COMP755-Lect11

October 1, 2018

1 COMP 755

Plan for today

1. Unsupervised learning
2. Mixture models
3. EM algorithm

2 Unsupervised learning

In supervised learning, data is given in form

$$\text{Data} = \{(\mathbf{x}_t, \mathbf{y}_t) \mid t = 1, ...T\}$$

There is a feature/predictor vector $\mathbf{x}$ and a target variable $\mathbf{y}$.

In unsupervised learning this distinction disappeares

$$\text{Data} = \{\mathbf{x}_t \mid t = 1, ...T\}$$

3 Examples of unsupervised learning

- Dimensionality reduction -- lossy compression
- Clustering -- assigning each point to a representative cluster
- Note: in classification groups are known, in clustering they are learned
- Deconvolution -- splitting mixed signals such as instruments or speakers in sound signal

Applications * Data summarization/compression * Denoising, outlier detection * Feature construction

4 Clustering

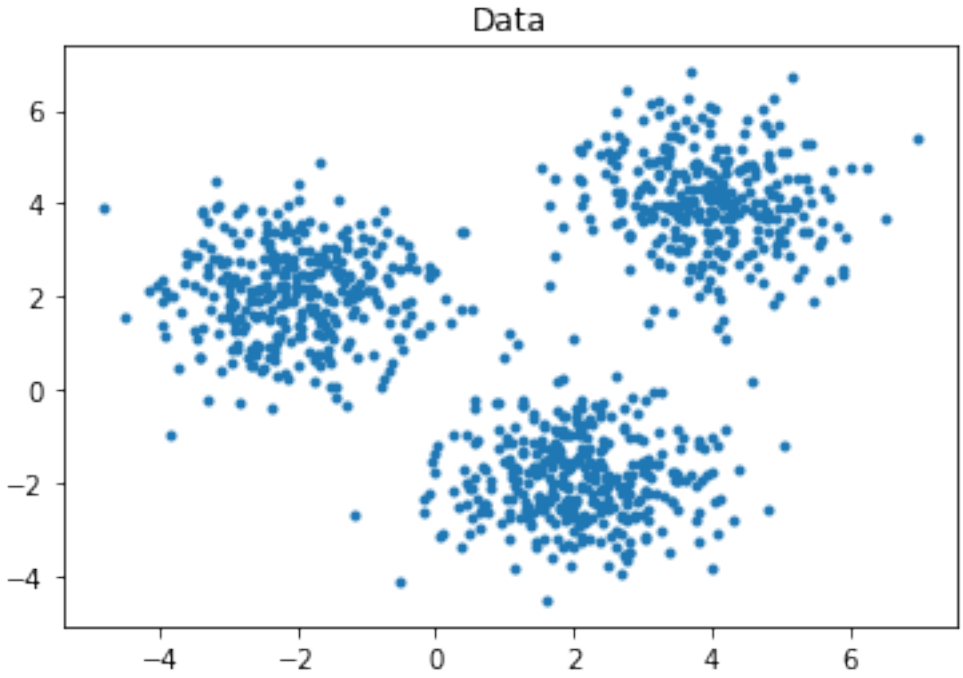
We will first look at a very simple -- and popular -- clustering algorithm called *K-means*

The algorithm iterates 1. assignment of samples to the closest of the **K** clusters 2. updates to clusters' **means**

In [1]:
```
import numpy
import matplotlib.pyplot as plt
%matplotlib inline
def generate_data(N,d,K,proby,mus,A=None):
    if A is None:
        A = numpy.eye(d)
    ys = [0]*N
    xs = numpy.zeros((d,N))
    for i in range(N):
        # Sample class according to the prior p(y)
        # in this case it is uniform
        ys[i] = numpy.random.choice(K,1)
        # Sample feature values according to p(x|y)
        # In this case, x ~ N(mmu[y[i]],sigma2*I)
        # To accomplish this, draw z1,z2 ~ N(0,I)
        z = numpy.random.randn(2,1)
        # transform by matrix A and shift by class mean
        x = numpy.dot(A,z) + mus[:,ys[i]]
        xs[:,i] = x[:,0]
    return xs,ys

def plot_samples(xs,ys,mus=None,colors=['r','g','b','k','c','m']):
    if not ys is None:
        K = numpy.max(ys)+1
        for c in range(K):
        # indices of samples assigned to class c
            ind = [i for i in range(N) if ys[i]==c]
            plt.plot(xs[0,ind],xs[1,ind],colors[c]+'.',label='Samples in cluster '+str(c
            if not mus is None:
                plt.plot(mus[0,c],mus[1,c],'kx',markersize=9,markeredgewidth=5)
                plt.plot(mus[0,c],mus[1,c],'wx',markersize=7,markeredgewidth=3)
        plt.legend(loc=2, bbox_to_anchor=(1,1))
    else:
        plt.plot(xs[0,:],xs[1,:],'.')


def plot_samples_post(xs,qs,mus=None,colors=['r','g','b','k','c','m']):
    K,N = qs.shape
    for i in range(N):
        plt.plot(xs[0,i],xs[1,i],'o',color=qs[:,i])
    for c in range(K):
    # indices of samples assigned to class c
        if not mus is None:
            plt.plot(mus[0,c],mus[1,c],'kx',markersize=9,markeredgewidth=5)
            plt.plot(mus[0,c],mus[1,c],'wx',markersize=7,markeredgewidth=3)
```

```
N = 1000 # 100 samples
K = 3   # 3 classes
d = 2   # x is 2d
proby = [1.0/K]*K # [1./3. , 1./3., 1./3.]
mus = 2.0*numpy.asarray([[-1.0,1.0,2],[1.0,-1.0,2.0]])

numpy.random.seed(1)
xs,ys = generate_data(N,d,K,proby,mus)
plot_samples(xs,None,mus)
plt.title('Data')
```

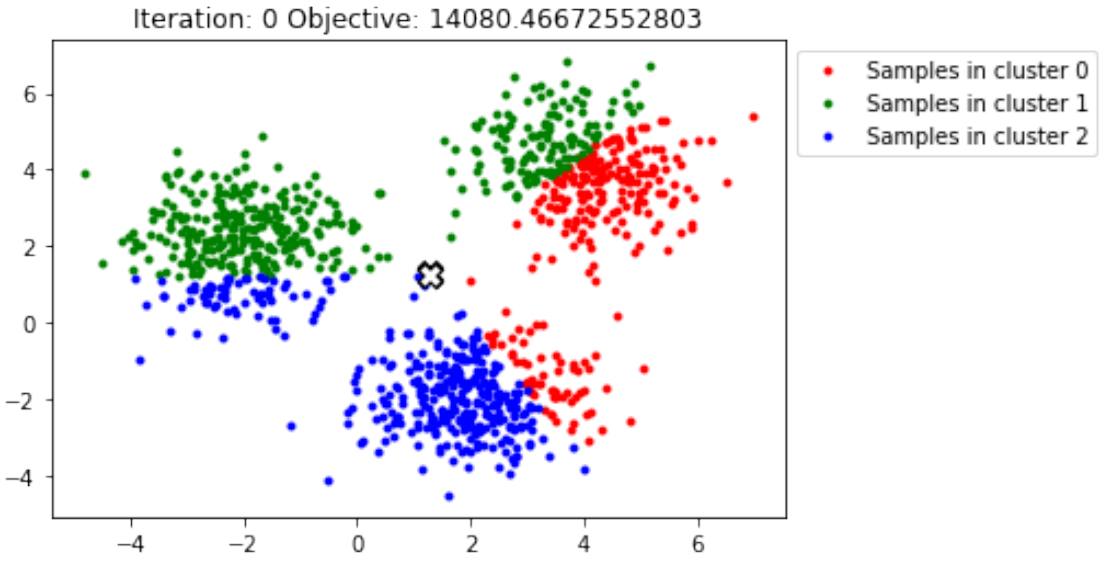
Out[1]: Text(0.5,1,'Data')

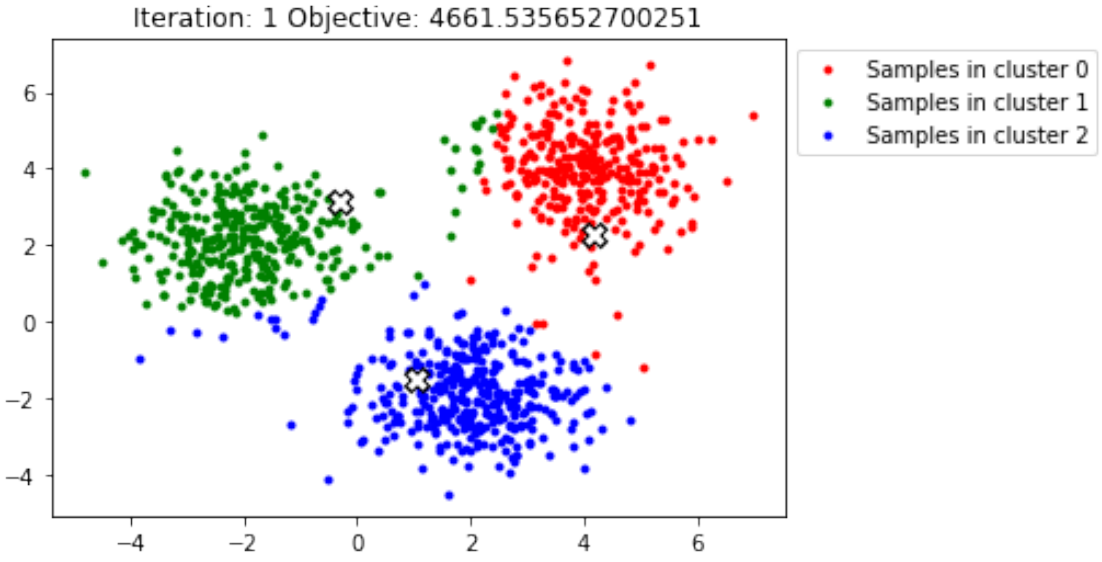


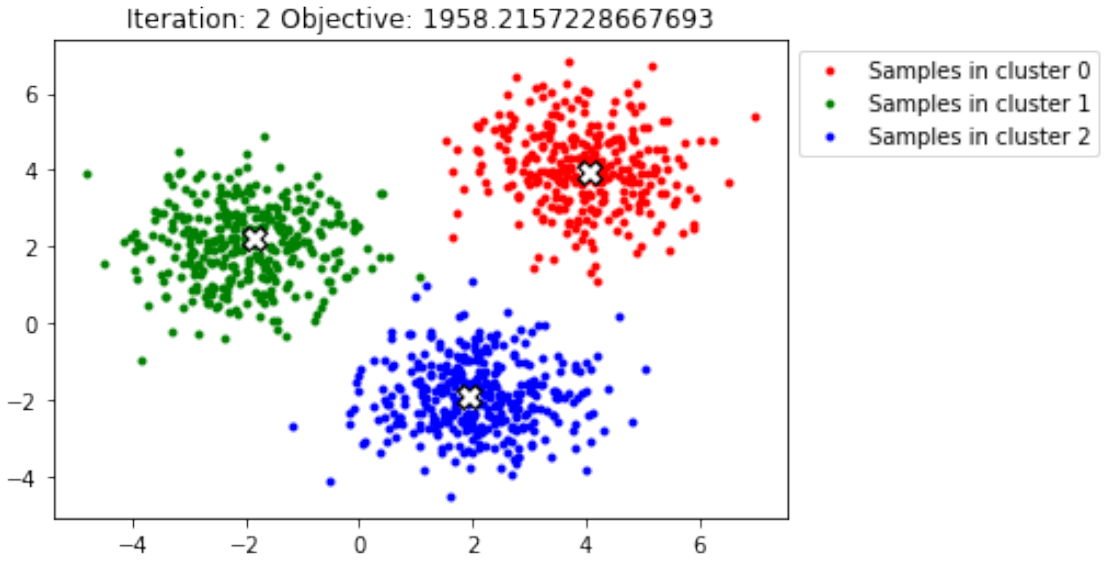
In [2]:
```
def kmeans(xs,K,iterations,tolerance=1e-7, just_last=False):
    # dimensions of data
    d,N = xs.shape

    # random initialization of centers
    data_mean = numpy.mean(xs,axis=1)[:,numpy.newaxis]
    mus = 0.01*numpy.random.randn(d,K) + data_mean

    # cluster assignments using 1-hot representation
    ph = numpy.zeros((K,N))
    # distance from each cluster center to each point
    last_objective = numpy.finfo('d').max
```

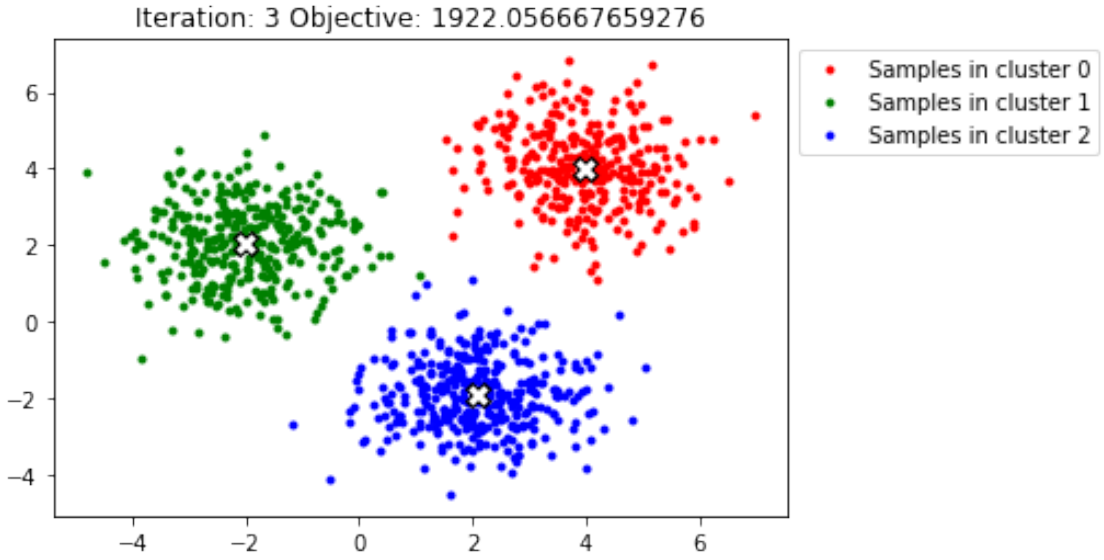
```
    for it in range(iterations):
        # compute distance between samples and cluster centers (mus)
        # recognize this as vectorized form of
        # x'x - 2.0 x'mu
        mus_sq = numpy.asmatrix(numpy.sum(mus**2.0,axis=0)).transpose()
        mus_xs = numpy.dot(mus.transpose(),xs)
        xs_sq = numpy.sum(xs**2.0,axis=0)
        distance =  mus_sq  - 2.0*mus_xs + xs_sq

        # objective is sum of distances from each sample
        # to its closest cluster
        objective = numpy.sum(numpy.min(distance,axis=0))

        # find closest clusters all at once
        h = numpy.argmin(distance,axis=0).transpose()

        # convert the closest cluster id to one-hot
        # representation
        ph[:] = 0
        for (i,v) in enumerate(h):
            ph[v,i] = 1.0

        # visualization
        if not just_last:
            plt.figure()
            plot_samples(xs,h,mus)
            plt.title('Iteration: {} Objective: {}'.format(it,objective))

        # check whether sufficient change has occurred
        if last_objective - objective < tolerance:
            break
        else:
            last_objective = objective

        # update each cluster center with mean of samples in that cluster
        # make sure not to divide by 0 -- in case of an empty cluster
        mus = numpy.dot(xs,ph.transpose())/(1e-5 + numpy.sum(ph,axis=1))

    if just_last:
        plt.figure()
        plot_samples(xs,h,mus)
        plt.title('Final after {} iterations with objective {}'.format(it,objective))
    return h,mus


numpy.random.seed(1)
xs,ys = generate_data(N,d,K,proby,mus)
numpy.random.seed(1)
```

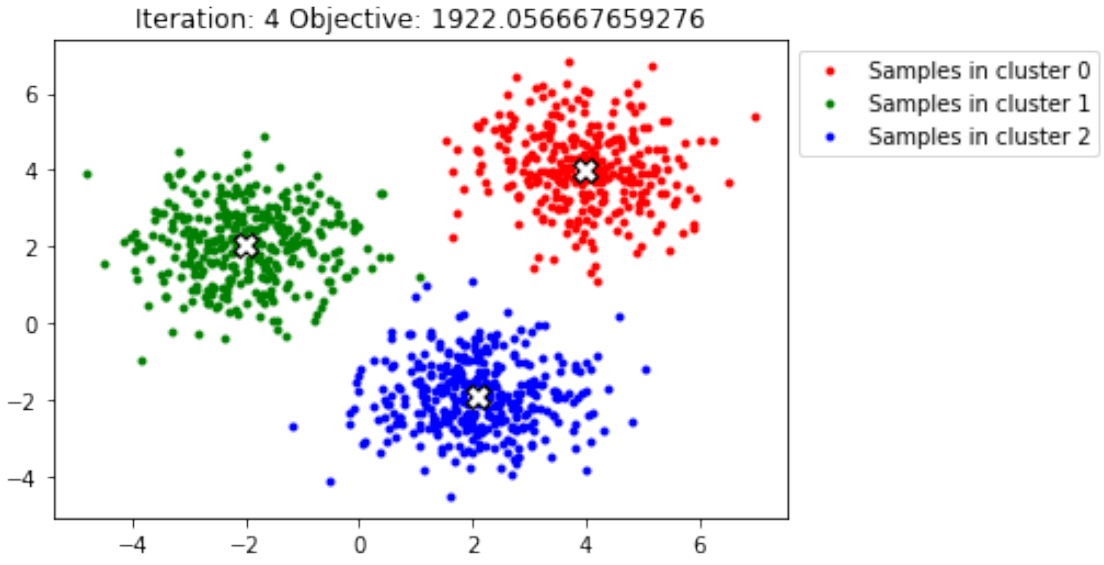
```
kmeans(xs,K=3,iterations=100,tolerance=1e-3);
```





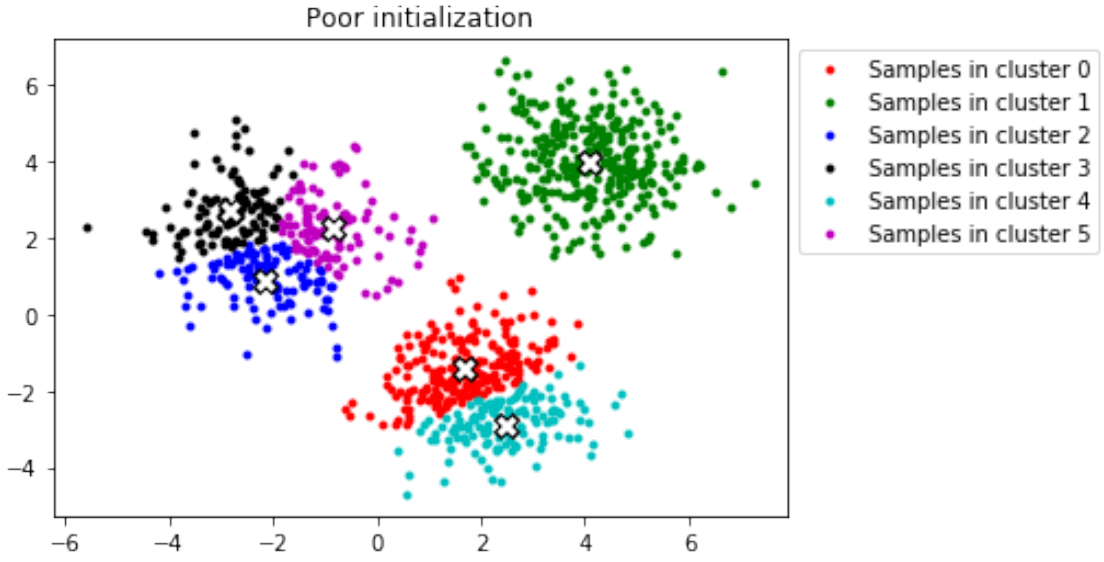

Iteration: 2 Objective: 1958.2157228667693
Samples in cluster 0
Samples in cluster 1
Samples in cluster 2
6
4
2
0
−2
−4
−4
−2
0
2
4
6


Iteration: 3 Objective: 1922.056667659276
Samples in cluster 0
Samples in cluster 1
Samples in cluster 2
6
4
2
0
−2
−4
−4
−2
0
2
4
6

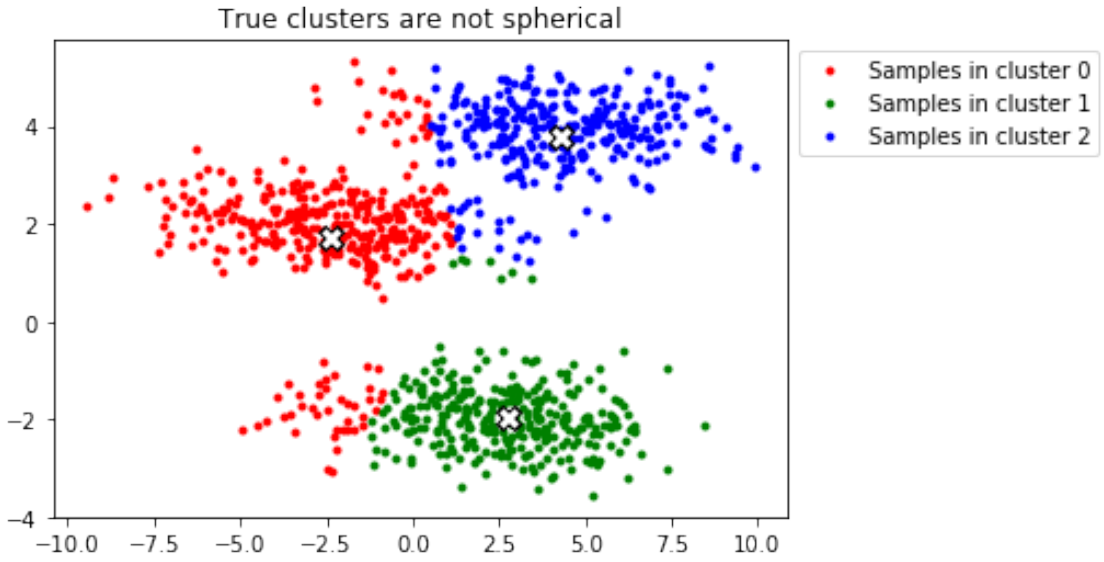


In [3]:
```
N = 1000 # 100 samples
K = 3    # 3 classes
d = 2    # x is 2d
proby = [1.0/K]*K # [1./3. , 1./3., 1./3.]
mus = 2.0*numpy.asarray([[-1.0,1.0,2],[1.0,-1.0,2.0]])

numpy.random.seed(6)
xs,ys = generate_data(N,d,K,proby,mus=mus)
kmeans(xs,K=6,iterations=30,tolerance=1e-7,just_last = True);
plt.title('Poor initialization')
```

Out[3]:
```
Text(0.5,1,'Poor initialization')
```



```
In [4]: numpy.random.seed(7)
        A = 1.4*numpy.random.randn(2,2)
        xs,ys = generate_data(N,d,K,proby,mus,A)
        kmeans(xs,K=3,iterations=10,tolerance=1e-3,just_last = True);
        plt.title('True clusters are not spherical');
```



5 K-means observations

1. Initialization is random -- means of the clusters are slightly preturbed versions of data mean.
2. Clusters are assumed to be spherical
3. Clusters can have zero members -- make sure there is no division with zero

   ```
   mus = numpy.dot(xs,ph.transpose())/(1e-5 + numpy.sum(ph,axis=1))
   ```

4. There are local minima

- Trivial: renaming of clusters
- Non-trivial: poor initialization, too small or too large K

5. Multiple restarts -- from different initializations -- can lead to better solutions

6 How do we come up with an algorithm such as K-means?

We will: 1. Write out a generative model for the data 2. Write out log-likelihood 3. Optimize log-likelihood

The twist compared to our previous model learning is in the fact that not all the variables are observed.

Labels, indicating cluster membership, are **hidden** from us.

7 Mixture models

Mixture models are suited to the data exhibit clusters.

Each cluster is called **mixture component**

Data is given to us as Data $= \{\mathbf{x}_t \mid t = 1, ...T\}$

We introduce a random variable h that tells us which cluster or mixture component the sample came from.

8 Mixture models -- generative story

Each sample $\mathbf{x}$ is generated by: 1. Selecting a cluster, according to some distribution $\pi = (\pi_1, ..., \pi_K)$

$$p(h) = \pi_h$$

2. Using parameters of cluster h generate the sample $\mathbf{x}$

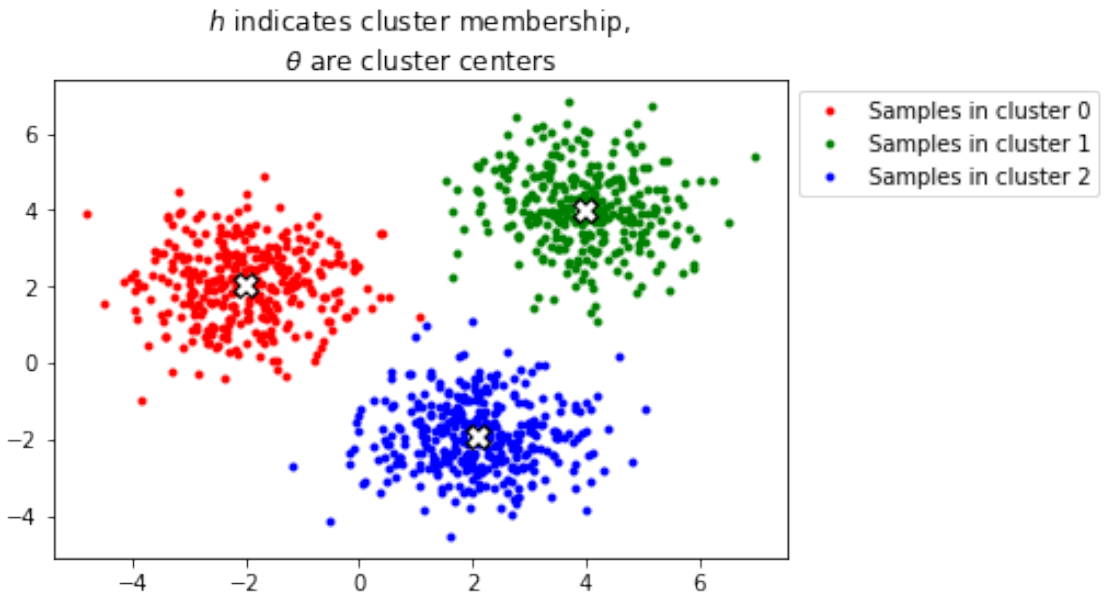
$$p(\mathbf{x} \mid h, \theta) = p(\mathbf{x} \mid \theta_h)$$

For example, you can think of θ_h as the mean of the cluster h

$$p(\mathbf{x} \mid \theta_h) = \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(x_i - \theta_{h,i})^2\right\}$$

```
In [5]: numpy.random.seed(1)
        xs,ys = generate_data(N,d,K,proby,mus)
        kmeans(xs,K=3,iterations=100,tolerance=1e-3,just_last=True);
        plt.title("$h$ indicates cluster membership,\n$\\theta$ are cluster centers")
```

```
Out[5]: Text(0.5,1,'$h$ indicates cluster membership,\n$\\theta$ are cluster centers')
```



9 Mixture models -- generative story

Note that generative model talks about how data might have been generated.

We want to fit a model under which that data is most probable.

To do so, we must write out log-likelihood

$$\mathcal{LL}(\Theta) = \sum_t \log p(\mathbf{x}_t \mid \Theta)$$

and maximize it with respect to parameters Θ.

10 Marginal Log-likelihood

For a single sample $\mathbf{x}$, we know how to compute $p(h)$ and $p(\mathbf{x} \mid h, \Theta)$ so we can obtain joint

$$p(\mathbf{x}, h \mid \Theta) = p(h)p(\mathbf{x} \mid h, \Theta).$$

This is probability of the full configuration $\mathbf{x}$ **and** cluster membership h.

Our data does not contain information about cluster membership, just vectors $\mathbf{x}$.

How do we compute $p(\mathbf{x} \mid \Theta)$?

11 Marginal Log-likelihood

We can use the fact that

$$p(\mathbf{x} \mid \Theta) = \sum_h p(\mathbf{x}, h \mid \Theta) = \sum_h p(h)p(\mathbf{x} \mid h, \Theta).$$

What is the interpretation of this sum?

12 Marginal Log-likelihood

Now, we can express log-likelihood in terms of probabilities in our model

$$\mathcal{LL}(\Theta) = \sum_t \log p(\mathbf{x}_t \mid \Theta) = \sum_{t=1}^{T} \log \sum_{h_t} p(\mathbf{x}_t, h_t \mid \Theta).$$

Observations 1. For each sample $\mathbf{x}_t$, we have corresponding cluster membership variable h_t 2. There is a sum under the log so we cannot push the log to probability terms

13 Dealing with difficult objectives

Typically, when we run into an objective that is difficult to work with (for example log of sums above), we seek a closely related objective that is easier.

Hence, we will not directly optimize the log-likelihood instead we will introduce a lower-bound on the log-likelihood which we will show is tight at the optimum.

To accomplish this we a bit of math that you may not be familar with 1. Convex and concave functions 2. Jensen's inequality

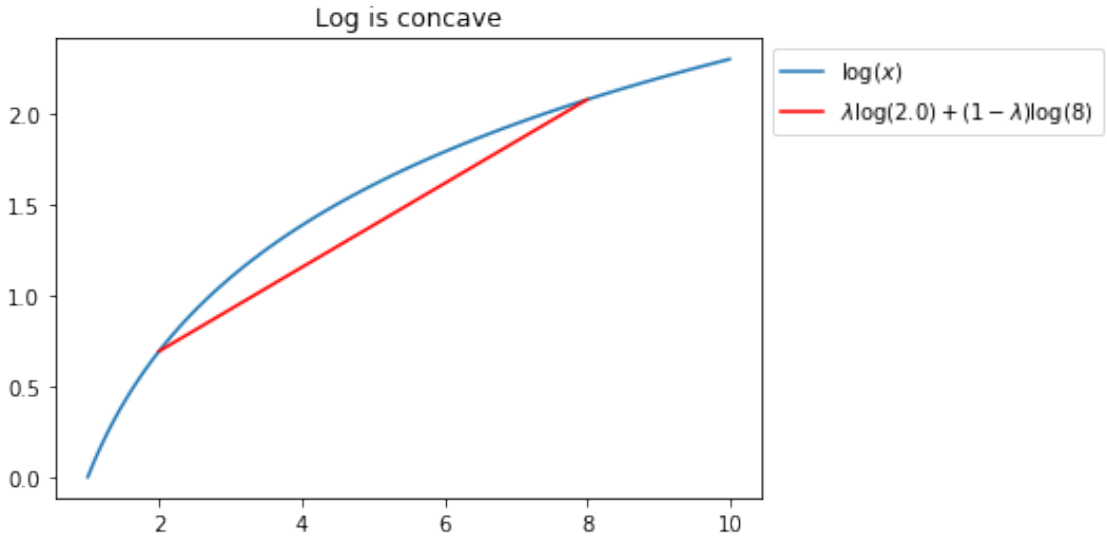
14 Concave functions

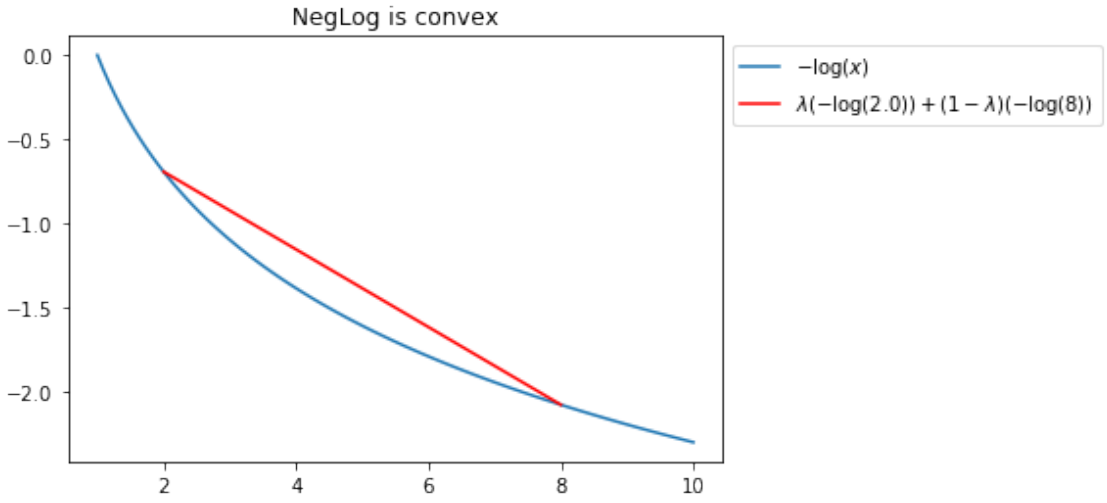
A function $f(x)$ is concave if

$$f(\lambda x + (1-\lambda)y) \geq \lambda f(x) + (1-\lambda) f(y)$$

for any $\lambda \in [0,1]$ Examples of concave functions are log, exp, square, etc.

```
In [6]: x = numpy.linspace(1.,10.0,100)
        px = [2.0,8.0]

        plt.plot(x,numpy.log(x),label ='$\log(x)$')
        plt.plot(px,numpy.log(px),'r',label = '$\lambda \log(2.0) + (1-\lambda) \log(8)$')
        plt.legend(loc=2, bbox_to_anchor=(1,1))
        plt.title('Log is concave')
        plt.figure()
        plt.plot(x,-numpy.log(x),label ='$-\log(x)$')
        plt.plot(px,-numpy.log(px),'r',label = '$\lambda (-\log(2.0)) + (1-\lambda) (-\log(8))$'
        plt.legend(loc=2, bbox_to_anchor=(1,1))
        plt.title('NegLog is convex')

Out[6]: Text(0.5,1,'NegLog is convex')
```





15 Jensen's inequality

Jensen's inequality

$$f(\mathbb{E}[H]) \geq \mathbb{E}[f(H)]$$

where

$$\mathbb{E}[H] = \sum_h p(H = h)h.$$

and f is concave.

16 Bounding log-likelihood

Starting with log-likelihood

$$\mathcal{LL}(\Theta) = \sum_t \log p(\mathbf{x}_t \mid \Theta) = \sum_{t=1}^{T} \log \sum_{h_t} p(\mathbf{x}_t, h_t \mid \Theta).$$

we introduce distributions $q_t(h_t)$ and multiply and divide by them

$$\begin{aligned}
\mathcal{LL}(\Theta) &= \sum_t \log p(\mathbf{x}_t \mid \Theta) = \sum_{t=1}^{T} \log \sum_{h_t} \frac{q_t(h_t)}{q_t(h_t)} p(\mathbf{x}_t, h_t \mid \Theta) \\
&= \sum_{t=1}^{T} \log \sum_{h_t} q_t(h_t) \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} \\
&= \sum_{t=1}^{T} \log \mathbb{E}_{q_t} \left[\frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} \right] \\
&\geq \sum_{t=1}^{T} \mathbb{E}_{q_t} \left[\log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} \right] \\
&= \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)}
\end{aligned}$$

17 Bounding log-likelihood

Starting with log-likelihood

$$\mathcal{LL}(\Theta) = \sum_t \log p(\mathbf{x}_t \mid \Theta) \geq \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} = \mathcal{B}(\Theta, q)$$

Natural questions that arise: 1. Where do we get q_ts? 2. Does optimizing bound result in the same Θ?

$$\operatorname*{argmax}_{\Theta} \mathcal{LL}(\Theta) \stackrel{?}{=} \operatorname*{argmax}_{\Theta} \mathcal{B}(\Theta, q)$$

18 Bounding log-likelihood

Before we start answering the questions we note that

$$\mathcal{LL}(\Theta) \geq \mathcal{B}(\Theta, q)$$

no matter which q_ts we choose so we can seek maximum of $\mathcal{B}(\Theta, q)$ with respect to a particular q_s and see what that gets us.

$$\operatorname*{argmax}_{q_s} \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} = \operatorname*{argmax}_{q_s} \underbrace{\sum_{h_s} q_s(h_s) \log \frac{p(h_s \mid \mathbf{x}_s, \Theta)}{q_s(h_s)}}_{\mathrm{KL}(q(h_s) || p(h_s | \mathbf{x}_s, \Theta)}$$

In words, optimal q_s is equal to $p(h_s \mid \mathbf{x}_s, \Theta)$, posterior probability of sample s's cluster membership.

19 Bounding log-likelihood

Further if we use optimal q_ts denoted by q_t^*

$$\mathcal{B}(\Theta, q^*) = \sum_{t=1}^{T} \sum_{h_t} p(h_t \mid \mathbf{x}_s, \Theta) \log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{p(h_t \mid \mathbf{x}_s, \Theta)} = \sum_{t=1}^{T} \log p(\mathbf{x}_t \mid \Theta) = \mathcal{LL}(\Theta)$$

Hence, if

$$q_t(h_t) = p(h_t \mid \mathbf{x}_t, \Theta)$$

the bound is tight.

20 Bounding log-likelihood

Natural questions that arise: * Where do we get q_ts? * A: We use posterior probabilities $p(h_t \mid \mathbf{x}_t, \Theta)$

- $\operatorname{argmax}_\Theta \mathcal{LL}(\Theta) \stackrel{?}{=} \operatorname{argmax}_\Theta \mathcal{B}(\Theta, q)$?
- A: Yes, if we use exact posterior probabilities in place of q_ts the two objectives coincide and optimal Θs are the same.

21 Expectation-Maximization (EM) algorithm

Hence we can maximize the bound $\mathcal{B}(\Theta)$ by iterating 1. (E-step) Computing the optimal

$$q_t^{\text{new}} = \operatorname*{argmax}_{q_t} \mathcal{B}(\Theta^{\text{old}}, q)$$

2. (M-step) Updating Θ given current $q_t(h_T)$

$$\Theta^{\text{new}} = \operatorname*{argmax}_{\Theta} \mathcal{B}(\Theta, q^{\text{new}})$$

Recall for a moment the K-means algorithm. It alternated analogous two steps: 1. Assigning each sample to a cluster 2. Cluster center computation based on assignments

22 Our first EM algorithm from scratch

The model

$$p(h) = \alpha_h$$
$$p(\mathbf{x} \mid h, \mu) = (2\pi)^{-\frac{d}{2}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \mu_h)^T(\mathbf{x} - \mu_h)\right\}$$

is a variant of ** Mixture of Gaussians. **

The bound

$$\begin{aligned}
\mathcal{B}(\Theta, q) &= \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \log \frac{p(\mathbf{x}_t, h_t \mid \Theta)}{q_t(h_t)} \\
&= \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \left[\log \alpha_{h_t} - \frac{d}{2} \log(2\pi) - \frac{1}{2}(\mathbf{x} - \mu_h)^T(\mathbf{x} - \mu_h)\right] \\
&- \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \log q_t(h_t)
\end{aligned}$$

In this case $\Theta = (\alpha_1, ..., \alpha_K, \mu_1, ..., \mu_K)$

23 Our first EM algorithm from scratch - E-step

The E-step

$$q_t(h_t = k) = p(h_t = k \mid \mathbf{x}_t, \mu) = \underbrace{\frac{p(\mathbf{x}_t, h_t = k \mid \mu)}{\sum_c p(\mathbf{x}_t, h_t = c \mid \mu)}}_{\text{same for all values of } k}$$

$$\propto p(\mathbf{x}_t, h_t = k \mid \mu)$$

$$= \alpha_{h_t} (2\pi)^{-\frac{d}{2}} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \mu_h)^T (\mathbf{x} - \mu_h) \right\}$$

24 E-step: Working in log-domain

If the data vectors are long, the computation of joint probabilities can yield very tiny probabilities.

Rather than working with probabilities we work with log-probabilities. Hence we store

$$\log q_t(h_t = k) = \log p(\mathbf{x}_t, h_t = k \mid \mu) - \log \sum_c p(\mathbf{x}_t, h_t = c \mid \mu)$$

If all the probabilities are stored in log-domain, then computation of their sum requires exponentation.

$$\log \sum_c p(\mathbf{x}_t, h_t = c \mid \mu) = \log \sum_c \exp \underbrace{\log p(\mathbf{x}_t, h_t = c \mid \mu)}_{\text{stored log-probability}}$$

```
In [7]: # Naive normalization
        # unnormalized log probability
        logp = numpy.array([-1000,-1000])
        # both should be equal to log(0.5) = -0.6931
        print("Incorrectly normalized probabilities:", logp - numpy.log(numpy.sum(numpy.exp(logp

        def logsumexp(vec):
            m = numpy.max(vec,axis=0)
            return numpy.log(numpy.sum(numpy.exp(vec-m),axis=0))+m

        # both should be equal to log(0.5) = -0.6931
        print("Correctly normalized probabilities:", logp - logsumexp(logp))

        # 2  x 3 , normalizing across the first dimension
        # all should be -0.69314
        logp = numpy.array([[-1000,+1000,-1000],[-1000,+1000,-1000]])
        print("Before column normalization:")
        print(logp)
        print("After column normalization:")
        print(logp - logsumexp(logp))
```

```
Incorrectly normalized probabilities: [ inf  inf]
Correctly normalized probabilities: [-0.69314718 -0.69314718]
Before column normalization:
[[-1000  1000 -1000]
 [-1000  1000 -1000]]
After column normalization:
[[-0.69314718 -0.69314718 -0.69314718]
 [-0.69314718 -0.69314718 -0.69314718]]


/Users/jgs/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:5: RuntimeWarning: divide
  """
```

25 E-step: Implementation

Given a function that computes $\log p(\mathbf{x}, h|\Theta)$ for all samples and all classes called `logjointp(x,Theta)`

```
q = numpy.zeros((K,N)) # clusters x samples
q = logjointp(x,Theta) # compute all joints at once
q = q - logsumexp(q)   # normalizing across clusters
```

26 M-step: Deriving updates

In M-step we optimize Θ given qs

$$\Theta^{\text{new}} = \operatorname*{argmax}_{\Theta} \mathcal{B}(\Theta, q^{\text{new}})$$

In general, we can take derivatives, equate them to zero, and solve:

$$\nabla_{\Theta} \mathcal{B}(\Theta, q^{\text{new}}) = 0$$

Relevant parts of the bound are

$$\sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \left[\log \alpha_{h_t} - \frac{1}{2} (\mathbf{x} - \mu_h)^T (\mathbf{x} - \mu_h) \right]$$

In case of αs we need to enforce the constraint that

$$\sum_c \alpha_c - 1 = 0.$$

27 M-step: Details of deriving α update

We need to solve the problem

$$\operatorname*{argmax}_{\alpha, \sum_c \alpha_c - 1 = 0} \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \left[\log \alpha_{h_t} - \frac{1}{2} (\mathbf{x} - \mu_h)^T (\mathbf{x} - \mu_h) \right]$$

This is acomplished by formulating a {**Lagrangian**}

$$L(\alpha, \lambda) = \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \left[\log \alpha_{h_t} - \frac{1}{2}(\mathbf{x} - \mu_h)^T (\mathbf{x} - \mu_h) \right] - \lambda \left(\underbrace{\sum_c \alpha_c - 1}_{\textbf{constraint}} \right).$$

We call λ Lagrange multiplier. It The optimality conditions for this problem are given by

$$\frac{\partial}{\partial_{\alpha_c}} L(\alpha, \lambda) = 0 \quad c \in \{1, ..., K\}$$
$$\frac{\partial}{\partial_{\lambda}} L(\alpha, \lambda) = 0$$

We will work this out on the board.

$$\alpha_c^* = \frac{\sum_t q_t(h_t = c)}{N}$$

28 An aside: Interpretation of the Lagrange multiplier

Constrainted optimization problems such as

$$\begin{array}{ll} \textbf{maximize}_x & f(x) \\ \textbf{subject to} & Ax = b \end{array}$$

are solved by constructing a Lagrangian function

$$L(x, \lambda) = f(x) - \lambda^T (Ax - b)$$

λ is a vector of multipliers which are adjusted so that the optimal solution of $L(x, \lambda)$ satisfies the constraint.

We can think of Lagrange multipliers λ as a price that you need to pay if you violate the constraint.

29 M-step: Details of deriving μ update

$$\mu_c^* = \underset{\mu_c}{\textbf{argmax}} \sum_{t=1}^{T} \sum_{h_t} q_t(h_t) \left[\log \alpha_{h_t} - \frac{1}{2}(\mathbf{x} - \mu_h)^T (\mathbf{x} - \mu_h) \right]$$

Take a gradient of the bound

$$\nabla_{\mu_c} \mathcal{B}(\Theta, q) = \sum_t q_t(c)(\mathbf{x}_t - \mu_c)$$

and equate it to zero

$$\sum_t q_t(c)(\mathbf{x}_t - \mu_c) = 0$$

to obtain

$$\mu_c^* = \frac{\sum_t q_t(c) \mathbf{x}_t}{\sum_t q_t(c)}$$

Reference: For all matrix calculus tricks http://www.ee.ic.ac.uk/hp/staff/dmb/matrix/intro.html

30 M-step: implementation

For our model -- mixture of Gaussians -- M-step updates μs an αs, given current q

$$\mu_c^* = \frac{\sum_t q_t(c)\mathbf{x}_t}{\sum_t q_t(c)}$$
$$\alpha_c^* = \frac{\sum_t q_t(h_t = c)}{N}$$

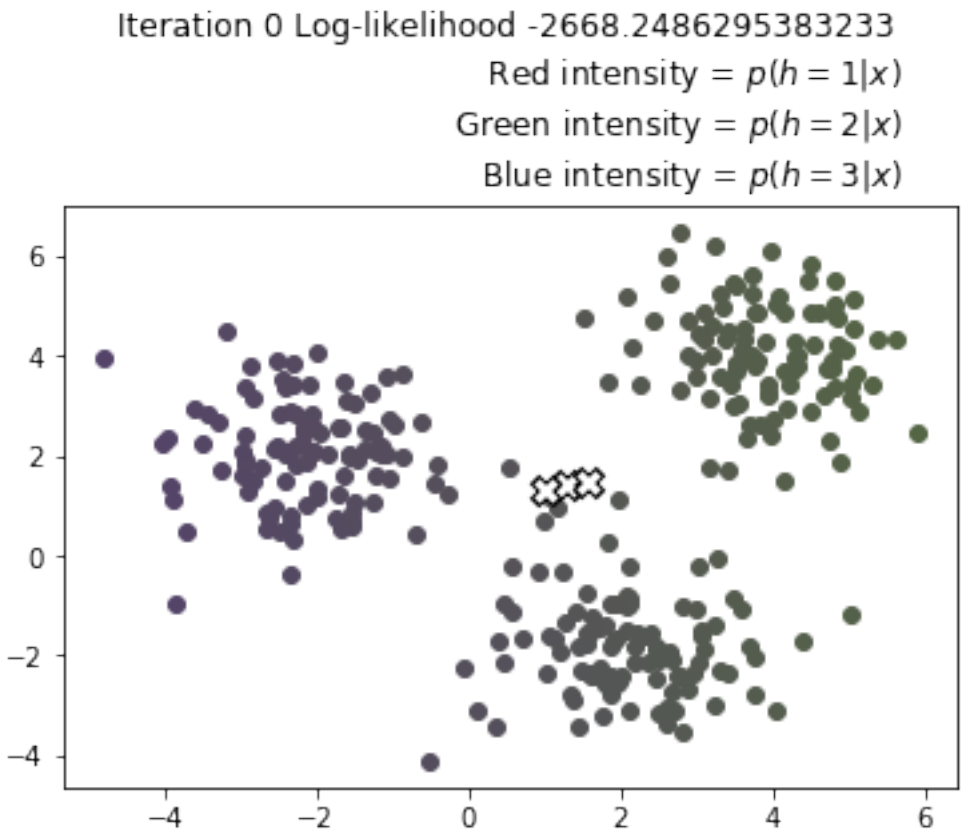
```
mus = numpy.dot(xs,q.transpose())/(1e-5 + numpy.sum(q,axis=1))
alpha = numpy.sum(q,axis=1)/N
```

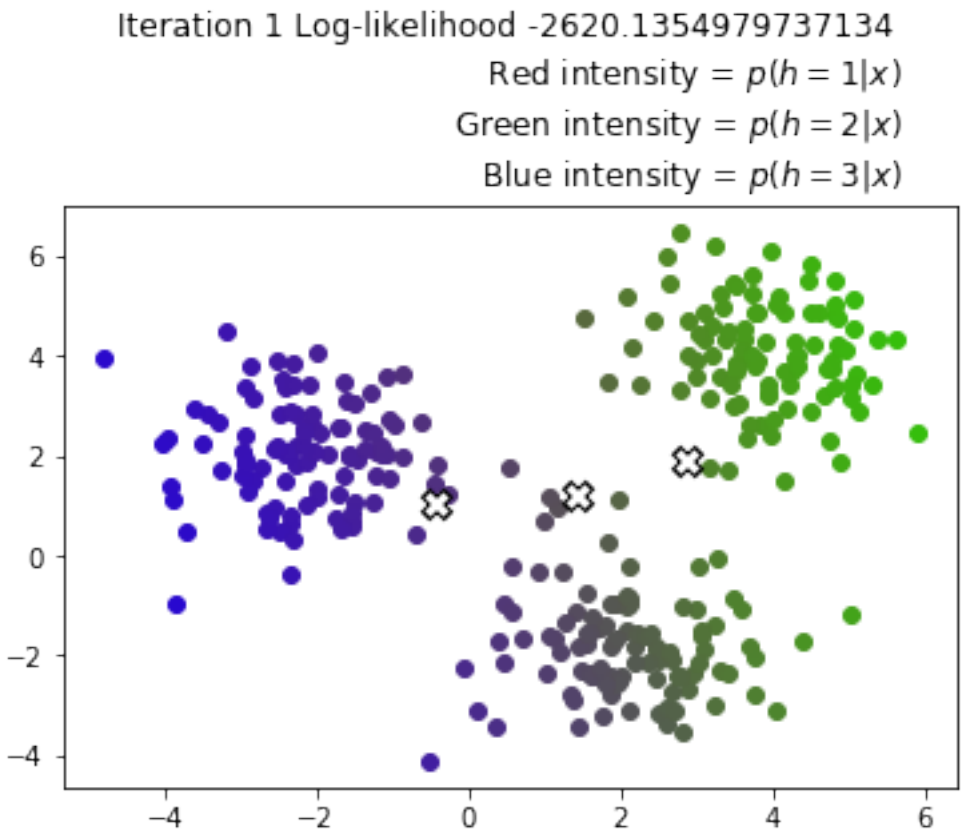
Note that `xs` **is of size** $d \times N$**,** `q` **is of size** $K \times N$**, hence** * `numpy.dot(xs,q.tranpose())` **computes** $\sum_t q_t(c)\mathbf{x}_t$ * `numpy.sum(q,axis=1)` **computes** $\sum_t q_t(c)$

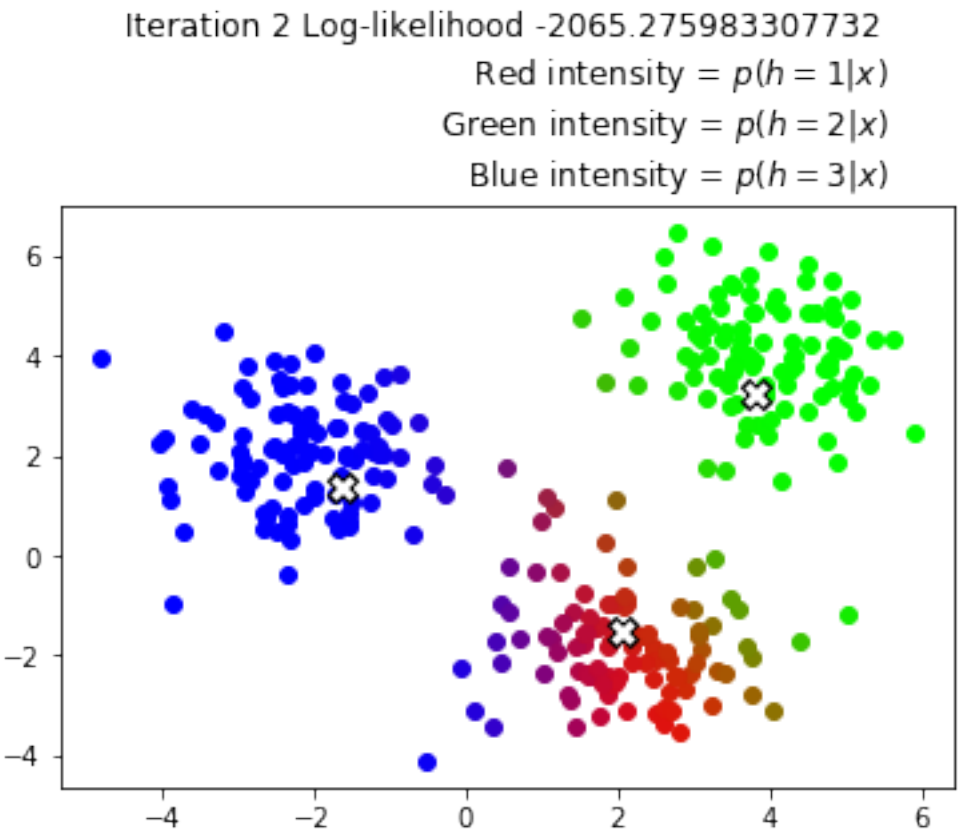
```
In [14]: def mog(xs,K,iterations=10, visualize=False):
             d,N = xs.shape
             # compute mean and std of data, and convert to
             # column vectors using numpy.newaxis trick.
             data_mean = numpy.mean(xs,axis=1)[:,numpy.newaxis]
             data_std = numpy.std(xs,axis=1)[:,numpy.newaxis]
             # initialize means around the data mean but
             # ensure they are not exactly the same by adding
             # small amount of noise
             mus = data_mean + 0.01*data_std*numpy.random.randn(d,K)
             xs_sq = numpy.sum(xs**2.0,axis=0)

             logalphas = numpy.array([-numpy.log(K)]*K)

             logconst = -(d/2.0)*numpy.log(2.0*numpy.pi)
             logliks = []
             for it in range(iterations):
                 #E-step:
                 mus_sq = numpy.sum(mus**2.0,axis=0)[:,numpy.newaxis]
                 mus_xs = numpy.dot(mus.transpose(),xs)
                 # compute log p(x,h) for all samples
                 q = logalphas[:,numpy.newaxis] + logconst - 0.5*(mus_sq - 2.0*mus_xs + xs_sq)

                 # loglikelihood is equal to sum(logsumexp(log(p(x,h))))
                 loglik = numpy.sum(logsumexp(q))

                 logliks.append(loglik)
                 # normalize columns to get log(p(h|x)) for all samples
                 q = numpy.exp(q - logsumexp(q))

                 # M-step:

                 mus = numpy.dot(xs,q.transpose())/(1e-5 + numpy.sum(q,axis=1))
                 logalphas = numpy.log(numpy.sum(q,axis=1)/N)
```

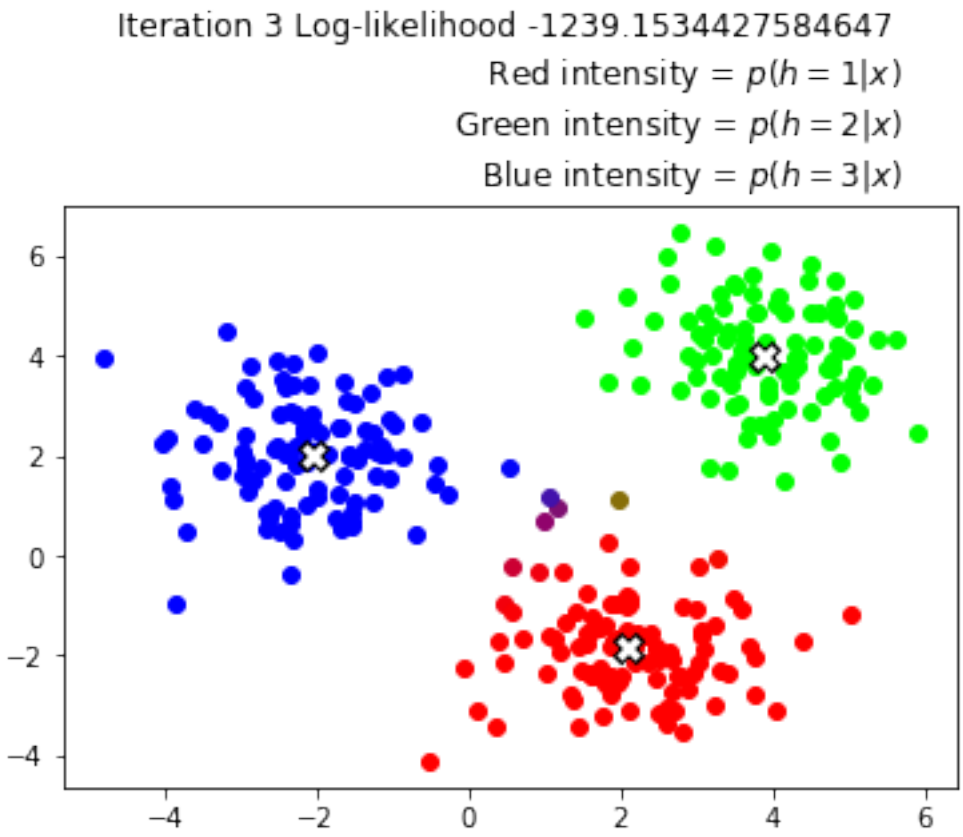
```
                if visualize:
                    print("Iteration: {} Log-likelihood: {} ".format(it,loglik))
                    plt.figure()
                    plot_samples_post(xs,q,mus)
                    plt.title(('Iteration {} Log-likelihood {} \n '+
                               'Red intensity = $p(h=1|x)$\nGreen intensity = $p(h=2|x)$\nBlue
                                multialignment='right')

            plt.figure()
            plt.plot(logliks)
            plt.xlabel('Iterations')
            plt.ylabel('Log-likelihood')
            alphas = numpy.exp(logalphas)
            return mus,alphas,q
        N = 300
        d = 2
        K = 3
        proby = [1./K]*K
        mus = 2.0*numpy.asarray([[-1.0,1.0,2],[1.0,-1.0,2.0]])
        numpy.random.seed(1)
        xs,ys = generate_data(N,d,K,proby,mus)

        mog(xs,3,iterations=5,visualize=True);
```

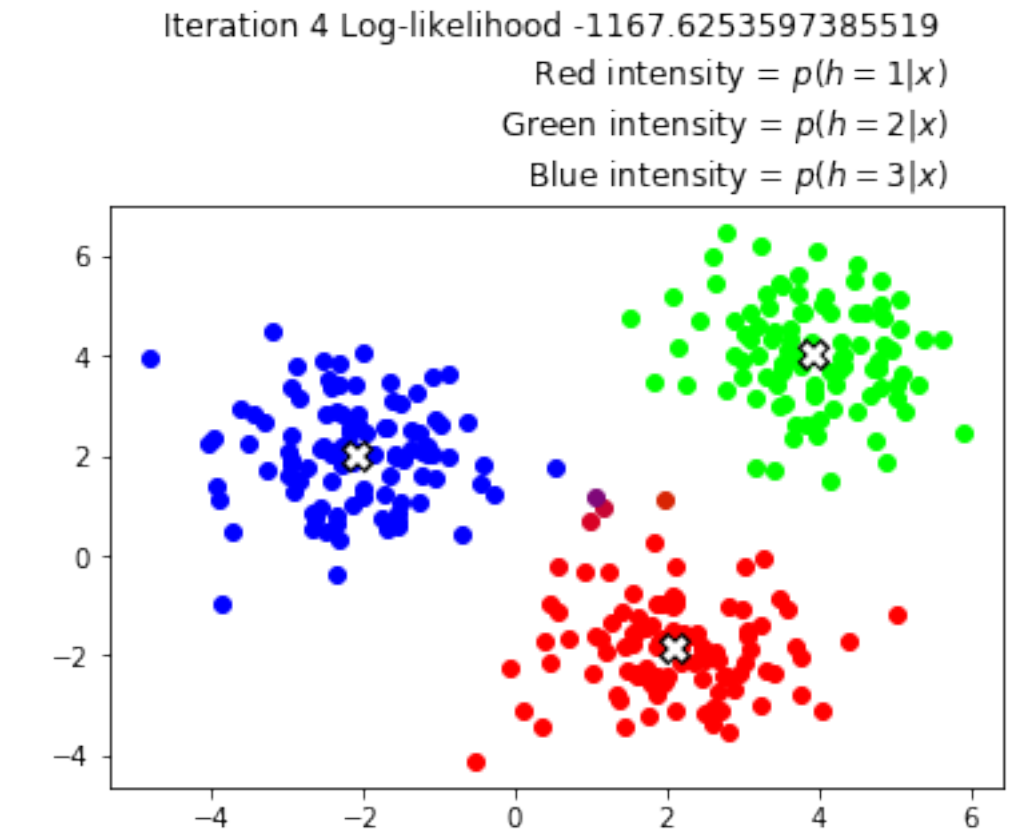
```
Iteration: 0 Log-likelihood: -2668.2486295383233
Iteration: 1 Log-likelihood: -2620.1354979737134
Iteration: 2 Log-likelihood: -2065.275983307732
Iteration: 3 Log-likelihood: -1239.1534427584647
Iteration: 4 Log-likelihood: -1167.6253597385519
```

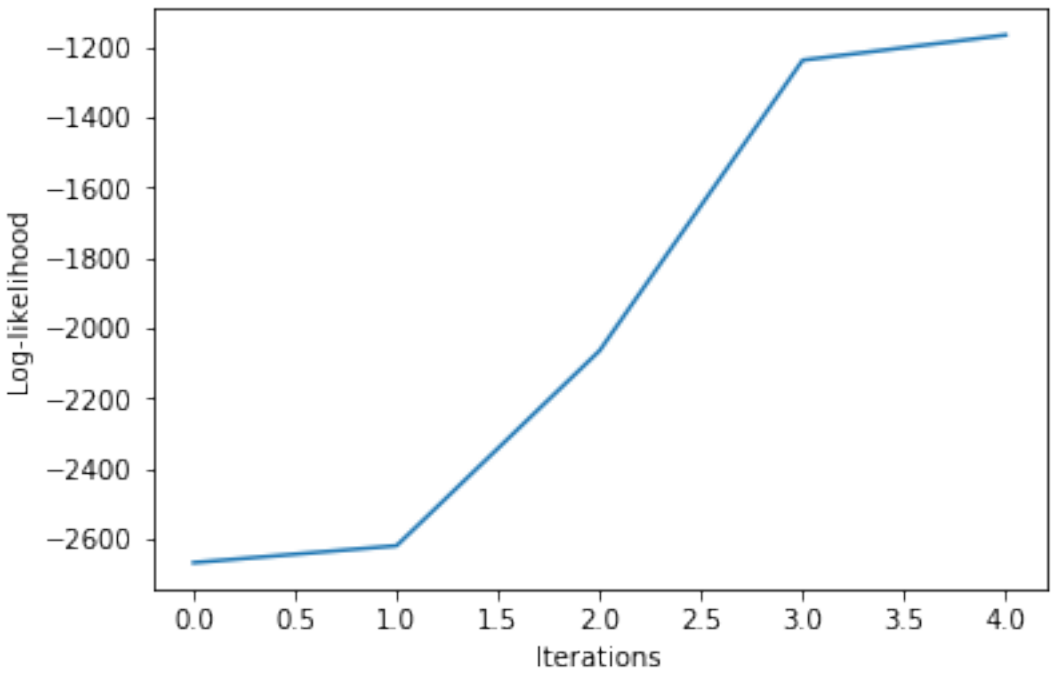

Iteration 0 Log-likelihood -2668.2486295383233
Red intensity = $p(h = 1|x)$
Green intensity = $p(h = 2|x)$
Blue intensity = $p(h = 3|x)$
6
4
2
0
−2
−4
−4
−2
0
2
4
6


Iteration 1 Log-likelihood -2620.1354979737134
Red intensity = $p(h = 1|x)$
Green intensity = $p(h = 2|x)$
Blue intensity = $p(h = 3|x)$
6
4
2
0
−2
−4
−4
−2
0
2
4
6

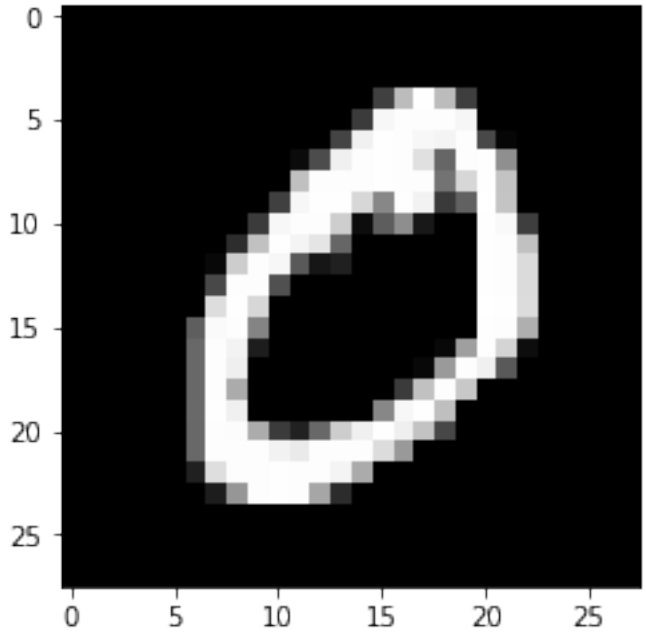

Iteration 2 Log-likelihood -2065.275983307732
Red intensity = $p(h = 1|x)$
Green intensity = $p(h = 2|x)$
Blue intensity = $p(h = 3|x)$
6
4
2
0
−2
−4
−4
−2
0
2
4
6

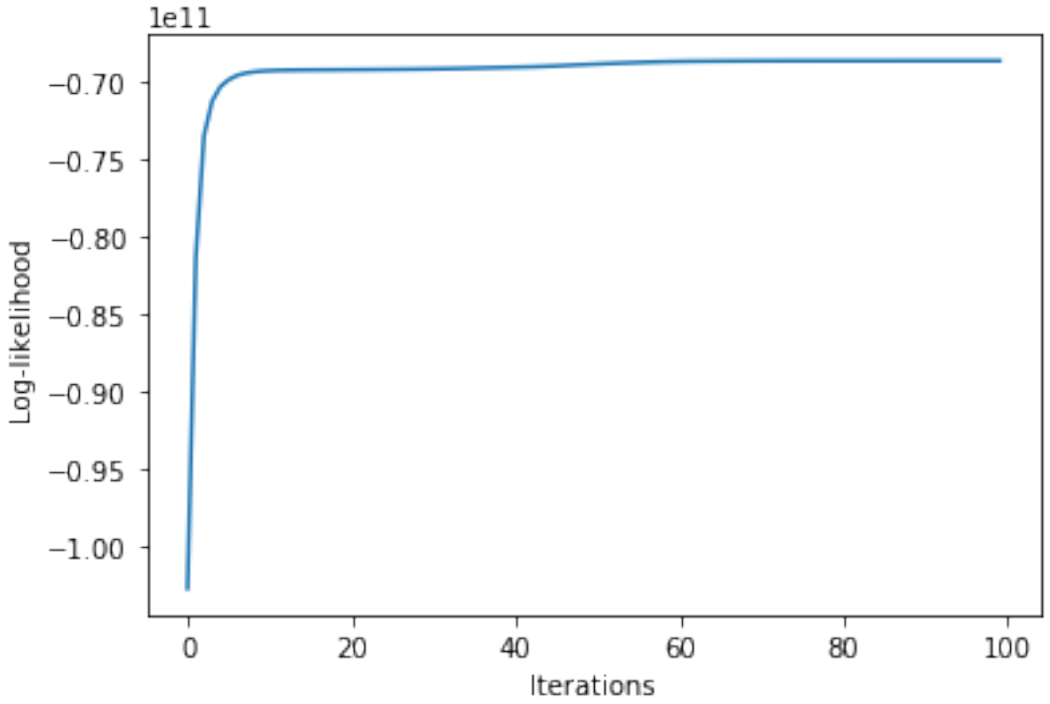

Iteration 3 Log-likelihood -1239.1534427584647
Red intensity = $p(h = 1|x)$
Green intensity = $p(h = 2|x)$
Blue intensity = $p(h = 3|x)$
6
4
2
0
−2
−4
−4
−2
0
2
4
6


Iteration 4 Log-likelihood -1167.6253597385519
Red intensity = $p(h = 1|x)$
Green intensity = $p(h = 2|x)$
Blue intensity = $p(h = 3|x)$
6
4
2
0
−2
−4
−4
−2
0
2
4
6


Log-likelihood
−1200
−1400
−1600
−1800
−2000
−2200
−2400
−2600
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Iterations

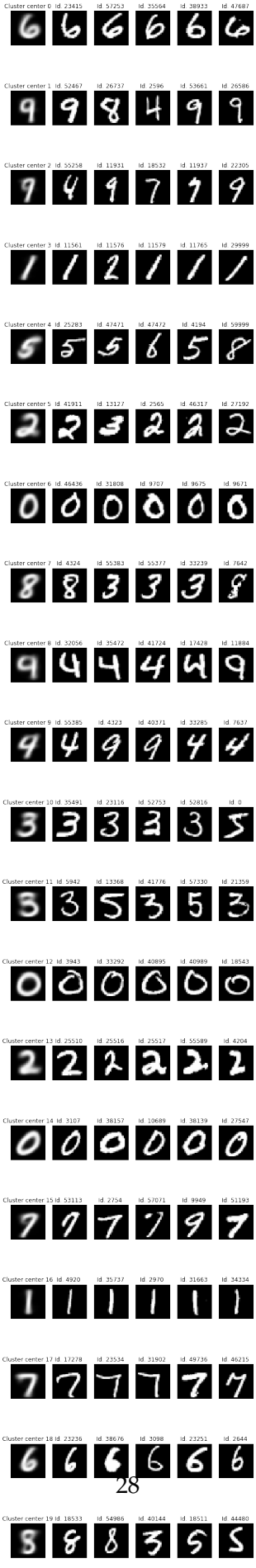
```
In [15]: import os, struct
         from array import array as pyarray
         from numpy import append, array, int8, uint8, zeros

         def load_mnist(dataset="training", digits=numpy.arange(10), path="."):
             if dataset == "training":
                 fname_img = os.path.join(path, 'train-images-idx3-ubyte')
                 fname_lbl = os.path.join(path, 'train-labels-idx1-ubyte')
             elif dataset == "testing":
                 fname_img = os.path.join(path, 't10k-images-idx3-ubyte')
                 fname_lbl = os.path.join(path, 't10k-labels-idx1-ubyte')
             else:
                 raise ValueError("dataset must be 'testing' or 'training'")

             flbl = open(fname_lbl, 'rb')
             magic_nr, size = struct.unpack(">II", flbl.read(8))
             lbl = pyarray("b", flbl.read())
             flbl.close()

             fimg = open(fname_img, 'rb')
             magic_nr, size, rows, cols = struct.unpack(">IIII", fimg.read(16))
             img = pyarray("B", fimg.read())
             fimg.close()

             ind = [ k for k in range(size) if lbl[k] in digits ]
             N = len(ind)

             images = zeros((N, rows, cols), dtype=uint8)
             labels = zeros((N, 1), dtype=int8)
             for i in range(len(ind)):
                 images[i] = array(img[ ind[i]*rows*cols : (ind[i]+1)*rows*cols ]).reshape((rows
                 labels[i] = lbl[ind[i]]

             return images, labels

         images,_ = load_mnist()

In [17]: plt.imshow(images[1,:,:],interpolation='None',cmap='Greys_r')
         sz = images.shape
         xs = numpy.reshape(images,(sz[0],sz[1]*sz[2])).transpose()

         means,alphas,qs = mog(xs,20,100)
```






```
In [18]: def show_digit(x):
             im = numpy.reshape(x,[28,28])
```

```
    plt.imshow(im,interpolation='None',cmap='Greys_r')
    plt.axis('off')

plt.figure(figsize=(9,60))
for k in range(20):
    plt.subplot(20,6,k*6+1)
    show_digit(means[:,k])
    plt.title('Cluster center {}'.format(k))
    lst = numpy.argsort(qs[k,:])[-5:]
    for j in range(5):
        plt.subplot(20,6,k*6+j+2)
        show_digit(xs[:,lst[j]])
        plt.title('Id. {} '.format(lst[j]))
```


Cluster center 0 Id: 23415 Id: 57253 Id: 35564 Id: 38933 Id: 47687
Cluster center 1 Id: 52467 Id: 26737 Id: 2596 Id: 52661 Id: 26586
Cluster center 2 Id: 55258 Id: 11931 Id: 18532 Id: 11937 Id: 22305
Cluster center 3 Id: 11561 Id: 11576 Id: 11579 Id: 11765 Id: 29999
Cluster center 4 Id: 25283 Id: 47471 Id: 47472 Id: 4194 Id: 59999
Cluster center 5 Id: 41911 Id: 13127 Id: 2565 Id: 46317 Id: 27192
Cluster center 6 Id: 46436 Id: 31808 Id: 9707 Id: 9675 Id: 9671
Cluster center 7 Id: 4324 Id: 55383 Id: 55377 Id: 33239 Id: 7642
Cluster center 8 Id: 32056 Id: 35472 Id: 41724 Id: 17428 Id: 11884
Cluster center 9 Id: 55385 Id: 4323 Id: 40371 Id: 33285 Id: 7637
Cluster center 10 Id: 35491 Id: 23116 Id: 52753 Id: 52816 Id: 0
Cluster center 11 Id: 5942 Id: 13368 Id: 41776 Id: 57330 Id: 21359
Cluster center 12 Id: 3943 Id: 33292 Id: 40895 Id: 40989 Id: 18543
Cluster center 13 Id: 25510 Id: 25516 Id: 25517 Id: 55589 Id: 4204
Cluster center 14 Id: 3107 Id: 38157 Id: 10689 Id: 38139 Id: 27547
Cluster center 15 Id: 53113 Id: 2754 Id: 57071 Id: 9949 Id: 51193
Cluster center 16 Id: 4920 Id: 35737 Id: 2970 Id: 31663 Id: 34334
Cluster center 17 Id: 17278 Id: 23534 Id: 31902 Id: 49736 Id: 46215
Cluster center 18 Id: 23236 Id: 38676 Id: 3098 Id: 23251 Id: 2644
Cluster center 19 Id: 18533 Id: 54986 Id: 40144 Id: 18511 Id: 44480

31 Video of parameter changes during learning

32 Covered

- **Mixture models**
- **EM algorithm**
- **K-means**