STAT545 HW4

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1. Problem 1: Exponential family distributions

1. Consider a random varibale x that can take D values and that is distributed according to the discrete distribution with parameters $\overrightarrow{\pi}$. We will wirte this as $p(x|\overrightarrow{\pi})$, with $p(x = c|\overrightarrow{\pi}) = \pi_c$ for $c \in \{1, \ldots, D\}$.

(a) Write $p(x|\overrightarrow{\pi})$ as an exponential family distribution and give the natural parameters $\overrightarrow{\eta}$ as a function of π (note this means you can also write π as a function of η though you don't have to). Also write a minimal feature vector ϕ (note $\pi_D = 1 - \sum_{i=1}^{D-1} \pi_i$).

(b) Write $E[\phi(x)]$, the expectation of the feature vector ϕ as a function of the natural parameters $\overrightarrow{\eta}$. Recall that given some data $X = (x_1, \ldots, x_N)$, maximum likelihood estimation (MLE) of η (and thus π) is moment matching (i.e. calculating the empirical average of π and setting η so that the population average and the empirical average match).

Solution:

1. For this discrete distribution, the exponential form is given as follows

(a)

$$\begin{aligned} p(x|\overrightarrow{\pi}) &= \prod_{k=1}^{D} \pi_k^{\delta(x=k)} \\ &= \exp(\sum_{k=1}^{D} \delta(x = k) \cdot \log(\pi_k)) \end{aligned}$$

The feature vector is given by $\phi(x) = [\delta(x = 1), \delta(x = 2), \cdots, \delta(x = D)]^\top$. The natural parameter is given by $\eta = [\log(\pi_1), \log(\pi_2), \cdots, \log(\pi_D)]^\top$. The minial exponential form is derived as follows, the minial feature vector is given by $\phi(x) = [\delta(x = 1), \delta(x = 2), \cdots, \delta(x = D - 1)]^\top$.

$$\begin{aligned} p(x|\overrightarrow{\pi}) &= \exp(\sum_{k=1}^{D} \delta(x = k) \cdot \log(\pi_k)) \\ &= \exp(\sum_{k=1}^{D-1} \delta(x = k) \log(\frac{\pi_k}{\pi_D}) + \sum_{k=1}^{D-1} \delta(x = k) \log(\pi_D) + \delta(x = D) \log(\pi_D)) \\ &= \pi_D \exp(\sum_{k=1}^{D-1} \delta(x = k) \log(\frac{\pi_k}{\pi_D})) \end{aligned}$$

(b) The expectation of the feature vector is given by

$$\mathbb{E}[\phi(x)] = \begin{bmatrix} \mathbb{E}[\delta(x = 1)] \\ \vdots \\ \mathbb{E}[\delta(x = D)] \end{bmatrix} = \begin{bmatrix} \pi_1 \\ \vdots \\ \pi_D \end{bmatrix} = \exp(\eta)$$

2. Let x be Poisson distributed with mean λ. Repeat parts (a), (b).

3. Let x be a 1-dimensional Gaussian with mean μ and variance σ^2. Repeat parts (a), (b) (Note: both μ and σ^2 are parameters).

4. Let x follow a geometric distribution with success probability p: ($Pr(X = k) = (1 - p)^k p$ for $k = 0, 1, 2, \ldots$). Repeat parts (a), (b).

Solution:

2. The Poisson distribution can be expressed in exponential form as follows

$$\begin{aligned} p(x|\lambda) &= \frac{\lambda^x \exp(-\lambda)}{x!} \\ &= \exp(-\lambda)\frac{1}{x!}\exp(\log(\lambda)x) \end{aligned}$$

The feature vector and the minimal feature vector are both $\phi(x) = x$, the natural parameter is $\eta = \log(\lambda)$. The expectation of the featrue vector is derived as follows

$$\mathbb{E}[\phi(x)] = \mathbb{E}[x] = \sum_{x=1}^{\infty} \frac{\lambda^x \exp(-\lambda)}{(x-1)!} = \lambda = \exp(\eta)$$

3. The 1-D normal distribution can be expressed in exponential form as follows,

$$\begin{aligned} p(x|\mu, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right) \\ &= \frac{\exp\left(-\frac{\mu^2}{2\sigma^2}\right)}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x\right) \end{aligned}$$

The feature vector and the minimal feature vector are both $\phi(x) = [x^2, x]^\top$, the natural parameter is $\eta = [-\frac{1}{2\sigma^2}, \frac{\mu}{\sigma^2}]^\top$. The expectation of the featrue vector is given by

$$\mathbb{E}[\phi(x)] = \begin{bmatrix} \mathbb{E}[x^2] \\ \mathbb{E}[x] \end{bmatrix} = \begin{bmatrix} \mu^2 + \sigma^2 \\ \mu \end{bmatrix} = \begin{bmatrix} -\frac{1}{2\eta_1} + \frac{\eta_2^2}{4\eta_1^2} \\ -\frac{1}{2\eta_1} \end{bmatrix}$$

4. The geometric distribution can be expressed in exponential form as follows,

$$\begin{aligned} Pr(X = k) &= (1-p)^X p \\ &= \exp(X\log(1-p) + \log(p)) \end{aligned}$$

The feature vector and the minimal feature vector are both x, and the natural parameter is $\log(1-p)$. The expectation of the feature vector is given by

$$\mathbb{E}[\phi(x)] = \mathbb{E}[x] = \sum_{k=0}^{\infty} k(1-p)^k p = \frac{1-p}{p} = \frac{\exp(\eta)}{1-\exp(\eta)}$$

2. Problem 2: EM for mixture of Bernoulli vectors

1. We looked at the MNIST dataset last assignment. Write code to create a new dataset of only twos and threes using the information in labels. Each pixel can take values from 1 to 256: now threshold the images to be binary (0 or 1). Use a threshold between 1 to 5 (whatever you think is best). Do not use a for loop.

We will model these binary images as a mixture of K Bernoulli vectors. Thus, we have K clusters, each of which is parametrized by a 784-dimensional vector with each component lying between 0 and 1. Call the kth cluster parameter μ^k, with $\mu^k \in [0,1]^{784}$. The probability over clusters is a k-component probability vector π. Thus, to generate an observation, we first sample a cluster c from π, and then generate a random binary image x by setting the ith pixel to 1 with probability μ_i^k for i from 1 to 784.

2. Given N observations $X = (x_1, \ldots, x_N)$ and their cluster assignments $C = (c_1, \ldots, c_N)$, write down the log joint-probability $\log p(X, C|\pi, \overrightarrow{\mu})$.

3. If we observed both X and C, what are the maximum likelihood estimates of π and the μ^ks?
4. Explain why $p(C|X, \pi, \overrightarrow{\mu}) = \prod_{i=1}^{N} p(c_i|x_i, \pi, \overrightarrow{\mu})$.. Write down $p(c_i|x_i, \pi, \overrightarrow{\mu})$. This is the q of the EM algorithm.
5. Write down the variational lower bound $\mathcal{F}(q, \pi, \overrightarrow{\mu})$ for the EM algorithm. Use the first expression in the slides involving the entropy $H(q)$.
6. For a given q, what are the π and $\overrightarrow{\mu}$ that maximize this? These expressions should be a simple relaxation of part (3).
7. Write an EM algorithm that maximizes $\mathcal{F}$ by alternately maximizing w.r.t. q (step 4) and $(\pi, \overrightarrow{\mu})$ (step 6). Although the algorithm doesn't require you to evaluate $\mathcal{F}$, your code should do this after each update. This is a useful diagnostic for debugging since $\mathcal{F}$ should never decrease. Your stopping criteria should be when the value of $\mathcal{F}$ stabilizes.
8. Run the EM algorithm on the binary digits data set for $K = 2$ and 3. Plot the cluster parameters using show_digit. Also plot the trace of the evolution of $\mathcal{F}$. Write down the final value of π and $\mathcal{F}$. What are the units of the latter?
9. The entropy of a distribution is a measure of how 'random' it is. For $K = 2$, calculate the entropy of the final $q(c_i|x_i, \overrightarrow{\mu}, \pi)$ of each digit, and plot the digit with the largest entropy. This is the digit with largest ambiguity about its correct cluster.

Solution:

1.

```
# Credit to https://gist.github.com/brendano/39760
# Load the MNIST digit recognition dataset into R

load_image_file <- function(filename) {
  ret = list()
  f = file(filename,'rb')
  readBin(f,'integer',n=1,size=4,endian='big')
  ret$n = readBin(f,'integer',n=1,size=4,endian='big')
  nrow = readBin(f,'integer',n=1,size=4,endian='big')
  ncol = readBin(f,'integer',n=1,size=4,endian='big')
  x = readBin(f,'integer',n=ret$n*nrow*ncol,size=1,signed=F)
  ret$x = matrix(x, ncol=nrow*ncol, byrow=T)
  close(f)
  ret
}
load_label_file <- function(filename) {
  f = file(filename,'rb')
  readBin(f,'integer',n=1,size=4,endian='big')
  n = readBin(f,'integer',n=1,size=4,endian='big')
  y = readBin(f,'integer',n=n,size=1,signed=F)
  close(f)
  y
}

show_digit <- function(arr784, col=gray(12:1/12), ...) {
  image(matrix(arr784, nrow=28)[,28:1], col=col,axes=F, ...)
}

# load the first 1000 digits and their labels
digits.list <- load_image_file('../HW3/data/train-images-idx3-ubyte')
```

```r
digits <- digits.list$x[1:1000,]
#digits <- digits / 255.0 # normalize pixels
digits <- ifelse(digits<4, 0, 1)
labels <- load_label_file('../HW3/data/train-labels-idx1-ubyte')
dim(digits)
```

```
## [1] 1000  784
```

```r
show_digit(digits[1,])
```

2. The joint probability is given by

$$p(X, C|\pi, \overrightarrow{\mu}) = \prod_{n=1}^{N}\prod_{k=1}^{K}\left[\pi_k \prod_{d=1}^{D}\left(\mu_d^k\right)^{x_{nd}}\left(1-\mu_d^k\right)^{1-x_{nd}}\right]^{\delta(c_n=k)}$$

$$\log p(X, C|\pi, \overrightarrow{\mu}) = \sum_{n=1}^{N}\sum_{k=1}^{K}\delta(c_n=k)\left\{\log\pi_k + \sum_{d=1}^{D}\left[x_{nd}\log\mu_d^k + (1-x_{nd})\log(1-\mu_d^k)\right]\right\}$$

3. Consider this constrained optimization problem, introduce the Lagrange multiplier λ, we have:

$$\arg\max \log p(X, C|\pi, \overrightarrow{\mu}) + \lambda(\sum_{k=1}^{K}\pi_k - 1)$$

Taking derivative to π_k, we have

$$\frac{\sum_{n=1}^{N}\delta(c_n=k)}{\pi_k} + \lambda = 0$$

Multiply both sides by π_k and sum over $k = 1, \ldots, K$, we have

$$\lambda = -\sum_{k=1}^{K}\sum_{n=1}^{N}\delta(c_n=k) = -N$$

Therefore, we have

$$\pi_k = \frac{\sum_{n=1}^{N}\delta(c_n=k)}{N}$$

Taking derivative to μ_d^k, we have

$$\sum_{n=1}^{N}\delta(c_n=k)\left[\frac{x_{nd}}{\mu_d^k} - \frac{1-x_{nd}}{1-\mu_d^k}\right] = 0$$

Therefore, we have

$$\mu_d^k = \frac{\sum_{n=1}^{N}x_{nd}\delta(c_n=k)}{\sum_{n=1}^{N}\delta(c_n=k)}$$

4. Each observation is independent to each other. The joint posterior probability is the product of the marginal posterior probability.

$$q_{n,k} = p(c_n = k|x_n, \pi, \overrightarrow{\mu}) = \frac{\pi_k p(x_n|\mu^k)}{\sum_{j=1}^{K} \pi_j p(x_n|\mu^j)}$$

5. The variational lower bound is given by

$$\begin{aligned} F(q, \pi, \overrightarrow{\mu}) &= \mathbb{E}_q[\log p(X, C|\pi, \overrightarrow{\mu})] + H(q) \\ &= \sum_{n=1}^{N}\sum_{k=1}^{K} q_{n,k} \left\{ \log \pi_k + \sum_{d=1}^{D} \left[x_{nd} \log \mu_d^k + (1 - x_{nd}) \log(1 - \mu_d^k) \right] \right\} - \sum_{n=1}^{N}\sum_{k=1}^{K} q_{n,k} \log q_{n,k} \end{aligned}$$

6. Analagous to part 3, the estimated parameters should be, given $N_k = \sum_{n=1}^{N} q_{n,k}$

$$\pi_k = \frac{N_k}{N}$$

$$\mu_d^k = \frac{\sum_{n=1}^{N} x_{nd} \cdot q_{n,k}}{N_k}$$

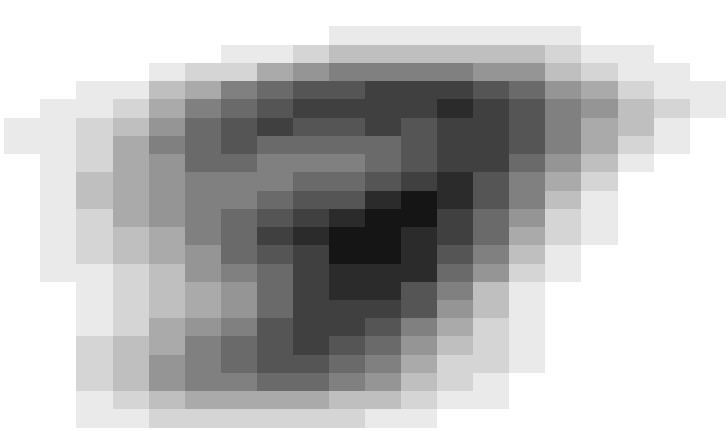
7. The algorithm is implemented as follows

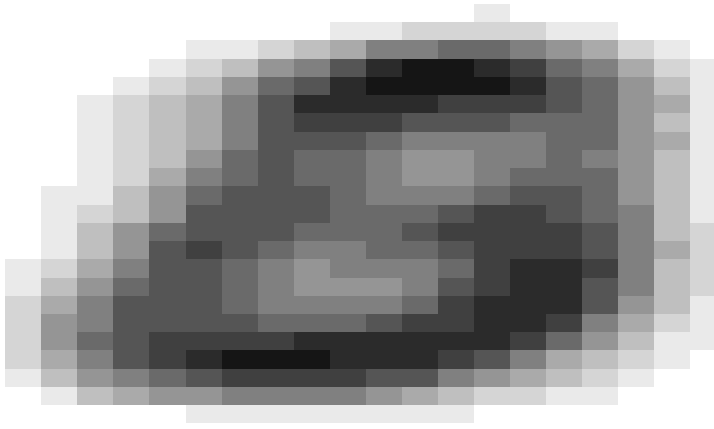
```
em <- function(Obs, K){
  # slog ignore zero logrithm
  slog <- function(val){
    pos <- val > 0
    val[pos] <- log(val[pos])
    return(val)
  }
  set.seed(12)
  # obtain sizes
  N <- nrow(Obs)
  D <- ncol(Obs)
  Pi <- runif(K,0,1)
  Pi <- Pi / sum(Pi)
  mu <- matrix(runif(D*K,0,1),nrow = D)
  q <- matrix(rep(0,N*K), nrow = N)
  temp <- rep(0,K)

  Tol <- 1e-2
  Change <- Tol + 1
  maxIter <- 100
  it <- 0
  Fvalue <- c()
  while (it <= maxIter && Tol <= Change) {
    # E step
    for (n in seq(1,N)){
      x <- Obs[n,]
      for (k in seq(1,K)){
        temp[k] = slog(Pi[k]) + sum(x*slog(mu[,k])) + sum((1 - x)*slog(1 - mu[,k]))
      }
      temp <- temp - max(temp)
      q[n,] <- exp(temp)/sum(exp(temp))
    }
```

```
    # M step
    Nk <- colSums(q)
    Pi <- Nk/N

    mu_update <- matrix(rep(0,D*K), nrow = D)
    for (kk in seq(1,K)){
      mu_update[,kk] <- colSums(q[,kk]*Obs)/Nk[kk]
    }
    Change <- max(abs(mu - mu_update))
    mu <- mu_update
    it <- it + 1

    # update F value
    fvalue <- 0
    for (n in seq(1,N)){
      x <- Obs[n,]
      for (k in seq(1,K)){
        temp[k] = slog(Pi[k]) + sum(x*slog(mu[,k])) + sum((1 - x)*slog(1 - mu[,k]))
        fvalue <- fvalue + q[n,k]*temp[k] - q[n,k]*slog(q[n,k])
      }
    }
    Fvalue <- c(Fvalue, fvalue)
  }

  return(list(Pi=Pi,mu=mu,q=q,Fvalue=Fvalue,it=it))
}
```

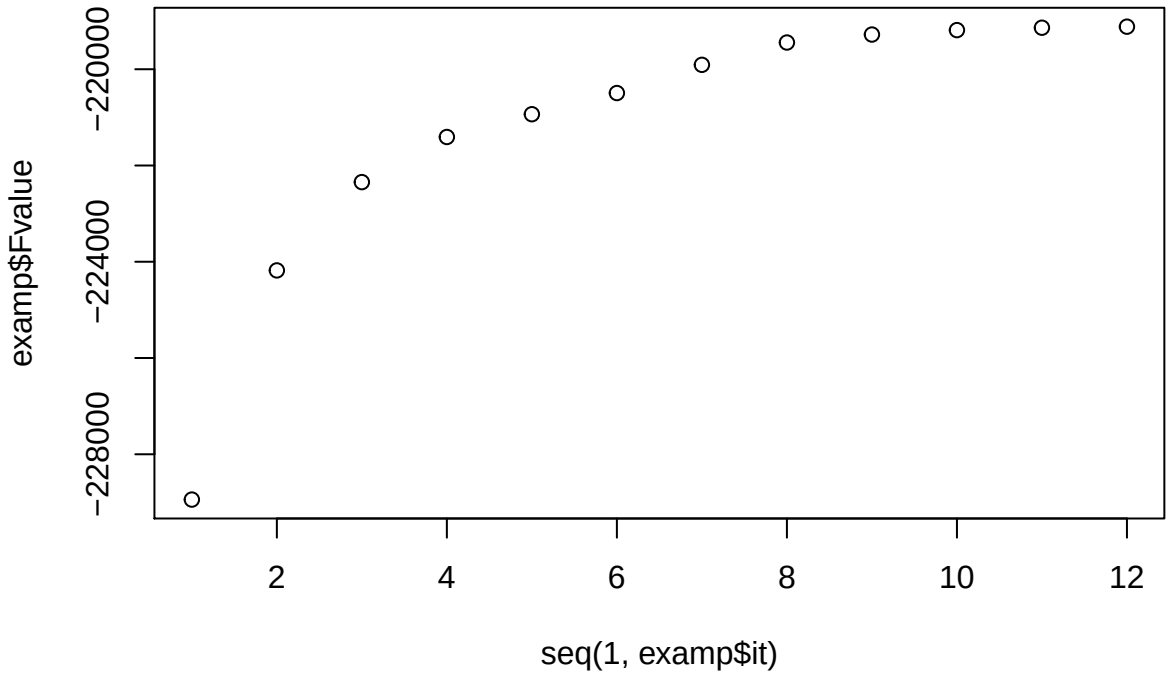
8.

```
#K = 2
examp <- em(digits,2)
for (id in seq(1,ncol(examp$mu))){
  show_digit(examp$mu[,id])
}
```





```
plot(seq(1,examp$it),examp$Fvalue)
```




```
cat(paste('Final value of pi and F:\n'))
```

```
## Final value of pi and F:
```

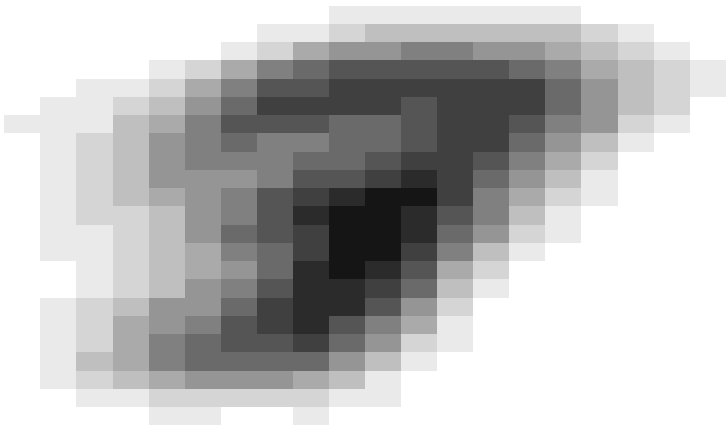
```
print(examp$Pi)
```

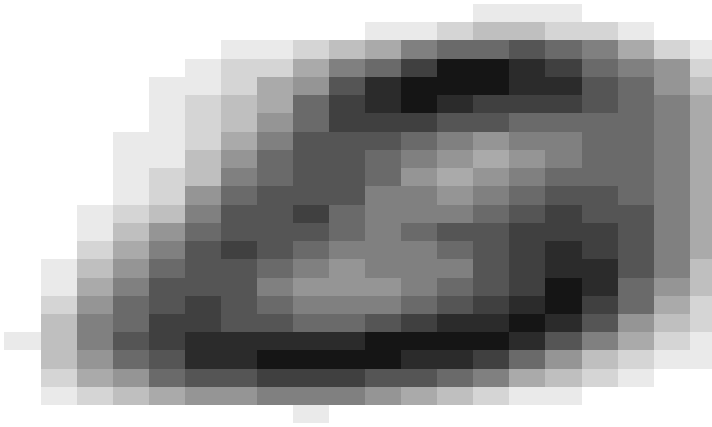
```
## [1] 0.5758176 0.4241824
```

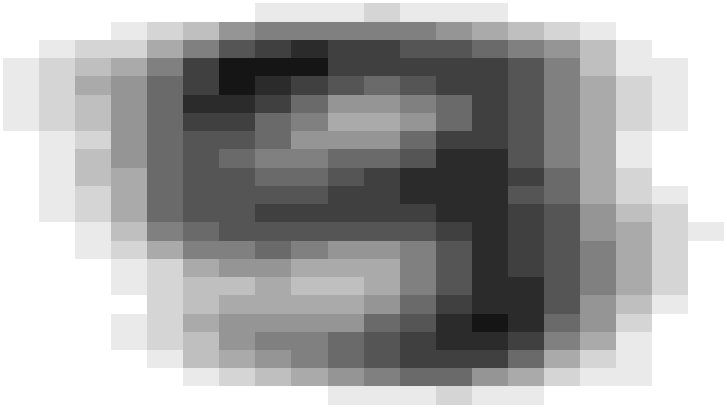
```
print(examp$Fvalue[examp$it])
```

```
## [1] -219116.1
```

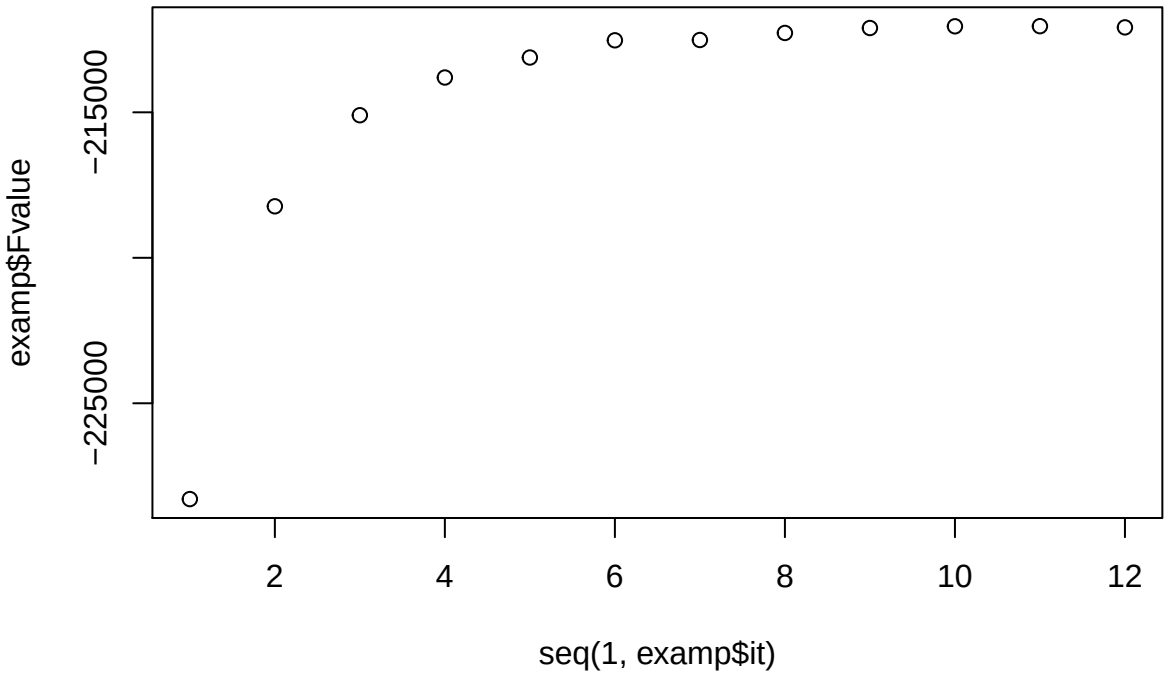
```
#K = 3
examp <- em(digits,3)
for (id in seq(1,ncol(examp$mu))){
  show_digit(examp$mu[,id])
}
```







```
plot(seq(1,examp$it),examp$Fvalue)
```




```
cat(paste('Final value of pi and F:\n'))
```

```
## Final value of pi and F:
```

```
print(examp$Pi)
```

```
## [1] 0.4569846 0.3563021 0.1867133
```

```
print(examp$Fvalue[examp$it])
```

```
## [1] -212080.2
```

The units of F is the same as the entropy, which is J/K.

9.

```
#examp <- em(digits,2)
#Q <- examp$q
#dim(Q)
#Entropy1 <- apply(Q,1,function(x) sum(-x*log(x)))
```

```
#Entropy <- rep(0,length(Entropy1))
#Entropy[Entropy1>0] <- Entropy1[Entropy1>0]
#show_digit(digits[which(Entropy==max(Entropy)),])
```