Principal Component Analysis

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STAT 4690–Applied Multivariate Analysis

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 $\|w\| = 1$)

Population PCA ii

- 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 $w_1^T \mathbf{Y}, \ldots, w_{j-1}^T \mathbf{Y}$.
- First, note that $\mathrm{Var}(w^T \mathbf{Y}) = w^T \Sigma w$. So our optimisation problem is

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

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

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

Population PCA iii

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

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

- From the first partial derivative, we conclude that

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

Population PCA iv

- 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.
- 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.

Population PCA v

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:
  - $\mathbf{Z}_i = w_i^T \mathbf{Y}$ 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

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

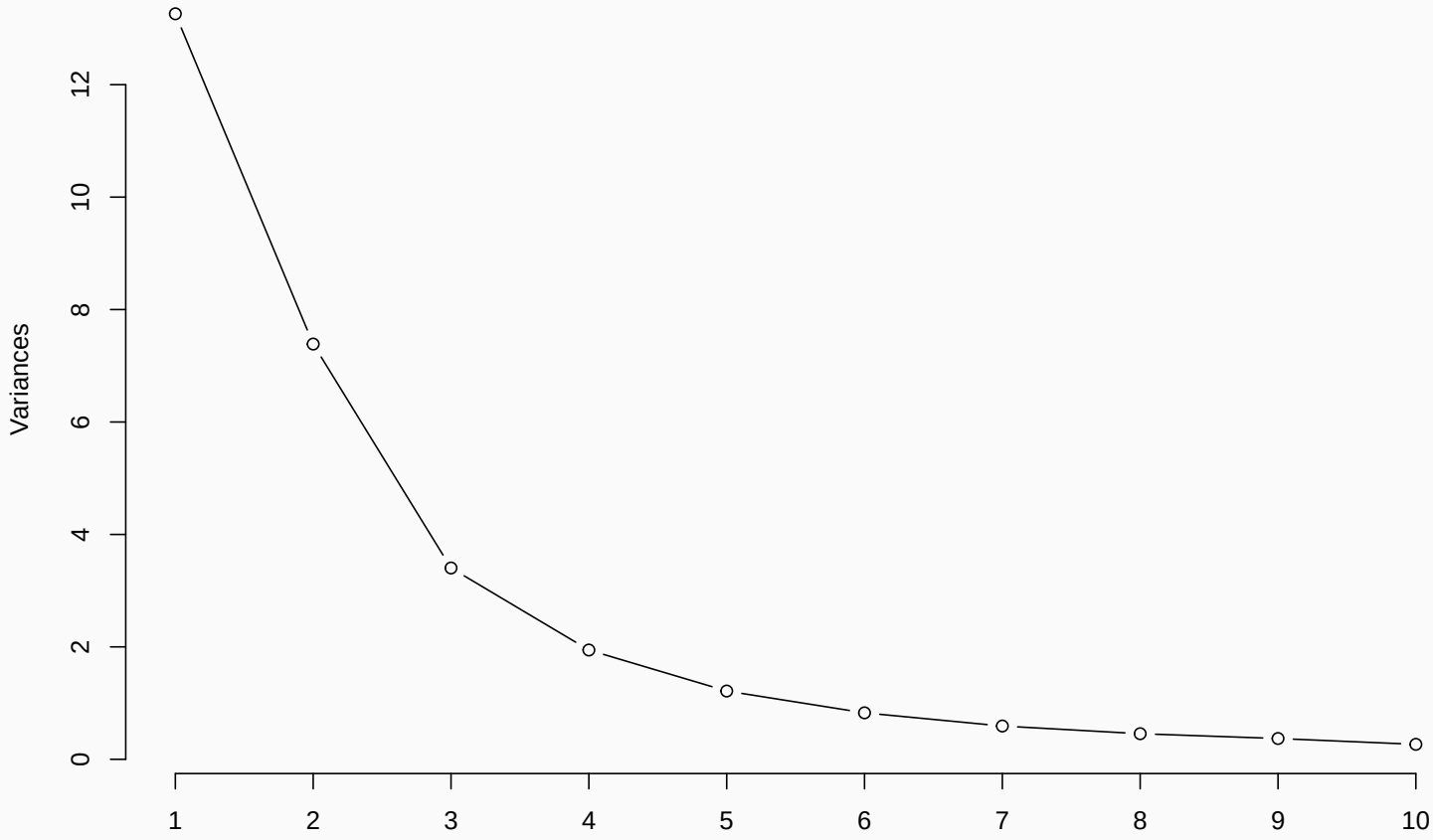
Properties of PCA ii

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

```
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)
```

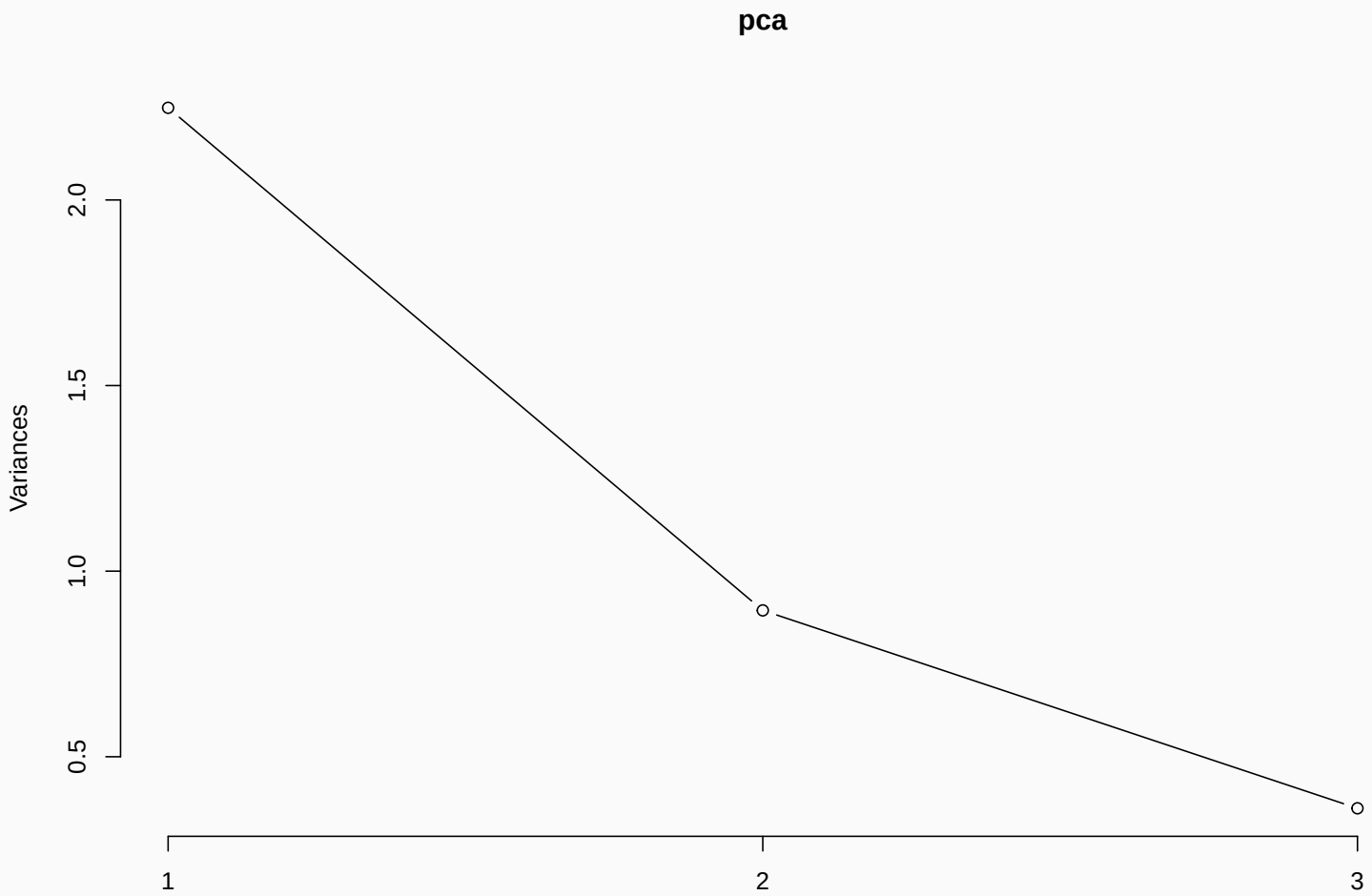
Example 1 ii

```
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
```

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

Example 1 iii



Example 2 i

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

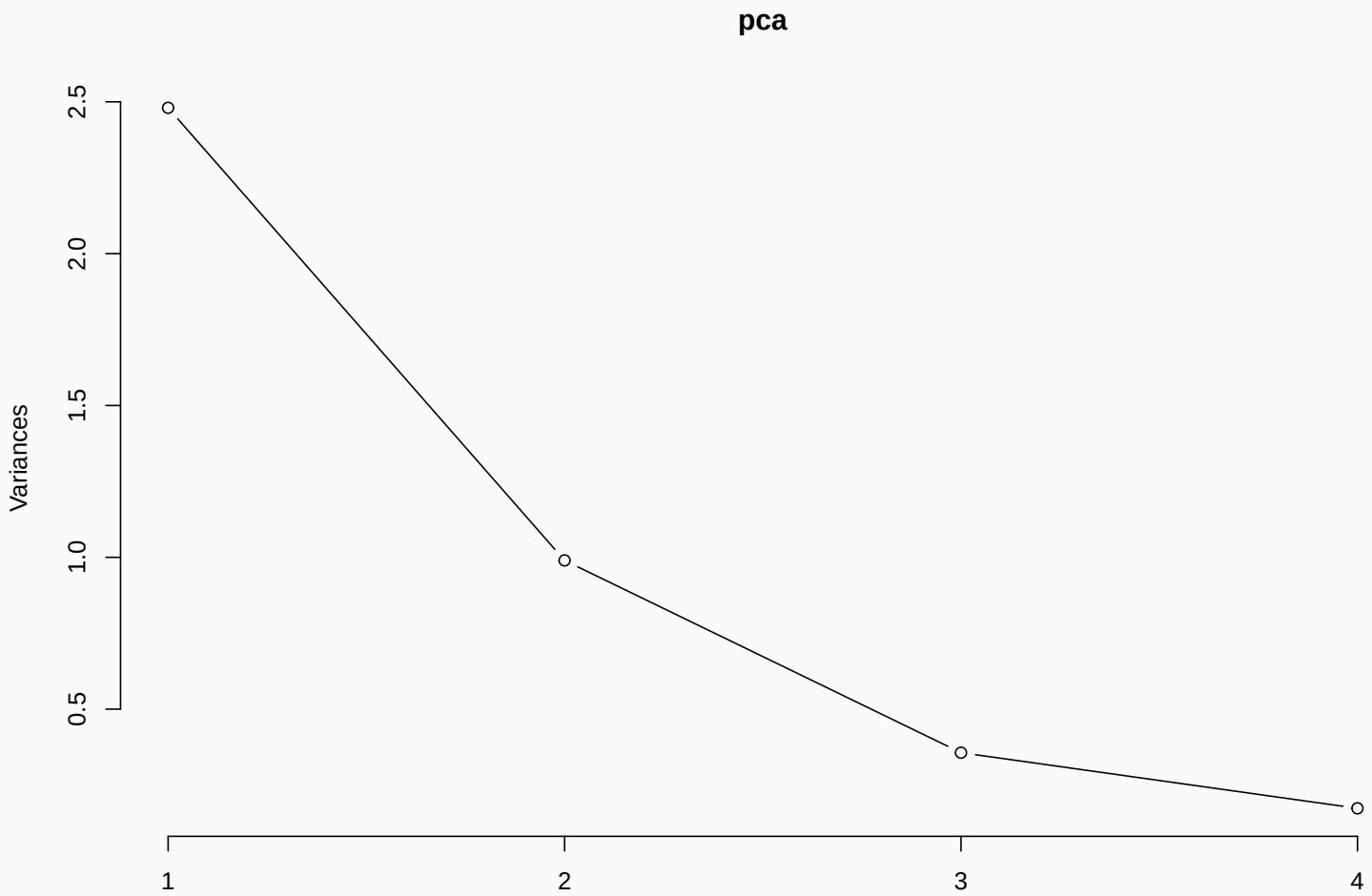
```
summary(pca)
```

```
## 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



Applications of PCA

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

```
library(ElemStatLearn)
library(tidyverse)
train <- subset(prostate, train == TRUE,
                select = -train)
test  <- subset(prostate, train == FALSE,
                select = -train)

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

Feature Extraction ii

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

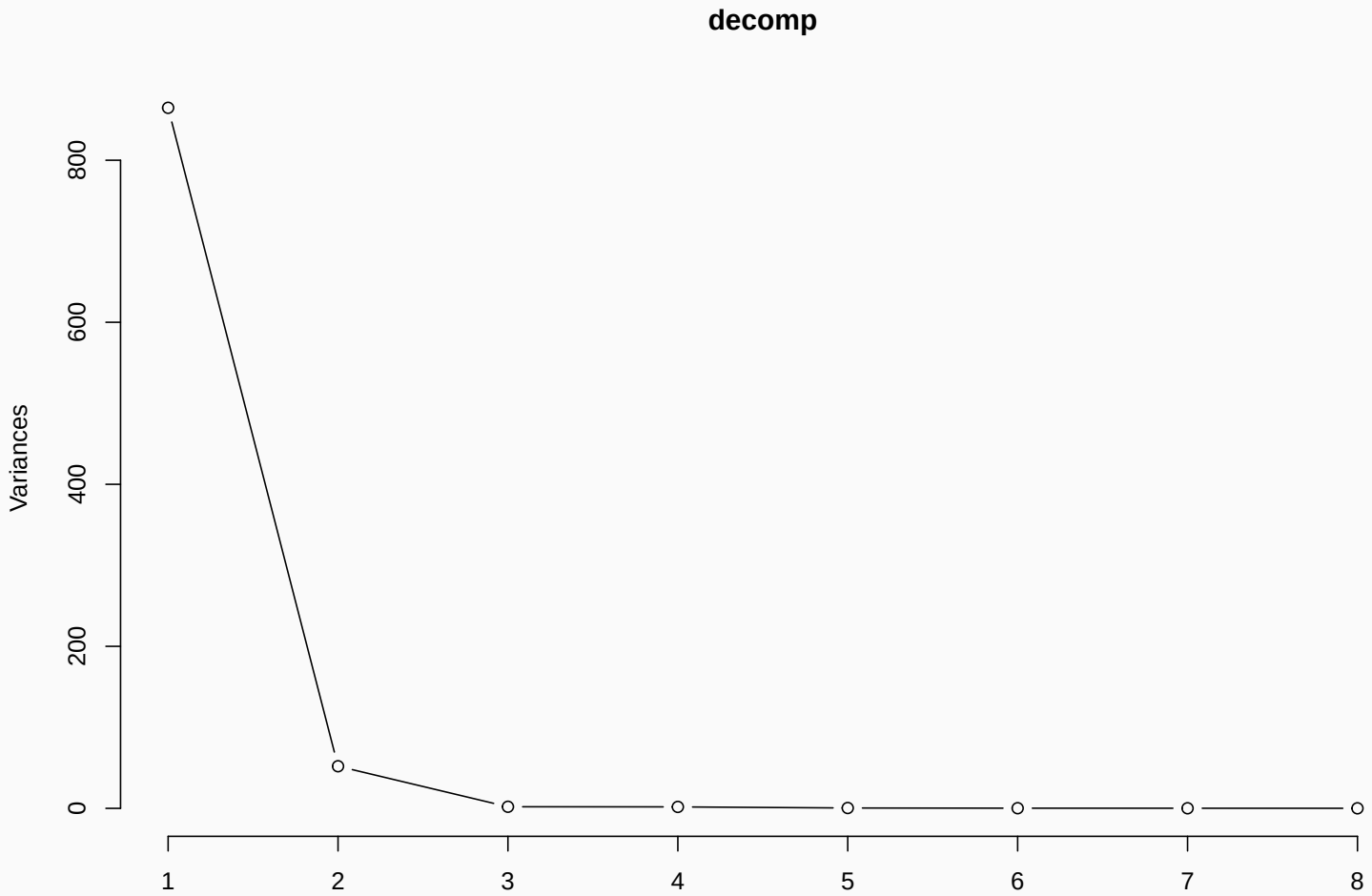
```
# PCA
decomp <- train %>%
  subset(select = -lpsa) %>%
  as.matrix() %>%
  prcomp
summary(decomp)$importance[,1:3]
```

Feature Extraction iii

```
##                             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
```

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

Feature Extraction iv



Feature Extraction v

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

test_pc <- as.data.frame(predict(decomp, test))
pc_pred <- predict(pc_model,
                   newdata = test_pc)
(pc_mse <- mean((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 = train[,c(keep, "lpsa")])
fs_pred <- predict(fs_model, newdata = test)
(fs_mse <- mean((test$lpsa - fs_pred)^2))
```

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

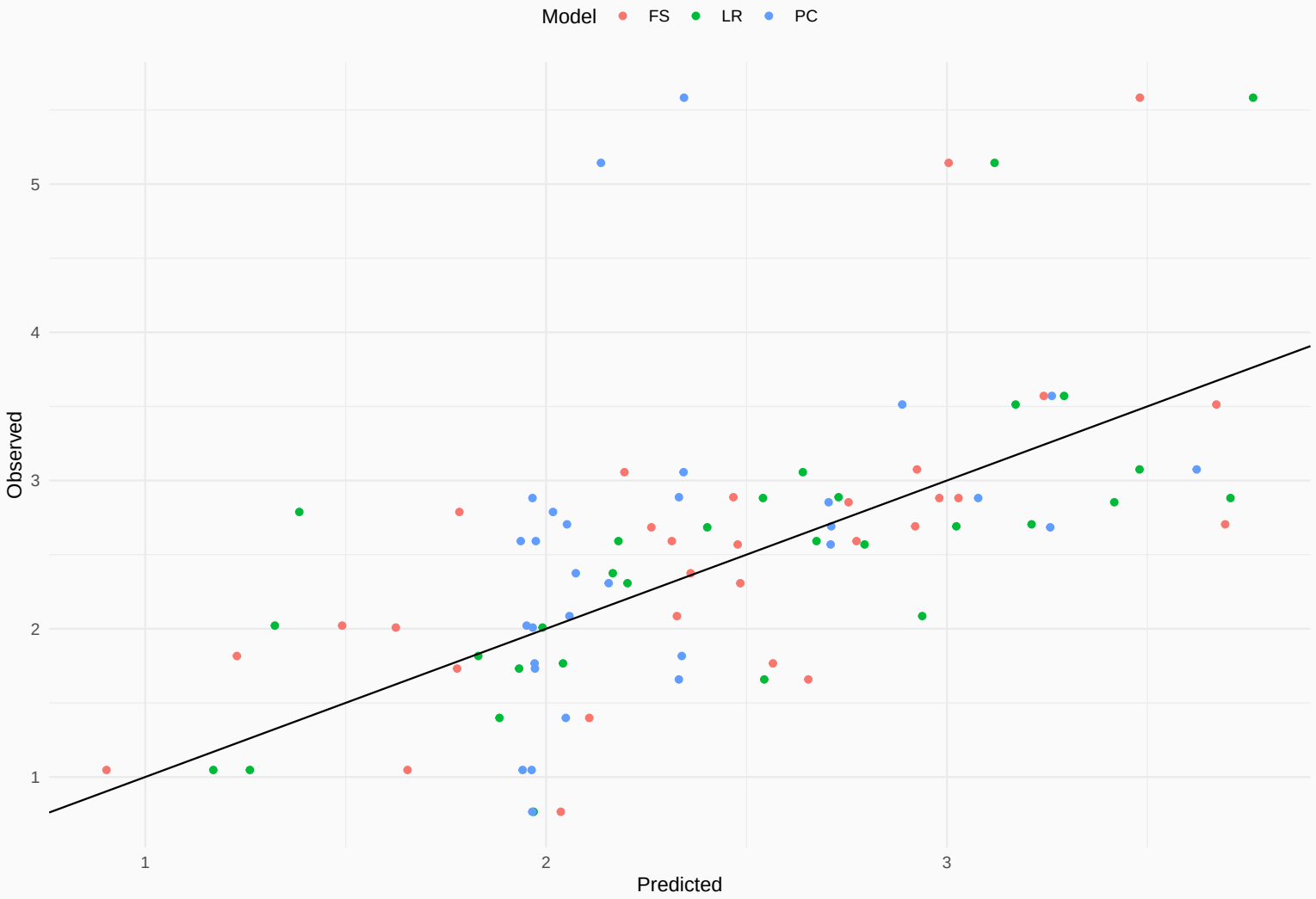
Feature Selection iii

```
model_plot <- data.frame(
  "obs" = 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.

Data Visualization i

```
library(dslabs)
```

```
mnist <- read_mnist()
```

```
dim(mnist$train$images)
```

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

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

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

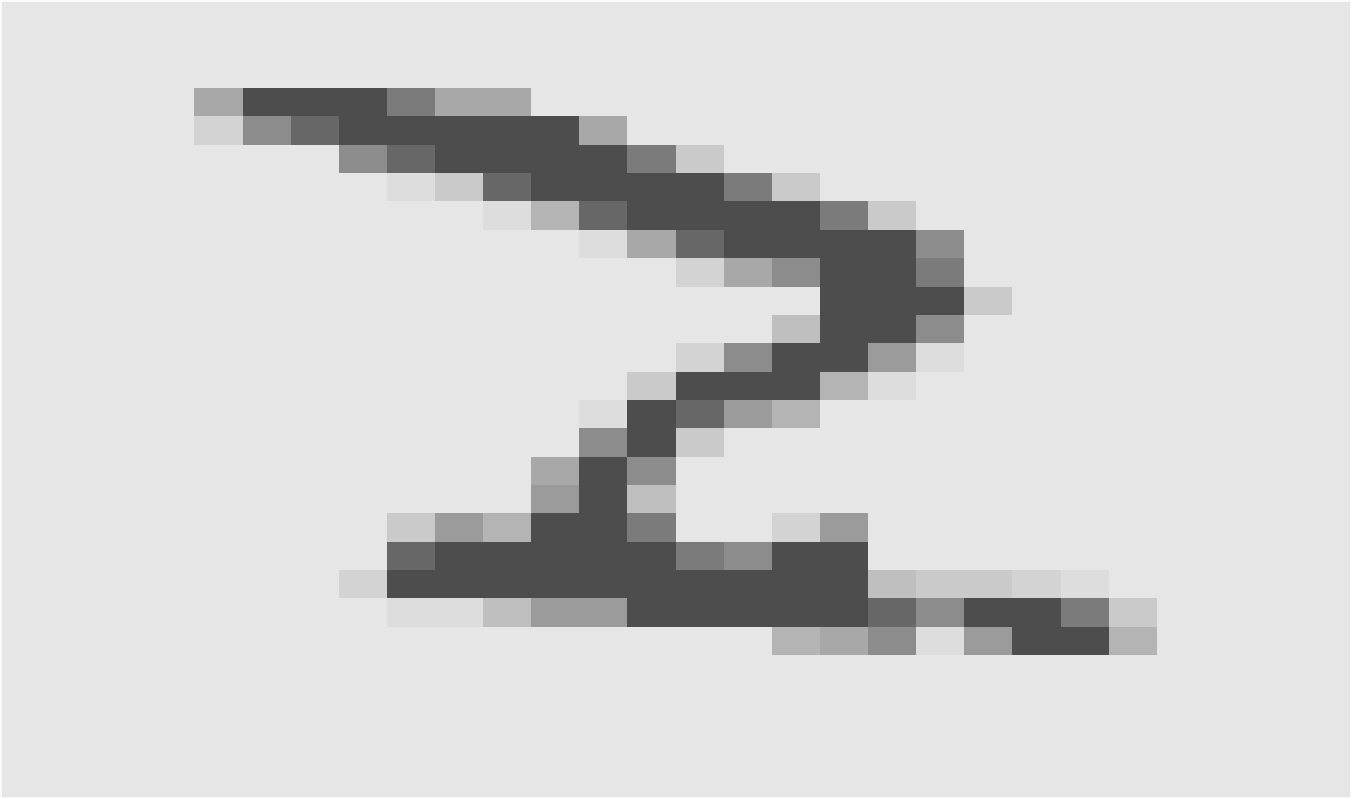
Data Visualization ii

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

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

```
matrix(mnist$train$images[1,], ncol = 28) %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE)
```

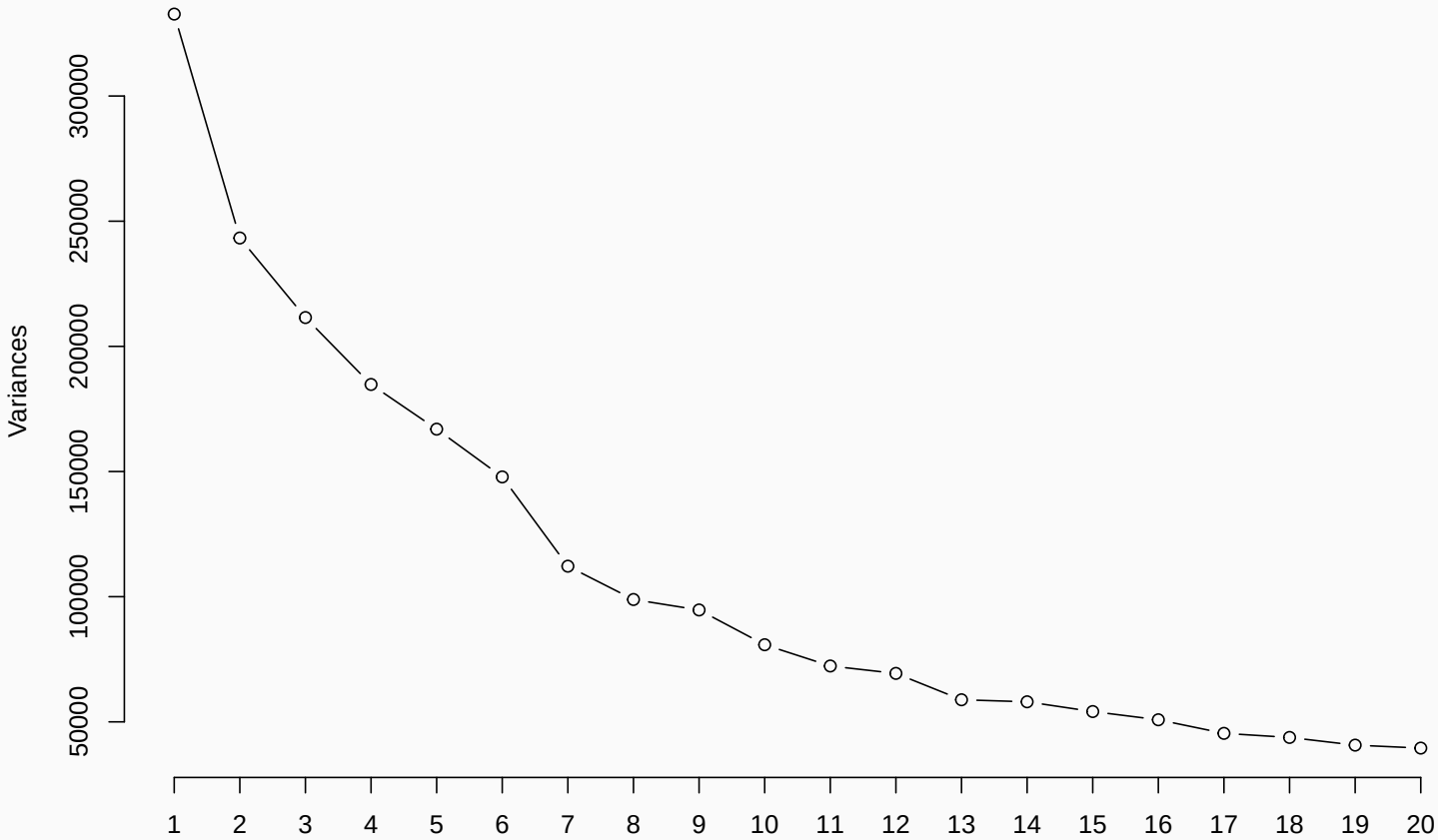
Data Visualization iii



Data Visualization iv

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

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

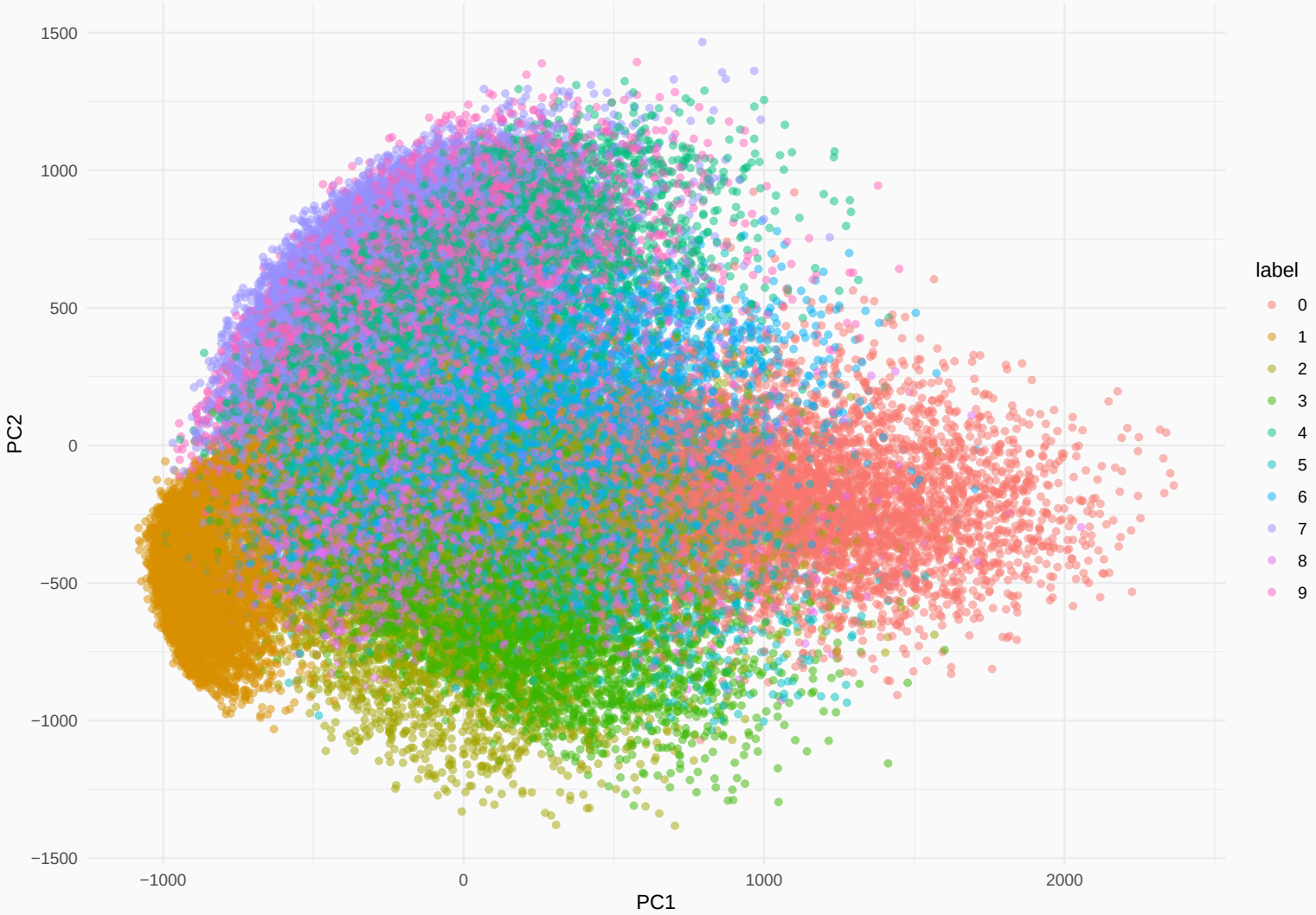
Data Visualization v



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()
```

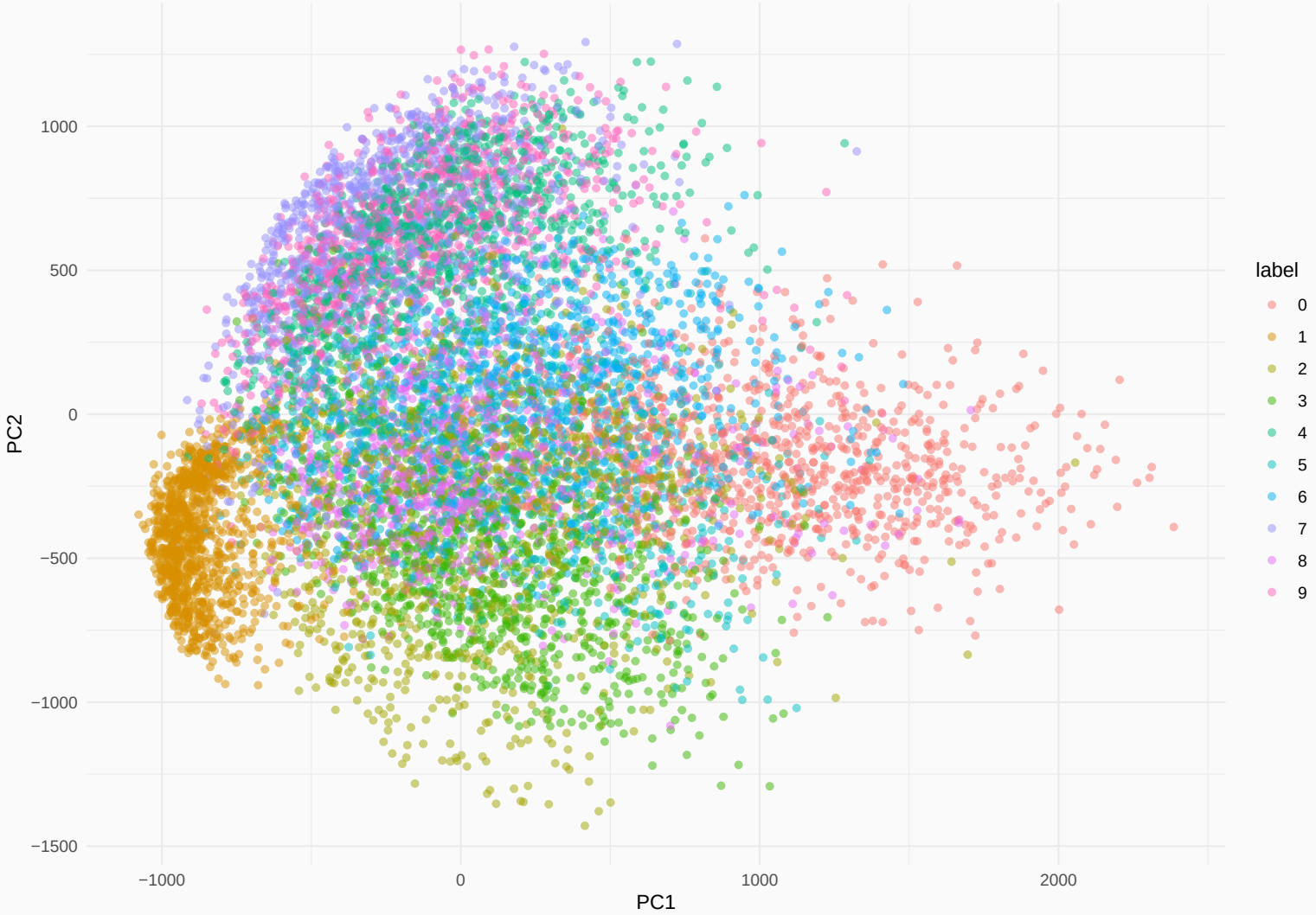
Data Visualization vii



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()
```

Data Visualization ix

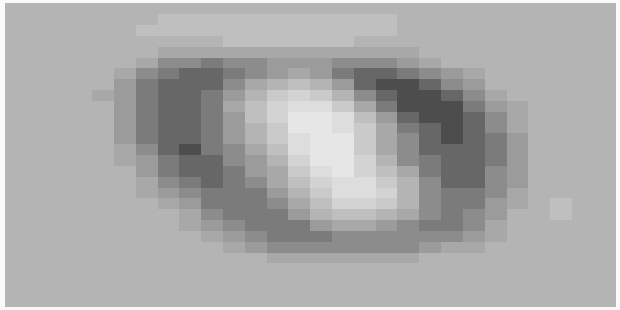


Data Visualization x

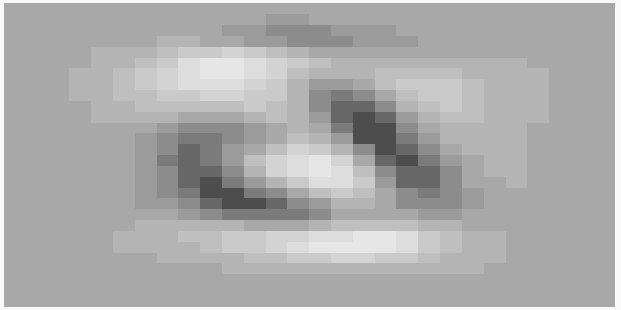
```
par(mfrow = c(2, 2))
for (i in seq_len(4)) {
  matrix(decomp$rotation[,i], ncol = 28) %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, main = paste0("PC", i))
}
```

Data Visualization xi

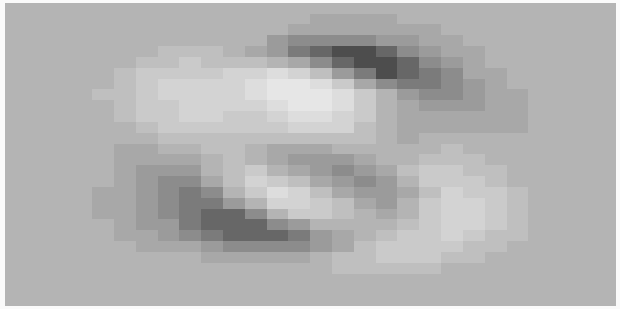
PC1



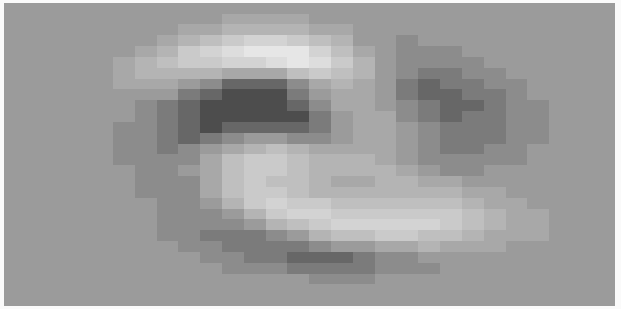
PC2



PC3



PC4

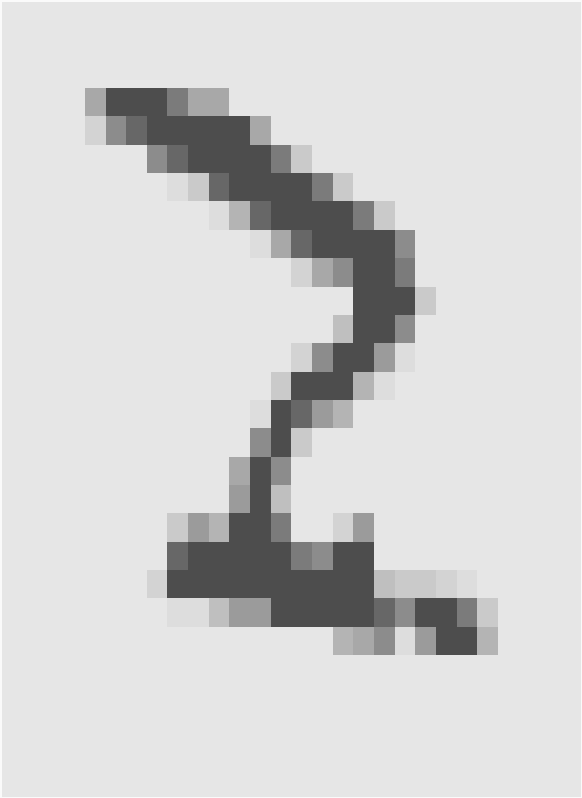


Data Visualization xii

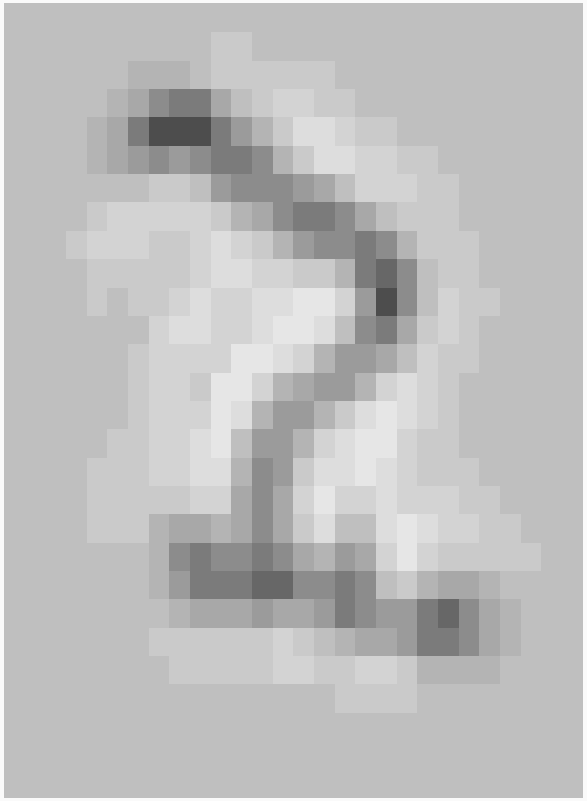
```
# Approximation with 90 PCs
approx_mnist <- decomp$rotation[, seq_len(90)] %*%
  decomp$x[1, seq_len(90)]
par(mfrow = c(1, 2))

matrix(mnist$train$images[1,], ncol = 28) %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, main = "Original")
matrix(approx_mnist, ncol = 28) %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, main = "Approx")
```

Data Visualization xiii

Original



Approx



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

```
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

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

colMeans(X)
```

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

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

Example 1 (revisited) iii

```
##             PC1             PC2             PC3
## -6.169544e-17  5.433154e-17  9.228729e-18
```

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

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

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.
- We want to find $\mu, W_k, \mathbf{Z}_i$ that minimises the **reconstruction error**:

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

Geometric interpretation of PCA iii

- First, treating W_k constant and minimising over $\mu, \mathbf{Z}_i$, we find

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

- Putting these quantities into the reconstruction error, we get

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

Geometric interpretation of PCA iv

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* or 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
```