



# CS 236756 - Technion - Intro to Machine Learning

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## Tutorial 09 - Expectation Maximization

- Based on **Pattern Recognition and Machine Learning** by *Christopher Bishop* (chapter 9) and slides by *Shai Fine*



### Agenda

- Demonstrations
  - K-means
  - Gaussian Mixture Models (GMM)
- Expectation-Maximization
  - Formalization
- Gaussian Mixture Models (GMM)
  - Overview
- Binomial Mixture Model (BMM)
- K-means as "Hard GMM"



### Great Video Explaining EM Algorithm

Just in case you need some more explanations and visualizations, a great series of videos covering GMMs and the EM algorithm:

- Part 1 (7:53 min) ([https://www.youtube.com/watch?v=REypj2sy\\_5U](https://www.youtube.com/watch?v=REypj2sy_5U)).
- Part 2 (10:39 min) (<https://www.youtube.com/watch?v=iQoXFmbXRJA>).
- Part 3 (3:05 min) (<https://www.youtube.com/watch?v=TG6Bh-NFhA0>).
- Part 4 (3:29 min) ([https://www.youtube.com/watch?v=zL\\_MHtT56S0](https://www.youtube.com/watch?v=zL_MHtT56S0)).
- Part 5 (10:53 min) (<https://www.youtube.com/watch?v=BWXd5dOkuTo>).



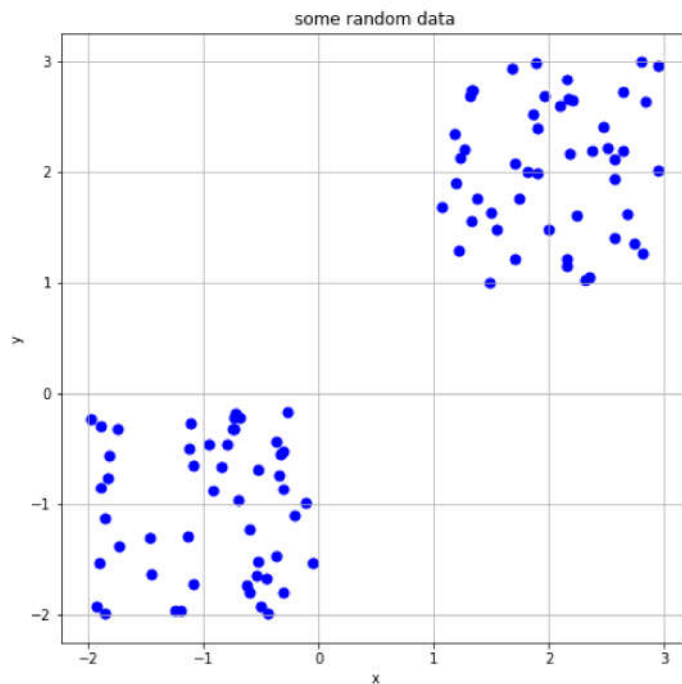
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```
In [1]: # imports for the tutorial
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib notebook
```

```
In [3]: # k-means example
from sklearn.cluster import KMeans
# generate random data
X = -2 * np.random.rand(100,2)
X[50:100, :] = 1 + 2 * np.random.rand(50,2)
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(1,1,1)
ax.scatter(X[:, 0], X[:, 1], s = 50, c = 'b')
ax.grid()
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_title("some random data")
```

Out[3]: Text(0.5,1,'some random data')



```

In [6]: k_mean = KMeans(n_clusters=2)
k_mean.fit(X)
print(k_mean)
# plot the centroids
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(1,1,1)
ax.scatter(X[:, 0], X[:, 1], s = 50, c = 'b', label="data")
ax.scatter(k_mean.cluster_centers_[0][0], k_mean.cluster_centers_[0][1], s=200, c='g', marker='s', label="center 1"
)
ax.scatter(k_mean.cluster_centers_[1][0], k_mean.cluster_centers_[1][1], s=200, c='r', marker='s', label="center 2"
)
ax.grid()
ax.legend()
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_title("some random data")

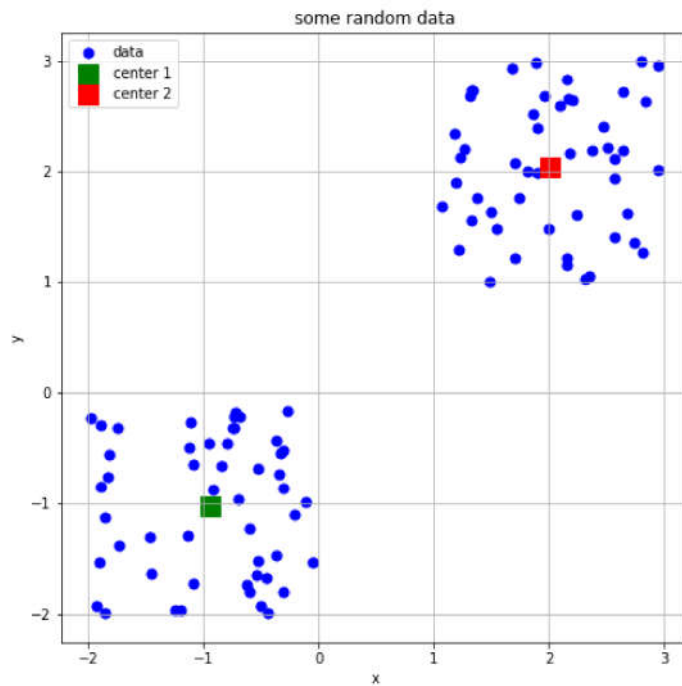
```

```

KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
       n_clusters=2, n_init=10, n_jobs=1, precompute_distances='auto',
       random_state=None, tol=0.0001, verbose=0)

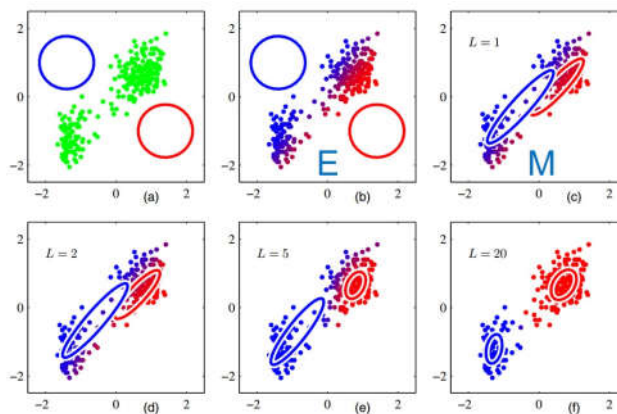
```

Out[6]: Text(0.5,1,'some random data')

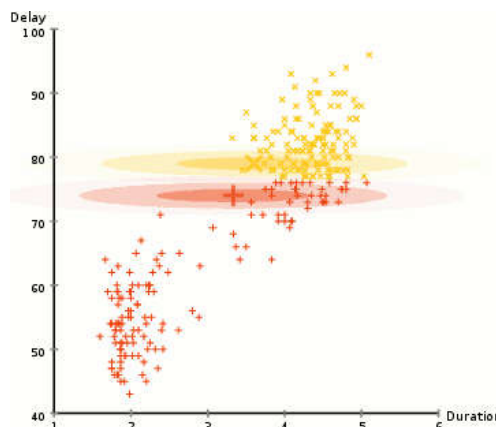


## Gaussian Mixture Models (GMMs)

- A Gaussian mixture model is a probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters.
- One can think of mixture models as generalizing k-means clustering to incorporate information about the covariance structure of the data as well as the centers of the latent Gaussians.
- The parameters of the model are the mean and covariance, which are unknown and will be learned by the EM algorithm.
- **Goal:** *Soft clustering* the data under the assumption that it is generated by a mixture of Gaussians.
  - The optimization method is called Expectation Maximization (EM) and will be used to achieve this goal.
- Illustration:

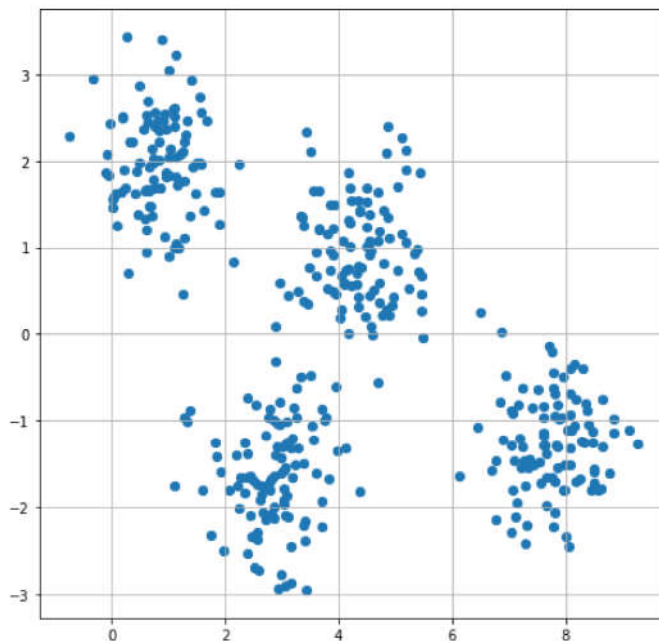


- Animation:



- Example: the following example is taken from [The Python Data Science Handbook \(https://jakevdp.github.io/PythonDataScienceHandbook/05.12-gaussian-mixtures.html\)](https://jakevdp.github.io/PythonDataScienceHandbook/05.12-gaussian-mixtures.html).

```
In [13]: # Generate some data
from sklearn.datasets.samples_generator import make_blobs
from sklearn.mixture import GaussianMixture
X, y_true = make_blobs(n_samples=400, centers=4,
                        cluster_std=0.60, random_state=0)
X = X[:, ::-1] # flip axes for better plotting
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(1,1,1)
ax.scatter(X[:, 0], X[:, 1], s=40, cmap='viridis')
ax.grid()
```



```
In [7]: # some helper functions for plotting
from matplotlib.patches import Ellipse

def draw_ellipse(position, covariance, ax=None, **kwargs):
    """Draw an ellipse with a given position and covariance"""
    ax = ax or plt.gca()

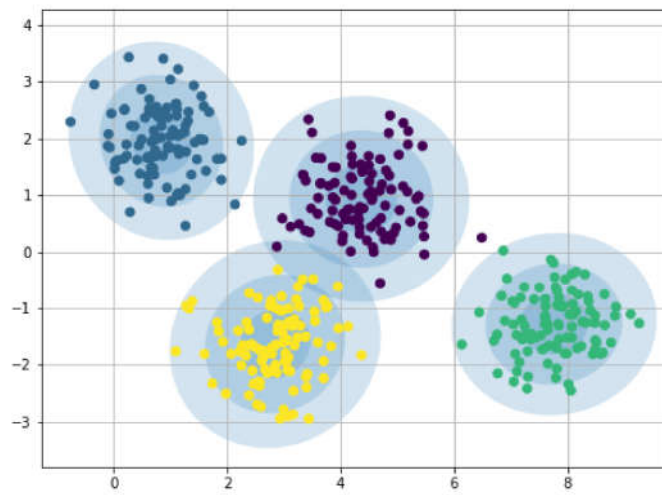
    # Convert covariance to principal axes
    if covariance.shape == (2, 2):
        U, s, Vt = np.linalg.svd(covariance)
        angle = np.degrees(np.arctan2(U[1, 0], U[0, 0]))
        width, height = 2 * np.sqrt(s)
    else:
        angle = 0
        width, height = 2 * np.sqrt(covariance)

    # Draw the Ellipse
    for nsig in range(1, 4):
        ax.add_patch(Ellipse(position, nsig * width, nsig * height,
                              angle, **kwargs))

def plot_gmm(gmm, X, label=True, ax=None):
    ax = ax or plt.gca()
    labels = gmm.fit(X).predict(X)
    if label:
        ax.scatter(X[:, 0], X[:, 1], c=labels, s=40, cmap='viridis', zorder=2)
    else:
        ax.scatter(X[:, 0], X[:, 1], s=40, zorder=2)
    ax.axis('equal')

    w_factor = 0.2 / gmm.weights_.max()
    for pos, covar, w in zip(gmm.means_, gmm.covariances_, gmm.weights_):
        draw_ellipse(pos, covar, alpha=w * w_factor)
```

```
In [12]: gmm = GaussianMixture(n_components=4, random_state=42)
fig = plt.figure(figsize=(8,6))
ax = fig.add_subplot(1,1,1)
ax.grid()
plot_gmm(gmm, X, ax=ax)
```





## Expectation Maximization (EM)

- Probabilistic method for **soft clustering**.
  - The "soft" version of K-means
- Assumes a probabilistic model of clusters that allows computing  $Pr(c_j|x)$  for each cluster  $c_j$  for a given example  $x$ .
  - If we had known for each data instance from what distribution it came from, we could have used a parametric estimation.
- We introduce *unobservable (latent)* variables which indicate source distribution.
- We run an iterative process:
  - Estimate latent variables from the data and the *current* estimation of distribution parameters.
  - Use current values of latent variables to refine parameter estimation.



## Formalization

- Log likelihood for a mixture model (under the *i.i.d* assumption):

$$\mathcal{L}(X|\Theta) = \log \prod_i Pr(x_i|\Theta) = \sum_i \log \sum_{j=1}^k Pr(x_i|C_j; \Theta) Pr(C_j; \Theta)$$

- Assume *latent* variables  $z$ , which when known make the optimization simpler:
  - **Complete** likelihood,  $\mathcal{L}_c(X, Z|\Theta)$ , in terms of  $x$  and  $z$
  - **Incomplete** likelihood,  $\mathcal{L}(X|\Theta)$ , in terms of  $x$

- However,  $z$  is *latent*, so we **can't compute**  $\mathcal{L}_c(X, Z|\Theta)$ 
  - But we can compute its **conditional expected value**, given  $X$  and old  $\theta^t$ :

$$Q(\Theta; \theta^t) = \mathbb{E}_Z[\mathcal{L}_c(X, Z|\Theta)|X, \theta^t] = \sum_Z Pr(Z|X, \theta^t) \log Pr(X, Z; \Theta)$$

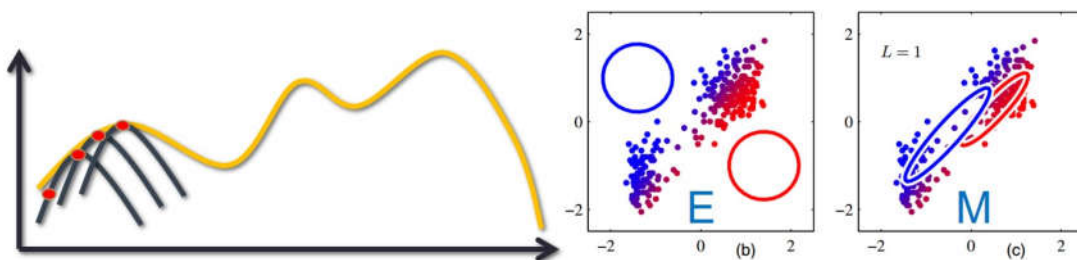
- From a computation viewpoint:
  - **The E-Step**: computes the **posterior probability**  $Pr(Z|X, \theta^t)$  using the *current* estimates (probability point  $i$  belongs to model  $j$ )
  - **The M-Step**: updates the **parameter estimates** to get  $\theta^{t+1}$  by maximizing  $Q(\Theta; \theta^t)$
- The EM Algorithm requires an **initial guess**  $\theta^0$  for the parameters.
- Each iteration of E-step and M-step is **guaranteed to increase the log-likelihood** of the observed data,  $\log Pr(X|\Theta)$  until a *local* maximum is reached.



## The Steps

- Iterate the two steps:
  - **E-step**: Estimate  $Z$  given  $X$  and current  $\Theta$ 
    - $Q(\Theta|\theta^t) = \mathbb{E}[\mathcal{L}(X, Z|\Theta)|X, \theta^t]$
  - **M-step**: Find new  $\Theta$  given  $Z$ ,  $X$  and old  $\Theta$ 
    - $\theta^{t+1} = \text{argmax}_{\Theta} Q(\Theta; \theta^t)$
- An increase in  $Q$  increases the incomplete likelihood

$$\mathcal{L}(X|\theta^t) \geq Q(\Theta|\theta^t)$$



## E Step - EM Recipe

Estimate  $Z$  given  $X$  and current  $\Theta$ :

$$Pr(z_i = j|x_i, \Theta) = \frac{Pr(x_i, z_i = j|\Theta)}{Pr(x_i|\Theta)} = \frac{Pr(x_i, z_i = j|\Theta)}{\sum_{j'} Pr(x_i, z_i = j'|\Theta)}$$

- Substitute the probabilities with the desired distribution.



## M Step (Derive Q) - EM Recipe

$$Q(\Theta|\theta^t) = \mathbb{E}[\mathcal{L}(X, Z|\Theta)|X, \theta^t] = \sum_Z Pr(Z|X, \theta^t) \log Pr(X, Z; \Theta) = \sum_i \sum_{j=1}^k Pr(z_i = j|x_i, \theta^t) \log Pr(x_i, z_i = j, \Theta) =$$

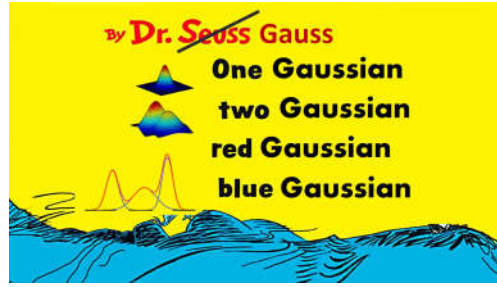


$$\sum_i \sum_{j=1}^k r_{ij} [\log Pr(z_i = j | \Theta) + \log Pr(x_i | z_i = j, \Theta)]$$

- $r_{ij} = Pr(z_i = j | x_i, \Theta)$  (from E step)
- Substitute  $Pr(x_i | z_i = j, \Theta)$  with the desired probability
- **Find MLE** (differentiate and compare to 0)



## Gaussian Mixture Models (GMMs) as EM



- One Gaussian:

$$\mathcal{N}(x|\mu, \Sigma) = Pr(x|\mu_j, \Sigma_j) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma_j|^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu_j)^T \Sigma_j^{-1} (x-\mu_j)}$$

- Gaussian **Mixture**:

$$Pr(x) = \sum_{j=1}^k \alpha_j \mathcal{N}(x|\mu_j, \Sigma_j)$$

- $\sum_{j=1}^k \alpha_j = 1$
  - Tha parameters of the model are:  $\alpha_j, \mu_j, \Sigma_j, \forall j \in \{1, \dots, k\}$
- The **log-likelihood** of a GMM:

$$\mathcal{L}(X|\Theta) = \log \prod_i Pr(x_i|\Theta) = \sum_i \log \sum_{j=1}^k \alpha_j \mathcal{N}(x_i|\mu_j, \Sigma_j)$$

- No closed form solution and not convex!**
- We introduce a **latent random variable**  $z$ 
  - $z \in \{0, 1\}^k$  - a one-hot random variable indicating the source Gaussian the sample belongs to
  - $Pr(z_k) = \alpha_k$  - the probability of that source
  - Reminder:  $\sum_{j=1}^k \alpha_j = 1$
- The marginal probability:

$$Pr(x) = \sum_z p(z)p(x|z) = \sum_{j=1}^k \alpha_j \mathcal{N}(x|\mu_j, \Sigma_j)$$

### GMM - E-Step

- The E-step computes the **posterior** probability of the missing data

$$Pr(z_i = j|x_i, \Theta) = \frac{Pr(x_i, z_i = j|\Theta)}{\sum_{j'} Pr(x_i, z_i = j'|\Theta)} = \frac{\alpha_j Pr(x_i|\mu_j, \Sigma_j)}{\sum_{j'} \alpha_{j'} Pr(x_i|\mu_{j'}, \Sigma_{j'})} = \frac{\alpha_j |\Sigma_j|^{-\frac{1}{2}} e^{-\frac{1}{2}(x_i-\mu_j)^T \Sigma_j^{-1} (x_i-\mu_j)}}{\sum_{j'} \alpha_{j'} |\Sigma_{j'}|^{-\frac{1}{2}} e^{-\frac{1}{2}(x_i-\mu_{j'})^T \Sigma_{j'}^{-1} (x_i-\mu_{j'})}}$$

- Denote:  $r_{ij} = Pr(z_i = j|x_i, \Theta)$

### GMM - Calculate $Q(\Theta; \Theta^t)$

$$\begin{aligned} Q(\Theta|\Theta^t) &= \mathbb{E}[\mathcal{L}(X, Z|\Theta)|X, \Theta^t] = \sum_Z Pr(Z|X, \Theta^t) \log Pr(X, Z; \Theta) = \sum_i \sum_{j=1}^k Pr(z_i = j|x_i, \Theta^t) \log Pr(x_i, z_i = j, \Theta) = \\ &= \sum_i \sum_{j=1}^k r_{ij} [\log Pr(z_i = j|\Theta) + \log Pr(x_i|z_i = j, \Theta)] = \\ &= \sum_i \sum_{j=1}^k r_{ij} [\log \alpha_j + \log Pr(x_i|\mu_j, \Sigma_j)] = \\ &= \sum_i \sum_{j=1}^k r_{ij} \log \alpha_j - \frac{1}{2} \sum_{j=1}^k \log |\Sigma_j| \sum_i r_{i,j} - \frac{1}{2} \sum_i \sum_{j=1}^k r_{ij} (x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j) + Const \end{aligned}$$

### GMM - M-Step

- To maximize  $Q(\Theta; \Theta^t)$  with respect to  $\mu_j$ , we set the gradient to zero.
- Reminder:  $\frac{\partial}{\partial s} (x - As)^T W (x - As) = -2A^T W (x - As)$
- Derive:

$$\frac{\partial}{\partial \mu_j} Q(\Theta; \Theta^t) = \sum_{i=1}^n r_{ij} \Sigma_j^{-1} (x_i - \mu_j) = 0 \rightarrow \hat{\mu}_j = \frac{\sum_{i=1}^n r_{ij} x_i}{\sum_{i=1}^n r_{ij}}$$

- Similarly:

$$\hat{\Sigma}_j = \frac{\sum_{i=1}^n r_{ij} (x_i - \mu_j)(x_i - \mu_j)^T}{\sum_{i=1}^n r_{ij}}$$

- To maximize  $Q(\Theta; \Theta^t)$  with respect to  $\alpha_j$ :
  - Use **Lagrange** multiplier:

- $\max Q(\Theta; \Theta^t)$  s.t.  $\sum_j \alpha_j = 1 \iff$
- $\mathcal{L} = Q(\Theta; \Theta^t) + \lambda(1 - \sum_j \alpha_j)$

▪  $\frac{\partial \mathcal{L}}{\partial \alpha_j} = \sum_i \frac{r_{ij}}{\alpha_j} - \lambda = 0$

- Find an expression for  $\lambda$  by **summing all partial derivatives** of  $\alpha_j$ :

$$\sum_i r_{ij}^{(t)} = \lambda \alpha_j \rightarrow \sum_j \sum_i r_{ij}^{(t)} = \lambda \sum_j \alpha_j \rightarrow \lambda = n$$

◦  $\sum_j \sum_i r_{ij}^{(t)} = \sum_j \sum_i \Pr(z_i = j | x_i, \Theta^t) = \sum_i \frac{\sum_j \Pr(x_i, z_i = j | \Theta)}{\sum_{j'} \Pr(x_i, z_i = j' | \Theta)} = \sum_{i=1}^n 1 = n$

- Substituting  $\lambda$  back in the *Lagrangian* derivative:

$$\frac{\partial \mathcal{L}}{\partial \alpha_j} = \sum_i \frac{r_{ij}}{\alpha_j} - \lambda = 0 \rightarrow \hat{\alpha}_j = \frac{\sum_{i=1}^n r_{ij}}{n}$$

- To sum up:

$$\hat{\mu}_j = \frac{\sum_{i=1}^n r_{ij} x_i}{\sum_{i=1}^n r_{ij}}$$

$$\hat{\Sigma}_j = \frac{\sum_{i=1}^n r_{ij} (x_i - \mu_j)(x_i - \mu_j)^T}{\sum_{i=1}^n r_{ij}}$$

$$\hat{\alpha}_j = \frac{\sum_{i=1}^n r_{ij}}{n}$$



## Bernoulli Mixture Models (BMMs) as EM

- We have  $k$  coins such that:
  - The probability of observing *heads* with the  $j^{th}$  coin is  $p_j$ .
  - We do not observe which coin was used.
  - We only observe  $x_i \in \{0, 1\}$ , which records whether we see a *heads* or *tails*.
- Let  $z_i \in \{1, \dots, k\}$  be the **missing information** of which coin was used on each flip (in other words, the *source* like in the GMM case).
  - The probability of using the  $j^{th}$  coin is  $Pr(z_i = j) = \alpha_j$  (which is a *parameter*)
- The complete data is given by  $(X, Z)$ 
  - Using the **law of total probability**, the (marginal) probability of the observed data  $X$ :

$$Pr(X) = \sum_j Pr(X|Z=j)Pr(Z=j)$$

- Thus, the *likelihood* of the full data set (incomplete likelihood) is:

$$\mathcal{L}(X|\Theta) = \prod_i \sum_j Pr(x_i|z_i=j)Pr(z_i=j) = \prod_i \sum_j \alpha_j p_j^{x_i} (1-p_j)^{1-x_i}$$

$$\Theta = (\alpha, p)$$

### BMM - E-Step

- The E-step computes the **posterior** probability of the missing data

$$Pr(z_i = j|x_i, \Theta) = \frac{Pr(x_i, z_i = j|\Theta)}{\sum_{j'} Pr(x_i, z_i = j'|\Theta)} = \frac{\alpha_j Pr(x_i|p_j)}{\sum_{j'} \alpha_{j'} Pr(x_i|p_{j'})} = \frac{\alpha_j p_j^{x_i} (1-p_j)^{1-x_i}}{\sum_{j'} \alpha_{j'} p_{j'}^{x_i} (1-p_{j'})^{1-x_i}}$$

- Denote:  $r_{ij} = Pr(z_i = j|x_i, \Theta)$

### BMM - Calculate $Q(\Theta; \Theta^t)$

$$\begin{aligned} Q(\Theta|\Theta^t) &= \mathbb{E}[\mathcal{L}(X, Z|\Theta)|X, \Theta^t] = \sum_Z Pr(Z|X, \Theta^t) \log Pr(X, Z; \Theta) = \sum_i \sum_{j=1}^k Pr(z_i = j|x_i, \Theta^t) \log Pr(x_i, z_i = j, \Theta) = \\ &= \sum_i \sum_{j=1}^k r_{ij} [\log Pr(z_i = j|\Theta) + \log Pr(x_i|z_i = j, \Theta)] = \\ &= \sum_i \sum_{j=1}^k r_{ij} [\log \alpha_j + \log Pr(x_i|p_j)] = \\ &= \sum_i \sum_{j=1}^k r_{ij} \log \alpha_j + \sum_i \sum_{j=1}^k r_{ij} \log (p_j^{x_i} (1-p_j)^{1-x_i}) = \\ &= \sum_i \sum_{j=1}^k r_{ij} \log \alpha_j + \sum_i \sum_{j=1}^k r_{ij} x_i \log(p_j) + r_{ij} (1-x_i) \log(1-p_j) \end{aligned}$$

### BMM - M-Step

- To maximize  $Q(\Theta; \Theta^t)$  with respect to  $p_j$ , we set the gradient to zero.
- Derive:

$$\frac{\partial}{\partial p_j} Q(\Theta; \Theta^t) = \sum_{i=1}^n r_{ij} \left( \frac{x_i}{p_j} - \frac{1-x_i}{1-p_j} \right) = 0 \rightarrow \hat{p}_j = \frac{\sum_{i=1}^n r_{ij} x_i}{\sum_{i=1}^n r_{ij}}$$

- To maximize  $Q(\Theta; \Theta^t)$  with respect to  $\alpha_j$ :

- Use **Lagrange** multiplier:
  - $\max Q(\Theta; \Theta^t)$  s.t.  $\sum_j \alpha_j = 1 \iff$
  - $\mathcal{L} = Q(\Theta; \Theta^t) + \lambda(1 - \sum_j \alpha_j)$

$$\frac{\partial \mathcal{L}}{\partial \alpha_j} = \sum_i \frac{r_{ij}}{\alpha_j} - \lambda = 0$$

- Find an expression for  $\lambda$  by **summing all partial derivatives** of  $\alpha_j$ :

$$\sum_i r_{ij}^{(t)} = \lambda \alpha_j \rightarrow \sum_j \sum_i r_{ij}^{(t)} = \lambda \sum_j \alpha_j \rightarrow \lambda = n$$

$$\circ \sum_j \sum_i r_{ij}^{(t)} = \sum_j \sum_i Pr(z_i = j|x_i, \Theta^t) = \sum_i \frac{\sum_j Pr(x_i, z_i = j|\Theta)}{\sum_{j'} Pr(x_i, z_i = j'|\Theta)} = \sum_{i=1}^n 1 = n$$

- Substituting  $\lambda$  back in the *Lagrangian* derivative:

$$\frac{\partial \mathcal{L}}{\partial \alpha_j} = \sum_i \frac{r_{ij}}{\alpha_j} - \lambda = 0 \rightarrow \hat{\alpha}_j = \frac{\sum_{i=1}^n r_{ij}}{n}$$

- To sum up:

$$\hat{p}_j = \frac{\sum_{i=1}^n r_{ij} x_i}{\sum_{i=1}^n r_{ij}}$$

$$\hat{\alpha}_j = \frac{\sum_{i=1}^n r_{ij}}{n}$$

- If all  $r_{ij} = \{0, 1\}$ , that is, deterministic, then:

- The component labels,  $z_i$ , are **known**
- The above update equations reduce to the standard formulas for *binomial distribution*.



## Relation to K-Means: K-Means as "Hard GMM"

- Recall the E-Step for GMM:

$$Pr(z_i = j | x_i, \Theta) = \frac{Pr(x_i, z_i = j | \Theta)}{\sum_{j'} Pr(x_i, z_i = j' | \Theta)} = \frac{\alpha_j Pr(x_i | \mu_j, \Sigma_j)}{\sum_{j'} \alpha_{j'} Pr(x_i | \mu_{j'}, \Sigma_{j'})} = \frac{\alpha_j e^{-\frac{1}{2}(x_i - \mu_j)^T \Sigma_j^{-1} (x_i - \mu_j)}}{\sum_{j'} \alpha_{j'} e^{-\frac{1}{2}(x_i - \mu_{j'})^T \Sigma_{j'}^{-1} (x_i - \mu_{j'})}}$$

- Let's assume all the Gaussians have the same  $\Sigma = \epsilon I$ :

$$Pr(z_i = j | x_i, \Theta) = \frac{Pr(x_i, z_i = j | \Theta)}{\sum_{j'} Pr(x_i, z_i = j' | \Theta)} = \frac{\alpha_j e^{-\frac{1}{2\epsilon} \|(x_i - \mu_j)\|_2^2}}{\sum_{j'} \alpha_{j'} e^{-\frac{1}{2\epsilon} \|(x_i - \mu_{j'})\|_2^2}}$$

- At the limit  $\epsilon \rightarrow 0$ :  $Pr(z_i = j | x_i, \Theta) = 1$  for  $j = \operatorname{argmin}\{x_i - \mu_j\}$  and  $Pr(z_i = j | x_i, \Theta) = 0$  for all others.
- Thus:

$$\begin{cases} r_{ij} = 1 & \text{if } j = \operatorname{argmin}_j \|x_i - \mu_j\|_2^2 \\ r_{ij} = 0 & \text{else} \end{cases}$$

- The GMM equations are now identical to the K-Means' equations:

$$\hat{\mu}_j = \frac{\sum_{i=1}^n r_{ij} x_i}{\sum_{i=1}^n r_{ij}}$$

$$\hat{\alpha}_j = \frac{\sum_{i=1}^n r_{ij}}{n}$$

- The  $\alpha$ s are not really required.



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- Examples and code snippets were taken from "Hands-On Machine Learning with Scikit-Learn and TensorFlow" (<http://shop.oreilly.com/product/0636920052289.do>).