CSCI-567: Assignment #5

Due on Tueday, November 17, 2015(One late day used)

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Contents

Problem 1

Problem 1: (a)

To find $\nabla_{y_t} L$:

$$\begin{aligned}
\nabla_{y_t} L &= \frac{\partial}{\partial y_t} \frac{1}{2} \sum_{i=1}^{N} (y_i - \hat{y_i})^T (y_i - \hat{y_i}) \\
&= \frac{\partial}{\partial y_t} \frac{1}{2} \sum_{i=1}^{N} (y_i^T y_i - 2 y_i^T \hat{y_i} + \hat{y_t}^2) \\
&= \frac{1}{2} (2y_t - 2\hat{y_t}) \\
&= y_t - \hat{y_t}
\end{aligned}$$

$$\boxed{\nabla_{y_t} L = y_t - \hat{y_t}}$$

Problem 1: (b)

To find $\nabla_{y_t} L$:

$$\nabla_{s_t} L = \sum_{k=1}^{T} \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t}$$

Let's define $z_t = W_{IH} x_t + W_{HH} s_{t-1}$
Thus,

$$\begin{aligned} z_k &= W_{IH} x_k + W_{HH} s_{k-1} \\ s_k &= \sigma(z_k) \\ y_k &= W_{HO} s_k \end{aligned}$$

Thus,

$$\frac{\partial y_k}{\partial s_k} = W_{HO} \tag{1}$$
$$\frac{\partial s_k}{\partial z_k} = \sigma(z_k)(1 - \sigma(z_k)) \tag{2}$$
$$\frac{\partial z_k}{\partial W_{IH}} = x_k \tag{3}$$
$$\frac{\partial y_k}{\partial W_{HH}} = y_{k-1} \tag{4}$$
$$\frac{\partial z_k}{\partial s_{k-1}} = W_{HH} \tag{5}$$
$$\frac{\partial s_k}{\partial s_{k-1}} = \frac{\partial s_k}{\partial z_k} \frac{\partial z_k}{\partial s_{k-1}} = \sigma(z_k)(1 - \sigma(z_k)) W_{HH} \tag{6}$$

Let's now consider $\frac{\partial s_k}{\partial s_t}$:
s_k depends on $s_{k-1}, s_{k-2}, \dots s_1$. And hence:

$$\frac{\partial s_k}{\partial s_t} = 0 \ \forall \ k < t$$

For $k \geq t$:

$$\frac{\partial s_k}{\partial s_t} = \frac{\partial s_k}{\partial s_{k-1}} \times \frac{\partial s_{k-1}}{\partial s_{k-2}} \times \frac{\partial s_{k-2}}{\partial s_{k-3}} \times \dots \frac{\partial s_{k-(k-t)+1}}{\partial s_{k-(k-t)}}$$

Thus, consider a special case of $t = T$:

$$\begin{aligned} \nabla_{s_T} L &= \sum_{k=T}^{T} \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t} \\ &= \frac{\partial L}{\partial y_T} \times \frac{\partial y_T}{\partial s_T} \\ &= (y_T - \hat{y_T}) W_{HO} \end{aligned}$$

Thus,

$$\boxed{\nabla_{S_T} L = (y_T - \hat{y_T}) W_{HO}}$$

Problem 1 [Problem 1: (b)] continued on next page...

Let's consider $\nabla_{s_t} L$ and $\nabla_{s_{t+1}} L$:

$$\nabla_{s_{t+1}} L = \sum_{k=t+1}^{T} \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t}$$

$$\nabla_{s_t} L = \sum_{k=t}^{T} \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t}$$

$$\implies \nabla_{s_t} L = \nabla_{s_{t+1}} L + \frac{\partial L}{\partial y_t} \times \frac{\partial y_t}{\partial s_t} \times \frac{\partial s_t}{\partial s_t}$$

$$\implies \nabla_{s_t} L = \nabla_{s_{t+1}} L + (y_t - \hat{y_t}) W_{HO}$$

Thus,

$$\boxed{\nabla_{s_t} L = \nabla_{s_{t+1}} L + (y_y - \hat{y_t}) W_{HO}}$$

Problem 1: (c)

$$\nabla_{W_{IH}} L = \sum_{k=1}^{T} \big(\frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k}\big) \times \frac{\partial s_k}{\partial z_k} \times \frac{\partial z_k}{\partial W_{IH}}$$

$$= \sum_{k=1}^{T} (y_k - \hat{y_k}) W_{HO} \times \sigma(z_k)(1 - \sigma(z_k)) \times x_k$$

Thus,

$$\nabla_{W_{IH}} L = \sum_{k=1}^{(} y_k - \hat{y_k}) W_{HO} \times \sigma(z_k)(1 - \sigma(z_k)) \times x_k$$

where $\nabla_{s_k} L = \nabla_{s_{k+1}} L + (y_k - \hat{y_k}) W_{HO}$

and $z_k = W_{IH} x_k + W_{HH} s_{k-1}$

boundary condition $\nabla_{S_T} L = (y_T - \hat{y_T}) W_{HO}$

$$\nabla_{W_{HH}} L = \sum_{k=1}^{T} \big(\frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k}\big) \times \frac{\partial s_k}{\partial z_k} \times \frac{\partial z_k}{\partial W_{HH}}$$

$$= \sum_{k=1}^{T} (y_k - \hat{y_k}) W_{HO} \times \sigma(z_k)(1 - \sigma(z_k)) \times s_{k-1}$$

Thus,

$$\nabla_{W_{IH}} L = \sum_{k=1}^{T} (y_k - \hat{y_k}) W_{HO} \times \sigma(z_k)(1 - \sigma(z_k)) \times s_{k-1}$$

where $\nabla_{s_k} L = \nabla_{s_{k+1}} L + (y_k - \hat{y_k}) W_{HO}$

and $z_k = W_{IH} x_k + W_{HH} s_{k-1}$

boundary condition $\nabla_{S_T} L = (y_T - \hat{y_T}) W_{HO}$

$$\nabla_{W_{HO}} L = \sum_{k=1}^{T} \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial W_{HO}}$$
$$= \sum_{k=1}^{T} (y_k - \hat{y_k}) s_k$$

Thus,

$$\nabla_{W_{HO}} L = \sum_{k=1}^{T} (y_k - \hat{y_k}) s_k$$

Problem 1: (d)

Leaky hidden units:

$$s_t = (1 - \tau) s_{t-1} + \tau \sigma(z_t)$$

Thus,

$$\frac{\partial s_t}{\partial s_{t-1}} = 1 - \tau + \tau \sigma(z_t)(1 - \sigma(z_t)) W_{HH}$$
$$\frac{\partial s_t}{\partial z_t} = \tau \sigma(z_t)(1 - \sigma(z_t))$$

For $\nabla_{W_{IH}} L$,

$$\nabla_{W_{IH}} L = \sum_{k=1}^{T} \big(\frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k}\big) \times \frac{\partial s_k}{\partial z_k} \times \frac{\partial z_k}{\partial W_{IH}}$$
$$= \sum_{k=1}^{T} (y_k - \hat{y_k}) W_{HO} \times \tau \sigma(z_k)(1 - \sigma(z_k)) \times x_k$$

For $\nabla_{W_{HH}} L$,

$$\nabla_{W_{IH}} L = \sum_{k=1}^{T} \big(\frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k}\big) \times \frac{\partial s_k}{\partial z_k} \times \frac{\partial z_k}{\partial W_{HH}}$$
$$= \sum_{k=1}^{T} (y_k - \hat{y_k}) W_{HO} \times \tau \sigma(z_k)(1 - \sigma(z_k)) \times s_{k-1}$$

For $\nabla_{W_{HO}} L$,

$$\nabla_{W_{HO}} L = \sum_{k=1}^{T} (y_k - \hat{y_k}) s_k$$
$$= \sum_{k=1}^{T} (y_k - \hat{y_k})((1 - \tau) s_{k-1} + \tau \sigma(z_k))$$

Problem 2

Problem 2: (a)

$$\tilde{D} = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}||\phi(x_n) - \tilde{\mu_k}||^2$$

where

$$\tilde{\mu_k} = \frac{\sum_{i=1}^{N} r_{ik}\phi(x_i)}{\sum_{i=1}^{N} r_{ik}}$$

Consider, $||\phi(x_n) - \tilde{\mu_k}||^2$

$$\begin{aligned}
||\phi(x_n) - \tilde{\mu_k}||^2 &= (\phi(x_n) - \tilde{\mu_k})^T(\phi(x_n) - \tilde{\mu_k}) \\
&= \phi(x_n)^T\phi(x_n) - 2\tilde{\mu}^T\phi(x_n) + \tilde{\mu}^T\tilde{\mu} \\
&= \phi(x_n)^T\phi(x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}\phi(x_i)^T\phi(x_n)}{\sum_{i=1}^{N} r_{ik}} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}\phi(x_i)^T\phi(x_j)}{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}}
\end{aligned}$$

Define $n_k = \sum_{i=1}^{N} r_{ik}$, so that it simplifies to:

$$\begin{aligned}
||\phi(x_n) - \tilde{\mu_k}||^2 &= \phi(x_n)^T\phi(x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}\phi(x_i)^T\phi(x_n)}{n_k} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}\phi(x_i)^T\phi(x_j)}{n_k^2} \\
&= K(x_n, x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}K(x_i, x_n)}{n_k} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}K(x_i, x_j)}{n_k^2}
\end{aligned}$$

Thus,

$$\tilde{D} = \sum_{n=1}^{N} K(x_n, x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}K(x_i, x_n)}{n_k} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}K(x_i, x_j)}{n_k^2}$$

Problem 2: (b)

1. For given point x_n calculate $K(x_n, x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}K(x_i, x_n)}{n_k} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}K(x_i, x_j)}{n_k^2}$ for all possible clusters k
2. Assign cluster to point x_n using:

$$r_{nk} = \begin{cases} 1 & k = \arg\min_k ||\phi(x_n) - \tilde{u_k}||_2^2 \\ 0 & \text{otherwise} \end{cases}$$

where

$$K(x_n, x_n) - 2\frac{\sum_{i=1}^{N} r_{ik}K(x_i, x_n)}{n_k} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} r_{ik}r_{jk}K(x_i, x_j)}{n_k^2}$$

and $n_k = \sum_{i=1}^{N} r_{ik}$

Problem 2 continued on next page...

Problem 2: (c)

Algorithm 1 Kernel k means

procedure KERNEL K MEANS
    mu[i] = x(random(1..N)) for $1 \leq i \leq k$ ▷ initialise cluster centroids[1..k] randomly choosing any k points of N (Sample without replacement)
    for i **do**:1 to N
        for j **do**:1 to N K[i,j] = $\phi(x_i)\phi(x_j)$
        end for
    end for
     r(n,k) $\longleftarrow$ [0]
    for i **do**:1 to N
        j = $\arg\min_k ||\phi(x_n) - \mu_k||^2$ ▷ Use the above formula to calculate distances
        r[i,j] = 1
        Update mu_j ▷ Recalculate centroids of assigned cluster j
    end for
end procedure

Problem 3

Given:

$$p(x_i) = \begin{cases} \pi + (1-\pi)e^{-\lambda} & x_i = 0 \\ (1-\pi)\frac{\lambda^{x_i}e^{-\lambda}}{x_i!} & x_i > 0 \end{cases}$$

Alternatively:

$$X_i = \begin{cases} 0 & \text{probability} = \pi + (1-\pi)e^{-\lambda} \\ x_i & \text{probability} = (1-\pi)\frac{\lambda^{x_i}e^{-\lambda}}{x_i!} \end{cases}$$

We define a *latent* variable Z_i for all cases where $X_i = 0$. It is latent because when we observed $X_i = 0$ we do not know if it came out of the 'Poisson' distribution or it came out the 'degenerate' distribution(which has a probability of 1 at point 0.). we cannot observe the following. So X_i comes out of a mixture of a degenerate distribution as follows:

$$Z_i = \begin{cases} 1 & X_i \text{ is from the degenerate distrbution} \\ 0 & \text{otherwise} \end{cases}$$

$$p(X_i = 0, Z_i = 1) = p(Z_i = 1) \times p(X_i = 0 | Z_i = 1) = \pi \times 1$$
$$P(X_i = 0, Z_i = 0) = p(Z_i = 0) \times p(X_i = 0 | Z_i = 0) = (1-\pi)e^{-\lambda} \times 1$$

$$L((\pi, \lambda)|(X, Z)) = \prod_{x_i=0} \pi^{z_i} \times ((1-\pi)e^{-\lambda})^{1-z_i} \times \prod_{x_i>0} (1-\pi)e^{\frac{\lambda_i^x e^{-\lambda}}{x_i!}}$$

$$\log L = \sum_{I(x_i=0)} z_i \log(\pi) + (1-z_i)\big(\log(1-\pi) - \lambda\big) + \sum_{I(x_i>0)} \big(\log(1-\pi) + x_i \log(\lambda_i) - \lambda - \log(x_i!)\big)$$

Notation $\theta = (\pi, \lambda)$ θ_0 represents a known parameter(as estimated from previous step, I don't use explicit indices for showing the E,M steps)

Problem 3 continued on next page...

E step:

$$Q(\theta, \theta_0) = \sum_{I(x_i=0)} E_{P(Z|X)}[z_i] \log(\pi) + (1 - E_{P(Z|X)}[z_i]) \big(\log(1-\pi) - \lambda \big) + \sum_{I(x_i>0)} \big(\log(1-\pi) + x_i \log(\lambda_i) - \lambda - \log(x_i!) \big)$$

$$\begin{aligned} E_{P(Z|X_i)}[z_i] &= 0 \times p(Z_i = 0|X) + 1 \times p(Z_i = 1|X_i = 0) \\ &= \frac{p(X_i = 0|Z_i = 1)p(Z_i = 1)}{p(X_i = 0|Z_i = 0)p(Z_i = 0) + p(X_i = 0|Z_i = 1)p(Z_i = 1)} \\ &= \frac{\pi_0}{\pi_0 + (1-\pi_0)e^{-\lambda_0}} \end{aligned}$$

Hence,

$$Q(\theta, \theta_0) = \sum_{I(x_i=0)} \frac{\pi_0}{\pi_0 + (1-\pi_0)e^{-\lambda_0}} \log(\pi) + (\frac{(1-\pi_0)e^{-\lambda_0}}{\pi_0 + (1-\pi_0)e^{-\lambda_0}}) \big(\log(1-\pi) - \lambda \big) + \sum_{I(x_i>0)} \big(\log(1-\pi) + x_i \log(\lambda) - \lambda - \log(x_i!) \big)$$

M step:

$$\begin{aligned} \frac{\partial Q}{\partial \lambda} &= 0 \\ &= \sum_{I(x_i=0)} (1 - E[z_i])(-1) + \sum_{I(x_i>0)} (\frac{x_i}{\lambda} - 1) = 0 \\ \implies \hat{\lambda} &= \frac{\sum_{I(x_i>0)} x_i}{n - \sum_{I(x_i=0)} E[z_i]} \\ \hat{\lambda} &= \frac{\sum_{I(x_i>0)} x_i}{n - \sum_{I(x_i=0)} \hat{z_i}} \\ \text{where } \hat{z} &= \frac{\pi_0}{\pi_0 + (1-\pi_0)e^{-\lambda_0}} \end{aligned}$$

$$\begin{aligned} \frac{\partial Q}{\partial \pi} &= 0 \\ &= \sum_{I(x_i=0)} (\frac{E[z_i]}{\pi} - \frac{1 - E[z_i]}{1-\pi}) - \sum_{I(x_i>0)} \frac{1}{1-\pi} = 0 \\ &= \sum_{I(x_i=0)} (\frac{E[z_i]}{\pi} + \frac{E[z_i]}{1-\pi}) - \frac{n}{1-\pi} = 0 \\ \implies \hat{\pi} &= \sum_{I(x_i=0)} \frac{\hat{z_i}}{n} \end{aligned}$$

Thus parameter updates are as follows:(subscript 1 indicates the next iteration and 0 indicates known parameter value from previous step)

$$\hat{z}_1 = \frac{\pi_0}{\pi_0 + (1-\pi_0)e^{-\lambda_0}}$$

$$\hat{\lambda}_1 = \frac{\sum_{I(x_i>0)} x_i}{n - \sum_{I(x_i=0)} \hat{z}_1}$$

$$\hat{\pi} = \sum_{I(x_i=0)} \frac{\hat{z_1}}{n}$$

Problem 4

Problem 4.2

As seen from Figure 2, k-means algorithm fails to separate the two circles. This happens because of the failure of the following assumption in this case: the dataset is linearly separable. The circular dataset is not really separable, and hence the clusters returned by k-means, have a linear boundary(making two halves of the circle)

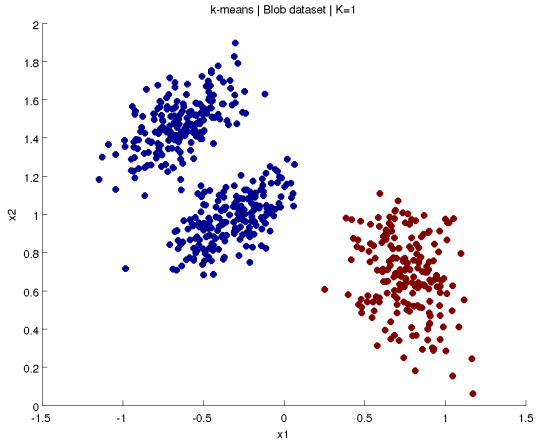

Figure 1: Problem 4.2 Blob Dataset $k = 2$

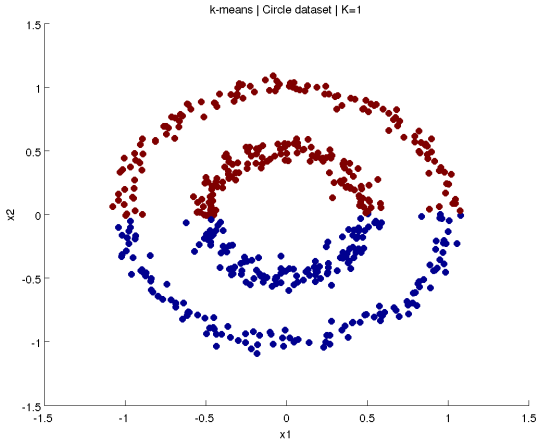

Figure 2: Problem 4.2 Circle Dataset $k = 2$

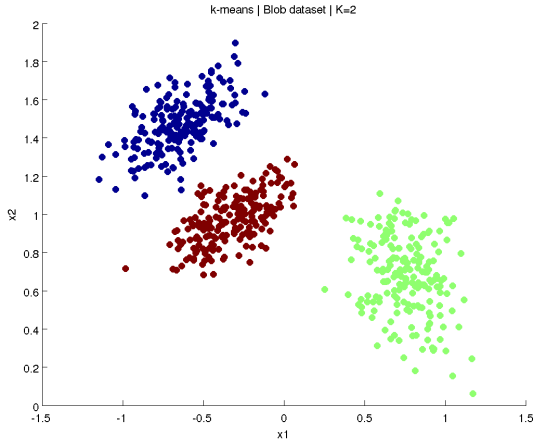

Figure 3: Problem 4.2 Blob Dataset $k = 3$

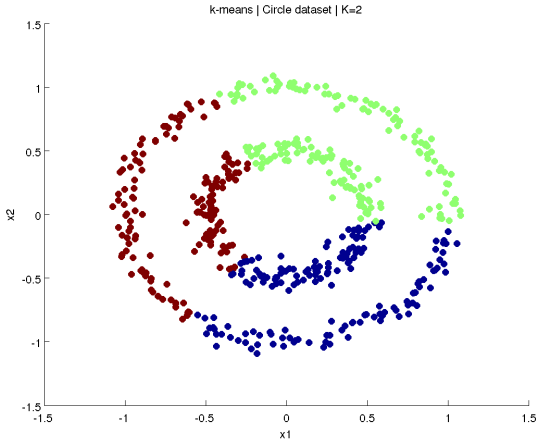

Figure 4: Problem 4.2 Circle Dataset $k = 3$

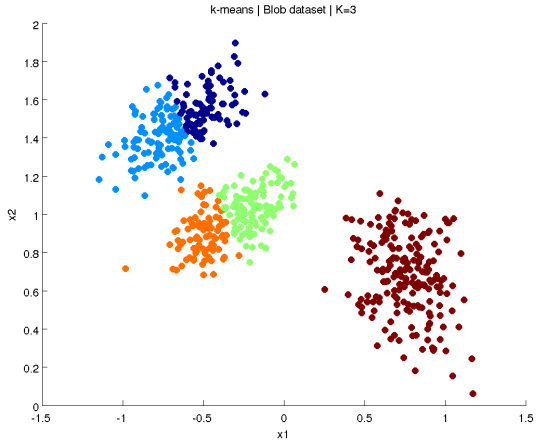

Figure 5: Problem 4.2 Blob Dataset $k = 5$

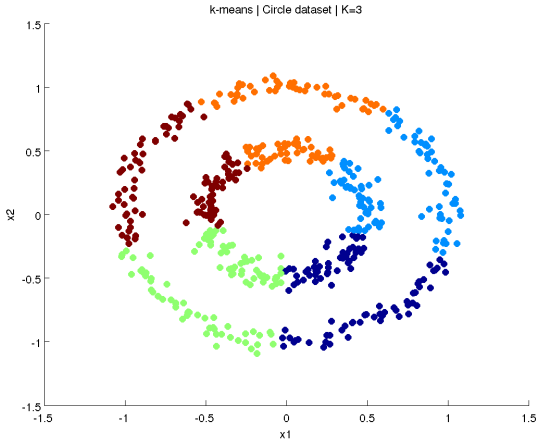

Figure 6: Problem 4.2 Circle Dataset $k = 5$

Problem 4 continued on next page. . .

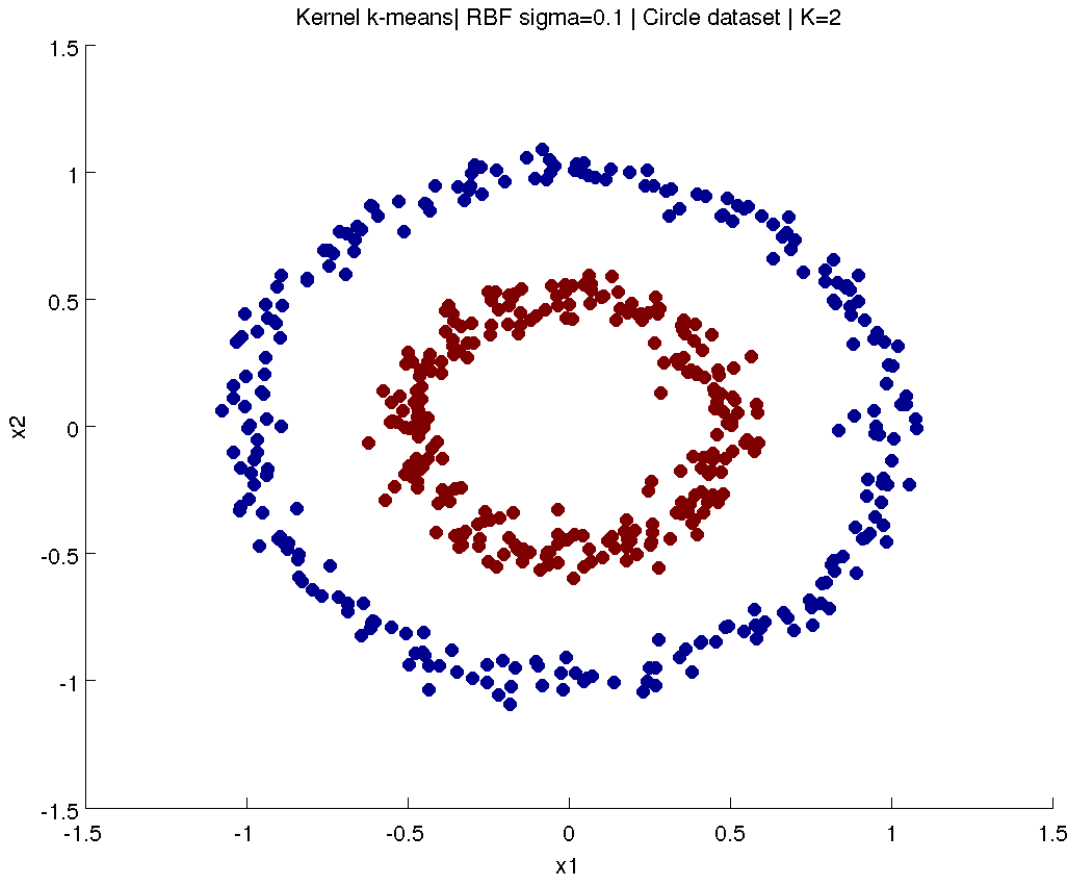

Figure 7: Problem 4.3(b) Kernel k-means with RBF kernel creates separate clusters

Problem 4.3(a)

Choice of Kernel = RBF:

$$K(x, x') = \exp(-\frac{||x - x'||^2}{2\sigma^2})$$

with $\sigma = 0.1$

Problem 4.3(b)

Problem 4.4(a)

Problem 4.4(b)

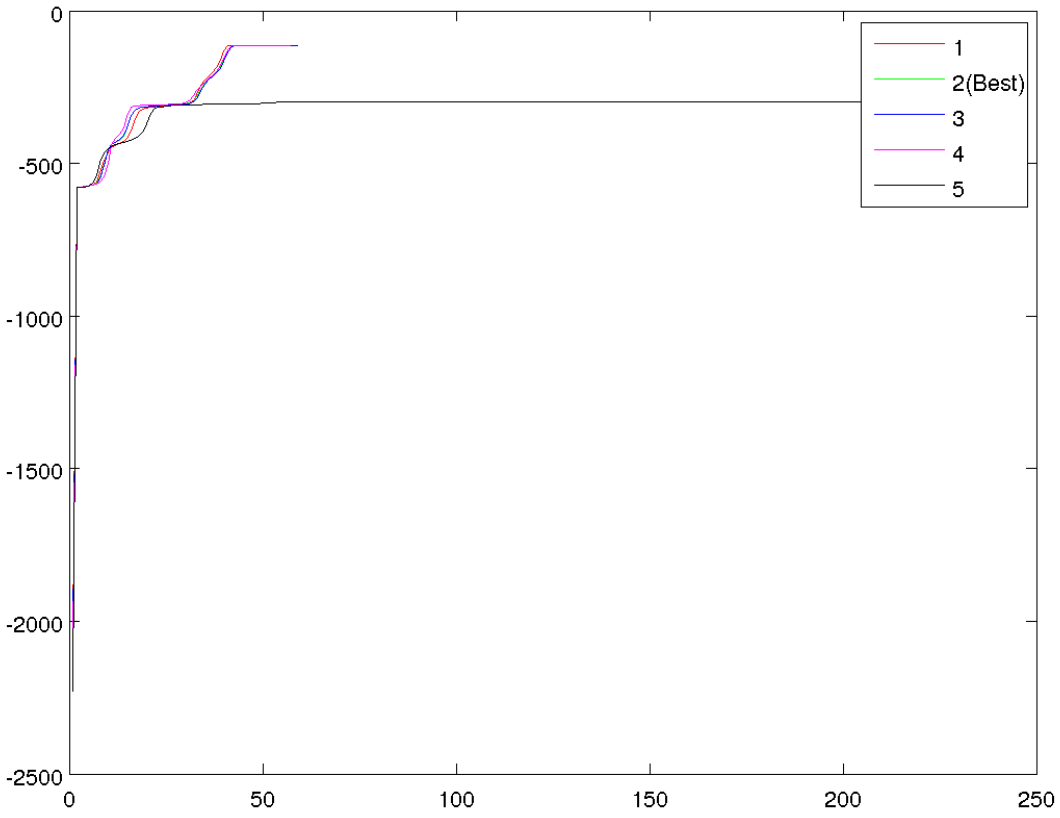

Figure 8: Problem 4.4(a) Log likelihood versus iteration for GMM with 3 mixtures and 5 different initializations

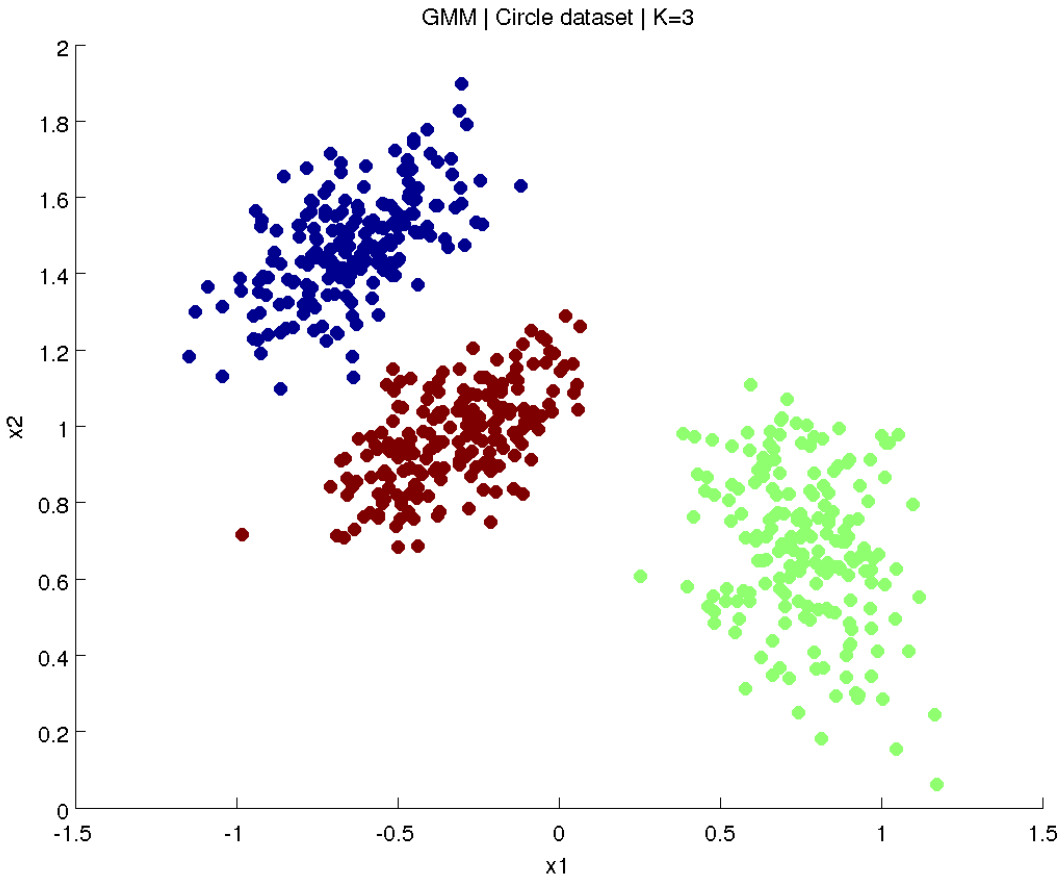

Figure 9: Problem 4.4(b) GMM showing most likely assignments

μ_i: Centroid of cluster i
σ_i: Covariance of cluster i

$$\mu_1 = (-0.6395, 1.4746)$$
$$\sigma_1 = \begin{pmatrix} 0.0360 & 0.0155 \\ 0.0155 & 0.0194 \end{pmatrix}$$

$$\mu_2 = (0.7590, 0.6798)$$
$$\sigma_2 = \begin{pmatrix} 0.0272 & -0.0084 \\ -0.0084 & 0.0404 \end{pmatrix}$$

$$\mu_3 = (-0.3259, 0.9713)$$
$$\sigma_3 = \begin{pmatrix} 0.0360 & 0.0146 \\ 0.0146 & 0.0163 \end{pmatrix}$$