

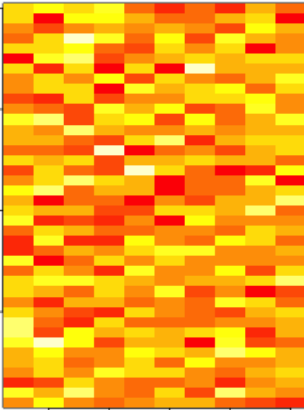


Principal Components Analysis and Singular Value Decomposition

Roger D. Peng, Associate Professor of Biostatistics
Johns Hopkins Bloomberg School of Public Health

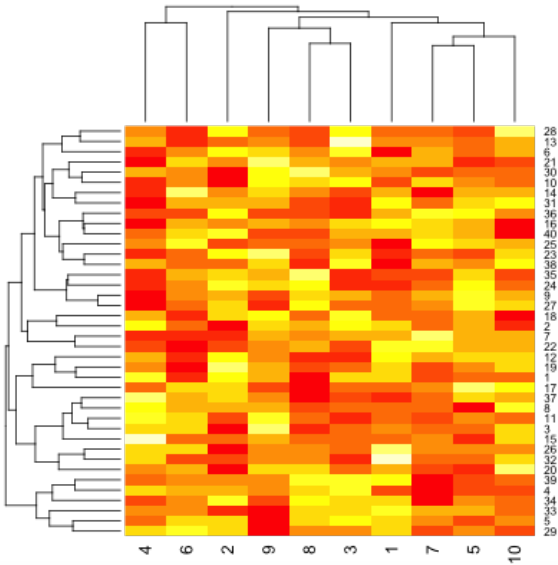
Matrix data

```
set.seed(12345)
par(mar = rep(0.2, 4))
dataMatrix <- matrix(rnorm(400), nrow = 40)
image(1:10, 1:40, t(dataMatrix)[, nrow(dataMatrix):1])
```



Cluster the data

```
par(mar = rep(0.2, 4))  
heatmap(dataMatrix)
```

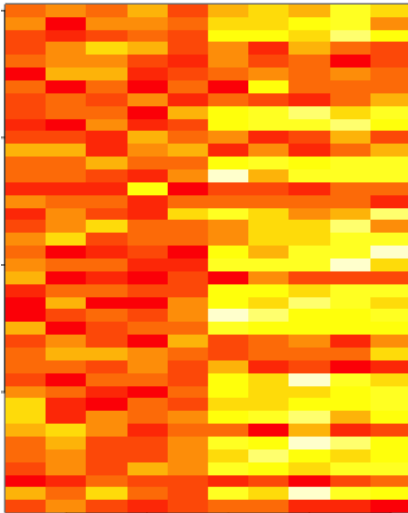


What if we add a pattern?

```
set.seed(678910)
for (i in 1:40) {
  # flip a coin
  coinFlip <- rbinom(1, size = 1, prob = 0.5)
  # if coin is heads add a common pattern to that row
  if (coinFlip) {
    dataMatrix[i, ] <- dataMatrix[i, ] + rep(c(0, 3), each = 5)
  }
}
```

What if we add a pattern? - the data

```
par(mar = rep(0.2, 4))  
image(1:10, 1:40, t(dataMatrix)[, nrow(dataMatrix):1])
```

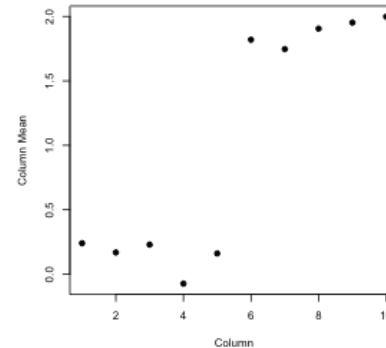
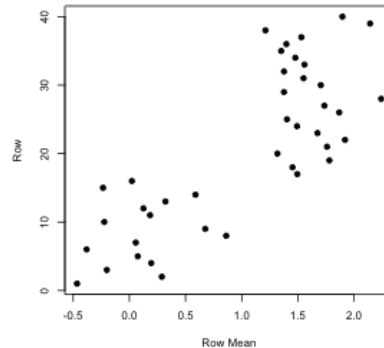
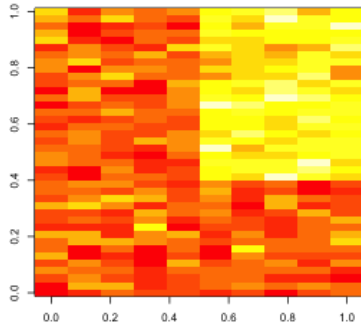


What if we add a pattern? - the clustered data

```
par(mar = rep(0.2, 4))  
heatmap(dataMatrix)
```

Patterns in rows and columns

```
hh <- hclust(dist(dataMatrix))
dataMatrixOrdered <- dataMatrix[hh$order, ]
par(mfrow = c(1, 3))
image(t(dataMatrixOrdered)[, nrow(dataMatrixOrdered):1])
plot(rowMeans(dataMatrixOrdered), 40:1, , xlab = "Row Mean", ylab = "Row", pch = 19)
plot(colMeans(dataMatrixOrdered), xlab = "Column", ylab = "Column Mean", pch = 19)
```



Related problems

You have multivariate variables X_1, \dots, X_n so $X_1 = (X_{11}, \dots, X_{1m})$

- Find a new set of multivariate variables that are uncorrelated and explain as much variance as possible.
- If you put all the variables together in one matrix, find the best matrix created with fewer variables (lower rank) that explains the original data.

The first goal is **statistical** and the second goal is **data compression**.

Related solutions - PCA/SVD

SVD

If X is a matrix with each variable in a column and each observation in a row then the SVD is a "matrix decomposition"

$$X = UDV^T$$

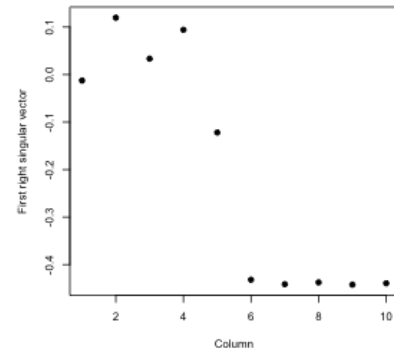
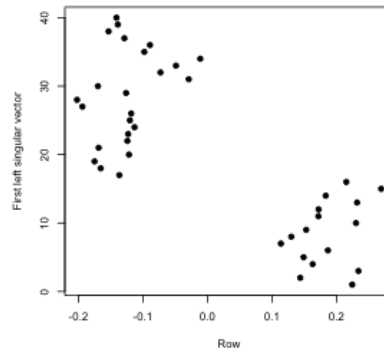
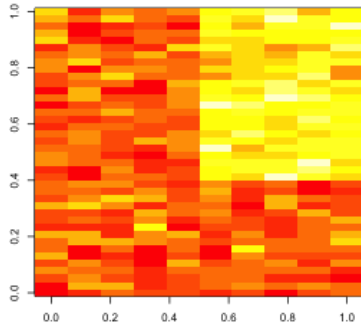
where the columns of U are orthogonal (left singular vectors), the columns of V are orthogonal (right singular vectors) and D is a diagonal matrix (singular values).

PCA

The principal components are equal to the right singular values if you first scale (subtract the mean, divide by the standard deviation) the variables.

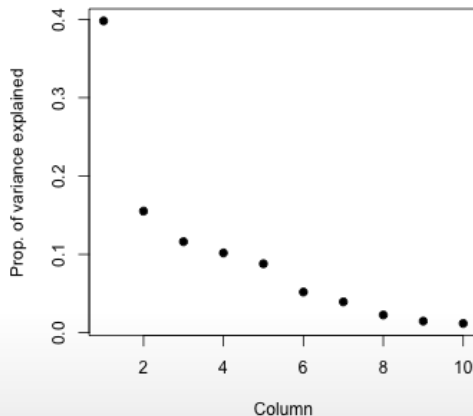
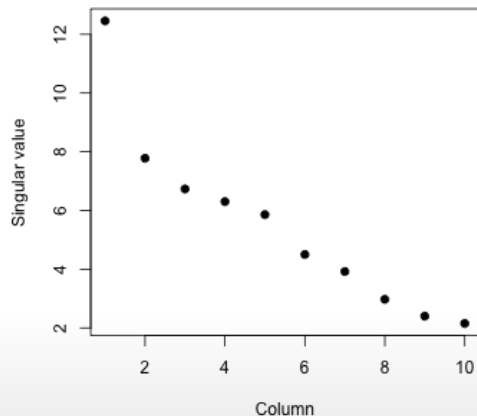
Components of the SVD - u and v

```
svd1 <- svd(scale(dataMatrixOrdered))  
par(mfrow = c(1, 3))  
image(t(dataMatrixOrdered)[, nrow(dataMatrixOrdered):1])  
plot(svd1$u[, 1], 40:1, , xlab = "Row", ylab = "First left singular vector",  
     pch = 19)  
plot(svd1$v[, 1], xlab = "Column", ylab = "First right singular vector", pch = 19)
```



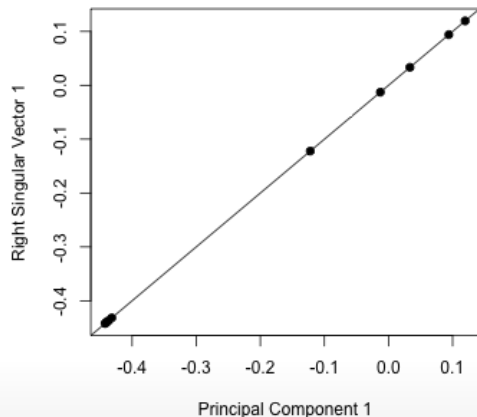
Components of the SVD - Variance explained

```
par(mfrow = c(1, 2))  
plot(svd1$d, xlab = "Column", ylab = "Singular value", pch = 19)  
plot(svd1$d^2/sum(svd1$d^2), xlab = "Column", ylab = "Prop. of variance explained",  
      pch = 19)
```



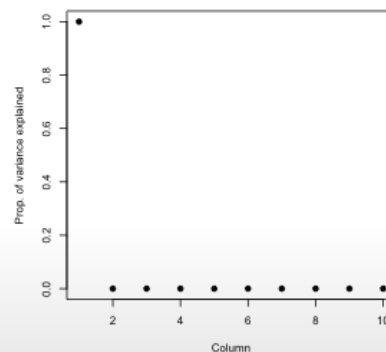
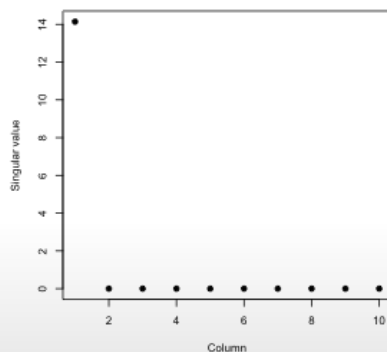
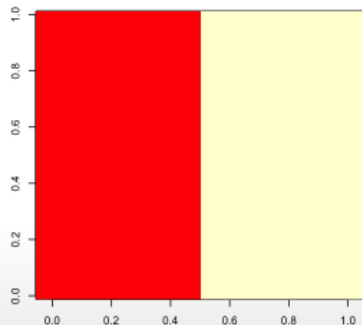
Relationship to principal components

```
svd1 <- svd(scale(dataMatrixOrdered))  
pca1 <- prcomp(dataMatrixOrdered, scale = TRUE)  
plot(pca1$rotation[, 1], svd1$v[, 1], pch = 19, xlab = "Principal Component 1",  
      ylab = "Right Singular Vector 1")  
abline(c(0, 1))
```



Components of the SVD - variance explained

```
constantMatrix <- dataMatrixOrdered*0
for(i in 1:dim(dataMatrixOrdered)[1]){constantMatrix[i,] <- rep(c(0,1),each=5)}
svd1 <- svd(constantMatrix)
par(mfrow=c(1,3))
image(t(constantMatrix)[,nrow(constantMatrix):1])
plot(svd1$d, xlab="Column", ylab="Singular value", pch=19)
plot(svd1$d^2/sum(svd1$d^2), xlab="Column", ylab="Prop. of variance explained", pch=19)
```

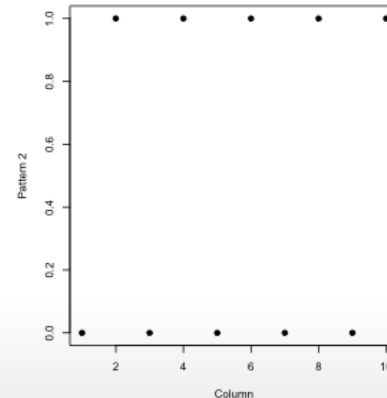
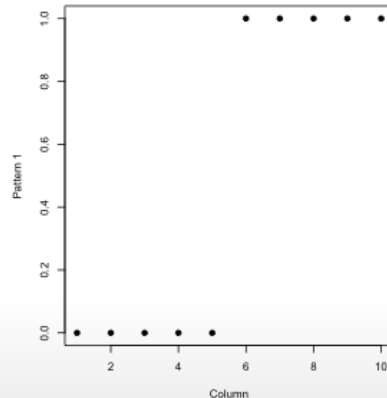
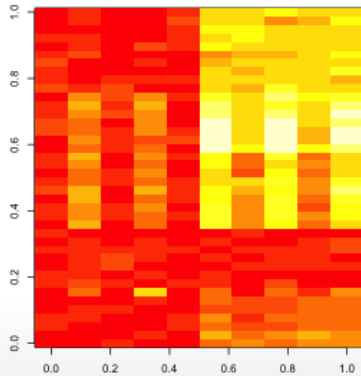


What if we add a second pattern?

```
set.seed(678910)
for (i in 1:40) {
  # flip a coin
  coinFlip1 <- rbinom(1, size = 1, prob = 0.5)
  coinFlip2 <- rbinom(1, size = 1, prob = 0.5)
  # if coin is heads add a common pattern to that row
  if (coinFlip1) {
    dataMatrix[i, ] <- dataMatrix[i, ] + rep(c(0, 5), each = 5)
  }
  if (coinFlip2) {
    dataMatrix[i, ] <- dataMatrix[i, ] + rep(c(0, 5), 5)
  }
}
hh <- hclust(dist(dataMatrix))
dataMatrixOrdered <- dataMatrix[hh$order, ]
```

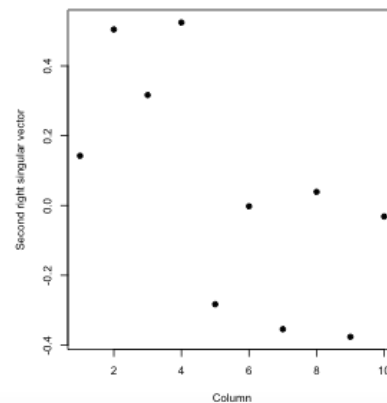
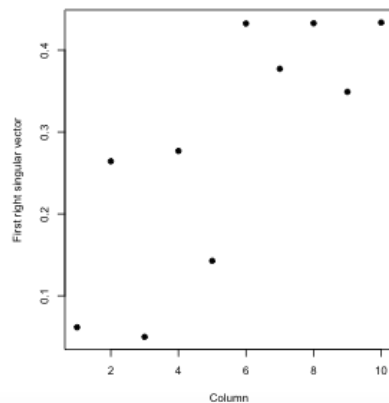
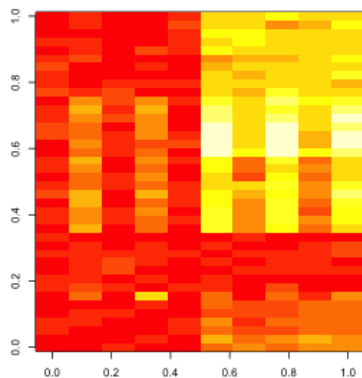
Singular value decomposition - true patterns

```
svd2 <- svd(scale(dataMatrixOrdered))  
par(mfrow = c(1, 3))  
image(t(dataMatrixOrdered)[, nrow(dataMatrixOrdered):1])  
plot(rep(c(0, 1), each = 5), pch = 19, xlab = "Column", ylab = "Pattern 1")  
plot(rep(c(0, 1), 5), pch = 19, xlab = "Column", ylab = "Pattern 2")
```



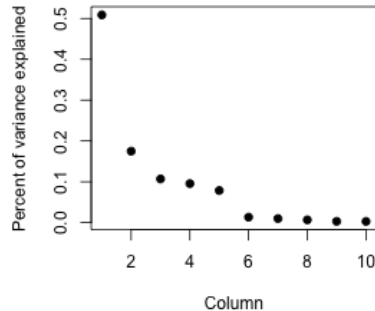
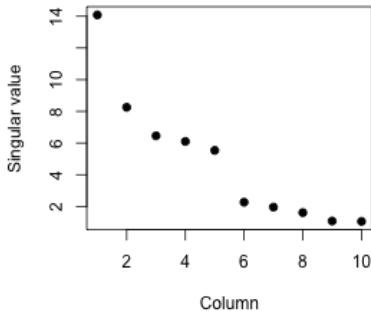
v and patterns of variance in rows

```
svd2 <- svd(scale(dataMatrixOrdered))  
par(mfrow = c(1, 3))  
image(t(dataMatrixOrdered)[, nrow(dataMatrixOrdered):1])  
plot(svd2$v[, 1], pch = 19, xlab = "Column", ylab = "First right singular vector")  
plot(svd2$v[, 2], pch = 19, xlab = "Column", ylab = "Second right singular vector")
```



d and variance explained

```
svd1 <- svd(scale(dataMatrixOrdered))  
par(mfrow = c(1, 2))  
plot(svd1$d, xlab = "Column", ylab = "Singular value", pch = 19)  
plot(svd1$d^2/sum(svd1$d^2), xlab = "Column", ylab = "Percent of variance explained",  
      pch = 19)
```



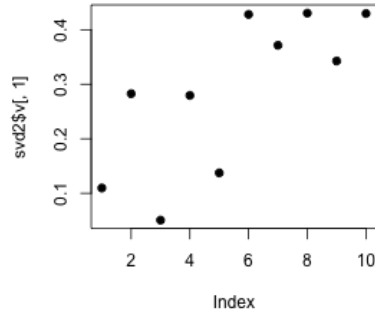
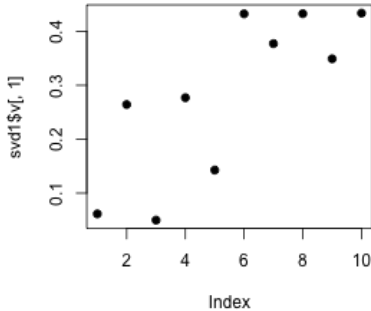
Missing values

```
dataMatrix2 <- dataMatrixOrdered
## Randomly insert some missing data
dataMatrix2[sample(1:100, size = 40, replace = FALSE)] <- NA
svd1 <- svd(scale(dataMatrix2)) ## Doesn't work!
```

```
## Error: infinite or missing values in 'x'
```

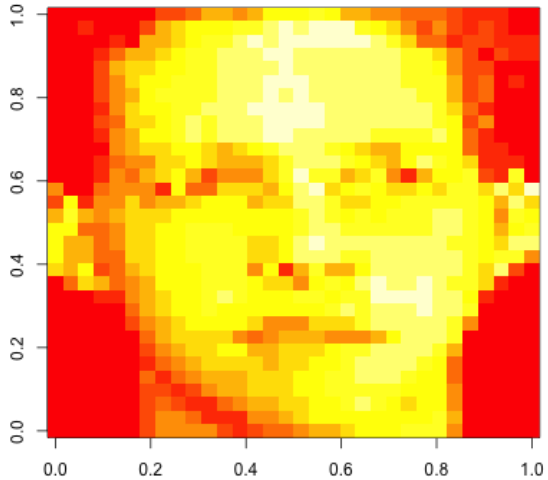
Imputing {impute}

```
library(impute) ## Available from http://bioconductor.org
dataMatrix2 <- dataMatrixOrdered
dataMatrix2[sample(1:100,size=40,replace=FALSE)] <- NA
dataMatrix2 <- impute.knn(dataMatrix2)$data
svd1 <- svd(scale(dataMatrixOrdered)); svd2 <- svd(scale(dataMatrix2))
par(mfrow=c(1,2)); plot(svd1$v[,1],pch=19); plot(svd2$v[,1],pch=19)
```



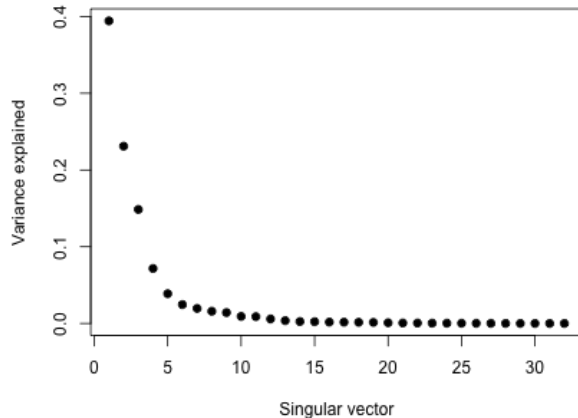
Face example

```
load("data/face.rda")  
image(t(faceData)[, nrow(faceData):1])
```



Face example - variance explained

```
svd1 <- svd(scale(faceData))  
plot(svd1$d^2/sum(svd1$d^2), pch = 19, xlab = "Singular vector", ylab = "Variance explained")
```

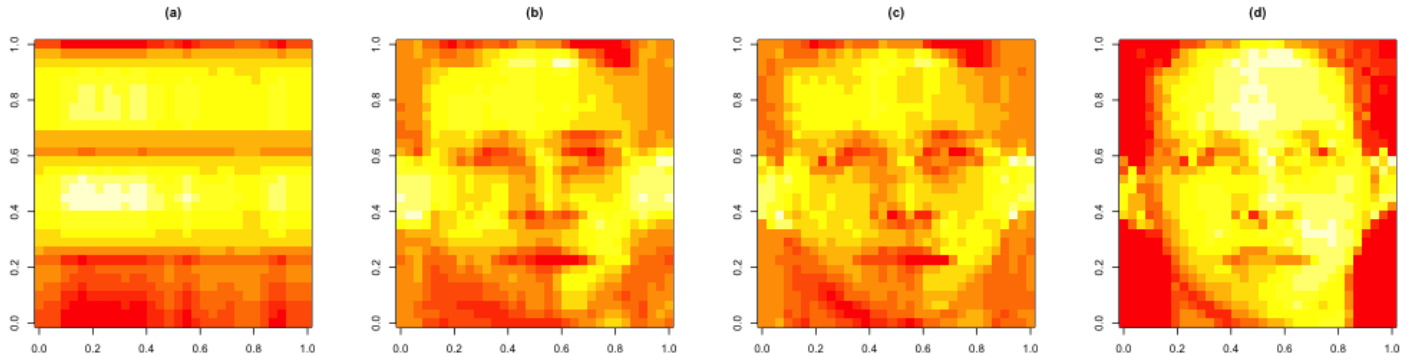


Face example - create approximations

```
svd1 <- svd(scale(faceData))  
## Note that %*% is matrix multiplication  
  
# Here svd1$d[1] is a constant  
approx1 <- svd1$u[, 1] %*% t(svd1$v[, 1]) * svd1$d[1]  
  
# In these examples we need to make the diagonal matrix out of d  
approx5 <- svd1$u[, 1:5] %*% diag(svd1$d[1:5]) %*% t(svd1$v[, 1:5])  
approx10 <- svd1$u[, 1:10] %*% diag(svd1$d[1:10]) %*% t(svd1$v[, 1:10])
```

Face example - plot approximations

```
par(mfrow = c(1, 4))  
image(t(approx1)[, nrow(approx1):1], main = "(a)")  
image(t(approx5)[, nrow(approx5):1], main = "(b)")  
image(t(approx10)[, nrow(approx10):1], main = "(c)")  
image(t(faceData)[, nrow(faceData):1], main = "(d)") ## Original data
```



Notes and further resources

- Scale matters
- PC's/SV's may mix real patterns
- Can be computationally intensive
- [Advanced data analysis from an elementary point of view](#)
- [Elements of statistical learning](#)
- Alternatives
 - [Factor analysis](#)
 - [Independent components analysis](#)
 - [Latent semantic analysis](#)