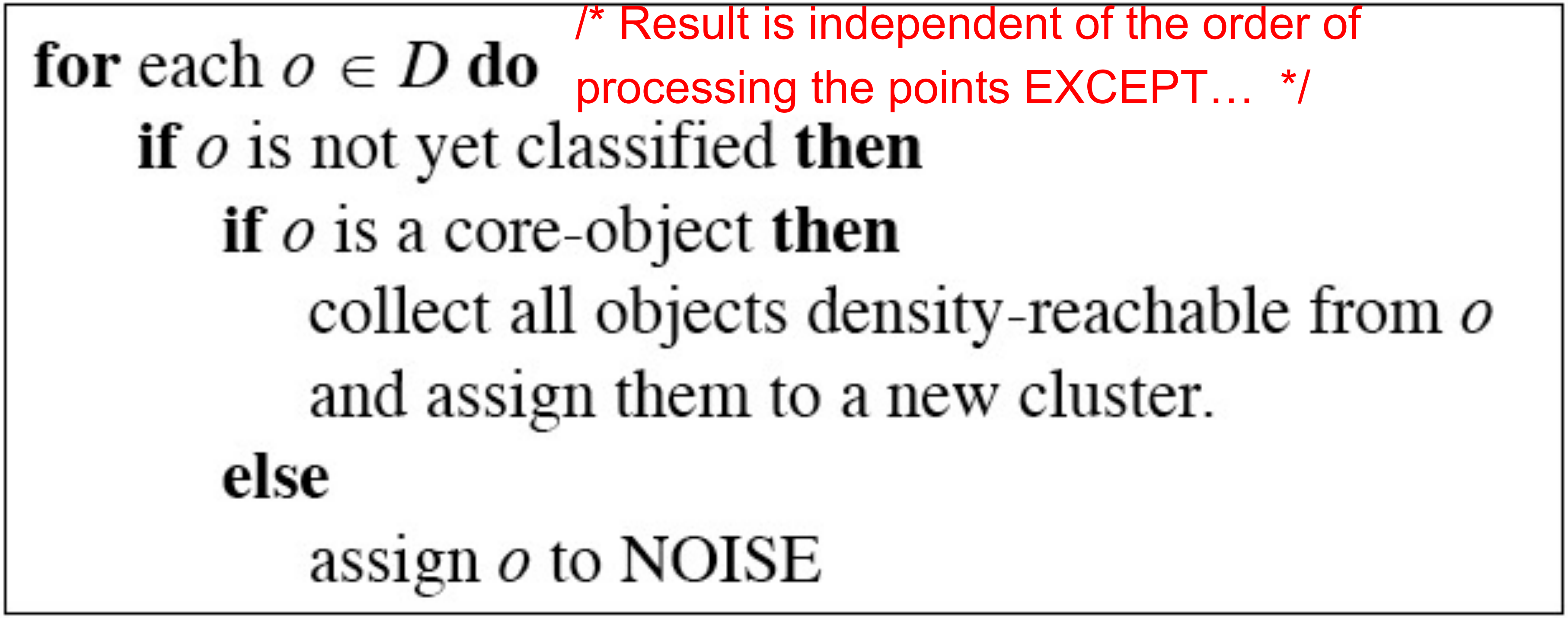
Connected: For all p,q in C: p and q are density-connected.

Maximal: For all p,q: if p in C and q is density-reachable from p, then q in C ;
also => each cluster has at least 1 Core point

- {o1, o10} alone is NOT a cluster by itself because NOT Maximal
- A Border point, e.g. o10, can belong to MULTIPLE clusters
- Clusters produced by DBSCAN is NOT necessarily disjoint !
- However, if p belongs to more than 1 cluster, it MUST BE a Border point

⇔ A core point always belongs to a Unique cluster, Why ?

DBSCAN: The Algorithm (Simplified)



/* Result is independent of the order of processing the points EXCEPT… */

```
for each $o \in D$ do
    if $o$ is not yet classified then
        if $o$ is a core-object then
            collect all objects density-reachable from $o$
            and assign them to a new cluster.
        else
            assign $o$ to NOISE
```

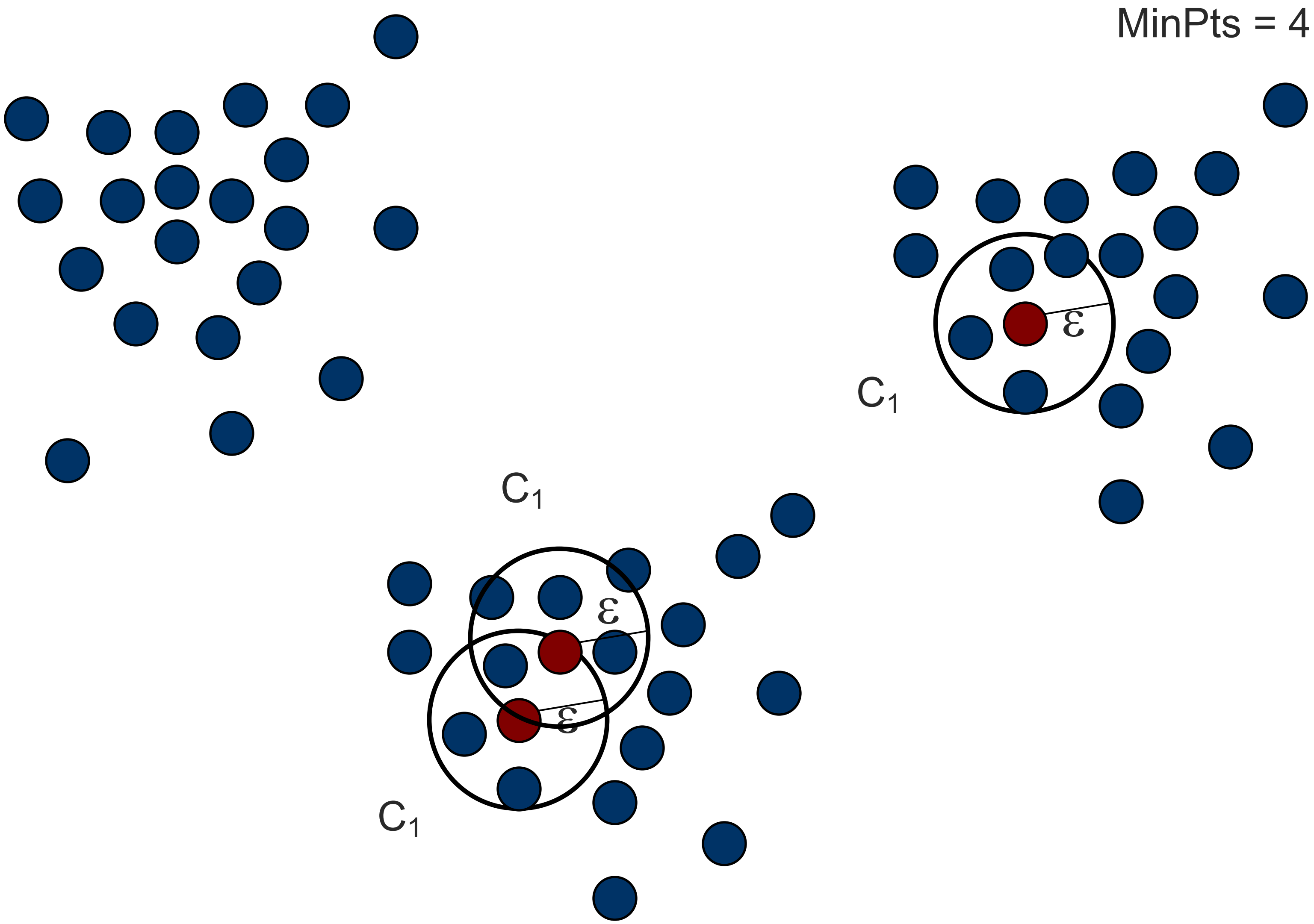
- Worst-case Time Complexity = $O(n^2)$! (trivial ?)
  - NOT O(n log n) Time as initially mis-claimed (for 17 years) !
- Time complexity = $\Omega(n^{4/3})$ for d > 2 [Gan&Tao 2015] ;
- O(n) space complexity
- O(n log n) Time only for 2-dimensional case [Gunawan 2013] ;
- ρ-approx DBSCAN runs in O(n) Time in Expectation for all dimensions [Gan&Tao 2015]

DBSCAN: The Algorithm (a more detail version)

```
DBSCAN(D, eps, MinPts)
    C = 0
    for each unvisited point P in dataset D
        mark P as visited
        N = regionQuery(P, eps)
        if sizeof(N) < MinPts
            mark P as NOISE
        else
            C = next cluster
            expandCluster(P, N, C, eps, MinPts)
```

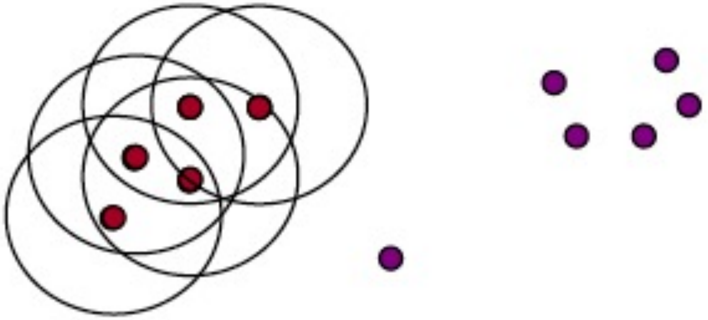
```
expandCluster(P,N,C,eps,MinPts)
    add P to cluster C
    for each point P' in N
        if P' is not visited
            mark P' as visited
            N' = regionQuery(P', eps)
            if sizeof(N') >= MinPts
                N = N joined with N'
        if P' is not yet member of any cluster
            add P' to cluster C
```

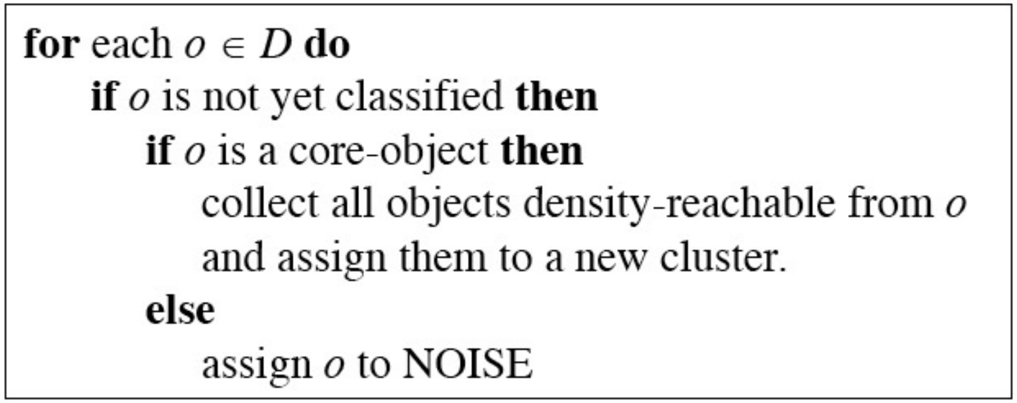
An Example



Running the DBSCAN Algorithm: An Example

- **Parameter**
    - $\varepsilon = 2$ cm
    - $MinPts = 3$





```
for each $o \in D$ do
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```

Running the DBSCAN Algorithm: An Example

- **Parameter**
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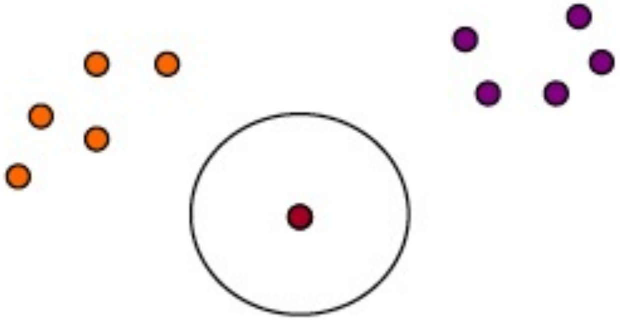

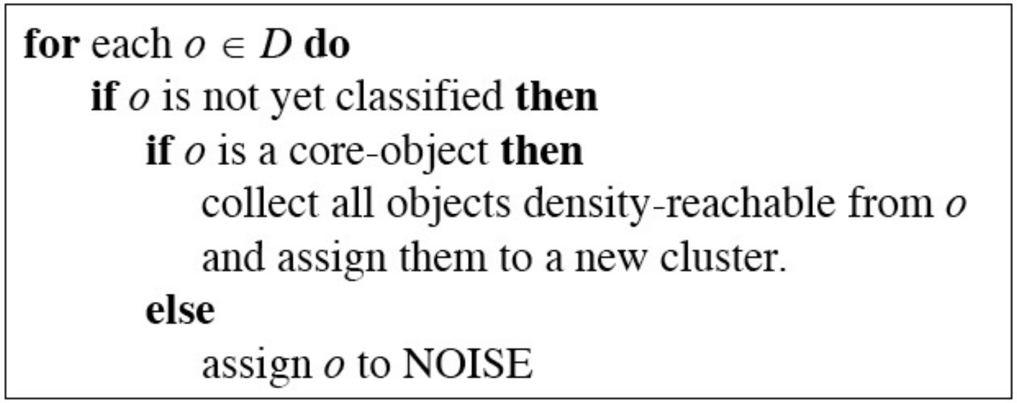

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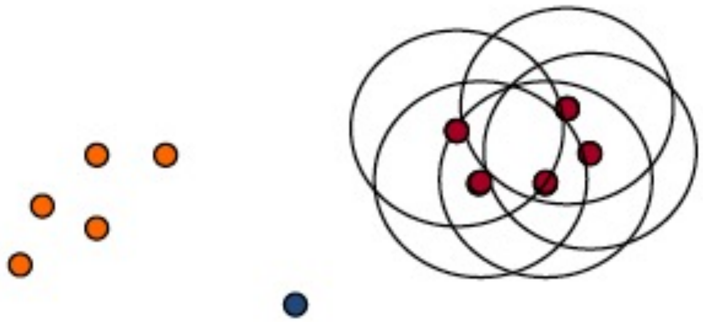
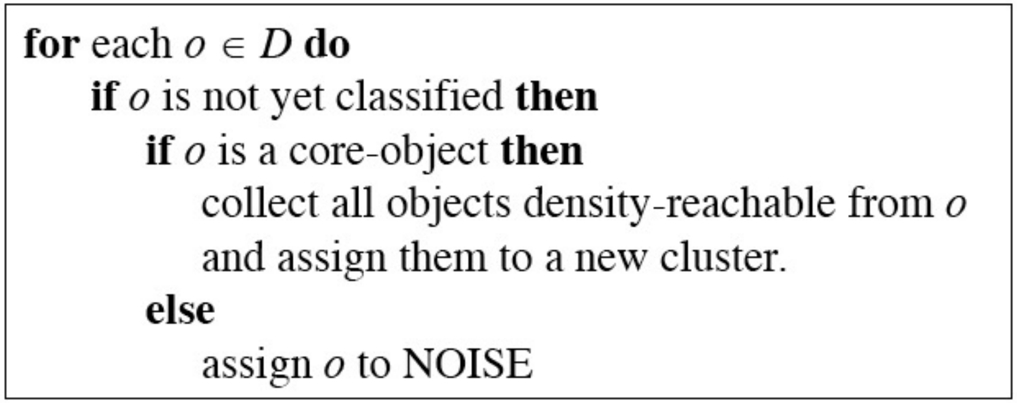
```

Running the DBSCAN Algorithm: An Example

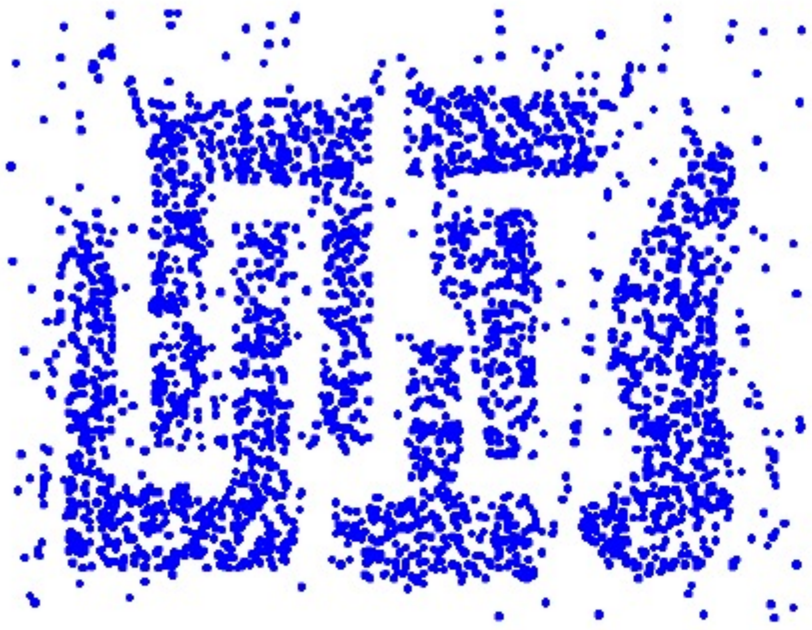
- **Parameter**
  - $\varepsilon = 2$ cm
  - $MinPts = 3$



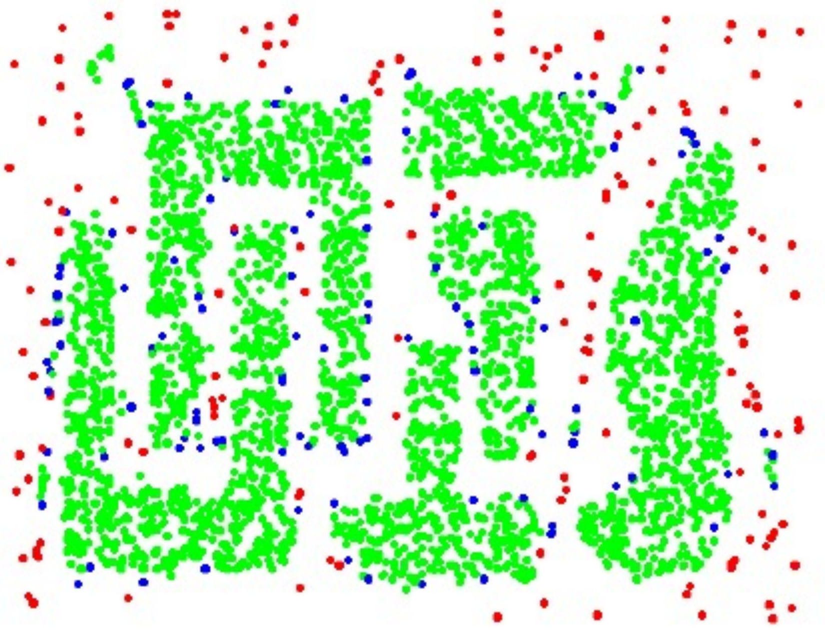


```
for each $o \in D$ do
    if $o$ is not yet classified then
        if $o$ is a core-object then
            collect all objects density-reachable from $o$
            and assign them to a new cluster.
        else
            assign $o$ to NOISE
```

Another Example



Original Points

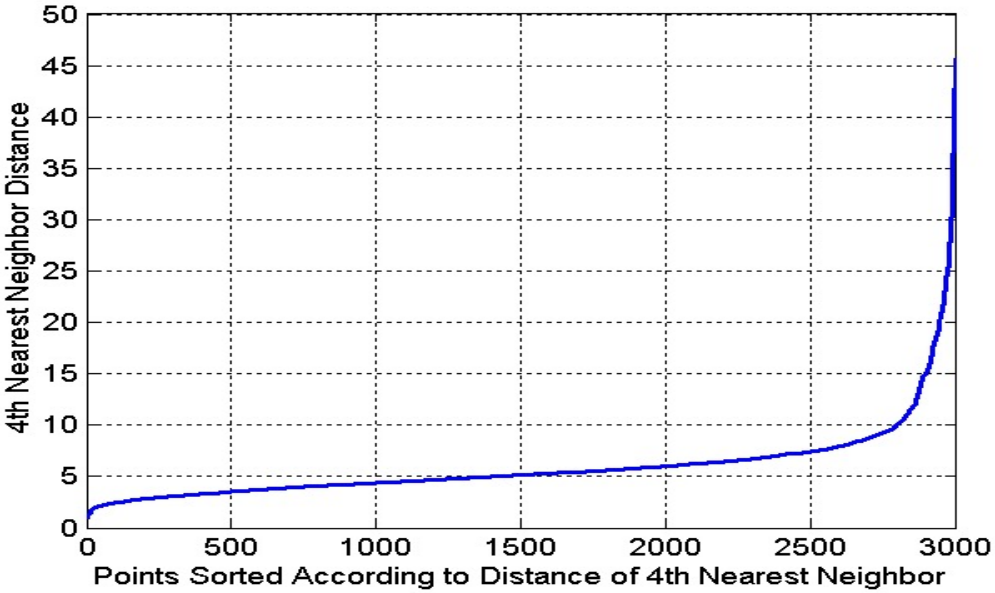


Point types: core, border and outliers

ε = 10, MinPts = 4

DBSCAN: Determining ε and MinPts

- Idea is that for points in a cluster, their k^th^ nearest neighbors are at roughly the same distance (BUT may NOT always be true !!)
- Noise points have the k^th^ nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^th^ nearest neighbor



DBSCAN: Determining ε and MinPts

- Distance from a point to its *k*th nearest neighbor=>k-dist
- For points that belong to some clusters, the value of k-dist will be small if k is not larger than cluster size
- For points that are not in a cluster such as noise points, the k-dist will be relatively large
- Compute k-dist for all points for some k
- Sort them in increasing order and plot sorted values
- A sharp change at the value of k-dist that corresponds to suitable value of ε and the value of k as MinPts

DBSCAN: Determining ε and MinPts

- A sharp change at the value of k-dist that corresponds to suitable value of ε and the value of k as MinPts
  - Points for which k-dist is less than ε will be labeled as core points while other points will be labeled as noise or border points.
- If k is too large=> small clusters (of size less than k) are likely to be labeled as noise
- If k is too small=> Even a small number of closely spaced that are noise or outliers will be incorrectly labeled as clusters

Sensitivity of DBSCAN w.r.t. the Choice of ε

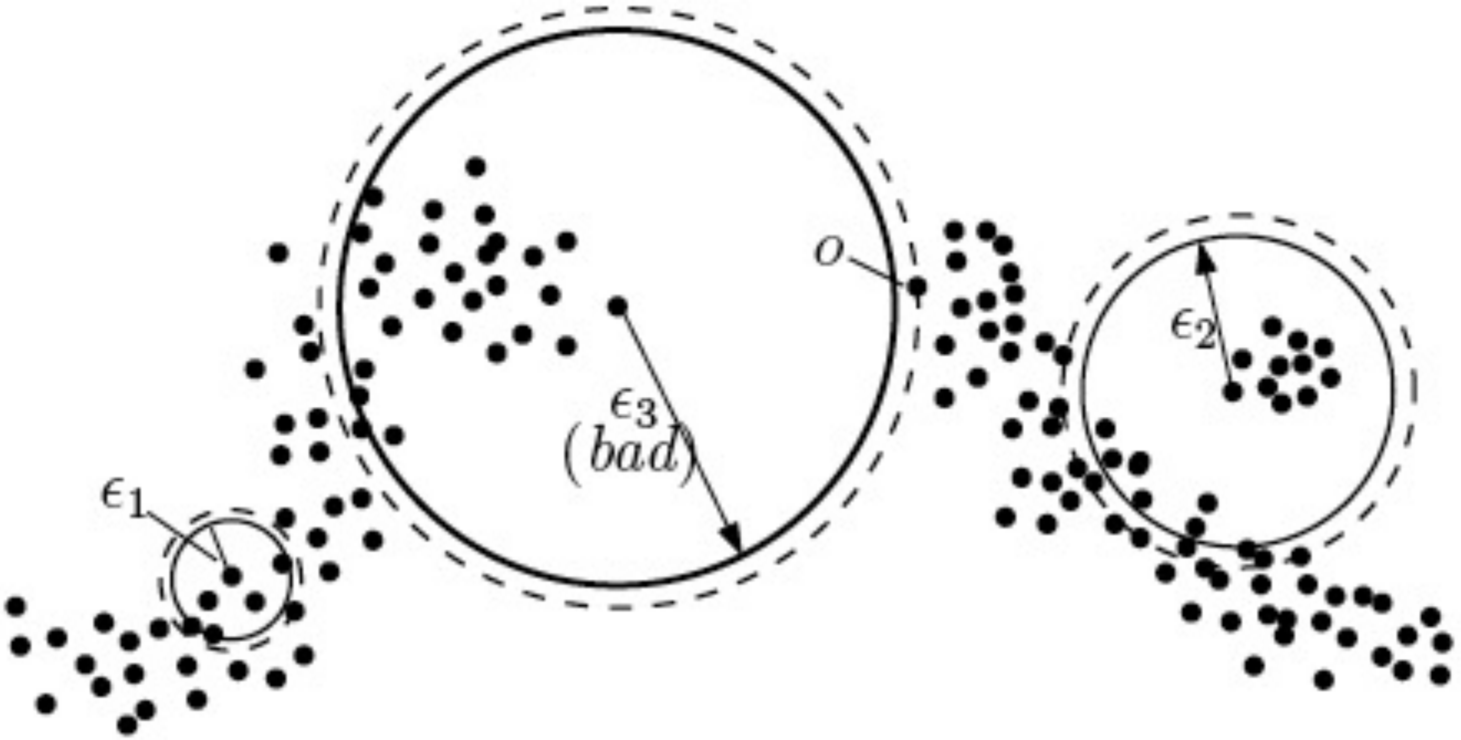


Figure 6: Good and bad choices of ϵ

- Choice of Eps1 will give 3 clusters and Eps2 will give 2 clusters ; these choices of Eps are robust w.r.t. minor perturbation ;

- Eps3 is a bad choice because a slight perturbation of eps3 will change the result from 2 clusters to 1 cluster ; Eps3 is TOO CLOSE to the distance between 2 clusters !!

DBSCAN results Sensitive to Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

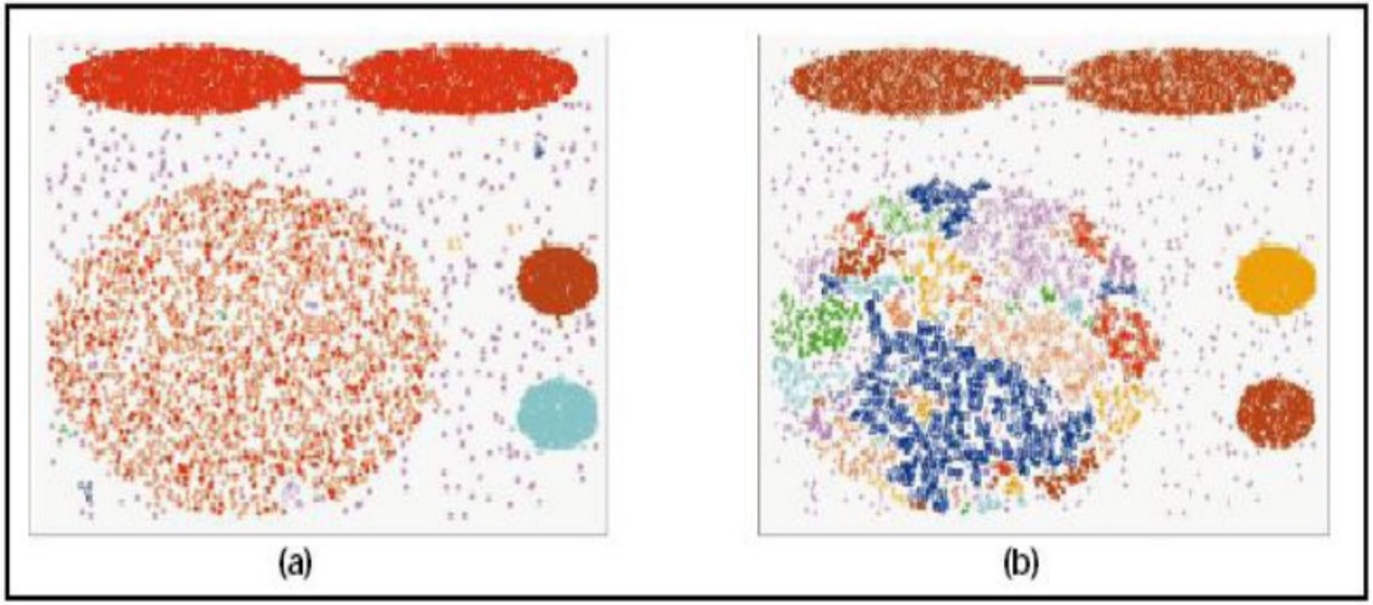
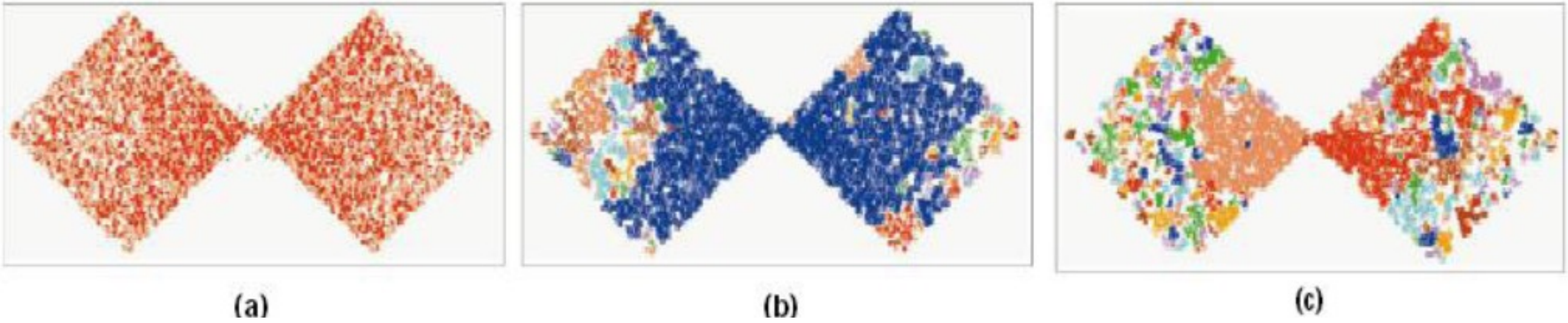
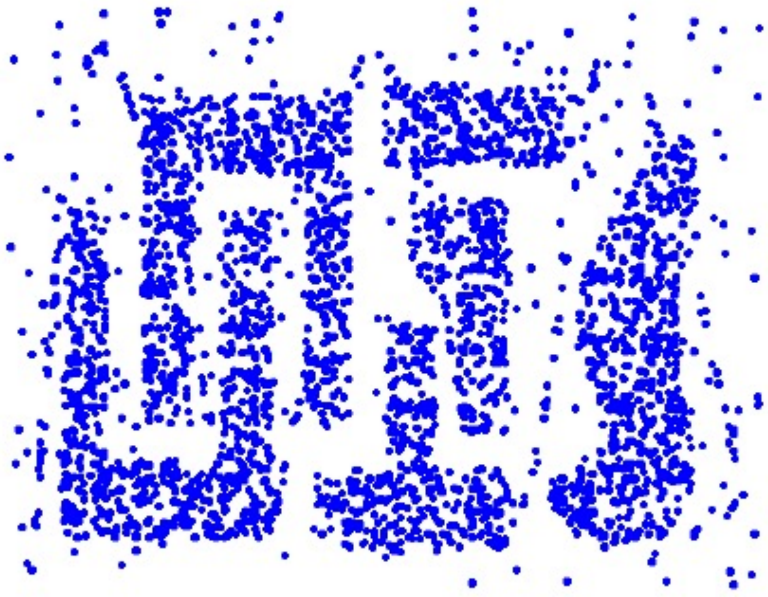


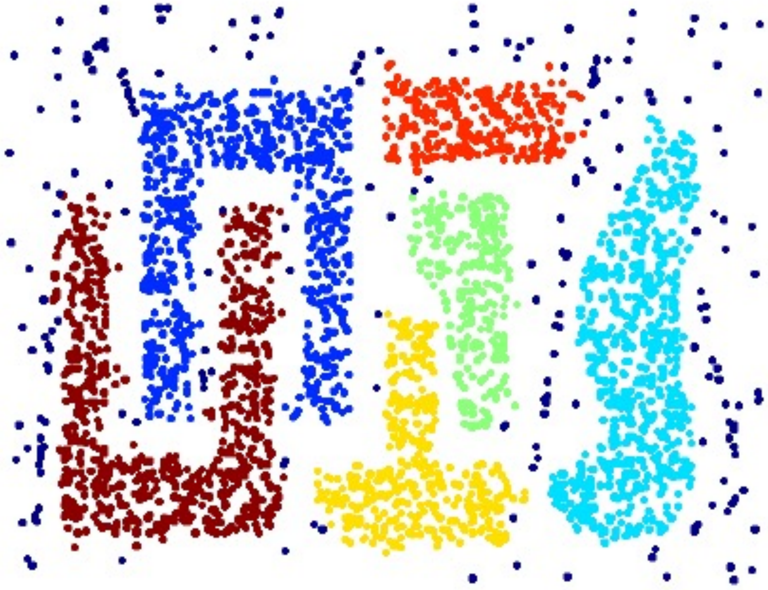
Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



When DBSCAN works well



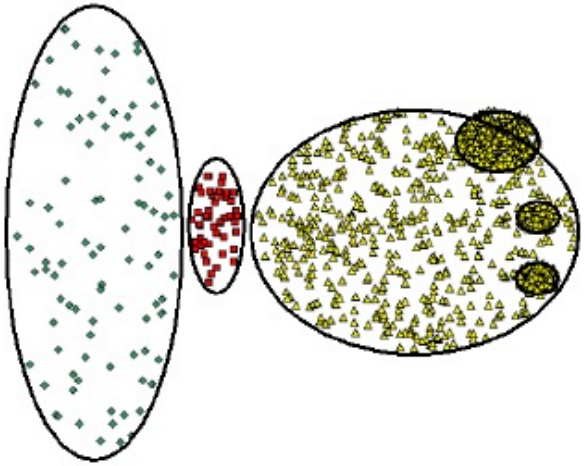
Original Points



Clusters

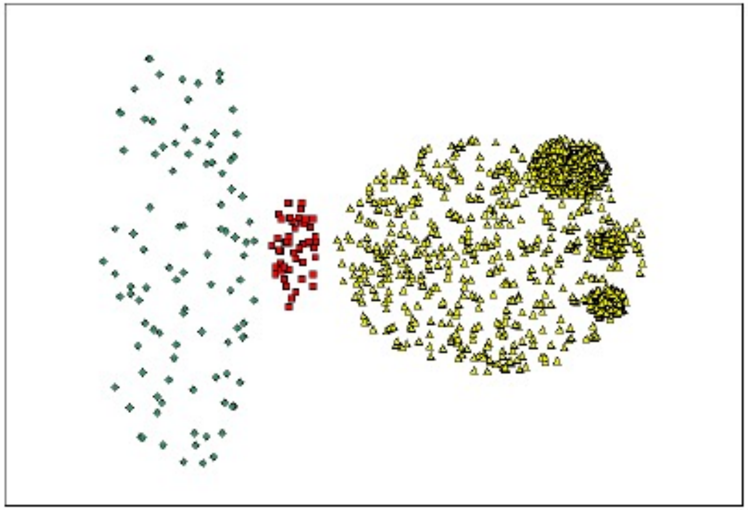
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN does NOT work well

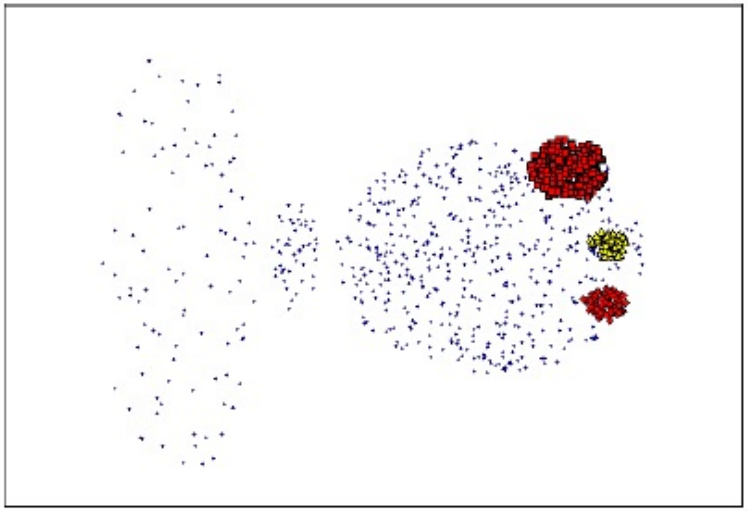


Original Points

- **Cannot handle varying densities**
- **sensitive to parameters—hard to determine the correct set of parameters**



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

Summary for DBSCAN

- DBSCAN depends on 2 critical parameters:
  - ε and Minpts
- The notion of ε-neighborhood w.r.t. Minpts threshold
- Definition of Core vs. Border vs. Noise (Outliner) points
- Density-Reachability vs. Density-Connectivity
- Defining a Cluster based on Density-Connectivity and MAXIMAL Density-Reachability
- Can be tricky to set the "correct" value of k (size of a cluster)
- Inability to handle highly variable density within the

Summary

- **Clustering:** Given a **set of points**, with a notion of **distance** between points, **group the points** into some number of ***clusters***
- **Algorithms:**
  - Agglomerative **hierarchical clustering**:
    - Centroid and clustroid
  - ***k*-means:**
    - Initialization, picking *k*
  - **EM for GMM**
  - **Density-based Clustering with DBSCAN for Clusters of arbitrary shapes**

Backup Slides

Backup Slides of the Derivation of MLE estimator for GMM

Maximum likelihood estimation of Gaussian

- Given data points x_n, n=1,…,N
- Find a single Gaussian distribution that maximizes data log-likelihood

$$L(\theta) = \sum_{n=1}^{N} \log p(x_n) = \sum_{n=1}^{N} \log N(x_n; m, C) = \sum_{n=1}^{N} \left[-\frac{d}{2}\log(2\pi) - \frac{1}{2}\log|C| - \frac{1}{2}(x_n - m)^T C^{-1}(x_n - m) \right]$$

- Set derivative of data log-likelihood w.r.t. parameters to zero

$$\frac{\partial}{\partial m} L(\theta) = C^{-1} \sum_{n=1}^{N} [x_n - m] = 0 \qquad \frac{\partial}{\partial C^{-1}} L(\theta) = \sum_{n=1}^{N} \left[\frac{1}{2} C - \frac{1}{2}(x_n - m)(x_n - m)^T \right] = 0$$

$$m = \frac{1}{N} \sum_{n=1}^{N} x_n \qquad C = \frac{1}{N} \sum_{n=1}^{N} (x_n - m)(x_n - m)^T$$

- Parameters set as data covariance and mean

Maximum likelihood estimation of Gaussian

$$P(x_n|\theta_k) = P(x_n|\mu_k, \Sigma_k) = \mathcal{N}(x_n|\mu_k, \Sigma_k) = (2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}$$

The derivative of a gaussian with respect to its mean

$$\frac{d}{d\mu_k}\{(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\} =$$

$$(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\frac{d}{d\mu_k}\{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\} =$$

$$(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\Sigma_k^{-1}(x-\mu_k) =$$

$$\mathcal{N}(x|\mu_k, \Sigma_k)\Sigma_k^{-1}(x-\mu_k)$$

Maximum likelihood estimation of GMM

Maximize for μ_k

$$\frac{d}{d\mu_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k,\Sigma_k))\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{d}{d\mu_k}P(x_n|\mu_k,\Sigma_k) = 0$$

Use the derivative that we previously found

Maximum likelihood estimation of GMM

Maximize for μ_k

$$\frac{d}{d\mu_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k, \Sigma_k))\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k, \Sigma_k)}\frac{d}{d\mu_k}P(x_n|\mu_k, \Sigma_k) = 0$$

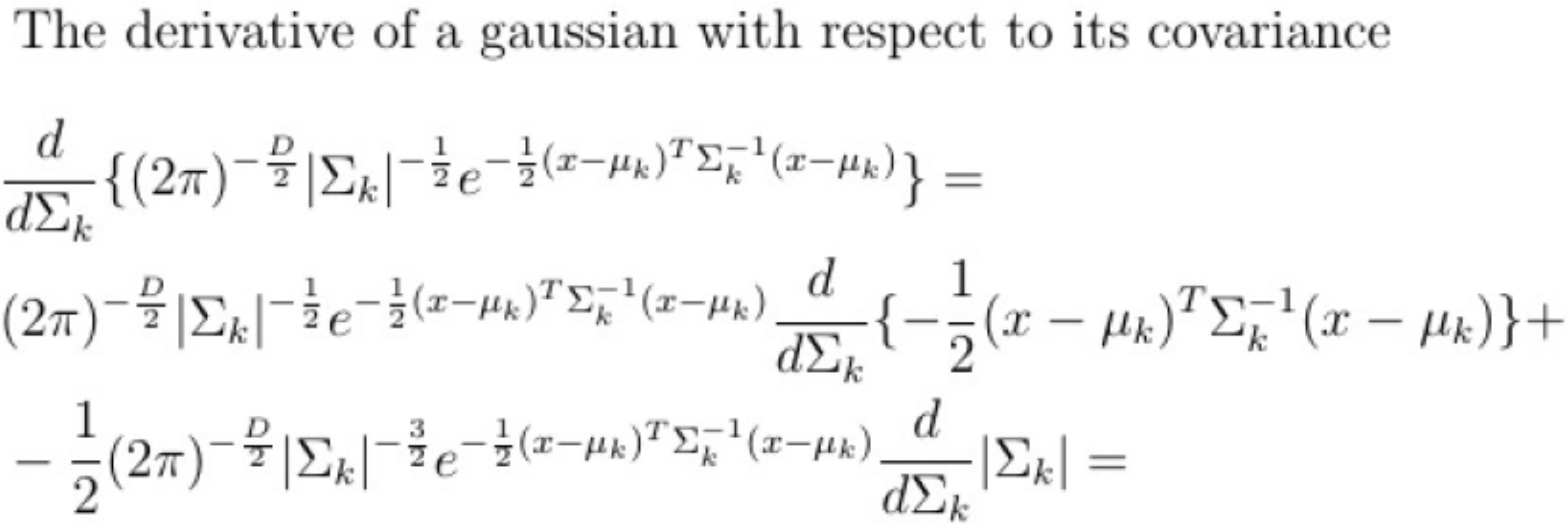
$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k, \Sigma_k)}P(x_n|\mu_k, \Sigma_k)\Sigma_k^{-1}(x_n - \mu_k) = 0$$

$$\sum_{n=1}^{N} z_{nk}(x_n - \mu_k) = 0$$

$$\mu_k\sum_{n=1}^{N} z_{nk} = \sum_{n=1}^{N} z_{nk}x_n$$

$$\mu_k = \frac{\sum_{n=1}^{N} z_{nk}x_n}{N_k}$$

Maximum likelihood estimation of Gaussian



The derivative of a gaussian with respect to its covariance

$$\frac{d}{d\Sigma_k}\{(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\} =$$

$$(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\frac{d}{d\Sigma_k}\{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\}+$$

$$-\frac{1}{2}(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{3}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\frac{d}{d\Sigma_k}|\Sigma_k| =$$

Product rule

Maximum likelihood estimation of Gaussian

The derivative of a gaussian with respect to its covariance

$$\frac{d}{d\Sigma_k}\{(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\} =$$

$$(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{1}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\frac{d}{d\Sigma_k}\{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\}+$$

$$-\frac{1}{2}(2\pi)^{-\frac{D}{2}}|\Sigma_k|^{-\frac{3}{2}}e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\frac{d}{d\Sigma_k}|\Sigma_k| =$$

$$\mathcal{N}(x|\mu_k,\Sigma_k)\frac{d}{d\Sigma_k}\{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\}$$

$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k,\Sigma_k)\frac{d}{d\Sigma_k}|\Sigma_k| =$$

Maximum likelihood estimation of Gaussian

$$\mathcal{N}(x|\mu_k, \Sigma_k)(-\frac{1}{2}(x-\mu_k)^T(x-\mu_k))\frac{d}{d\Sigma_k}\Sigma_k^{-1}$$
$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k, \Sigma_k)|\Sigma_k|\Sigma_k^{-1} =$$

Maximum likelihood estimation of Gaussian

$$\mathcal{N}(x|\mu_k,\Sigma_k)(-\frac{1}{2}(x-\mu_k)^T(x-\mu_k))\frac{d}{d\Sigma_k}\Sigma_k^{-1}$$

$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k,\Sigma_k)|\Sigma_k|\Sigma_k^{-1}=$$

Derivative of inverse

$$\mathcal{N}(x|\mu_k,\Sigma_k)(-\frac{1}{2}(x-\mu_k)^T(x-\mu_k))(-\Sigma_k^{-1}\Sigma_k^{-1})$$

$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k,\Sigma_k)|\Sigma_k|\Sigma_k^{-1}=$$

Maximum likelihood estimation of Gaussian

$$\mathcal{N}(x|\mu_k,\Sigma_k)(-\frac{1}{2}(x-\mu_k)^T(x-\mu_k))\frac{d}{d\Sigma_k}\Sigma_k^{-1}$$

$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k,\Sigma_k)|\Sigma_k|\Sigma_k^{-1} =$$

$$\mathcal{N}(x|\mu_k,\Sigma_k)(-\frac{1}{2}(x-\mu_k)^T(x-\mu_k))(-\Sigma_k^{-1}\Sigma_k^{-1})$$

$$-\frac{1}{2}|\Sigma_k|^{-1}\mathcal{N}(x|\mu_k,\Sigma_k)|\Sigma_k|\Sigma_k^{-1} =$$

$$\mathcal{N}(x|\mu_k,\Sigma_k)\frac{1}{2}(x-\mu_k)^T(x-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1}$$

$$-\frac{1}{2}\mathcal{N}(x|\mu_k,\Sigma_k)\Sigma_k^{-1} =$$

$$\frac{1}{2}\mathcal{N}(x|\mu_k,\Sigma_k)\{(x-\mu_k)^T(x-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1}-\Sigma_k^{-1}\}$$

Maximum likelihood estimation of GMM

Set derivative with respect to Σ_k equal to 0:

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k,\Sigma_k))\} = 0$$

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}ln(P(x_n|\mu_k,\Sigma_k)) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{d}{d\Sigma_k}P(x_n|\mu_k,\Sigma_k) = 0$$

Use derivative of gaussian

Maximum likelihood estimation of GMM

Set derivative with respect to Σ_k equal to 0:

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k,\Sigma_k))\} = 0$$

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}ln(P(x_n|\mu_k,\Sigma_k)) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{d}{d\Sigma_k}P(x_n|\mu_k,\Sigma_k) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{1}{2}P(x_n|\mu_k,\Sigma_k)\{(x_n-\mu_k)^T(x_n-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1} - \Sigma_k^{-1}\} = 0$$

Drop distributions

Maximum likelihood estimation of GMM

Set derivative with respect to Σ_k equal to 0:

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k,\Sigma_k))\} = 0$$

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} ln(P(x_n|\mu_k,\Sigma_k)) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{d}{d\Sigma_k}P(x_n|\mu_k,\Sigma_k) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{1}{2}P(x_n|\mu_k,\Sigma_k)\{(x_n-\mu_k)^T(x_n-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1} - \Sigma_k^{-1}\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\{(x_n-\mu_k)^T(x_n-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1} - \Sigma_k^{-1}\} = 0$$

Multiply with Σ_k Σ_k

Maximum likelihood estimation of GMM

Set derivative with respect to Σ_k equal to 0:

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\{ln(\pi_k) + ln(P(x_n|\mu_k,\Sigma_k))\} = 0$$

$$\frac{d}{d\Sigma_k}\sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} ln(P(x_n|\mu_k,\Sigma_k)) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{d}{d\Sigma_k}P(x_n|\mu_k,\Sigma_k) = 0$$

$$\sum_{n=1}^{N} z_{nk}\frac{1}{P(x_n|\mu_k,\Sigma_k)}\frac{1}{2}P(x_n|\mu_k,\Sigma_k)\{(x_n-\mu_k)^T(x_n-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1} - \Sigma_k^{-1}\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\{(x_n-\mu_k)^T(x_n-\mu_k)\Sigma_k^{-1}\Sigma_k^{-1} - \Sigma_k^{-1}\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\{(x_n-\mu_k)^T(x_n-\mu_k) - \Sigma_k\} = 0$$

$$\sum_{n=1}^{N} z_{nk}\Sigma_k = \sum_{n=1}^{N} z_{nk}(x_n-\mu_k)^T(x_n-\mu_k)$$

$$N_k\Sigma_k = \sum_{n=1}^{N} z_{nk}(x_n-\mu_k)^T(x_n-\mu_k)$$

$$\Sigma_k = \frac{\sum_{n=1}^{N} z_{nk}(x_n-\mu_k)^T(x_n-\mu_k)}{N_k}$$