Assignment #6 – Machine Learning – Professor Haugh

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Question 1

Demonstrating by induction,

Base case $i = 1$:

The optimization model is,

$$\max_{a} Var(a^T x)$$
$$subject\ to \quad a^T a = 1$$

The Lagrangean is,

$$L(a, \lambda) = Var(a^T x) + \lambda(1 - a^T a)$$

Differentiating and equaling to zero, to find the maximizer,

$$\frac{dL}{da} = \Sigma a - \lambda a = 0$$
$$\Sigma a = \lambda a$$

This is the equation that solves for the Eigen-value λ and Eigen-vector $a = \gamma_1$, therefore for the base case, the proposed model solves for γ_1.

Base case $i = 2$:

The optimization model corresponds to

$$\max_{a} Var(a^T x)$$
$$subject\ to \quad a^T a = 1$$
$$a^T \gamma_1 = 0$$

The Lagrangean is,

$$L(a, \lambda, \mu) = Var(a^T x) + \lambda(1 - a^T a) - \mu_1 a^T \gamma_1$$

Differentiating and equaling to zero,

$$\frac{dL}{da} = \Sigma a - \lambda a - \mu_1 \gamma_1 = 0$$

Question 2

(a) Optimizing Z for fixed B, the model to optimize is

$$\min_{Z} \sum_{i=1}^{n} \sum_{j=1}^{d} \gamma_{j,i} \left[x_{j,i} - \sum_{k=1}^{M} z_{k,i} b_{j,k} \right]^2$$

Calculating the first order conditions,

$$\sum_{j=1}^{d} \gamma_{j,i} \left(x_{j,i} - \sum_{l=1}^{M} z_{l,i} \hat{b}_{j,l} \right) \hat{b}_{j,k} = 0 \;\; \forall \, i = 1, \dots, n$$

Having B constant, for each $i = 1, \dots, n$, we have a system of M equations, defined by the vector of equations above.

It is not a problem is the system of equations is under-determined (there are less observations in the nth data column of X than there are components of B). We can use the pseudo-inverse of the matrix to provide a minimal solution.

(b) Optimizing for B for fixed Z, the first order conditions yield,

$$\sum_{i=1}^{n} \gamma_{j,i} \left(x_{j,i} - \sum_{l=1}^{M} \hat{z}_{l,i} b_{j,l} \right) \hat{z}_{k,i} = 0 \;\; \forall \, j = 1, \dots, d$$

Having Z constant, for each $j = 1, \dots, d$, we have a system of M equations, defined by the vector of equations above.

(c) To code the function, I will use the following logic to construct the systems of equations.

For the first step, create $i = 1, \dots, n$ systems of equations, of size M, of the form $c^{(i)} = M^{(i)} z^{(i)}$, where

$$\left[z^{(i)} \right]_l = z_{l,i}$$

$$\left[M^{(i)} \right]_{kl} = \sum_{j=1}^{d} \gamma_{j,i} \, \hat{b}_{j,l} \hat{b}_{j,k}$$

$$\left[c^{(i)} \right]_l = \sum_{j=1}^{d} \gamma_{j,i} x_{j,i} \hat{b}_{j,l}$$

For the second step, create $j = 1, .., d$ systems of equations of the form $m^{(j)} = F^{(j)} b^{(j)}$, where

$$\left[b^{(j)} \right]_l = b_{j,l}$$

$$\left[F^{(j)} \right]_{kl} = \sum_{i=1}^{n} \gamma_{j,i} \, \hat{z}_{l,i} \hat{z}_{k,i}$$

$$\left[m^{(j)} \right]_l = \sum_{i=1}^{n} \gamma_{j,i} x_{j,i} \hat{z}_{l,i}$$

The convergence criteria will be based on parameter ϵ. Let $Z_{i,j}^{(t)}, B_{i,j}^{(t)}$ represent the elements of Z and B on iteration t.

We will stop iterating when,

$$Convergence = \sum_{k,i} \left(Z_{k,i}^{t+1} - Z_{k,i}^{t} \right)^2 + \sum_{j,k} \left(B_{j,k}^{t+1} - B_{j,k}^{t} \right)^2 \leq \epsilon$$

Question 3

(a) To make the problem manageable, I decided to use $d = 300$ users, $n = 600$ movies, and will apply the formulas with total number of PCA dimensions $M = 5$.

The data matrix x, has shape $d\ x\ n$: the users is the dimensionality of the dataset, and n as number of observations.

The initial basis B^0 was chosen as $B^0_{i,j} = \begin{cases} 1 & if\ j = (i\ mod(M)) + 1 \\ 0 & \sim \end{cases}$

The tolerance criteria was set at $\epsilon = 1$. The tolerance indicator is detailed in question 2.(c).

The script took $1168[s] \approx 20[min]$ to run. The RMSE is 24549.7

The output of the script was the following:

```
[1] "Starting Iterations"
[1] "-----------"
Iteration =  1
Tolerance =  1
Convergence =  2900.13
RMSE =  24577.08
Iteration Time =  30.21 0 30.26 NA NA
Total Time =  30.21 0 30.26 NA NA
[1] "-----------"
Iteration =  2
Tolerance =  1
Convergence =  22099.94
RMSE =  24567.16
Iteration Time =  27.4 0 27.47 NA NA
Total Time =  57.61 0 57.73 NA NA
[1] "-----------"
Iteration =  3
Tolerance =  1
Convergence =  1407.341
RMSE =  24558.37
Iteration Time =  30.2 0 30.36 NA NA
Total Time =  87.81 0 88.09 NA NA
[1] "-----------"
```

... Iteration 4 to 36...

```
Iteration =  37
Tolerance =  1
Convergence =  1.296265
RMSE =  24549.54
Iteration Time =  32.06 0 32.17 NA NA
Total Time =  1116.56 0.24 1120.51 NA NA
[1] "-----------"
Iteration =  38
Tolerance =  1
Convergence =  1.13819
RMSE =  24549.62
Iteration Time =  29.52 0 29.58 NA NA
Total Time =  1146.08 0.24 1150.09 NA NA
[1] "-----------"
Iteration =  39
Tolerance =  1
Convergence =  0.9894758
RMSE =  24549.7
Iteration Time =  22.34 0 22.34 NA NA
Total Time =  1168.42 0.24 1172.43 NA NA
```

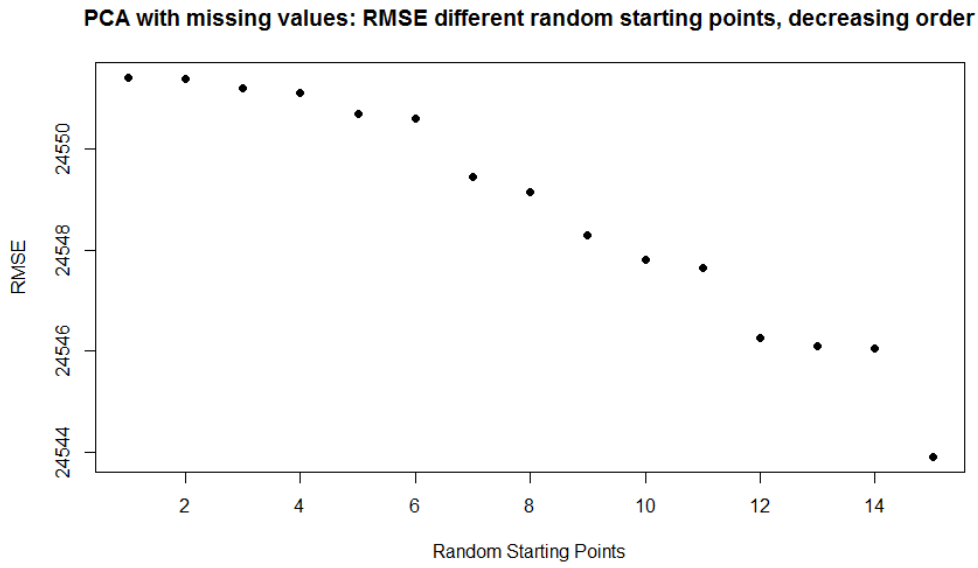
(b) I ran the code with $K = 15$ different starting points. We can clearly reach better local minima if we try different starting points, therefore this must be of recurring practice in the industry. On the other hand, I see that this is a very intensive task from a computational standpoint.

This process took is around 5 hours of computer time.

I generated the random initial basis drawing each element of the matrix from a standard normal distribution.

The RMSE obtained are in the following list, and plotted below.

```
> RMSE
 [1] 24551.40 24549.45 24551.20 24550.71 24546.27 24551.41 24549.14 24551.11 24550.
60 24547.82 24546.10 24543.92 24547.64
[14] 24546.05 24548.29
```



(c) Using this code,

The output matrix $\hat{B}$ is an approximation for the first $M = 5$ columns of the matrix of factor loadings, in the lecture notes represented with the Greek Letter Γ.

The output matrix $\hat{Z}$ is an estimated reconstruction of each data point in the PCA space.

To estimate the full matrix of ratings of $Users\ x\ Movies$, which we will call R, we can do

$$\hat{R} \approx \hat{B} \cdot \hat{Z}$$

If we want to look at movies to recommend to user d,

1. Extract the d^{th} row of the matrix $\hat{R}$, represented as $\hat{R}_{i,}$. This is a row vector of dimension n.
2. We create a new row vector r_d, containing only the unrated movies. We would calculate it with pair-wise multiplication, for each movie i as follows,

$$(r_d)_i = \hat{R}_{d,i} \cdot (1 - \gamma_{d,i})$$

$$(r_i)$$

3. Within this subset, recommend the movies with the highest rating.

If we want to recommend a movie of a specific genre, using the definition of matrix $G_{i,j}$, add two steps:

4. If we want to recommend a specific genre $\bar{g}$ to user d, we get the column vector $G_{.,\bar{g}}$, and make pairwise multiplication,

$$(r_d)_i \leftarrow (r_d)_i \cdot G_{i,\bar{g}} \; \forall i \in N$$

Recall that N is the set of movies.

5. The final vector represents all the recommended movies i from genre $\bar{g}$, for user d.

Question 4

(a) I wrote the code that can be found in the appendix. The function I wrote is callable through the following syntax:

```
pageRank(connections, epsilon, start.vector, convergence)
```

- Connections: square matrix of length d, containing 0's and 1's. The 1's indicate that webpage of row i has a link to page of column j.
- Epsilon: scalar value that allows to have an irreducible matrix
- Start.vector: Row vector of size d, to stat off the iterations.
- Convergence: stopping criteria for the iterations

(b) The resulting vector with $\epsilon = 0.15$ is displayed below. The output makes a lot of sense, for example:

- Page 3 has the highest rank, and it makes sense because it has the highest amount of inbound links.
- Page 1 has a very high rank, similar to Page 3, because it is basically the only page leading out of 3.
- Pages 4 and 6 have the lowest rank, and we can see that they have no inbound links.

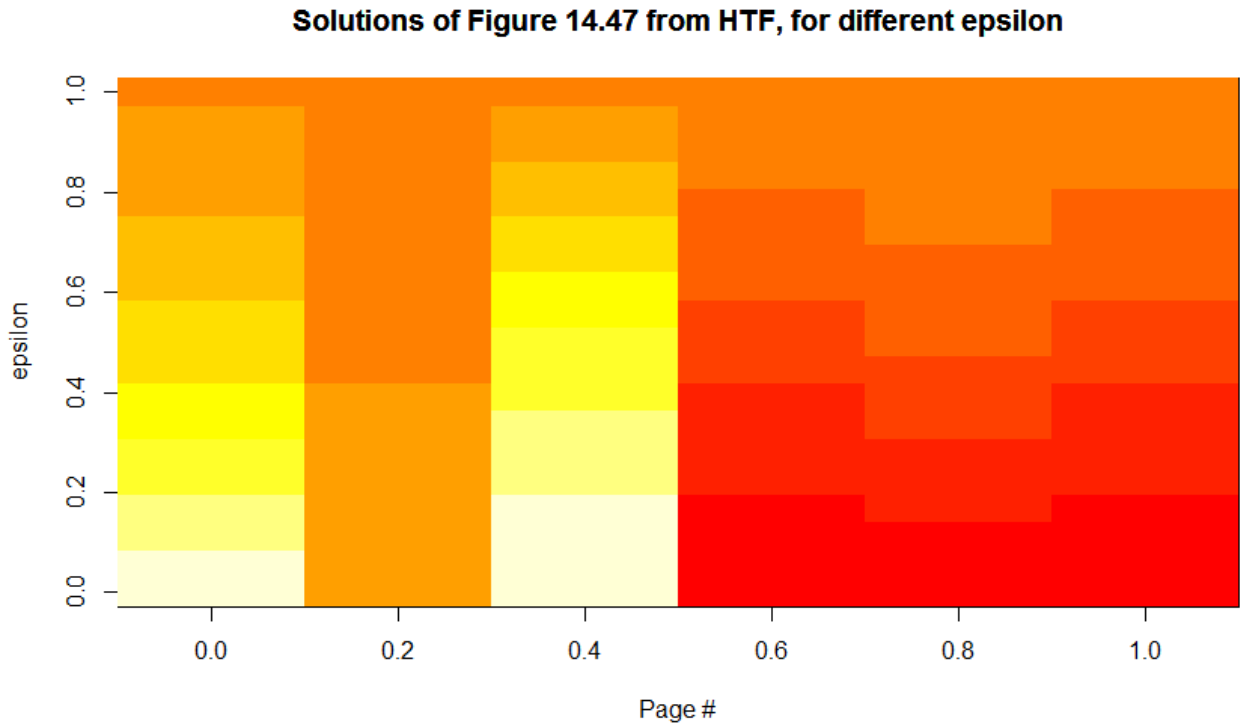
```
> pi
          [,1]      [,2]      [,3]  [,4]     [,5]  [,6]
[1,] 0.3538667 0.1860446 0.3744637 0.025 0.035625 0.025
```

(c) The impact of ϵ is extremely relevant. I solved the model for values of ϵ ranging from 0.1 to 1, in steps of 0.5.

The resulting vectors are represented below, as numbers, and as colors.

- When epsilon is close to zero, the webpage links are relevant.
- The closer we get to $\epsilon \to 1$, the values for the limiting probabilities are more similar to each other.
- At $\epsilon = 1$, all of the pages have the same rank.

```
> pi.matrix
           [,1]      [,2]      [,3]       [,4]       [,5]       [,6]
 [1,] 0.3690412 0.1902649 0.3831939 0.01666667 0.02416667 0.01666667
 [2,] 0.3538667 0.1860446 0.3744637 0.02500000 0.03562500 0.02500000
 [3,] 0.3390041 0.1822408 0.3654218 0.03333333 0.04666667 0.03333333
 [4,] 0.3243365 0.1789440 0.3560946 0.04166667 0.05729167 0.04166667
 [5,] 0.3100062 0.1760022 0.3464916 0.05000000 0.06750000 0.05000000
 [6,] 0.2960187 0.1735199 0.3365031 0.05833333 0.07729167 0.05833333
 [7,] 0.2823941 0.1713934 0.3262125 0.06666667 0.08666667 0.06666667
 [8,] 0.2691870 0.1696405 0.3155475 0.07500000 0.09562500 0.07500000
 [9,] 0.2564290 0.1682739 0.3044637 0.08333333 0.10416667 0.08333333
[10,] 0.2441521 0.1672259 0.2929970 0.09166667 0.11229167 0.09166667
[11,] 0.2324352 0.1664768 0.2810880 0.10000000 0.12000000 0.10000000
[12,] 0.2213324 0.1660213 0.2686879 0.10833333 0.12729167 0.10833333
[13,] 0.2108980 0.1658082 0.2557938 0.11666667 0.13416667 0.11666667
[14,] 0.2012329 0.1657715 0.2423706 0.12500000 0.14062500 0.12500000
[15,] 0.1923533 0.1659000 0.2284133 0.13333333 0.14666667 0.13333333
[16,] 0.1843698 0.1661194 0.2138858 0.14166667 0.15229167 0.14166667
[17,] 0.1773750 0.1663687 0.1987562 0.15000000 0.15750000 0.15000000
[18,] 0.1714427 0.1665781 0.1830208 0.15833333 0.16229167 0.15833333
[19,] 0.1666667 0.1666667 0.1666667 0.16666667 0.16666667 0.16666667
```



Appendix

Code for Q2

```
PCA_missing <- function(numBasis, data, data.avail, tolerance, startB){

library("corpcor")

# On the data matrix, the rows are the features, and columns are the observations.
# Get n = columns of X (number of data points)
n = ncol(data)
# Get d = rows of x (number of features, dimension of x)
d = nrow(data)

# Initialize matrices
Z <- mat.or.vec(numBasis,n)
B <- mat.or.vec(d,numBasis)
B <- startB

cat('Starting Iterations\n')
convergence <- 1000000
iter <- 1
ptm <- 0
ttm <- proc.time()
while (convergence > tolerance) {
  ptm <- proc.time()
  cat("-----------\n")
  cat('Iteration = ', iter, "\n")
  ## First Step, solve i = 1,...,n systems of equations with B fixed. We get Z.
  for (i in 1:n){
  # System of equations M_i * z_i = c_i
    # Define the matrix M_i
    M <- mat.or.vec(numBasis, numBasis)
    for (k in 1:numBasis){
      for (l in 1:numBasis){
        # Sum over dimension of x
        for (j in 1:d){
          M[k,l] <- M[k,l] + data.avail[j,i]*B[j,l]*B[j,k]
        }
      }
    }
    # Define the vector c_i
    c <- mat.or.vec(numBasis,1)
    # Sum over dimension of x
    for (l in 1:numBasis){
        c[l] = 0
      # Sum over dimension of x
      for (j in 1:d){
        if (data.avail[j,i] == 1) {
          c[l] <- c[l] + data.avail[j,i]*data[j,i]*B[j,l]
        }
      }
    }
    # Save z.old
    Z.old <- Z


    # Solve for z_i
#    print("M = ")
#    print(M)
#    cat("c = ", c, "\n")
    Z[,i] <- pseudoinverse(M) %*% c
#    print("Z = ")
#    print(Z)

  }

  ## Second Step, solve j = 1,...,d systems of equations with Z fixed. We get B.
  for (j in 1:d){

    # System of equations F_j * b_j = m_j
    # Define the matrix F_j
    Fmat <- mat.or.vec(numBasis, numBasis)
    for (k in 1:numBasis){
      for (l in 1:numBasis){
        # Sum over dimension of x
```

```
        for (i in 1:n){
          Fmat[k,l] <- Fmat[k,l] + data.avail[j,i]*Z[l,i]*Z[k,i]
        }
      }
    }
    # Define the vector c_i
    m <- mat.or.vec(numBasis,1)
    # Sum over dimension of x
    for (l in 1:numBasis){
      # Sum over dimension of x
      for (i in 1:n){
        if(data.avail[j,i] == 1){
          m[l] <- m[l] + data.avail[j,i]*data[j,i]*Z[l,i]
        }
      }

    }
    # Save B.old
    B.old <- B
    # Solve for b_j
#    B[,j] <- solve(Fmat, m)
    B[j,] <- pseudoinverse(Fmat) %*% m
#    print("B = ")
#    print(Z)

  }

  # Calculate convergence criteria
  # Squared difference between iteration results
  convergence <- 0
  for(l in 1:numBasis) {
    for(i in 1:n) {
      convergence <- convergence + (Z[l,n]-Z.old[l,n])^2
    }
    for(j in 1:d) {
      convergence <- convergence + (B[j,l]-B.old[j,l])^2
    }
  }
  iter <- iter+1

  ### Calculate Root-mean-squared-error (RMSE)
  # RMSE Compute objective function
  RMSE <- 0
  temp.RMSE <- 0
  for(i in 1:n){
    for(j in 1:d){
      if(data.avail[j,i] == 1){
        for(k in 1:numBasis){
          temp.RMSE <- temp.RMSE + B[j,k]*Z[k,i]
        }
        RMSE <- RMSE + (data[j,i]-temp.RMSE)^2
      }

    }
  }
  # RMSE Count number of observations, and divide
  data.avail.count <- 0
  for(i in 1:n){
    for(j in 1:d){
      data.avail.count <- data.avail.count + data.avail[j,i]
    }
  }
  # RMSE Divide and apply square root
  RMSE <- RMSE / data.avail.count
  RMSE <- RMSE^(1/2)

  ### Output
  # Convergence Measures
  cat('Tolerance =\t', tolerance, "\n")
  cat('Convergence =\t', convergence, "\n")
  cat('RMSE =\t\t', RMSE, "\n")
  # Timing
  cat("Iteration Time =\t", proc.time() - ptm, "\n")
  cat("Total Time  =\t\t", proc.time() - ttm, "\n\n")
}
returnList <- list("Convergence" = convergence, "RMSE" = RMSE, "Total Time" = proc.time() - ttm,
                   "Basis" = B)
return(returnList)
}
```

Code for Q3

```
source("Q2.R") # Function PCA with missing data.

# Input Parameters
num.users = 200 # Max 943
num.movies = 400 # Max 1682
num.pca.basis = 5
convergence = 1


### Prepare the database (snippet from Q2 HW5)
movies <- read.table("u.item", sep = "|", header = FALSE, stringsAsFactors = FALSE, quote="")
movies <- movies[,c(1,2)]
names(movies) <- c("movieid","movie")
rank   <- read.table("u.data", sep = "\t", header = FALSE, stringsAsFactors = FALSE,
                     col.names = c("userid","movieid","rating","ts"))
critics <- merge(movies, rank, by = "movieid")
critics$movie <- NULL
critics$ts <- NULL
names(critics) <- c("movieid","person","rank")

### Prepare matrices
# Data matrix
data = matrix(nrow = num.users, ncol = num.movies)
gamma = matrix(nrow = num.users, ncol = num.movies)
for(i in 1:nrow(critics)) {
  if (critics[i,2] <= num.users & critics[i,1] <= num.movies) {
    data[critics[i,2] , critics[i,1]] <- critics[i,3]
  }
}
# Gamma matrix
for(i in 1:ncol(data)){
  for(d in 1:nrow(data)){
    if(is.na(data[d,i]) ){
      gamma[d,i] = 0
    } else {
      gamma[d,i] = 1
    }
  }
}
# Starting Basis
start.pca.basis = matrix(0, nrow = nrow(data), ncol = num.pca.basis)

# Part A
for(d in 1:nrow(data)){
  start.pca.basis[d,d %% num.pca.basis + 1] = 1
}
finalB <- PCA_missing(num.pca.basis, data, gamma, convergence, start.pca.basis)
finalB

# Part B

K = 15
RMSE <- mat.or.vec(K,1)
iter = 1
for(iter in 1:K){
  start.pca.basis <- matrix( rnorm(nrow(data)*num.pca.basis,mean=0,sd=1), nrow(data), num.pca.basis)
  output <- PCA_missing(num.pca.basis, data, gamma, convergence, start.pca.basis)
  RMSE[iter] <- output$RMSE
}
RMSE
plot(RMSE)
RMSE.sorted <- sort(RMSE, decreasing = TRUE)
plot(RMSE.sorted, pch = 19, xlab = "Random Starting Points", ylab = "RMSE",
     main = "PCA with missing values: RMSE different random starting points, decreasing order")
```

Code for Q4

```
pageRank <- function(connections, epsilon, start.vector, convergence){
  d <- nrow(connections)

  ## Create transition matrix as Q_jk = 1/c(j)
  ## Where c(j) is the number of outbout links from page i

  # Initialize transition matrix as zeros.
  trans.mat <- matrix(0, nrow = d, ncol = d)

  # Compute c(j)
  c <- rowSums(connections)

  # Populate transition matrix
  for(j in 1:d){
    for(k in 1:d){
      if (connections[j,k] == 1){
        trans.mat[j,k] <- 1 / c[j]
      }
    }
  }

  # Create irreductible transition matrix by adding epsilon to all elements
  ones <- matrix(data = 1, nrow = d, ncol = d)
  trans.mat.irr <- (1-epsilon) * trans.mat + epsilon/d*ones

  # Initialize the iterating vector
  mu = start.vector
  mu.old = start.vector


  check <- 10000
  iter <- 1
  while(check > convergence){
    # Update mu
    mu <- mu.old %*% trans.mat.irr
    # Calculate convergence criteria
    check <- dist(rbind(mu,mu.old))
    # Record old mu
    mu.old <- mu
    # Output stats
    cat('Done with iteration:', iter, '\n')
    cat('Convergence:', check, ' / ', convergence, '\n')
    iter <- iter + 1
  }
return(mu)
}
connections <- matrix(c(0,0,1,1,0,0,
                        1,0,0,0,0,1,
                        1,1,0,1,1,0,
                        0,0,0,0,0,0,
                        0,0,0,0,0,1,
                        0,0,0,0,0,0),
                      nrow = 6, ncol = 6)
initial <- matrix(1/nrow(connections), nrow = 1, ncol = nrow(connections))
epsilon <- 0.15
convergence <- 0.0001

# Question b
pi <- pageRank(connections,epsilon,initial,convergence)
pi

# Question c

epsilon.values <- matrix(seq(0.1, 1, 0.05), nrow = 19)
pi.matrix <- matrix(0, nrow = nrow(epsilon.values), ncol = nrow(connections))

for(iter in 1:nrow(epsilon.values)){
  pi.matrix[iter,] <- pageRank(connections,epsilon.values[iter,1],initial,convergence)
}

pi.matrix

a <-image(t(pi.matrix))
title(main = 'Solutions of Figure 14.47 from HTF, for different epsilon',
      xlab = 'Page #', ylab = 'epsilon')
```