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**.

Lagrange Multipliers i

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.

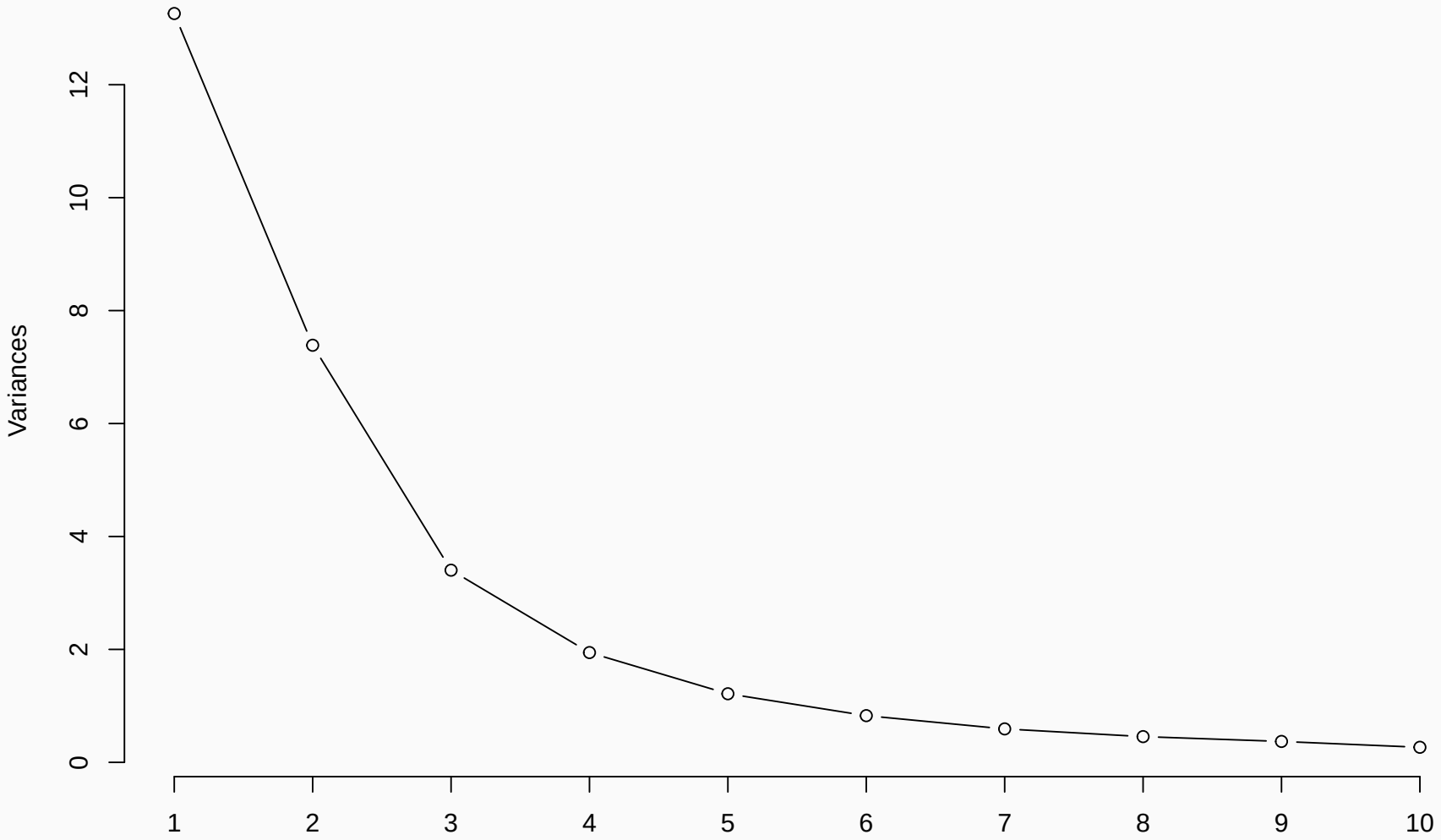
Properties of PCA ii

- **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)
```

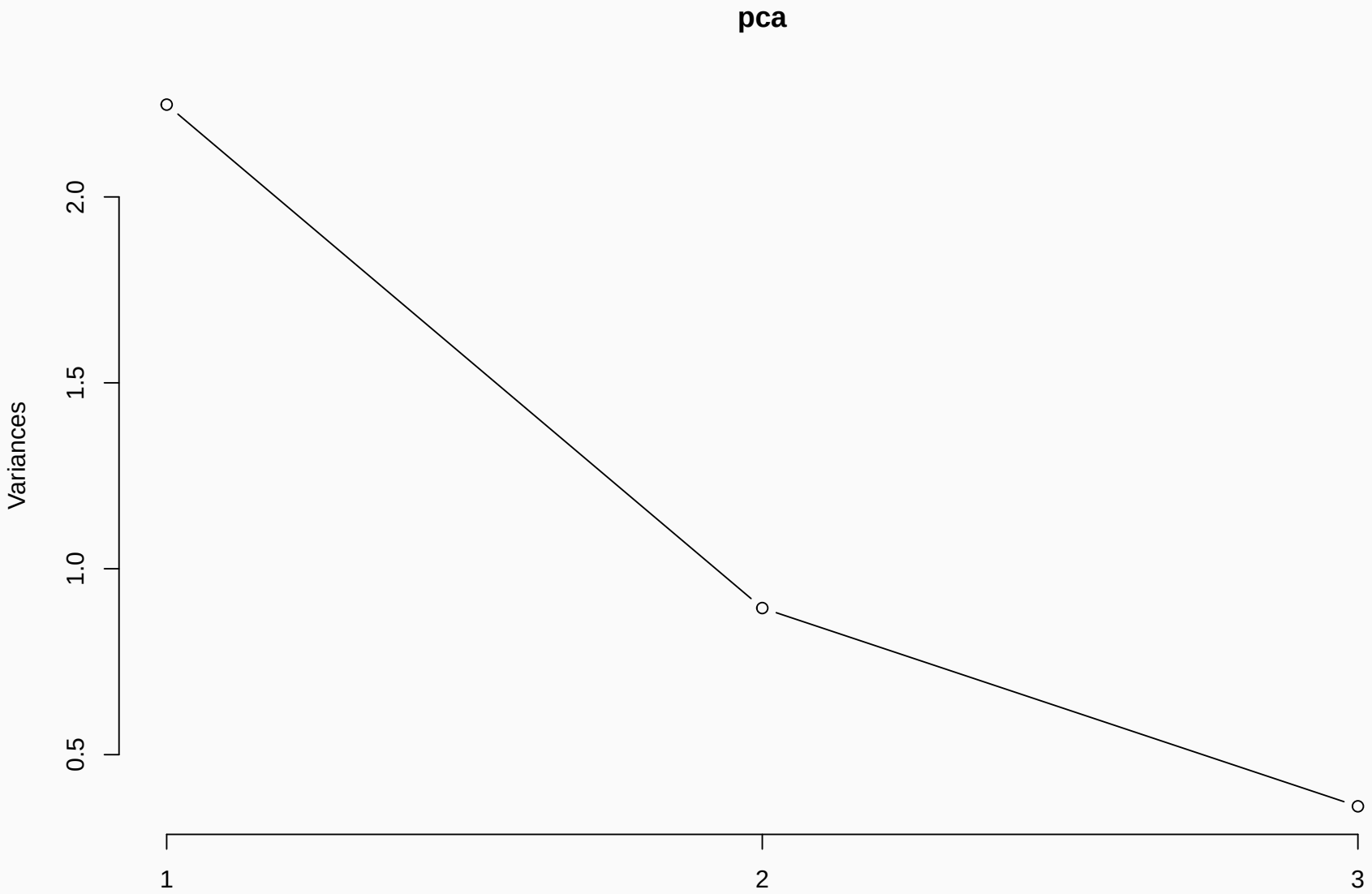
Example 1 ii

```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

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

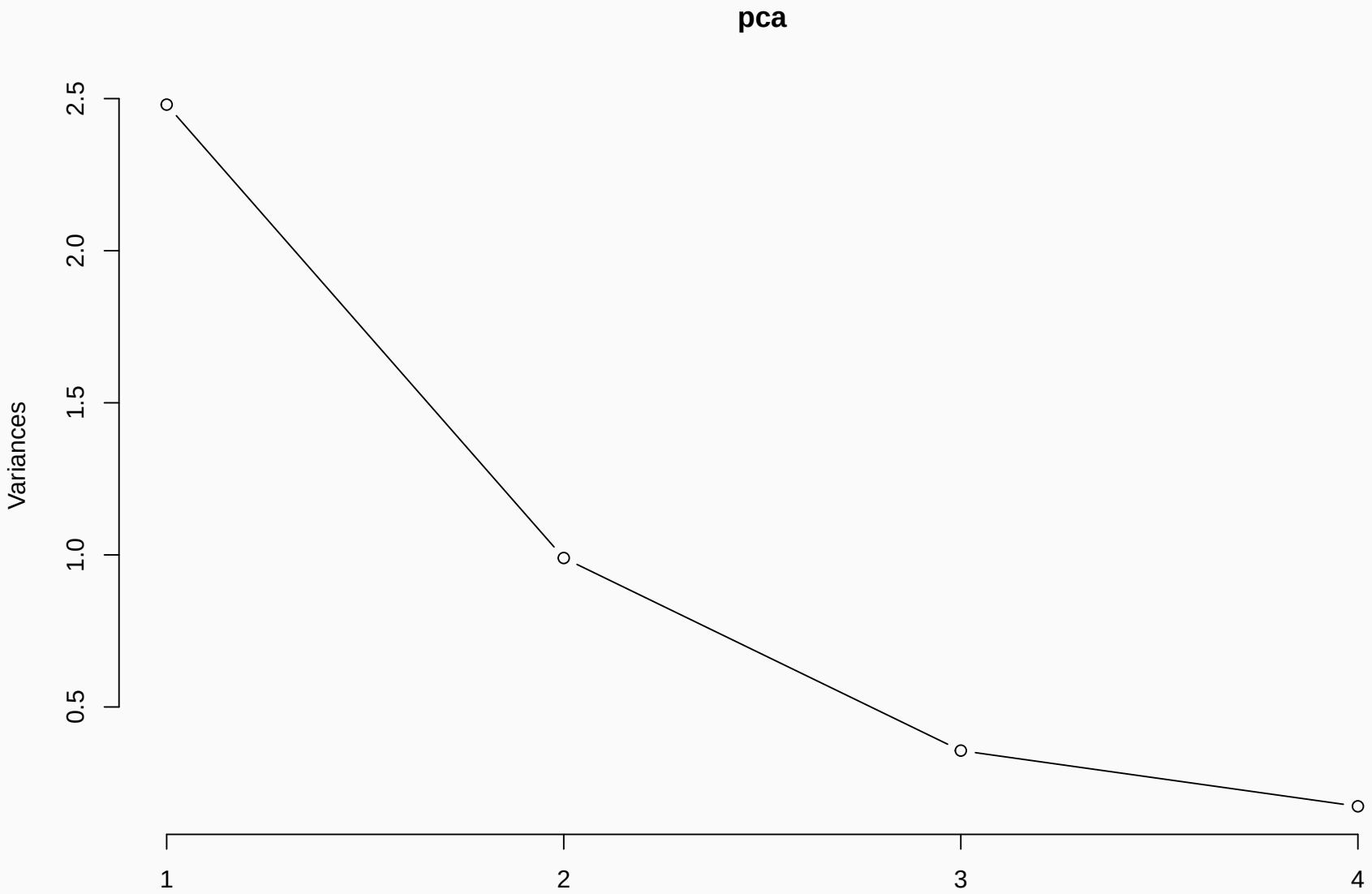
```
summary(pca)
```

```
## 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

```
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
```

Data Visualization i

```
library(tidyverse)
library(dslabs)

mnist <- read_mnist()

dim(mnist$train$images)
```

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

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

Data Visualization ii

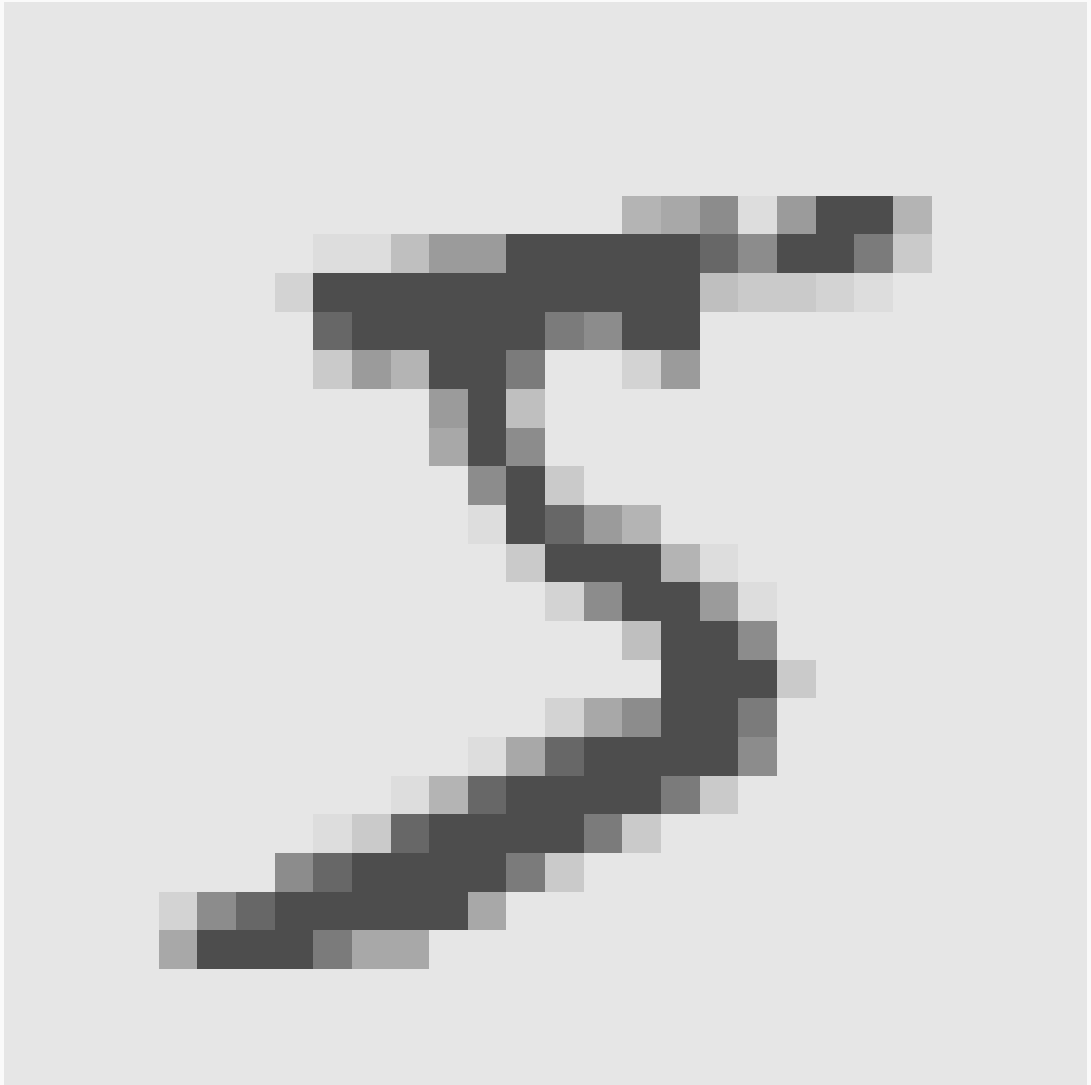
```
## [1] 10000   784
```

```
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)
```

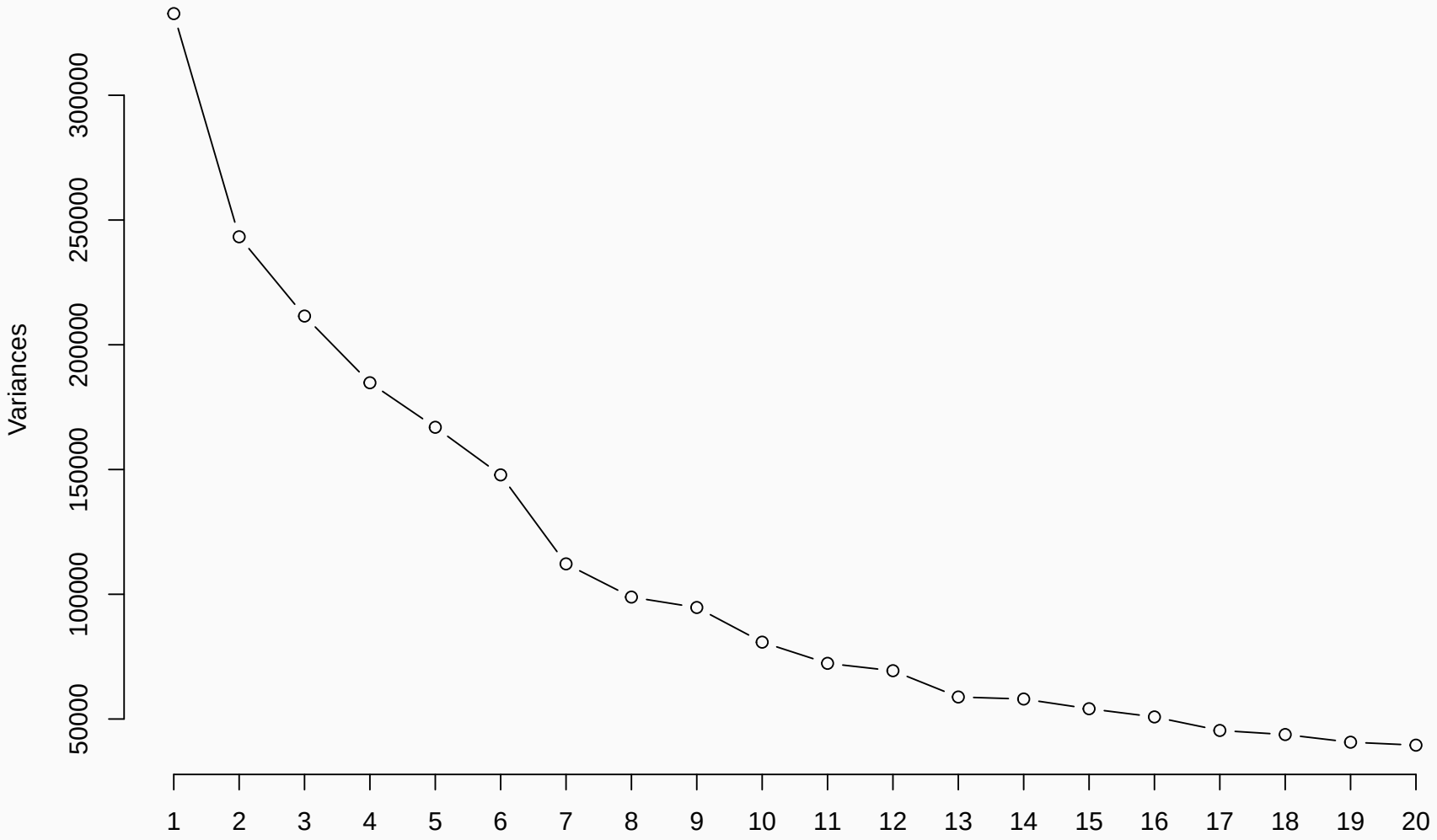
Data Visualization iii



Data Visualization iv

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

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

Data Visualization v



Data Visualization vi

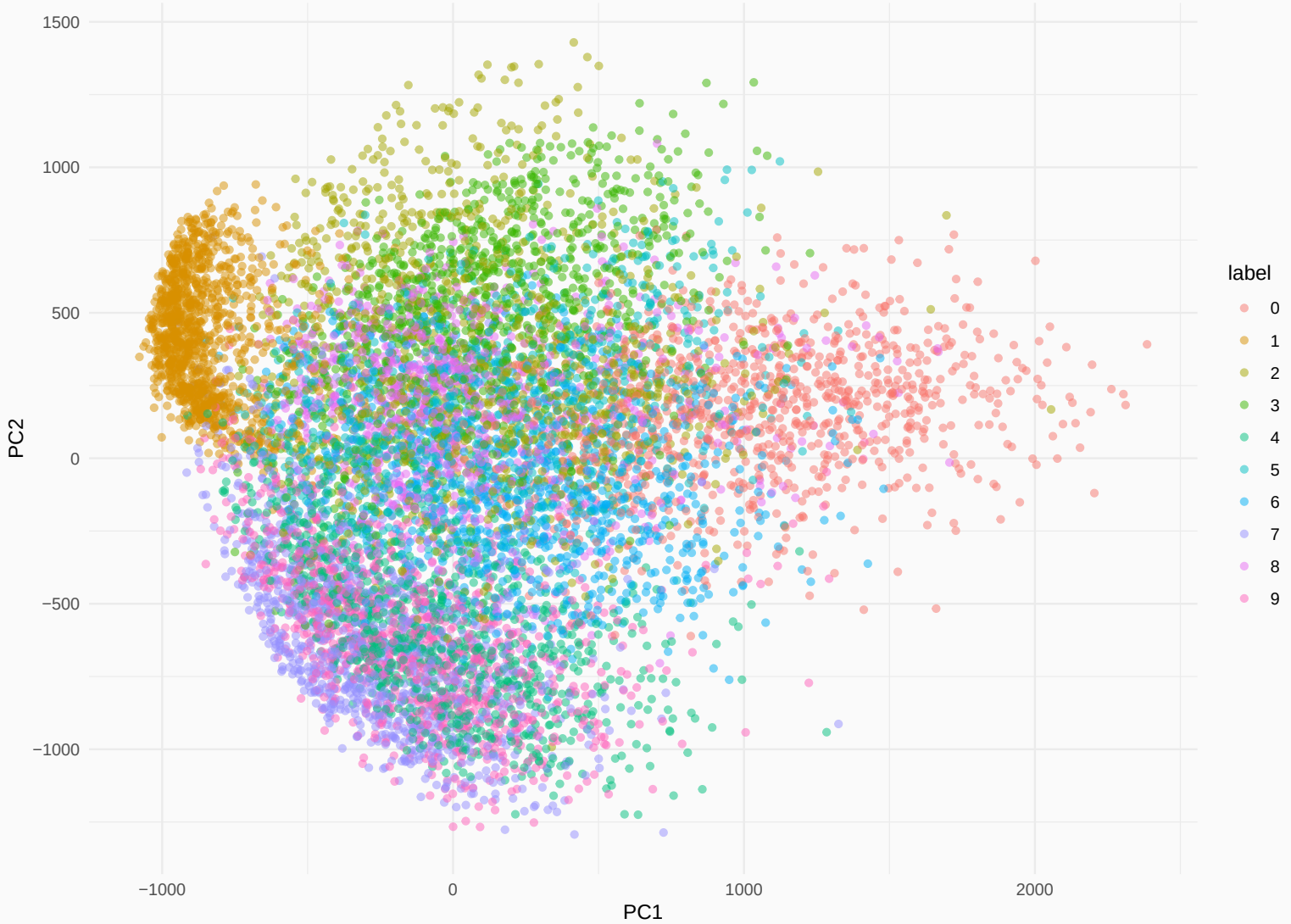
```
decomp$x[,1:2] %>%
  as.data.frame() %>%
  mutate(label = factor(mnist$train$labels)) %>%
  ggplot(aes(PC1, PC2, colour = label)) +
  geom_point(alpha = 0.5) +
  theme_minimal() +
  coord_fixed()
```

Data Visualization vii

Data Visualization viii

```
# 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

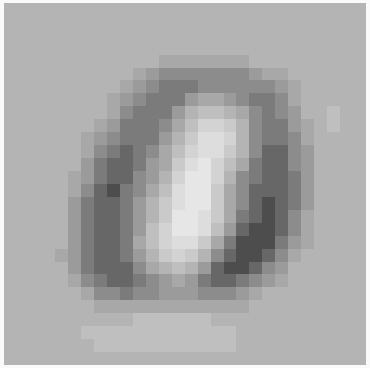


Data Visualization x

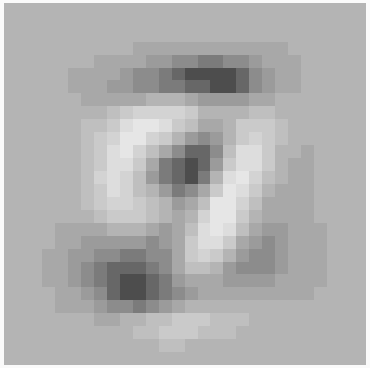
```
par(mfrow = c(2, 2))
for (i in seq_len(4)) {
  img <- matrix(decomp$rotation[,i], ncol = 28)
  img <- img[,rev(1:28)]
  image(img, col = gray.colors(12, rev = TRUE),
        axes = FALSE, main = paste0("PC", i), asp = 1)
}
```

Data Visualization xi

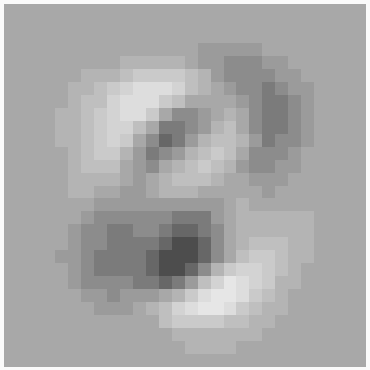
PC1



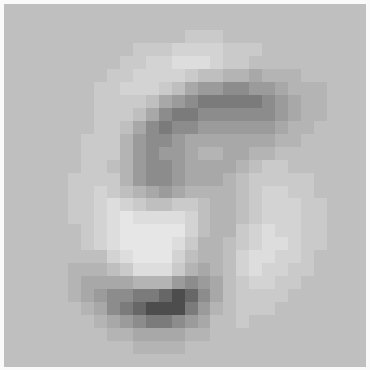
PC2



PC3



PC4



```
# 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)]
```

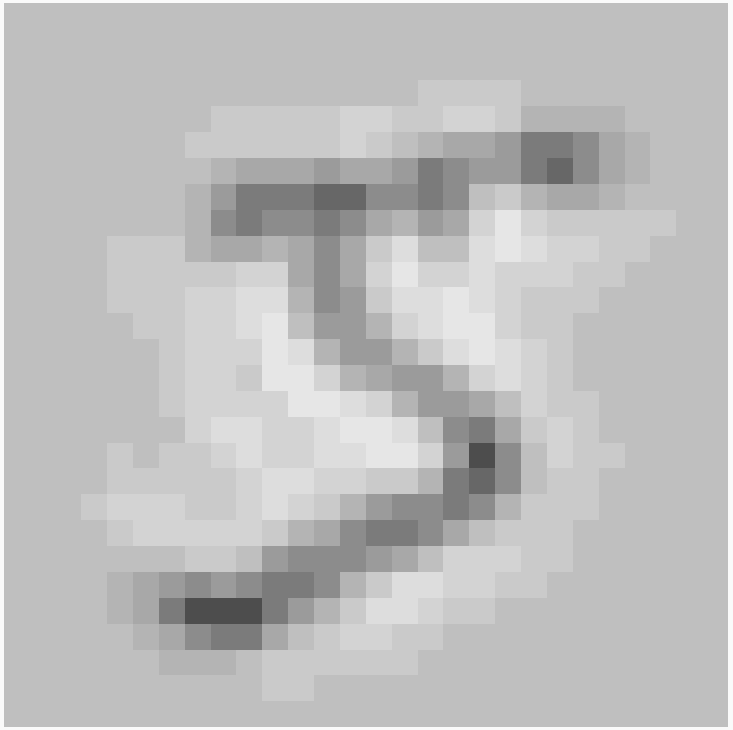
Data Visualization xiii

```
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)
```

Data Visualization xiv

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:

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

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

Geometric interpretation of PCA iv

- 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

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

Geometric interpretation of PCA v

- 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:

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

Geometric interpretation of PCA vi

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

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

- Putting these quantities into the reconstruction error, we get

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

Geometric interpretation of PCA vii

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

```
# 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)

# 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.

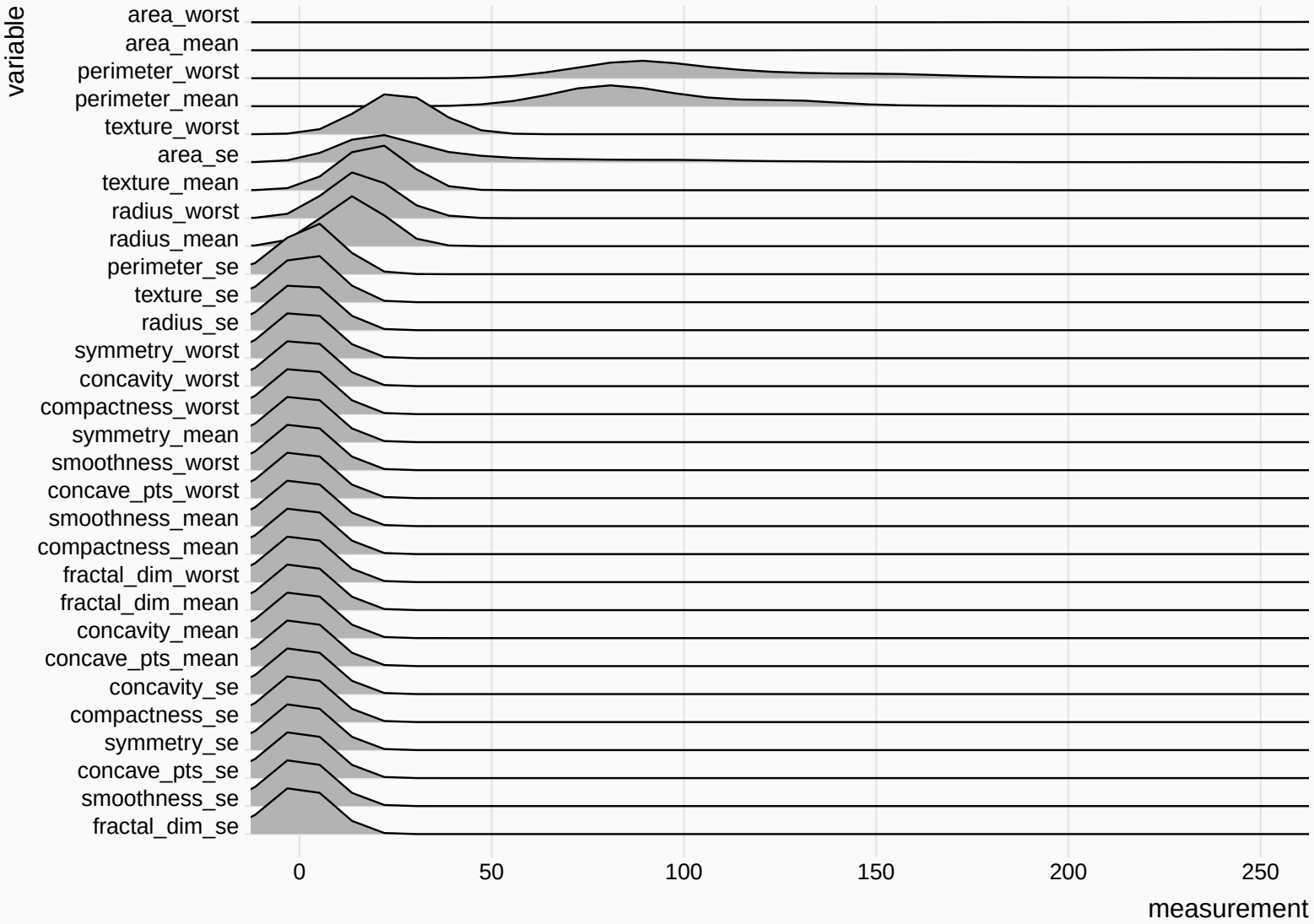
Comments ii

- 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 $\Longrightarrow$ smaller correlation

Example i

```
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

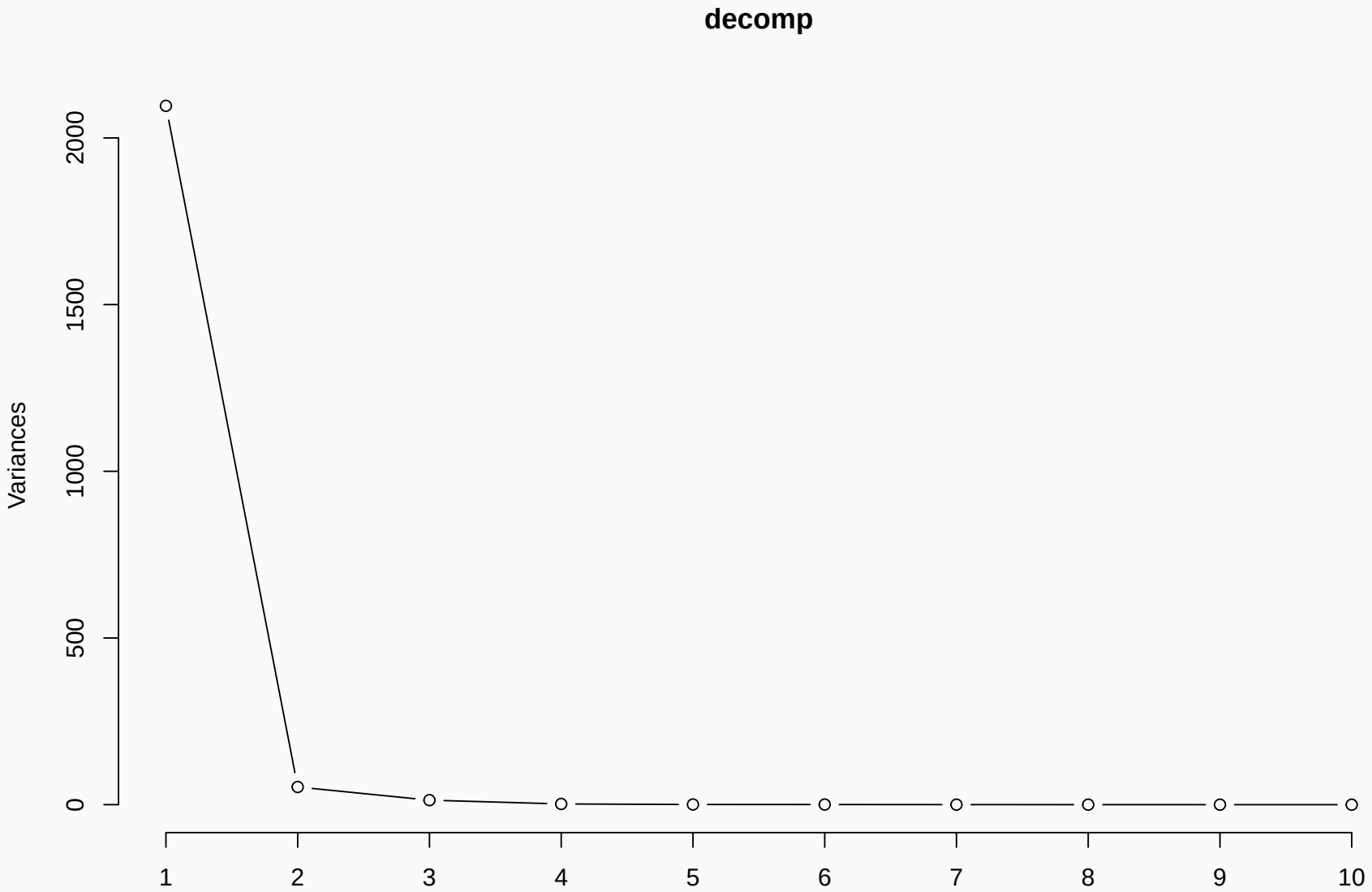
```
# Remove some variables
rem_index <- which(colnames(brca$x) %in%
                     c("area_worst", "area_mean",
                       "perimeter_worst",
                       "perimeter_mean"))
dataset <- brca$x[,-rem_index]
decomp <- prcomp(dataset)
summary(decomp)$importance[,1:3]
```

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
```

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

Example v



Example vi

```r
# 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
```

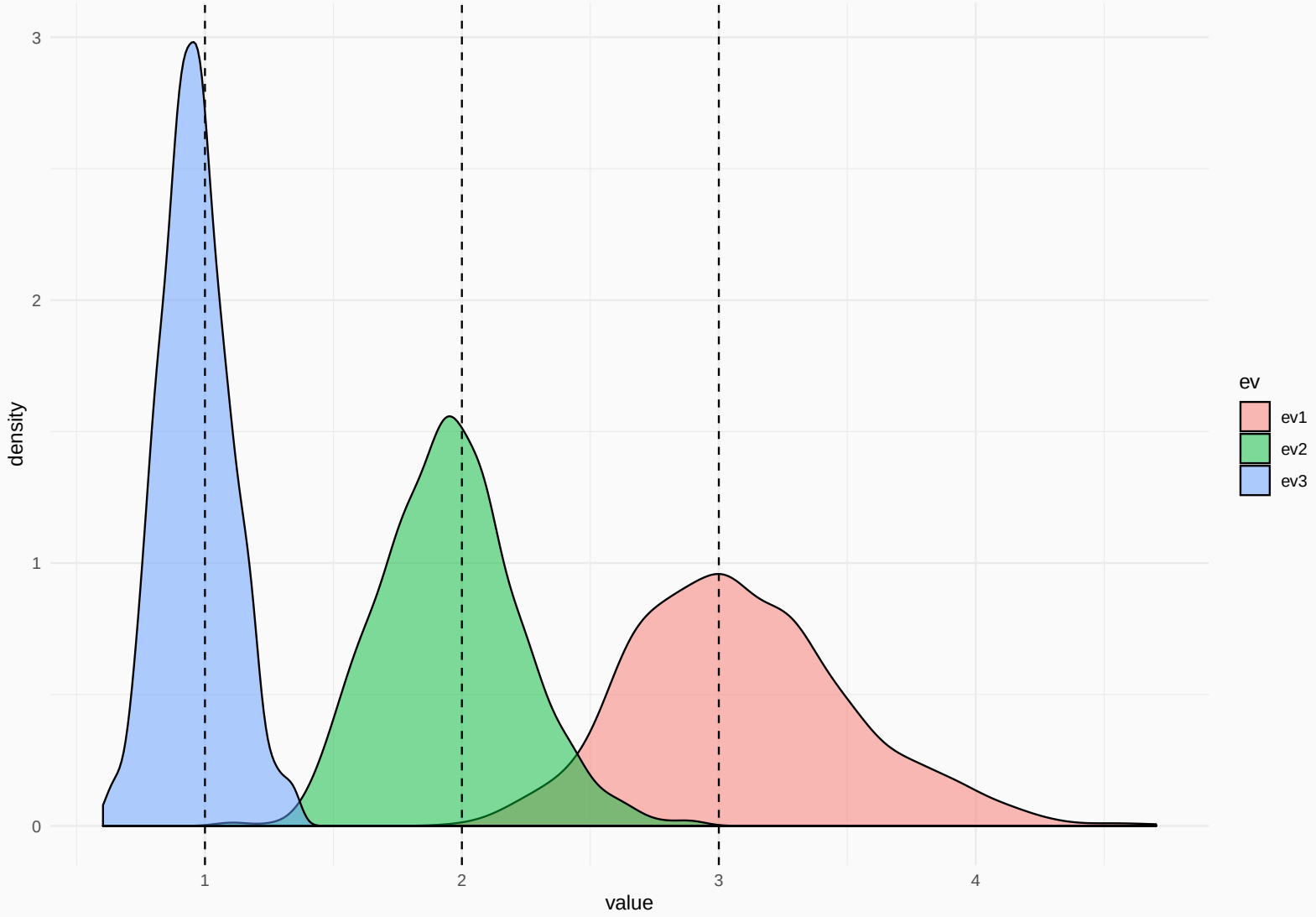
Simulations i

```
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

```
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

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

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

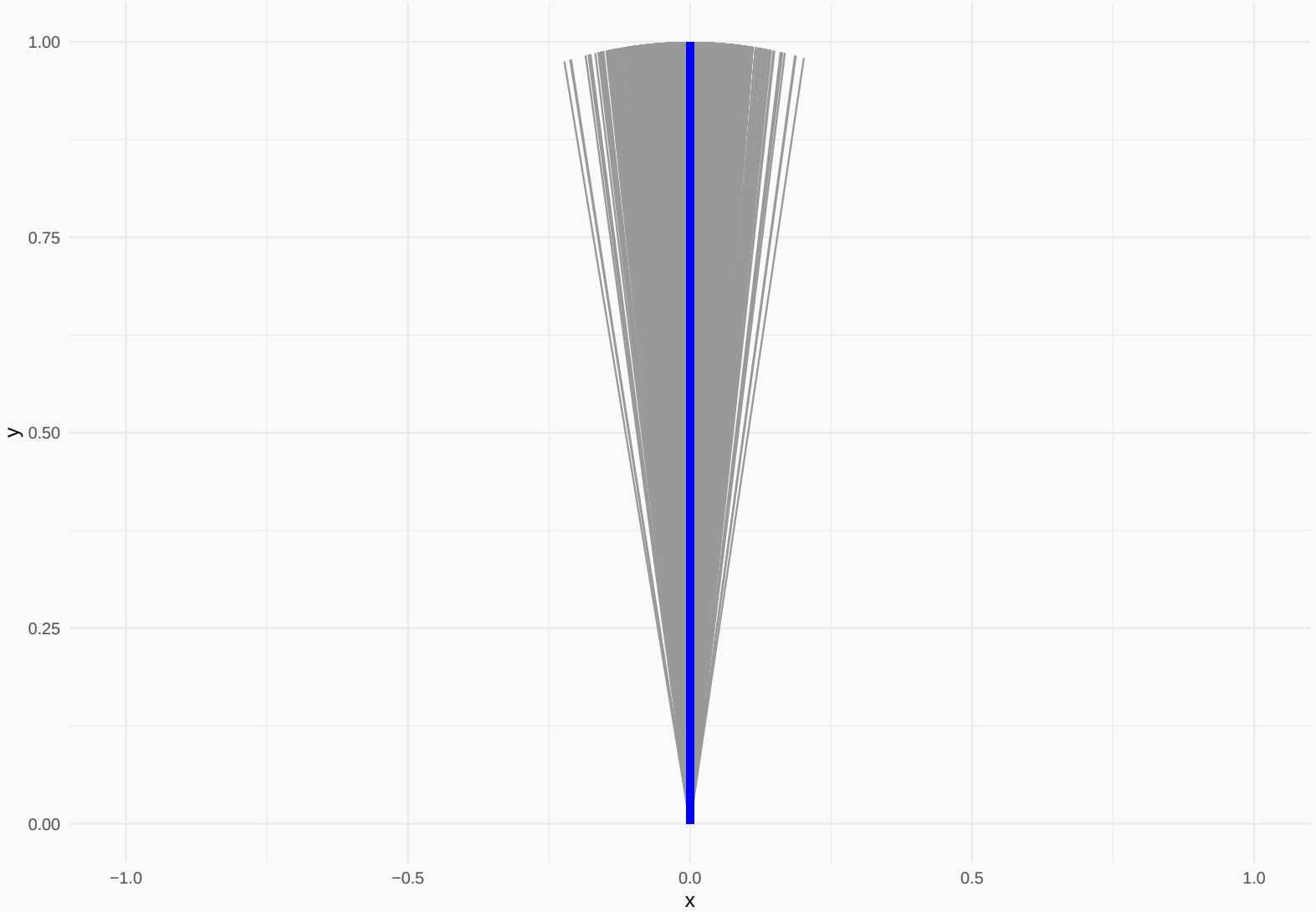
Simulations v

```r
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 vi

```
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()
```

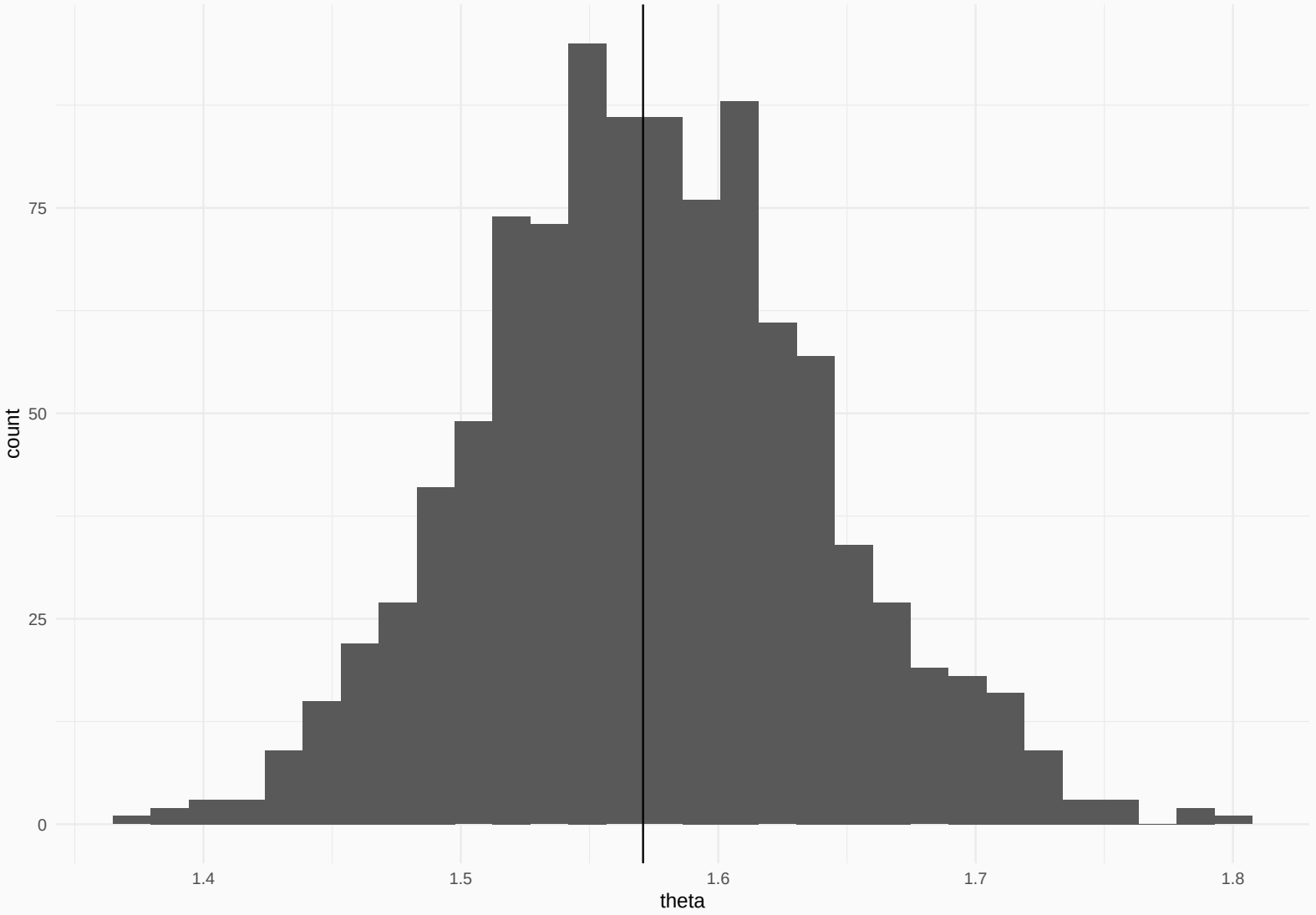
Simulations vii



Simulations viii

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

Simulations ix



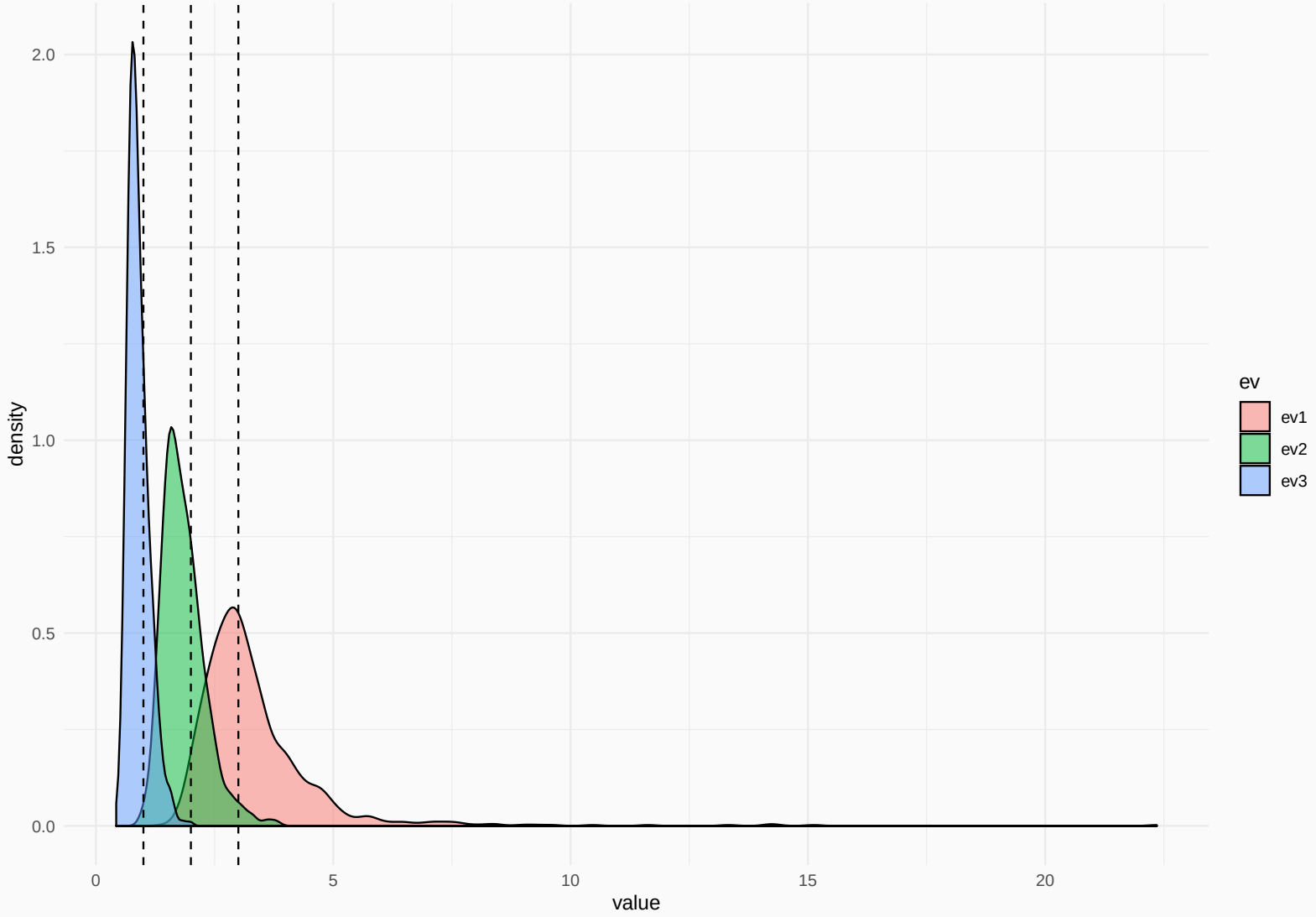
Simulations x

```r
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])
})
```

Simulations xi

```
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 xii

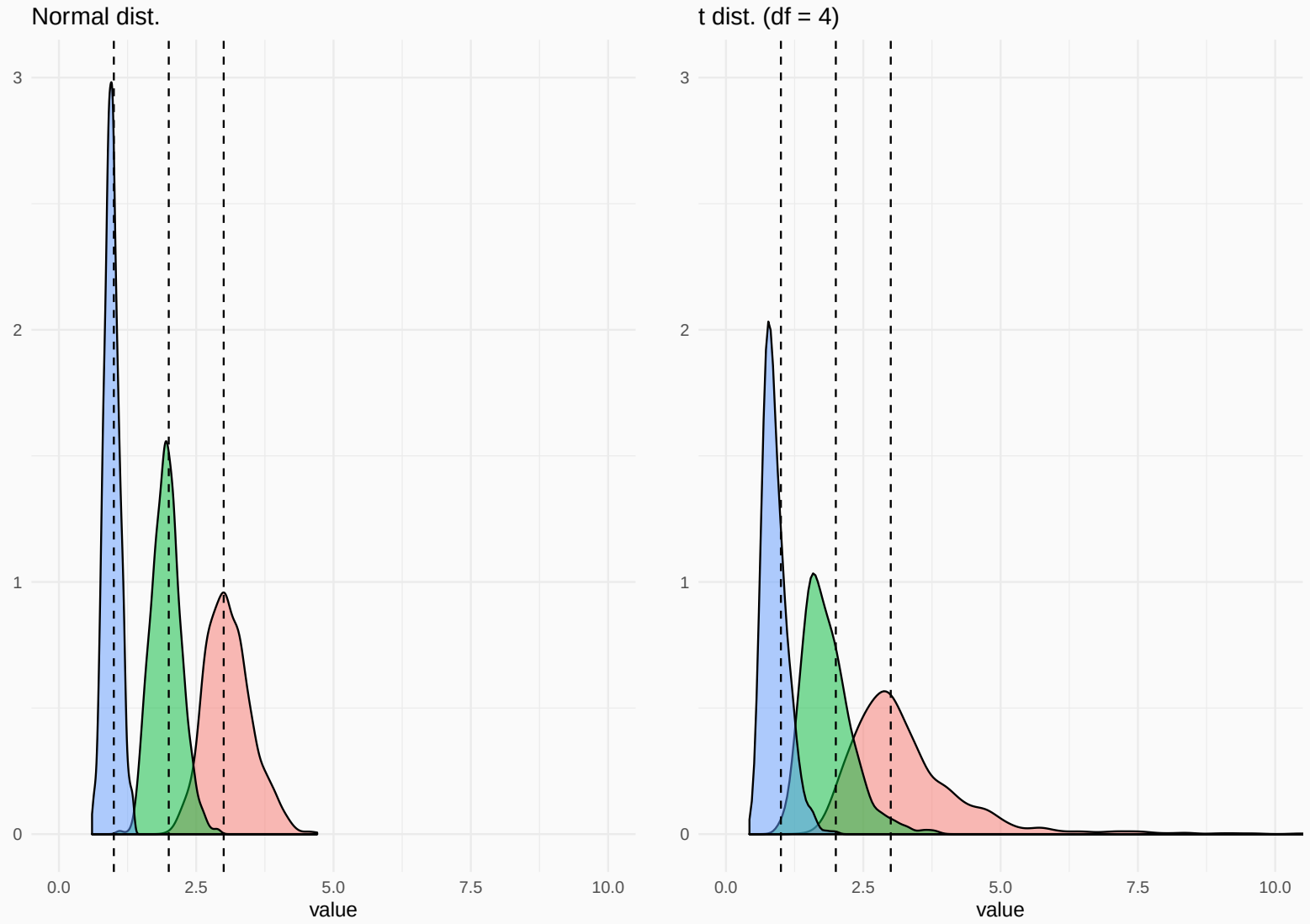


Simulations xiii

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

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

Simulations xiv



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

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

- 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

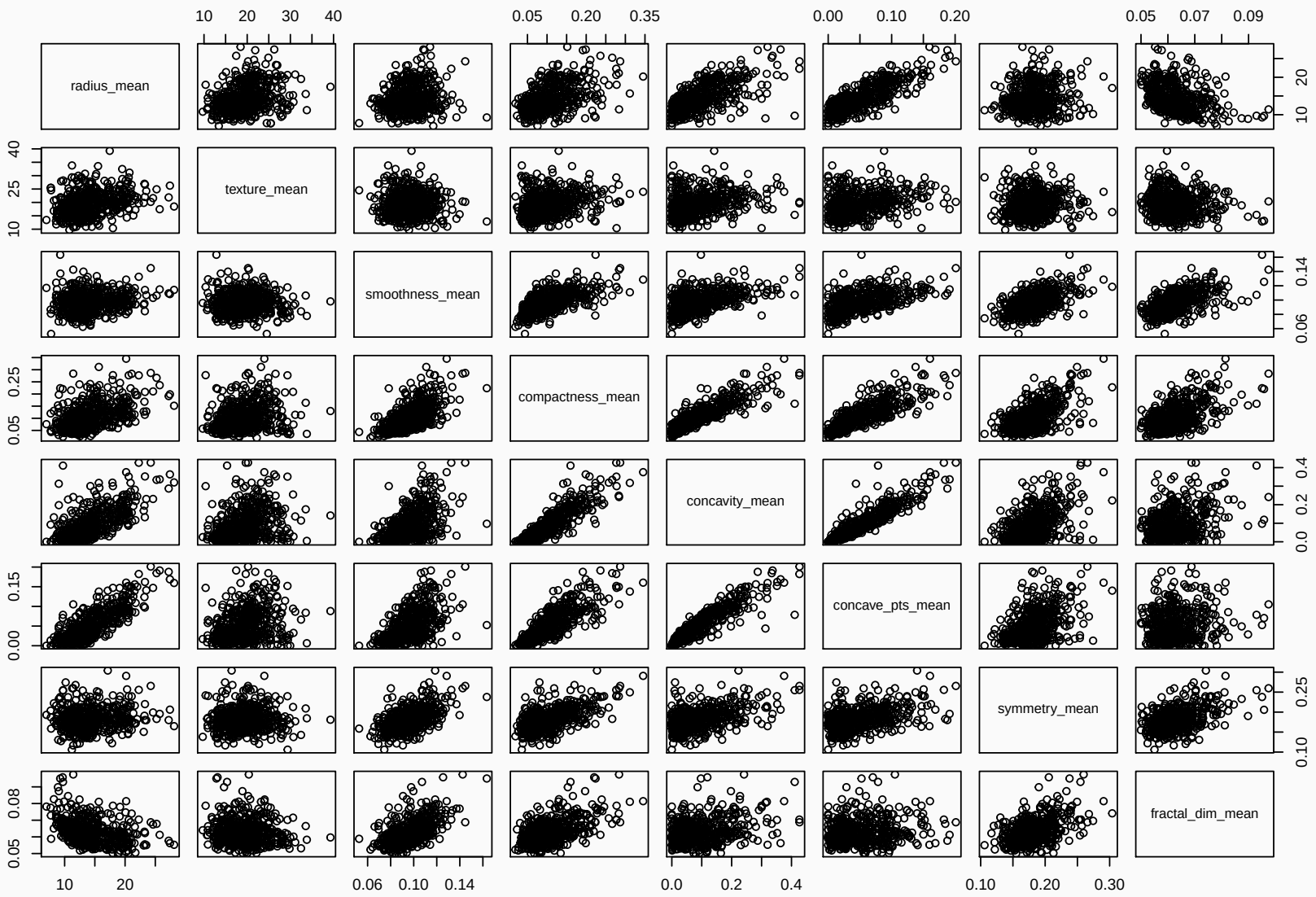
- Let $\bar{r} = \frac{2}{p(p-1)} \sum_{i<j} r_{ij}$ be the average of all off-diagonal elements (we are only looking at entries below the diagonal).
- Finally, let $\hat{\gamma} = \frac{(p-1)^2[1-(1-\bar{r})^2]}{p-(p-2)(1-\bar{r})^2}$.
- We reject the null hypothesis that the correlation matrix is equal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

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

```
# 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)

Selecting the number of PCs ii

- 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

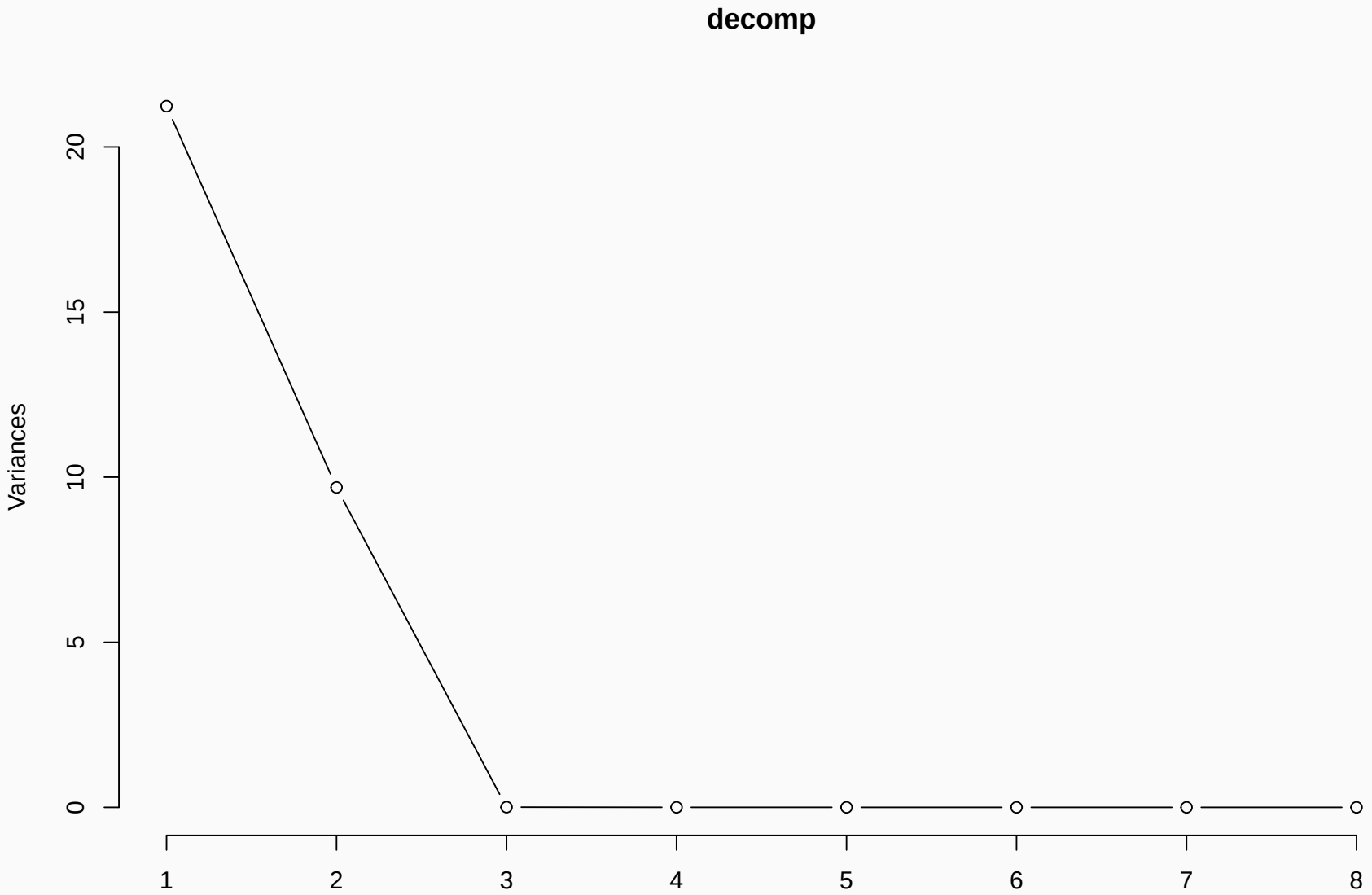
```
decomp <- prcomp(dataset)

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

```
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

```
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.

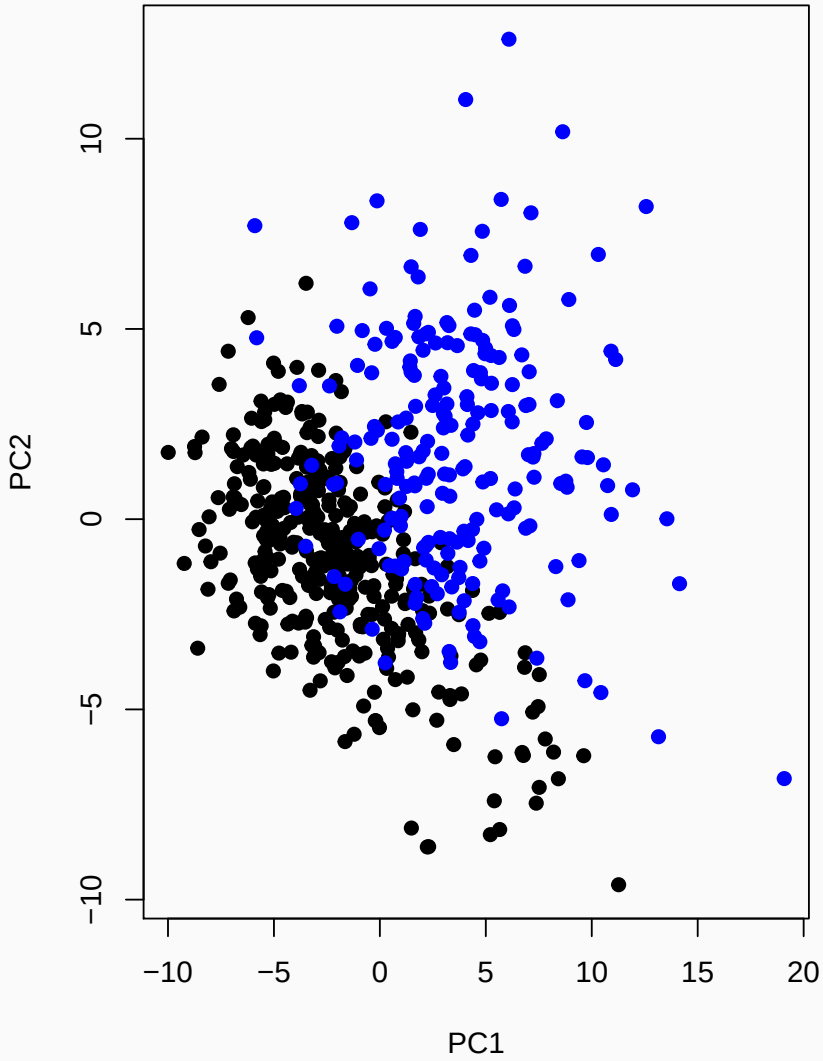
Example (cont'd) i

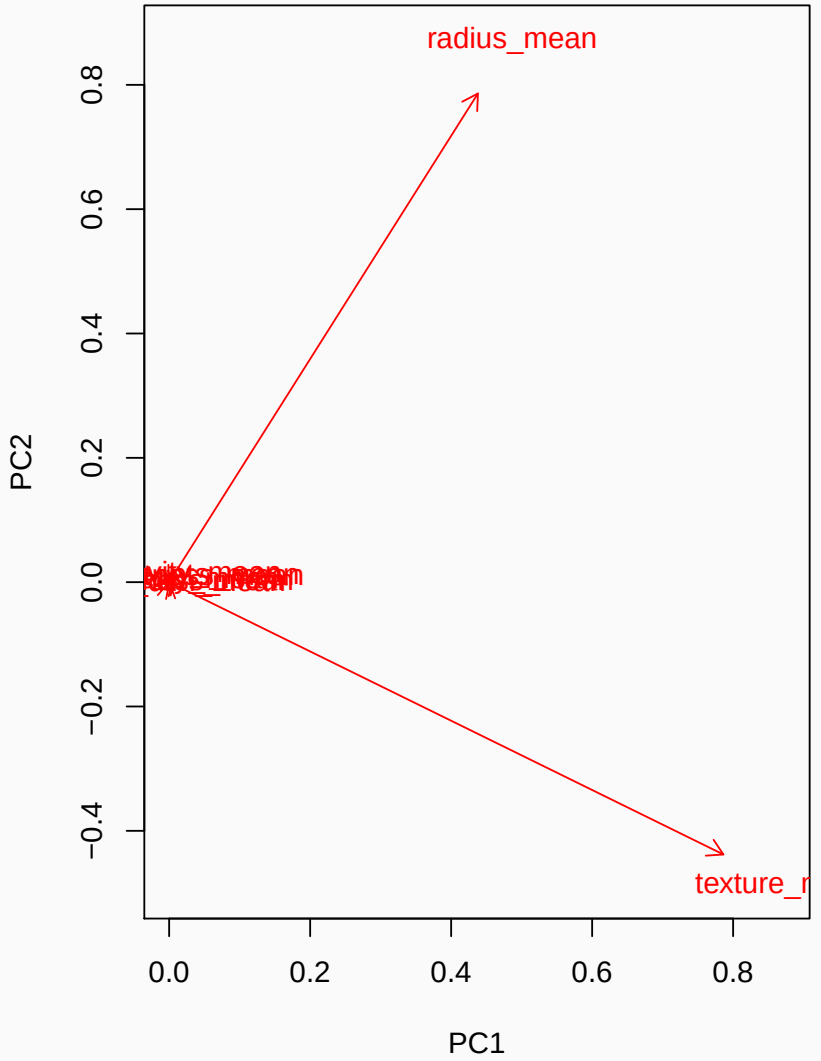
```
# Continuing with our example on breast cancer
decomp <- prcomp(dataset)

# 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

```
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)
```

Example (cont'd) iii

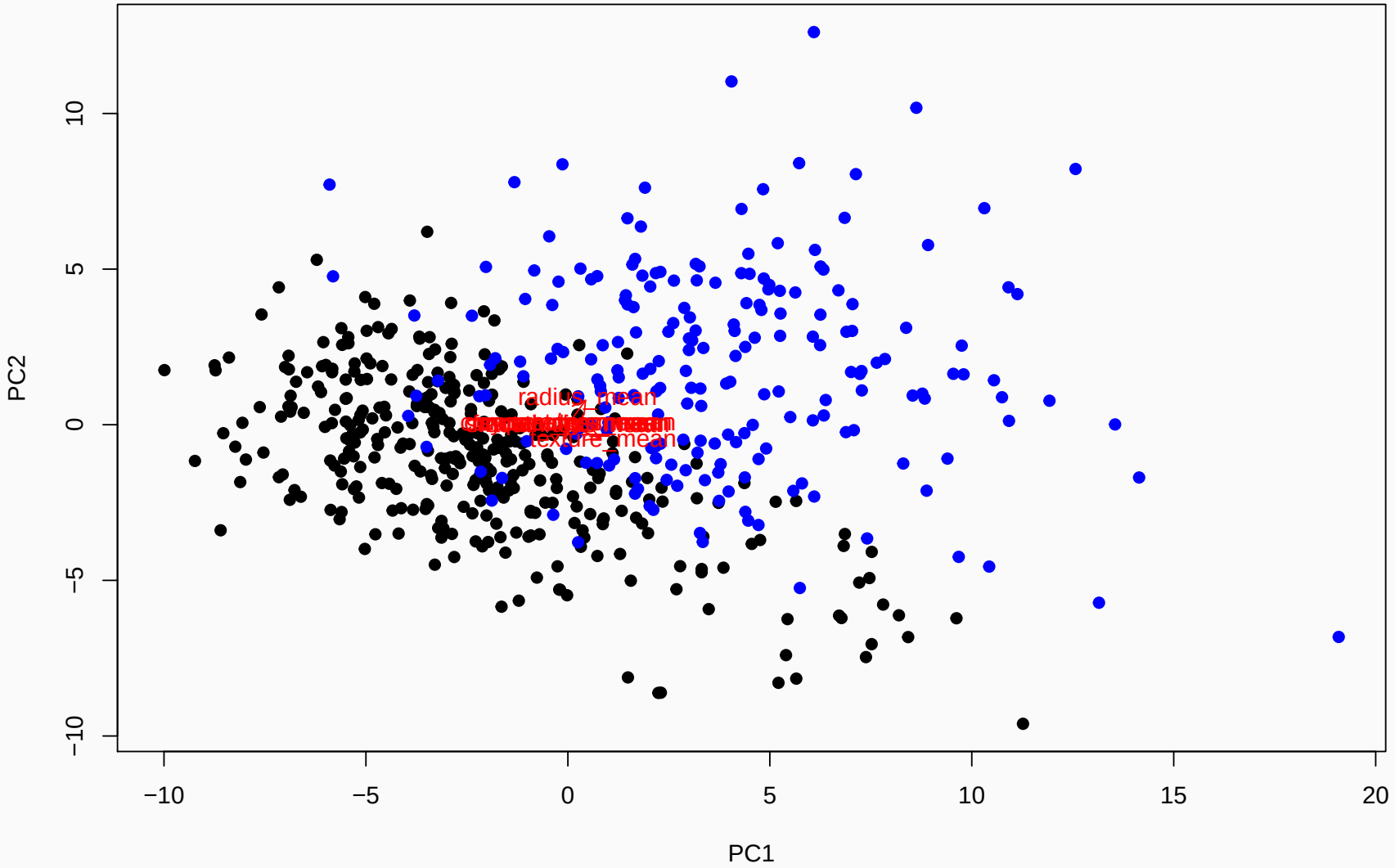




Example (cont'd) iv

```
# 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)
```

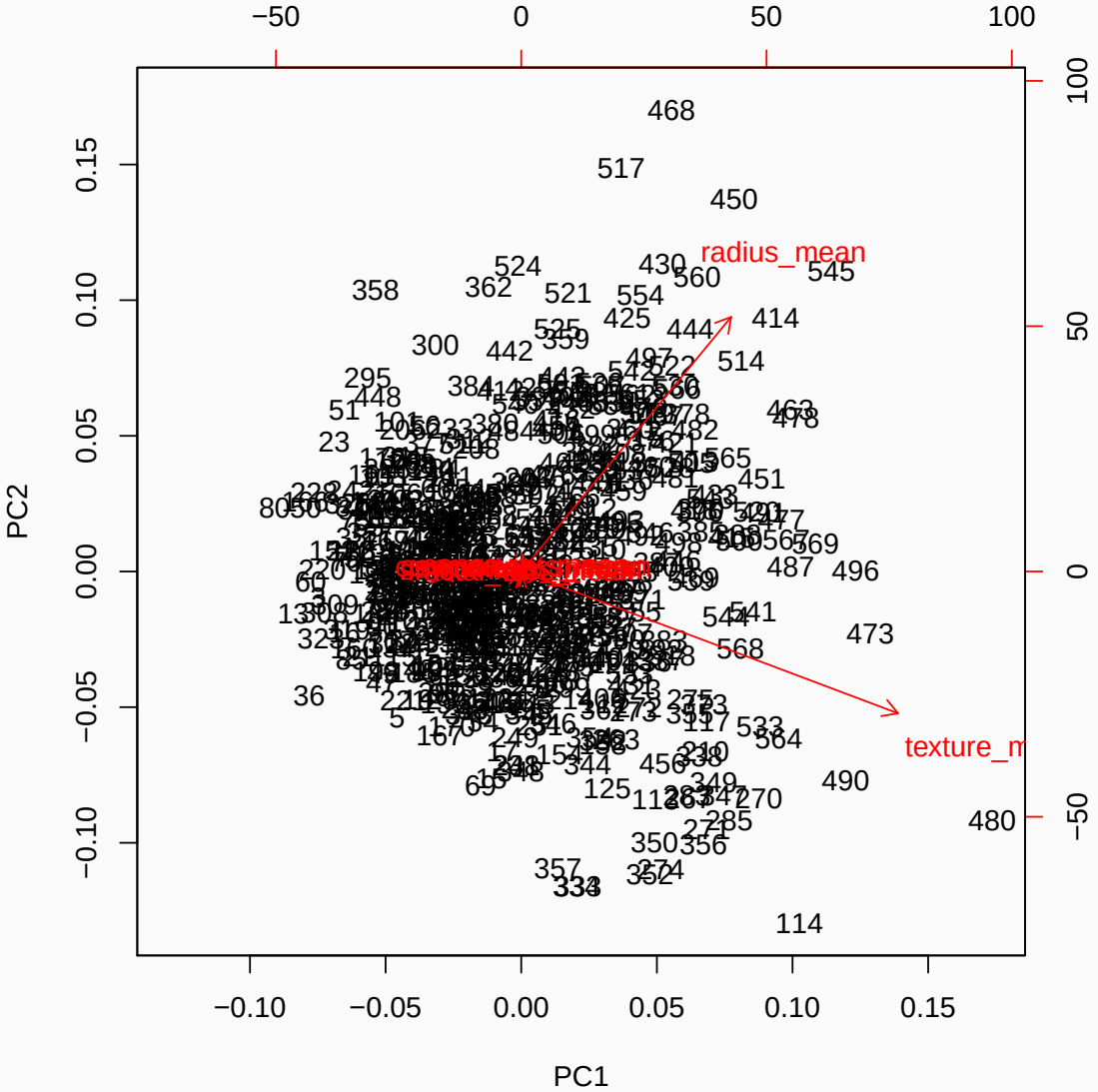
Example (cont'd) v



Example (cont'd) vi

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

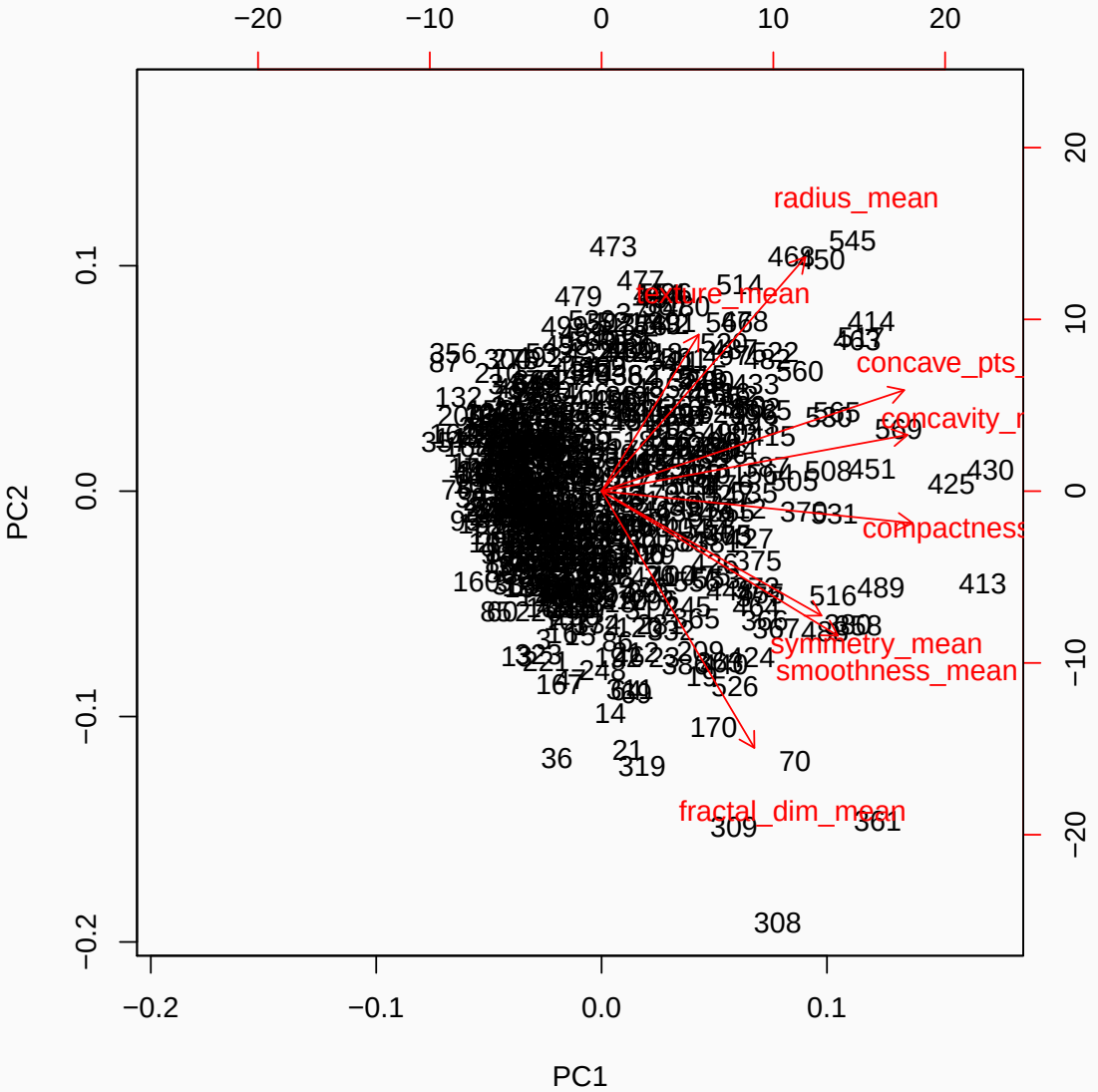
Example (cont'd) vii



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.

Feature Extraction i

Feature Extraction ii

```
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)

# 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))
```

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)
```

Feature Selection iv

```
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.