深蓝学院
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3D Point Clouds
Lecture 3 – Clustering

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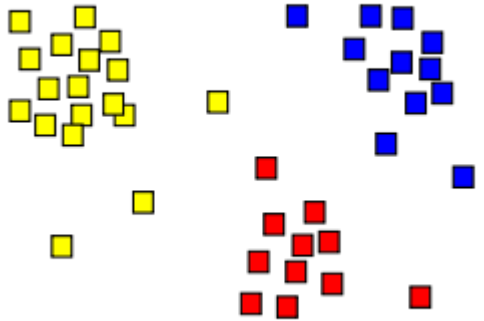
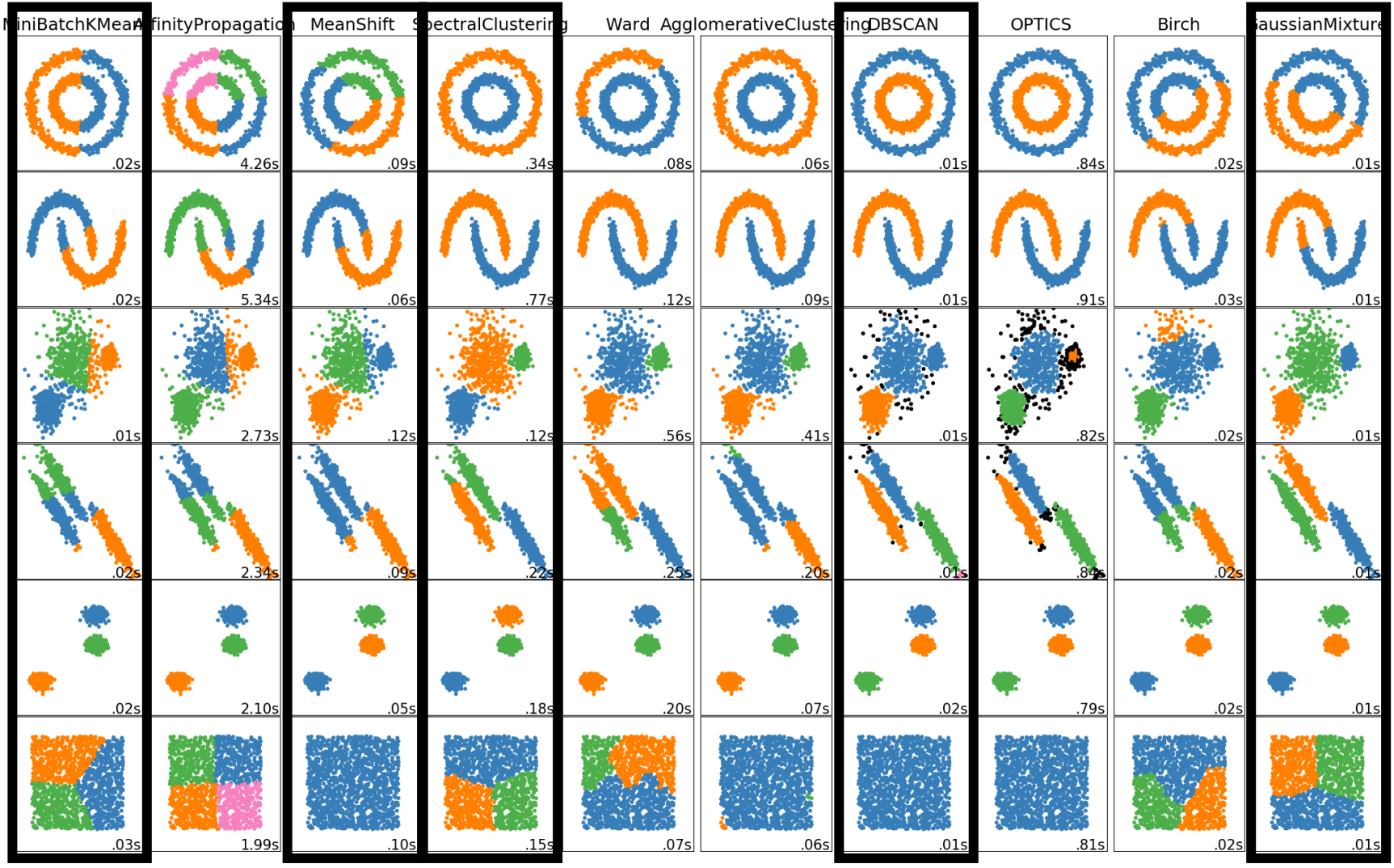
- 1、Math Prerequisite
- 2、K-Means
- 3、Gaussian Mixture Models (GMM)
- 4、Expectation Maximization (EM)
- 5、Spectral Clustering
- 6、Others – Mean Shift, DBSCAN

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
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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, …)

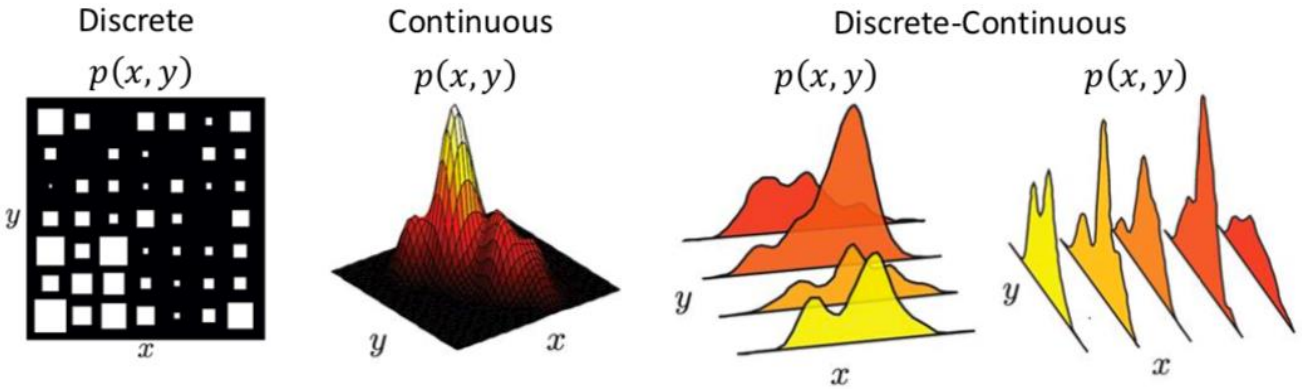

Image Source: "Computer Vision: Models, Learning, and Inference", Simon Prince
Content source: Uncertainty Modeling in AI, Lee Gim Hee

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:

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

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

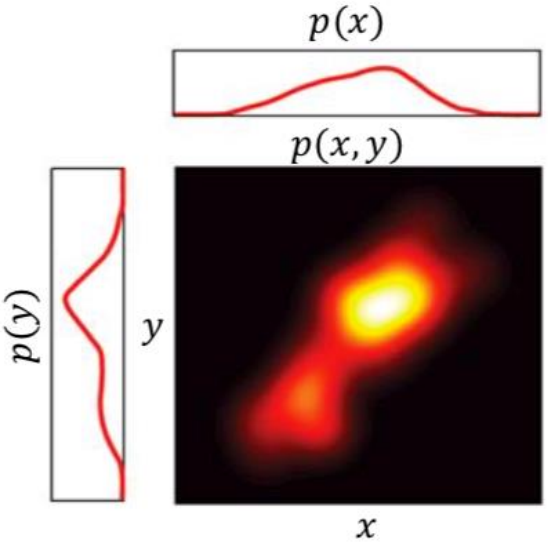

Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince
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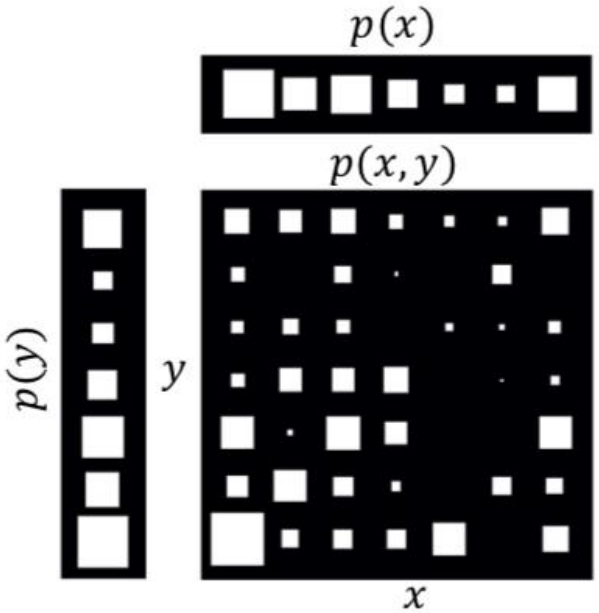
Probability - Marginalization

Discrete:

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

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



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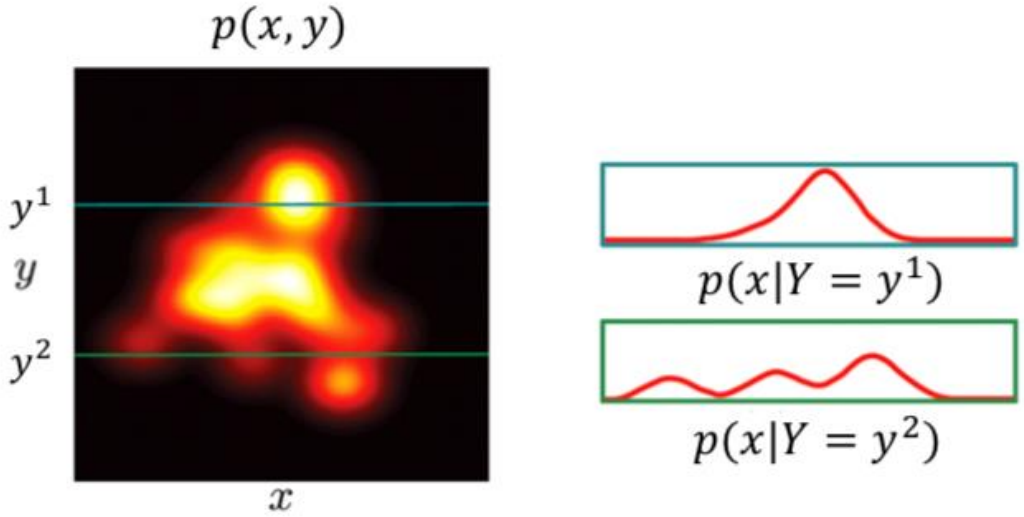
Probability – Conditional Probability

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



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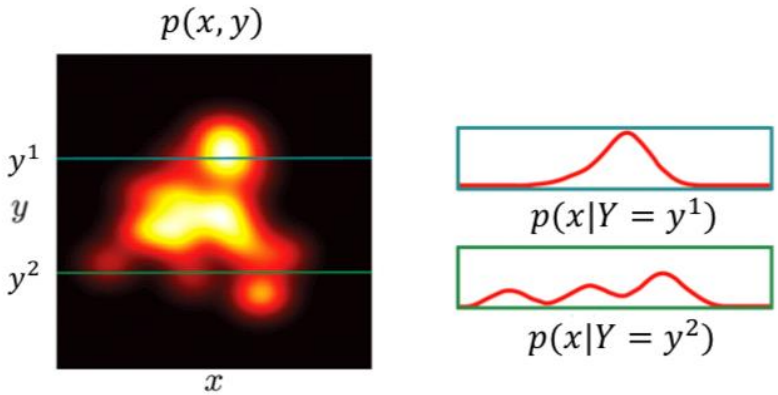
Probability – Conditional Probability

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

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



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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

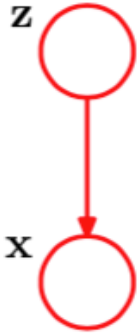
Probability – Conditional Probability

- 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

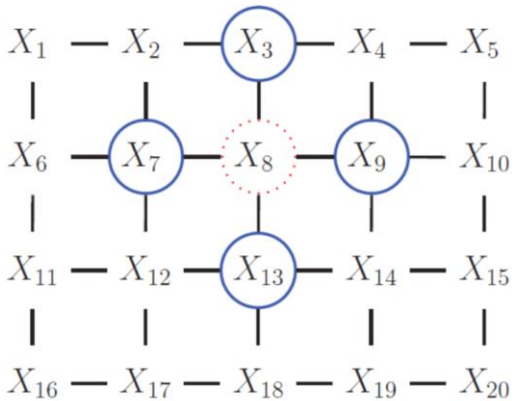
Graphical Modeling - Directed Graphical Model (DGM)



- 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



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Optimization – Lagrange multiplier

- Consider the optimization problem

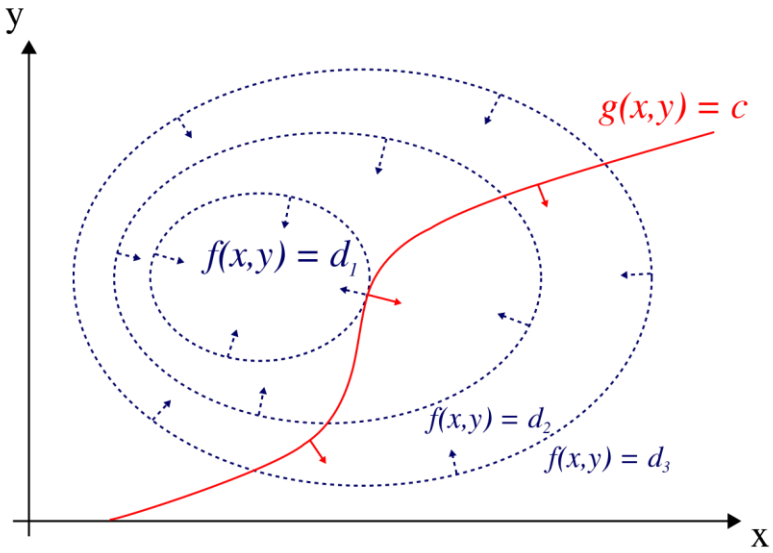
$$\max\ f(x,y),\ s.t.:\ g(x,y)=0$$

- 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:

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

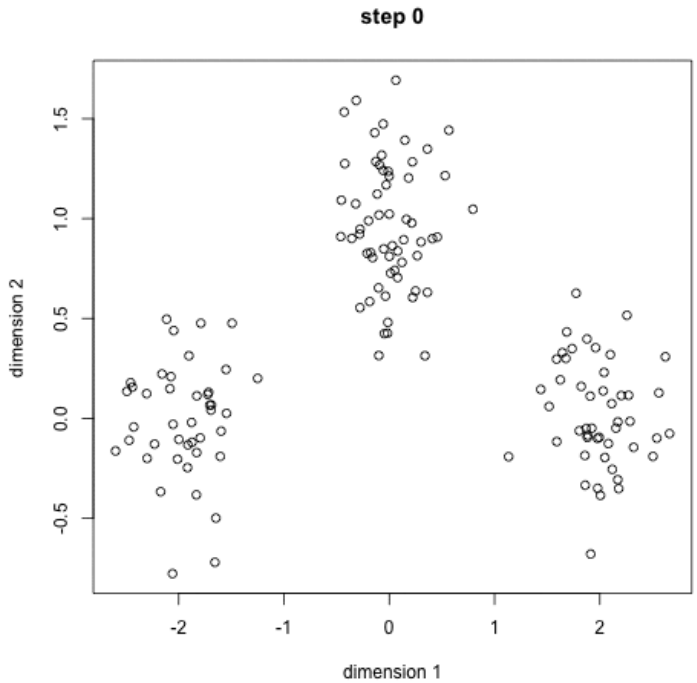
- The above equation means
  (1) $g(x, y) = 0$
  (2) gradient of *f* and *g* are parallel

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

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)

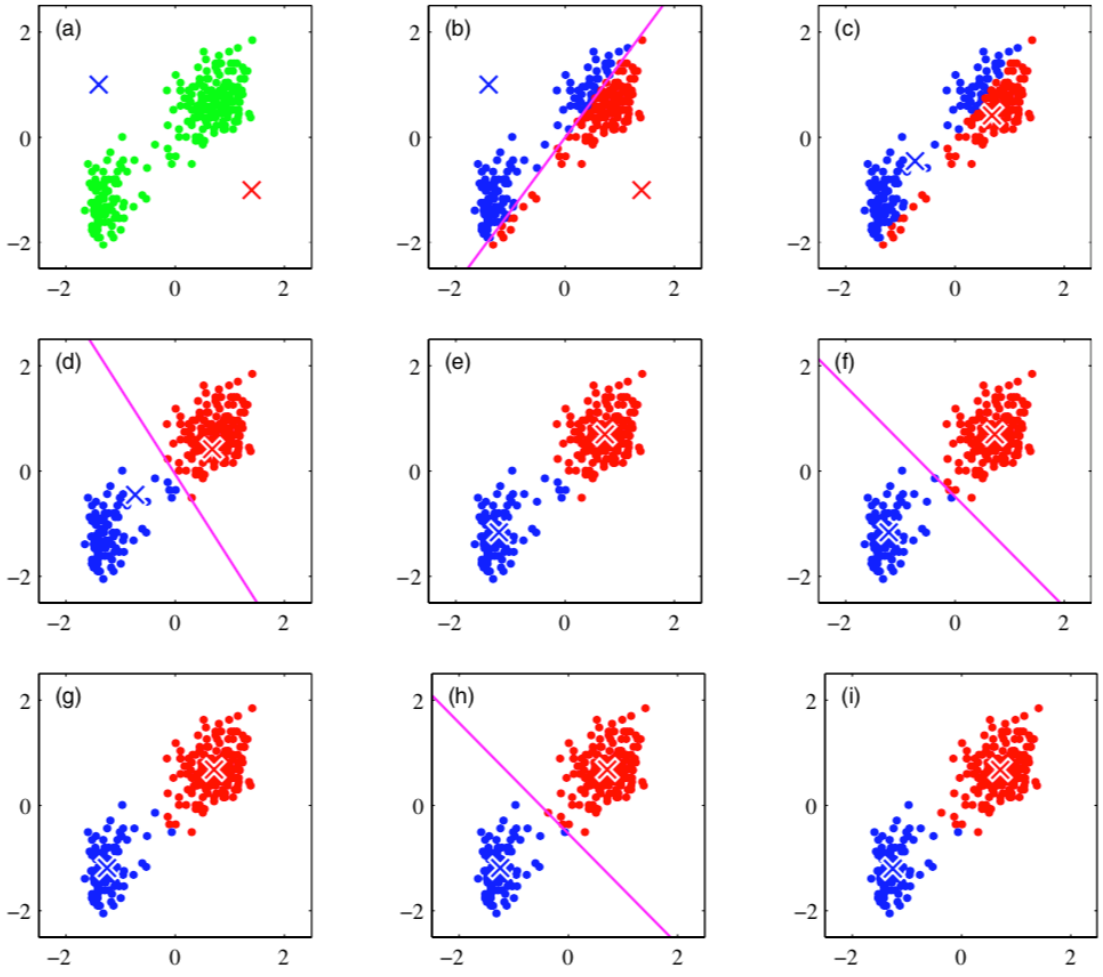


Figure source: Pattern Recognition and Machine Learning, Bishop Dataset: re-scaled Old Faithful dataset

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

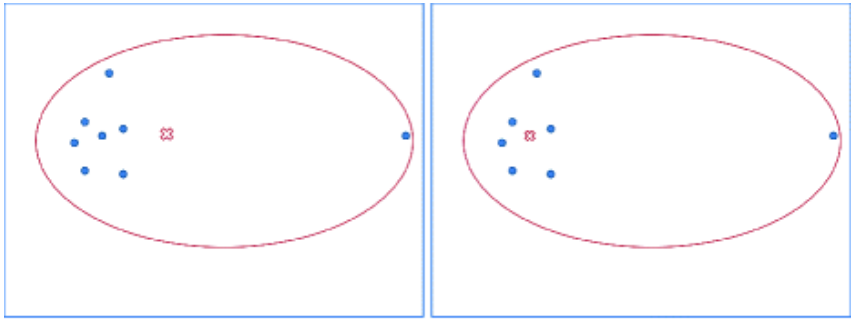
- Mini-batch version of this is the mini-batch K-Means mentioned in previous slice

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

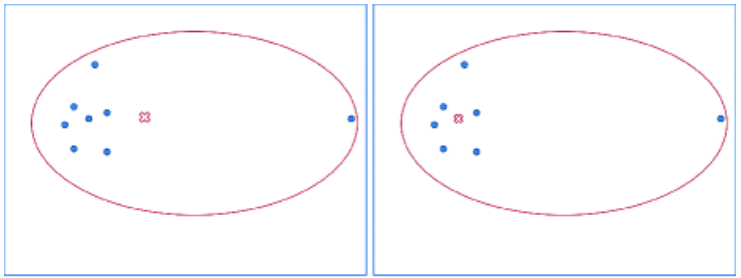
E step

- 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

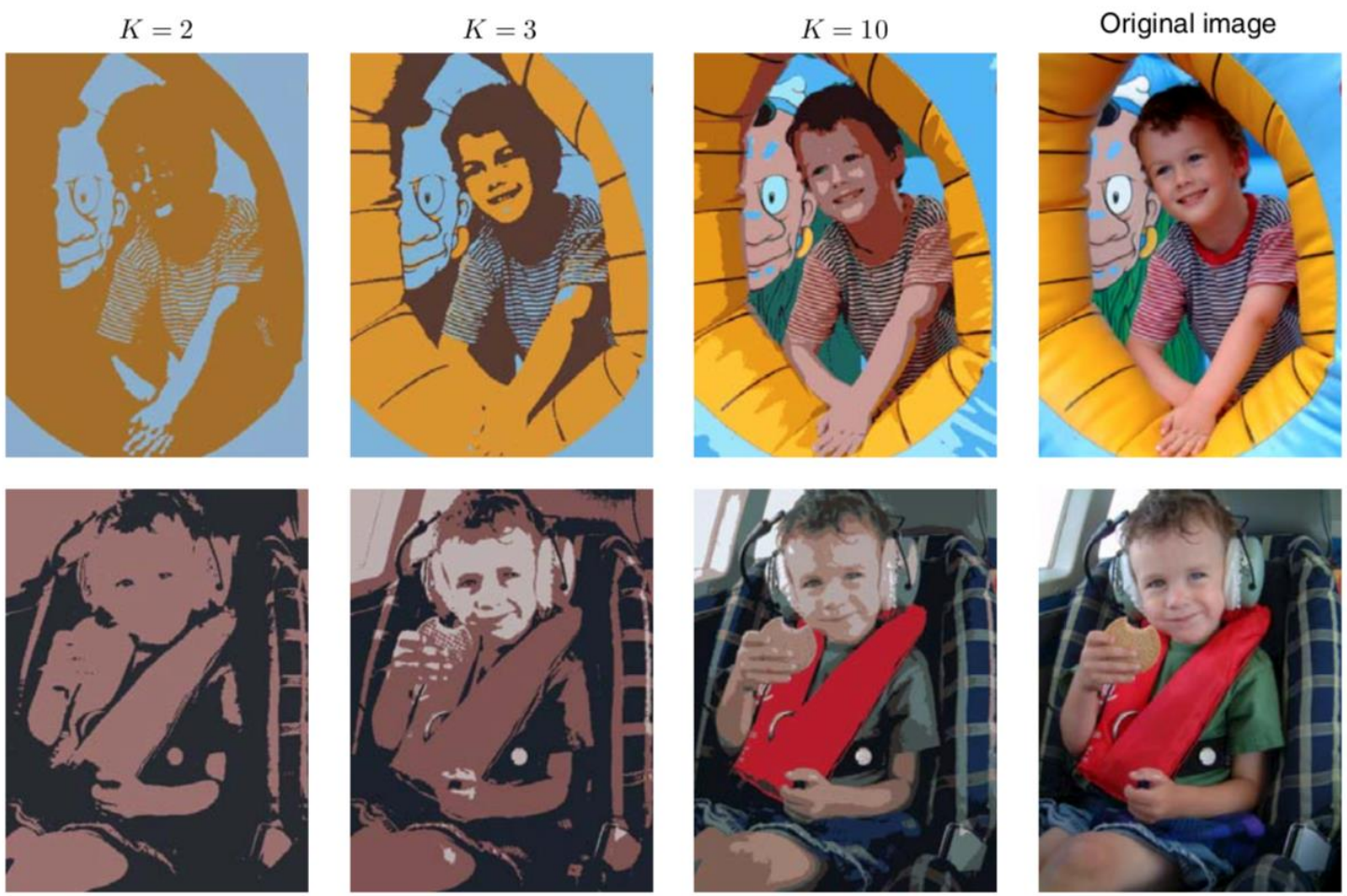


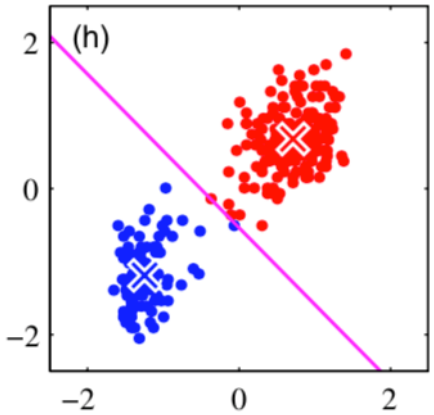
Figure source: Pattern Recognition and Machine Learning, Bishop

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

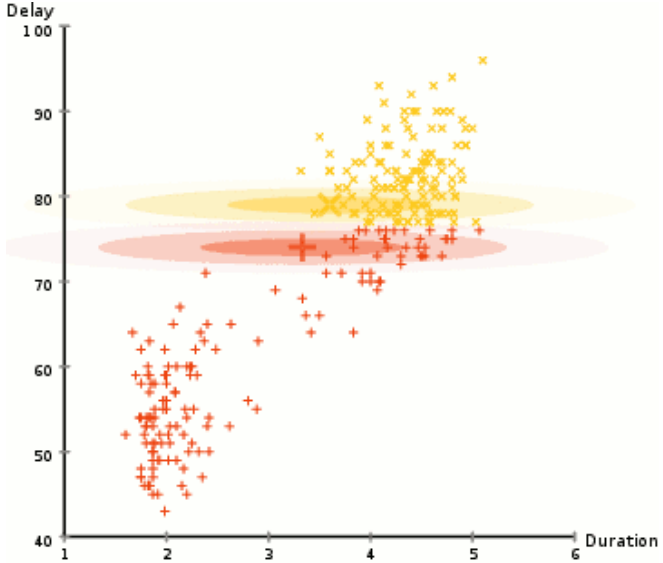
K-Means – Limitations

- 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)

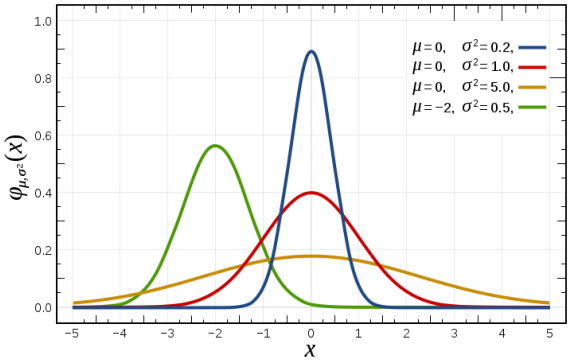
- Represent a cluster by a Gaussian Distribution $\mathcal{N}(\mu, \sigma)$
- GMM tells the probability of a point belonging to each cluster



Gaussian Distribution

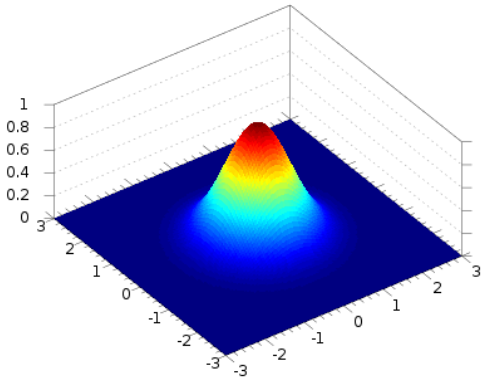
Single variable Gaussian

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



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

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

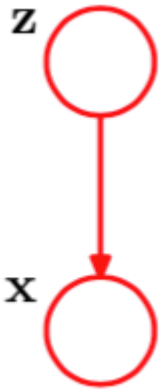
GMM

- 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

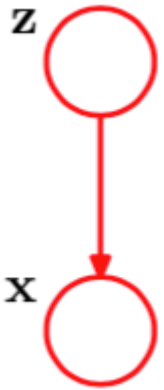
$$p(x|z_k = 1) = \mathcal{N}(x|\mu_k, \Sigma_k)$$

- 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 $p(x) = \sum_z p(x, z)$

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



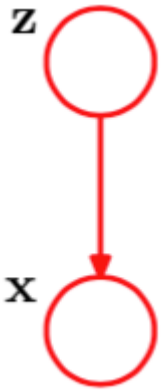
GMM

- 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

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

这里公式不全,对于Nk等参数的介绍,参考该ppt的后面部分

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.

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

上式表示N个点中某一个点n,属于第k类的概率

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

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

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

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

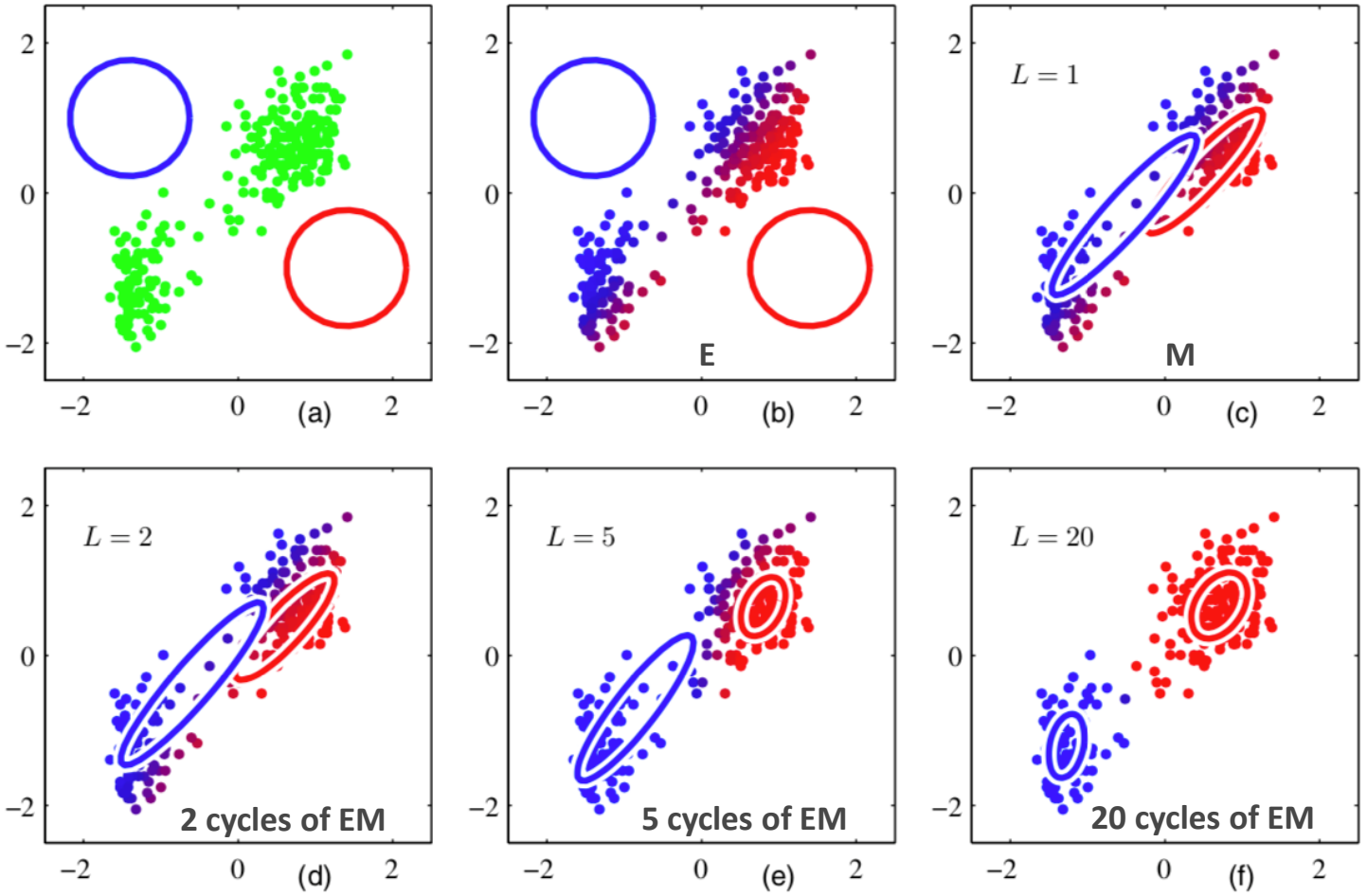


Figure source: Pattern Recognition and Machine Learning, Bishop

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

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

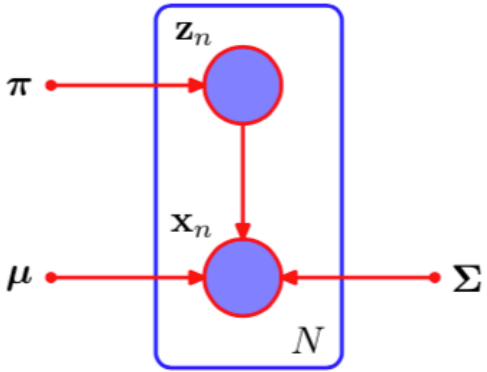
GMM revisited

- 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

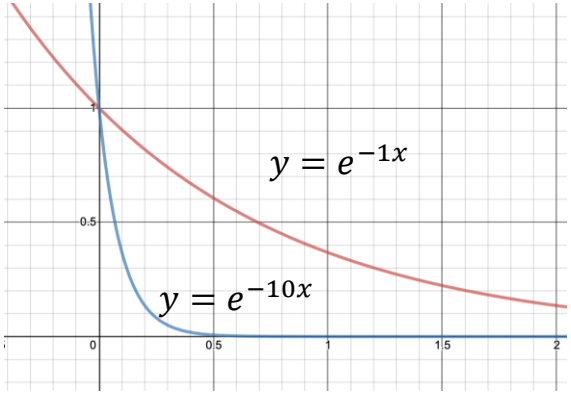
$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\mu_j, \Sigma_j)}$$

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

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

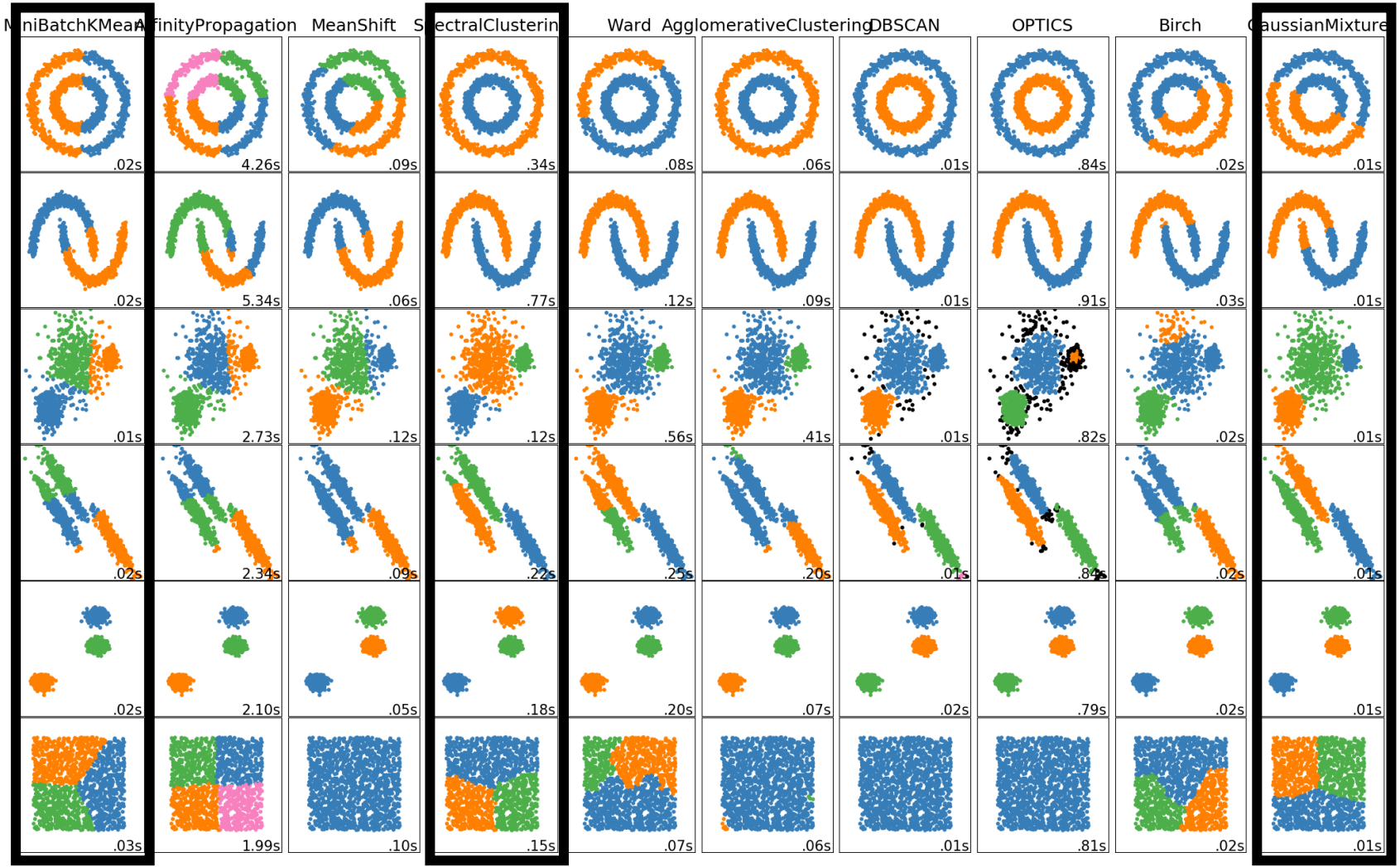
- The soft assignment becomes hard $\gamma(z_{nk}) \to r_{nk}$
- The variance is zero $\Sigma_k \to 0$

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
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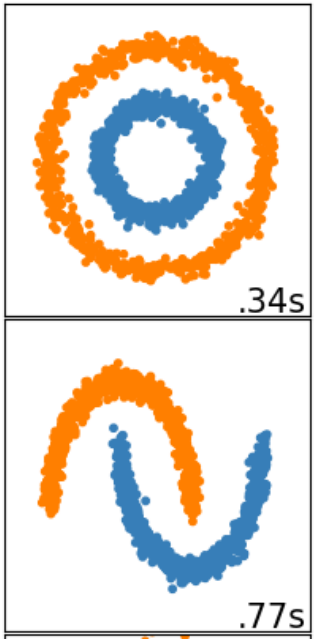
.01s

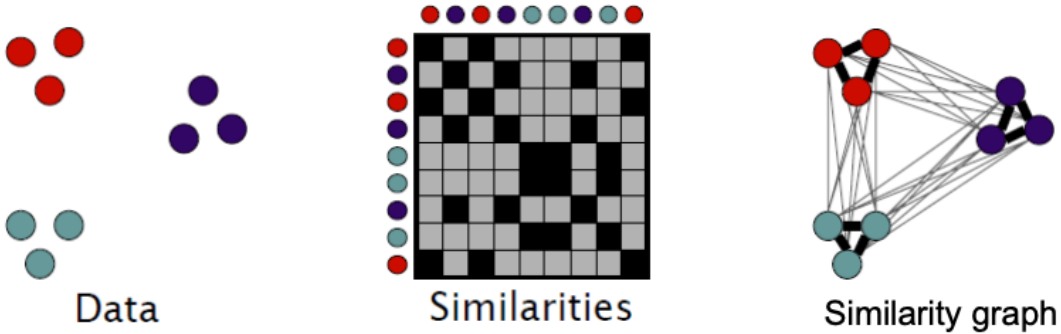
Spectral Clustering

- 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

权重是距离的倒数

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

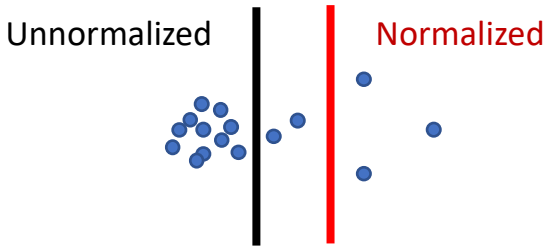
1. Build the graph to get adjacency matrix $W \in \mathbb{R}^{n \times n}$
2. Compute unnormalized Laplacian L
3. Compute the first (smallest) k eigenvectors $v_1, \cdots, v_k$ of L
4. Let $V \in \mathbb{R}^{n \times k}$ be the matrix contraining the vectors $v_1, \cdots, v_k$ as columns
5. For $i = 1, \cdots n$, 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 $A_i = \{j | y_j \in C_i\}$

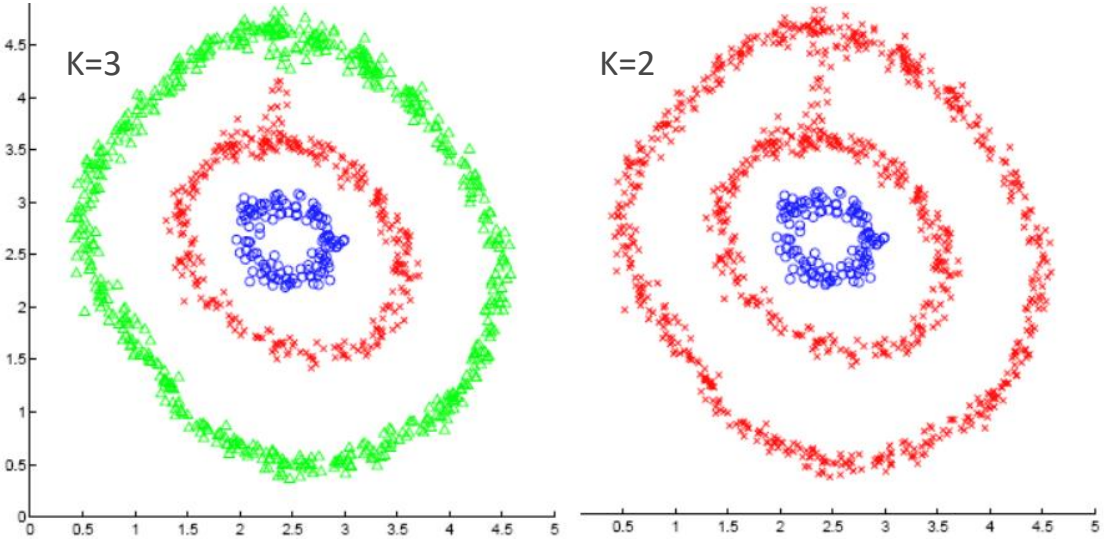
Unnormalized vs. Normalized

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



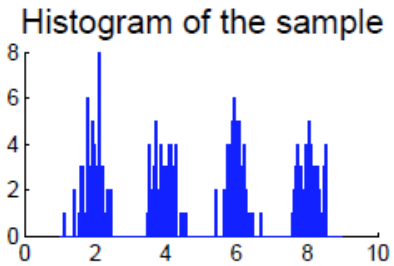
Spectral Clustering

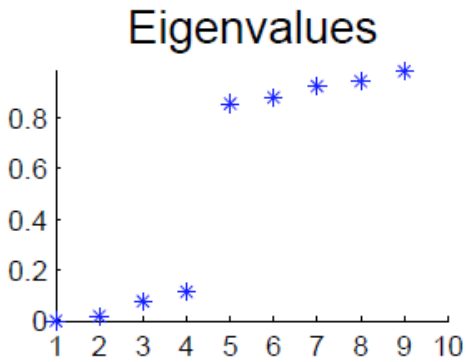
- Usually normalized spectral clustering works well with un-uniform point density.
- Selection of number of clusters k



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
  - $\Delta_k = |\lambda_k - \lambda_{k-1}|$



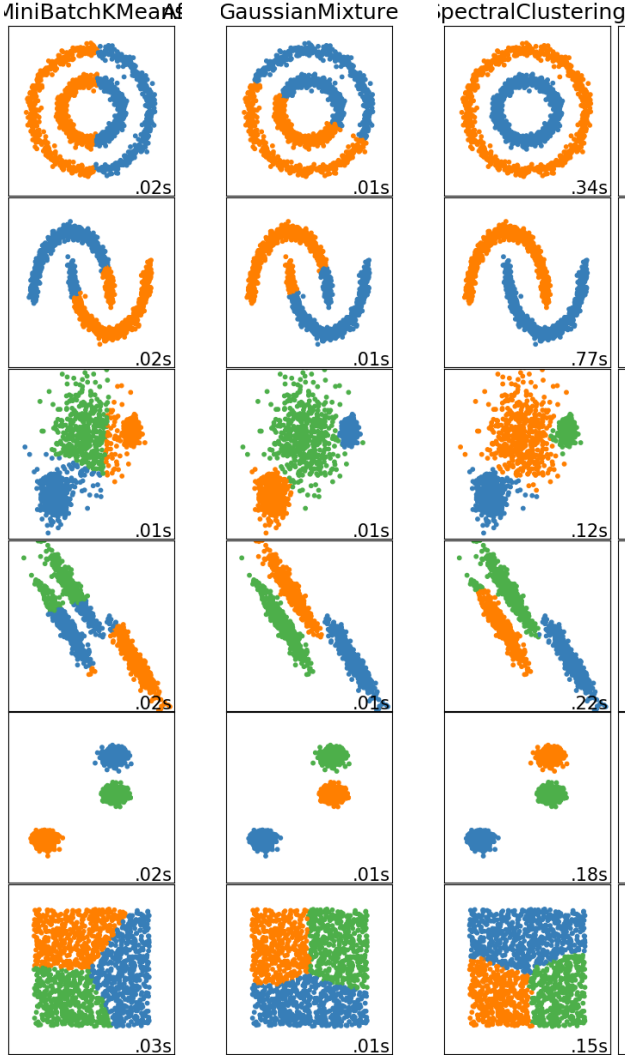


Spectral Clustering

- 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