Principal Component Analysis

Max Turgeon

STAT 7200–Multivariate Statistics

Objectives

- Discuss population and sample principal component analysis.
- Explain how PCA can be used for visualizing high-dimensional data.
- Present a geometric view on PCA.
- Discuss asymptotic results about PCA.
- Explain how PCA can be used for model selection.

Population PCA i

- **PCA**: Principal Component Analysis
- Dimension reduction method:
    - Let $\mathbf{Y} = (Y_1, \ldots, Y_p)$ be a random vector with covariance matrix Σ. We are looking for a transformation $h : \mathbb{R}^p \to \mathbb{R}^k$, with $k \ll p$ such that $h(\mathbf{Y})$ retains "as much information as possible" about $\mathbf{Y}$.
- In PCA, we are looking for a **linear transformation** $h(y) = w^T y$ with **maximal variance** (where $\|w\| = 1$)
- More generally, we are looking for k linear transformations $w_1, \ldots, w_k$ such that $w_j^T \mathbf{Y}$ has maximal variance and is uncorrelated with $w_1^T \mathbf{Y}, \ldots, w_{j-1}^T \mathbf{Y}$.

Population PCA ii

- First, note that $\mathrm{Var}(w^T\mathbf{Y}) = w^T\Sigma w$. So our optimisation problem is

$$\max_w w^T\Sigma w, \quad \text{with } w^T w = 1.$$

- We will solve this constrained optimisation problem using the method of **Lagrange multipliers**.

Let $f, g : \mathbb{R}^p \to \mathbb{R}$ be differentiable functions. Let c be a real number, and assume that we are looking for an extremum point $\mathbf{y}_0 \in \mathbb{R}^p$ of f subject to the constraint $g(\mathbf{y}_0) = 0$. If such an extremum point exists, then there exists a scalar λ such that

$$\nabla f(\mathbf{y}_0) = \lambda \nabla g(\mathbf{y}_0).$$

Lagrange Multipliers ii

- In practice, this means that we can replace the constrained optimisation problem in p variables

$$\max_{\mathbf{y}} f(\mathbf{y}), \qquad \text{such that } g(\mathbf{y}) = c,$$

with the *unconstrained* optimisation problem in $p+1$ variables

$$\max_{\mathbf{y},\lambda} \left\{ f(\mathbf{y}) - \lambda \left(g(\mathbf{y}) - c \right) \right\}.$$

Population PCA (cont'd) i

- From the theory of Lagrange multipliers, we can look at the *unconstrained* problem

$$\max_{w,\lambda} w^T \Sigma w - \lambda(w^T w - 1).$$

- Write $\phi(w, \lambda)$ for the function we are trying to optimise. We have

$$\begin{aligned}\frac{\partial}{\partial w}\phi(w,\lambda) &= \frac{\partial}{\partial w} w^T \Sigma w - \lambda(w^T w - 1)\\ &= 2\Sigma w - 2\lambda w;\\ \frac{\partial}{\partial \lambda}\phi(w,\lambda) &= w^T w - 1.\end{aligned}$$

Population PCA (cont'd) ii

- From the first partial derivative, we conclude that

$$\Sigma w = \lambda w.$$

- From the second partial derivative, we conclude that $w \neq 0$; in other words, w is an eigenvector of Σ with eigenvalue λ.
- Moreover, at this stationary point of $\phi(w, \lambda)$, we have

$$\mathrm{Var}(w^T\mathbf{Y}) = w^T\Sigma w = w^T(\lambda w) = \lambda w^T w = \lambda.$$

- In other words, to maximise the variance $\mathrm{Var}(w^T\mathbf{Y})$, we need to choose λ to be the *largest* eigenvalue of Σ.

Population PCA (cont'd) iii

- By induction, and using the extra constraints $w_i^T w_j = 0$, we can show that all other linear transformations are given by eigenvectors of Σ.

PCA Theorem

Let $\lambda_1 \geq \cdots \geq \lambda_p$ be the eigenvalues of Σ, with corresponding unit-norm eigenvectors $w_1, \ldots, w_p$. To reduce the dimension of $\mathbf{Y}$ from p to k such that every component of $W^T\mathbf{Y}$ is uncorrelated and each direction has maximal variance, we can take $W = \begin{pmatrix} w_1 & \cdots & w_k \end{pmatrix}$, whose j-th column is w_j.

Properties of PCA i

- Some vocabulary:
  - $Z_i = w_i^T \mathbf{Y}$ is called the i-th **principal component** of $\mathbf{Y}$.
  - w_i is the i-th vector of **loadings**.
- Note that we can take $k = p$, in which case we do not reduce the dimension of $\mathbf{Y}$, but we *transform* it into a random vector with *uncorrelated* components.
- Let $\Sigma = P\Lambda P^T$ be the eigendecomposition of Σ. We have

$$\sum_{i=1}^p \mathrm{Var}(w_i^T \mathbf{Y}) = \sum_{i=1}^p \lambda_i = \mathrm{tr}(\Lambda) = \mathrm{tr}(\Sigma) = \sum_{i=1}^p \mathrm{Var}(Y_i).$$

- Therefore, each linear transformation $w_i^T \mathbf{Y}$ contributes $\lambda_i / \sum_j \lambda_j$ as percentage of the overall variance.

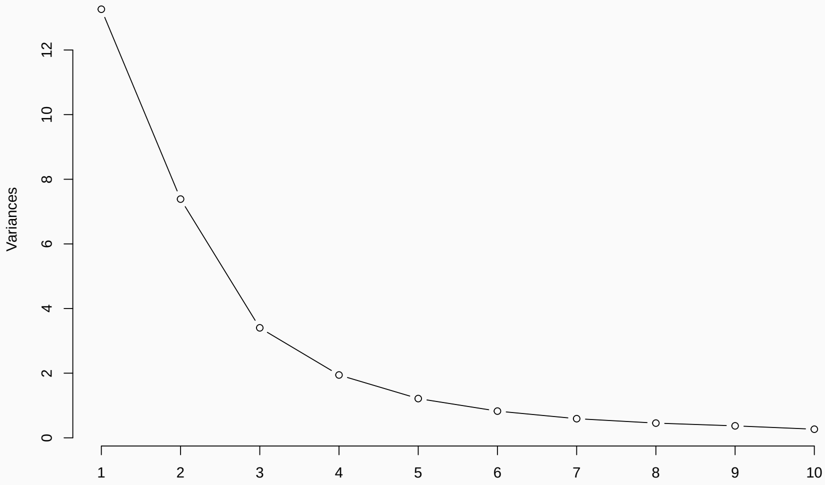
Properties of PCA ii

- Selecting k: One common strategy is to select a threshold (e.g. $c = 0.9$) such that

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

Scree plot

- A **scree plot** is a plot with the sequence $1, \ldots, p$ on the x-axis, and the sequence $\lambda_1, \ldots, \lambda_p$ on the y-axis.
- Another common strategy for selecting k is to choose the point where the curve starts to flatten out.
    - **Note**: This inflection point does not necessarily exist, and it may be hard to identify.


Variances
0
2
4
6
8
10
12
1
2
3
4
5
6
7
8
9
10

Correlation matrix

- When the observations are on the different scale, it is typically more appropriate to normalise the components of $\mathbf{Y}$ before doing PCA.
    - The variance depends on the units, and therefore without normalising, the component with the "smallest" units (e.g. centimeters vs. meters) could be driving most of the overall variance.
- In other words, instead of using Σ, we can use the (population) correlation matrix R.
- **Note**: The loadings and components we obtain from Σ are **not** equivalent to the ones obtained from R.

Sample PCA

- In general, we do not the population covariance matrix Σ.
- Therefore, in practice, we estimate the loadings w_i through the eigenvectors of the sample covariance matrix S_n.
- As with the population version of PCA, if the units are different, we should normalise the components or use the sample correlation matrix.

Example 1 i

```r
library(mvtnorm)
Sigma <- matrix(c(1, 0.5, 0.1,
                  0.5, 1, 0.5,
                  0.1, 0.5, 1),
                ncol = 3)

set.seed(17)
X <- rmvnorm(100, sigma = Sigma)
pca <- prcomp(X)
```

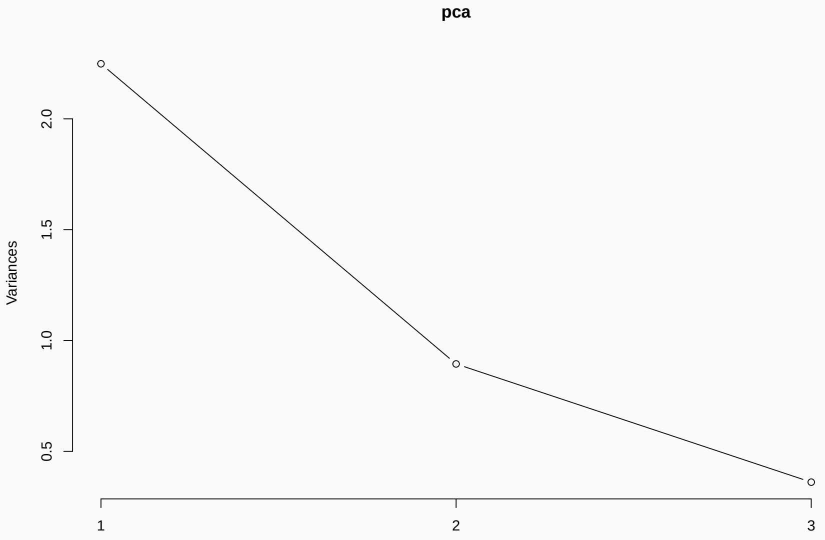
Example 1 ii

```r
summary(pca)
```

```
## Importance of components:
##                           PC1    PC2    PC3
## Standard deviation     1.4994 0.9457 0.6009
## Proportion of Variance 0.6417 0.2552 0.1031
## Cumulative Proportion  0.6417 0.8969 1.0000
```

```r
screeplot(pca, type = 'l')
```

Example 1 iii



Example 2 i

```r
pca <- prcomp(USArrests, scale = TRUE)
```

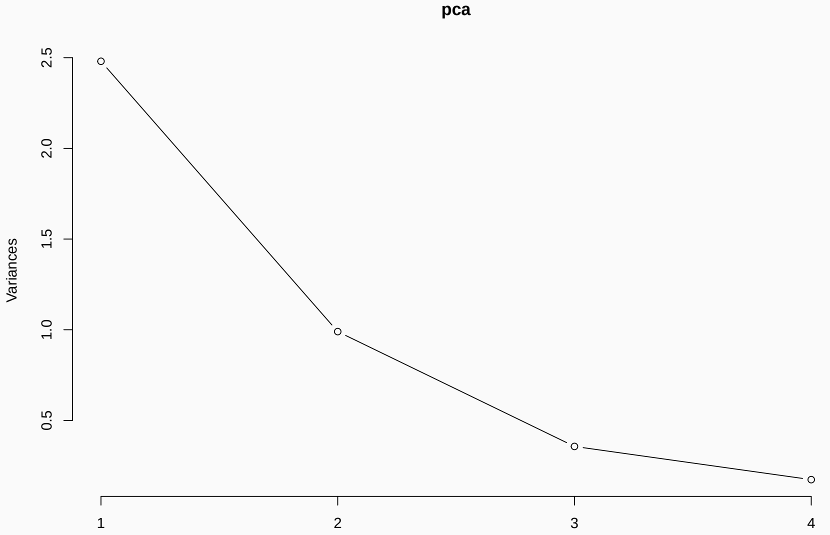
```r
summary(pca)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4
## Standard deviation     1.5749 0.9949 0.59713 0.41645
## Proportion of Variance 0.6201 0.2474 0.08914 0.04336
## Cumulative Proportion  0.6201 0.8675 0.95664 1.00000
```

Example 2 ii

```r
screeplot(pca, type = 'l')
```

Example 2 iii



Additional comments about sample PCA i

- Let $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ be a sample from a distribution with covariance matrix Σ. Write $\mathbb{Y}$ for the $n \times p$ matrix whose i-th row is $\mathbf{Y}_i$.
- Let S_n be the sample covariance matrix, and write W_k for the matrix whose columns are the first k eigenvectors of S_n.
- You can define the matrix of k principal components as

$$\mathbb{Z} = \mathbb{Y}W_k.$$

Additional comments about sample PCA ii

- On the other hand, it is much more common to define it as

$$\mathbb{Z} = \tilde{\mathbb{Y}} W_k,$$

where $\tilde{\mathbb{Y}}$ is the centered version of $\mathbb{Y}$ (i.e. the sample mean has been subtracted from each row).

  - This leads to sample principal components with mean zero.

Example 1 (revisited) i

```r
library(mvtnorm)
Sigma <- matrix(c(1, 0.5, 0.1,
                  0.5, 1, 0.5,
                  0.1, 0.5, 1),
                ncol = 3)
mu <- c(1, 2, 2)
```

Example 1 (revisited) ii

```r
set.seed(17)
X <- rmvnorm(100, mean = mu,
             sigma = Sigma)
pca <- prcomp(X)

colMeans(X)
```

```
## [1] 0.8789229 2.0517403 2.0965127
```

```r
colMeans(pca$x)
```

Example 1 (revisited) iii

```
##           PC1           PC2           PC3
## -5.523360e-17  4.454770e-17  7.077672e-18
```

```
# On the other hand
pca <- prcomp(X, center = FALSE)
colMeans(pca$x)
```

```
##         PC1         PC2         PC3
## 3.058960918 0.142358612 0.001050088
```

```r
library(tidyverse)
library(dslabs)

mnist <- read_mnist()

dim(mnist$train$images)
```

```
## [1] 60000   784
```

```r
dim(mnist$test$images)
```

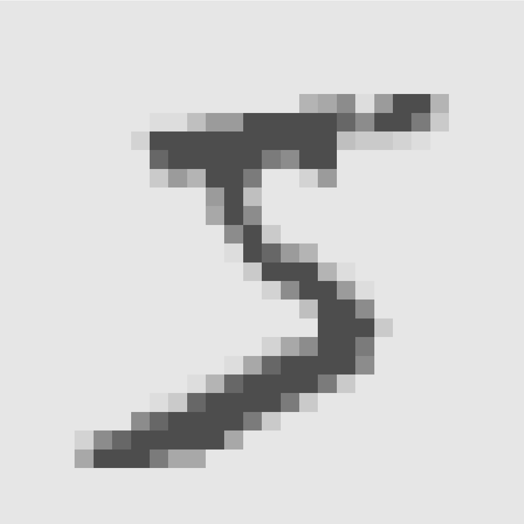
```
## [1] 10000   784
```

```
head(mnist$train$labels)
```

```
## [1] 5 0 4 1 9 2
```

```
img <- matrix(mnist$train$images[1,], ncol = 28)
# Switch columns
img <- img[,rev(1:28)]
image(img, col = gray.colors(12, rev = TRUE),
      axes = FALSE, asp = 1)
```

Data Visualization iii

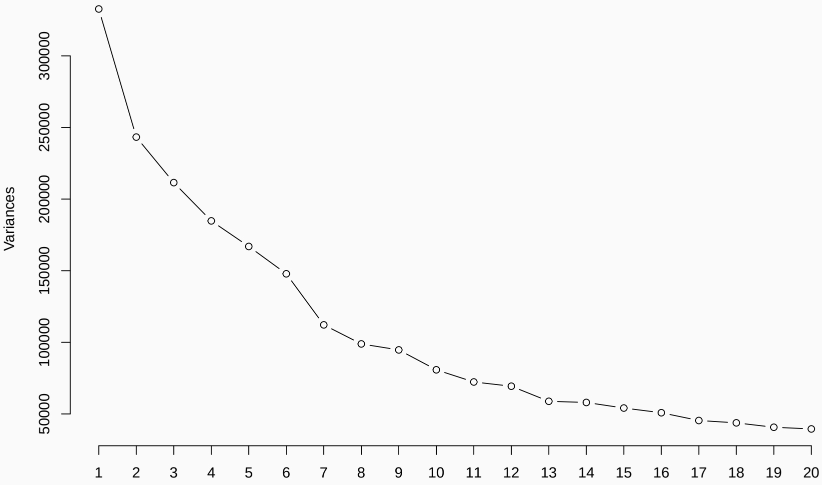


Data Visualization iv

```r
decomp <- prcomp(mnist$train$images)
```

```r
screeplot(decomp, type = 'lines',
          npcs = 20, main = "")
```

Data Visualization v

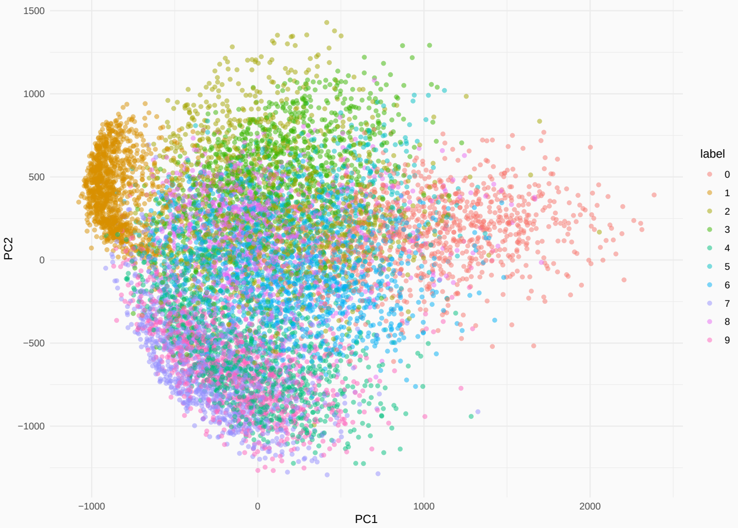


```
decomp$x[,1:2] %>%
  as.data.frame() %>%
  mutate(label = factor(mnist$train$labels)) %>%
  ggplot(aes(PC1, PC2, colour = label)) +
  geom_point(alpha = 0.5) +
  theme_minimal() +
  coord_fixed()
```

Data Visualization vii

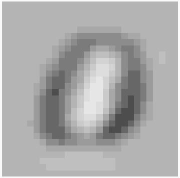
```r
# And on the test set
decomp %>%
  predict(newdata = mnist$test$images) %>%
  as.data.frame() %>%
  mutate(label = factor(mnist$test$labels)) %>%
  ggplot(aes(PC1, PC2, colour = label)) +
  geom_point(alpha = 0.5) +
  theme_minimal() +
  coord_fixed()
```

Data Visualization ix

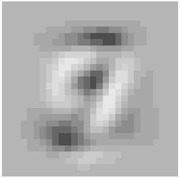


```r
par(mfrow = c(2, 2))
for (i in seq_len(4)) {
  img <- matrix(decomp$rotation[,i], ncol = 28)
  img <- img[,rev(1:28)]
  image(img, col = gray.colors(12, rev = TRUE),
        axes = FALSE, main = paste0("PC", i), asp = 1)
}
```

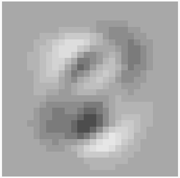
PC1



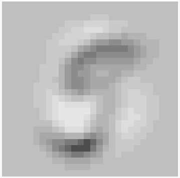
PC2



PC3



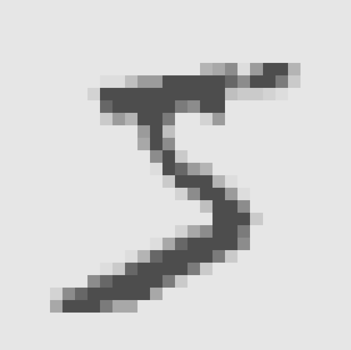
PC4



```r
# Approximation with 90 PCs
approx_mnist <- decomp$rotation[, seq_len(90)] %*%
  decomp$x[1, seq_len(90)]

# Original image
img1 <- matrix(mnist$train$images[1,], ncol = 28)
img1 <- img1[,rev(1:28)]
# Approximation
img2 <- matrix(approx_mnist, ncol = 28)
img2 <- img2[,rev(1:28)]
```

```r
par(mfrow = c(1, 2))
image(img1, col = gray.colors(12, rev = TRUE),
      axes = FALSE, main = "Original", asp = 1)
image(img2, col = gray.colors(12, rev = TRUE),
      axes = FALSE, main = "Approx", asp = 1)
```

Original



Approx

Geometric interpretation of PCA i

- The definition of PCA as a linear combination that maximises variance is due to Hotelling (1933).
- But PCA was actually introduced earlier by Pearson (1901)
    - *On Lines and Planes of Closest Fit to Systems of Points in Space*
- He defined PCA as the **best approximation of the data by a linear manifold**
- Let's suppose we have a lower dimension representation of $\mathbb{Y}$, denoted by a $n \times k$ matrix $\mathbb{Z}$.

Geometric interpretation of PCA ii

- We want to *reconstruct* $\mathbb{Y}$ using an affine transformation

$$f(z) = \mu + W_k z,$$

  where W_k is a $p \times k$ matrix whose columns are orthogonal vectors of unit length.
- We want to find $\mu, W_k, \mathbf{Z}_i$ that minimises the **reconstruction error**:

$$\min_{\mu, W_k, \mathbf{Z}_i} \sum_{i=1}^n \|\mathbf{Y}_i - \mu - W_k\mathbf{Z}_i\|_2^2.$$

- First, we can treat W_k constant and minimise over $\mu, \mathbf{Z}_i$. Write

$$\phi(\mu, \mathbf{Z}_i) = \sum_{i=1}^n \|\mathbf{Y}_i - \mu - W_k\mathbf{Z}_i\|_2^2.$$

Geometric interpretation of PCA iii

- We will take the derivative of ϕ with respect to both μ and $\mathbf{Z}_i$. Using the chain rule (and remembering that the derivatives should be a p- and a k-dimension column vector, respectively), we get:

$$\frac{\partial}{\partial \mu}\phi(\mu, \mathbf{Z}_i) = \sum_{i=1}^{n} -2(\mathbf{Y}_i - \mu - W_k\mathbf{Z}_i), \quad (1)$$

$$\frac{\partial}{\partial \mathbf{Z}_i}\phi(\mu, \mathbf{Z}_i) = -2W_k^T(\mathbf{Y}_i - \mu - W_k\mathbf{Z}_i). \quad (2)$$

- Equation 1 gives us

$$\frac{\partial}{\partial \mu}\phi(\mu, \mathbf{Z}_i) = -2\left(\sum_{i=1}^{n}\mathbf{Y}_i\right) + 2n\mu + 2W_k\left(\sum_{i=1}^{n}\mathbf{Z}_i\right).$$

Setting this equal to zero and solving for μ, we get

$$\mu = \bar{\mathbf{Y}} - W_k\bar{\mathbf{Z}}.$$

- Similarly, Equation 2 gives us

$$\frac{\partial}{\partial \mathbf{Z}_i}\phi(\mu, \mathbf{Z}_i) = -2W_k^T(\mathbf{Y}_i - \mu) + 2\mathbf{Z}_i.$$

Setting this equal to zero and solving for $\mathbf{Z}_i$, we get

$$\mathbf{Z}_i = W_k^T(\mathbf{Y}_i - \mu).$$

- Now, observe that our system of equations is *overdetermined*, i.e. our equations are not independent. Indeed, if we take the sample average of both sides of the equality $\mathbf{Z}_i = W_k^T(\mathbf{Y}_i - \mu)$, we get a tautology:

$$\begin{aligned}
\bar{\mathbf{Z}} &= W_k^T(\bar{\mathbf{Y}} - \mu) \\
&= W_k^T(\bar{\mathbf{Y}} - \bar{\mathbf{Y}} + W_k\bar{\mathbf{Z}}) \qquad \text{(since } \mu = \bar{\mathbf{Y}} - W_k\bar{\mathbf{Z}}\text{)} \\
&= W_k^T(W_k\bar{\mathbf{Z}}) \\
&= \bar{\mathbf{Z}}.
\end{aligned}$$

- Since we have many solutions to this system of equations, we will choose one by requiring that $\bar{\mathbf{Z}} = 0$. This gives us

$$\begin{aligned}\hat{\mu} &= \bar{\mathbf{Y}},\\ \hat{\mathbf{Z}}_i &= W_k^T(\mathbf{Y}_i - \bar{\mathbf{Y}}).\end{aligned}$$

- Putting these quantities into the reconstruction error, we get

$$\min_{W_k} \sum_{i=1}^n \|(\mathbf{Y}_i - \bar{\mathbf{Y}}) - W_k W_k^T(\mathbf{Y}_i - \bar{\mathbf{Y}})\|_2^2.$$

Eckart–Young theorem

The reconstruction error is minimised by taking W_k to be the matrix whose columns are the first k eigenvectors of the sampling covariance matrix S_n.

Equivalently, we can take the matrix whose columns are the first k *right singular vectors* of the centered data matrix $\tilde{\mathbb{Y}}$.

Example i

```r
set.seed(1234)
# Random measurement error
sigma <- 5

# Exact relationship between
# Celsius and Fahrenheit
temp_c <- seq(-40, 40, by = 1)
temp_f <- 1.8*temp_c + 32
```

Example ii

```r
# Add measurement error
temp_c_noise <- temp_c + rnorm(n = length(temp_c),
                               sd = sigma)
temp_f_noise <- temp_f + rnorm(n = length(temp_f),
                               sd = sigma)
```

```r
# Linear model
(fit <- lm(temp_f_noise ~ temp_c_noise))
```

Example iii

```
##
## Call:
## lm(formula = temp_f_noise ~ temp_c_noise)
##
## Coefficients:
##  (Intercept)  temp_c_noise
##       34.256         1.662
```

```
confint(fit)
```

Example iv

```
##                     2.5 %   97.5 %
## (Intercept)  32.152891 36.35921
## temp_c_noise  1.577228  1.74711
```

```
# PCA
pca <- prcomp(cbind(temp_c_noise, temp_f_noise))
pca$rotation
```

```
##                    PC1        PC2
## temp_c_noise 0.5012360 -0.8653106
## temp_f_noise 0.8653106  0.5012360
```

Example v

```
pca$rotation[2,"PC1"]/pca$rotation[1,"PC1"]
```

```
## [1] 1.726354
```

Large sample inference i

- If we impose distributional assumptions on the data $\mathbf{Y}$, we can derive the sampling distributions of the sample principal components.
- Assume $\mathbf{Y} \sim N_p(\mu, \Sigma)$, with Σ positive definite. Let $\lambda_1 > \cdots > \lambda_p$ be the eigenvalues of Σ; in particular we assume they are *distinct*. Finally let $w_1, \ldots, w_p$ be the corresponding eigenvectors.
- Given a random sample of size n, let S_n be the sample covariance matrix, $\hat{\lambda}_1, \ldots, \hat{\lambda}_p$ its eigenvalues, and $\hat{w}_1, \ldots, \hat{w}_p$ the corresponding eigenvectors.

Large sample inference ii

- Define Λ to be the diagonal matrix whose entries are $\lambda_1, \ldots, \lambda_p$, and define

$$\Omega_i = \lambda_i \sum_{k=1, k \neq i}^{p} \frac{\lambda_k}{(\lambda_k - \lambda_i)^2} w_k w_k^T.$$

Large sample inference iii

Asymptotic results

1. Write $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_p)$ and similarly for $\hat{\boldsymbol{\lambda}}$. As $n \to \infty$, we have
$$\sqrt{n}\left(\hat{\boldsymbol{\lambda}} - \boldsymbol{\lambda}\right) \to N_p(0, 2\Lambda^2).$$
2. As $n \to \infty$, we have
$$\sqrt{n}\left(\hat{w}_i - w_i\right) \to N_p(0, \Omega_i).$$
3. Each $\hat{\lambda}_i$ is distributed independently of $\hat{w}_i$.

Comments i

- These results **only** apply to principal components derived from the covariance matrix.
    - Some asymptotic results are available for those derived from the correlation matrix, but we will not cover them in class.
- Asymptotically, all eigenvalues of S_n are independent.
- You can get a confidence interval for λ_i as follows:

$$\frac{\hat{\lambda}_i}{(1 + z_{\alpha/2}\sqrt{2/n})} \leq \lambda_i \leq \frac{\hat{\lambda}_i}{(1 - z_{\alpha/2}\sqrt{2/n})}.$$

    - Use Bonferroni correction if you want CIs that are simultaneously valid for all eigenvalues.

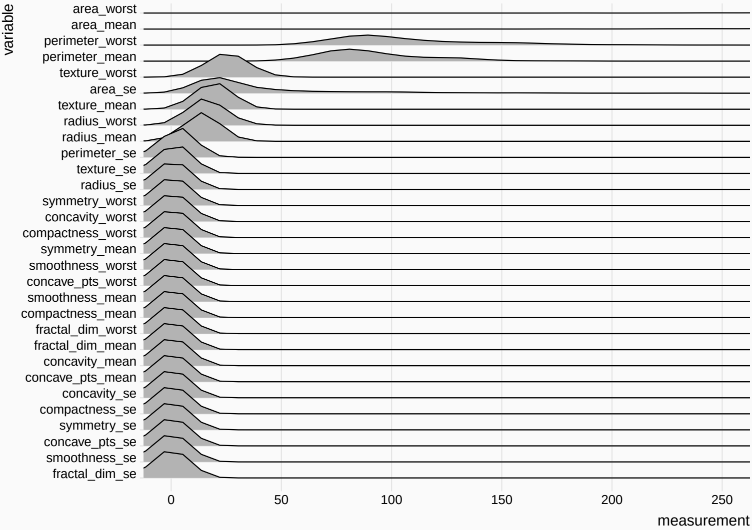
Comments ii

- The matrices Ω_i have rank $p-1$, and therefore they are *singular*.
- The entries of $\hat{w}_i$ are correlated, and this correlation depends on the *separation* between the eigenvalues.
    - Good separation $\implies$ smaller correlation

Example i

```r
library(dslabs)
library(ggridges)

# Data on Breast Cancer
as.data.frame(brca$x) %>%
  gather(variable, measurement) %>%
  mutate(variable = reorder(variable, measurement,
                            median)) %>%
  ggplot(aes(x = measurement, y = variable)) +
  geom_density_ridges() + theme_ridges() +
  coord_cartesian(xlim = c(0, 250))
```

Example ii


variable
area_worst
area_mean
perimeter_worst
perimeter_mean
texture_worst
area_se
texture_mean
radius_worst
radius_mean
perimeter_se
texture_se
radius_se
symmetry_worst
concavity_worst
compactness_worst
symmetry_mean
smoothness_worst
concave_pts_worst
smoothness_mean
compactness_mean
fractal_dim_worst
fractal_dim_mean
concavity_mean
concave_pts_mean
concavity_se
compactness_se
symmetry_se
concave_pts_se
smoothness_se
fractal_dim_se
0
50
100
150
200
250
measurement

Example iii

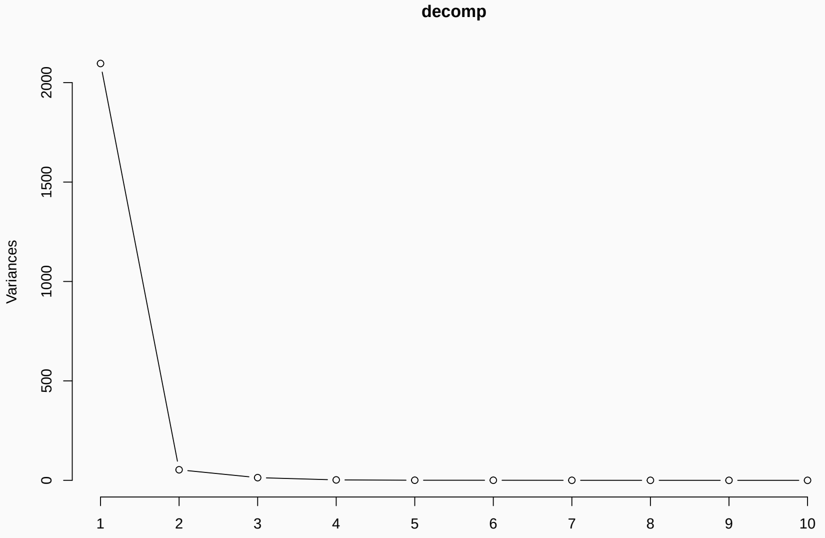
```r
# Remove some variables
rem_index <- which(colnames(brca$x) %in%
                     c("area_worst", "area_mean",
                       "perimeter_worst",
                       "perimeter_mean"))
dataset <- brca$x[,-rem_index]
decomp <- prcomp(dataset)
summary(decomp)$importance[,1:3]
```

Example iv

```
##                               PC1      PC2      PC3
## Standard deviation     45.78445 7.281664 3.677815
## Proportion of Variance  0.96776 0.024480 0.006240
## Cumulative Proportion   0.96776 0.992240 0.998490
```

```r
screeplot(decomp, type = 'l')
```

Example v



Example vi

```
# Let's put a CI around the first eigenvalue
first_ev <- decomp$sdev[1]^2
n <- nrow(dataset)

# Recall that TV = 2166
c("LB" = first_ev/(1+qnorm(0.975)*sqrt(2/n)),
  "Est." = first_ev,
  "UP" = first_ev/(1-qnorm(0.975)*sqrt(2/n)))
```

```
##       LB     Est.       UP
## 1877.992 2096.216 2371.822
```

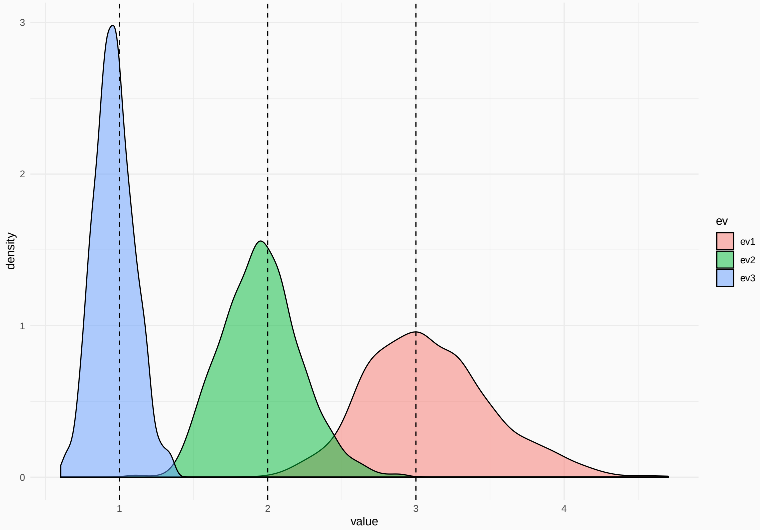
Simulations i

```r
B <- 1000; n <- 100; p <- 3

results <- purrr::map_df(seq_len(B), function(b) {
    X <- matrix(rnorm(p*n, sd = sqrt(c(1, 2, 3))),
                ncol = p, byrow = TRUE)
    tmp <- eigen(cov(X), symmetric = TRUE,
                 only.values = TRUE)
    tibble(ev1 = tmp$values[1],
           ev2 = tmp$values[2],
           ev3 = tmp$values[3])
})
```

Simulations ii

```r
results %>%
  gather(ev, value) %>%
  ggplot(aes(value, fill = ev)) +
  geom_density(alpha = 0.5) +
  theme_minimal() +
  geom_vline(xintercept = c(1, 2, 3),
             linetype = 'dashed')
```

Simulations iii



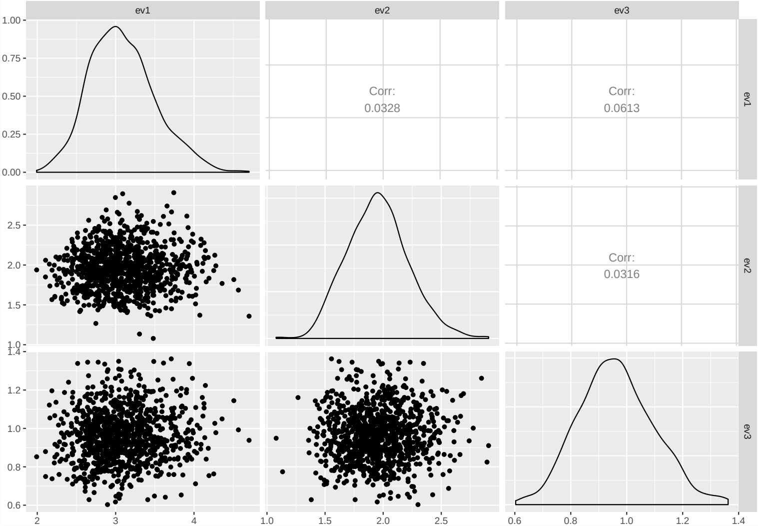
Simulations iv

```r
summarise_all(results, mean)
```

```
## # A tibble: 1 x 3
##      ev1   ev2   ev3
##    <dbl> <dbl> <dbl>
## 1  3.09  1.95 0.963
```

```r
# Is there some correlation?
GGally::ggpairs(results)
```

Simulations v



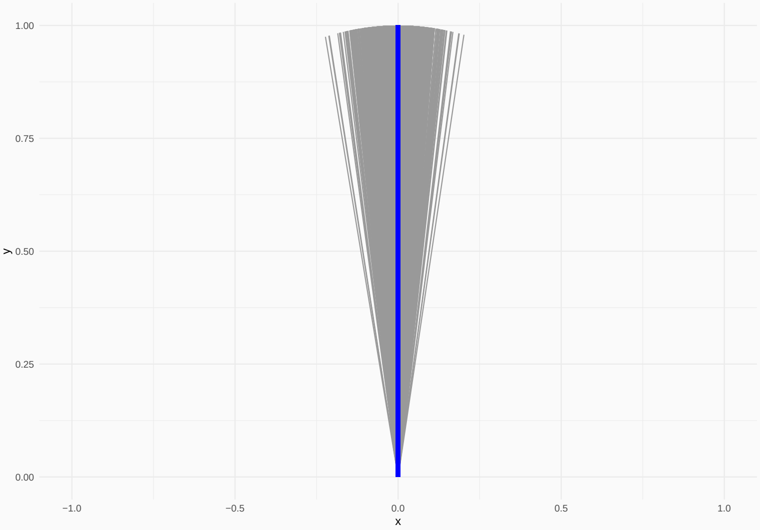
Simulations vi

```
p <- 2
results_vect <- purrr::map_df(seq_len(B), function(b) {
  X <- matrix(rnorm(p*n, sd = c(1, 2)), ncol = p,
              byrow = TRUE)
  tmp <- eigen(cov(X), symmetric = TRUE)

  tibble(
    xend = tmp$vectors[1,1],
    yend = tmp$vectors[2,1]
  )
})
```

Simulations vii

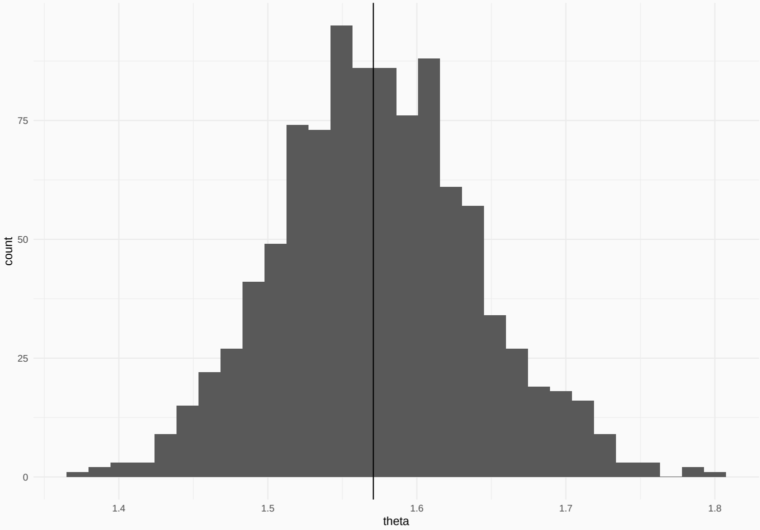
```
ggplot(results_vect) +
  geom_segment(aes(xend = xend, yend = yend),
               x = 0, y = 0, colour = 'grey60') +
  geom_segment(x = 0, xend = 0,
               y = 0, yend = 1,
               colour = 'blue', size = 2) +
  expand_limits(y = 0, x = c(-1, 1)) +
  theme_minimal()
```

Simulations viii



```r
# Or looking at angles
transmute(results_vect,
          theta = atan2(yend, xend)) %>%
  ggplot(aes(theta)) +
  geom_histogram() +
  theme_minimal() +
  geom_vline(xintercept = pi/2)
```

Simulations x

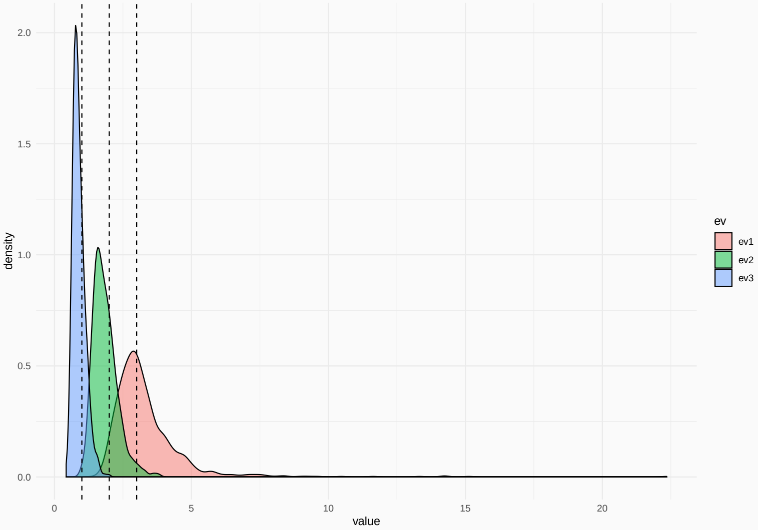


Simulations xi

```
library(mvtnorm)
# What about the t distribution
results_t <- purrr::map_df(seq_len(B), function(b) {
    X <- rmvt(n, sigma = diag(2*c(1, 2, 3)/4),
              df = 4)
    tmp <- eigen(cov(X), symmetric = TRUE,
                 only.values = TRUE)
    tibble(ev1 = tmp$values[1],
           ev2 = tmp$values[2],
           ev3 = tmp$values[3])
})
```

```
results_t %>%
  gather(ev, value) %>%
  ggplot(aes(value, fill = ev)) +
  geom_density(alpha = 0.5) +
  theme_minimal() +
  geom_vline(xintercept = c(1, 2, 3),
             linetype = 'dashed')
```

Simulations xiii

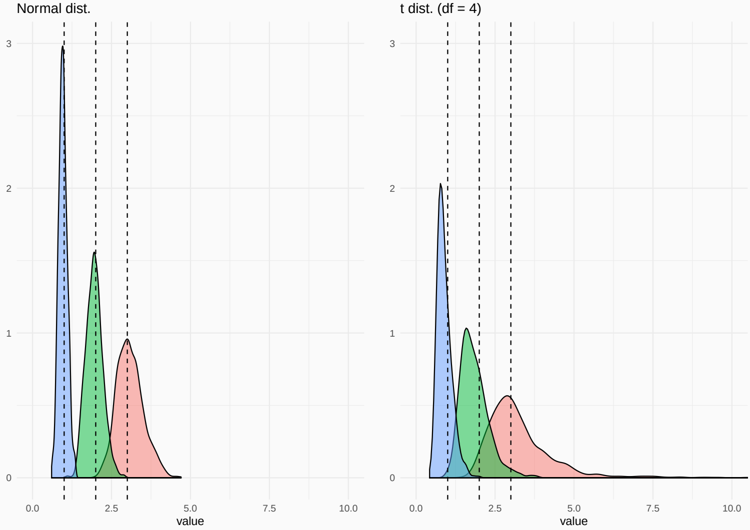


Simulations xiv

```
summarise_all(results_t, mean)
```

```
## # A tibble: 1 x 3
##     ev1   ev2   ev3
##   <dbl> <dbl> <dbl>
## 1  3.34  1.85 0.896
```

Simulations xv



Test for structured covariance i

- The asymptotic results above assumed distinct eigenvalues.
- But we may be interested in *structured* covariance matrices; for example:

$$\Sigma_0 = \sigma^2 \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{pmatrix}.$$

- This is called an **exchangeable** correlation structure.

Test for structured covariance ii

- Assuming $\rho > 0$, the eigenvalues of Σ_0 are

$$\begin{aligned}\lambda_1 &= \sigma^2(1 + (p-1)\rho),\\ \lambda_2 &= \sigma^2(1-\rho),\\ \vdots \quad & \quad \vdots\\ \lambda_p &= \sigma^2(1-\rho).\end{aligned}$$

- Let's assume $\sigma^2 = 1$. We are interested in testing whether the correlation matrix is equal to Σ_1.
- Let $\bar{r}_k = \frac{1}{p-1}\sum_{i=1,i\neq k}^{p} r_{ik}$ be the average of the off-diagonal value of the k-th column of the sample correlation matrix.

Test for structured covariance iii

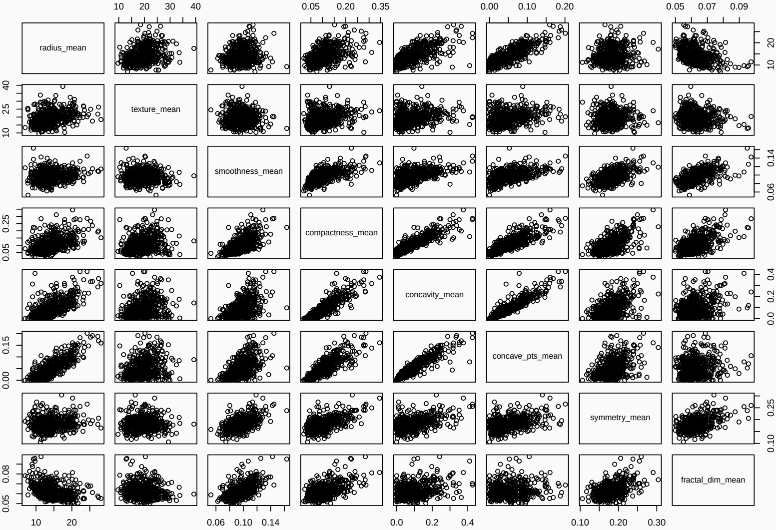
- Let $\bar{r} = \frac{2}{p(p-1)} \sum_{i<j} r_{ij}$ be the average of all off-diagonal elements (we are only looking at entries below the diagonal).
- Finally, let $\hat{\gamma} = \frac{(p-1)^2[1-(1-\bar{r})^2]}{p-(p-2)(1-\bar{r})^2}$.
- We reject the null hypothesis that the correlation matrix is equal to Σ_0 if

$$\frac{(n-1)}{(1-\bar{r})^2}\left[\sum_{i<j}(r_{ij}-\bar{r})^2 - \hat{\gamma}\sum_{k=1}^{p}(\bar{r}_k-\bar{r})^2\right] > \chi^2_\alpha((p+1)(p-2)/2)$$

Example i

```
# Keep only mean measurements
rem_index2 <- grep("mean", colnames(brca$x),
                    invert = TRUE)
dataset <- brca$x[,-c(rem_index,
                      rem_index2)]
R <- cor(dataset)

pairs(dataset)
```

Example ii


radius_mean
texture_mean
smoothness_mean
compactness_mean
concavity_mean
concave_pts_mean
symmetry_mean
fractal_dim_mean
10 20 30 40
0.05 0.20 0.35
0.00 0.10 0.20
0.05 0.07 0.09
10 20
10 25 40
0.06 0.14
0.05 0.25
0.0 0.2 0.4
0.00 0.15
0.10 0.25
0.05 0.08
0.06 0.10 0.14
0.10 0.20 0.30

Example iii

```
# Overall mean
r_bar <- mean(R[upper.tri(R, diag = FALSE)])

# Column specific means
r_cols <- (colSums(R) - 1)/(nrow(R) - 1)

# Extra quantities
p <- ncol(dataset)
n <- nrow(dataset)
gamma_hat <- (p - 1)^2*(1 - (1 - r_bar)^2)/
  (p - (p - 2)*(1 - r_bar)^2)
```

Example iv

```r
# Test statistic
Tstat <- sum((R[upper.tri(R,
                          diag = FALSE)] - r_bar)^2) -
  gamma_hat*sum((r_cols - r_bar)^2)
Tstat <- (n-1)*Tstat/(1-r_bar)^2

Tstat > qchisq(0.95, 0.5*(p+1)*(p-2))
```

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

Selecting the number of PCs i

- We already discussed two strategies for selecting the number of principal components:
    - Look at the scree plot and find where the curve starts to be flat;
    - Retain as many PCs as required to explain the desired proportion of variance.
- There is a vast literature on different strategies for selecting the number of components. Two good references:
    - Peres-Neto *et al.* (2005) *How many principal components? stopping rules for determining the number of non-trivial axes revisited*
    - Jolliffe (2012) *Principal Component Analysis* (2nd ed)

- We will discuss one more technique based on resampling.
- The idea is to try to estimate the distribution of eigenvalues if there was no correlation between the variables.

Algorithm

1. Permute the observations of each column **independently**.
2. Perform PCA on the permuted data.
3. Repeat B times and collect the eigenvalues $\hat{\lambda}_1^{(b)}, \ldots, \hat{\lambda}_p^{(b)}$.
4. Keep the components whose observed $\hat{\lambda}_i$ is greater than $(1-\alpha)$% of the values $\hat{\lambda}_i^{(b)}$ obtained through permutations.

Example (cont'd) i

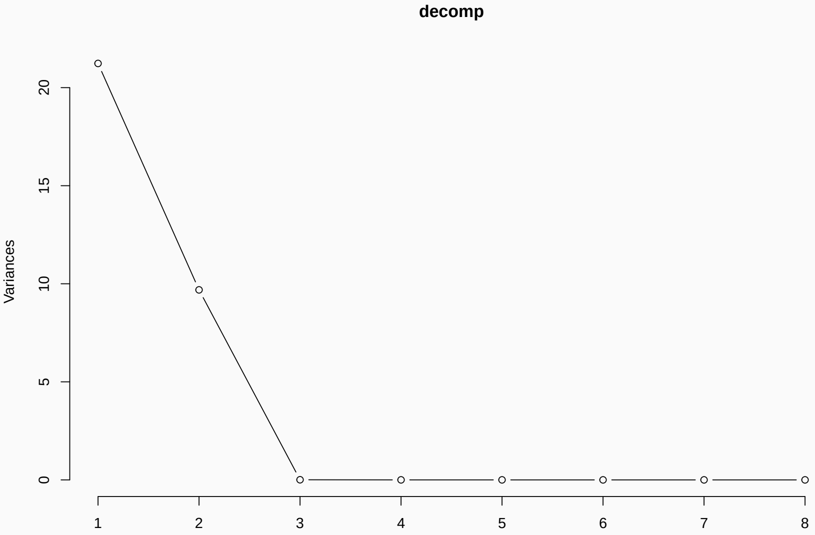
```r
decomp <- prcomp(dataset)

summary(decomp)$importance[,seq_len(3)]
```

```
##                            PC1      PC2        PC3
## Standard deviation     4.60806 3.112611 0.07664969
## Proportion of Variance 0.68654 0.313240 0.00019000
## Cumulative Proportion  0.68654 0.999780 0.99997000
```

Example (cont'd) ii

```
screeplot(decomp, type = 'l')
```

Example (cont'd) iii



Example (cont'd) iv

```r
permute_data <- function(data) {
  p <- ncol(data)
  data_perm <- data
  for (i in seq_len(p)) {
    ind_sc <- sample(nrow(data))
    data_perm[,i] <- data[ind_sc, i]
  }
  return(data_perm)
}
```

Example (cont'd) v

```r
set.seed(123)
B <- 1000
alpha <- 0.05
results <- matrix(NA, ncol = B,
                  nrow = ncol(dataset))

results[,1] <- decomp$sdev
results[,-1] <- replicate(B - 1, {
  data_perm <- permute_data(dataset)
  prcomp(data_perm)$sdev
})
```

Example (cont'd) vi

```r
cutoff <- apply(results, 1, function(row) {
  mean(row >= row[1])
})
which(cutoff < alpha)
```

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

Biplots i

- In our example with the MNIST dataset, we plotted the first principal component against the second component.
    - This gave us a sense of how much discriminatory ability each PC gave us.
    - E.g. the first PC separated 1s from 0s
- What was missing from that plot was how the PCs were related to the original variables.
- A **biplot** is a graphical display of both the original observations and original variables *together* on one scatterplot.
    - The prefix “bi” refers to two modalities (i.e. observations and variables), not to two dimensions.

Biplots ii

- One approach to biplots relies on the Eckart-Young theorem:
    - The “best” 2-dimensional representation of the data passes through the plane containing the first two eigenvectors of the sample covariance matrix.

Biplots iii

Construction

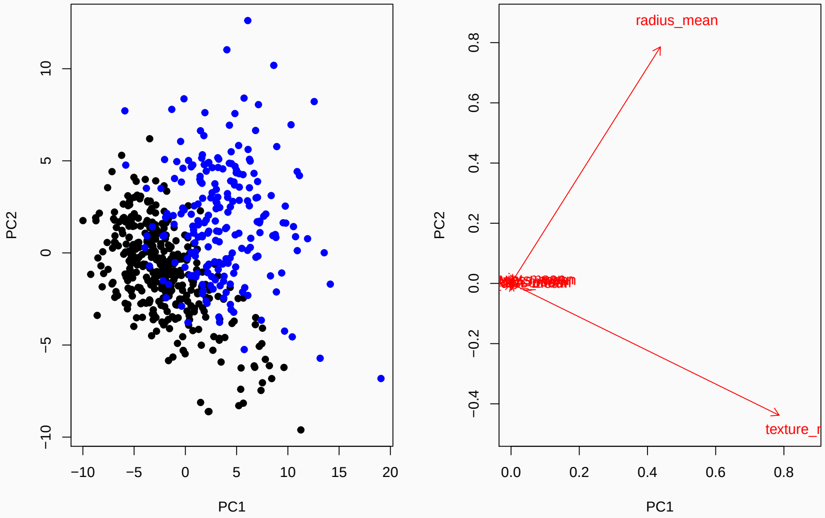
- Let $\tilde{\mathbb{Y}}$ be the $n \times p$ matrix of centered data, and let $w_1, \ldots, w_p$ be the p eigenvectors of $\tilde{\mathbb{Y}}^T \tilde{\mathbb{Y}}$.
- For each row $\mathbf{Y}_i$ of $\mathbb{Y}$, add the point $\left(w_1^T \mathbf{Y}_i, w_2^T \mathbf{Y}_i\right)$ to the plot.
- The j-th column of $\mathbb{Y}$ is represented by an arrow from the origin to the point (w_{1j}, w_{2j}).
- It may be necessary to rescale the PCs and/or the loadings in order to see the relationship better.

Example (cont'd) i

```r
# Continuing with our example on breast cancer
decomp <- prcomp(dataset)

# Extract PCs and loadings
PCs <- decomp$x[, 1:2]
loadings <- decomp$rotation[, 1:2]

# Extract data on tumour type
colour <- ifelse(brca$y == "B", "black", 'blue')
```

Example (cont'd) ii

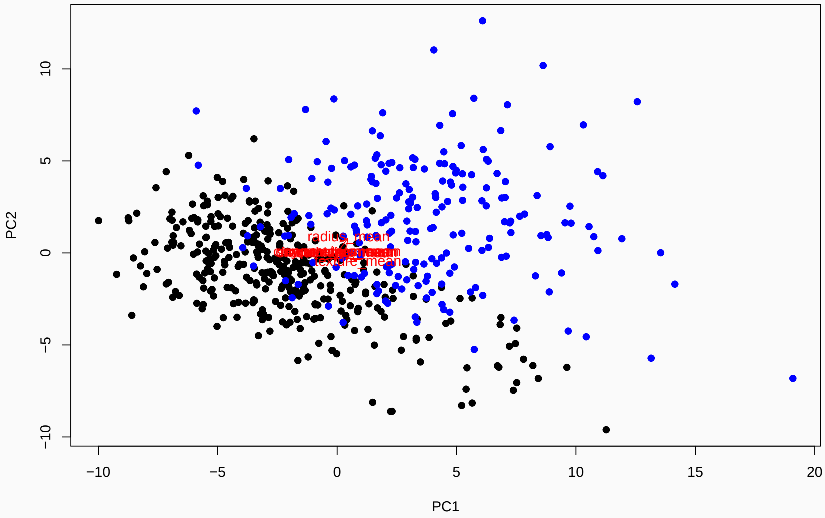
```r
par(mfrow = c(1,2))
plot(PCs, pch = 19, col = colour)
plot(loadings, type = 'n')
text(loadings,
     labels = colnames(dataset),
     col = 'red')
arrows(0, 0, 0.9 * loadings[, 1],
       0.9 * loadings[, 2],
       col = 'red',
       length = 0.1)
```


PC2
PC1
10
5
0
−5
−10
15
20
radius_mean
texture_r
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4

Example (cont'd) iv

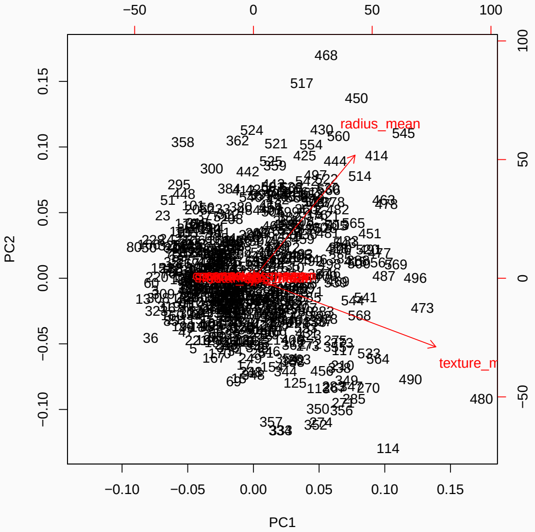
```r
# Or both on the same plot
plot(PCs, pch = 19, col = colour)
text(loadings,
     labels = colnames(dataset),
     col = 'red')
arrows(0, 0, 0.9 * loadings[, 1],
       0.9 * loadings[, 2],
       col = 'red',
       length = 0.1)
```

Example (cont'd) v



```r
# The biplot function rescales for us
biplot(decomp)
```

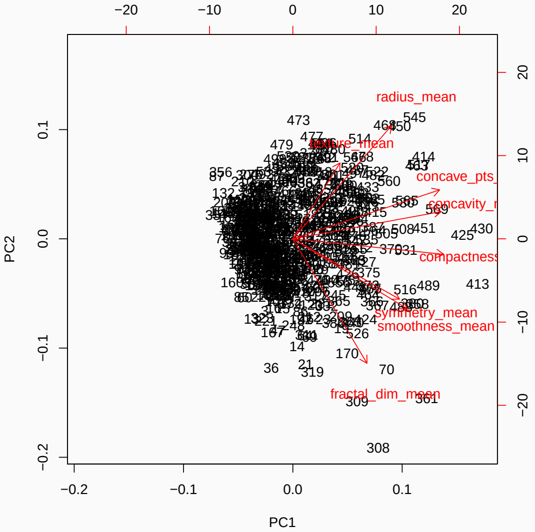
Example (cont’d) vii



Example (cont'd) viii

```r
# With scaled data
biplot(prcomp(dataset, scale = TRUE))
```

Example (cont’d) ix



Summary of graphical displays

- When we plot the first PC against the second PC, we are looking for similarity between *observations*.
- When we plot the first loading against the second loading, we are looking for similarity between *variables*.
    - Orthogonal loadings $\Longrightarrow$ Uncorrelated variables
    - Obtuse angle between loadings $\Longrightarrow$ Negative correlation
- A **biplot** combines both pieces of information.
    - You can think of it as a projection of the p-dimensional scatter plot (points and axes) onto a 2-dimensional plane.
- A **scree plot** displays the amount of variation in each principal component.

Applications of PCA to Model Building

Training and testing i

- Recall: **Mean Squared Error**

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2,$$

  where $Y_i, \hat{Y}_i$ are the *observed* and *predicted* values.
- It is good practice to separate your dataset in two:
  - **Training** dataset, that is used to build and fit your model (e.g. choose covariates, estimate regression coefficients).
  - **Testing** dataset, that it used to compute the MSE or other performance metrics.

Training and testing ii

- PCA can be used for predictive model building in (univariate) linear regression:
  - **Feature extraction**: Perform PCA on the covariates, extract the first k PCs, and use them as predictors in your model.
  - **Feature selection**: Perform PCA on the covariates, look at the first PC, find the covariates whose loadings are the largest (in absolute value), and only use those covariates as predictors.

```r
library(tidyverse)
url <- "https://maxturgeon.ca/w20-stat7200/prostate.csv"
prostate <- read_csv(url)

# Separate into training and testing sets
data_train <- filter(prostate, train == TRUE) %>%
  dplyr::select(-train)
data_test <- filter(prostate, train == FALSE) %>%
  dplyr::select(-train)
```

```r
# First model: Linear regression
lr_model <- lm(lpsa ~ ., data = data_train)
lr_pred <- predict(lr_model, newdata = data_test)
(lr_mse <- mean((data_test$lpsa - lr_pred)^2))
```

```
## [1] 0.521274
```

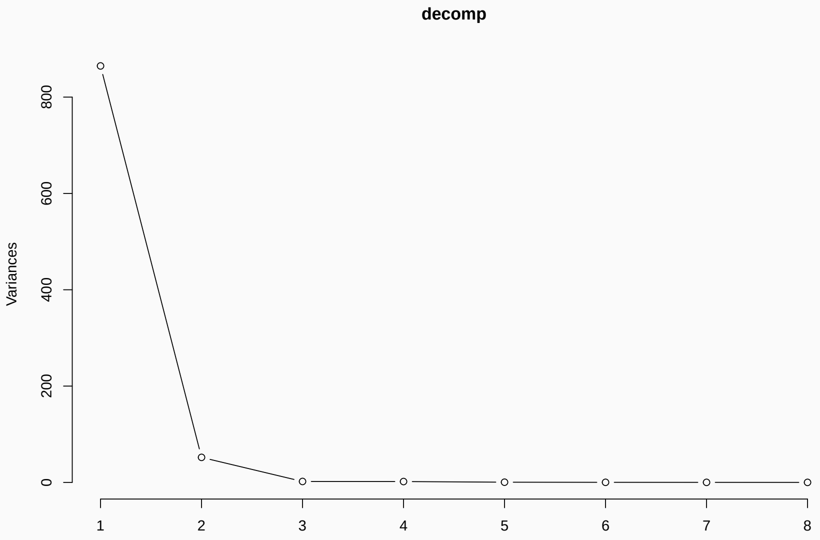
Feature Extraction iii

```
# PCA
decomp <- data_train %>%
  subset(select = -lpsa) %>%
  as.matrix() %>%
  prcomp
summary(decomp)$importance[,1:3]
```

```
##                             PC1      PC2      PC3
## Standard deviation     29.40597 7.211721 1.410789
## Proportion of Variance  0.93844 0.056440 0.002160
## Cumulative Proportion   0.93844 0.994890 0.997050
```

```r
screeplot(decomp, type = 'lines')
```

Feature Extraction v



Feature Extraction vi

```r
# Second model: PCs for predictors
train_pc <- data_train
train_pc$PC1 <- decomp$x[,1]
pc_model <- lm(lpsa ~ PC1, data = train_pc)
```

```r
test_pc <- as.data.frame(predict(decomp, data_test))
pc_pred <- predict(pc_model,
                   newdata = test_pc)
(pc_mse <- mean((data_test$lpsa - pc_pred)^2))
```

```
## [1] 0.9552741
```

Feature Selection i

```
contribution <- decomp$rotation[,"PC1"]
round(contribution, 3)[1:6]
```

```
##   lcavol lweight     age    lbph     svi     lcp
##    0.021   0.001   0.075  -0.001   0.007   0.032
```

```
round(contribution, 3)[7:8]
```

```
## gleason   pgg45
##    0.018   0.996
```

Feature Selection ii

```
(keep <- names(which(abs(contribution) > 0.01)))
```

```
## [1] "lcavol"  "age"     "lcp"     "gleason" "pgg45"
```

```
fs_model <- lm(lpsa ~ ., data = data_train[,c(keep, "lpsa
fs_pred <- predict(fs_model, newdata = data_test)
(fs_mse <- mean((data_test$lpsa - fs_pred)^2))
```

```
## [1] 0.5815571
```

Feature Selection iii

```
model_plot <- data.frame(
  ”obs” = data_test$lpsa,
  ”LR” = lr_pred,
  ”PC” = pc_pred,
  ”FS” = fs_pred
) %>%
  gather(Model, pred, -obs)
```

```r
ggplot(model_plot,
       aes(pred, obs, colour = Model)) +
  geom_point() +
  theme_minimal() +
  geom_abline(slope = 1, intercept = 0) +
  theme(legend.position = 'top') +
  xlab("Predicted") + ylab("Observed")
```

Feature Selection v

Comments

- The full model performed better than the ones we created with PCA
    - It had a lower MSE
- On the other hand, if we had multicollinearity issues, or too many covariates ($p > n$), the PCA models could outperform the full model.
- However, note that PCA does not use the association between the covariates and the outcome, so it will never be the most efficient way of building a model.