EM_algorithm

February 21, 2015

```
In [1]: import os
        import sys
        import glob
        import matplotlib.pyplot as plt
        import numpy as np
        import pandas as pd
        %matplotlib inline
        plt.style.use('ggplot')
        np.random.seed(1234)

        np.set_printoptions(formatter={'all':lambda x: '%.3f' % x})
```

```
In [2]: from IPython.display import Image
        from numpy.core.umath_tests import matrix_multiply as mm
```

```
In [3]: from scipy.optimize import minimize
        from scipy.stats import bernoulli, binom
```

0.1 Outline

- Review of Jensen's inequality
- Concavity of log function
- Example of coin tossing with missing informaiton to provide context
- Derivation of EM equations
- Illustration of EM convergence
- Derivation of update equations of coin tossing example
- Code for coin tossing example
- Derivation of update equatiosn for mixture of Gaussians
- Code for mixture of Gaussians

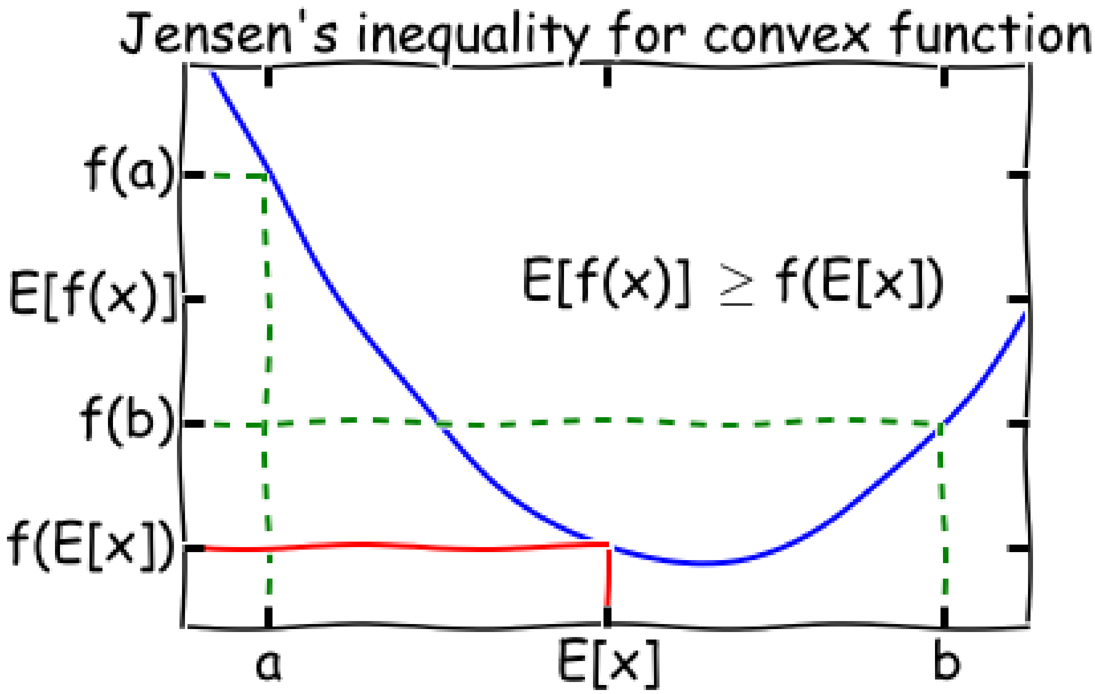
0.2 Jensen's inequality

For a convex function f, $E[f(x) \geq f(E[x])$. Flip the signe for a concave function.

A function $f(x)$ is convex if $f''(x) \geq 0$ everywhere in its domain. For example, if $f(x) = \log x$, $f''(x) = -1/x^2$, so the log function is concave for $x \in (0, \infty]$. A visual illustration of Jensen's inequality is shown below.

```
In [4]: Image(filename='figs/jensen.png')
```

Out[4]:



When is Jensen's inequality an equality? From the diagram, we can see that this only happens if the function $f(x)$ is a constant! We will make use of this fact later on in the lecture.

0.3 Maximum likelihood with complete information

Consider an experiment with coin A that has a probability θ_A of heads, and a coin B that has a probability θ_B of tails. We draw m samples as follows - for each sample, pick one of the coins at random, flip it n times, and record the number of heads and tails (that sum to n). If we recorded which coin we used for each sample, we have *complete* information and can estimate θ_A and θ_B in closed form. To be very explicit, suppose we drew 5 samples with the number of heads and tails represented as a vector x, and the sequence of coins chosen was A, A, B, A, B. Then the complete log likelihood is

$$\log p(x_1; \theta_A) + \log p(x_2; \theta_A) + \ logp(x_3; \theta_B) + \log p(x_4; \theta_A) + \log p(x_5; \theta_B)$$

where $p(x_i; \theta)$ is the binomial distribtion PMF with $n = m$ and $p = \theta$. We will use z_i to indicate the label of the i^{th} coin, that is - whether we used coin A or B to gnerate the i^{th} sample.

Coin toss example from What is the expectation maximization algorithm?

0.3.1 Solving for complete likelihood using minimization

```
In [5]: def neg_loglik(thetas, n, xs, zs):
            return -np.sum([binom(n, thetas[z]).logpmf(x) for (x, z) in zip(xs, zs)])
```

```
In [6]: m = 10
        theta_A = 0.8
        theta_B = 0.3
        theta_0 = [theta_A, theta_B]
```

```
coin_A = bernoulli(theta_A)
coin_B = bernoulli(theta_B)

xs = map(sum, [coin_A.rvs(m), coin_A.rvs(m), coin_B.rvs(m), coin_A.rvs(m), coin_B.rvs(m)])
zs = [0, 0, 1, 0, 1]
```

Exact solution

```
In [7]: xs = np.array(xs)
        xs

Out[7]: array([7.000, 9.000, 2.000, 6.000, 0.000])

In [8]: ml_A = np.sum(xs[[0,1,3]])/(3.0*m)
        ml_B = np.sum(xs[[2,4]])/(2.0*m)
        ml_A, ml_B

Out[8]: (0.73333333333333328, 0.10000000000000001)
```

Numerical estimate

```
In [9]: bnds = [(0,1), (0,1)]
        minimize(neg_loglik, [0.5, 0.5], args=(m, xs, zs),
                 bounds=bnds, method='tnc', options={'maxiter': 100})

Out[9]:   status: 1
         success: True
            nfev: 19
             fun: 7.6552677541114456
               x: array([0.733, 0.100])
         message: 'Converged (|f_n-f_(n-1)| ~= 0)'
             jac: array([0.000, -0.000])
             nit: 7
```

0.4 Incomplete information

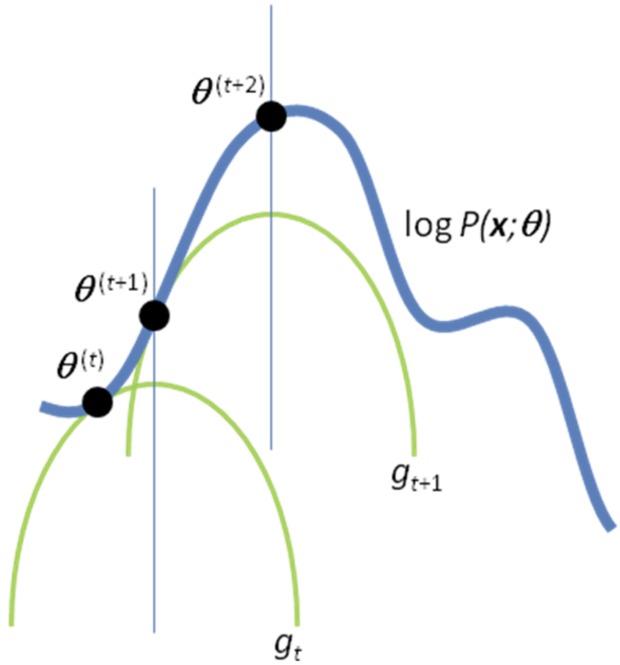
However, if we did not record the coin we used, we have *missing* data and the problem of estimating θ is harder to solve. One way to approach the problem is to ask - can we assign weights w_i to each sample according to how likely it is to be generated from coin A or coin B?

With knowledge of w_i, we can maximize the likelihod to find θ. Similarly, given w_i, we can calculate what θ should be. So the basic idea behind Expectation Maximization (EM) is simply to start with a guess for θ, then calculate z, then update θ using this new value for z, and repeat till convergence. The derivation below shows why the EM algorithm using this "alternating" updates actually works.

A verbal outline of the derivtion - first consider the log likelihood function as a curve (surface) where the base is θ. Find another function Q of θ that is a lower bound of the log-likelihood but touches the log likelihodd function at some θ (E-step). Next find the value of θ that maximizes this function (M-step). Now find yet antoher function of θ that is a lower bound of the log-likelihood but touches the log likelihodd function at this new θ. Now repeat until convergence - at this point, the maxima of the lower bound and likelihood functions are the same and we have found the maximum log likelihood. See illustratioin below.

```
In [10]: # Image from http://www.nature.com/nbt/journal/v26/n8/extref/nbt1406-S1.pdf
         Image(filename='figs/em.png', width=800)

Out[10]:
```



Supplementary Figure 1 Convergence of the EM algorithm. Starting from initial parameters $\theta^{(t)}$, the E-step of the EM algorithm constructs a function g_t that lower-bounds the objective function $\log P(\mathbf{x};\theta)$. In the M-step, $\theta^{(t+1)}$ is computed as the maximum of g_t. In the next E-step, a new lower-bound g_{t+1} is constructed; maximization of g_{t+1} in the next M-step gives $\theta^{(t+2)}$, etc.

The only remaining step is how to find the functions that are lower bounds of the log likelihood. This will require a little math using Jensen's inequality, and is shown in the next section.

0.4.1 Derivation

In the E-step, we identify a function which is a lower bound for the log-likelikelihood

$$\begin{aligned}
ll &= \sum_i \log p(x_i;\theta) && \text{definition of log likelihood} && (1)\\
&= \sum_i \log \sum_{z_i} p(x_i, z_i;\theta) && \text{augment with latent variables } z && (2)\\
&= \sum_i \log \sum_{z_i} Q_i(z_i)\frac{p(x_i, z_i;\theta)}{Q_i(z_i)} && Q_i \text{ is a distribution for } z_i && (3)\\
&= \sum_i \log E_{z_i}[\frac{p(x_i, z_i;\theta)}{Q_i(z_i)}] && \text{taking expectations - hence the E in EM} && (4)\\
&\geq \sum E_{z_i}[\log \frac{p(x_i, z_i;\theta)}{Q_i(z_i)}] && \text{Using Jensen's rule for log which is concave} && (5)\\
&\geq \sum_i \sum_{z_i} Q_i(z_i) \log \frac{p(x_i, z_i;\theta)}{Q_i(z_i)} && \text{Q function} && (6)
\end{aligned}$$

How do we choose the distribution Q_i? We want the Q function to touch the log-likelihood, and know that Jensen's inequality is an equality only if the function is constant. So

$$\begin{aligned}
\frac{p(x_i, z_i; \theta)}{Q_i(z_i)} &= c && (7)\\
\implies Q_i(z_i) &\propto p(x_i, z_i; \theta) && (8)\\
\implies Q_i(z_i) &= \frac{p(x_i, z_i; \theta)}{\sum_{z_i} p(x_i, z_i; \theta)} && \text{Since } Q \text{ is a distribution and sums to 1} \quad (9)\\
\implies Q_i(z_i) &= \frac{p(x_i, z_i; \theta)}{p(x_i, \theta)} && \text{marginalizing } z_i \quad (10)\\
\implies Q_i(z_i) &= p(z_i|x_i; \theta) && \text{by definition} \quad (11)
\end{aligned}$$

So Q_i is just the posterior distribution of z_i, and this completes the E-step.

In the M-step, we find the value of θ that maximizes the Q function, and then we iterate over the E and M steps until convergence.

So we see that EM is an algorihtm for maximum likelikhood optimization when there is missing inforrmaiton - or when it is useful to add latent augmented variables to simplify maximum likelihood calculatoins.

0.4.2 EM for coin toss example

- i indicates the sample
- j indicates the coin
- l is an index running through each of the coins
- θ is the probability of the coin being heads
- ϕ is the probability of choosing a particular coin
- h is the number of heads in a sample
- n is the number of coin tosses in a sample
- k is the number of coins
- m is the number of samples

For the E-step, with each sample we have

$$\begin{aligned}
w_j &= Q_i(z_i = j) && (12)\\
&= p(z_i = j|x_i; \theta) && (13)\\
&= \frac{p(x_i|z_i = j; \theta)p(z_i = j; \phi)}{\sum_{l=1}^{k} p(x_i|z_i = l; \theta)p(z_i = l; \phi)} && \text{Baye's rule } P(A|B) = \frac{P(B|A)P(B)}{P(A)} \quad (14)\\
&= \frac{\theta_j^h (1-\theta_j)^{n-h} \phi_j}{\sum_{l=1}^{k} \theta_l^h (1-\theta_l)^{n-h} \phi_l} && (15)\\
\text{[EQN 1]} &= \frac{\theta_j^h (1-\theta_j)^{n-h}}{\sum_{l=1}^{k} \theta_l^h (1-\theta_l)^{n-h}} && \text{assume } \phi \text{ is fixed since we are equally likely to choose each coin} \quad (16)
\end{aligned}$$

For the M-step, we need to find the value of θ that maximises the Q function

$$\sum_i \sum_{z_i} Q_i(z_i) \log \frac{p(x_i, z_i; \theta)}{Q_i(z_i)} \tag{17}$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{k} w_j \log \frac{p(x_i | z_i = j; \theta)\, p(z_i = j; \phi)}{w_j} \tag{18}$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{k} w_j \log \frac{\theta_j^h (1-\theta_j)^{n-h} \phi_j}{w_j} \tag{19}$$

$$[\text{EQN } 2] = \sum_{i=1}^{m} \sum_{j=1}^{k} w_j \left(h \log \theta_j + (n-h) \log(1-\theta_j) + \log \phi_j - \log w_j\right) \tag{20}$$

We can differentiate and solve for each component θ_s where the derivative vanishes

$$\sum_{i=1}^{m} w_s \left(\frac{h}{\theta_s} - \frac{n-h}{1-\theta_s} \right) = 0 \tag{21}$$

$$\implies \theta_s = \frac{\sum_{i=1}^{m} w_s h}{\sum_{i=1}^{m} w_s n} \tag{22}$$

0.4.3 First explicit solution

In [11]:
```
xs = np.array([(5,5), (9,1), (8,2), (4,6), (7,3)])
thetas = np.array([[0.6, 0.4], [0.5, 0.5]])

tol = 0.01
max_iter = 100

ll_old = 0
for i in range(max_iter):
    ws_A = []
    ws_B = []

    vs_A = []
    vs_B = []

    ll_new = 0

    # E-step: calculate probability distributions over possible completions
    for x in xs:

        # multinomial (binomial) log likelihood
        ll_A = np.sum([x*np.log(thetas[0])])
        ll_B = np.sum([x*np.log(thetas[1])])

        # [EQN 1]
        denom = np.exp(ll_A) + np.exp(ll_B)
        w_A = np.exp(ll_A)/denom
        w_B = np.exp(ll_B)/denom

        ws_A.append(w_A)
        ws_B.append(w_B)
```

```
                # used for calculating theta
                vs_A.append(np.dot(w_A, x))
                vs_B.append(np.dot(w_B, x))

                # update complete log likelihood
                ll_new += w_A * ll_A + w_B * ll_B

            # M-step: update values for parameters given current distribution
            # [EQN 2]
            thetas[0] = np.sum(vs_A, 0)/np.sum(vs_A)
            thetas[1] = np.sum(vs_B, 0)/np.sum(vs_B)
            # print distribution of z for each x and current parameter estimate

            print "Iteration: %d" % (i+1)
            print "theta_A = %.2f, theta_B = %.2f, ll = %.2f" % (thetas[0,0], thetas[1,0], ll_new)

            if np.abs(ll_new - ll_old) < tol:
                break
            ll_old = ll_new
```

```
Iteration: 1
theta_A = 0.71, theta_B = 0.58, ll = -32.69
Iteration: 2
theta_A = 0.75, theta_B = 0.57, ll = -31.26
Iteration: 3
theta_A = 0.77, theta_B = 0.55, ll = -30.76
Iteration: 4
theta_A = 0.78, theta_B = 0.53, ll = -30.33
Iteration: 5
theta_A = 0.79, theta_B = 0.53, ll = -30.07
Iteration: 6
theta_A = 0.79, theta_B = 0.52, ll = -29.95
Iteration: 7
theta_A = 0.80, theta_B = 0.52, ll = -29.90
Iteration: 8
theta_A = 0.80, theta_B = 0.52, ll = -29.88
Iteration: 9
theta_A = 0.80, theta_B = 0.52, ll = -29.87
```

0.4.4 Vectorizing . . .

In [12]:
```
xs = np.array([(5,5), (9,1), (8,2), (4,6), (7,3)])
thetas = np.array([[0.6, 0.4], [0.5, 0.5]])

tol = 0.01
max_iter = 100

ll_old = -np.infty
for i in range(max_iter):
    ll_A = np.sum(xs * np.log(thetas[0]), axis=1)
    ll_B = np.sum(xs * np.log(thetas[1]), axis=1)
    denom = np.exp(ll_A) + np.exp(ll_B)
    w_A = np.exp(ll_A)/denom
    w_B = np.exp(ll_B)/denom
```

```
        vs_A = w_A[:, None] * xs
        vs_B = w_B[:, None] * xs

        thetas[0] = np.sum(vs_A, 0)/np.sum(vs_A)
        thetas[1] = np.sum(vs_B, 0)/np.sum(vs_B)

        ll_new = w_A.dot(ll_A) + w_B.dot(ll_B)

        print "Iteration: %d" % (i+1)
        print "theta_A = %.2f, theta_B = %.2f, ll = %.2f" % (thetas[0,0], thetas[1,0], ll_new)

        if np.abs(ll_new - ll_old) < tol:
            break
        ll_old = ll_new
```

```
Iteration: 1
theta_A = 0.71, theta_B = 0.58, ll = -32.69
Iteration: 2
theta_A = 0.75, theta_B = 0.57, ll = -31.26
Iteration: 3
theta_A = 0.77, theta_B = 0.55, ll = -30.76
Iteration: 4
theta_A = 0.78, theta_B = 0.53, ll = -30.33
Iteration: 5
theta_A = 0.79, theta_B = 0.53, ll = -30.07
Iteration: 6
theta_A = 0.79, theta_B = 0.52, ll = -29.95
Iteration: 7
theta_A = 0.80, theta_B = 0.52, ll = -29.90
Iteration: 8
theta_A = 0.80, theta_B = 0.52, ll = -29.88
Iteration: 9
theta_A = 0.80, theta_B = 0.52, ll = -29.87
```

0.4.5 Writing as a function

In [13]:
```
def em(xs, thetas, max_iter=100, tol=1e-6):
    """Expectation-maximization for coin sample problem."""

    ll_old = -np.infty
    for i in range(max_iter):
        ll = np.array([np.sum(xs * np.log(theta), axis=1) for theta in thetas])
        lik = np.exp(ll)
        ws = lik/lik.sum(0)
        vs = np.array([w[:, None] * xs for w in ws])
        thetas = np.array([v.sum(0)/v.sum() for v in vs])
        ll_new = np.sum([w*l for w, l in zip(ws, ll)])
        if np.abs(ll_new - ll_old) < tol:
            break
        ll_old = ll_new
    return i, thetas, ll_new
```

0.4.6 Checking

```
In [14]: xs = np.array([(5,5), (9,1), (8,2), (4,6), (7,3)])
         thetas = np.array([[0.6, 0.4], [0.5, 0.5]])

         i, thetas, ll = em(xs, thetas)
         print i
         for theta in thetas:
             print theta
         print ll
```

```
18
[0.797 0.203]
[0.520 0.480]
-29.868676155
```

0.4.7 Make up some data

```
In [15]: np.random.seed(1234)

         n = 100
         p0 = 0.8
         p1 = 0.35
         xs = np.concatenate([np.random.binomial(n, p0, n/2), np.random.binomial(n, p1, n/2)])
         xs = np.column_stack([xs, n-xs])
         np.random.shuffle(xs)
```

0.4.8 EM with multiple random starts

```
In [16]: results = [em(xs, np.random.random((2,2))) for i in range(10)]
         i, thetas, ll =  sorted(results, key=lambda x: x[-1])[-1]
         print i
         for theta in thetas:
             print theta
         print ll
```

```
4
[0.352 0.648]
[0.798 0.202]
-5756.59565198
```

0.5 Gaussian mixture models

```
In [17]: import scipy.stats as st
```

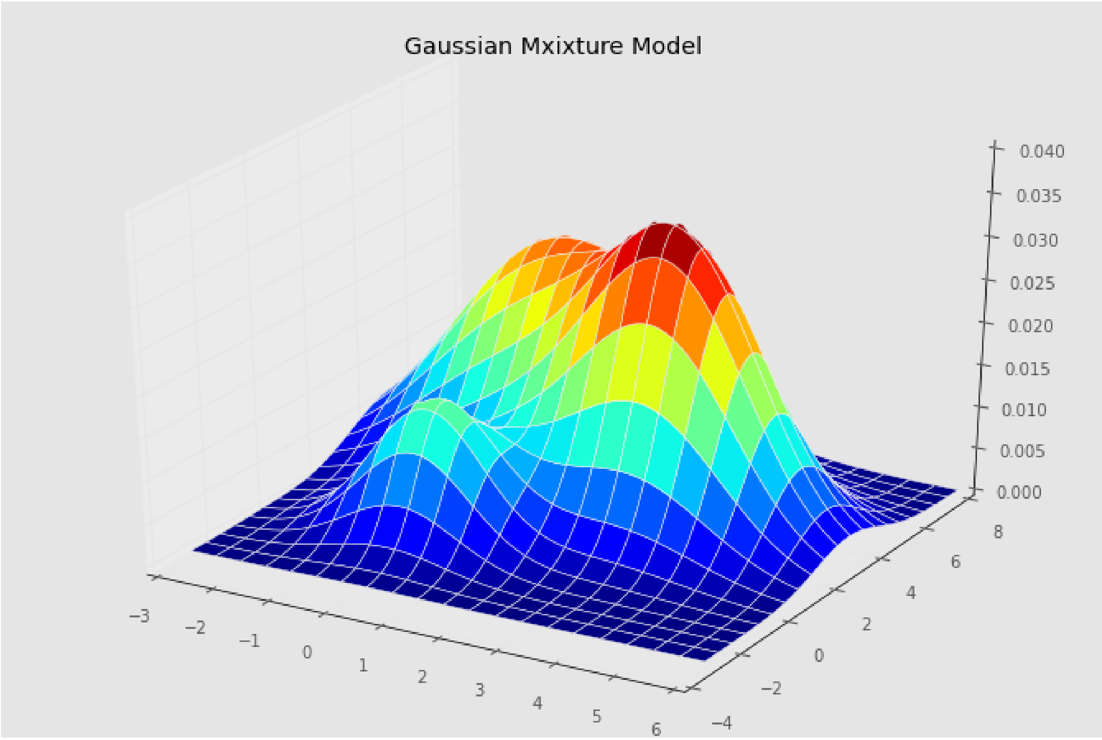
```
In [18]: def f(x, y):
             z = np.column_stack([x.ravel(), y.ravel()])
             return (0.1*st.multivariate_normal([0,0], 1*np.eye(2)).pdf(z) +
                     0.4*st.multivariate_normal([3,3], 2*np.eye(2)).pdf(z) +
                     0.5*st.multivariate_normal([0,5], 3*np.eye(2)).pdf(z))
```

```
In [19]: f(np.arange(3), np.arange(3))
```

```
Out[19]: array([0.017, 0.012, 0.023])
```

```
In [20]: s = 200
         x = np.linspace(-3, 6, s)
         y = np.linspace(-3, 8, s)
         X, Y = np.meshgrid(x, y)
         Z = np.reshape(f(X, Y), (s, s))

         from mpl_toolkits.mplot3d import Axes3D
         fig = plt.figure(figsize=(12,8))
         ax = fig.add_subplot(111, projection='3d')
         ax.plot_surface(X, Y, Z, cmap='jet')
         plt.title('Gaussian Mxixture Model');
```



A mixture of k Gaussians has the following PDF

$$p(x) = \sum_{j=1}^{k} \alpha_j \phi(x; \mu_j, \Sigma_j) \tag{23}$$

where α_j is the weight of the j^{th} Gaussain component and

$$\phi(x; \mu, \Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right) \tag{24}$$

Suppose we observe $y_1, y_2, \ldots, y_n$ as a sample from a mixture of Gaussians. The log-likeihood is then

$$l(\theta) = \sum_{i=1}^{n} \log\left(\sum_{j=1}^{k} \alpha_j \phi(y_i; \mu_j, \Sigma_j)\right) \tag{25}$$

where $\theta = (\alpha, \mu, \Sigma)$

There is no closed form for maximizing the parameters of this log-likelihood, and it is hard to maximize directly.

0.6 Using EM

Suppose we augment with the latent variable z that indicates which of the k Gaussians our observation y came from. The derivation of the E and M steps are the same as for the toy example, only with more algebra.

For the E-step, we have

$$
\begin{aligned}
w_j^i &= Q_i(z^i = j) && (26)\\
&= p(z^i = j | y^i; \theta) && (27)\\
&= \frac{p(y^i | z^i = j; \mu, \Sigma) p(z^i = j; \alpha)}{\sum_{l=1}^k p(y^i | z^i = l; \mu, \Sigma) p(z^i = l; \alpha)} && \text{Baye's rule} \quad (28)\\
&= \frac{\phi(y^i; \mu_j, \Sigma_j)\alpha_j}{\sum_{l=1}^k \phi(y^i; \mu_l, \Sigma_l)\alpha_l} && (29)
\end{aligned}
$$

For the M-step, we have to find $\theta = (w, \mu, \Sigma)$ that maximizes Q

$$
\sum_{i=1}^m \sum_{j=1}^k Q(z^i = j) \log \frac{p(x^i | z^i = j; \mu, \Sigma) p(z^i = j; \alpha)}{Q(z^i = j)} \tag{30}
$$

By taking derivatives with respect to (w, μ, Σ) respectively and solving (remember to use Lagrange multipliers for the constraint that $\sum_{j=1}^k w_j = 1$), we get

$$
\begin{aligned}
\alpha_j &= \frac{1}{m} \sum_{i=1}^m w_j^i && (31)\\
\mu_j &= \frac{\sum_{i=1}^m w_j^i x^i}{\sum_{i=1}^m w_j^i} && (32)\\
\Sigma_j &= \frac{\sum_{i=1}^m w_j^i (x^i - \mu)(x^i - \mu)^T}{\sum_{i1}^m w_j^i} && (33)
\end{aligned}
$$

```
In [21]: from scipy.stats import multivariate_normal as mvn
```

```
In [22]: def em_gmm_orig(xs, pis, mus, sigmas, tol=0.01, max_iter=100):

             n, p = xs.shape
             k = len(pis)

             ll_old = 0
             for i in range(max_iter):
                 exp_A = []
                 exp_B = []
                 ll_new = 0

                 # E-step
                 ws = np.zeros((k, n))
                 for j in range(len(mus)):
                     for i in range(n):
```

```
                ws[j, i] = pis[j] * mvn(mus[j], sigmas[j]).pdf(xs[i])
        ws /= ws.sum(0)

        # M-step
        pis = np.zeros(k)
        for j in range(len(mus)):
            for i in range(n):
                pis[j] += ws[j, i]
        pis /= n

        mus = np.zeros((k, p))
        for j in range(k):
            for i in range(n):
                mus[j] += ws[j, i] * xs[i]
            mus[j] /= ws[j, :].sum()

        sigmas = np.zeros((k, p, p))
        for j in range(k):
            for i in range(n):
                ys = np.reshape(xs[i]- mus[j], (2,1))
                sigmas[j] += ws[j, i] * np.dot(ys, ys.T)
            sigmas[j] /= ws[j,:].sum()

        # update complete log likelihoood
        ll_new = 0.0
        for i in range(n):
            s = 0
            for j in range(k):
                s += pis[j] * mvn(mus[j], sigmas[j]).pdf(xs[i])
            ll_new += np.log(s)

        if np.abs(ll_new - ll_old) < tol:
            break
        ll_old = ll_new

    return ll_new, pis, mus, sigmas
```

0.7 Vectorized version

```
In [23]: def em_gmm_vect(xs, pis, mus, sigmas, tol=0.01, max_iter=100):

             n, p = xs.shape
             k = len(pis)

             ll_old = 0
             for i in range(max_iter):
                 exp_A = []
                 exp_B = []
                 ll_new = 0

                 # E-step
                 ws = np.zeros((k, n))
                 for j in range(k):
                     ws[j, :] = pis[j] * mvn(mus[j], sigmas[j]).pdf(xs)
```

```
        ws /= ws.sum(0)

        # M-step
        pis = ws.sum(axis=1)
        pis /= n

        mus = np.dot(ws, xs)
        mus /= ws.sum(1)[:, None]

        sigmas = np.zeros((k, p, p))
        for j in range(k):
            ys = xs - mus[j, :]
            sigmas[j] = (ws[j,:,None,None] * mm(ys[:,:,None], ys[:,None,:])).sum(axis=0)
        sigmas /= ws.sum(axis=1)[:,None,None]

        # update complete log likelihoood
        ll_new = 0
        for pi, mu, sigma in zip(pis, mus, sigmas):
            ll_new += pi*mvn(mu, sigma).pdf(xs)
        ll_new = np.log(ll_new).sum()

        if np.abs(ll_new - ll_old) < tol:
            break
        ll_old = ll_new

    return ll_new, pis, mus, sigmas
```

0.8 Vectorization with Einstein summation notation

```
In [24]: def em_gmm_eins(xs, pis, mus, sigmas, tol=0.01, max_iter=100):

             n, p = xs.shape
             k = len(pis)

             ll_old = 0
             for i in range(max_iter):
                 exp_A = []
                 exp_B = []
                 ll_new = 0

                 # E-step
                 ws = np.zeros((k, n))
                 for j, (pi, mu, sigma) in enumerate(zip(pis, mus, sigmas)):
                     ws[j, :] = pi * mvn(mu, sigma).pdf(xs)
                 ws /= ws.sum(0)

                 # M-step
                 pis = np.einsum('kn->k', ws)/n
                 mus = np.einsum('kn,np -> kp', ws, xs)/ws.sum(1)[:, None]
                 sigmas = np.einsum('kn,knp,knq -> kpq', ws,
                     xs-mus[:,None,:], xs-mus[:,None,:])/ws.sum(axis=1)[:,None,None]

                 # update complete log likelihoood
                 ll_new = 0
```

```
            for pi, mu, sigma in zip(pis, mus, sigmas):
                ll_new += pi*mvn(mu, sigma).pdf(xs)
            ll_new = np.log(ll_new).sum()

            if np.abs(ll_new - ll_old) < tol:
                break
            ll_old = ll_new

        return ll_new, pis, mus, sigmas
```

0.9 Comparison of EM routines

In [25]:
```
np.random.seed(123)

# create data set
n = 1000
_mus = np.array([[0,4], [-2,0]])
_sigmas = np.array([[[3, 0], [0, 0.5]], [[1,0],[0,2]]])
_pis = np.array([0.6, 0.4])
xs = np.concatenate([np.random.multivariate_normal(mu, sigma, int(pi*n))
                    for pi, mu, sigma in zip(_pis, _mus, _sigmas)])

# initial guesses for parameters
pis = np.random.random(2)
pis /= pis.sum()
mus = np.random.random((2,2))
sigmas = np.array([np.eye(2)] * 2)
```

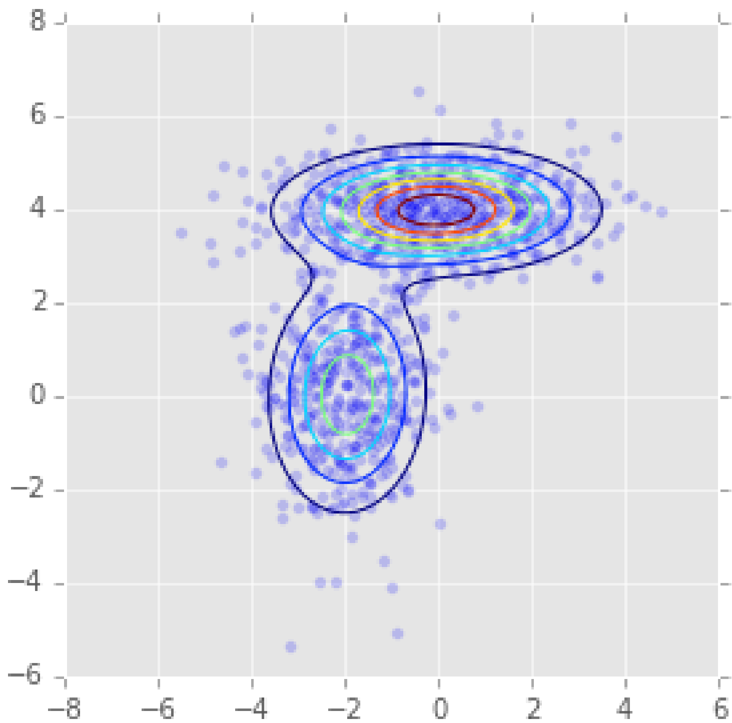
In [26]:
```
%%time
ll1, pis1, mus1, sigmas1 = em_gmm_orig(xs, pis, mus, sigmas)
```

```
CPU times: user 33.8 s, sys: 243 ms, total: 34.1 s
Wall time: 34.3 s
```

In [27]:
```
intervals = 101
ys = np.linspace(-8,8,intervals)
X, Y = np.meshgrid(ys, ys)
_ys = np.vstack([X.ravel(), Y.ravel()]).T

z = np.zeros(len(_ys))
for pi, mu, sigma in zip(pis1, mus1, sigmas1):
    z += pi*mvn(mu, sigma).pdf(_ys)
z = z.reshape((intervals, intervals))

ax = plt.subplot(111)
plt.scatter(xs[:,0], xs[:,1], alpha=0.2)
plt.contour(X, Y, z, N=10)
plt.axis([-8,6,-6,8])
ax.axes.set_aspect('equal')
plt.tight_layout()
```



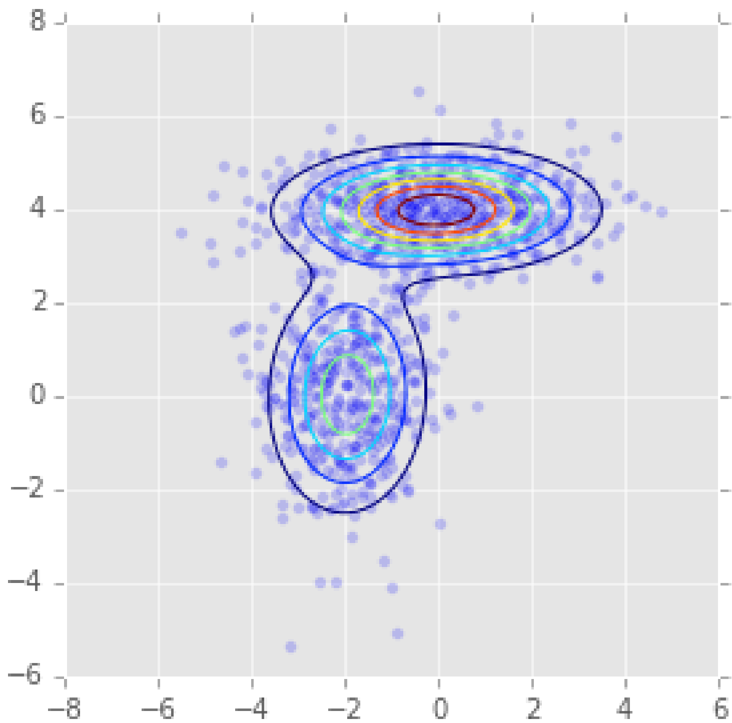

```
In [28]: %%time
         ll2, pis2, mus2, sigmas2 = em_gmm_vect(xs, pis, mus, sigmas)
```

```
CPU times: user 131 ms, sys: 5.03 ms, total: 136 ms
Wall time: 78.1 ms
```

```
In [29]: intervals = 101
         ys = np.linspace(-8,8,intervals)
         X, Y = np.meshgrid(ys, ys)
         _ys = np.vstack([X.ravel(), Y.ravel()]).T

         z = np.zeros(len(_ys))
         for pi, mu, sigma in zip(pis2, mus2, sigmas2):
             z += pi*mvn(mu, sigma).pdf(_ys)
         z = z.reshape((intervals, intervals))

         ax = plt.subplot(111)
         plt.scatter(xs[:,0], xs[:,1], alpha=0.2)
         plt.contour(X, Y, z, N=10)
         plt.axis([-8,6,-6,8])
         ax.axes.set_aspect('equal')
         plt.tight_layout()
```




```
In [30]: %%time
         ll3, pis3, mus3, sigmas3 = em_gmm_eins(xs, pis, mus, sigmas)
```

```
CPU times: user 68.3 ms, sys: 3.26 ms, total: 71.6 ms
Wall time: 71.9 ms
```

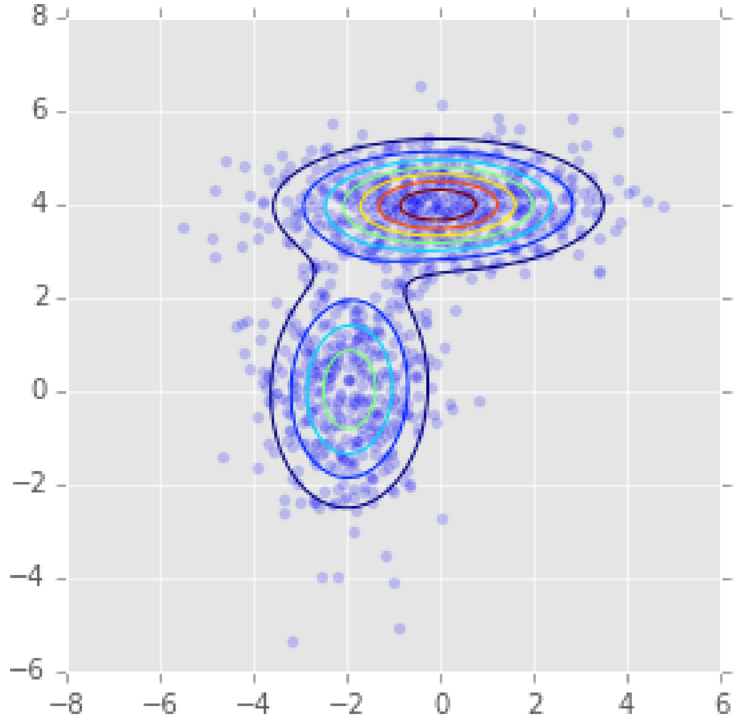
```
In [31]: # %timeit em_gmm_orig(xs, pis, mus, sigmas)
         %timeit em_gmm_vect(xs, pis, mus, sigmas)
         %timeit em_gmm_eins(xs, pis, mus, sigmas)
```

```
10 loops, best of 3: 85.1 ms per loop
10 loops, best of 3: 54 ms per loop
```

```
In [32]: intervals = 101
         ys = np.linspace(-8,8,intervals)
         X, Y = np.meshgrid(ys, ys)
         _ys = np.vstack([X.ravel(), Y.ravel()]).T

         z = np.zeros(len(_ys))
         for pi, mu, sigma in zip(pis3, mus3, sigmas3):
             z += pi*mvn(mu, sigma).pdf(_ys)
         z = z.reshape((intervals, intervals))

         ax = plt.subplot(111)
         plt.scatter(xs[:,0], xs[:,1], alpha=0.2)
         plt.contour(X, Y, z, N=10)
         plt.axis([-8,6,-6,8])
         ax.axes.set_aspect('equal')
         plt.tight_layout()
```


8
6
4
2
0
−2
−4
−6
−8
−6
−4
−2
0
2
4
6