CSCI-567: Assignment #5

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

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Contents

Problem 1																			3
Problem 1:	(a)	 	 																3
Problem 1:	(b)	 	 																4
Problem 1:	(c)	 	 																5
Problem 1:	(d)	 	 																6
Problem 2																			7
Problem 2:	(a)	 	 																7
Problem 2:	(b)	 	 																7
Problem 2:	(c)	 	 		•	 •													8
Problem 3																			9
Problem 4																			11
Problem 4.2	2	 	 																11
Problem 4.3	3(a)	 	 																13
Problem 4.3	3(b)	 	 																13
Problem 4.4	. ,																		
Droblom 4	1(b)																		12

Problem 1

Problem 1: (a)

To find $\nabla_{y_t} L$:

$$\nabla_{y_t} L = \frac{\partial}{\partial y_t} \frac{1}{2} \sum_{i=1}^{N} (y_i - \hat{y}_i)^T (y_i - \hat{y}_i)$$

$$= \frac{\partial}{\partial y_t} \frac{1}{2} \sum_{i=1}^{N} (y_i^T y_i - 2y_i^T \hat{y}_i + \hat{y}_t^2)$$

$$= \frac{1}{2} (2y_t - 2\hat{y}_t)$$

$$= y_t - \hat{y}_t$$

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

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,

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

$$s_k = \sigma(z_k)$$

$$y_k = W_{HO}s_k$$

Thus,

$$\frac{\partial y_k}{\partial s_k} = W_{HO} \tag{1}$$

$$\frac{\partial s_k}{\partial z_k} = \sigma(z_k)(1 - \sigma(z_k)) \tag{2}$$

$$\frac{\partial z_k}{\partial W_{IH}} = x_k \tag{3}$$

$$\frac{\partial y_k}{\partial W_{HH}} = y_{k-1} \tag{4}$$

$$\frac{\partial z_k}{\partial s_{k-1}} = W_{HH} \tag{5}$$

$$\frac{\partial s_k}{\partial s_{k-1}} = \frac{\partial s_k}{\partial z_k} \frac{\partial z_k}{\partial s_{k-1}} = \sigma(z_k) (1 - \sigma(z_k)) W_{HH}$$
(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:

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

Thus,

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

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

$$\begin{split} \nabla_{s_{t+1}} L &= \sum_{k=t+1}^T \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t} \\ \nabla_{s_t} L &= \sum_{k=t}^T \frac{\partial L}{\partial y_k} \times \frac{\partial y_k}{\partial s_k} \times \frac{\partial s_k}{\partial s_t} \\ &\Longrightarrow \nabla_{s_t} L = \nabla_{s_{t+1}} L + \frac{\partial L}{\partial y_t} \times \frac{\partial y_t}{\partial s_t} \times \frac{\partial s_t}{\partial s_t} \\ &\Longrightarrow \nabla_{s_t} L = \nabla_{s_{t+1}} L + (y_t - \hat{y_t}) W_{HO} \end{split}$$

Thus,

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

Problem 1: (c)

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

Thus,

$$\begin{split} \nabla_{W_{IH}} L &= \sum_{k=1}^{(} y_k - \hat{y_k}) W_{HO} \times \sigma(z_k) (1 - \sigma(z_k)) \times x_k \\ & \text{where } \nabla_{s_k} L = \nabla_{s_{k+1}} L + (y_k - \hat{y_k}) W_{HO} \\ & \text{and } z_k = W_{IH} x_k + W_{HH} s_{k-1} \\ & \text{boundary condition } \nabla_{S_T} L = (y_T - \hat{y_T}) W_{HO} \end{split}$$

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

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,

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

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

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

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

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

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

$$||\phi(x_n) - \tilde{\mu_k}||^2 = (\phi(x_n) - \tilde{\mu_k})^T (\phi(x_n) - \tilde{\mu_k})$$

$$= \phi(x_n)^T \phi(x_n) - 2\tilde{\mu}^T \phi(x_n) + \tilde{\mu}^T \tilde{\mu}$$

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

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

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

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

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: (c)

Algorithm 1 Kernel k means

```
1: procedure Kernel K means
        mu[i] = x(random(1..N)) for 1 \le i \le k
                                                          \triangleright initialise cluster centroids[1..k] randomly choosing any k
    points of N (Sample without replacement)
        \textbf{for} \ i \ \textbf{do}{:}1 \ to \ N
3:
            for j do:1 to N K[i,j] = \phi(x_i)\phi(x_j)
 4:
            end for
 5:
        end for
6:
         r(n,k) \leftarrow [0]
        for i do:1 to N
7:
            j = \arg\min_{k} ||\phi(x_n) - \mu_k||^2
 8:
                                                                        \triangleright Use the above formula to calculate distances
            r[i,j] = 1
9:
            Update mu_j
                                                                           \triangleright Recalculate centroids of assigned cluster j
10:
        end for
11:
12: 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:

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

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

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

Notation $\theta = (\pi, \lambda) \theta_0$ represents a known parameter (as estimated from previous step, I don't use explicit indices for showing the E,M steps)

E step:

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

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

Hence,

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

M step:

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

$$\begin{split} \frac{\partial Q}{\partial \pi} &= 0 \\ &= \sum_{I(x_i = 0)} \left(\frac{E[z_i]}{\pi} - \frac{1 - E[z_i]}{1 - \pi} \right) - \sum_{I(x_i > 0)} \frac{1}{1 - \pi} = 0 \\ &= \sum_{I(x_i = 0)} \left(\frac{E[z_i]}{\pi} + \frac{E[z_i]}{1 - \pi} \right) - \frac{n}{1 - \pi} = 0 \\ \Longrightarrow \hat{\pi} &= \sum_{I(x_i = 0)} \frac{\hat{z}_i}{n} \end{split}$$

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

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

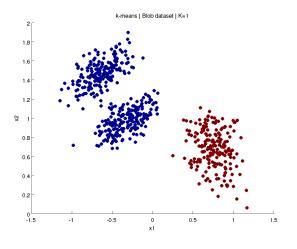
$$\hat{\lambda}_1 = \frac{\sum_{I(x_i > 0)} x_i}{n - \sum_{I(x_i = 0)} \hat{z_1}}$$

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

Problem 4

Problem 4.2

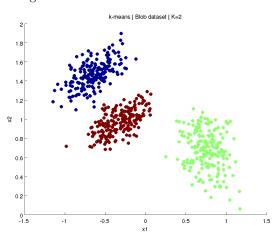
As seen from Figure 2, k-means algorithm fails to separate the two circles. This happens because of the failure of the following assumption in this case: the dataset is linearly separable. The circular dataset is not really separable, and hence the clusters returned by k-means, have a linear boundary(making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



N-means | Circle dataset | K=1

Figure 1: Problem 4.2 Blob Dataset k=2

Figure 2: Problem 4.2 Circle Dataset k = 2



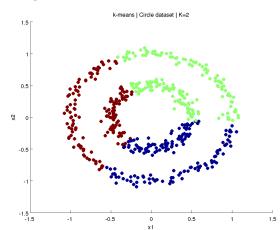
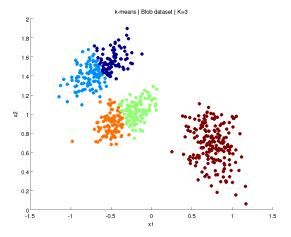


Figure 3: Problem 4.2 Blob Dataset k=3

Figure 4: Problem 4.2 Circle Dataset k=3



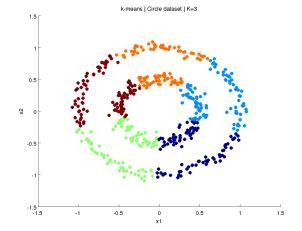


Figure 5: Problem 4.2 Blob Dataset k=5

Figure 6: Problem 4.2 Circle Dataset k=5

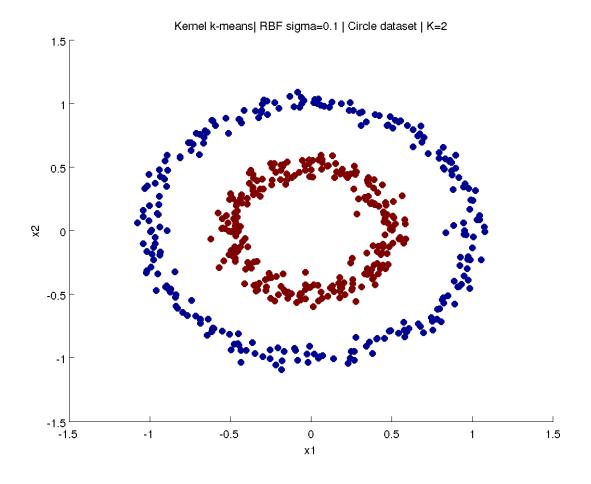


Figure 7: Problem 4.3(b) Kernel k-means with RBF kernel creates separate clusters

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)

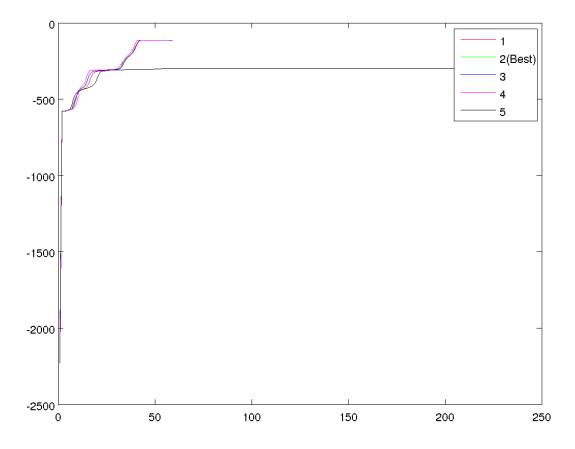


Figure 8: Problem 4.4(a) Log likelihood versus iteration for GMM with 3 mixtures and 5 different initializations

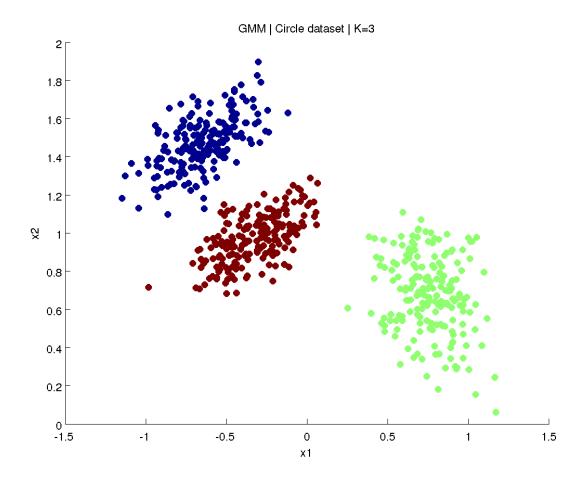


Figure 9: Problem 4.4(b) GMM showing most likely assignments

 μ_i : Centroid of cluster i

 $\sigma_i \colon$ Covariance of cluster i

$$\mu_1 = (-0.6395, 1.4746)$$

$$\sigma_1 = \begin{pmatrix} 0.0360 & 0.0155 \\ 0.0155 & 0.0194 \end{pmatrix}$$

$$\mu_2 = (0.7590, 0.6798)$$

$$\sigma_2 = \begin{pmatrix} 0.0272 & -0.0084 \\ -0.0084 & 0.0404 \end{pmatrix}$$

$$\mu_3 = (-0.3259, 0.9713)$$

$$\sigma_3 = \begin{pmatrix} 0.0360 & 0.0146 \\ 0.0146 & 0.0163 \end{pmatrix}$$