In [1]:
```
from IPython.core.display import display, HTML
display(HTML("<style>.container { width:100% !important; }</style>"))
```

# Expectation-Maximization

## Definitions

Let $\mathcal{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ be a sample ($\mathbf{x}_i \in \mathbb{R}^d$) of $n$ i.i.d. observations from a mixture of two distinct $d$-dimensional multivariate Gaussian distributions. Let $\mathcal{Y} = (y_1, y_2, \ldots, y_n)$ be the set of group labels, that is $y \in \{1, 2\}$ which indicate from which Gaussian mixture each observation $\mathbf{x}_i$ was truly sampled from. The set $\mathcal{Y}$ is sometimes called "latent" indicating that the gourp labels $y_i$ are unknown beforehand. That is, we do not know into which Gaussians the samples belong to. Furthermore, we define $\boldsymbol{\theta} = (\boldsymbol{\tau}, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2)$ to be a set of parameters which fully describe the distributions of the data. The parameters $\boldsymbol{\tau} = (\tau_1, \tau_2)$ are the "mixing parameters" with $\tau_1 + \tau_2 = 1$ which determine the weights of "how much" each sample $\mathbf{x}_i$ came from either Gaussian. We treat these "mixing values" as the prior probabilities that a given sample $\mathbf{x}_i$ "belongs" to either Gaussian 1 or Gaussian 2. Explicitly put, we state this as $P(y_i = 1|\boldsymbol{\theta}) = \tau_1$ and $P(y_2 = 1|\boldsymbol{\theta}) = \tau_2 = 1 - \tau_1$.

If sample $\mathbf{x}_i$ was generated by Gaussian 1, then $\mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$ and if it was generated by Gaussian 2, then $\mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$. Explicitly put:

$$p(\mathbf{x}_i|y_i = 1, \boldsymbol{\theta}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_1|}} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_1)\right), \quad \text{if } \mathbf{x}_i \text{ is known to be generated by Gaussian 1}$$

$$p(\mathbf{x}_i|y_i = 2, \boldsymbol{\theta}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_2|}} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_2)\right), \quad \text{if } \mathbf{x}_i \text{ is known to be generated by Gaussian 2.}$$

If $\mathbf{x}_i$ is generated by the mixture of these two Gaussians, then the probability density of $\mathbf{x}_i$ is:

$$p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{j=1}^{2} p(\mathbf{x}_i, y_i = j|\boldsymbol{\theta}) = \sum_{j=1}^{2} P(y_i = j|\boldsymbol{\theta})\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta}) = \tau_1 \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_1|}} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_1)\right) + \tau_2 \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_2|}} \exp\left(-\frac{1}{2}\right.$$

If we integrate the mixture density of $\mathbf{x}_i$:

$$\int_{-\infty}^{\infty} p(\mathbf{x}_i|\boldsymbol{\theta})\, d\mathbf{x} = \int_{-\infty}^{\infty} \sum_{j=1}^{2} P(y_i = j|\boldsymbol{\theta})\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta})\, d\mathbf{x} = \tau_1 \underbrace{\int_{-\infty}^{\infty} p(\mathbf{x}_i|y_i = 1, \boldsymbol{\theta})\, d\mathbf{x}}_{=1} + \tau_2 \underbrace{\int_{-\infty}^{\infty} p(\mathbf{x}_i|y_i = 2, \boldsymbol{\theta})\, d\mathbf{x}}_{=1} = \tau_1 + \tau_2 = 1$$

as it should.

## Incomplete data likelihood

Let us first define the "incomplete" data likelihood (with symbol $L$ as likelihood, since it's not the same as probability):

$$L(\mathcal{X}|\boldsymbol{\theta}) = L(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \prod_{i=1}^{n}\sum_{j=1}^{2} P(y_i = j|\boldsymbol{\theta})\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta}) = \prod_{i=1}^{n}\sum_{j=1}^{2} \tau_j\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta}),$$

This "incomplete data likelihood" means the likelihood of observing the data set $\mathcal{X}$ prior to not having any information about the labels in $\mathcal{Y}$ assuming that both Gaussians contribute in the generation of the samples.

## Complete data likelihood

The "complete data likelihood" is the likelihood of observing the pair $(\mathcal{X}, \mathcal{Y})$ from the Gaussian mixture. In this case, since the set $\mathcal{Y}$ is given we know for sure that either Gaussian 1 or Gaussian 2 completely generated a given sample $\mathbf{x}_i$. Thus we can write the complete data likelihood as:

$$L(\mathcal{X}, \mathcal{Y}|\boldsymbol{\theta}) = L(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n, y_1, y_2, \ldots, y_n|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{x}_i, y_i|\boldsymbol{\theta}) = \prod_{i=1}^{n}\sum_{j=1}^{2} P(y_i = j|\boldsymbol{\theta})\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta})\, \mathbb{I}(y_i = j) = \prod_{i=1}^{n}\sum_{j=1}^{2} \tau_j\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta})\, \mathbb{I}(y_i =$$

where $\mathbb{I}(y_i = j) \in \{0, 1\}$ is the indicator function. Why is the indicator function added here? Lets take a look at the joint density above, that is $p(\mathbf{x}_i, y_i|\boldsymbol{\theta})$. What is this function saying? If we did not care from which Gaussian the observation $\mathbf{x}_i$ was sampled from, then the density of $\mathbf{x}_i$ would be described by $p(\mathbf{x}_i|\boldsymbol{\theta}) = \sum_{j=1}^{2} p(\mathbf{x}_i, y_i = j|\boldsymbol{\theta})$, that is by the combination of the two Gaussians. Now, with the function $p(\mathbf{x}_i, y_i|\boldsymbol{\theta})$ the density depends on from which Gaussian $\mathbf{x}_i$ was generated from. Thus if $y_i = 1$, then the "part" of the mixture density belonging to Gaussian 2 had no probabilistic effect on the sampling of $\mathbf{x}_i$ and thus only the density caused by Gaussian 1 had a part to play.

Lets open up the incomplete likelihood more:

$$L(\mathcal{X}, \mathcal{Y}|\boldsymbol{\theta}) = \prod_{i=1}^{n}\sum_{j=1}^{2} \tau_j\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta})\, \mathbb{I}(y_i = j) = \prod_{i=1}^{n}\sum_{j=1}^{2} \exp\big(\ln \tau_j\big)\, \exp\left(\ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}}\right) \exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_j)\right) \mathbb{I}(y_i = j)$$

$$= \prod_{i=1}^{n}\sum_{j=1}^{2} \exp\left(\ln \tau_j + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_j)\right) \mathbb{I}(y_i = j)$$

At this point, lets take a look at the inner sum:

$$\sum_{j=1}^{2} \exp\left( \ln \tau_j + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_j) \right) \mathbb{I}(y_i = j)$$

$$= \exp\left( \ln \tau_1 + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_1|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_1) \right) \mathbb{I}(y_i = 1) + \exp\left( \ln \tau_2 + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_2|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_2) \right) \mathbb{I}(y_i =$$

Because $\mathbb{I}(y_i = j)$ equals either $0$ or $1$ we know for sure that one of the above terms is always zero. Getting back to the complete likelihood, this is why it is true that:

$$p(\mathcal{X}, \mathcal{Y}|\boldsymbol{\theta}) = \prod_{i=1}^{n} \underbrace{\sum_{j=1}^{2} \exp\left( \ln \tau_j + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_j) \right) \mathbb{I}(y_i = j)}_{\text{Only one term in this sum}} = \exp\left( \sum_{i=1}^{n} \sum_{j=1}^{2} \left\{ \ln \tau_j + \ln \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}} - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}$$

$$= \exp\left( \sum_{i=1}^{n} \sum_{j=1}^{2} \left\{ \ln \tau_j - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_j| - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_j) \right\} \mathbb{I}(y_i = j) \right),$$

and furthermore, since only one of the functions $\mathbb{I}(y_i = j)$ equals 1 and the rest are zero, we can safely omit the indicator from the equation without affecting the results. Thus:

$$p(\mathcal{X}, \mathcal{Y}|\boldsymbol{\theta}) = \exp\left( \sum_{i=1}^{n} \sum_{j=1}^{2} \left\{ \ln \tau_j - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_j| - \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_j) \right\} \right).$$

As a next step, let us look at the density $p(y_i = j | \mathbf{x}_i, \boldsymbol{\theta})$. By applying the Bayes theorem (where distributions can be discrete and continuous) we have that:

$$p(y_i = j | \mathbf{x}_i, \boldsymbol{\theta}) = \frac{p(\mathbf{x}_i | y_i = j, \boldsymbol{\theta}) P(y_i = j | \boldsymbol{\theta})}{p(\mathbf{x}_i | \boldsymbol{\theta})} = \frac{p(\mathbf{x}_i | y_i = j, \boldsymbol{\theta}) \tau_j}{\sum_{k=1}^{2} p(\mathbf{x}_i, y_i = k | \boldsymbol{\theta})} = \frac{p(\mathbf{x}_i | y_i = j, \boldsymbol{\theta}) \tau_j}{\sum_{k=1}^{2} p(\mathbf{x}_i | y_i = k, \boldsymbol{\theta}) \tau_k} = \frac{\frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j|}} \exp\left( -\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x}_i - \right.}{\sum_{k=1}^{2} \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \exp\left( -\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\right.}$$

## Finding the MLE solution

Next, let us define the function:

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = E_{Y|X,\boldsymbol{\theta}^{(t)}}\left[\ln p(\mathcal{X},\mathcal{Y}|\boldsymbol{\theta})\right],$$

where $X$ and $Y$ refer to the random variables of $\mathbf{x}$ and $y$, and $\boldsymbol{\theta}^{(t)}$ referes to the parameter set $\boldsymbol{\theta}$ at (time) step $t$, that is $\boldsymbol{\theta}^{(t)} = (\boldsymbol{\tau}^{(t)}, \boldsymbol{\mu}_1^{(t)}, \boldsymbol{\mu}_2^{(t)}, \boldsymbol{\Sigma}_1^{(t)}, \boldsymbol{\Sigma}_2^{(t)})$. Let us continue with this function:

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = E_{Y|X,\boldsymbol{\theta}^{(t)}}\left[\ln p(\mathcal{X},\mathcal{Y}|\boldsymbol{\theta})\right] = E_{Y|X,\boldsymbol{\theta}^{(t)}}\left[\ln \prod_{i=1}^{n} p(\mathbf{x}_i, y_i|\boldsymbol{\theta})\right] = E_{Y|X,\boldsymbol{\theta}^{(t)}}\left[\sum_{i=1}^{n} \ln p(\mathbf{x}_i, y_i|\boldsymbol{\theta})\right] = \sum_{i=1}^{n} E_{Y|X,\boldsymbol{\theta}^{(t)}}\left[\ln p(\mathbf{x}_i, y_i|\boldsymbol{\theta})\right] = \sum_{i=1}^{n}\sum_{j=1}^{2} p(y_i =$$

## The mixing parameters

Let us first find the optimal mixing parameters. To do so, recall that we had the constraint $\tau_1 + \tau_2 = 1$ so we need to use Langrange multipliers and thus our optimization function becomes:

$$f(\lambda, \boldsymbol{\tau}) = Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) + \lambda(\tau_1 + \tau_2 - 1),$$

and thus by taking the derivative, setting to zero, etc.:

$$\frac{\partial f(\lambda, \boldsymbol{\tau})}{\partial \tau_k} = \frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \tau_k} + \lambda = 0 \Leftrightarrow \lambda = -\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \tau_k}.$$

So what is $\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \tau_k}$? Lets calculate it:

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \tau_k} = \frac{\partial}{\partial \tau_k}\left(\sum_{i=1}^{n}\sum_{j=1}^{2} p(y_i = j|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \ln p(\mathbf{x}_i, y_i = j|\boldsymbol{\theta})\right) = \underbrace{\frac{\partial}{\partial \tau_k}\left(\sum_{i=1}^{n}\sum_{j=1}^{2} p(y_i = j|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \ln p(\mathbf{x}_i, y_i = j|\boldsymbol{\theta})\right)}_{\text{Notice that } p(y_i=j|\,\mathbf{x}_i,\boldsymbol{\theta}^{(t)}) \text{ is a function of the old } \boldsymbol{\theta}^{(t)} \text{ parameters}} = \sum_{i=1}^{n}\sum_{j=1}^{2} p(y_i = j|\,\mathbf{x}_i, \boldsymbol{\theta}$$

Lets look at the partial derivative of the log function:

$$\frac{\partial}{\partial \tau_k}(\ln p(\mathbf{x}_i, y_i = j|\boldsymbol{\theta})) = \frac{\partial}{\partial \tau_k}(\ln P(y_i = j|\boldsymbol{\theta})\, p(\mathbf{x}_i|y_i = j, \boldsymbol{\theta})) = \frac{\partial}{\partial \tau_k}\left(\ln\left\{\tau_j \frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}_j|}}\exp\left(-\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_j)^T\boldsymbol{\Sigma}_j^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_j)\right)\right\}\right)$$

$$= \frac{\partial}{\partial \tau_k}\left(\ln \tau_j + \ln\left\{\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}_j|}}\exp\left(-\frac{1}{2}(\mathbf{x}_i-\boldsymbol{\mu}_j)^T\boldsymbol{\Sigma}_j^{-1}(\mathbf{x}_i-\boldsymbol{\mu}_j)\right)\right\}\right) = \frac{\partial}{\partial \tau_k}(\ln \tau_j) + \underbrace{\frac{\partial}{\partial \tau_k}\left(\ln\left\{\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}_j|}}\exp\left(-\frac{1}{2}(\mathbf{x}_i-\boldsymbol{\mu}_j)^T\boldsymbol{\Sigma}_j^{-1}(\mathbf{x}_i-\right.\right.\right.}_{\text{Does not depend on } \tau_k \text{ so equals 0}}$$

Thus we have:

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \tau_k} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)})\frac{1}{\tau_k},$$

from which it follows:

$$\lambda = -\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)})\frac{1}{\tau_k} \Leftrightarrow \lambda\tau_k = -\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}).$$

Let us now sum both sides for $k = 1, 2$ and we get:

$$\lambda\underbrace{\sum_{k=1}^{2}\tau_k}_{=1} = -\sum_{i=1}^{n}\underbrace{\sum_{k=1}^{2} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)})}_{=1} \Leftrightarrow \lambda = -\sum_{i=1}^{n} 1 \Leftrightarrow \lambda = -n.$$

Subsituting the $\lambda = -n$ to the previous equation we get:

$$\lambda\tau_k = -\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \Leftrightarrow -n\tau_k = -\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \Leftrightarrow \tau_k = \frac{1}{n}\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}).$$

Thus we get that optimal next time step parameter for $\tau_k$ (which we denote by $\tau_k^{(t+1)}$) is:

$$\boxed{\tau_k^{(t+1)} = \frac{1}{n}\sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) = \frac{1}{n}\sum_{i=1}^{n} \frac{\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}_k^{(t)}|}}\exp\left(-\frac{1}{2}(\mathbf{x}_i-\boldsymbol{\mu}_k^{(t)})^T(\boldsymbol{\Sigma}_k^{(t)})^{-1}(\mathbf{x}_i-\boldsymbol{\mu}_k^{(t)})\right)\tau_k^{(t)}}{\sum_{j=1}^{2}\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}_j^{(t)}|}}\exp\left(-\frac{1}{2}(\mathbf{x}_i-\boldsymbol{\mu}_j^{(t)})^T(\boldsymbol{\Sigma}_j^{(t)})^{-1}(\mathbf{x}_i-\boldsymbol{\mu}_j^{(t)})\right)\tau_j^{(t)}}}$$

## The mean parameters

Next, let us find the optimal $\boldsymbol{\mu}_k = (\mu_{k1}, \mu_{k2}, \ldots, \mu_{kd})$:

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \mu_{kp}} = \frac{\partial}{\partial \mu_{kp}} \left( \sum_{i=1}^{n} \sum_{j=1}^{2} p(y_i = j | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \ln p(\mathbf{x}_i, y_i = j | \boldsymbol{\theta}) \right) = \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} (\ln p(\mathbf{x}_i, y_i = k | \boldsymbol{\theta})) = \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left( \ln \left\{ \tau_k \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \exp\left( -\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) \right\} \right) = \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left( \ln \tau_k + \ln \left\{ \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \right.\right.$$

$$= \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left( \ln \tau_k - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_k| - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right)$$

$$= \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left( -\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right)$$

$$= -\frac{1}{2} \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} (\mathbf{x}_i^T \boldsymbol{\Sigma}_k^{-1} \mathbf{x}_i - \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}_k^{-1} \mathbf{x}_i - \mathbf{x}_i^T \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\mu}_k + \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\mu}_k)$$

$$= -\frac{1}{2} \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} (-\boldsymbol{\mu}_k^T \boldsymbol{\Sigma}_k^{-1} \mathbf{x}_i - \mathbf{x}_i^T \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\mu}_k + \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\mu}_k),$$

at this point let us denote $\boldsymbol{\Sigma}_k^{-1} = \begin{pmatrix} a_{11} & \cdots & a_{1d} \\ \vdots & \ddots & \vdots \\ a_{d1} & \cdots & a_{dd} \end{pmatrix} = [\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_d]$, where $\mathbf{a}_j = \begin{pmatrix} a_{1j} \\ \vdots \\ a_{dj} \end{pmatrix}$ and continue:

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \mu_{kp}} = -\frac{1}{2} \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left[ -\boldsymbol{\mu}_k^T \begin{pmatrix} \mathbf{a}_1^T \mathbf{x}_i \\ \vdots \\ \mathbf{a}_d^T \mathbf{x}_i \end{pmatrix} - \mathbf{x}_i^T \begin{pmatrix} \mathbf{a}_1^T \boldsymbol{\mu}_k \\ \vdots \\ \mathbf{a}_d^T \boldsymbol{\mu}_k \end{pmatrix} + \boldsymbol{\mu}_k^T \begin{pmatrix} \mathbf{a}_1^T \boldsymbol{\mu}_k \\ \vdots \\ \mathbf{a}_d^T \boldsymbol{\mu}_k \end{pmatrix} \right]$$

$$= -\frac{1}{2} \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \mu_{kp}} \left[ -2\mu_{kp} \mathbf{x}_i^T \mathbf{a}_p + \mu_{kp} \boldsymbol{\mu}_k^T \mathbf{a}_p \right] = -\frac{1}{2} \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \left[ -2\mathbf{x}_i^T \mathbf{a}_p + 2\boldsymbol{\mu}_k^T \mathbf{a}_p \right]$$

$$= \sum_{i=1}^{n} p(y_i = k | \, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \, \mathbf{a}_p^T (\mathbf{x}_i - \boldsymbol{\mu}_k).$$

Setting this to zero we get:

$$\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, \mathbf{a}_p^T (\mathbf{x}_i - \boldsymbol{\mu}_k) = 0,$$

and noting that we can group all the optimal $\mu_{kp}$ values into vector equation as:

$$\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) = \mathbf{0},$$

and thus:

$$\boldsymbol{\Sigma}_k \sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) = \boldsymbol{\Sigma}_k \mathbf{0} \Leftrightarrow \sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, \boldsymbol{\Sigma}_k \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) = \mathbf{0} \Leftrightarrow \sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, (\mathbf{x}_i - \boldsymbol{\mu}_k) = \mathbf{0},$$

from which we get that the next step optimal mean vector $\boldsymbol{\mu}_k^{(t+1)}$ is

$$\boxed{\boldsymbol{\mu}_k^{(t+1)} = \frac{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, \mathbf{x}_i}{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})}},$$

thus with the components:

$$\boxed{\mu_{kp}^{(t+1)} = \frac{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})\, x_{ip}}{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})}},$$

where:

$$p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) = \frac{\frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k^{(t)}|}} \exp\left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k^{(t)})^T (\boldsymbol{\Sigma}_k^{(t)})^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k^{(t)})\right) \tau_k^{(t)}}{\sum_{j=1}^{2} \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_j^{(t)}|}} \exp\left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_j^{(t)})^T (\boldsymbol{\Sigma}_j^{(t)})^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_j^{(t)})\right) \tau_j^{(t)}}.$$

## The covariance parameters

Denote $\boldsymbol{\Sigma}_k = \begin{pmatrix} s_{11}^k & \cdots & s_{1d}^k \\ \vdots & \ddots & \vdots \\ s_{d1}^k & \cdots & s_{dd}^k \end{pmatrix}$

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial s_{rp}^k} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial s_{rp}^k} \left( \ln \tau_k + \ln \left\{ \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \exp\left( -\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) \right\} \right)$$

$$= \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial s_{rp}^k} \left( \ln \tau_k - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\boldsymbol{\Sigma}_k| - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right)$$

$$= \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial s_{rp}^k} \left( -\frac{1}{2} \ln |\boldsymbol{\Sigma}_k| - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right).$$

At this point I will list few matrix differentiation rules which state (you can check these up from matrix differentiation literature, e.g. wiki):

$$\frac{\partial \ln |A|}{\partial A_{ij}} = A_{ij}^{-1} \rightarrow \frac{\partial \ln |A|}{\partial A} = A^{-1}$$

$$\frac{\partial \mathbf{x}^T A \mathbf{x}}{\partial A_{ij}} = -(A^{-1} \mathbf{x} \mathbf{x}^T A^{-1})_{ij} \rightarrow \frac{\partial \mathbf{x}^T A \mathbf{x}}{\partial A} = -A^{-1} \mathbf{x} \mathbf{x}^T A^{-1},$$

where I have used the subscripts $()_{ij}$ to denote the $ij$th element of the corresponding matrix. Using these results we get:

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial s_{rp}^k} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial s_{rp}^k} \left( -\frac{1}{2} \ln |\boldsymbol{\Sigma}_k| - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \left( -\frac{1}{2} (\boldsymbol{\Sigma}_k^{-1})_{rp} + \frac{1}{2} \left( \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k \right.\right.$$

$$\Leftrightarrow \frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\Sigma}_k} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \frac{\partial}{\partial \boldsymbol{\Sigma}_k} \left( -\frac{1}{2} \ln |\boldsymbol{\Sigma}_k| - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right) = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \left( -\frac{1}{2} \boldsymbol{\Sigma}_k^{-1} + \frac{1}{2} \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)( \right.$$

$$\frac{\partial Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})}{\partial \boldsymbol{\Sigma}_k} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \left( -\frac{1}{2} \boldsymbol{\Sigma}_k^{-1} + \frac{1}{2} \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} \right) = 0$$

$$\Leftrightarrow \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \boldsymbol{\Sigma}_k^{-1} = \sum_{i=1}^{n} p(y_i = k|\,\mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}$$

$$\Leftrightarrow \sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \boldsymbol{\Sigma}_k \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\Sigma}_k = \sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \boldsymbol{\Sigma}_k \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} \boldsymbol{\Sigma}_k$$

$$\Leftrightarrow \boldsymbol{\Sigma}_k = \frac{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T}{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})}.$$

We can replace the the old mean parameters (here $\boldsymbol{\mu}_k = \boldsymbol{\mu}_k^{(t)}$) with the newly found mean parameters $\boldsymbol{\mu}_k^{(t+1)}$, and so we get the next optimal time step covariance matrix as:

$$\boxed{\boldsymbol{\Sigma}_k^{(t+1)} = \frac{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)}) \left(\mathbf{x}_i - \boldsymbol{\mu}_k^{(t+1)}\right) \left(\mathbf{x}_i - \boldsymbol{\mu}_k^{(t+1)}\right)^T}{\sum_{i=1}^{n} p(y_i = k|\, \mathbf{x}_i, \boldsymbol{\theta}^{(t)})}}$$

The newly updated matrix is a symmetric and positive-semidefinite matrix.

# Summary of the key steps of the EM-algorithm (upcoming)

# Summary of the key steps of the EM-algorithm for Gaussian mixture model (upcoming)

# Python implementation (upcoming)

In [87]:
```
import numpy as np
from scipy import random, linalg
import matplotlib.pyplot as plt
import matplotlib
from matplotlib import animation, rc
from IPython.display import HTML
import time


def gaussianpdf(mu, sigma, x):
    const = 1/np.sqrt(np.power(2*np.pi, len(mu)) * np.linalg.det(sigma))
    #print(mu, "\n", sigma, "\n", x)
    return const * np.exp(-1/2 * np.dot(np.transpose(x-mu), np.dot(np.linalg.inv(sigma), x-mu)))
```

```
def createRandomGaussianParams(number_of_dimensions):
    mu = random.uniform(0, 1, size=(number_of_dimensions, 1))
    A = random.rand(number_of_dimensions, number_of_dimensions)
    sigma = np.dot(A,A.transpose())
    return mu,sigma

import numpy as np
from scipy.interpolate import griddata
import matplotlib.pyplot as plt
import numpy.ma as ma
from numpy.random import uniform, seed
from matplotlib import cm
def gauss(x,y,Sigma,mu):
    X=np.vstack((x,y)).T
    mat_multi=np.dot((X-mu[None,...]).dot(np.linalg.inv(Sigma)),(X-mu[None,...]).T)
    return  np.diag(np.exp(-1*(mat_multi)))
def plot_countour(x,y,z):
    # define grid.
    xi = np.linspace(-2.1, 2.1, 100)
    yi = np.linspace(-2.1, 2.1, 100)
    ## grid the data.
    zi = griddata((x, y), z, (xi[None,:], yi[:,None]), method='cubic')
    levels = [0.2, 0.4, 0.6, 0.8, 1.0]
    # contour the gridded data, plotting dots at the randomly spaced data points.
    CS = plt.contour(xi,yi,zi,len(levels),linewidths=0.5,colors='k', levels=levels)
    #CS = plt.contourf(xi,yi,zi,15,cmap=plt.cm.jet)
    CS = plt.contourf(xi,yi,zi,len(levels),cmap=cm.Greys_r, levels=levels)
    plt.colorbar() # draw colorbar
    # plot data points.
    # plt.scatter(x, y, marker='o', c='b', s=5)
    plt.xlim(-2, 2)
    plt.ylim(-2, 2)
    plt.title('griddata test (%d points)' % npts)
    plt.show()


# make up some randomly distributed data
#seed(1234)
npts = 1000
mu, sigma = createRandomGaussianParams(2)



x = uniform(-2, 2, npts)
```

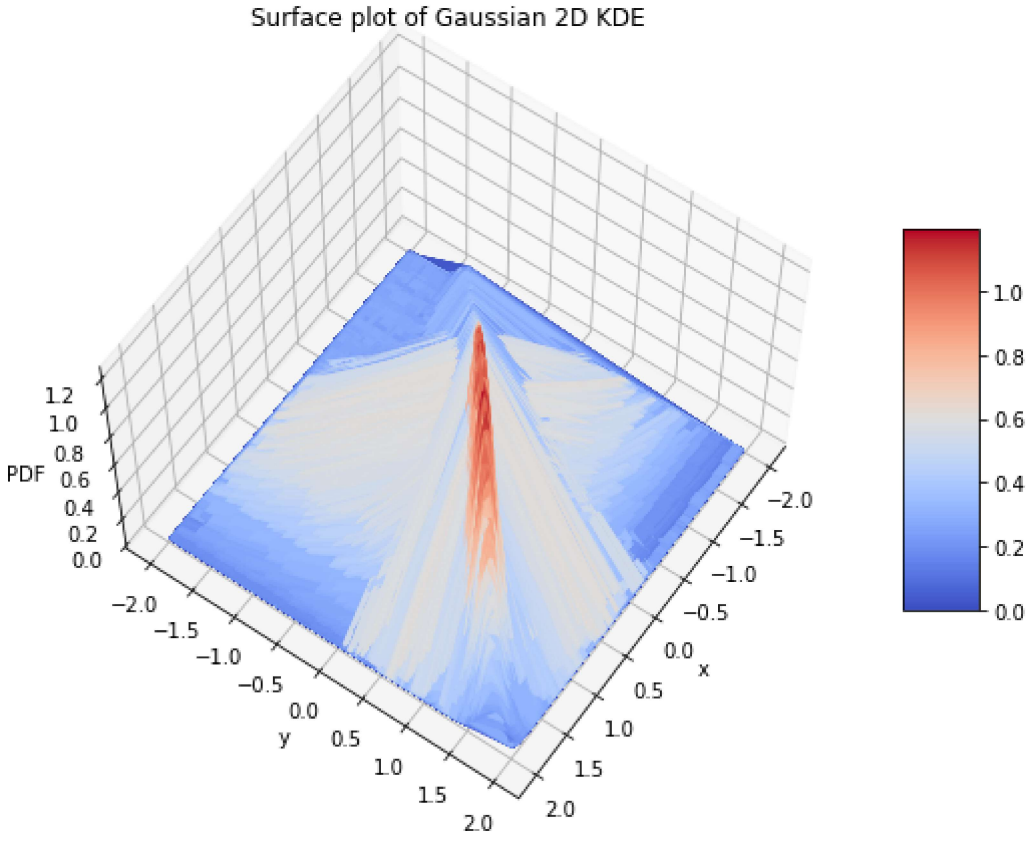
```
y = uniform(-2, 2, npts)

X, Y = np.meshgrid(x,y)
Z = np.zeros(X.shape)
#print(Z.shape)
for i in range(Z.shape[0]):
   for j in range(Z.shape[1]):
        #print(np.asarray([[X[i,j]],[Y[i,j]]]))
        Z[i,j] = gaussianpdf(mu, sigma, np.asarray([[X[i,j]],[Y[i,j]]]))[0][0]
        #print(gaussianpdf(mu, sigma, np.asarray([[X[i,j]],[Y[i,j]]])))
        #time.sleep(1)

#z = gauss(x, y, Sigma=sigma, mu=mu[0])
#plot_countour(x, y, z)
```

In [88]:

```
%matplotlib inline
fig = plt.figure(figsize=(13, 7))
ax = plt.axes(projection='3d')
surf = ax.plot_surface(X,Y,Z, rstride=1, cstride=1, cmap='coolwarm', edgecolor='none')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('PDF')
ax.set_title('Surface plot of Gaussian 2D KDE')
fig.colorbar(surf, shrink=0.5, aspect=5) # add color bar indicating the PDF
ax.view_init(60, 35)
```


Surface plot of Gaussian 2D KDE
PDF
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
y
x
1.0
0.8
0.6
0.4
0.2
0.0