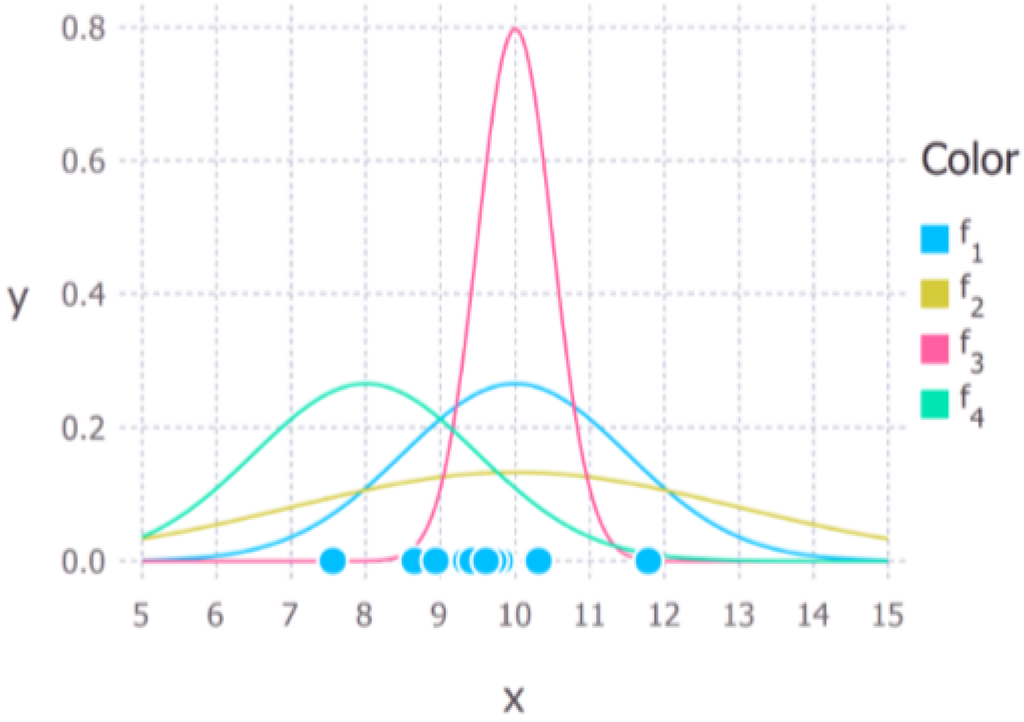
Mixtures of Gaussians

Single Gaussian

We want to know which curve was most likely responsible for creating the data points that we observed?



Maximum Likelihood Estimates

Important assumption

Each data point is generated independently of the others.

Gaussian distribution

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

Joint Gaussian Distribution

$$P(9,9.5,11;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(9-\mu)^2}{2\sigma^2}) \times \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(9.5-\mu)^2}{2\sigma^2}) \times \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(11-\mu)^2}{2\sigma^2})$$

Calculating Maximum Likelihood Estimates

- We need to find the values of μ and σ that results in giving the maximum value of the above expression.
- The above expression for the total probability is difficult to differentiate.
- It is almost always simplified by taking the **natural logarithm** of the expression.

Log Likelihood

This is absolutely fine because the **natural logarithm** is a monotonically increasing function.

Taking logs of the original expression gives us:

$$\ln(P(9, 9.5, 11; \mu, \sigma)) = \ln(\frac{1}{\sigma\sqrt{2\pi}}) - \frac{(9-\mu)^2}{2\sigma^2} + \ln(\frac{1}{\sigma\sqrt{2\pi}}) - \frac{(9.5-\mu)^2}{2\sigma^2} + \ln(\frac{1}{\sigma\sqrt{2\pi}}) - \frac{(11-\mu)^2}{2\sigma^2}$$

By simplifying it, we get:

$$\ln(P(9, 9.5, 11; \mu, \sigma)) = -3\ln(\sigma) - \frac{3}{2}\ln(2\pi) - \frac{1}{2\sigma^2}[(9-\mu)^2 + (9.5-\mu)^2 + (11-\mu)^2]$$

Computing μ_{ML} and σ_{ML}

Take partial derivative of μ and σ_{ML} and set them to zero.

$$\frac{\partial \ln(P(x; \mu, \sigma))}{\partial \mu} = \frac{1}{\sigma^2}[9 + 9.5 + 11 - 3\mu] = 0$$

$$\mu_{ML} = 9.833$$

Do the same thing to σ.

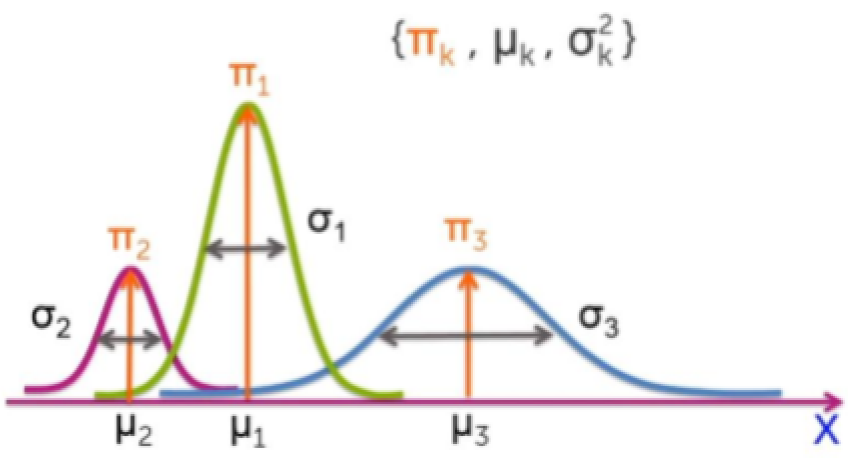
Mixtures of Gaussians

GMM (Gaussians Mixed Model)

$$p(x) = \sum_{k=1}^{K} \pi_k [\frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{(x-\mu_k)^2}{2\sigma_k^2})]$$

where $\sum_{k=1}^{K}\pi_k = 1$ and $0 \le \pi_k \le 1$.

Associate **a weight π_k** with each Gaussian Component: **"The mixing coefficients"**.



Higher Dimension

Multivariate normal distribution:

$$f(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{(2\pi)^N|\Sigma|}}\exp(-\frac{1}{2}(X-\mu)^T\Sigma^{-1}(X-\mu))$$

where ${\Sigma}$ is the **covariance matrix** of ${X}$, X and μ are N by 1 matrice.

$$X = (x_1, x_2, \ldots, x_N)^T$$

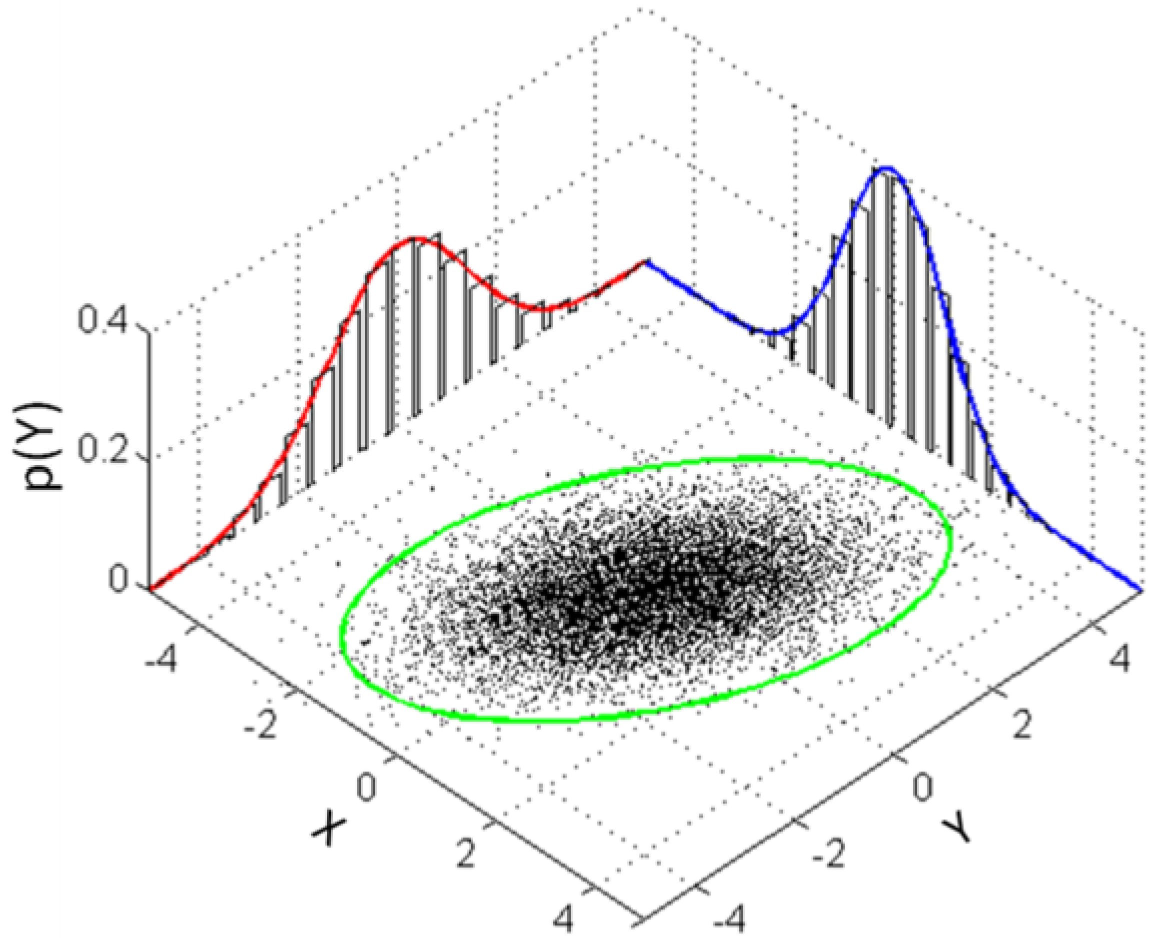
Then, we will have the covariance matrix:

$$\Sigma_{i,j} = cov(x_i, x_j) = E[(x_i - E[x_i])(x_j - E[x_j])] = E[x_i x_j] - E[x_i][x_j]$$

Correlation coefficient: $$ \rho_{x_i, x_j} = \frac{cov(x_i, x_j)}{\sigma_{x_i}\sigma_{x_j}}

$$

Two Dimension



$$f(x_1, x_2) = \frac{1}{2\pi\sigma_{x_1}\sigma_{x_2}\sqrt{1-\rho^2}}\exp(-\frac{1}{2(1-\rho^2)}[\frac{(x_1-\mu_{x_1})}{\sigma_{x_1}^2} + \frac{(x_2-\mu_{x_2})}{\sigma_{x_2}^2} - \frac{2\rho(x_i-\mu_{x_i})(x_j-\mu_{x_j})}{\sigma_{x_i}\sigma_{x_j}}])$$

where

$$\Sigma = [\sigma_{x_1}^2 \quad \rho\sigma_{x_1}\sigma_{x_2}, \rho\sigma_{x_1}\sigma_{x_2} \quad \sigma_{x_1}^2]$$

Maximum Likelihood

Mixture of Gaussians:

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

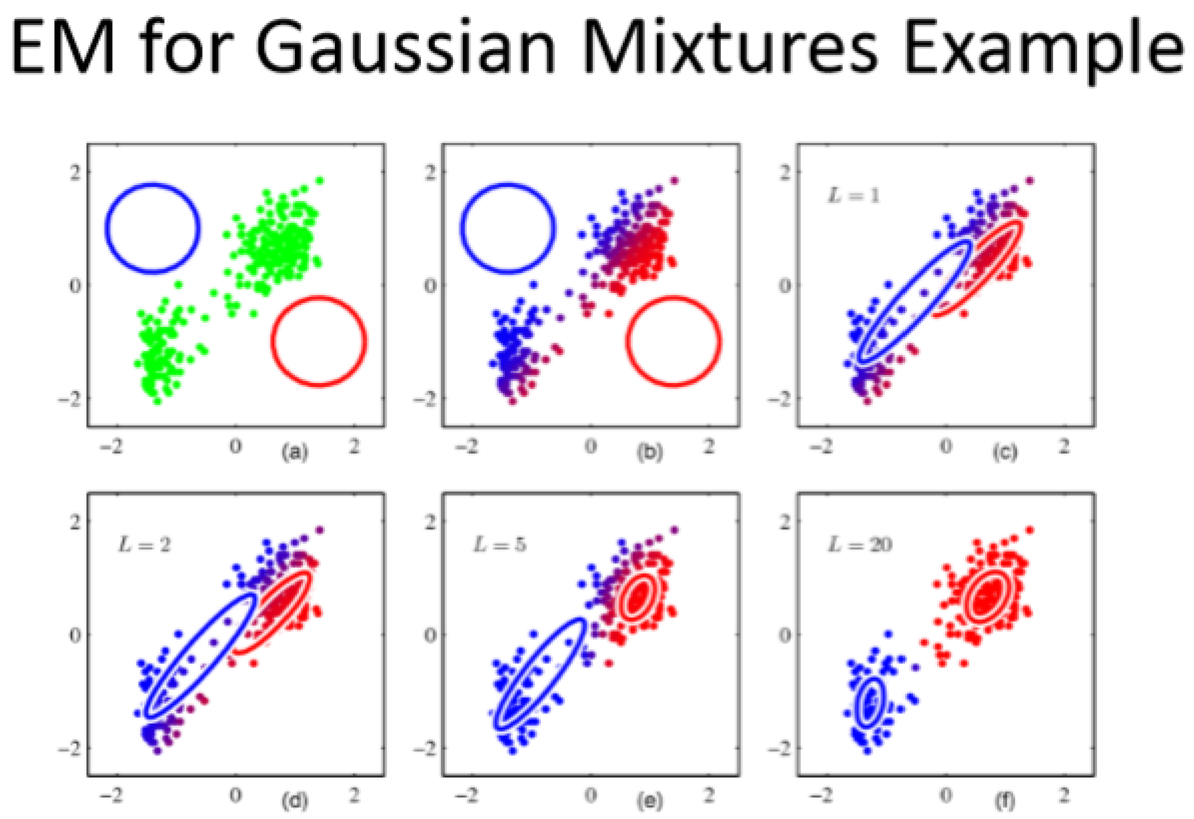
The dimension of each Gaussian is N. We have K Gaussian distrubutions in all.

We can estimate parameters using Maximum Likelihood, i.e. maximize

$$\ln(p(X|\pi, \mu, \Sigma)) = \ln p(x^1, x^2, \dots, x^N | \pi_1, \dots, \pi_K, \mu_1, \dots, \mu_k, \Sigma_1, \dots, \Sigma_K)$$

This algorithm is called **Expectation Maximization (EM)**.

Expectation Maximization



1. Initialize the means μ_k, covariances Σ_k and mixing coefficients π_k and evaluate the initial value of the log likelihood.

2. E step. Evaluate the responsibility value using the current parameter values.

$$p(z_k|x_i) = \frac{\pi_k N(x_i|\mu_k, \Sigma_k)}{\Sigma_{j=1}^{K} N(x_i|\mu_j, \sigma_j)}$$

   其中，$i = 1, 2, 3, ..., m$，m为总样本数，K为高斯分布的个数。计算各个数据样本x_i属于第k个cluster的概率。

3. M step. Re-estimate the parameters using the current responsibilities. 根据刚刚得出的概率，重新计算means μ_k, covariances Σ_k and mixing coefficients π_k.

重新计算各个高斯分布的权重(mixing coefficients)

$$\pi_k = \frac{1}{m} \Sigma_{i=1}^{m} p(z_k|x_i)$$

均值的计算，例如，第k个高斯分布的均值：

$$\mu_k^{new} = \frac{\Sigma_{i=1}^m p(z_k|x_i)x_i}{\Sigma_{i=1}^m p(z_k|x_i)}$$

协方差矩阵的计算，

$$\Sigma_k^{new} = \frac{\Sigma_{i=1}^m p(z_k|x_i)(x_i - \mu_k^{new})(x_i - u_k^{new})^T}{\Sigma_{i=1}^m p(z_k|x_i)}$$

4. 重复E-step and M-step直到收敛。

那这跟Maximum Likelihood又有什么关系呢？ 我们的每一步，实际上都是在maximize p(x).