Multivariate Analysis Lecture 11: Applications of PCA

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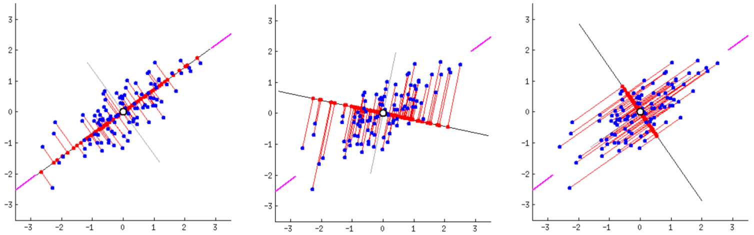
Section 1

Review of PCA

PCA: Different Directions Have Different Variances

- PCA projects the original data onto a lower-dimensional space using linear combinations of the original features.
- Click the link to see the animated version!



The Spectral Decomposition of A Covariance Matrix

- Let $\mathbf{\Sigma}_{p\times p}$ be the covariance matrix of a random vector $\mathbf{X} \in \mathbb{R}$.
- A Covariance matrix is a positive definite or positive semi-definite.
- Spectral decomposition:

$$\mathbf{\Sigma} = \Gamma\Lambda\Gamma^T$$

  where Λ is the diagonal matrix of the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_p \geq 0$
- The Eigenvectors are the columns of $\Gamma = (\gamma_1, \cdots, \gamma_p)$, where γ_i is the *i*th eigenvector.

First PC

- Let $Y_1 = a^T \mathbf{X}$ denote the first principal component, which is defined as the linear combination reaches the maximum variance subject to $||a|| = 1$. Mathematically, we are looking for a s.t.
$$a = \underset{a^T a = 1}{\arg\max}\ a^T \mathbf{\Sigma} a$$
- First Principal Component. Among all the linear combinations of $\mathbf{X}$, the one with the maximum variance is $Y_1 = \gamma_1^T \mathbf{X}$ and the corresponding variance is λ_1.

2nd PC

- Second Principal Component. Mathematically, we are looking for a s.t.

$$a = \underset{a^T a=1, a^T \gamma_1=0}{\arg\max} \; a^T \mathbf{\Sigma} a$$

- The second PC is

$$Y_2 = \gamma_2^T \mathbf{X}$$

ith PC

- For the *i*th principal component, we are looking for a linear combination in terms of $a^T\mathbf{X}$ such as

$$a = \underset{a^T a=1, a^T\gamma_1=0,\cdots,a^T\gamma_{i-1}=0}{\arg\max} a^T\mathbf{\Sigma}a$$

- The *i*th principal component is

$$Y_i = \gamma_i^T\mathbf{X}$$

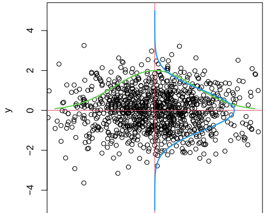
Example

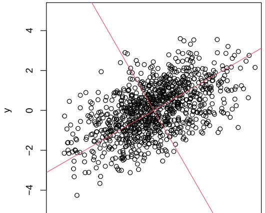
```r
n=1000; set.seed(1)
Sigma1=diag(c(4,1), 2, 2); Sigma2=diag(c(1,4), 2, 2)
theta=pi/6
R1=matrix(c(cos(theta), sin(theta), -sin(theta), cos(theta)), 2,2)
R2=matrix(c(cos(theta), sin(theta), -sin(theta), cos(theta)), 2,2)
Sigma3=R1%*%Sigma1%*%t(R1)
Sigma4=R2%*%Sigma1%*%t(R2)
set.seed(1)
X1=data.frame(mvrnorm(n, rep(0,2), Sigma1)); names(X1)=c("x","y")
X2=data.frame(mvrnorm(n, rep(0,2), Sigma2)); names(X2)=c("x","y")
X3=data.frame(mvrnorm(n, rep(0,2), Sigma3)); names(X3)=c("x","y")
X4=data.frame(mvrnorm(n, rep(0,2), Sigma4)); names(X4)=c("x","y")
Sigma3
```

```
##          [,1]     [,2]
## [1,] 3.250000 1.299038
## [2,] 1.299038 1.750000
```

Simulated Data

```r
par(mfrow=c(1,2),pty="s")
plot(X1, xlim=c(-5,5), ylim=c(-5,5));
abline(0,0, col=2); abline(v=0, col=2)
lines(seq(-5,5,0.1), 10*dnorm(seq(-5,5,0.1), 0, 2), col=3, lwd=2)
lines(10*dnorm(seq(-5,5,0.1), 0, 1), seq(-5,5,0.1), col=4, lwd=2)
plot(X3, xlim=c(-5,5), ylim=c(-5,5));
abline(0,1/sqrt(3), col=2); abline(0, -sqrt(3), col=2)
```





Example: 1st PC and 2nd PC

```
gamma1=eigen(Sigma3)$vectors[,1]
gamma1
```

```
## [1] -0.8660254 -0.5000000
```

```
gamma2=eigen(Sigma3)$vectors[,2]
gamma2
```

```
## [1]  0.5000000 -0.8660254
```

- 1st PC: $-0.8660254x - 0.5y$, in the direction of γ_1.
- 2nd PC: $0.5x - 0.8660254y$, in the direction of γ_2.

Example: Project An Observation to 1st PC

- Consider a, the first observation in X_3:

```
a=as.matrix(X3[1,],1,2)
a
```

```
##          x        y
## 1 1.20705 2.447848
```

- We project it to the direction of $\gamma_1 = (-0.8660254, -0.5)^T$. Because γ_1 is a unit vector

Example: Project An Observation to 1st PC

```
a
```

```
##          x        y
## 1 1.20705 2.447848
```

```
gamma1
```

```
## [1] -0.8660254 -0.5000000
```

```
a%*%gamma1 #inner product
```

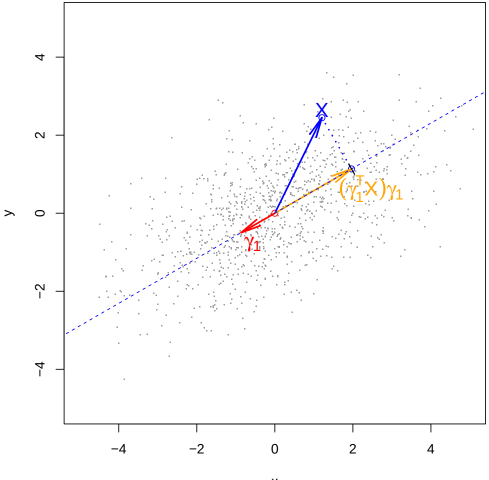
```
##        [,1]
## 1 -2.26926
```

```
a[1]*gamma1[1]+a[2]*gamma1[2] #inner product
```

```
## [1] -2.26926
```

```
(a%*%gamma1)%*%gamma1 #projection
```

Example: Project An Observation to 1st PC



Example: Project All Observations to 1st PC

- The data matrix X_3 is a 1000×2 matrix, where each row is an observation.
- The projected values of all observations to the first PC is given by

$$Y_1 = \mathbf{X}_3 \gamma_1,$$

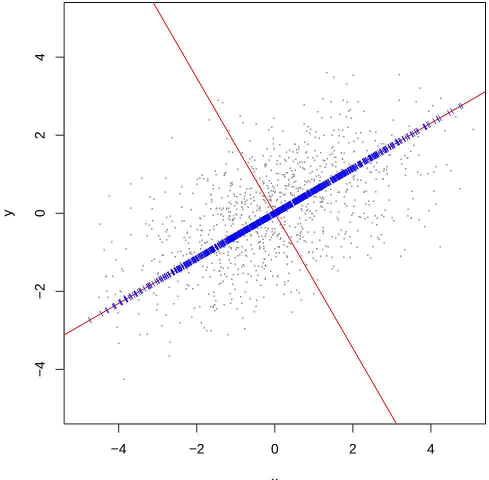
where

- X_3 is 1000-by-2
- γ_1 is 2-by-1, the first eigenvector of the covariance matrix $\mathbf{\Sigma}$.

Example: Project All Observations to 1st PC

```
par(mfrow=c(1,1),pty="s")
plot(X3, xlim=c(-5,5), ylim=c(-5,5), col=8, pch=".");
abline(0,1/sqrt(3), col="red"); abline(0, -sqrt(3), col="red")
points(x=0,y=0, col="red")
proj=as.matrix(X3)%*%gamma1 %*%gamma1
text(x=proj[,1],y=proj[,2], labels="|", col="blue", srt=30, cex=0.5)
```

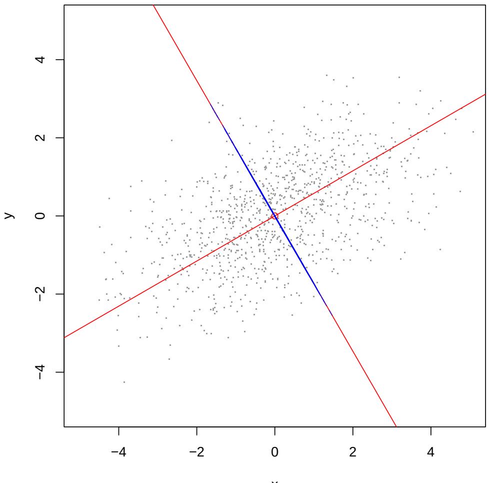
Example: Project All Observations to 1st PC



Example: Project All Observations to 2nd PC

```
par(mfrow=c(1,1),pty="s")
plot(X3, xlim=c(-5,5), ylim=c(-5,5), col=8, pch=".");
abline(0,1/sqrt(3), col="red"); abline(0, -sqrt(3), col="red")
points(x=0,y=0, col="red")
proj=as.matrix(X3)%*%gamma2 %*%gamma2
text(x=proj[,1],y=proj[,2], labels="|", col="blue", srt=30, cex=0.5)
```

Example: Project All Observations to 2nd PC



Example: The Two PCs

- The projected values on the first and second PCs are given by

$$PC_1 = \mathbf{X}_3\gamma_1,$$

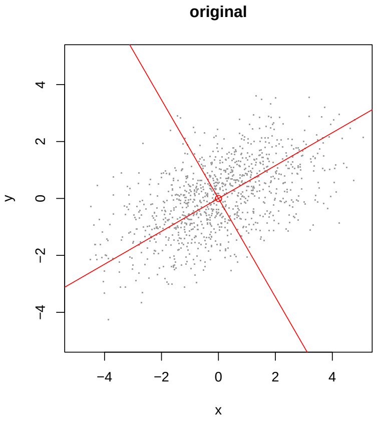
$$PC_2 = \mathbf{X}_3\gamma_2$$

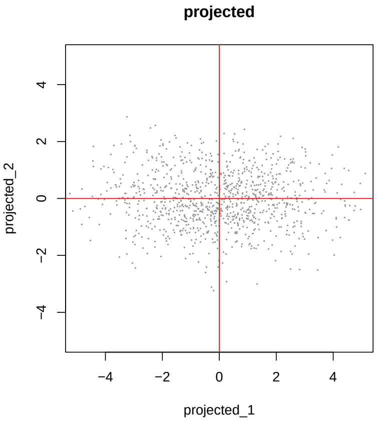
- Note, the above are values on the two directions, not the projections; in other words, the directional information is not included.

Example: The Two PCs

```
par(mfrow=c(1,2),pty="s")
plot(X3, xlim=c(-5,5), ylim=c(-5,5), col=8, pch=".", main="original");
abline(0,1/sqrt(3), col="red"); abline(0, -sqrt(3), col="red")
points(x=0,y=0, col="red")
projected_1=as.matrix(X3)%*%gamma1
projected_2=as.matrix(X3)%*%gamma2

plot(projected_1, projected_2, xlim=c(-5,5), ylim=c(-5,5), col=8, pch="
abline(h=0, v=0, col="red")
```

Example: The Two PCs





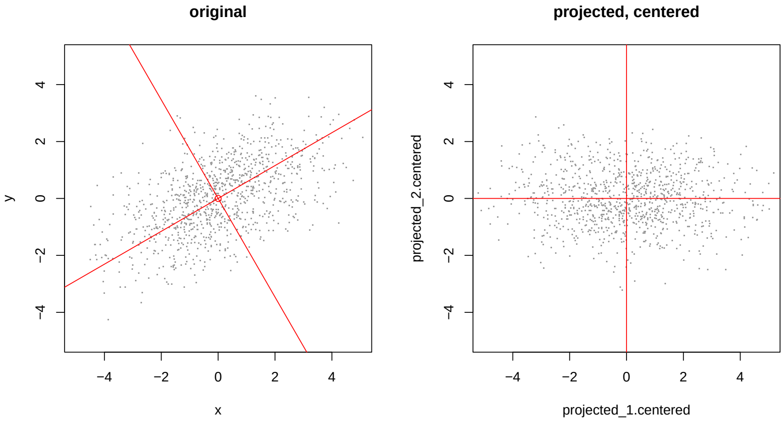
Example: Centered Data

- In the example, the data were generated from mean 0.
- In practice, the data may not be centered. Although the center information is not essential for PCA, it is often useful to center the data before applying PCA.
- Centering the data is equivalent to subtracting the mean from each observation.

Example: Centered Data

```
X3_centered=scale(X3, scale=FALSE)
projected_1.centered=as.matrix(X3_centered)%*%gamma1
projected_2.centered=as.matrix(X3_centered)%*%gamma2

par(mfrow=c(1,2),pty="s")
plot(X3, xlim=c(-5,5), ylim=c(-5,5), col=8, pch=".", main="original");
abline(0,1/sqrt(3), col="red"); abline(0, -sqrt(3), col="red")
points(x=0,y=0, col="red")

plot(projected_1.centered, projected_2.centered, xlim=c(-5,5), ylim=c(-
abline(h=0, v=0, col="red")
```

Example: Centered Data



Section 2

Variance Exaplained

Dimensionality Reduction Using PCA

- PCA aims to reduce the dimensionality of a dataset while preserving as much variance as possible.
- Dimensionality reduction using PCA can
  - ease visualization and analysis
  - help identify underlying patterns or structure in the data.
  - improve the performance of machine learning algorithms by reducing noise and collinearity.
- PCA is most effective when the majority of the variance can be captured by a small number of principal components.

Total Variance

- There are at least two justifications to use $\sum_{i=1}^{p} \lambda_i$ as the total variance:
  1. One way to quantify the total variance in $\mathbf{X}$ is the trace of the covariance matrix $\mathbf{\Sigma}$
     - Recall that $tr(\mathbf{\Sigma}) = \sum_{i=1}^{n} \lambda_i$
  2. The variance of ith PC is $Var(Y_i) = Var(\gamma_i^T \mathbf{X}) = \lambda_i$. Thus, the total variance of PCs is

$$\sum_{i=1}^{p} Var(Y_i) = \sum_{i=1}^{p} \lambda_i$$

Variance Explained

- The proportion of the variance explained by *i*th PC explains is

$$\lambda_i / \sum_{i=1}^{p} \lambda_i$$

- Cumulative Explained Variance is the proportion of the total variance explained by the first k PCs is

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{p} \lambda_i}$$

Variance Explained: Example

```r
lambda=eigen(Sigma3)$values
# Prop of Variance explained by 1st PC
lambda[1]/sum(lambda)
```

```
## [1] 0.8
```

```r
# Prop of Cumulative Variance explained by two PCs
sum(lambda[1:2])/sum(lambda)
```

```
## [1] 1
```

- In this example, 1st PC explains 80% of variance, 2nd PC explains 20% of variance.

Section 3

Apply PCA to Data

Estimate $\boldsymbol{\Sigma}$.

- We have discussed how to find PCs for a random vector $\mathbf{X}_{p\times 1} \sim (0, \boldsymbol{\Sigma})$, where $\boldsymbol{\Sigma}$ is a known covariance matrix.
- In practice,
    - the observed data is an $n \times p$ data matrix $\mathbf{X}_{n\times p}$
    - $\boldsymbol{\Sigma}$ is unknown, which can be estimated by the sample covariance matrix $\mathbf{S}$.

Apply PCA to A Data Set: Steps

1. Estimate $\mathbf{\Sigma}$ by the sample covariance matrix $\mathbf{S}$
2. Compute the eigenvectors of $\mathbf{S}$, and denote them by $\gamma_1, \cdots, \gamma_p$
3. Compute the PCs

- PC1: $Y_1 = \mathbf{X}\gamma_1$, which is a $n \times 1$ vector
- PC2: $Y_2 = \mathbf{X}\gamma_2$, which is a $n \times 1$ vector
- $\cdots\cdots$
- PCi: $Y_i = \mathbf{X}\gamma_i$, which is a $n \times 1$ vector
- Equivalently, compute

$$Y_{pc} = \mathbf{X}\Gamma$$

which is the $n \times p$ matrix with the ith column being the ith PC.

Section 4

Example: Iris Data

Outline

- PCA using raw data
- PCA using centered data
- PCA using standardized data
- Scree plot
- Biplot

Subsection 1

PCA Using Raw Data

Estimate Σ

```
############################################################
## iris data
##rearrange the data such as the response matrix is an n-by-p matrix
Y=cbind(SepalL=c(iris3[,1,1],iris3[,1,2],iris3[,1,3]),
SepalW=c(iris3[,2,1],iris3[,2,2],iris3[,2,3]),
PetalL=c(iris3[,3,1],iris3[,3,2],iris3[,3,3]),
PetalW=c(iris3[,4,1],iris3[,4,2],iris3[,4,3]))
#for unknown reasons, data.frame won't work but cbind works
#alternatively, we can use the following way to define y
#y=aperm(iris3,c(1,3,2));dim(y)=c(150,4)
S=cov(Y)
```

Compute PCs

```
eigen.vec=eigen(S)$vectors
eigen.val=eigen(S)$values
gamma1=eigen.vec[,1]
gamma2=eigen.vec[,2]
gamma3=eigen.vec[,3]
gamma4=eigen.vec[,4]
# The four pcs:
pc1=Y%*%gamma1
pc2=Y%*%gamma2
pc3=Y%*%gamma3
pc4=Y%*%gamma4
# Equivalently, we can obtain the nx4 matrix of PCs
PCs=Y%*%eigen.vec
```

The Loadings (Weights)

```
gamma1
```

```
## [1]  0.36138659 -0.08452251  0.85667061  0.35828920
```

```
gamma2
```

```
## [1] -0.65658877 -0.73016143  0.17337266  0.07548102
```

```
gamma3
```

```
## [1] -0.58202985  0.59791083  0.07623608  0.54583143
```

```
gamma4
```

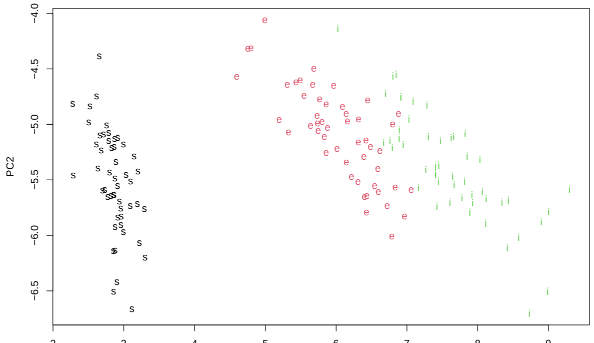
```
## [1]  0.3154872 -0.3197231 -0.4798390  0.7536574
```

The Four PCs

- PC 1: $Y_1 = 0.36SL - 0.08SW + 0.86PL + 0.36PL$
- PC 2: $Y_2 = -0.66SL - 0.73SW + 0.17PL + 0.08PL$
- PC 3: $Y_3 = -0.60SL - 0.60SW + 0.08PL + 0.55PL$
- PC 4: $Y_4 = 0.32SL - 0.32SW - 0.48PL + 0.75PL$
- Note that PC1 loads the most on PL. This is not surprising because PL has the largest variance among all the four features.

Visualize PC1 and PC2

```
plot(pc1,pc2,xlab="PC1", ylab="PC2", type="n")
points(pc1[1:50], pc2[1:50], col=1, pch="s")
points(pc1[51:100], pc2[51:100], col=2, pch="e")
points(pc1[101:150], pc2[101:150], col=3, pch="i")
```

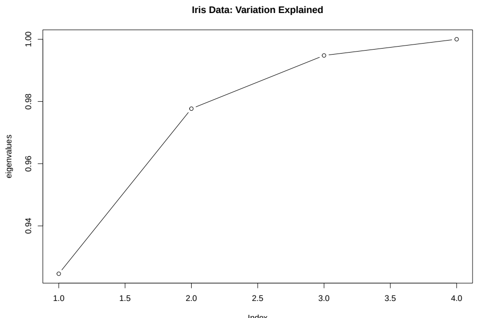


Proportions of Variation Explained (Cumulative)

```r
cumsum(eigen.val/sum(eigen.val))
```

```
## [1] 0.9246187 0.9776852 0.9947878 1.0000000
```

```r
plot(cumsum(eigen.val)/sum(eigen.val), type="b", main="Iris Data: Varia
ylab="eigenvalues")
```



Subsection 2

PCA Using Centered Data

PCA Using Centered Data

```
# The four pcs:
pc1_c=scale(Y, scale=FALSE)%*%gamma1
pc2_c=scale(Y, scale=FALSE)%*%gamma2
pc3_c=scale(Y, scale=FALSE)%*%gamma3
pc4_c=scale(Y, scale=FALSE)%*%gamma4
# or
PCs_c=scale(Y, scale=FALSE)%*%eigen(S)$vectors
```

The PCs from R

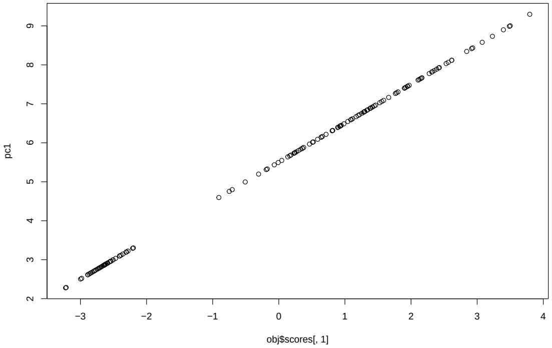
```
#help(princomp), pay attention to fix_sign
obj=princomp(Y)
names(obj)
```

```
## [1] "sdev"     "loadings" "center"   "scale"    "n.obs"    "scores"
```

```
#help(loadings), pay attention to cutoff
#check loadings and scores to verify that
#they are same as what we calculated
```

The PCs from R vs our PCs

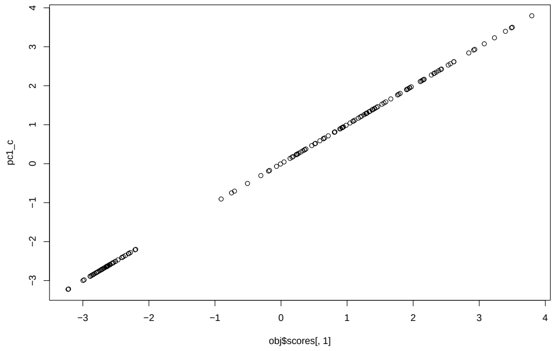
```r
plot(obj$scores[,1], pc1)
```



- The diffence is due to not centering vs centering

R Uses Centered Data to Compute PCA

```
plot(obj$scores[,1], pc1_c)
```



- They are identical

Subsection 3

PCA Using Standardized Data

Covariance of Standardized Data

- The covariance matrix using standardized data

```
cov(scale(Y, scale=TRUE))
```

```
##           SepalL     SepalW     PetalL     PetalW
## SepalL  1.0000000 -0.1175698  0.8717538  0.8179411
## SepalW -0.1175698  1.0000000 -0.4284401 -0.3661259
## PetalL  0.8717538 -0.4284401  1.0000000  0.9628654
## PetalW  0.8179411 -0.3661259  0.9628654  1.0000000
```

Correlation Matrix

- The correlation matrix is the covariance matrix of standardized data

```r
cor(Y)
```

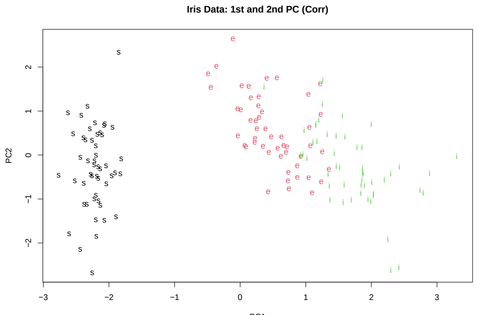
```
##            SepalL     SepalW     PetalL     PetalW
## SepalL  1.0000000 -0.1175698  0.8717538  0.8179411
## SepalW -0.1175698  1.0000000 -0.4284401 -0.3661259
## PetalL  0.8717538 -0.4284401  1.0000000  0.9628654
## PetalW  0.8179411 -0.3661259  0.9628654  1.0000000
```

PCA Based on Correlation Matrix

```
gamma1_s=eigen(cor(Y))$vectors[,1]
gamma2_s=eigen(cor(Y))$vectors[,2]
gamma3_s=eigen(cor(Y))$vectors[,3]
gamma4_s=eigen(cor(Y))$vectors[,4]
```

The PCs based on Correlation Matrix

```
PCs_s=scale(Y)%*% eigen(cor(Y))$vectors
plot(PCs_s[,1:2], xlab="PC1", ylab="PC2",
     main="Iris Data: 1st and 2nd PC (Corr)", type="n")
points(PCs_s[1:50, 1:2], col=1, pch="s")
points(PCs_s[51:100, 1:2], col=2, pch="e")
points(PCs_s[101:150, 1:2], col=3, pch="i")
```



PCA with Standardized Data in R

- The princomp function in R has an option to use correlation matrix rather than covariance matrix

```
obj.cor=princomp(Y, cor=TRUE)
```

Standardized vs Not-Standardized

- Loadings

```
obj$loadings[,1:4]
```

```
##               Comp.1      Comp.2      Comp.3     Comp.4
## SepalL  0.36138659  0.65658877  0.58202985  0.3154872
## SepalW -0.08452251  0.73016143 -0.59791083 -0.3197231
## PetalL  0.85667061 -0.17337266 -0.07623608 -0.4798390
## PetalW  0.35828920 -0.07548102 -0.54583143  0.7536574
```

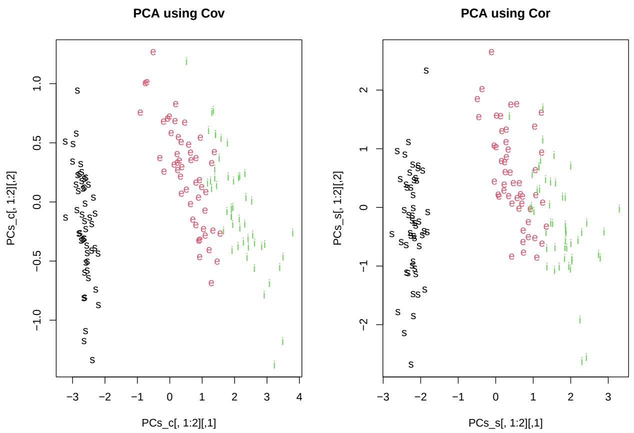
```
obj.cor$loading[,1:4]
```

```
##             Comp.1     Comp.2     Comp.3     Comp.4
## SepalL  0.5210659 0.37741762  0.7195664  0.2612863
## SepalW -0.2693474 0.92329566 -0.2443818 -0.1235096
## PetalL  0.5804131 0.02449161 -0.1421264 -0.8014492
## PetalW  0.5648565 0.06694199 -0.6342727  0.5235971
```

PCA based on Cov vs Cor: 1st and 2nd PC

```
par(mfrow=c(1,2))
plot(PCs_c[,1:2], main="PCA using Cov", type="n")
points(PCs_c[1:50, 1:2], col=1, pch="s")
points(PCs_c[51:100, 1:2], col=2, pch="e")
points(PCs_c[101:150, 1:2], col=3, pch="i")
plot(PCs_s[,1:2], main="PCA using Cor", type="n")
points(PCs_s[1:50, 1:2], col=1, pch="s")
points(PCs_s[51:100, 1:2], col=2, pch="e")
points(PCs_s[101:150, 1:2], col=3, pch="i")
```

PCA Using Standardized Data

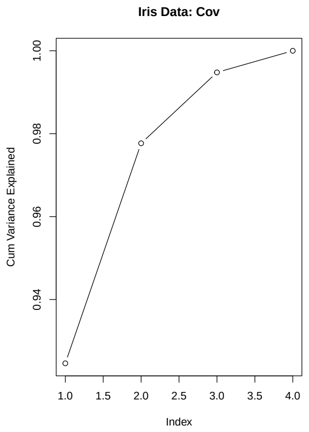


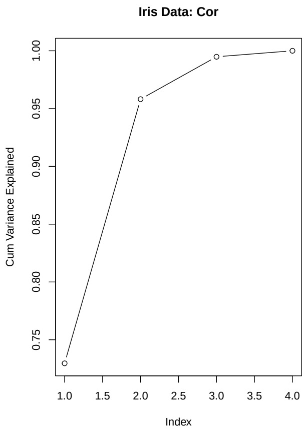
PCA based on Cov vs Cor: Variance Explained (Cumulatively)

```
par(mfrow=c(1,2))
cumsum(eigen(cov(Y))$values)/sum(eigen(cov(Y))$values)
plot(cumsum(eigen(cov(Y))$values)/sum(eigen(cov(Y))$values),
     type="b", main="Iris Data: Cov",ylab="Cum Variance Explained")
cumsum(eigen(cor(Y))$values)/sum(eigen(cor(Y))$values)
plot(cumsum(eigen(cor(Y))$values)/sum(eigen(cor(Y))$values),
     type="b", main="Iris Data: Cor",ylab="Cum Variance Explained")
```

PCA Using Standardized Data

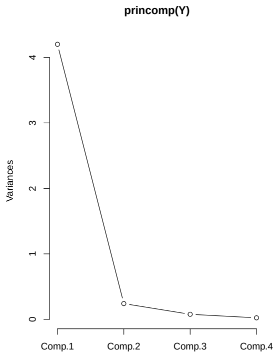
```
## [1] 0.9246187 0.9776852 0.9947878 1.0000000

## [1] 0.7296245 0.9581321 0.9948213 1.0000000
```

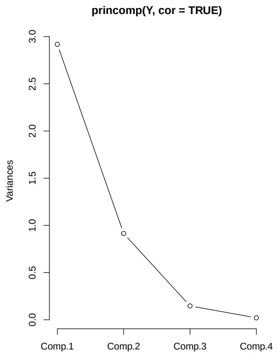




PCA based on Cov vs Cor: Variances (Scree Plot)

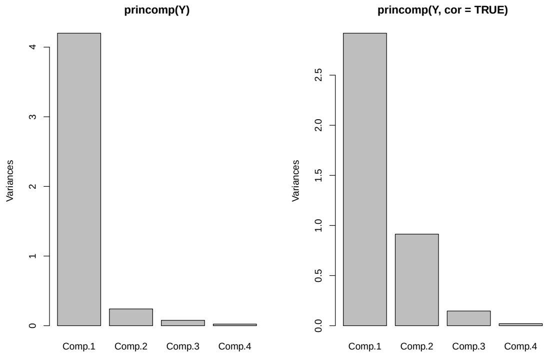
```r
par(mfrow=c(1,2))
plot(princomp(Y), type="l")
plot(princomp(Y, cor=TRUE), type="l")
```





PCA based on Cov vs Cor: Variances (Scree Plot)

```r
par(mfrow=c(1,2))
plot(princomp(Y))
plot(princomp(Y, cor=TRUE))
```



Visualizing PCA

- We have seen scree plots for visualizing the variance explained by each PC
- Biplots are another way to visualize PCA results
- A biplot is a visualization tool that combines:
  - Scores (projected data points)
  - Loadings (variable vectors) from Principal Component Analysis (PCA).
- A biplot shows relationships between observations and between variables in reduced dimensions (e.g., PC1 vs. PC2).

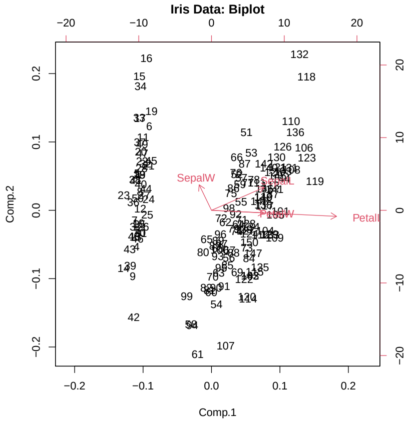
Biplot: loadings

```
obj$loadings
```

```
##
## Loadings:
##        Comp.1 Comp.2 Comp.3 Comp.4
## SepalL  0.361  0.657  0.582  0.315
## SepalW         0.730 -0.598 -0.320
## PetalL  0.857 -0.173        -0.480
## PetalW  0.358        -0.546  0.754
##
##                Comp.1 Comp.2 Comp.3 Comp.4
## SS loadings      1.00   1.00   1.00   1.00
## Proportion Var   0.25   0.25   0.25   0.25
## Cumulative Var   0.25   0.50   0.75   1.00
```

Biplot

```
biplot(obj, main="Iris Data: Biplot")
```



Biplot: the scale parameter

- The loadings and scores often have very different scales.
- The scale parameter harmonizes them for visualization.
- The default value is 1, which means the loadings are scaled by 1 and the scores are scaled by 1, i.e., cores and loadings are scaled equally.
- Make scale < 1 if variable arrows are too small to interpret.
- Use scale > 1 if data points are too crowded.

Section 5

Example: Wine Data

The Wine Data

```
wine = read.csv("http://archive.ics.uci.edu/ml/machine-learning-databas
dim(wine)
```

```
## [1] 4898   12
```

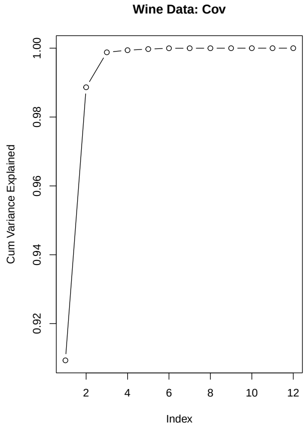
```
head(wine)
```

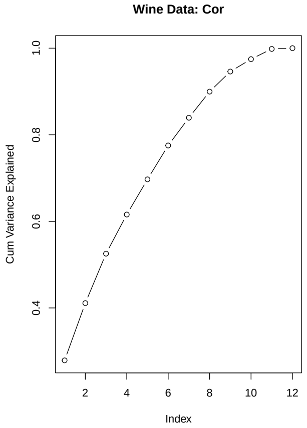
```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chloride
## 1           7.0             0.27        0.36           20.7      0.04
## 2           6.3             0.30        0.34            1.6      0.04
## 3           8.1             0.28        0.40            6.9      0.05
## 4           7.2             0.23        0.32            8.5      0.05
## 5           7.2             0.23        0.32            8.5      0.05
## 6           8.1             0.28        0.40            6.9      0.05
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates al
## 1                  45                  170  1.0010 3.00      0.45
## 2                  14                  132  0.9940 3.30      0.49
## 3                  30                   97  0.9951 3.26      0.44
```

PCA based on Cov vs Cor: Variance Explained

```r
par(mfrow=c(1,2))
cumsum(eigen(cov(wine))$values)/sum(eigen(cov(wine))$values)
plot(cumsum(eigen(cov(wine))$values)/sum(eigen(cov(wine))$values),
     type="b", main="Wine Data: Cov",ylab="Cum Variance Explained")
cumsum(eigen(cor(wine))$values)/sum(eigen(cor(wine))$values)
plot(cumsum(eigen(cor(wine))$values)/sum(eigen(cor(wine))$values),
     type="b", main="Wine Data: Cor",ylab="Cum Variance Explained")
```

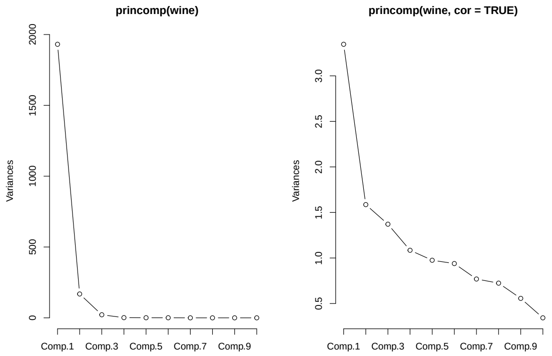
```
## [1] 0.9093312 0.9886453 0.9987968 0.9994164 0.9997397 0.9999753 0.9
## [8] 0.9999906 0.9999960 0.9999998 1.0000000 1.0000000

## [1] 0.2788891 0.4110633 0.5253276 0.6157327 0.6970063 0.7752366 0.8
## [8] 0.8996651 0.9460402 0.9746180 0.9982942 1.0000000
```





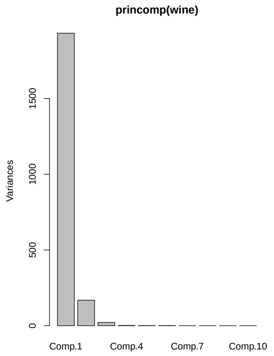
PCA based on Cov vs Cor: Variances (Scree Plot)

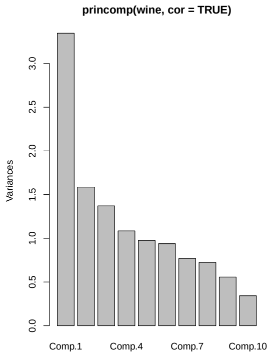
```
par(mfrow=c(1,2))
plot(princomp(wine), type="l")
plot(princomp(wine, cor=TRUE), type="l")
```



PCA based on Cov vs Cor: Variances (Scree Plot)

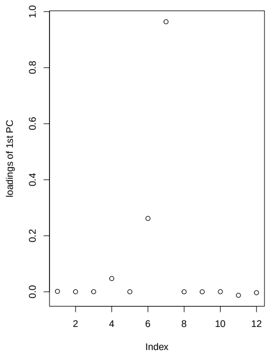
```
par(mfrow=c(1,2))
plot(princomp(wine))
plot(princomp(wine, cor=TRUE))
```

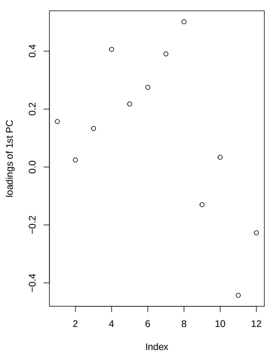




PCA based on Cov vs Cor: Loadings of 1st PC

```
par(mfrow=c(1,2))
plot(princomp(wine)$loadings[,1], ylab="loadings of 1st PC")
plot(princomp(wine, cor=TRUE)$loadings[,1], ylab="loadings of 1st PC")
```





Wine Data: PCA_COV and PCA_COR Are Different

- In the wine data, raw data and standardized data give very different results
- Raw Data: the first PC dominants the rest
- Standardized data: the variances of the PCs are less different
- Why?

Wine Data: The measurements

- There are 12 measurements / features in the wine data
- The variances are very different

```r
apply(wine, 2, var)
```

```
##        fixed.acidity     volatile.acidity          citric.acid
##         7.121136e-01         1.015954e-02         1.464579e-02
##       residual.sugar            chlorides  free.sulfur.dioxide
##         2.572577e+01         4.773337e-04         2.892427e+02
## total.sulfur.dioxide              density                   pH
##         1.806085e+03         8.945524e-06         2.280118e-02
##            sulphates              alcohol              quality
##         1.302471e-02         1.514427e+00         7.843557e-01
```

Standardized vs Not-Standardized

- PCA depends on the measurement scale
- When features are not standardized, the leading PCs tend to give larger loadings for features with large variances
- When similar variables are measured using different units, standardization is typically recommended before PCA

Section 6

Choose k

Choose the Number of PCs

- A rule of thumb? Choose the PC's that contain more information than the average amount of information per PC.
- People often choose k such that at least a certain percentage of the total variance is explained. E.g., 80%, 90%, 95%, 99%
- Scree Plots:
    - A scree plot is a plot of the eigenvalues against the number of PCs
    - we look for an "elbow point" where the decrease in eigenvalues becomes less steep. The number of PCs corresponding to the elbow point can be chosen.
- No unified solution. The choice of the number of PCs may depend on the specific problem

Choose the Number of PCs

- Balancing dimensionality reduction and information retention.
- Too few PCs may result in significant loss of information
- Too many PCS is not efficient in dimension reduction application or research question

The Remaining Lectures Will Cover

- Lec 12: Linear Discriminant Analysis
- Lec 13: Linear Discriminant Analysis
- Lec 14: Factor Analysis
- Lec 15: Cluster Analysis
- Lec 16: Canonical Analysis
- Lec 17: Structural Equation Modeling
- Lec 18: Conclusion