深蓝学院
shenlanxueyuan.com

3D Point Clouds
Lecture 3 – Clustering

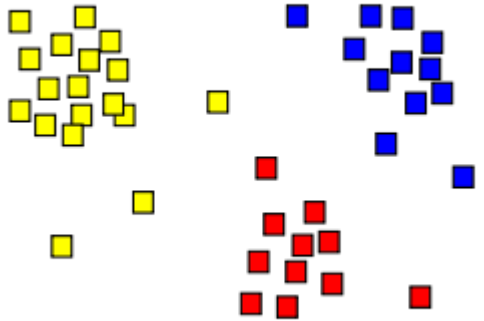
主讲人 黎嘉信

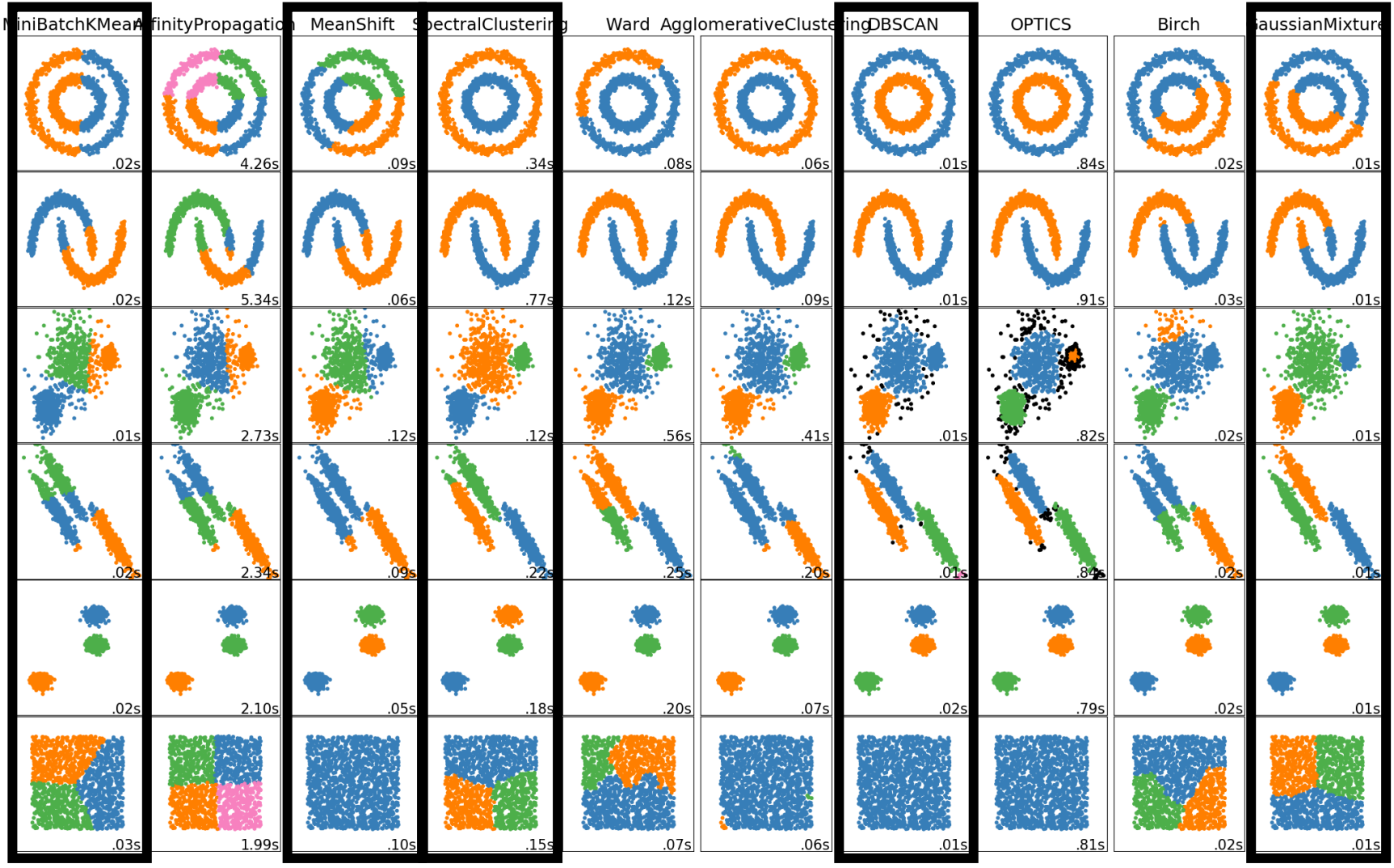
Aptiv 自动驾驶
新加坡国立大学 博士
清华大学 本科

- 1、Math Prerequisite
- 2、K-Means
- 3、Gaussian Mixture Models (GMM)
- 4、Expectation Maximization (EM)
- 5、Spectral Clustering
- 6、Others – Mean Shift, DBSCAN

Introduction Clustering

- Clustering is to group objects such that objects in the same group (called a cluster) are similar, while objects belong to different groups are dis-similar.
- There are many clustering algorithms
- We focus on two types:
  - Theoretically profound
    - K-Means,
    - GMM (Gaussian Mixture Model)
    - EM (Expectation-Maximation)
    - Spectral Clustering
  - Practically useful
    - Mean-Shift
    - DBSCAN (Density-Based Spatial Clustering of Applications with Noise)




MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
OPTICS
Birch
GaussianMixture
.02s
4.26s
.09s
.34s
.08s
.06s
.01s
.84s
.02s
.01s
.02s
5.34s
.06s
.77s
.12s
.09s
.01s
.91s
.03s
.01s
.01s
2.73s
.12s
.12s
.56s
.41s
.01s
.82s
.02s
.01s
.02s
2.34s
.09s
.22s
.25s
.20s
.01s
.84s
.02s
.01s
.02s
2.10s
.05s
.18s
.20s
.07s
.02s
.79s
.02s
.01s
.03s
1.99s
.10s
.15s
.07s
.06s
.01s
.81s
.02s
.01s

Math Prerequisite

Need some background knowledge to understand K-Means, GMM, EM, Spectral Clustering

- Linear Algebra
  - SVD
  - Rayleigh Quotient
- Probability
  - Bayes rule
  - Conditional Probability
- Graphical Modeling
  - Directed graph
  - Undirected graph
- Lagrange Multiplier

Spectral Theorem

Let $A \in R^{n,n}$ be symmetric, and $\lambda_i \in R, i = 1, 2, \cdots, n$ be the eigenvalues of A. There exists a set of orthonormal vectors $u_i \in R_n, i = 1, 2, \cdots, n$, such that $Au_i = \lambda_i u_i$. Equivalently, there exists an orthogonal matrix $U = [u_1, \cdots, u_n]$ (i.e., $UU^T = U^T U = I_n$), such that,

$$A = U\Lambda U^T = \sum_{i=1}^{n} \lambda_i u_i u_i^T, \Lambda = \text{diag}(\lambda_1, \cdots, \lambda_n)$$

Rayleigh Quotients

Given a symmertric matrix $A \in S^n$,

Physical meaning of SVD!

$$\lambda_{\min}(A) \leq \frac{x^T A x}{x^T x} \leq \lambda_{\max}(A), \forall x \neq 0$$

$$\lambda_{max}(A) = \max_{x:\|x\|_2=1} x^T A x$$

$$\lambda_{min}(A) = \min_{x:\|x\|_2=1} x^T A x$$

The maximum and minimum are attained for $x = u_1$ and for $x = u_n$, respectively, where u_1 and u_n are the largest and smallest eigenvector of A, respectively.

Probability – Joint Probability

- Consider all combinations events of two random variables X and Y
- This is captured in the *joint probability* distribution p(x, y)
- Read as "*probability of X and Y*"
- Can be more than two random variables, i.e., p(a, b, c, …)

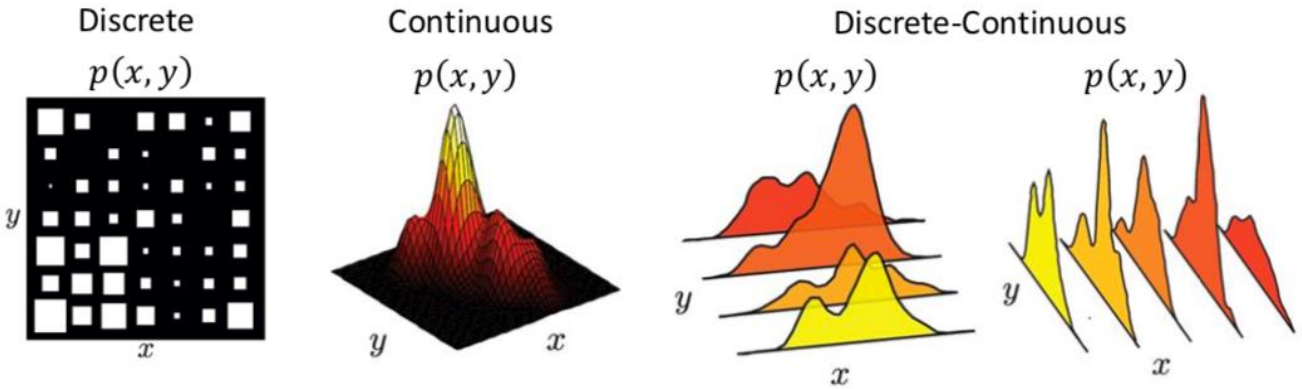


Image Source: "Computer Vision: Models, Learning, and Inference", Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

Probability - Marginalization

- Recover probability distribution of any variable in a joint distribution by integrating (or summing) over all other variables.
- “sum rule” of probability

Continuous:

$$p(x) = \int p(x, y)\, dy$$

$$p(y) = \int p(x, y)\, dx$$

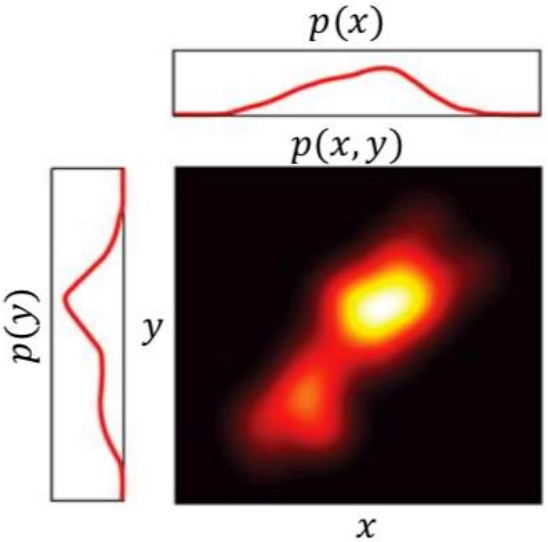


Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

Probability - Marginalization

Discrete:

$$p(x) = \sum_{y} p(x, y)$$

$$p(y) = \sum_{x} p(x, y)$$

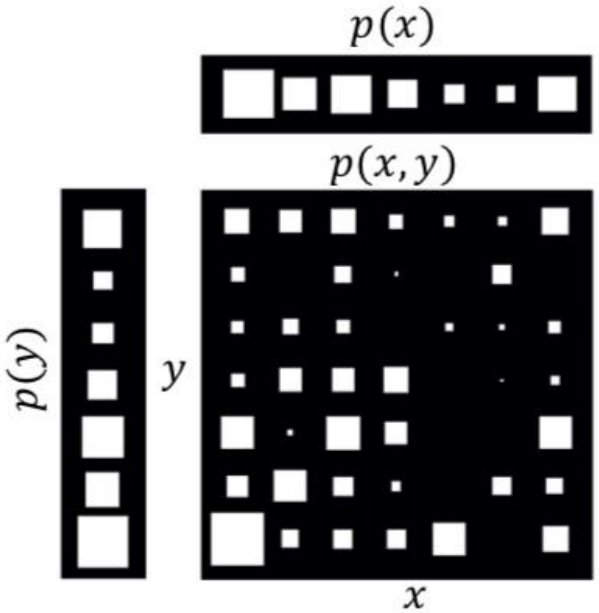


Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

Probability – Conditional Probability

$p(x|Y = y^*)$: probability of X given $Y = y^*$

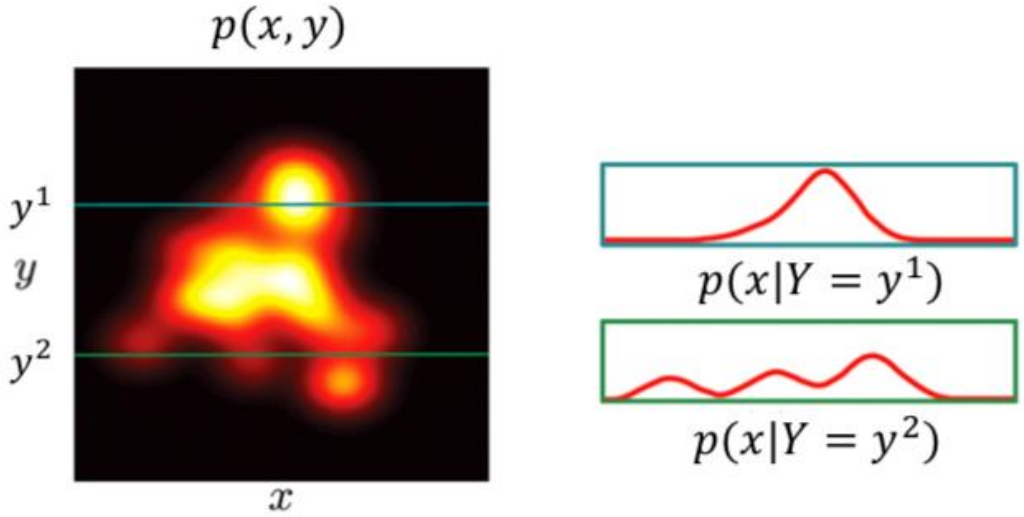


Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

Probability – Conditional Probability

- Conditional probability can be extracted from joint probability
- Extract appropriate slice and normalize (sum to 1)

$$P(x|Y=y^*) = \frac{p(x, Y=y^*)}{\int p(x, Y=y^*)dx} = \frac{p(x, Y=y^*)}{p(Y=y^*)}$$

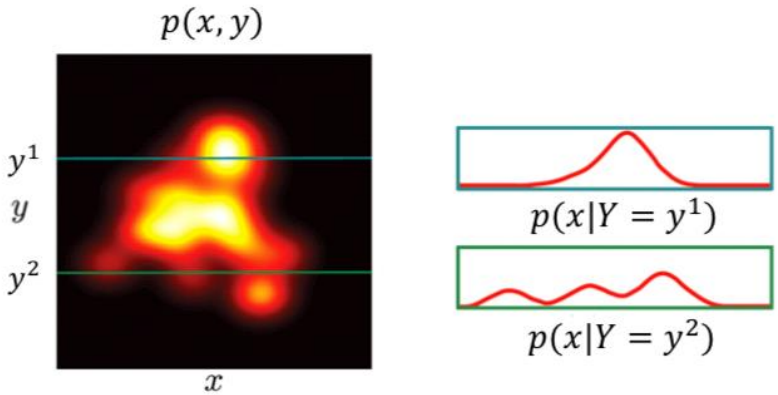


Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

Probability – Conditional Probability

- Conditional probability:

$$P(x|Y = y^*) = \frac{p(x, Y = y^*)}{\int p(x, Y = y^*)dx} = \frac{p(x, Y = y^*)}{p(Y = y^*)}$$

- Can be written in compact form:

$$p(x|y) = \frac{p(x, y)}{p(y)}$$

- Which leads to:

$$p(x, y) = p(x|y)p(y)$$
$$p(x, y) = p(y|x)p(x)$$

Hence, the name “product rule”!

Content source: Uncertainty Modeling in AI, Lee Gim Hee

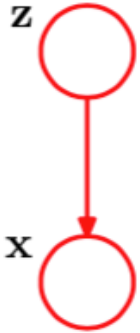
Probability – Conditional Probability

- The product rule works for higher dimensions as well

$$
\begin{aligned}
p(w,x,y,z) &= p(w,x,y|z)p(z) \\
&= p(w,x|y,z)p(y|z)p(z) \\
&= p(w|x,y,z)p(x|y,z)p(y|z)p(z)
\end{aligned}
$$

Content source: Uncertainty Modeling in AI, Lee Gim Hee

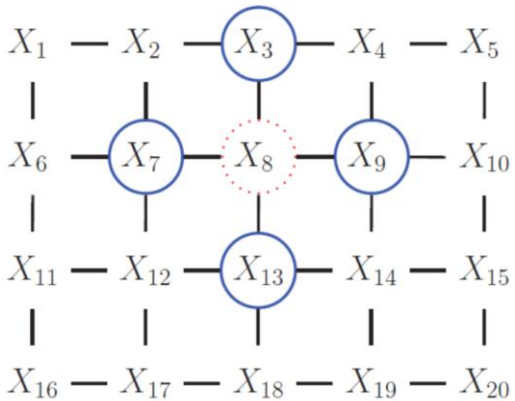
Graphical Modeling - Directed Graphical Model (DGM)



- DGM is used to represent conditional independence
- DGM is represented by $G(V, E)$
  V is a set of nodes. One node is one variable.
  E is a set of oriented edges. One edge is one conditional relationship.
- Markov assumption – a random variable X is independent of its non-descendants given its parents
  - E.g., the joint distribution is $p(x, z) = p(z)p(x|z)$
  - E.g., z → "age of a person", x → "hair white or black"
    $p(x|z)$ means the probability of white/black hair given a person's age
    It is different to $p(x)$, which means the probability of white/black hair without other info

Graphical Modeling - Undirected Graphical Model (UGM)

- It is called Markov Random Field (MRF) or Markov Network as well
- UGM is represented by $G(V, E)$, where V is a set of nodes, E is a set of undirected edges
  - E.g., below can be a map, X_i are cities, the edges are roads.
  - E.g., with UGM, I know the shortest path from X_1 to X_8



Content source: Uncertainty Modeling in AI, Lee Gim Hee

Optimization – Lagrange multiplier

- Consider the optimization problem

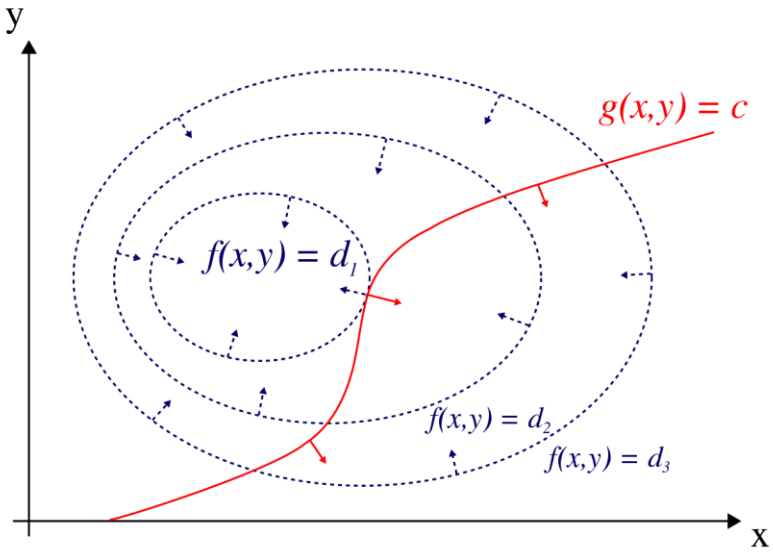
$$\max\ f(x,y),\ s.t.:\ g(x,y)=0$$

- Assume that both f and g have continuous first partial derivatives

Intuition

- The circles are level sets of $f(x,y)$
- $g(x,y)=0$ means x, y have to be on the red line
- At a (local) maximum, *f(x, y)* can NOT be increasing along the direction (tangent) of $g(x,y)=0$

$$\nabla_{x,y} f = \lambda \nabla_{x,y} g$$



Optimization – Lagrange multiplier

- Introduce a new variable λ called *Lagrange multiplier*
- Let's study the Lagrange function:

$$\mathcal{L}(x, y, \lambda) = f(x, y) - \lambda g(x, y)$$

- And solve:

$$\nabla_{x,y,\lambda} \mathcal{L}(x, y, \lambda) = 0.$$

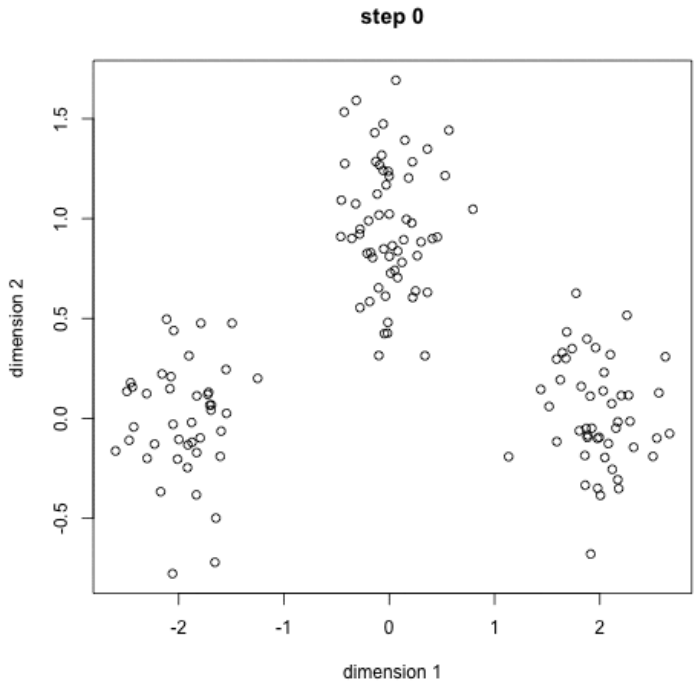
- The above equation means
  (1) $g(x, y) = 0$
  (2) gradient of *f* and *g* are parallel

$$\nabla_{x,y,\lambda} \mathcal{L}(x, y, \lambda) = 0 \iff \begin{cases} \nabla_{x,y} f(x, y) = \lambda \nabla_{x,y} g(x, y) \\ g(x, y) = 0 \end{cases}$$

K-Means

N input data points, find K clusters.

1. Randomly select *K* center points
2. Each data point is assigned to one of the *K* centers.
3. Re-compute the *K* centers by the mean of each group
4. Iterate step 2 & 3.



K-Means - Definition

- Data set $\{x_1, \cdots, x_N\}, x_n \in \mathbb{R}^D$
- Cluster center $\mu_k, k = 1, \cdots K$
  - μ_k is the center of k^{th} cluster
- Binary variable $r_{nk} \in \{0, 1\}$
  - x_n belong to which cluster
- Objective of K-Means is to minimize the distortion measure

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

K-Means

- Iteratively optimize r_{nk} and μ_k
- For some fixed values for μ_k, minimize J with respect to r_{nk}
  - This is the E (expectation) step of the EM algorithm
- For some fixed values of r_{nk}, minimize J with respect to μ_k
  - This is the M (maximization) step of the EM algorithm

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

K-Means E step

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

- N data points are independent, so we can optimize for each n separately.
- Simply assign the n^{th} data point to the closest cluster center, which will minimize $||x_n - \mu_k||^2$
- Formally

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$

K-Means M step

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

- With r_{nk} fixed, the objective function J is a quadratic function of μ_k
- Compute its first order derivative and make it to 0
- Consider each center μ_k separately

$$2 \sum_{n=1}^{N} r_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k) = 0$$

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \mathbf{x}_n}{\sum_n r_{nk}}$$

K-Means

- Illustration of the K=2
  a) Initialization
  b) Expectation – find r_{nk}
  c) Maximization – find μ_k

Other figures are repeating (b)(c)

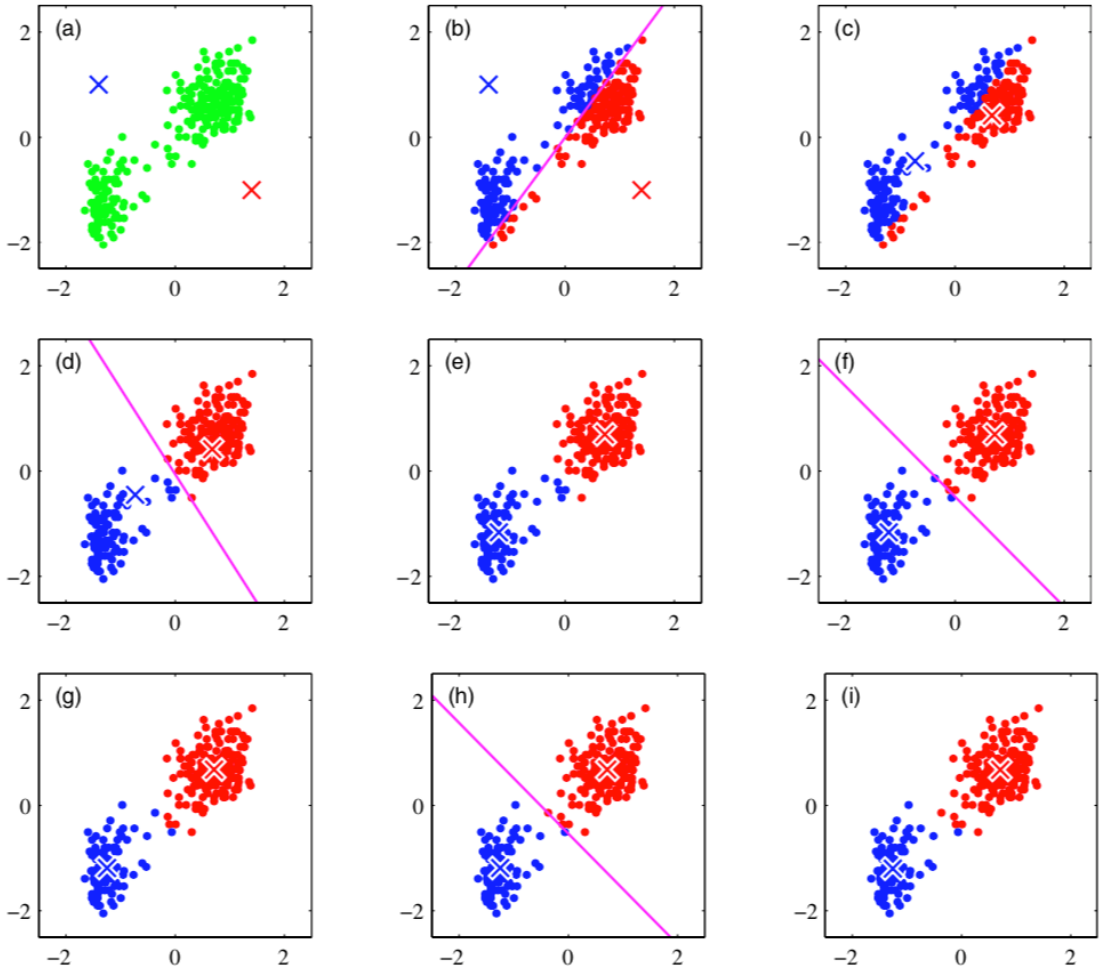


Figure source: Pattern Recognition and Machine Learning, Bishop Dataset: re-scaled Old Faithful dataset

K-Means Practical Tricks

- Randomly select K points as the initial μ_k
- Run K-Means multiple times with random initialization, select the one with the lowest cost J
- In E-step, it is necessary to compute distance between x_n and μ_k
  - Nearest Neighbor algorithms in Lecture 2
- Mini-batch K-Means: In each E&M iteration, select a subset of the data points.
  - Reduce the compute time
  - Converges faster
  - The final result may be slightly worse.

K-Means: Sequential Update

- The E / M step are performed for each data point x_n
  1. For each data point x_n, find the nearest center μ_k^{old}
  2. Update the center into

$$\boldsymbol{\mu}_k^{\text{new}} = \boldsymbol{\mu}_k^{\text{old}} + \eta_n(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{old}})$$

  where η_n is the learning rate

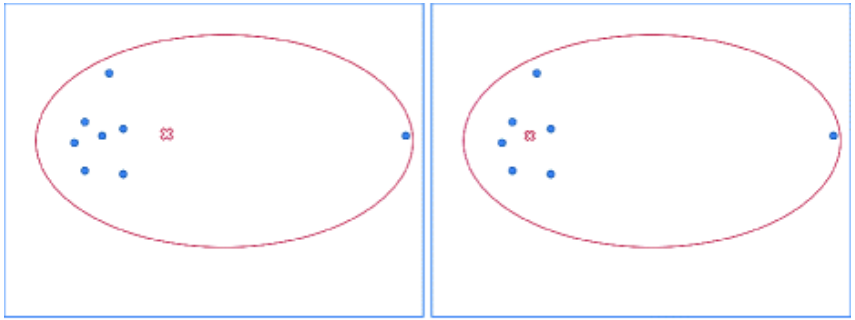
- Mini-batch version of this is the mini-batch K-Means mentioned in previous slice

K-Medoids

- Standard K-Means with Euclidean distance is problematic in some cases.
  - Outlier – outliers will drag the centers away
  - Limits the type of data points – E.g., Euclidean distance is not for categorical labels
- Apply general dissimilarity metric

K-Medoids $$\widetilde{J} = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$

K-Means $$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$



(a) Mean (b) Medoid

K-Medoids

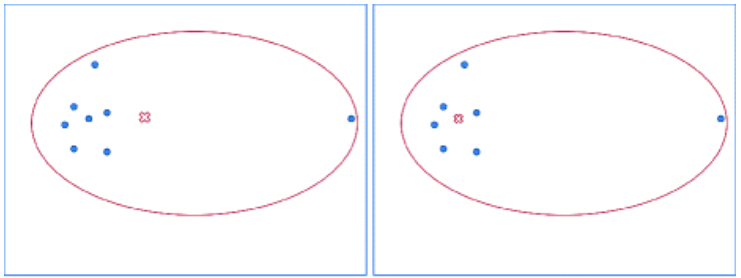
E step

- Same, just need to evaluate the dissimilarity measure $V(\cdot,\cdot)$ instead of Euclidean distance
- $O(KN)$ complexity

$$\widetilde{J} = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$

M step

- First order derivative over $V(\cdot,\cdot)$ can be intractable
- Therefore, assign μ_k to be one of the data point that has smallest $\tilde{J}$
- Can be implemented as discrete search over the N_k points of that cluster
- $O\left(N_k^2\right)$ complexity



(a) Mean (b) Medoid

K-Means Application – Compression

- Illustrated as image compression, can be easily applied to point cloud (XYZRGB) compression
  1. A $H \times W \times 3$ image is represented as $N \times 3$ points
  2. Cluster them into K clusters
  3. Now the $N \times 3$ points can be represented by N labels.

- Similarly, a [XYZRGB] point cloud can be compressed into [XYZL], where L is the cluster label

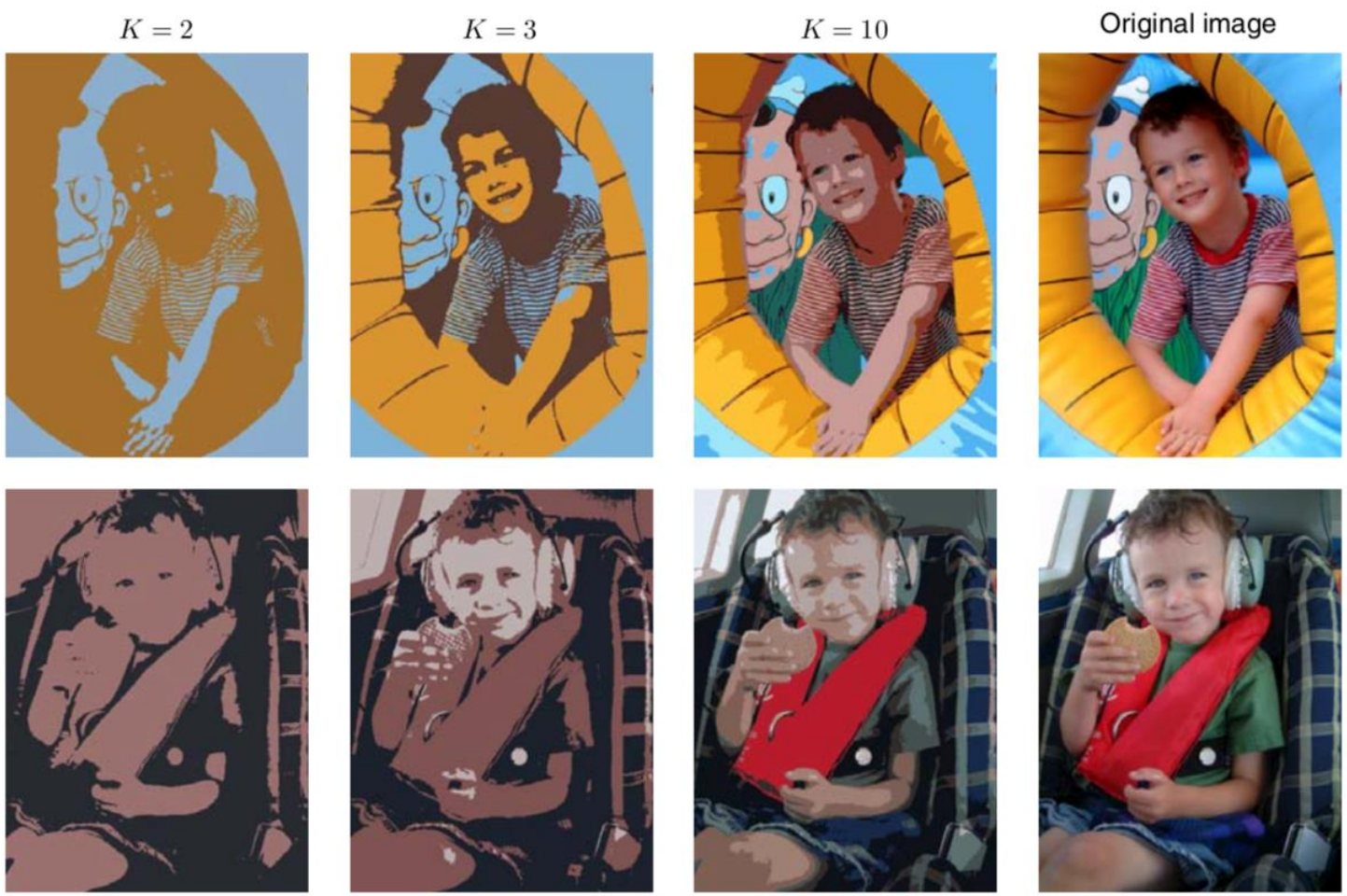


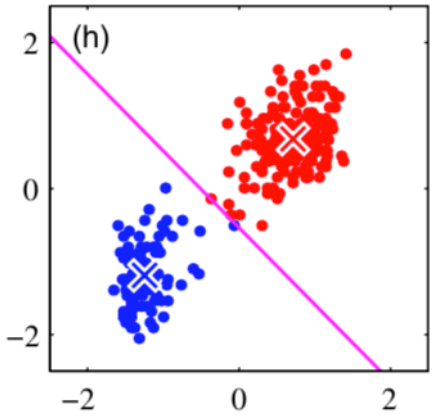
Figure source: Pattern Recognition and Machine Learning, Bishop

K-Means Compression

- Original Image have N pixels, 3 channels
  - Each channel is 8bits
  - In total $24N$ bits
- Compressed Image have N labels + cluster centers
  - N labels -> $\lceil N \log_2 K \rceil$ bits (Note that M bits can represent 2^M integers)
  - Cluster centers -> $24K$ bits
    - K clusters, each is [R,G,B]
  - In total $\lceil N \log_2 K \rceil + 24K$ bits
- $K \ll N$ therefore compression is effective

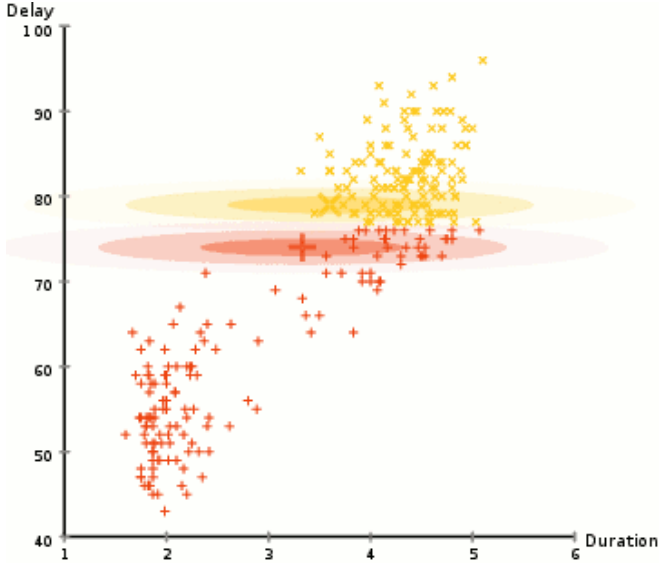
K-Means – Limitations

- Hard assignment, i.e., $\mu_k \in \{0, 1\}$ is binary label.
  - Sometimes a data point lies around the border line between centers
  - Lack of uncertainty measure for the assignments
- K is unknown



Gaussian Mixture Model (GMM)

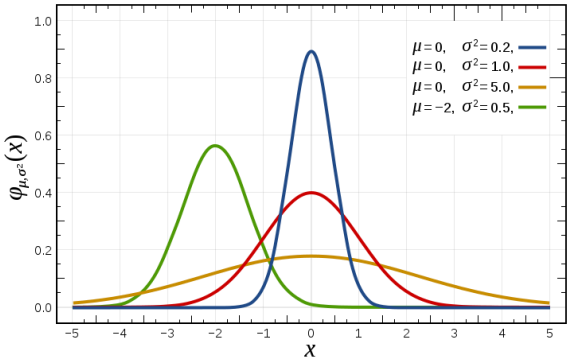
- Represent a cluster by a Gaussian Distribution $\mathcal{N}(\mu, \sigma)$
- GMM tells the probability of a point belonging to each cluster



Gaussian Distribution

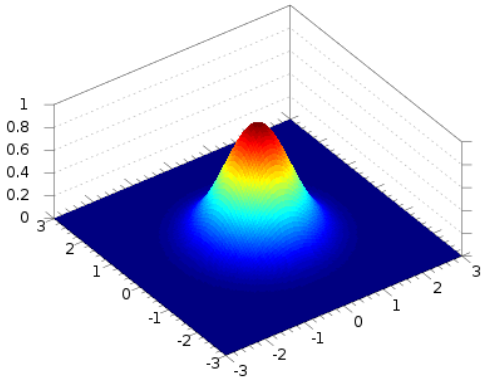
Single variable Gaussian

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



Multivariate Gaussian with D-dimensional vector

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$



GMM

- Formally, a Gaussian mixture distribution can be written as a linear combination of single Gaussians $\mathcal{N}(\mu_k, \Sigma_k)$ using weights π_k

$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

- The $\{\mu_k, \Sigma_k, \pi_k\}, k = 1, \cdots, K$ describes the GMM built from the data points. In another word, we can "generate" points using this $p(x)$

- But we want clustering! That is, the probability of each data point belongs to each single Gaussian $\mathcal{N}(\mu_k, \Sigma_k)$

GMM

- Let's introduce a K-dimensional binary variable *z* having a *1-of-K* representation.

$$z_k \in \{0, 1\}, \qquad \Sigma_k z_k = 1$$

- This $p(z_k = 1)$ is the prior probability of Gaussian distribution $\mathcal{N}(\mu_k, \Sigma_k)$

$$p(z_k = 1) = \pi_k$$

- The conditional probability $p(z|x)$ is the clustering "label probability" we want, given a data point x

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)}, \qquad p(x) = \sum_z p(z)p(x|z)$$

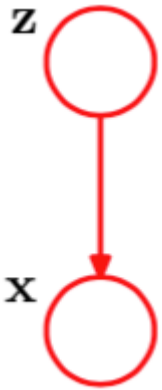
GMM

- Gaussian Mixture Model is represented by a graphical model, where the joint distribution $p(x, z) = p(z)p(x|z)$

- $p(z_k = 1) = \pi_k$, $z = [z_1, \cdots, z_k, \cdots, z_K]$, 1-of-K representation
  Constraints: $0 \leq \pi_k \leq 1$, $\sum_{k=1}^{K} \pi_k = 1$

- Alternatively,

$$p(z) = \prod_{k=1}^{K} \pi_k^{z_k}$$



GMM

- $p(x|z_k = 1)$ is a single Gaussian distribution

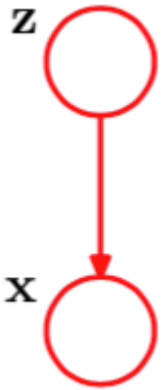
$$p(x|z_k = 1) = \mathcal{N}(x|\mu_k, \Sigma_k)$$

- Alternatively,

$$p(x|z) = \prod_{k=1}^{K} \mathcal{N}(x|\mu_k, \Sigma_k)^{z_k}$$

- The marginal distribution of x is given by $p(x) = \sum_z p(x, z)$

$$p(x) = \sum_z p(z)p(x|z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$



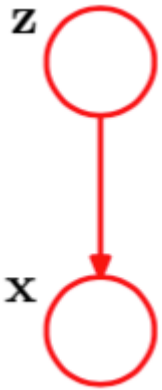
GMM

- Now we can get the posterior $p(z|x)$
  - Given a data point x, which cluster it belongs to?
- Denote $p(z_k = 1|x)\ as\ \gamma(z_k)$
- Use Bayes' rule and Total Probability Rule

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{z}|\mathbf{x})}{p(\mathbf{x})} = \frac{p(\mathbf{z})p(\mathbf{x}|\mathbf{z})}{\sum_{j=1}^{K} p(\mathbf{x}|z_j)p(z_j)}$$

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)}$$

$$= \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_j, \Sigma_j)}$$



GMM – Maximum Likelihood (MLE)

- Now we know how to get $\gamma(z_k)$, given GMM parameters $\{\pi_k, \mu_k, \Sigma_k\}$
- But how do we estimate $\{\pi_k, \mu_k, \Sigma_k\}, \gamma(z_k)$ given data points $\{\mathrm{x}_1, \cdots, \mathrm{x}_N\}$
- Maximum likelihood!

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

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

GMM – Maximum Likelihood (MLE)

- Maximum likelihood formulation suffers from singularity problem
- Assume that the GMM has the covariance matrix represented as $\Sigma_k = \sigma_k^2 I$, where *I* is identity matrix
- Assume that there is a data point $x_n = \mu_j$, the likelihood contributed by x_n is:

$$\mathcal{N}\left(\mathrm{x}_n \middle| \mathrm{x}_n, \sigma_j^2 \mathbf{I}\right) = \frac{1}{(2\pi)^{1/2}} \frac{1}{\sigma_j}$$

- What if σ_j is very small?
- So in GMM maximum likelihood formulation, we can put a Gaussian over a single point, and this leads to very large likelihood.

GMM – Maximum Likelihood (MLE)

- There are methods to avoid singularity
- Tricks
  - If a Gaussian component is collapsing into very small Σ_k, reset its mean μ_k to randomly chosen values, and Σ_k to a large value
- Systematic methods
  - Maximum-a-Posterior (MAP) – Add prior constraints to the parameters
  - Bayesian approach – Prior and proper uncertainty estimation of the parameters

Solve the MLE

- Maximum Likelihood Formulation of GMM

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

- Solve π, μ, Σ iteratively, fixed the others, solve one
- Let's look at μ_k first
- Compute the first order derivatives with respect to μ_k

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \mathbf{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \mathbf{\Sigma}_j)}}_{\gamma(z_{nk})} \mathbf{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

Solve the MLE

- Here N_k can be interpreted as the effective number of points assigned to cluster *k*
- μ_k is the weighted average of all point in the data set
- The weight is the posterior probability $\gamma(z_{nk})$
- The denominator is the effective number N_k

$$0 = -\sum_{n=1}^{N} \gamma(z_{nk}) \boldsymbol{\Sigma}_k (\mathbf{x}_n - \mu_k)$$

Solve the MLE

- Compute the first order derivatives with respect to Σ_k, we can solve Σ_k similarly,

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

- Σ_k is the weighted average of all point's variance centered by μ_k
- The weight is the posterior probability $\gamma(z_{nk})$
- The denominator is the effective number N_k

Solve the MLE

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

- Now let's solve for π_k
- However, there is a constraint $\sum_{k=1}^{K} \pi_k = 1$
- Lagrange Multiplier λ

$$\ln p(\mathbf{X}|\pi,\mu,\Sigma) + \lambda\left(\sum_{k=1}^{K} \pi_k - 1\right)$$

- Compute first order derivate with respect to π_k and make it 0

$$0 = \sum_{n=1}^{N} \frac{\mathcal{N}(\mathbf{x}_n|\mu_k,\Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_k,\Sigma_k)} + \lambda$$

Solve the MLE

Solve λ first

$$0 = \sum_{n=1}^{N} \frac{\mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)} + \lambda$$

$$0 = \sum_{k=1}^{K} \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)} + \sum_{k=1}^{K} \pi_k \lambda$$

$$0 = \left(\sum_{n=1}^{N} 1 \right) + \lambda$$

$$\lambda = -N$$

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

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

Solve the MLE

- Solve π_k
- Intuitively, π_k is the effective cluster member number over data set size.

$$0 = \sum_{n=1}^{N} \frac{\mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)} + \lambda$$

$$0 = \frac{1}{\pi_k} \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)} - N$$

$$0 = \frac{1}{\pi_k} \sum_{n=1}^{N} \gamma_{nk} - N$$

$$\pi_k = \frac{N_k}{N}$$

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

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

Summary for GMM MLE

1. Initialize the means μ_k, covariances Σ_k and weights π_k

2. E-step. Evaluate the posterior $p(z_{nk} = 1|x_n)$, intuitively this is the probability of x_n being assigned to each of the K clusters.

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

Summary for GMM MLE

3. M-Step. Estimate the parameters using MLE.

4. Evaluate the log likelihood, if converges, stop. Otherwise go back to E-step

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

$$\begin{aligned}
\boldsymbol{\mu}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \\
\boldsymbol{\Sigma}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}} \\
\pi_k^{\text{new}} &= \frac{N_k}{N}
\end{aligned}$$

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

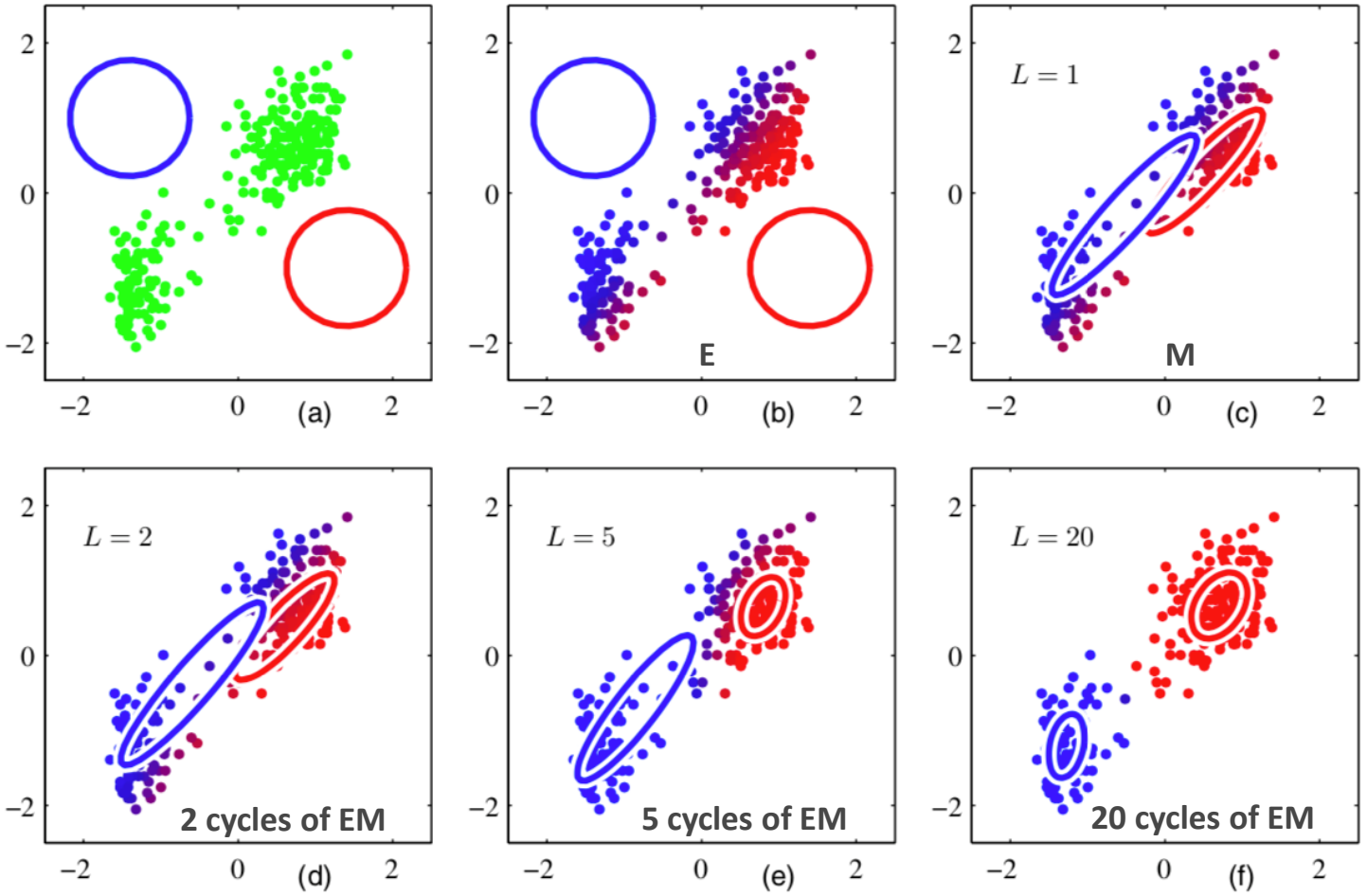


Figure source: Pattern Recognition and Machine Learning, Bishop

Expectation – Maximization (EM)

Given a joint distribution $p(X, Z|\theta)$ over observed variables X and latent variables Z, governed by parameters θ, the goal is to maximize the likelihood function $p(X|\theta)$ with respect to θ

$$p(\mathbf{X}|\boldsymbol{\theta}) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$

1. Choose an initial parameter θ^{old}
2. E-step. Evaluate $p(Z|X, \theta^{old})$
3. M-step. Evaluate θ^{new} by solving the optimization problem

$$\theta^{\text{new}} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{\text{old}})$$

$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) = \mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\theta)]$$

4. Check for convergence, if not, go back to E-step

$$\theta^{old} \leftarrow \theta^{new}$$

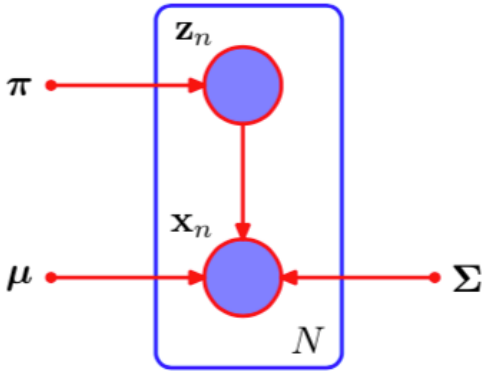
GMM revisited

- In GMM, we have the joint distribution $p(x,z) = p(z)p(x|z)$

$$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k} \qquad p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$$

- Alternatively

$$p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}$$



where z_{nk} denotes the k^{th} component of $\mathbf{z}_n$

- Take the logarithm, we have

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

GMM revisited

Let's recall the M-step of EM algorithm

$$\theta^{\text{new}} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{\text{old}})$$

$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) = \mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\theta)]$$

In the context of GMM, we have

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

$$\mathbb{E}_z[\ln p(\mathbf{X}, \mathbf{Z}|\mu, \Sigma, \pi)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{E}[z_{nk}] \{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)\}$$

GMM revisited

Recall the posterior in GMM

$$p(z_{nk}=1|\mathbf{x}_n,\mu_k,\Sigma_k,\pi_k)=\gamma(z_{nk})=\frac{\pi_k\mathcal{N}(\mathbf{x}_n|\mu_k,\Sigma_k)}{\sum_{j=1}^{K}\pi_j\mathcal{N}(\mathbf{x}_n|\mu_j,\Sigma_j)}$$

So we have

$$\begin{aligned}\mathbb{E}[z_{nk}] &= \sum_{z_{nk}} z_{nk}p(z_{nk}|\mathbf{x}_n,\mu_k,\Sigma_k,\pi_k)\\ &= 0\cdot p(z_{nk}=0|\mathbf{x}_n,\mu_k,\Sigma_k,\pi_k)+1\cdot p(z_{nk}=1|\mathbf{x}_n,\mu_k,\Sigma_k,\pi_k)\\ &= \gamma(z_{nk})\end{aligned}$$

GMM revisited

$$\theta^{\text{new}} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{\text{old}}) \qquad \text{M-step}$$

$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) = \mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\theta)]$$

- Now we have $\mathcal{Q}$ function for the GMM problem

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}$$

- Solving for the maximum we have the same result as the previous GMM solution

$$\begin{aligned}
\boldsymbol{\mu}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \\
\boldsymbol{\Sigma}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^{\mathrm{T}} \\
\pi_k^{\text{new}} &= \frac{N_k}{N}
\end{aligned}$$

GMM revisited

In summary, we derivate the GMM result using two methods

1. Standard MLE formulation

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

2. EM algorithm

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \mathbf{\Sigma}, \boldsymbol{\pi})] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \mathbf{\Sigma}_k)\}$$

K-Means revisited

- K-Means is a special of the GMM
  - The soft assignment becomes hard $\gamma(z_{nk}) \rightarrow r_{nk}$
  - The variance is zero $\Sigma_k \rightarrow 0$
- In the case that $\Sigma_k = \epsilon I$, the original $\gamma(z_{nk})$ becomes

$$\gamma(z_{nk}) = \frac{\pi_k \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2/2\epsilon\right\}}{\sum_j \pi_j \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2/2\epsilon\right\}}$$

- Why? Let's look at the two equations below

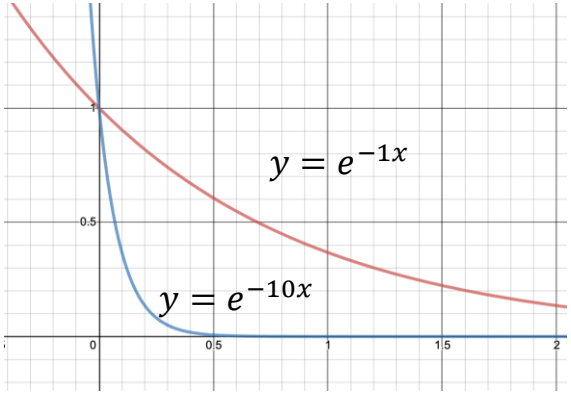
$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_j, \Sigma_j)}$$

$$p(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \frac{1}{(2\pi\epsilon)^{1/2}} \exp\left\{-\frac{1}{2\epsilon}\|\mathbf{x} - \boldsymbol{\mu}_k\|^2\right\}$$

K-Means revisited

$$\gamma(z_{nk}) = \frac{\pi_k \exp\{-\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2/2\epsilon\}}{\sum_j \pi_j \exp\{-\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2/2\epsilon\}}$$

- Let's consider the limit $\epsilon \to 0$
- Look at the denominator
- The j that $\|x_n - \mu_j\|^2$ is smallest goes to zero most slowly
- All other j goes to zero quickly
- Therefore $\gamma(z_{nk}) \to r_{nk}$



$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$

K-Means revisited

- The M-step of GMM/EM gives the following

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] = \sum_{n=1}^{N}\sum_{k=1}^{K} \gamma(z_{nk}) \{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}$$

- Given $\Sigma_k = \epsilon I, \quad \epsilon \to 0, \ \gamma(z_{nk}) \to r_{nk}$

- It can be written as

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] \to -\frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2 + \text{const}$$

- Which is the same as the distortion measure J in the K-means algorithm

$$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

Conclusion for K-Means, GMM, EM

GMM is a special application of EM

- The latent variable $\{z_{nk}\}$ and the model parameters $\{\mu_k, \Sigma_k, \pi_k\}$ are estimated in the E-step and M-step
- The clustering probability is given by $\gamma(z_{nk}) = p(z_{nk} = 1|x_n, \mu_k, \Sigma_k, \pi_k)$

K-Means is a special case of GMM, where

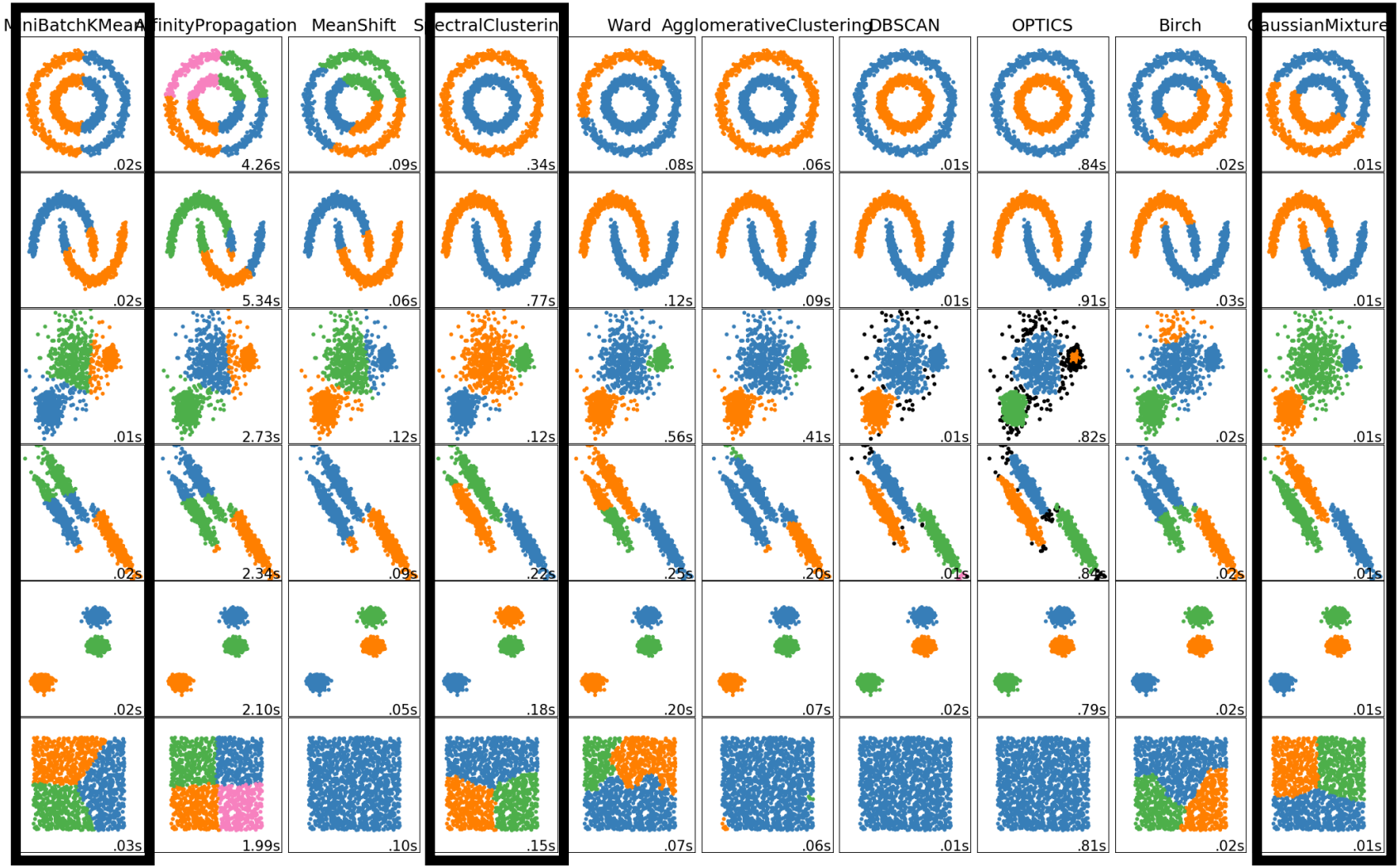
- The soft assignment becomes hard $\gamma(z_{nk}) \to r_{nk}$
- The variance is zero $\Sigma_k \to 0$

K-Means Summary

- Complexity $O(t \cdot k \cdot n \cdot d)$
  - t- number of iteration, k- number of clusters, n- number of points, d- number of dimension
- Advantage
  - Simple
  - Fast
- Disadvantage
  - Assumes circle/sphere-like data – same variance in all directions
  - Need to provide number of clusters
  - Sensitive to initialization
  - Sensitive to outlier
    - Can be alleviated by K-Medoids

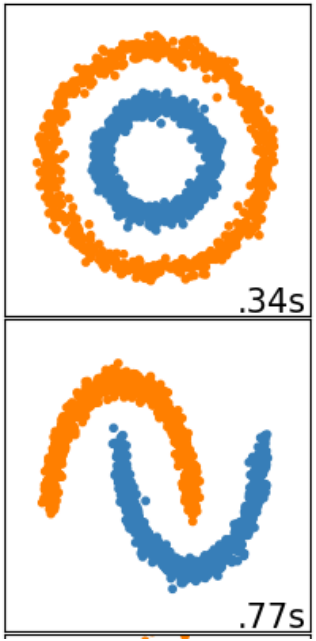
GMM Summary

- Complexity $O(t \cdot k \cdot n \cdot d)$
  - t- number of iteration, k- number of clusters, n- number of points, d- number of dimension
- Advantage
  - Provides uncertainty estimation – soft assignment
  - More robust to outlier
- Disadvantage
  - Need to provide number of clusters
  - Mainly works with convex clusters
    - Gaussian distributions are in the shape of ellipsoid
  - Singularity problem


MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
OPTICS
Birch
GaussianMixture
.02s
4.26s
.09s
.34s
.08s
.06s
.01s
.84s
.02s
.01s
.02s
5.34s
.06s
.77s
.12s
.09s
.01s
.91s
.03s
.01s
.01s
2.73s
.12s
.12s
.56s
.41s
.01s
.82s
.02s
.01s
.02s
2.34s
.09s
.22s
.25s
.20s
.01s
.84s
.02s
.01s
.02s
2.10s
.05s
.18s
.20s
.07s
.02s
.79s
.02s
.01s
.03s
1.99s
.10s
.15s
.07s
.06s
.01s
.81s
.02s
.01s

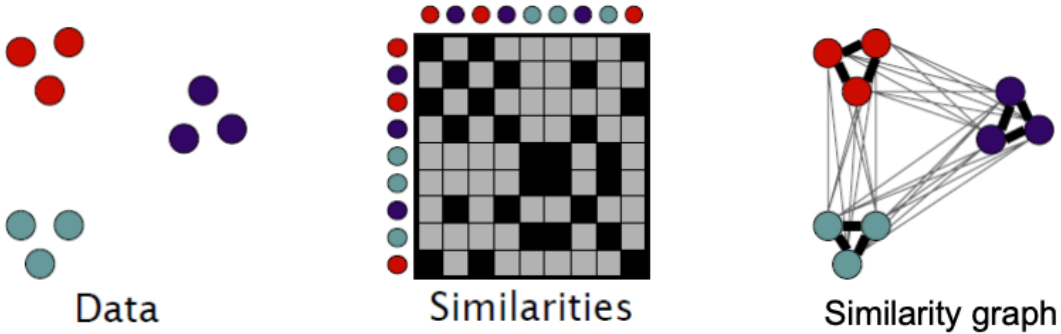
Spectral Clustering

- K-Means fails row 1, 2, 3, 4
- GMM fails row 1, 2
- Why? They are based on Euclidean distance!
- How about other metric? E.g., connectivity?
- Spectral Clustering works with connectivity!



Spectral Clustering

- Works for a (Weighted) Undirected Graph $G = (V, E)$, where $V = \{v_1, \cdots, v_n\}$,
- The edge between two vertices v_i, v_j carries weight $w_{ij} \geq 0$.
  - Two vertices are not connected if $w_{ij} = 0$
  - Specially, $w_{ii} = 0$
- The weighted adjacency matrix / similarity matrix is represented by $W = (w_{ij})_{i,j=1,\cdots,n}$



Spectral Clustering – How to build the Graph

- Every point is a vertex
- There are 3 common graphs built for Spectral Clustering

1. ϵ-neighborhood graph. Radius nearest neighbor search. $w_{ij} = d(v_i, v_j)$
2. k-neighborhood graph. KNN search. $w_{ij} = d(v_i, v_j)$
   a) Build an edge if v_i is one of the knn of v_j OR v_j is one of the knn of v_i
   b) Build an edge if v_i is one of the knn of v_j AND v_j is one of the knn of v_i
3. Fully connected graph. Connect every point.

Spectral Clustering – Laplacian Matrix

- Degree matrix D
  - A diagonal matrix with degrees $d_1, \cdots, d_n$ on the diagonal
  - $d_i = \sum_{j=1}^{n} w_{ij}$ is the row sum of adjacency matrix W
- Unnormalized graph Laplacian matrix $L = D - W$
- Normalized graph Laplacian matrix
  - $L_{sym} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}$
  - $L_{rw} = D^{-1} L = I - D^{-1} W$

Unnormalized Spectral Clustering

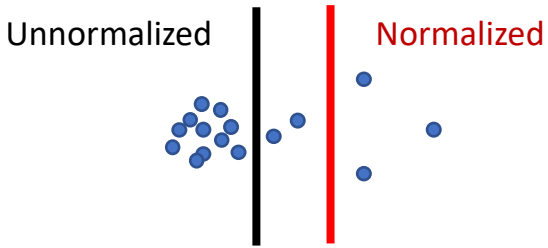
1. Build the graph to get adjacency matrix $W \in \mathbb{R}^{n \times n}$
2. Compute unnormalized Laplacian L
3. Compute the first (smallest) k eigenvectors $v_1, \cdots, v_k$ of L
4. Let $V \in \mathbb{R}^{n \times k}$ be the matrix contraining the vectors $v_1, \cdots, v_k$ as columns
5. For $i = 1, \cdots n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of V
6. Cluster the points $\{y_i \in \mathbb{R}^k\}$ with k-means algorithm into clusters $C_1, \cdots, C_k$
7. The final output clusters are $A_1, \cdots, A_k$ where $A_i = \{j | y_j \in C_i\}$

Normalized Spectral Clustering

1. Build the graph to get adjacency matrix $W \in \mathbb{R}^{n \times n}$
2. Compute normalized Laplacian $L' = L_{rw}$
3. Compute the first (smallest) k eigenvectors $v_1, \cdots, v_k$ of L'
4. Let $V \in \mathbb{R}^{n \times k}$ be the matrix contraining the vectors $v_1, \cdots, v_k$ as columns
5. For $i = 1, \cdots n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of V
6. Cluster the points $\{y_i \in \mathbb{R}^k\}$ with k-means algorithm into clusters $C_1, \cdots, C_k$
7. The final output clusters are $A_1, \cdots, A_k$ where $A_i = \{j | y_j \in C_i\}$

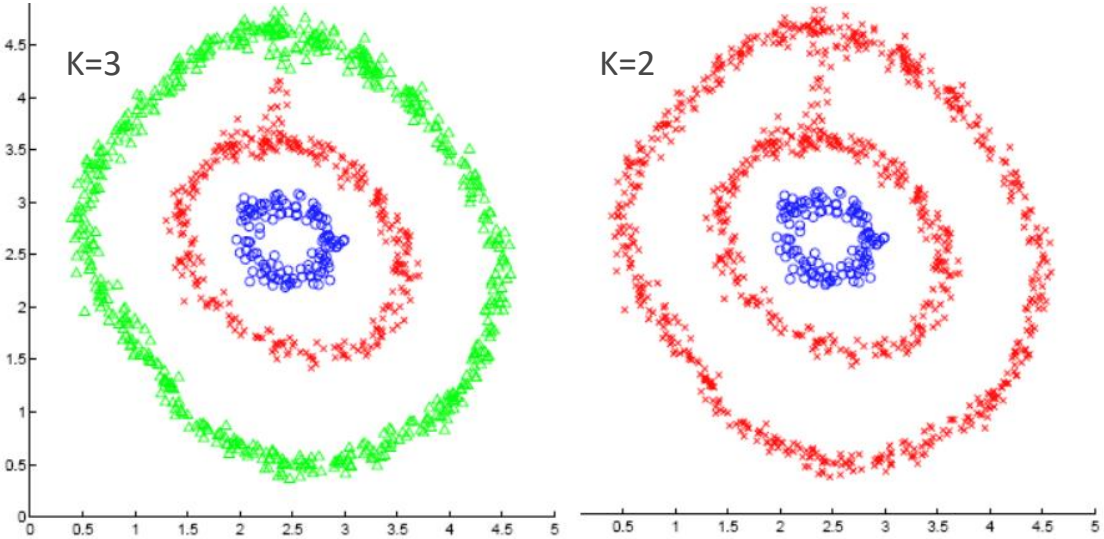
Unnormalized vs. Normalized

- Unnormalized spectral clustering tends to make clusters have equal number of vertices
- Normalized tends to group same density clusters
- Why? Lecture-4



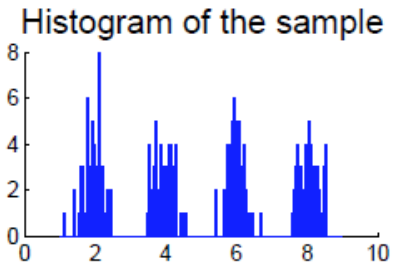
Spectral Clustering

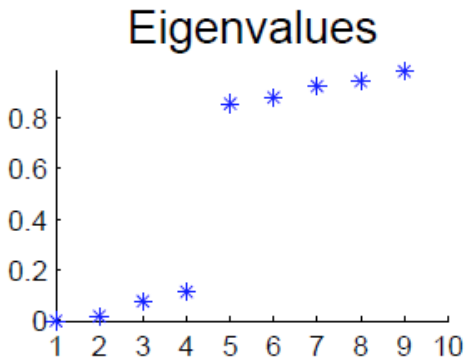
- Usually normalized spectral clustering works well with un-uniform point density.
- Selection of number of clusters k



Spectral Clustering

- Selection of k can be done by eigenvalue analysis
- Most stable clustering is given by the value of k that maximizes the eigen-gap
  - Eigengap is the difference between consecutive eigenvalues
  - $\Delta_k = |\lambda_k - \lambda_{k-1}|$



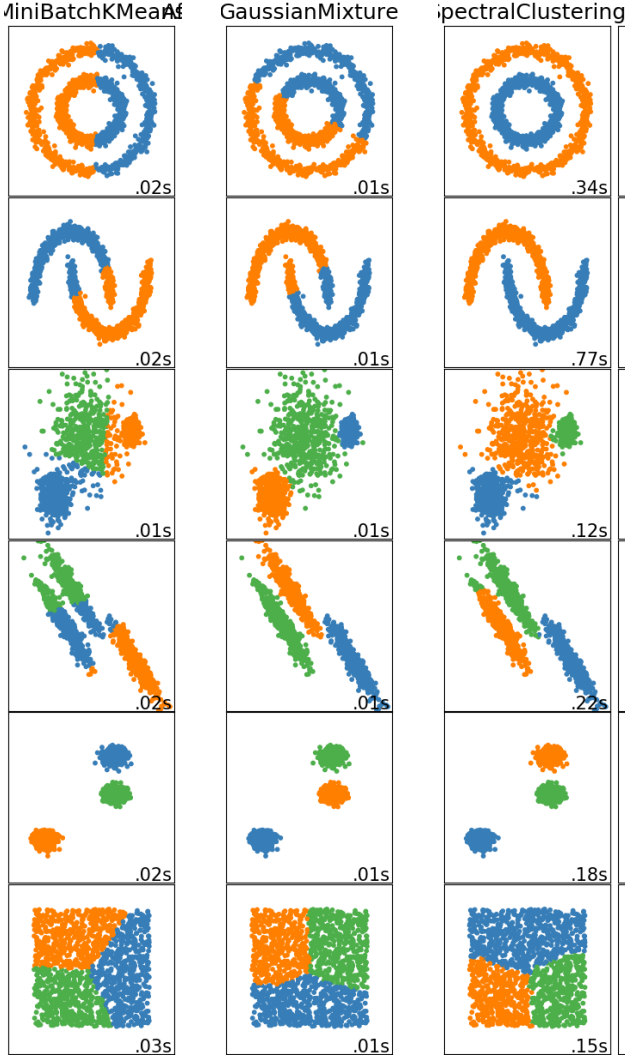


Spectral Clustering

- Complexity: $O(n^3)$
  - This is the complexity of eigen decomposition
  - K-means complexity is $O(t \cdot k \cdot n \cdot d)$
- Advantage
  - No assumption on cluster shape
  - Works with similarity, including Euclidean, connectivity
  - Works with any dimensional data
  - Able to estimate the number of clusters
- Disadvantage
  - Computational expensive
    - Can be alleviated using sparse similarity matrix and sparse eigen solver

Summary

- K-Means
  - Euclidean distance
  - Hard assignment
  - No modeling for a cluster
  - Pre-defined cluster number k
- GMM
  - Euclidean distance
  - Probability formulation – soft clustering
  - Mean and variance estimation for each cluster
  - Pre-defined cluster number k
- Spectral Clustering
  - Works with connectivity
  - Heuristic to determine cluster number k



Next Lecture

- First half of next lecture covers other Clustering algorithms:
  - Proof and intuition of Spectral Clustering
  - DBSCAN
  - Mean-Shift
- Second half covers Model Fitting:
  - Hough Transform
  - Sample Consensus

Homework

- Generate clustering dataset using sklearn
  - https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html
- Implement your own version of
  - K-Means
  - GMM
  - Spectral Clustering
- Visualize and compare the results with the standard results
  - https://scikit-learn.org/stable/modules/clustering.html#overview-of-clustering-methods

感谢各位聆听！

Thanks for Listening