Machine Learning: Cross-Validation & Regularisation

ACTL3142 & ACTL5110 Statistical Machine Learning for Risk Applications

Lecture Outline

- **Linear Regression Recap**
- Generalised Linear Models Recap
- Glassdoor Dataset
- Statistical Model Evaluation
- Validation Set Approach
- k-Fold Cross-Validation
- Leave-One-Out Cross-Validation
- Regularisation
- Regularisation Plots
- Regularisation Demos
- Ridge and Lasso Intuition

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Single Linear Regression (SLR)

Scenario: use *head circumference (mm)* to predict *age (weeks)* of a fetal baby

$$\boldsymbol{x} = \begin{pmatrix} 105 \\ 120 \\ 110 \\ 117 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 20 \\ 24 \\ 22 \\ 23 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 20.3 \\ 24.0 \\ 21.5 \\ 23.2 \end{pmatrix}$$

$$\hat{y}(x) = \beta_0 + \beta_1 x$$

```r
circumference <- c(105, 120, 110, 117)
age <- c(20, 24, 22, 23)
model <- lm(age ~ circumference)
print(coef(model))
```

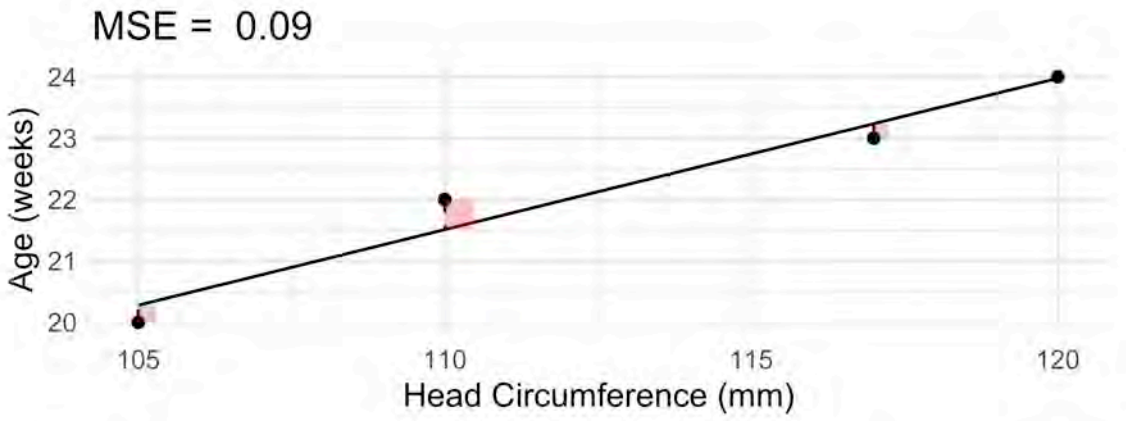
```
(Intercept) circumference
 -5.5905797     0.2463768
```

```r
predict(model, newdata = data.frame(circumference))
```

```
       1        2        3        4
20.27899 23.97464 21.51087 23.23551
```

Mean squared error

$$\boldsymbol{y} = \begin{pmatrix} 20 \\ 24 \\ 22 \\ 23 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 20.3 \\ 24.0 \\ 21.5 \\ 23.2 \end{pmatrix}, \quad \boldsymbol{y} - \hat{\boldsymbol{y}} = \begin{pmatrix} -0.3 \\ 0 \\ 0.5 \\ -0.2 \end{pmatrix}.$$

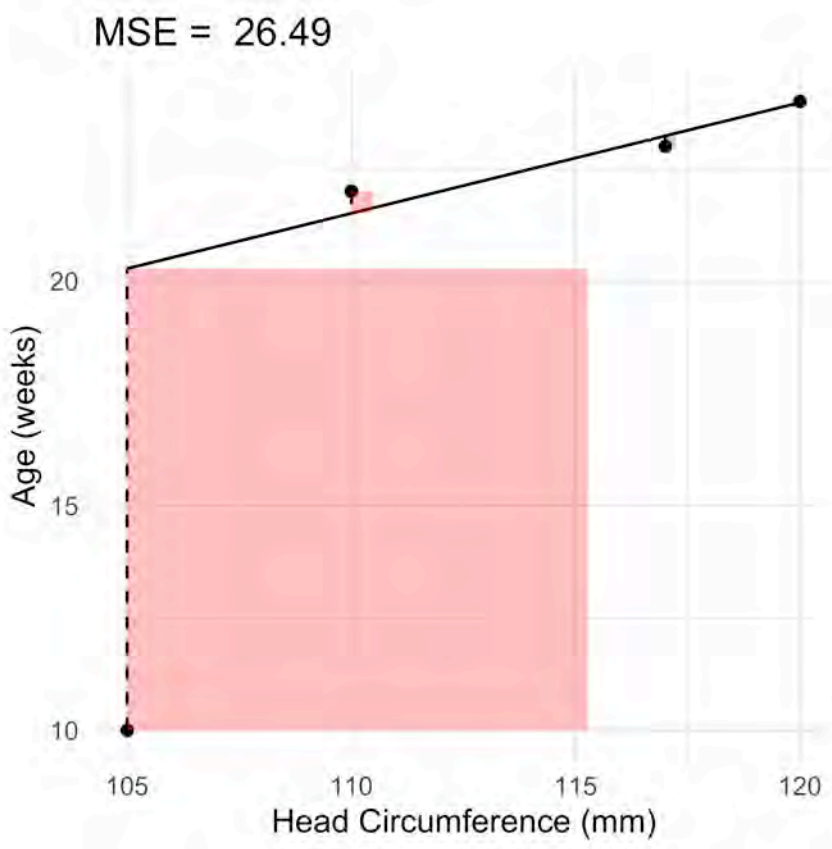


$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{4}\left[(-0.3)^2 + 0^2 + 0.5^2 + (-0.2)^2\right] = 0.09.$$

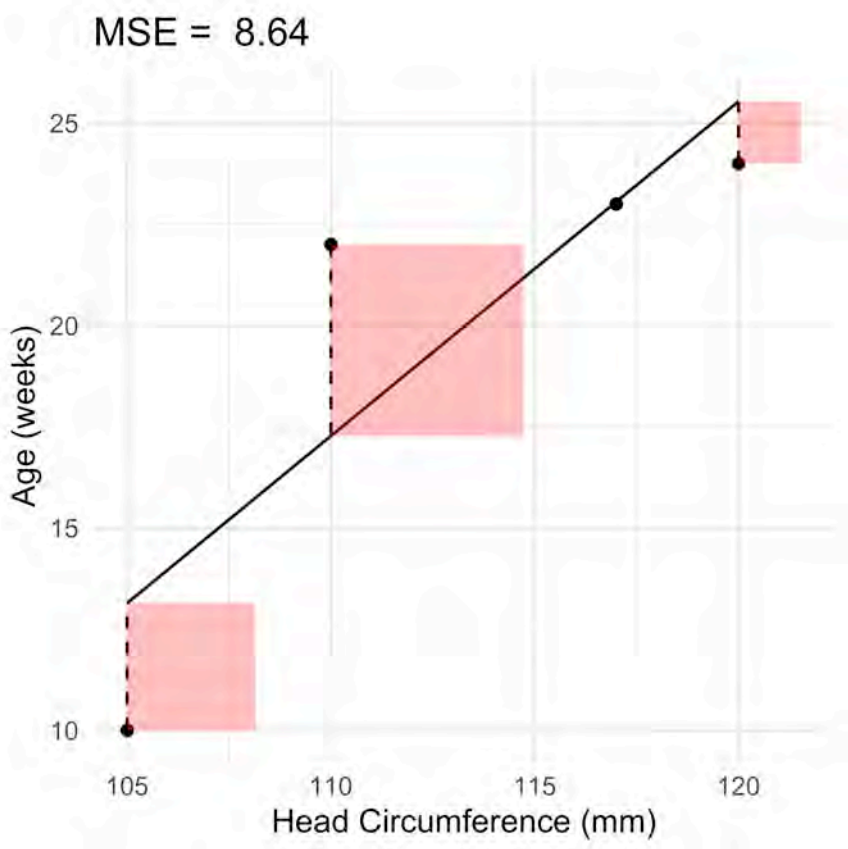
$\text{RSS} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = 0.38.$

Sensitive to outliers

If we instead had $\boldsymbol{y} = \begin{pmatrix} 10 & 24 & 22 & 23 \end{pmatrix}^\top$.



The previous model



New model after training

Multiple Linear Regression (MLR)

Scenario: use *temperature* ($°C$) **and** *humidity* ($\%$) to predict *rainfall* (mm)

$$\boldsymbol{X} = \begin{pmatrix} 27 & 80 \\ 32 & 70 \\ 28 & 72 \\ 22 & 86 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 6 \\ 7 \\ 6 \\ 4 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 5.7 \\ 7.2 \\ 5.9 \\ 4.2 \end{pmatrix}$$

$$\hat{y}(\boldsymbol{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p = \beta_0 + \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle$$

```r
weather <- data.frame(temperature = c(27, 32, 28, 22), humidity = c(80, 70, 72, 86))
rainfall <- c(6, 7, 6, 4)
model <- lm(rainfall ~ temperature + humidity, data = weather)
summary(model)$coefficients
```

```
              Estimate  Std. Error    t value  Pr(>|t|)
(Intercept) -5.51001821 10.45422801 -0.5270612 0.6912003
temperature  0.34244080  0.15162225  2.2585129 0.2653588
humidity     0.02504554  0.08434494  0.2969418 0.8162405
```

```r
predict(model, newdata = weather)
```

```
       1        2        3        4
5.739526 7.201275 5.881603 4.177596
```

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MLR's design matrix

Scenario: use *temperature* ($°C$) **and** *humidity* ($\%$) to predict *rainfall* (mm)

$$\boldsymbol{X} = \begin{pmatrix} 1 & 27 & 80 \\ 1 & 32 & 70 \\ 1 & 28 & 72 \\ 1 & 22 & 86 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 6 \\ 7 \\ 6 \\ 4 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 5.7 \\ 7.2 \\ 5.9 \\ 4.2 \end{pmatrix}$$

$$\hat{y}(\boldsymbol{x}) = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p = \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle$$

```r
as.matrix(weather)
```

```
     temperature humidity
[1,]          27       80
[2,]          32       70
[3,]          28       72
[4,]          22       86
```

```r
X <- model.matrix(rainfall ~ temperature + humidity, data = weather)
X
```

```
  (Intercept) temperature humidity
1           1          27       80
2           1          32       70
3           1          28       72
4           1          22       86
attr(,"assign")
[1] 0 1 2
```

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MLR is just matrix equations

$$\boldsymbol{\beta} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

```
model <- lm(rainfall ~ temperature +
        humidity, data = weather)
coef(model)
```

```
(Intercept) temperature    humidity
-5.51001821  0.34244080  0.02504554
```

```
y <- rainfall
beta <- solve(t(X) %*% X) %*% t(X) %*% y
beta
```

```
                    [,1]
(Intercept) -5.51001821
temperature  0.34244080
humidity     0.02504554
```

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\beta}.$$

```
predict(model, newdata = weather)
```

```
       1        2        3        4
5.739526 7.201275 5.881603 4.177596
```

```
X %*% beta
```

```
     [,1]
1 5.739526
2 7.201275
3 5.881603
4 4.177596
```

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MLR after normalising the inputs

Scenario: use *temperature (z-score)* **and** *humidity (z-score)* to predict *rainfall (mm)*

$$\boldsymbol{X} = \begin{pmatrix} 1 & -0.06 & 0.41 \\ 1 & 1.15 & -0.95 \\ 1 & 0.18 & -0.68 \\ 1 & -1.28 & 1.22 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 6 \\ 7 \\ 6 \\ 4 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 5.7 \\ 7.2 \\ 5.9 \\ 4.2 \end{pmatrix}$$

$$\hat{y}(\boldsymbol{x}) = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p = \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle$$

```r
weather <- data.frame(temperature = c(27, 32, 28, 22), humidity = c(80, 70, 72, 86))
weather <- data.frame(scale(weather))
rainfall <- c(6, 7, 6, 4)
model <- lm(rainfall ~ temperature + humidity, data = weather)
summary(model)$coefficients
```

```
            Estimate Std. Error    t value   Pr(>|t|)
(Intercept) 5.750000  0.1961608 29.3126889 0.02170981
temperature 1.408455  0.6236204  2.2585129 0.26535876
humidity    0.185179  0.6236204  0.2969418 0.81624051
```

```r
predict(model, newdata = weather)
```

```
       1        2        3        4
5.739526 7.201275 5.881603 4.177596
```

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SLR with categorical inputs

Scenario: use *property type* to predict its *sale price ($)*

$$\boldsymbol{x} = \begin{pmatrix} \text{Unit} \\ \text{TownHouse} \\ \text{TownHouse} \\ \text{House} \end{pmatrix} \longrightarrow \boldsymbol{X} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 300000 \\ 500000 \\ 510000 \\ 700000 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 300000 \\ 505000 \\ 505000 \\ 700000 \end{pmatrix}$$

$$\hat{y}(x) = \beta_0 + \beta_1 \underbrace{I(x = \text{Unit})}_{=:x_1} + \beta_2 \underbrace{I(x = \text{TownHouse})}_{=:x_2} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

```r
type <- factor(c("Unit", "TownHouse", "TownHouse", "House"))
price <- c(300000, 500000, 510000, 700000)
model <- lm(price ~ type)
summary(model)$coefficients
```

```
             Estimate Std. Error   t value    Pr(>|t|)
(Intercept)    700000   7071.068  98.99495 0.006430612
typeTownHouse -195000   8660.254 -22.51666 0.028254710
typeUnit      -400000  10000.000 -40.00000 0.015912180
```

```r
predict(model, newdata = data.frame(type))
```

```
     1      2      3      4
300000 505000 505000 700000
```

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Changing the base case

Scenario: use *property type* to predict its *sale price ($)*

$$\boldsymbol{x} = \begin{pmatrix} \text{Unit} \\ \text{TownHouse} \\ \text{TownHouse} \\ \text{House} \end{pmatrix} \longrightarrow \boldsymbol{X} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 300000 \\ 500000 \\ 510000 \\ 700000 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 300000 \\ 505000 \\ 505000 \\ 700000 \end{pmatrix}$$

$$\hat{y}(x) = \beta_0 + \beta_1 \underbrace{I(x = \text{TownHouse})}_{=:x_1} + \beta_2 \underbrace{I(x = \text{House})}_{=:x_2} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

```r
type <- factor(c("Unit", "TownHouse", "TownHouse", "House"), levels = c("Unit", "TownHouse", "House"))
price <- c(300000, 500000, 510000, 700000)
model <- lm(price ~ type)
summary(model)$coefficients
```

```
             Estimate Std. Error  t value   Pr(>|t|)
(Intercept)    300000   7071.068 42.42641 0.01500249
typeTownHouse  205000   8660.254 23.67136 0.02687811
typeHouse      400000  10000.000 40.00000 0.01591218
```

```r
predict(model, newdata = data.frame(type))
```

```
     1      2      3      4
300000 505000 505000 700000
```

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Changing the target's units

Scenario: use *property type* to predict its *sale price ($000,000's)*

$$\boldsymbol{x} = \begin{pmatrix} \text{Unit} \\ \text{TownHouse} \\ \text{TownHouse} \\ \text{House} \end{pmatrix} \longrightarrow \boldsymbol{X} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 0.3 \\ 0.5 \\ 0.51 \\ 0.7 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} 0.3 \\ 0.505 \\ 0.505 \\ 0.7 \end{pmatrix}$$

$$\hat{y}(x) = \beta_0 + \beta_1 \underbrace{I(x = \text{TownHouse})}_{=:x_1} + \beta_2 \underbrace{I(x = \text{House})}_{=:x_2} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

```r
type <- factor(c("Unit", "TownHouse", "TownHouse", "House"), levels = c("Unit", "TownHouse", "House"))
price <- c(0.3, 0.5, 0.51, 0.7)
model <- lm(price ~ type)
summary(model)$coefficients
```

```
             Estimate  Std. Error  t value   Pr(>|t|)
(Intercept)     0.300 0.007071068 42.42641 0.01500249
typeTownHouse   0.205 0.008660254 23.67136 0.02687811
typeHouse       0.400 0.010000000 40.00000 0.01591218
```

```r
predict(model, newdata = data.frame(type))
```

```
    1     2     3     4
0.300 0.505 0.505 0.700
```

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Dates as categorical inputs

Imagine you had dataset with 157,209 rows and one covariate column was ‘date of birth’. There were 27,485 unique values for the date of birth column. You make a linear regression with the date of birth as an input, and treat it as a categorical variable (the default behaviour for text data in R).

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MLR with categorical targets

Scenario: use *tumour radius (mm)* and *ages (years)* to predict *benign* **or** *malignant*

$$\boldsymbol{X} = \begin{pmatrix} 1 & 14.8 & 48 \\ 1 & 16.4 & 49 \\ 1 & 15.5 & 47 \\ 1 & 14.2 & 46 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} \text{Benign} \\ \text{Malignant} \\ \text{Benign} \\ \text{Malignant} \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$$

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Binomial regression

Scenario: use *tumour radius (mm)* and *ages (years)* to predict *benign* **or** *malignant*

$$\boldsymbol{X} = \begin{pmatrix} 1 & 14.8 & 48 \\ 1 & 16.4 & 49 \\ 1 & 15.5 & 47 \\ 1 & 14.2 & 46 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} \text{Benign} \\ \textbf{Malignant} \\ \text{Benign} \\ \textbf{Malignant} \end{pmatrix}, \quad \boldsymbol{X\beta} = \begin{pmatrix} -0.46 \\ 0.18 \\ 0.37 \\ -0.09 \end{pmatrix}$$

```r
df <- data.frame(radius = c(14.8, 16.4, 15.5, 14.2), age = c(48, 49, 47, 46))
tumour <- factor(c("Benign", "Malignant", "Benign", "Malignant"))
model <- glm(tumour ~ radius + age, data = df, family = binomial)
```

Step 1: Make a linear prediction

```r
linear <- predict(model, newdata = df, type = "link")
linear
```

```
         1          2          3          4
-0.46393923  0.18380161  0.36575186 -0.08928047
```

```r
X <- model.matrix(~ radius + age, data = df)
beta <- coef(model)
t(X %*% beta)
```

```
             1         2         3          4
[1,] -0.4639392 0.1838016 0.3657519 -0.08928047
```

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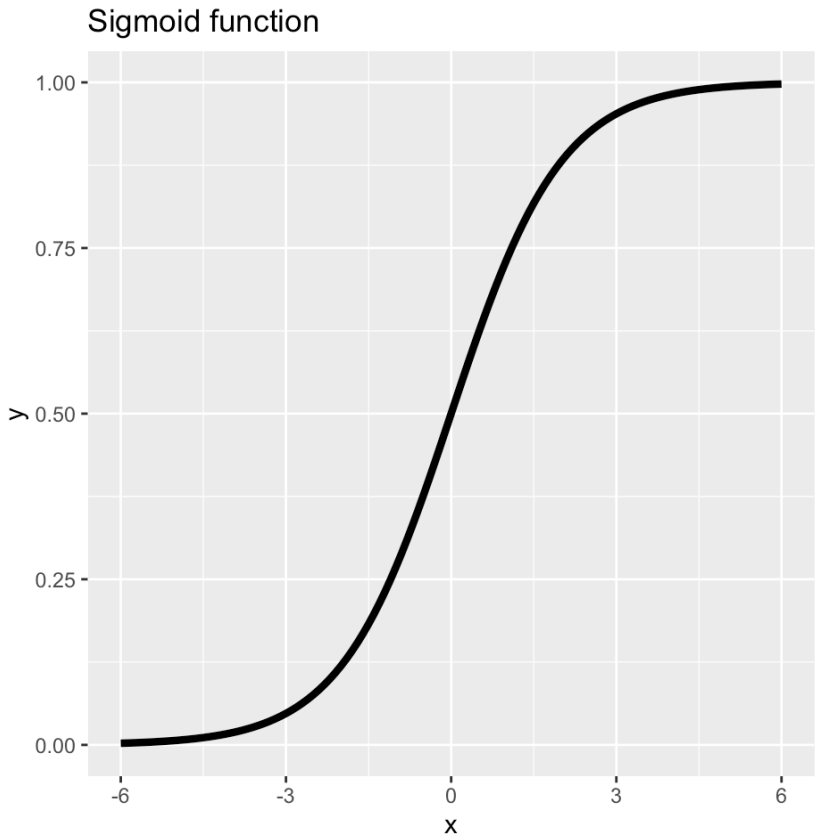
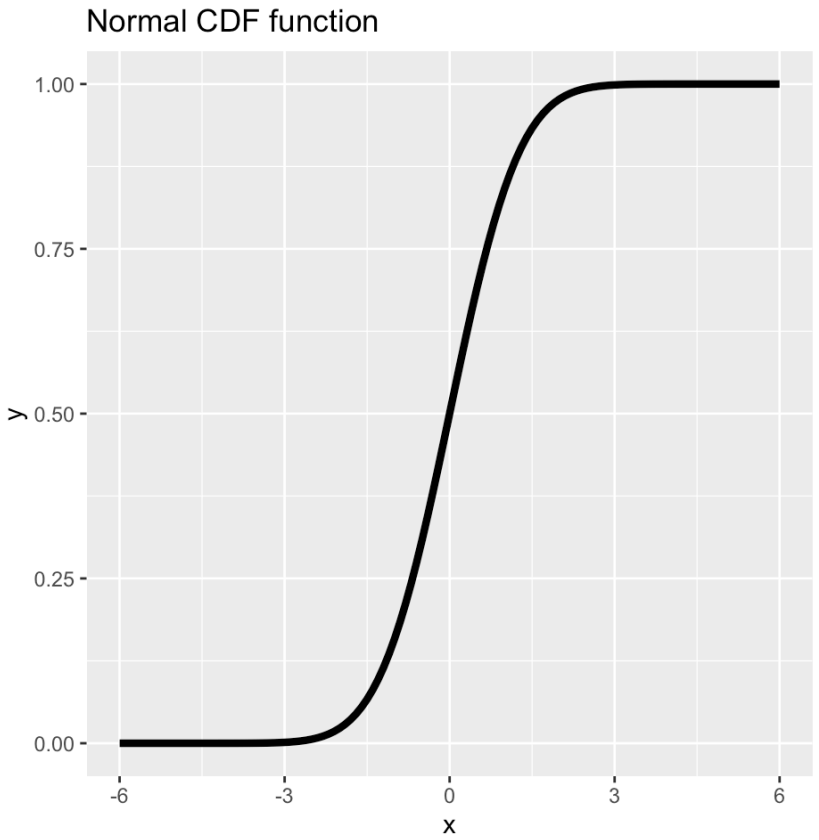
Logistic regression and probit regression





This give you **logistic regression**.

This gives you **probit regression**.

Logistic Regression

Scenario: use *tumour radius (mm)* and *ages (years)* to predict *benign* **or** *malignant*

$$\boldsymbol{y} = \begin{pmatrix} \text{Benign} \\ \textbf{Malignant} \\ \text{Benign} \\ \textbf{Malignant} \end{pmatrix}, \quad \boldsymbol{X\beta} = \begin{pmatrix} -0.46 \\ 0.18 \\ 0.37 \\ -0.09 \end{pmatrix}, \quad \sigma(\boldsymbol{X\beta}) = \begin{pmatrix} 39\% \\ 55\% \\ 59\% \\ 48\% \end{pmatrix}$$

```r
df <- data.frame(radius = c(14.8, 16.4, 15.5, 14.2), age = c(48, 49, 47, 46))
tumour <- factor(c("Benign", "Malignant", "Benign", "Malignant"))
model <- glm(tumour ~ radius + age, data = df, family = binomial)
```

Step 2: Shove it through some function to make it a probability

```r
sigmoid <- function(x) 1 / (1 + exp(-x))
sigmoid(linear)
```

```
        1         2         3         4
0.3860517 0.5458215 0.5904321 0.4776947
```

```r
predict(model, newdata = df, type = "response")
```

```
        1         2         3         4
0.3860517 0.5458215 0.5904321 0.4776947
```

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Predicting categories

Scenario: use *tumour radius (mm)* and *ages (years)* to predict *benign* **or** *malignant*

$$\boldsymbol{y} = \begin{pmatrix} \text{Benign} \\ \textbf{Malignant} \\ \text{Benign} \\ \textbf{Malignant} \end{pmatrix}, \quad \sigma(\boldsymbol{X}\boldsymbol{\beta}) = \begin{pmatrix} 39\% \\ 55\% \\ 59\% \\ 48\% \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} \text{Benign} \\ \text{Malignant} \\ \text{Malignant} \\ \text{Benign} \end{pmatrix}$$

```r
df <- data.frame(radius = c(14.8, 16.4, 15.5, 14.2), age = c(48, 49, 47, 46))
tumour <- factor(c("Benign", "Malignant", "Benign", "Malignant"))
model <- glm(tumour ~ radius + age, data = df, family = binomial)
```

```r
predict_probs <- predict(model, newdata = df, type = "response")
round(100 * predict_probs, 2)
```

```
    1     2     3     4
38.61 54.58 59.04 47.77
```

```r
cutoff <- 0.5
predicted_tumours <- ifelse(predict_probs > cutoff, "Malignant", "Benign")
print(predicted_tumours)
```

```
       1           2           3           4
"Benign" "Malignant" "Malignant"    "Benign"
```

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Assessing accuracy in classification problems

Scenario: use *tumour radius (mm)* and *ages (years)* to predict *benign* **or** *malignant*

$$\boldsymbol{y} = \begin{pmatrix} \text{Benign} \\ \text{Malignant} \\ \text{Benign} \\ \text{Malignant} \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} \text{Benign} \\ \text{Malignant} \\ \text{Malignant} \\ \text{Benign} \end{pmatrix}$$

Accuracy:

$$\frac{1}{n}\sum_{i=1}^{n} I(y_i = \hat{y}_i)$$

Error rate:

$$\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$$

Note

The word "accuracy" is used often used loosely when discussing models, particularly regression models. In the context of classification it has this specific meaning.

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Poisson regression

Scenario: use *population density* to predict the daily **count of** *gun violence incidents*

$$\boldsymbol{X} = \begin{pmatrix} 1 & 10 \\ 1 & 15 \\ 1 & 12 \\ 1 & 18 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 155 \\ 208 \\ 116 \\ 301 \end{pmatrix}, \quad \hat{\boldsymbol{y}} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$$

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Predict the mean of a Poisson distribution

Scenario: use *population density* to predict the daily **count of** *gun violence incidents*

$$\boldsymbol{X} = \begin{pmatrix} 1 & 10 \\ 1 & 15 \\ 1 & 12 \\ 1 & 18 \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} 155 \\ 208 \\ 116 \\ 301 \end{pmatrix}, \quad \boldsymbol{X\beta} = \begin{pmatrix} 4.82 \\ 5.35 \\ 5.03 \\ 5.67 \end{pmatrix}, \quad \hat{\boldsymbol{\mu}} = \begin{pmatrix} 125.1 \\ 211.3 \\ 154.3 \\ 289.4 \end{pmatrix}$$

```r
guns <- data.frame(density = c(10, 15, 12, 18))
incidents <- c(155, 208, 116, 301)
model <- glm(incidents ~ density, data = guns, family = poisson)
summary(model)$coefficients
```

```
             Estimate Std. Error   z value     Pr(>|z|)
(Intercept) 3.7803729 0.17881503 21.141248 3.321765e-99
density     0.1048546 0.01190339  8.808802 1.264908e-18
```

```r
predict(model, newdata = guns, type = "link")
```

```
       1        2        3        4
4.828919 5.353192 5.038628 5.667756
```

```r
predict(model, newdata = guns, type = "response")
```

```
       1        2        3        4
125.0757 211.2817 154.2583 289.3844
```

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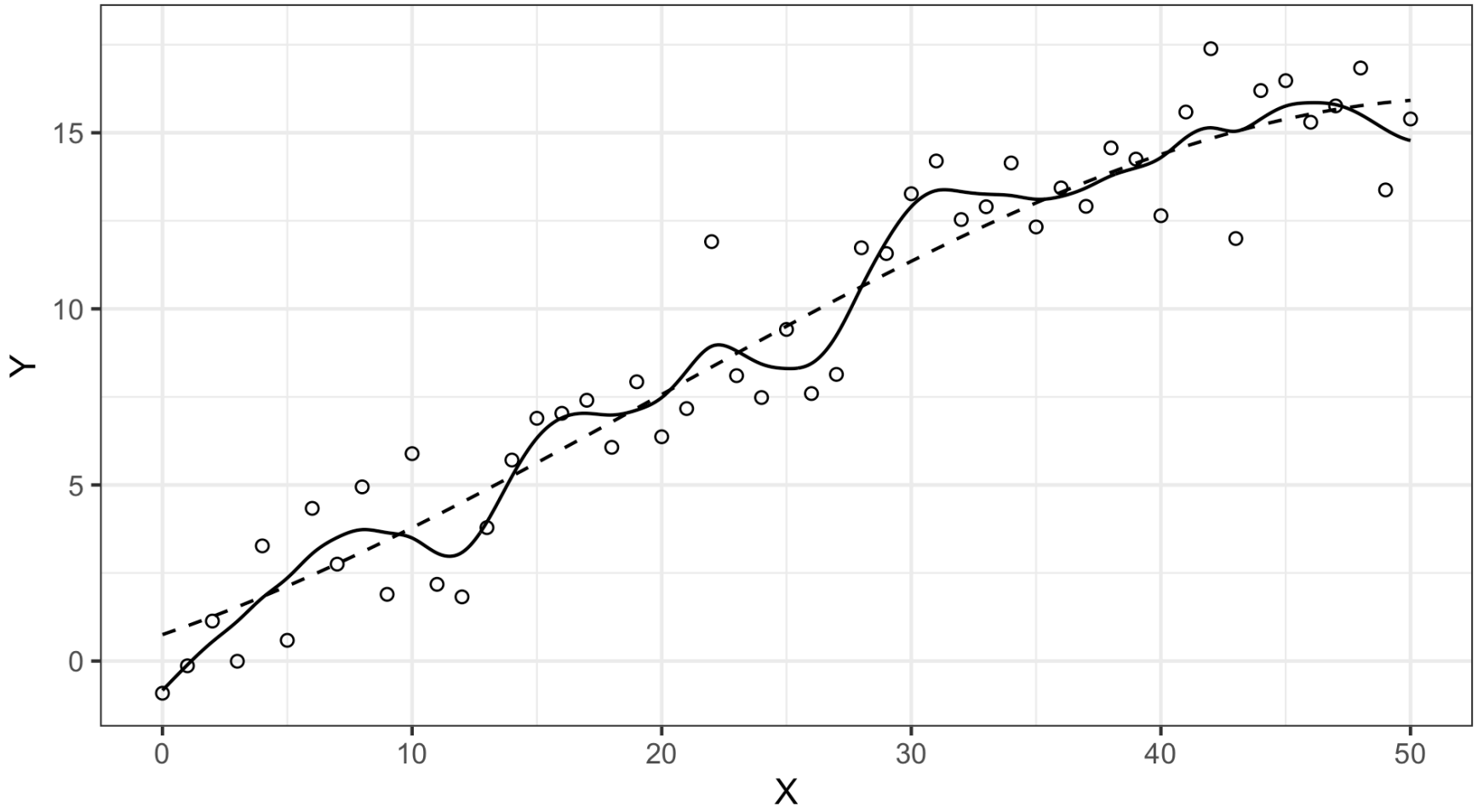
Splines (Week 8)



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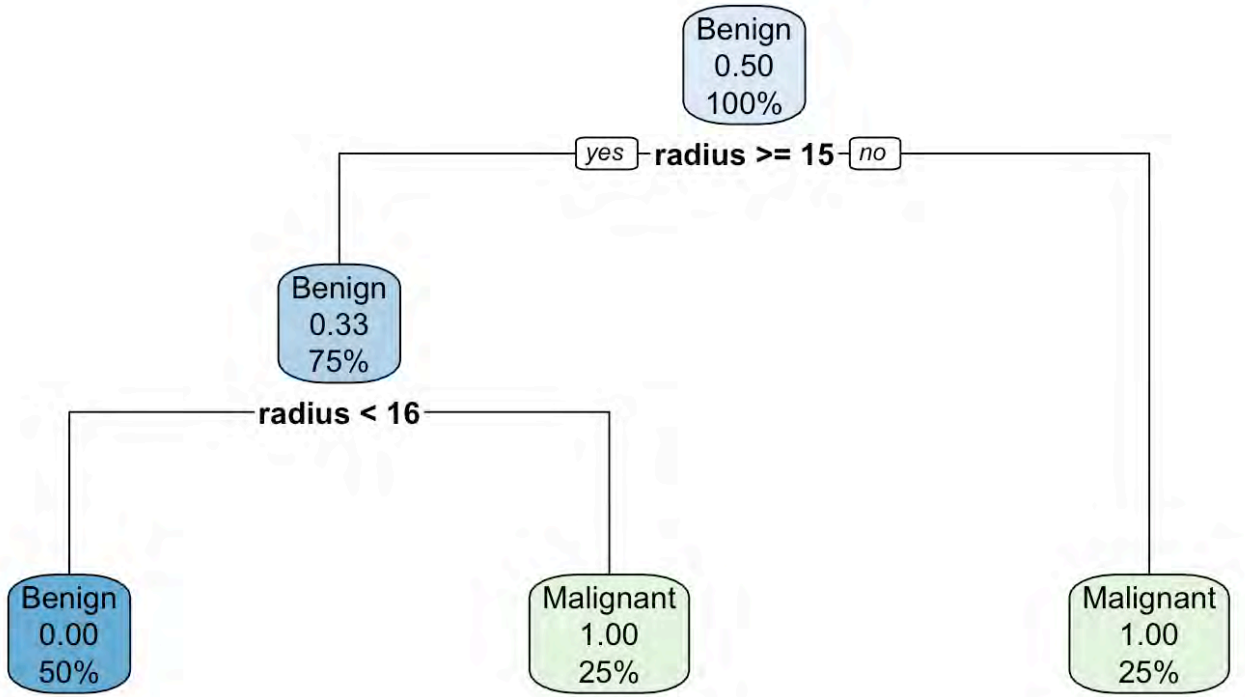
Trees (Week 9)

```r
model <- rpart(tumour ~ radius + age, data = df, control = rpart.control(minsplit = 2))
rpart.plot(model)
```



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Glassdoor Job Reviews

> "This large dataset contains job descriptions and rankings among various criteria such as work-life balance, income, culture, etc. The data covers the various industries in the UK. Great dataset for multidimensional sentiment analysis."

Dall-E 2 rendition of this dataset

Source: Kaggle, Glassdoor Job Reviews

The columns

Rankings are 1–5:

- `overall_rating`: rating for the job (target)
- `work_life_balance`: sub-rating: work-life balance
- `culture_values`: sub-rating: culture
- `diversity_inclusion`: sub-rating: diversity and inclusion
- `career_opp`: sub-rating: career opportunities
- `comp_benefits`: sub-rating: compensation and benefits
- `senior_mgmt`: sub-rating: senior management

Last two are coded: `v` - Positive, `r` - Mild, `x` - Negative, `o` - No opinion

- `recommend`: recommend the firm
- `ceo_approv`: approves firm's CEO

Source: Kaggle, Glassdoor Job Reviews

Load the data

Available at https://laub.au/ml/data/uni_reviews.csv.

```
df_uni <- read.csv("uni_reviews.csv")
df_uni
```

```
# A tibble: 18,358 × 18
   firm  date_review job_title current location overall_rating work_life_balance
   <chr> <chr>       <chr>     <chr>   <chr>              <int>             <dbl>
 1 Birm… 2012-06-28  " Operat… Curren… "Birmin…               5                 4
 2 Birm… 2014-04-23  " Inform… Curren… "Birmin…               4                 5
 3 Birm… 2014-05-05  " "       Curren… ""                     4                 3
 4 Birm… 2014-07-18  " Out Re… Curren… "Birmin…               2                 5
 5 Birm… 2014-12-05  " Profes… Curren… "Birmin…               5                 5
 6 Birm… 2015-07-28  " Anonym… Curren… ""                     3                 2
 7 Birm… 2015-08-20  " Anonym… Former… ""                     4                 5
 8 Birm… 2015-11-05  " Studen… Curren… "Birmin…               5                 5
 9 Birm… 2015-11-19  " Senior… Curren… ""                     3                 3
10 Birm… 2016-01-04  " Operat… Former… "Birmin…               4                 5
# ℹ 18,348 more rows
# ℹ 11 more variables: culture_values <dbl>, diversity_inclusion <dbl>,
#   career_opp <dbl>, comp_benefits <dbl>, senior_mgmt <dbl>, recommend <chr>,
#   ceo_approv <chr>, outlook <chr>, headline <chr>, pros <chr>, cons <chr>
```

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Bird's eye view of the data

```
1 summary(df_uni)
```

```
    firm           date_review         job_title           current
Length:18358       Length:18358       Length:18358       Length:18358
Class :character   Class :character   Class :character   Class :character
Mode  :character   Mode  :character   Mode  :character   Mode  :character



  location         overall_rating  work_life_balance culture_values
Length:18358       Min.   :1.000   Min.   :1.00      Min.   :1.000
Class :character   1st Qu.:4.000   1st Qu.:3.00      1st Qu.:3.000
Mode  :character   Median :4.000   Median :4.00      Median :4.000
                   Mean   :4.136   Mean   :3.89      Mean   :3.962
                   3rd Qu.:5.000   3rd Qu.:5.00      3rd Qu.:5.000
                   Max.   :5.000   Max.   :5.00      Max.   :5.000
                                   NA's   :5316      NA's   :5782
diversity_inclusion   career_opp    comp_benefits    senior_mgmt
Min.   :1.000       Min.   :1.000   Min.   :1.000   Min.   :1.000
1st Qu.:4.000       1st Qu.:3.000   1st Qu.:3.000   1st Qu.:3.000
Median :5.000       Median :4.000   Median :4.000   Median :4.000
Mean   :4.146       Mean   :3.649   Mean   :3.542   Mean   :3.484
3rd Qu.:5.000       3rd Qu.:5.000   3rd Qu.:5.000   3rd Qu.:5.000
```

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Look for common jobs and universities

```
1 table(df_uni$firm) %>% sort(decreasing = TRUE) %>% head(10)
```

```
  University-of-Michigan University-College-London        Oxford-University
                    4185                      1259                      1238
 University-of-Cambridge  University-of-Manchester   University-of-Edinburgh
                    1199                       861                       682
University-of-Nottingham     University-of-Warwick       University-of-Leeds
                     678                       590                       548
 University-of-Sheffield
                     518
```

```
1 table(df_uni$job_title) %>% sort(decreasing = TRUE) %>% head(10)
```

```
            Anonymous Employee
                          3817                                      1581
                       Student                            PhD Student
                           992                                       940
            Research Assistant                       Research Associate
                           592                                       577
Postdoctoral Research Associate                       Student Ambassador
                           325                                       317
                      Lecturer                          Research Fellow
                           262                                       216
```

UNSW SYDNEY

Look at the textual data

```r
# Print a random sample of 'pros' and 'cons'
set.seed(123)
sample(df_uni$pros, 5)
```

```
[1] "Good Staff and Work Environment, Cheap cost of living."
[2] "Amazing people, depts vary. Some research groups are disfunctional, some are amazing places. The one
I am is amazing."
[3] "Amazing University. As well as working within the area I was assigned it was encouraged that interns
seek out people from other parts of the company in order to learn more about the different areas within
RR.\n- Supportive Team\n- Loads of Feedback\n- Interesting Projects"
[4] "It was a great learning experience among many experienced professionals in the health care industry."
[5] "Great city, great campus, good relationships between academic and administrative/technical staff,
strong NSS results and a desire to maintain the student experience and grow the high quality research
output."
```

```r
sample(df_uni$cons, 5)
```

```
[1] "poor management and divide and rule tactics have driven most staff to leave their jobs"
[2] "Not much work to do which result in limited experience."
[3] "Not enough pay for the work you do in certain departments"
[4] "long job hours sometimes go past 40hrs a week"
[5] "Bureaucratic. There are support mechanisms but sometimes, needs lots of approval. IT is also slow.
Needs better balance in workloads."
```

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Change some bizarre coding scheme

Two columns had: v - Positive, r - Mild, x - Negative, o - No opinion

```r
table(df_uni$recommend)
```

```
   o    v    x
7458 9202 1698
```

```r
table(df_uni$ceo_approv)
```

```
   o    r    v    x
9869 3646 4042  801
```

```r
df_uni <- df_uni %>%
  mutate(
    recommend = factor(recode(recommend,
                              "v" = "Positive",
                              "r" = "Mild",
                              "x" = "Negative",
                              "o" = "No opinion"),
                       levels = c("No opinion", "Positive", "Mild", "Negative")),
    ceo_approv = factor(recode(ceo_approv,
                               "v" = "Positive",
                               "r" = "Mild",
                               "x" = "Negative",
                               "o" = "No opinion"),
                        levels = c("No opinion", "Positive", "Mild", "Negative"))
  )
```

```r
table(df_uni$recommend)
```

```
No opinion   Positive       Mild   Negative
      7458       9202          0       1698
```

```r
table(df_uni$ceo_approv)
```

```
No opinion   Positive       Mild   Negative
      9869       4042       3646        801
```

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Removing missing values

```
df_uni <- df_uni[complete.cases(df_uni[, c("work_life_balance", "culture_values", "career_opp",
        "comp_benefits", "senior_mgmt", "overall_rating", "recommend", "ceo_approv")]), ]
df_uni
```

```
# A tibble: 12,124 × 18
   firm  date_review job_title current location overall_rating work_life_balance
   <chr> <chr>       <chr>     <chr>   <chr>              <int>             <dbl>
 1 Birm… 2012-06-28  " Operat… Curren… "Birmin…               5                 4
 2 Birm… 2014-04-23  " Inform… Curren… "Birmin…               4                 5
 3 Birm… 2014-05-05  " "       Curren… ""                     4                 3
 4 Birm… 2014-07-18  " Out Re… Curren… "Birmin…               2                 5
 5 Birm… 2014-12-05  " Profes… Curren… "Birmin…               5                 5
 6 Birm… 2015-07-28  " Anonym… Curren… ""                     3                 2
 7 Birm… 2015-08-20  " Anonym… Former… ""                     4                 5
 8 Birm… 2015-11-05  " Studen… Curren… "Birmin…               5                 5
 9 Birm… 2015-11-19  " Senior… Curren… ""                     3                 3
10 Birm… 2016-01-04  " Operat… Former… "Birmin…               4                 5
# ℹ 12,114 more rows
# ℹ 11 more variables: culture_values <dbl>, diversity_inclusion <dbl>,
#   career_opp <dbl>, comp_benefits <dbl>, senior_mgmt <dbl>, recommend <fct>,
#   ceo_approv <fct>, outlook <chr>, headline <chr>, pros <chr>, cons <chr>
```

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Make a model

Regress over the sub-rankings

```r
model_subrankings <- lm(overall_rating ~ work_life_balance + culture_values +
        career_opp + comp_benefits + senior_mgmt, data = df_uni)
summary(model_subrankings)
```

```
Call:
lm(formula = overall_rating ~ work_life_balance + culture_values +
    career_opp + comp_benefits + senior_mgmt, data = df_uni)

Residuals:
    Min      1Q  Median      3Q     Max
-4.1733 -0.2923 -0.0585  0.3605  3.3510

Coefficients:
                  Estimate Std. Error t value Pr(>|t|)
(Intercept)       0.767970   0.022694   33.84   <2e-16 ***
work_life_balance 0.087806   0.005854   15.00   <2e-16 ***
culture_values    0.305204   0.007081   43.10   <2e-16 ***
career_opp        0.208360   0.005867   35.52   <2e-16 ***
comp_benefits     0.071375   0.005619   12.70   <2e-16 ***
senior_mgmt       0.208329   0.006618   31.48   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5906 on 12118 degrees of freedom
Multiple R-squared:  0.6873,    Adjusted R-squared:  0.6872
```

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Make another model

Regress over the `recommend` and `ceo_approv`

```r
model_recommend <- lm(overall_rating ~ recommend + ceo_approv, data = df_uni)
summary(model_recommend)
```

```
Call:
lm(formula = overall_rating ~ recommend + ceo_approv, data = df_uni)

Residuals:
    Min      1Q  Median      3Q     Max
-3.5708 -0.5220 -0.0557  0.5978  3.0196

Coefficients:
                  Estimate Std. Error t value Pr(>|t|)
(Intercept)        4.05573    0.01583 256.264  < 2e-16 ***
recommendPositive  0.34650    0.02180  15.894  < 2e-16 ***
recommendNegative -1.53373    0.02916 -52.589  < 2e-16 ***
ceo_approvPositive  0.16852    0.02062   8.173 3.31e-16 ***
ceo_approvMild    -0.18989    0.02065  -9.196  < 2e-16 ***
ceo_approvNegative -0.54163    0.03505 -15.454  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.7865 on 12118 degrees of freedom
Multiple R-squared:  0.4454,    Adjusted R-squared:  0.4452
F-statistic:  1947 on 5 and 12118 DF,  p-value: < 2.2e-16
```

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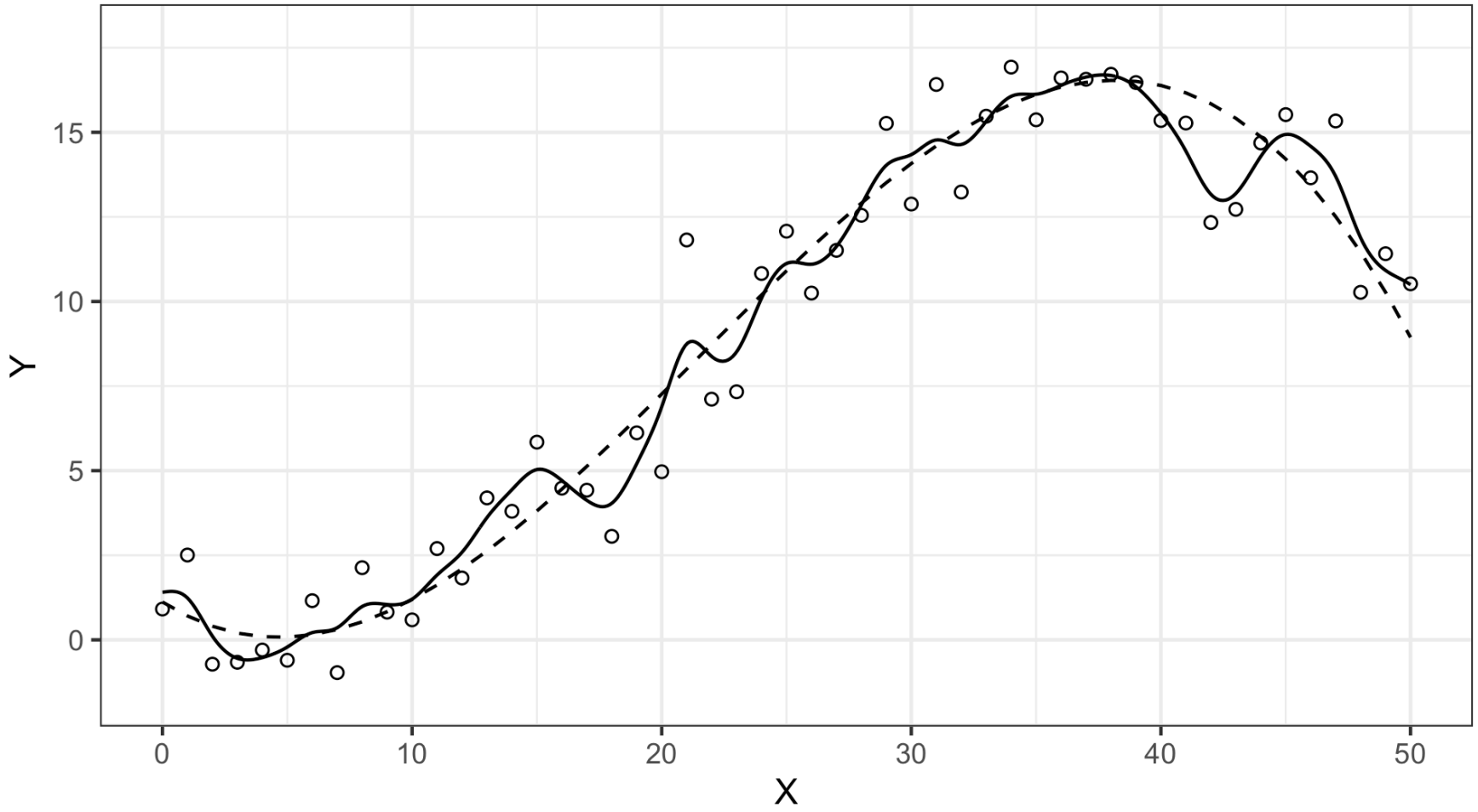
Model evaluation

You fit a few models, then ask:

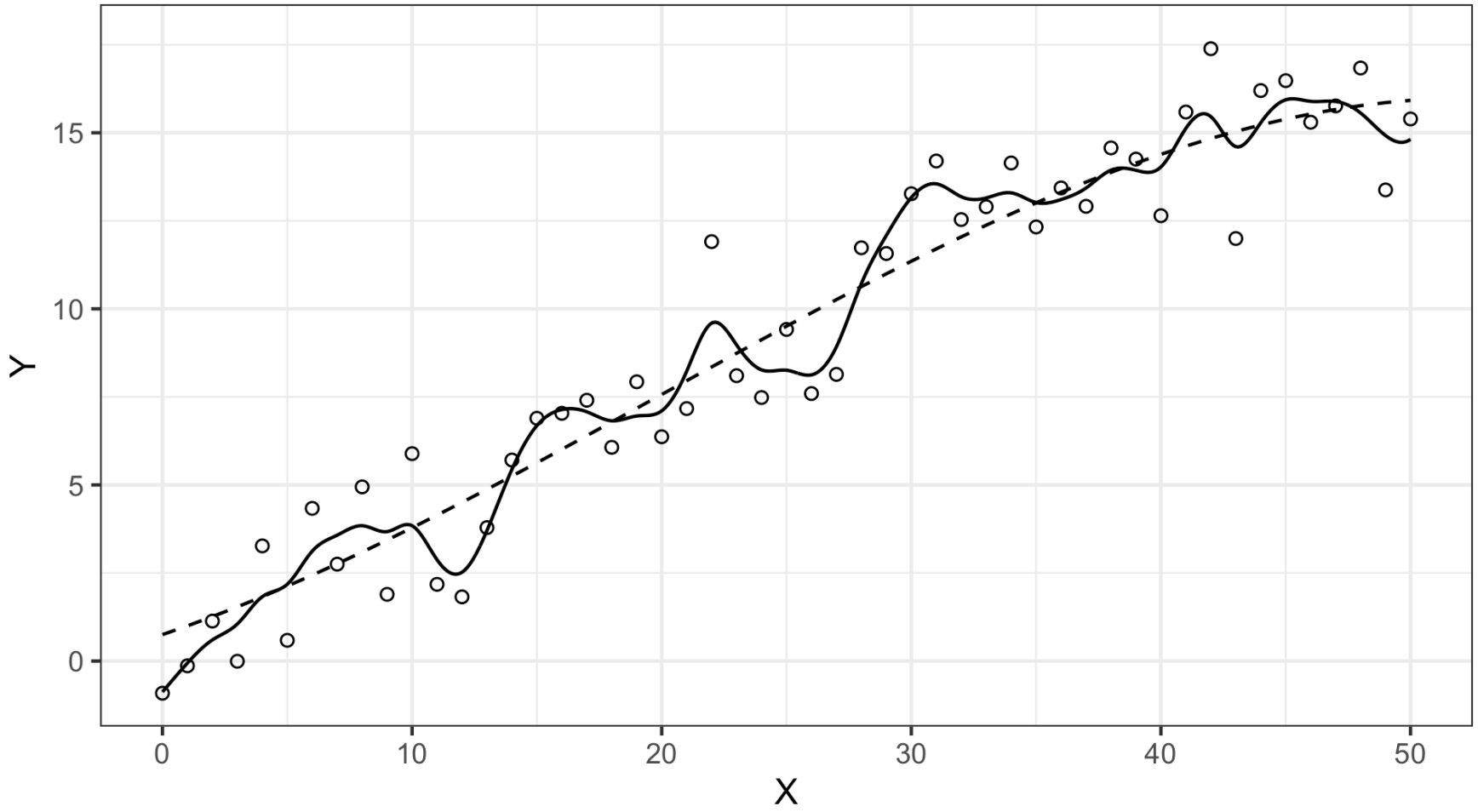
1. **Model Selection:** Which of these models is the best?
2. **Future Performance:** How good should we expect the final model to be on unseen data?

If we make a claim about a model's performance, we prefer to be pessimistic (underestimate) rather than optimistic (overestimate).

Overfitting I



Overfitting II



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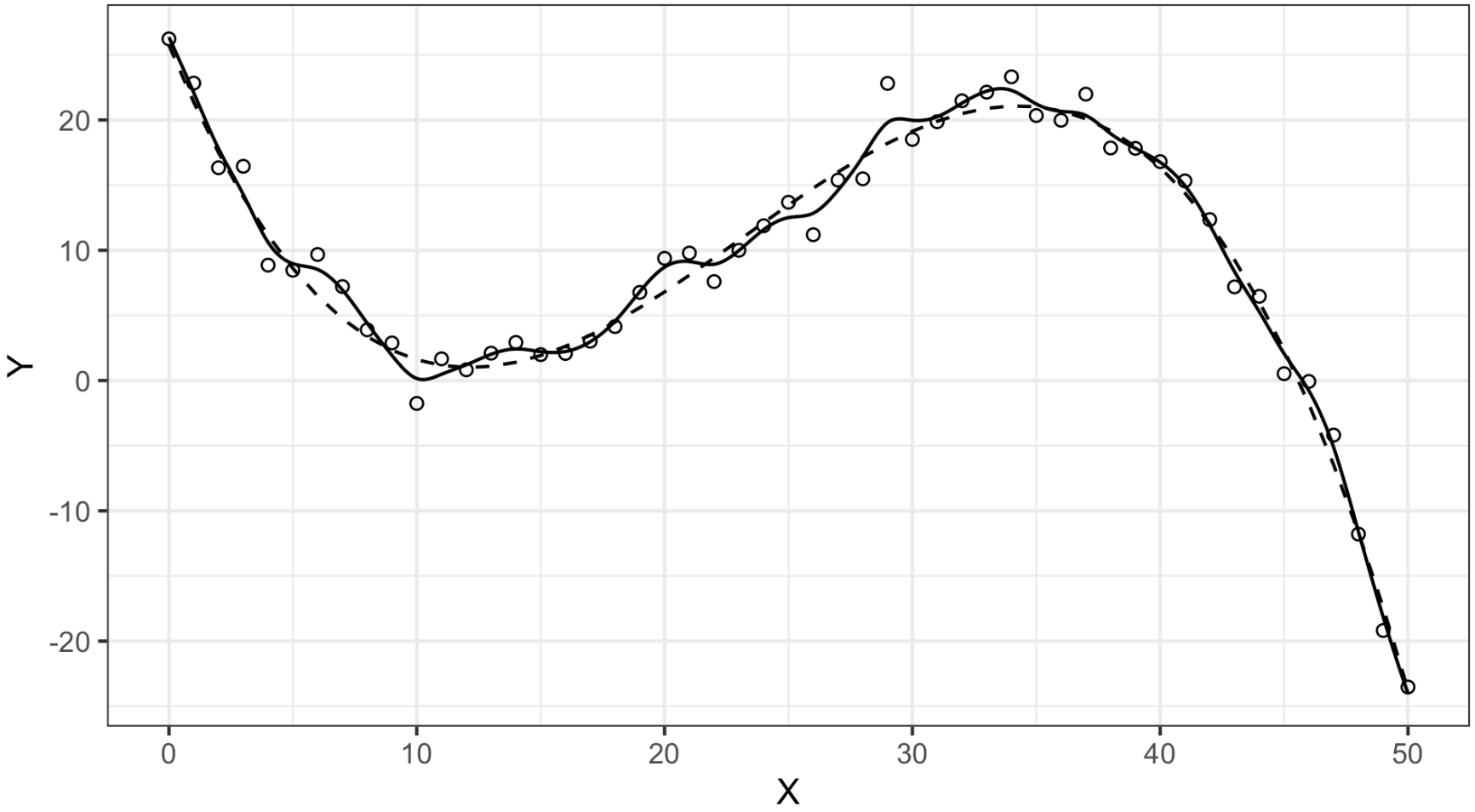
Overfitting III



The ‘statistical’ or ‘indirect’ approach

Bragging about a good RSS is like saying “I can predict with 100% accuracy what I had for lunch yesterday”.

Combine RSS with a penalty for the complexity of the model (p predictors):

$$C_p = \frac{1}{n}(\text{RSS} + 2p\hat{\sigma}^2)$$

$$\text{AIC} = \frac{1}{n}(\text{RSS} + 2p\hat{\sigma}^2)$$

$$\text{BIC} = \frac{1}{n}(\text{RSS} + \log(n)\, p\hat{\sigma}^2)$$

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-p-1)}{\text{TSS}/(n-1)}$$

For the Glassdoor models

Model 1

```
AIC(model_subrankings)
```

```
[1] 21646.59
```

```
BIC(model_subrankings)
```

```
[1] 21698.41
```

```
summary(model_subrankings)$adj.r.squared
```

```
[1] 0.6871576
```

Model 2

```
AIC(model_recommend)
```

```
[1] 28592.3
```

```
BIC(model_recommend)
```

```
[1] 28644.12
```

```
summary(model_recommend)$adj.r.squared
```

```
[1] 0.4452108
```

Which is the better model (according to this 'indirect' approach)?

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The ML approach

Just make predictions on new data

Set aside a fraction after *shuffling*.

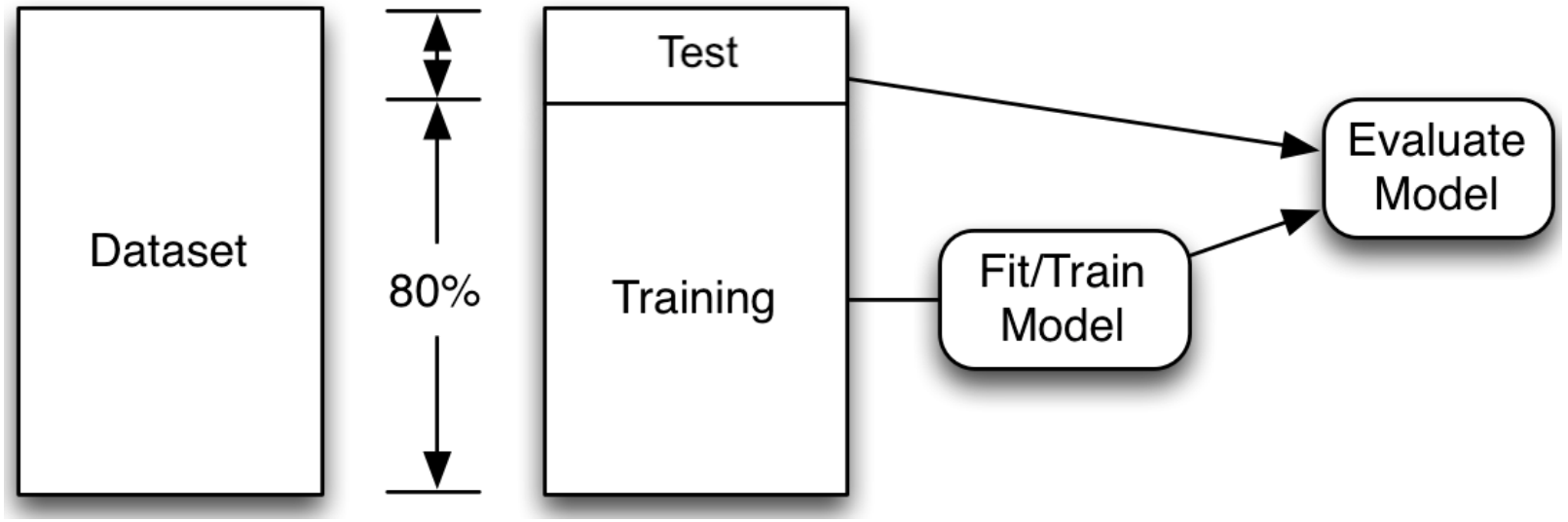
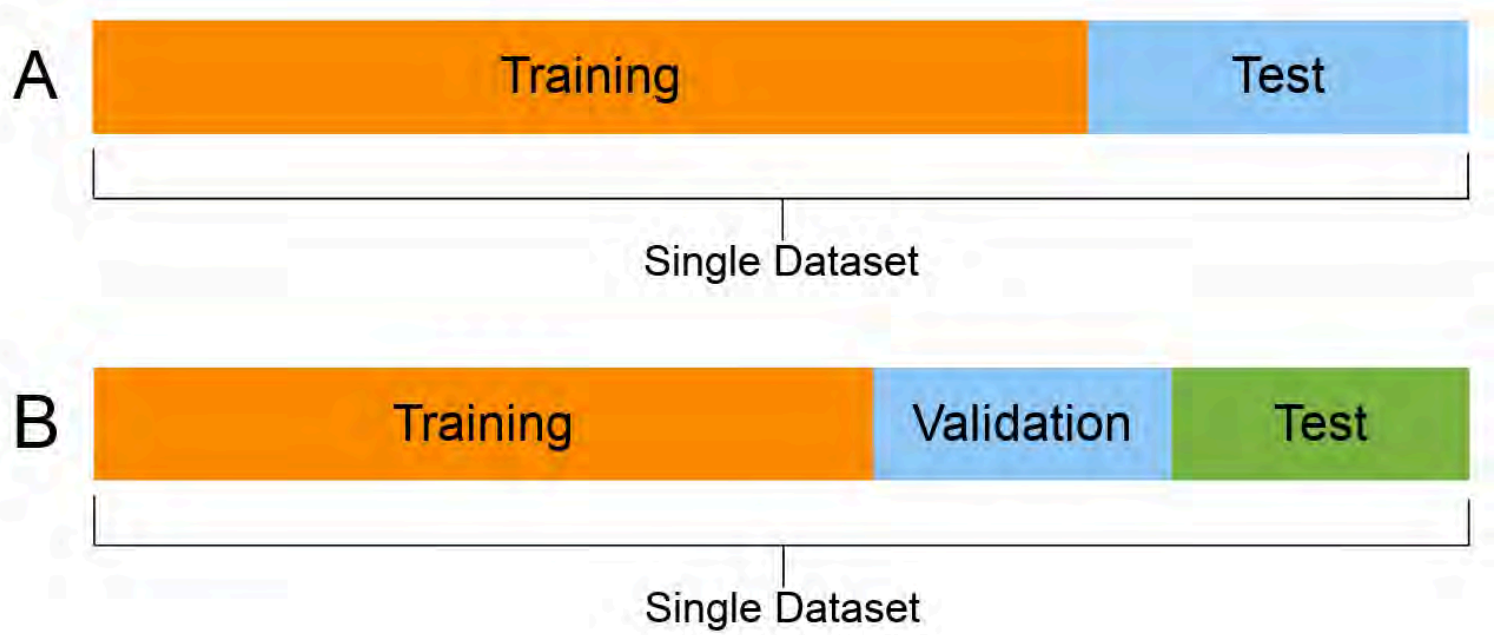


Illustration of a typical training/test split.

Note

The model's metrics on the test set are the *test set error*. Note, there is also the term *test error* which is the model's error on unseen data. So, test set error is an estimate of the test error.

The *validation set approach*



Splitting the data.

1. For each model, fit it to the *training set*.
2. Compute the error for each model on the *validation set*.
3. Select the model with the lowest validation error.
4. Compute the error of the final model on the *test set*.

Source: Wikipedia.

Getting random rows

```
df_toy <- data.frame(thing = c("croissant", "coffee", "gadgets", "books", "music"),
                     cost = c(9, 5, 100, 20, 40))
```

Using the `sample` function:

```
set.seed(42)
sample(df_toy$thing, 3)
```

```
[1] "croissant" "music"     "books"
```

You can use `1:nrow(df_toy)` to get all the possible indices of the data frame.

```
three_indices <- sample(1:nrow(df_toy), 3)
three_indices
```

```
[1] 1 2 4
```

```
df_toy[three_indices, ]
```

```
# A tibble: 3 × 2
  thing      cost
  <chr>     <dbl>
1 croissant     9
2 coffee        5
3 books        20
```

```
df_toy[-three_indices, ]
```

```
# A tibble: 2 × 2
  thing    cost
  <chr>   <dbl>
1 gadgets   100
2 music      40
```

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Split the data

First extract the test dataset:

```
set.seed(123)
test_index <- sample(1:nrow(df_uni), 0.2 * nrow(df_uni))
test <- df_uni[test_index, ]
train_val <- df_uni[-test_index, ]
```

Then split the rest into validation and test sets:

```
val_index <- sample(1:nrow(train_val), 0.25 * nrow(train_val))
val <- train_val[val_index, ]
train <- train_val[-val_index, ]
```

```
dim(train)
```

```
[1] 7275   18
```

```
dim(val)
```

```
[1] 2425   18
```

```
dim(test)
```

```
[1] 2424   18
```

Remember, models *tend to* be improve with more data (not always!).

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Train on train, compare on val, test on test

Train on training set:

```
model_subrankings <- lm(overall_rating ~ work_life_balance + culture_values +
        career_opp + comp_benefits + senior_mgmt, data = train)
model_recommend <- lm(overall_rating ~ recommend + ceo_approv, data = train)
```

Pick the model with the lowest validation error:

```
val_pred_subrankings <- predict(model_subrankings, newdata = val)
mean((val_pred_subrankings - val$overall_rating)^2)
```

```
[1] 0.3484431
```

```
val_pred_recommend <- predict(model_recommend, newdata = val)
mean((val_pred_recommend - val$overall_rating)^2)
```

```
[1] 0.6313695
```

Take **only the selected** model, and calculate the test set error:

```
test_pred_subrankings <- predict(model_subrankings, newdata = test)
mean((test_pred_subrankings - test$overall_rating)^2)
```

```
[1] 0.346846
```

Expect training set error $<$ validation set error $<$ test set error (but not always!).

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Why shuffle the data?

Let's create a toy dataset where the target values are separated.

```
train_toy <- df_toy_classification[1:6, ]
test_toy <- df_toy_classification[7:10, ]
```

```
train_toy
```

```
# A tibble: 6 × 3
  feature1 feature2 target
     <dbl>    <dbl>  <dbl>
1        1      2.5      0
2        2      3        0
3        3      3.9      0
4        4      5.1      0
5        5      6.6      0
6        6      7        0
```

```
test_toy
```

```
# A tibble: 4 × 3
  feature1 feature2 target
     <dbl>    <dbl>  <dbl>
1        7      7.5      1
2        8      9.2      1
3        9     10.4      1
4       10     11.1      1
```

```
model <- glm(target ~ ., data = train_toy, family = binomial)
coef(model)
```

```
  (Intercept)      feature1      feature2
-2.456607e+01 -1.638022e-14  1.377780e-14
```

```
predict(model, newdata = test_toy, type = "response")
```

```
           7            8            9           10
2.143345e-11 2.143345e-11 2.143345e-11 2.143345e-11
```

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Why not use validation set for both?

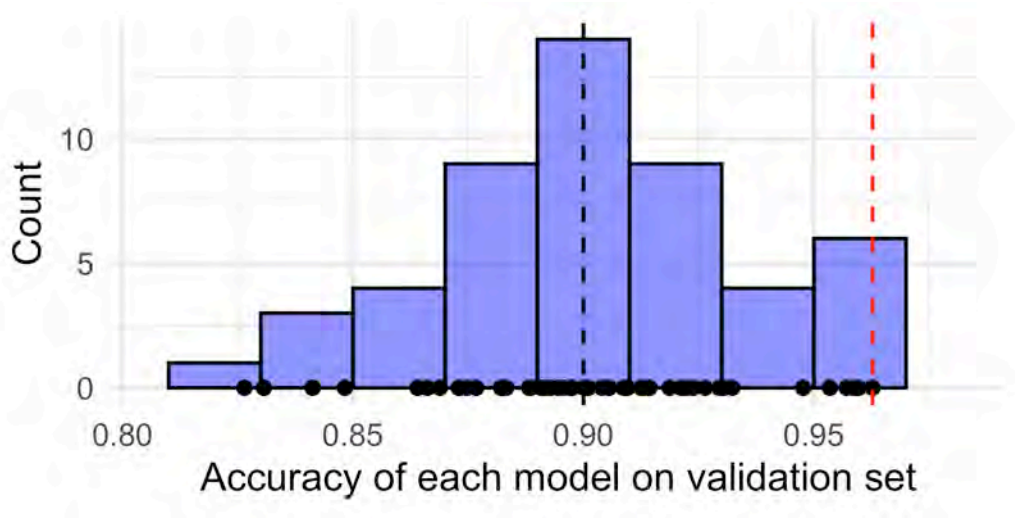
Thought experiment: have m classifiers: $f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x})$.

They are just as good as each other in the long run

$$\mathbb{P}(\, f_i(\boldsymbol{X}) = Y \,) \;=\; 90\%, \quad \text{for } i = 1, \ldots, m.$$

Evaluate each model on the validation set, some will be better than others.

If you just took the best, you'd think it has $\approx 98\%$ accuracy!



You get *unbiased estimates* for each model's accuracy.

However, you get a *biased estimate* for the best model's future performance.

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Optionally, you can retrain once or twice

Your best validation set model only trained on a fraction (e.g. 60%) of the data.

Retrain on the train and validation set combined (often 80%):

```
model_subrankings_train_val <- update(model_subrankings, data = rbind(train, val))
```

Can still estimate the test error for this new model:

```
test_pred_subrankings_train_val <- predict(model_subrankings_train_val, newdata = test)
mean((test_pred_subrankings_train_val - test$overall_rating)^2)
```

```
[1] 0.3471235
```

Warning

Lastly, if you want the best possible model, you can retrain on the entire dataset:

```
model_subrankings_all <- update(model_subrankings, data = df_uni)
```

But we have no unseen data to test this on!

In theory, some outlier in the test set could make this model worse than the previous one.

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Validation Set Approach

> "In statistics, sometimes we only use a single data set. To still be able to evaluate the performance of the developed prediction model on the same data, sophisticated methods have developed over a long period of time and are still in use in some parts of the statistics community. These methods account for the fact that the model saw the data during fitting and applied corrections to account for that. These methods include, for example, the Akaike Information Criterion (AIC) or the Bayesian Information Criterion (BIC). Don't get confused. If you have a validation set, you don't need these methods."

Source: Sic & Duerr (2020), Probabilistic Deep Learning, Chapter 5.

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Illustration

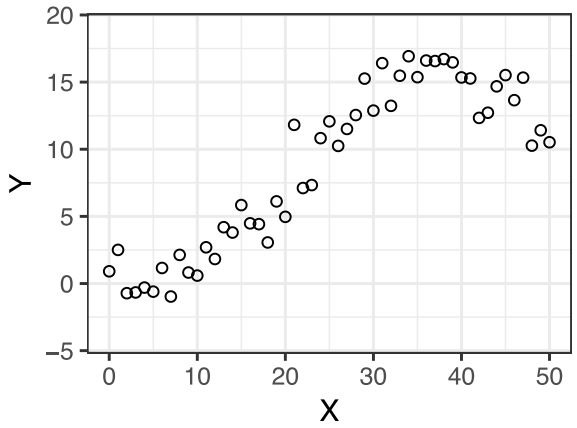
Illustration of 5-fold cross-validation.

Idea

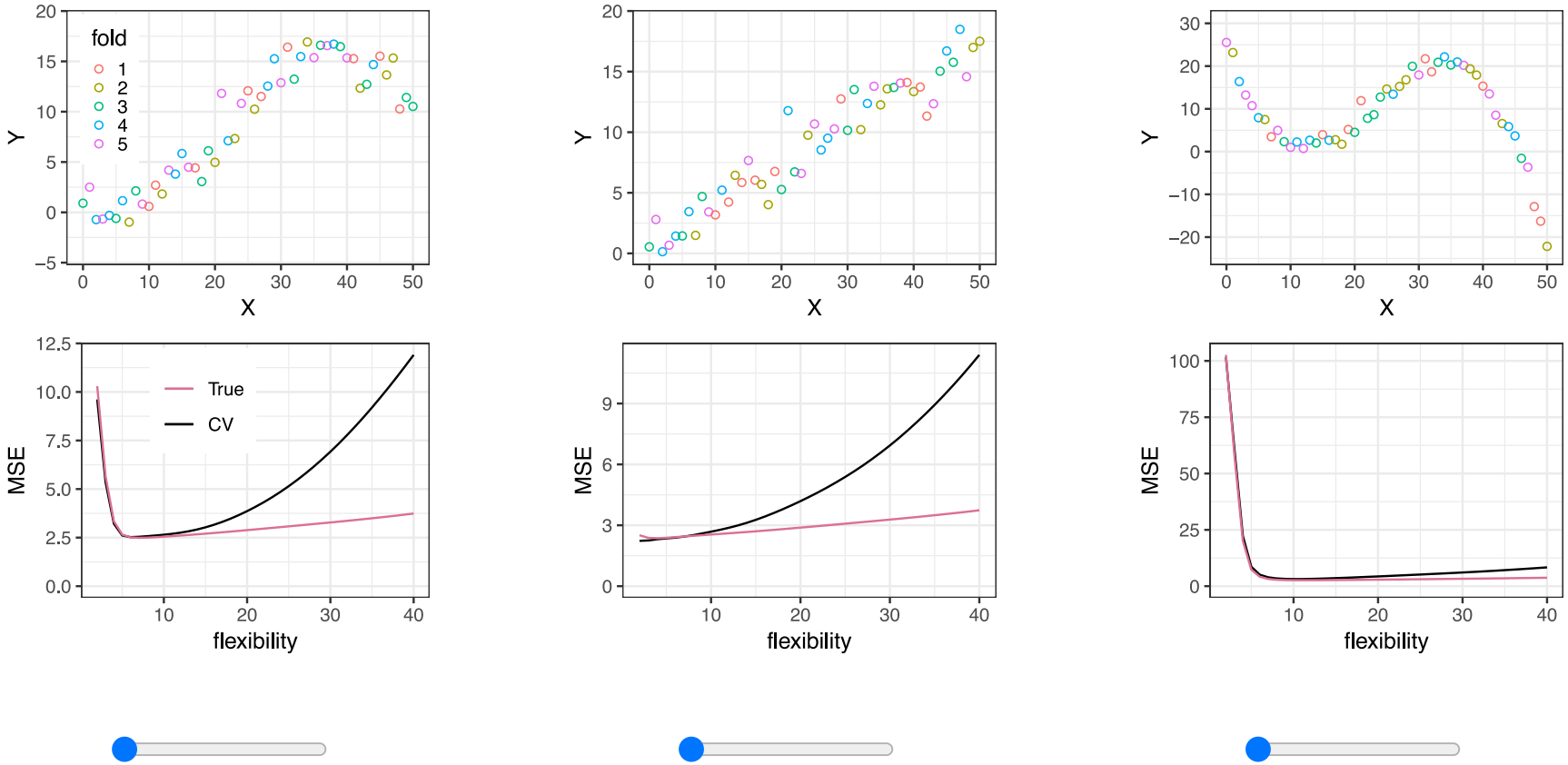
- Randomly divided the set of observations into K groups, or folds of about equal size
  - the k^{th} fold is treated as a validation set
  - the remaining $K-1$ folds make up the training set
- Repeat K times resulting K estimates of the test error

$$\text{CV}_{(K)} = \frac{1}{K}\sum_{k=1}^{K}\text{MSE}_k$$

- In practice $K = 5$ or $K = 10$
- LOOCV is a special case where $K = n$



Simulated Examples



Cross-Validation

```r
set.seed(123)
train_val <- rbind(train, val)
train_val_shuffle <- train_val[sample(1:nrow(train_val)), ]

k <- 5
fold_size <- floor(nrow(train_val) / k)
mse_subrankings <- numeric(k)
mse_recommend <- numeric(k)

for (i in 1:k) {
  val_indices <- ((i - 1) * fold_size + 1):(i * fold_size)
  val <- train_val_shuffle[val_indices, ]
  train <- train_val_shuffle[-val_indices, ]

  model_subrankings <- lm(overall_rating ~ work_life_balance + culture_values +
                            career_opp + comp_benefits + senior_mgmt, data = train)
  model_recommend <- lm(overall_rating ~ recommend + ceo_approv, data = train)

  mse_subrankings[i] <- mean((predict(model_subrankings, newdata = val) - val$overall_rating)^2)
  mse_recommend[i] <- mean((predict(model_recommend, newdata = val) - val$overall_rating)^2)
}
mse_subrankings
```

```
[1] 0.3084817 0.3520156 0.3816378 0.3468752 0.3592670
```

```r
mse_recommend
```

```
[1] 0.6047533 0.6084730 0.6381717 0.6427707 0.6503017
```

```r
c(mean(mse_subrankings), mean(mse_recommend))
```

```
[1] 0.3496555 0.6288941
```

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A linear model is a (Gaussian) GLM

```r
model_recommend <- lm(
    overall_rating ~ recommend + ceo_approv,
    data = train_val)
summary(model_recommend)
```

```
Call:
lm(formula = overall_rating ~ recommend +
ceo_approv, data = train_val)

Residuals:
    Min      1Q  Median      3Q     Max
-3.5616 -0.5616 -0.0527  0.6026  3.0055

Coefficients:
                   Estimate Std. Error t value
Pr(>|t|)
(Intercept)         4.05265    0.01787 226.808  <
2e-16 ***
recommendPositive   0.34473    0.02456  14.036  <
2e-16 ***
recommendNegative  -1.52585    0.03269 -46.682  <
2e-16 ***
ceo_approvPositive  0.16426    0.02323   7.071
1.64e-12 ***
ceo_approvMild     -0.18919    0.02323  -8.145
4.25e-16 ***
```

```r
model_recommend <- glm(
    overall_rating ~ recommend + ceo_approv,
    data = train_val)
summary(model_recommend)
```

```
Call:
glm(formula = overall_rating ~ recommend +
ceo_approv, data = train_val)

Coefficients:
                   Estimate Std. Error t value
Pr(>|t|)
(Intercept)         4.05265    0.01787 226.808  <
2e-16 ***
recommendPositive   0.34473    0.02456  14.036  <
2e-16 ***
recommendNegative  -1.52585    0.03269 -46.682  <
2e-16 ***
ceo_approvPositive  0.16426    0.02323   7.071
1.64e-12 ***
ceo_approvMild     -0.18919    0.02323  -8.145
4.25e-16 ***
ceo_approvNegative -0.53227    0.03941 -13.506  <
2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05
```

Using `cv.glm`

Typically wouldn't write your own loop, but use a function like `cv.glm`:

```
library(boot)

set.seed(123)

# Fit the models as 'glm's first
model_subrankings <- glm(overall_rating ~ work_life_balance + culture_values + career_opp +
    comp_benefits + senior_mgmt, data = train_val)
model_recommend <- glm(overall_rating ~ recommend + ceo_approv, data = train_val)

# Pass them to 'cv.glm'
cv_subrankings <- cv.glm(train_val, model_subrankings, K = 10)
cv_recommend <- cv.glm(train_val, model_recommend, K = 10)

(cv_mse_subrankings <- cv_subrankings$delta[1])
```

```
[1] 0.3496653
```

```
(cv_mse_recommend <- cv_recommend$delta[1])
```

```
[1] 0.6287906
```

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Lecture Outline

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LOOCV: Idea

- Split the set of observations into two parts:
  - a single observation (x_i, y_i) for the validation set
  - the remaining observations make up the training set: $\{(x_1, y_1), \ldots, (x_{i-1}, y_{i-1}), (x_{i+1}, y_{i+1}), \ldots, (x_n, y_n)\}$
- Fit the model on the $n - 1$ training observations
- Predict $\hat{y}_i$ for the validation set
  - $\text{MSE}_i = (y_i - \hat{y}_i)^2$ provides an approximately unbiased estimate for the test error
- Repeat the procedure n times
- The resulting LOOCV estimate for the test error is:

$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \text{MSE}_i$$

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Validation set vs LOOCV - Discussion

Discuss how LOOCV performs relative to the Validation set approach - focusing in particular on the drawbacks of the Validation set approach identified previously.

LOOCV for least square linear models

- For linear (or polynomial) regression, LOOCV is extremely cheap to compute:

$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$

- where
  - $\hat{y}_i$ is the original least squares fit
  - h_i is the leverage defined in Chapter 3 (M2)
- This simplification generally does not apply in general

> **Note**
>
> LOOCV and this simplification is cute & historically important, but less practically so.

Harry Potter dataset

```r
(movies <- read.csv("Movies.csv"))
```

```
# A tibble: 8 × 6
  Movie.ID Movie.Title                    Release.Year Runtime Budget Box.Office
     <int> <chr>                                 <int>   <int> <chr>  <chr>
1        1 Harry Potter and the Philosop…         2001     152 "$125… "$1,002,0…
2        2 Harry Potter and the Chamber …         2002     161 "$100… "$880,300…
3        3 Harry Potter and the Prisoner…         2004     142 "$130… "$796,700…
4        4 Harry Potter and the Goblet o…         2005     157 "$150… "$896,400…
5        5 Harry Potter and the Order of…         2007     138 "$150… "$942,000…
6        6 Harry Potter and the Half-Blo…         2009     153 "$250… "$943,200…
7        7 Harry Potter and the Deathly …         2010     146 "$200… "$976,900…
8        8 Harry Potter and the Deathly …         2011     130 "$250… "$1,342,0…
```

```r
# Clean the dataset and convert relevant columns to numerical format
movies$Budget <- as.numeric(gsub("[\\$,]", "", movies$Budget))
movies$Box.Office <- as.numeric(gsub("[\\$,]", "", movies$Box.Office))
```

```r
# Grab just one movie as a test set
test_index <- sample(1:nrow(movies), 1)
train_val <- movies[-test_index, ]
(test <- movies[test_index, ])
```

```
# A tibble: 1 × 6
  Movie.ID Movie.Title                    Release.Year Runtime Budget Box.Office
     <int> <chr>                                 <int>   <int>  <dbl>      <dbl>
1        4 Harry Potter and the Goblet o…         2005     157  1.5e8  896400000
```

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LOOCV for the Harry Potter dataset

```r
model_year <- glm(Box.Office ~ Budget + Release.Year, data = train_val)
model_runtime <- glm(Box.Office ~ Budget + Runtime, data = train_val)

cv_year <- cv.glm(train_val, model_year) # cv.glm defaults to LOOCV
cv_runtime <- cv.glm(train_val, model_runtime)
```

```r
cv_year$delta[1]
```

```
[1] 6.153881e+16
```

```r
cv_runtime$delta[1]
```

```
[1] 5.905452e+16
```

```r
# Test error for the runtime model
test_pred_runtime <- predict(model_runtime, newdata = test)
(mean((test_pred_runtime - test$Box.Office)^2))
```

```
[1] 1.575889e+14
```

```r
summary(model_runtime)$coefficients
```

```
                Estimate   Std. Error   t value  Pr(>|t|)
(Intercept)  1.708822e+09 1.040374e+09  1.642508 0.1758294
Budget       1.275637e+00 1.089689e+00  1.170643 0.3067254
Runtime     -6.473381e+06 6.444243e+06 -1.004522 0.3719641
```

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Exam question 2023

```r
# Load dataset
library(mlbench)
data(BostonHousing)

# Split the data into training and test sets
set.seed(123)
train_index <- sample(nrow(BostonHousing),
    0.8 * nrow(BostonHousing))
train <- BostonHousing[train_index, ]
test <- BostonHousing[-train_index, ]

# Fit a linear regression model
lm_model <- lm(medv ~ ., data = train)

# Calculate the training and test errors
train_pred <- predict(lm_model, newdata = train)
train_error <- mean((train_pred - train$medv)^2)
lm_model <- lm(medv ~ ., data = test)
test_pred <- predict(lm_model, newdata = test)
test_error <- mean((test_pred - test$medv)^2)

# Print the training and test errors
cat("Training Error (MSE):", train_error, "\n")
```

```
Training Error (MSE): 21.60875
```

```r
cat("Test Error (MSE):", test_error, "\n")
```

```
Test Error (MSE): 20.26994
```

3a) Which do you expect to be lower on average, the training loss or the test loss? Why?

3b) Describe why, in this case, the test error is less than the training error.

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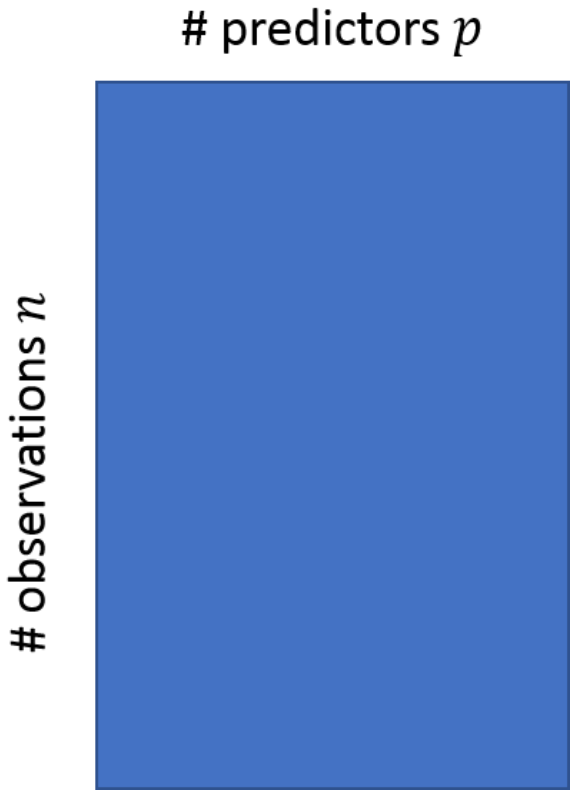
Tall data vs wide data



A tall dataset ($n \gg p$)

Traditional linear regression methods

A wide dataset ($p \gg n$)

Traditional methods break, regularisation methods can help

LMs with $p > n$

If $p > n$, R will just fit the first n parameters and give NA for the rest.

```r
first_few_rows <- df_uni[1:3, ]
model_subrankings <- lm(overall_rating ~ work_life_balance + culture_values +
        career_opp + comp_benefits + senior_mgmt, data = first_few_rows)
summary(model_subrankings)
```

```
Call:
lm(formula = overall_rating ~ work_life_balance + culture_values +
    career_opp + comp_benefits + senior_mgmt, data = first_few_rows)

Residuals:
ALL 3 residuals are 0: no residual degrees of freedom!

Coefficients: (3 not defined because of singularities)
                  Estimate Std. Error t value Pr(>|t|)
(Intercept)         3.6667        NaN     NaN      NaN
work_life_balance  -0.3333        NaN     NaN      NaN
culture_values      0.6667        NaN     NaN      NaN
career_opp              NA         NA      NA       NA
comp_benefits           NA         NA      NA       NA
senior_mgmt             NA         NA      NA       NA

Residual standard error: NaN on 0 degrees of freedom
Multiple R-squared:      1, Adjusted R-squared:    NaN
F-statistic:   NaN on 2 and 0 DF,  p-value: NA
```

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Shrinkage methods

- Alternative to subset selection is to fit model using all p predictors, but *constraints*, or *regularizes* the coefficients (='shrinks' the coefficients)
- Two main types:
  - Ridge regression: pushes estimates towards zero, but all predictors included
  - Lasso regression: pushes estimates towards zero, some predictors excluded
  - (There's also the elastic net, a which is a combination of ridge and lasso)
- Allows us to fit models with $n < p$

Ridge regression

Minimise on β:

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 = \text{RSS} + \lambda\sum_{j=1}^{p}\beta_j^2$$

- The shrinkage penalty $\lambda\sum_{j=1}^{p}\beta_j^2$ restricts the growth of coefficient estimates.
- $\lambda = 0$: Parameter estimates not penalised at all, reduces to simple linear regression - obtain the best model which includes all parameters
- $\lambda \to \infty$: Parameter estimates heavily penalised, coefficients pushed to zero, model is $y_i = \hat{\beta}_0$
- Note that β_0's estimate is not penalised: Coefficient estimates are heavily scale-variant
- Also called "L^2 regularisation" as the penalty is the square of the β_j's L^2 norm

Lasso regression

Minimise on β:

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \text{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|$$

- Only difference: penalties placed on absolute value of coefficient estimates
- Can force some of them to exactly zero: significantly easier to interpret model
- Has the effect of also performing some variable selection, like best-subset
- Also called "L^1 regularisation" as the penalty is the β_j's L^1 norm

Note

Before calculating the ridge & lasso penalties, we should standardise all of $\boldsymbol{X}$'s columns so their sample variances are one. Otherwise we would be penalising some β_i's simply because the ith covariate's values are relatively bigger or smaller numbers. The R package we use for ridge & lasso regression will do this for you.

Elastic net model

Combines ridge and lasso penalties, so you minimise

$$\text{RSS} + \lambda \Big[\alpha \sum_{j=1}^{p} |\beta_j| + (1-\alpha) \sum_{j=1}^{p} \beta_j^2 \Big]$$

- $\alpha = 1$ is lasso, $\alpha = 0$ is ridge
- $0 < \alpha < 1$ is elastic net, a compromise between ridge and lasso

The `glmnet` package fits elastic net models, so you have to choose $\alpha = 0$ or $\alpha = 1$ to get ridge or lasso. It fits GLMs with the penalties described above.

- "Ridge regression" is just linear regression with a ridge penalty
- "Lasso regression" is just linear regression with a lasso penalty
- Can also do logistic regression, Poisson regression, etc. with a ridge or lasso penalty (the RSS term would change to match the specific GLM model)

Ridge closed-form solution

$$\boldsymbol{\beta}_{\text{LM}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

```
model_subrankings <- lm(overall_rating ~ work
coef(model_subrankings)
```

```
      (Intercept) work_life_balance
culture_values         career_opp
        3.6666667         -0.3333333
0.6666667                  NA
    comp_benefits        senior_mgmt
               NA                  NA
```

```
X <- model.matrix(~ work_life_balance + cultu
X <- cbind(rep(1, nrow(X)), scale(X[, -1])) #
y <- first_few_rows$overall_rating
beta <- solve(t(X) %*% X) %*% t(X) %*% y
```

```
Error in solve.default(t(X) %*% X): system is
computationally singular: reciprocal condition
number = 7.39832e-34
```

$$\boldsymbol{\beta}_{\text{Ridge}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

```
ridge <- glmnet(X[,-1], y, alpha = 0, lambda=
coef(ridge, s=0.01)
```

```
6 x 1 sparse Matrix of class "dgCMatrix"
                             s1
(Intercept)         4.33333333
work_life_balance -0.02139038
culture_values      0.12750285
career_opp          0.15892194
comp_benefits       0.17324706
senior_mgmt        -0.15706300
```

```
beta <- solve(t(X) %*% X + 0.01 * diag(ncol(X
beta
```

```
                            [,1]
                       4.3189369
work_life_balance -0.0252433
culture_values      0.1338977
career_opp          0.1591410
comp_benefits       0.1691859
senior_mgmt        -0.1581698
```

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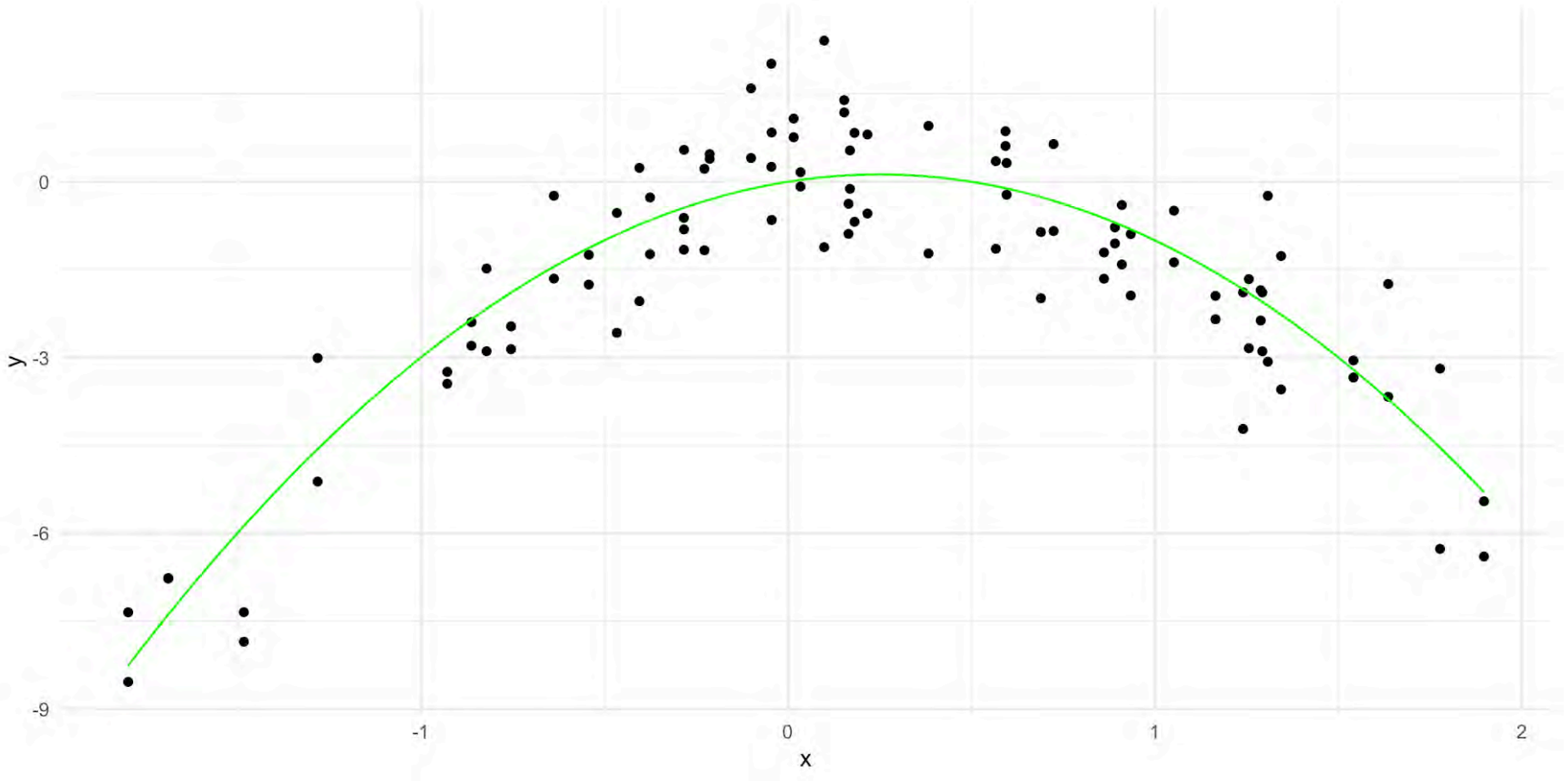
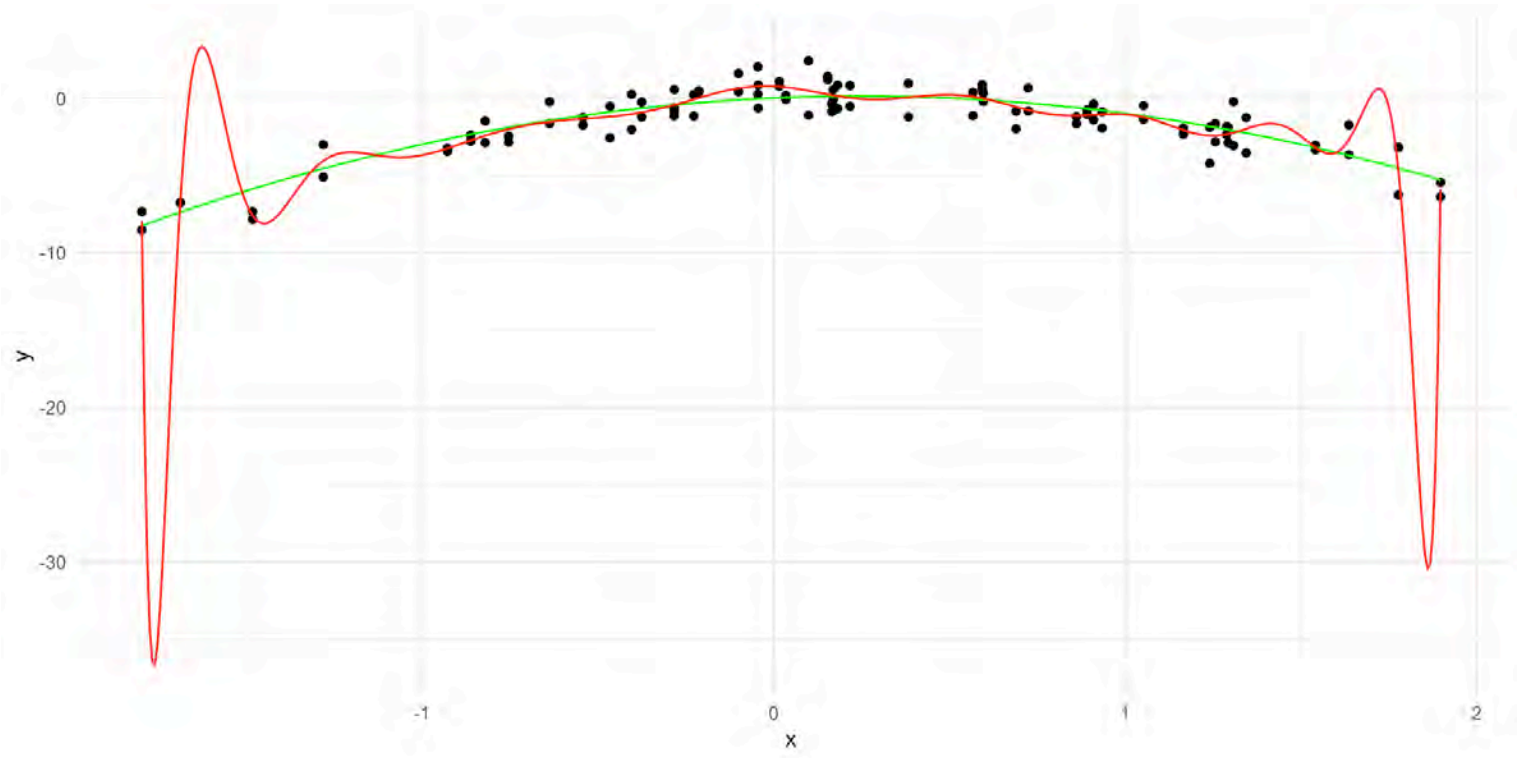
Synthetic data example



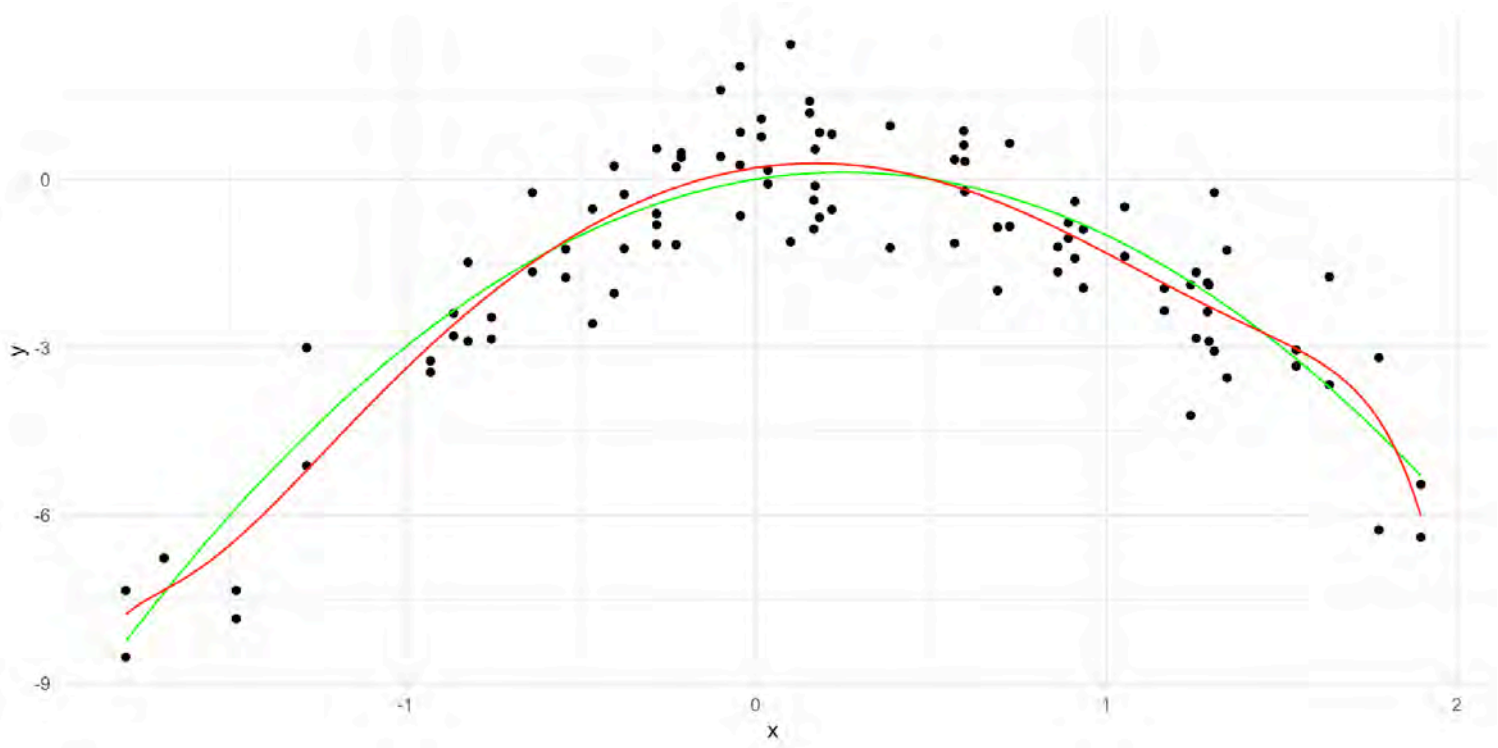
Polynomial regression



$$\hat{y}(x) = 0.76 - 1.09x - 22.91x^2 + \cdots - 1.77x^{19} + 2.15x^{20}$$

The $\sum_{j=1}^{20} \hat{\beta}_j^2$ is 6970618.

Ridge regression with $\lambda = 0.01$



$$\hat{y}(x) = 0.20 + 0.92x - 2.73x^2 + \cdots + 0.000007x^{19} - 0.000003x^{20}$$

The $\sum_{j=1}^{20} \hat{\beta}_j^2$ is 8.31.

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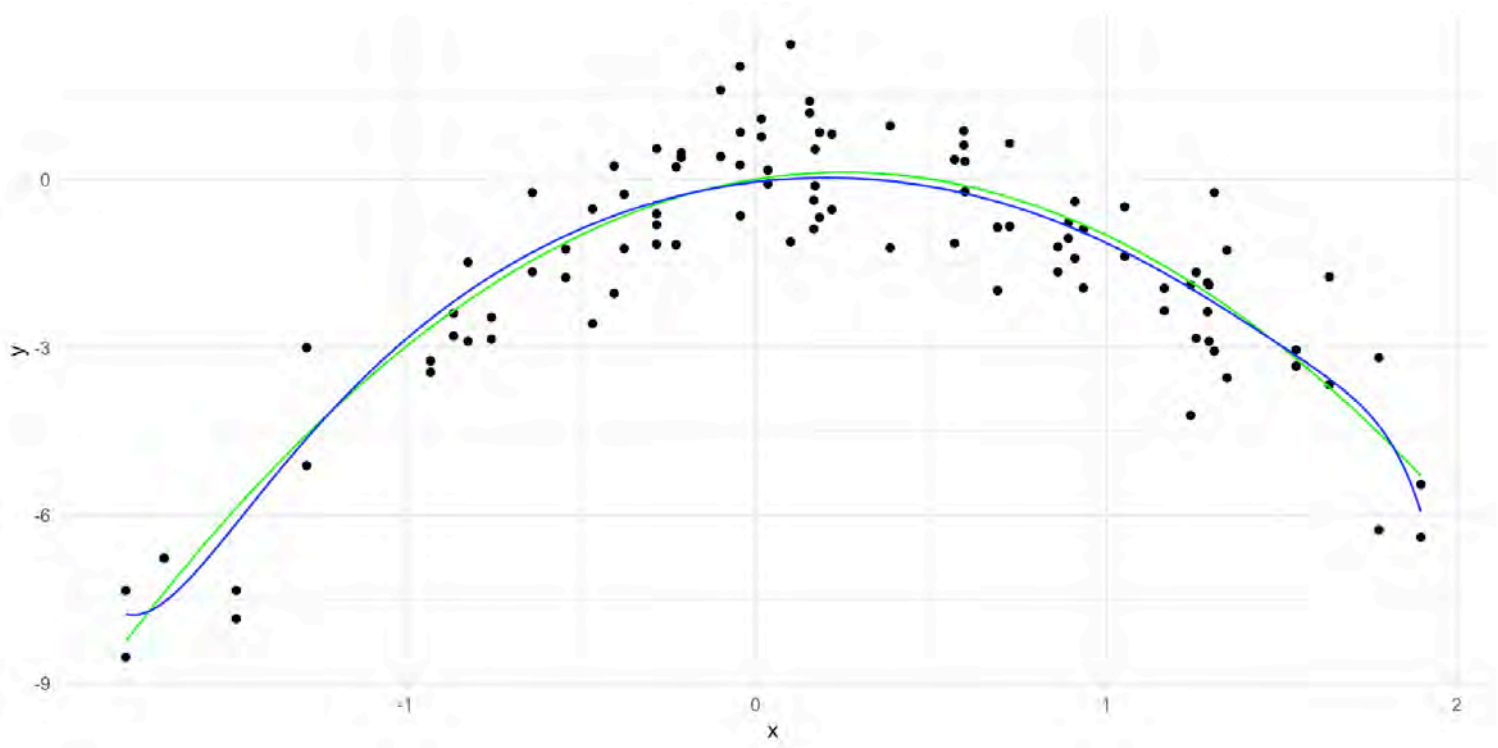
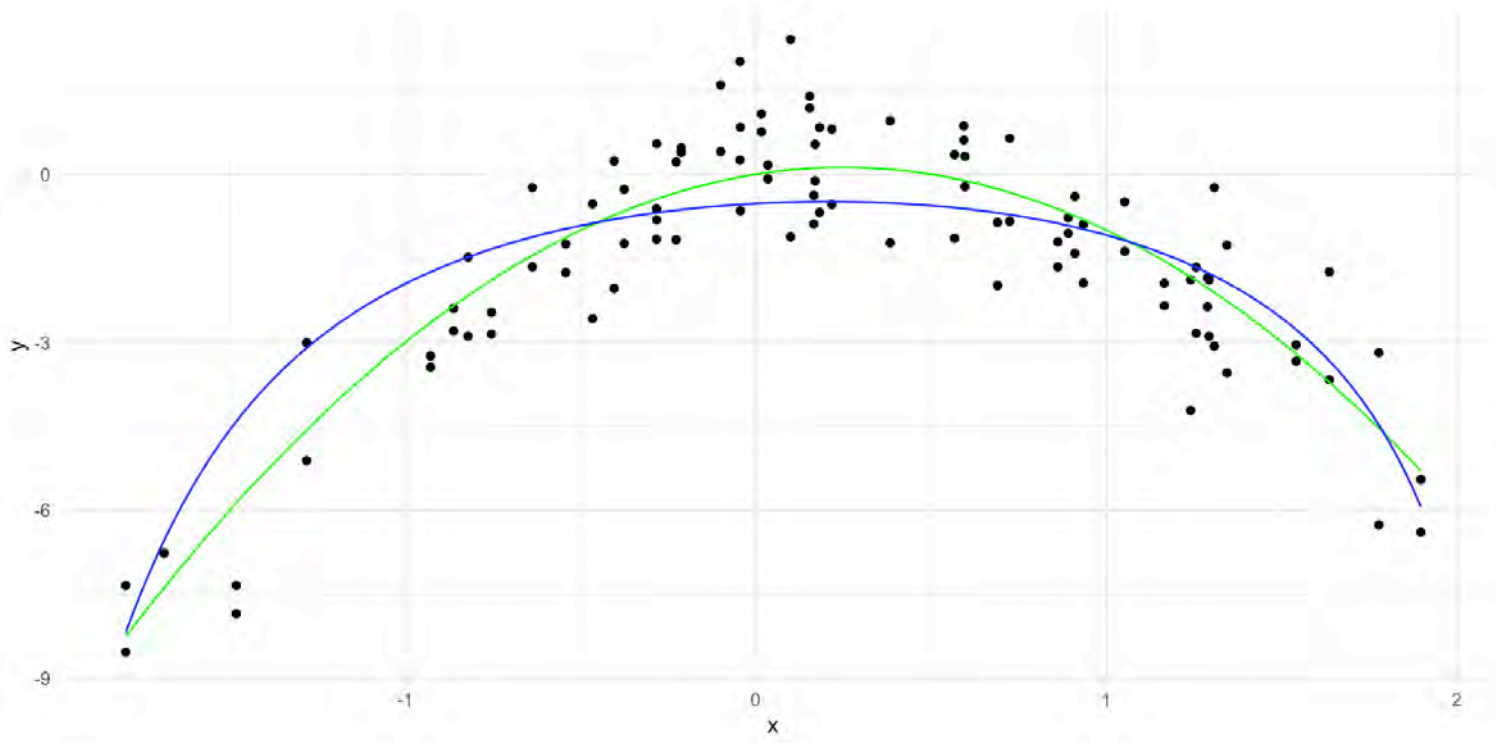
Ridge regression with $\lambda = 0.1$



$$\hat{y}(x) = -0.05 + 0.73x - 1.82x^2 + \cdots - 0.000004x^{19} - 0.000001x^{20}$$

The $\sum_{j=1}^{20} \hat{\beta}_j^2$ is 3.86.

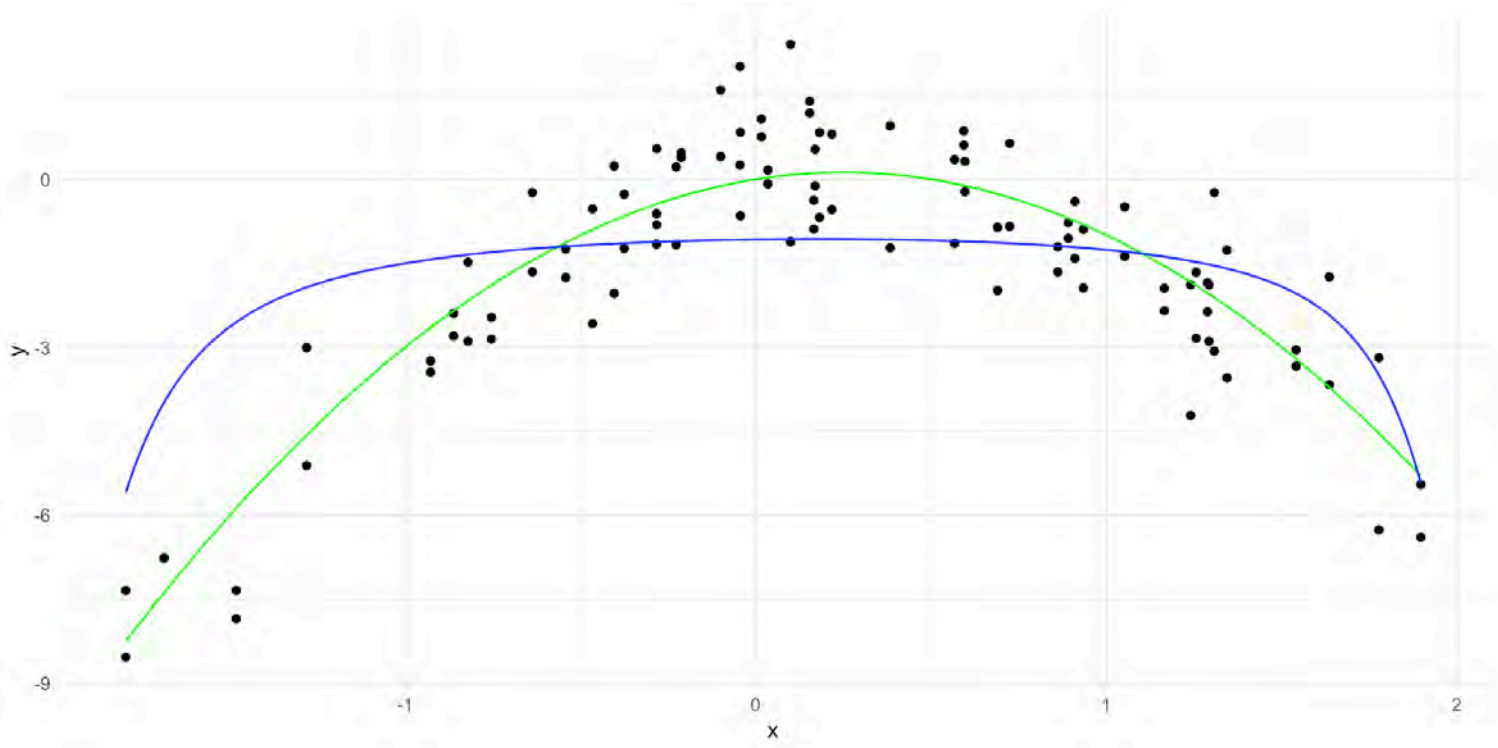
Ridge regression with $\lambda = 1$



$$\hat{y}(x) = -0.52 + 0.34x - 0.82x^2 + \cdots - 0.0000006x^{19} + 0.00000007x^{20}$$

The $\sum_{j=1}^{20} \hat{\beta}_j^2$ is 0.818.

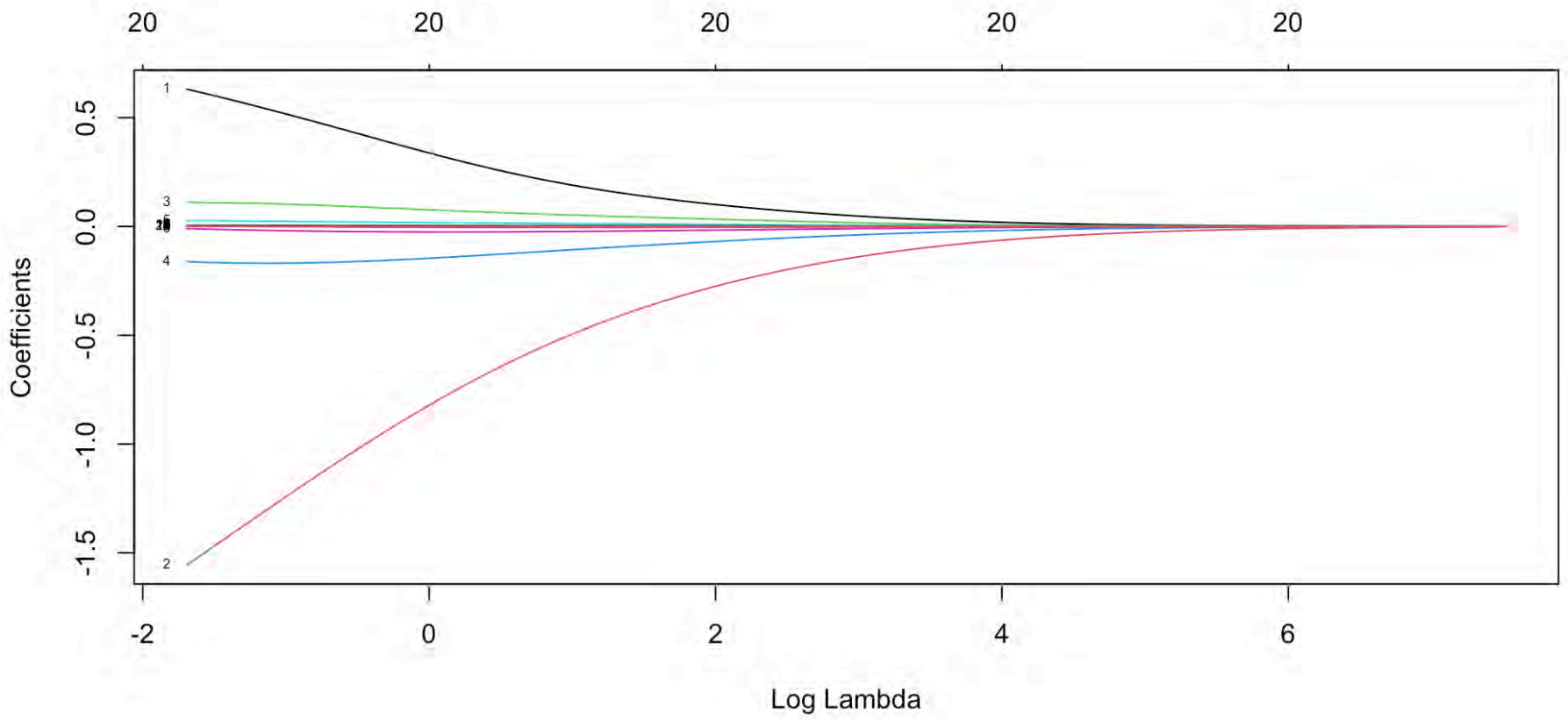
Ridge regression with $\lambda = 10$



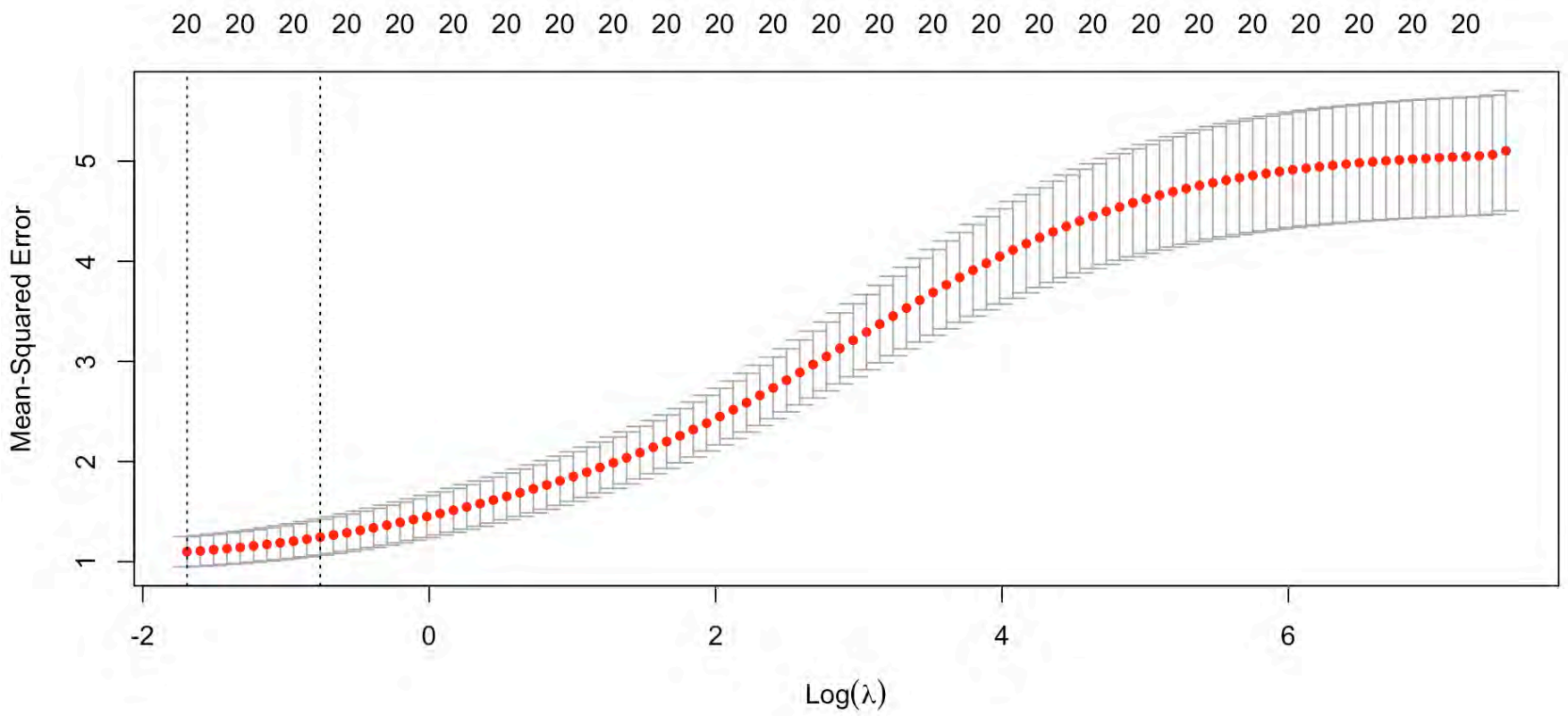
$$\hat{y}(x) = -1.08 + 0.08x - 0.23x^2 + \cdots + 0.0000003x^{19} - 0.000001x^{20}$$

The $\sum_{j=1}^{20} \hat{\beta}_j^2$ is 0.0624.

Regularisation path plots

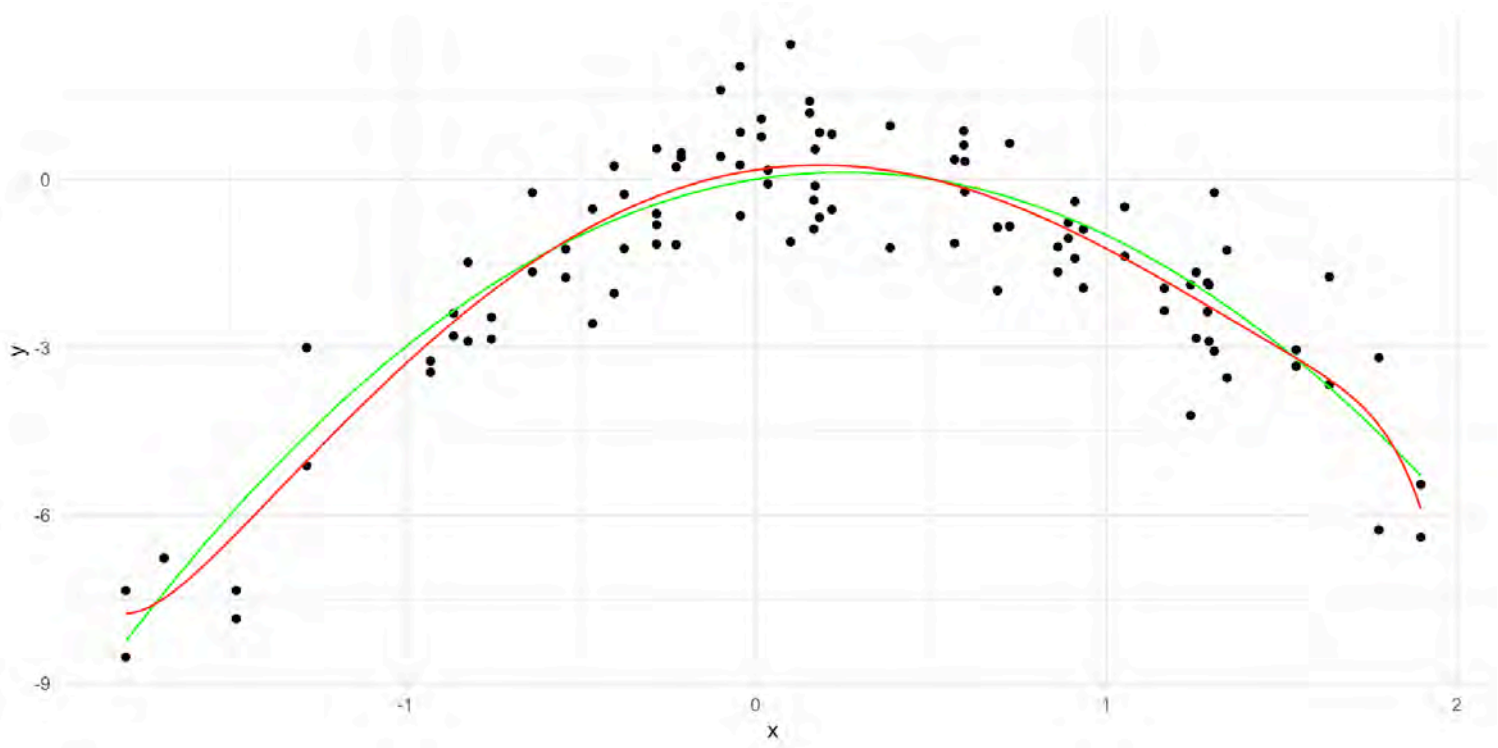


Cross-validation errors



The λ which minimises the CV MSE is 0.1842555 ($\log(\lambda)$ is -1.6914321).

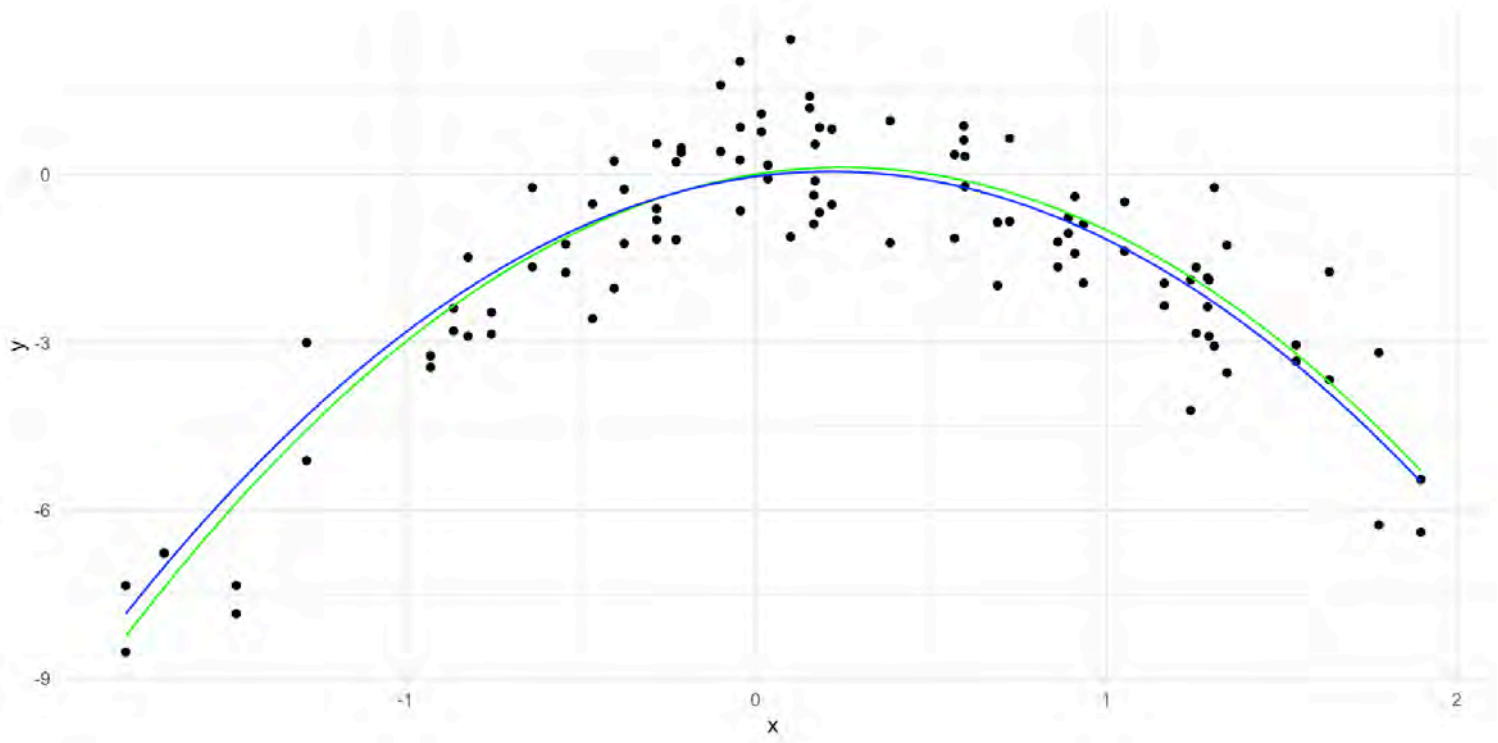
Lasso regression with $\lambda = 0.01$



$$\hat{y}(x) = 0.17 + 0.93x - 2.60x^2 + \cdots - 3.29 \times 10^{-6}x^{19} - 5.95 \times 10^{-7}x^{20}$$

The $\sum_{j=1}^{20} |\hat{\beta}_j|$ is 3.79 and there are 8 non-zero coefficients.

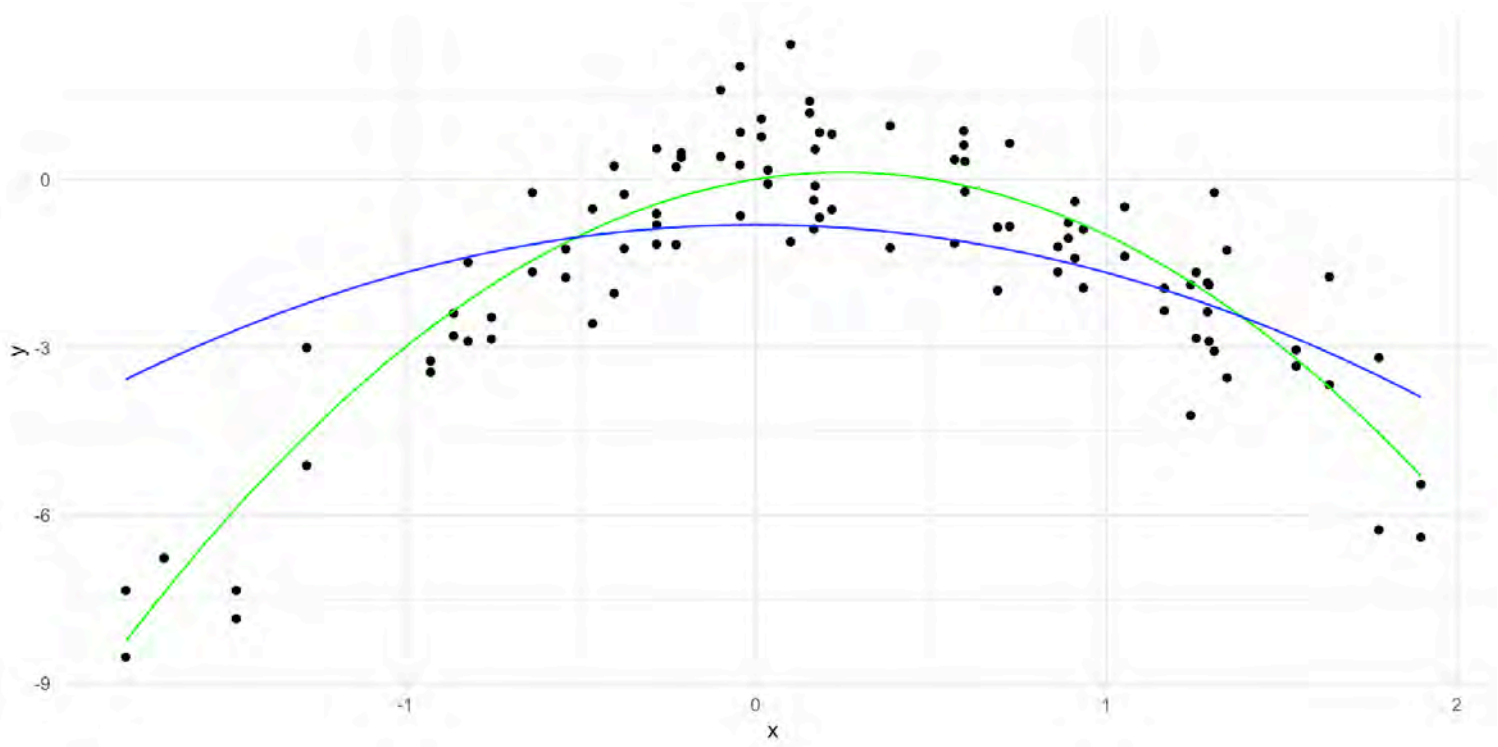
Lasso regression with $\lambda = 0.1$



$$\hat{y}(x) = -0.04 + 0.83x - 1.96x^2$$

The $\sum_{j=1}^{20} |\hat{\beta}_j|$ is 2.79 and there are 2 non-zero coefficients.

Lasso regression with $\lambda = 1$



$$\hat{y}(x) = -0.81 - 0.86x^2$$

The $\sum_{j=1}^{20} |\hat{\beta}_j|$ is 0.855 and there are 1 non-zero coefficients.

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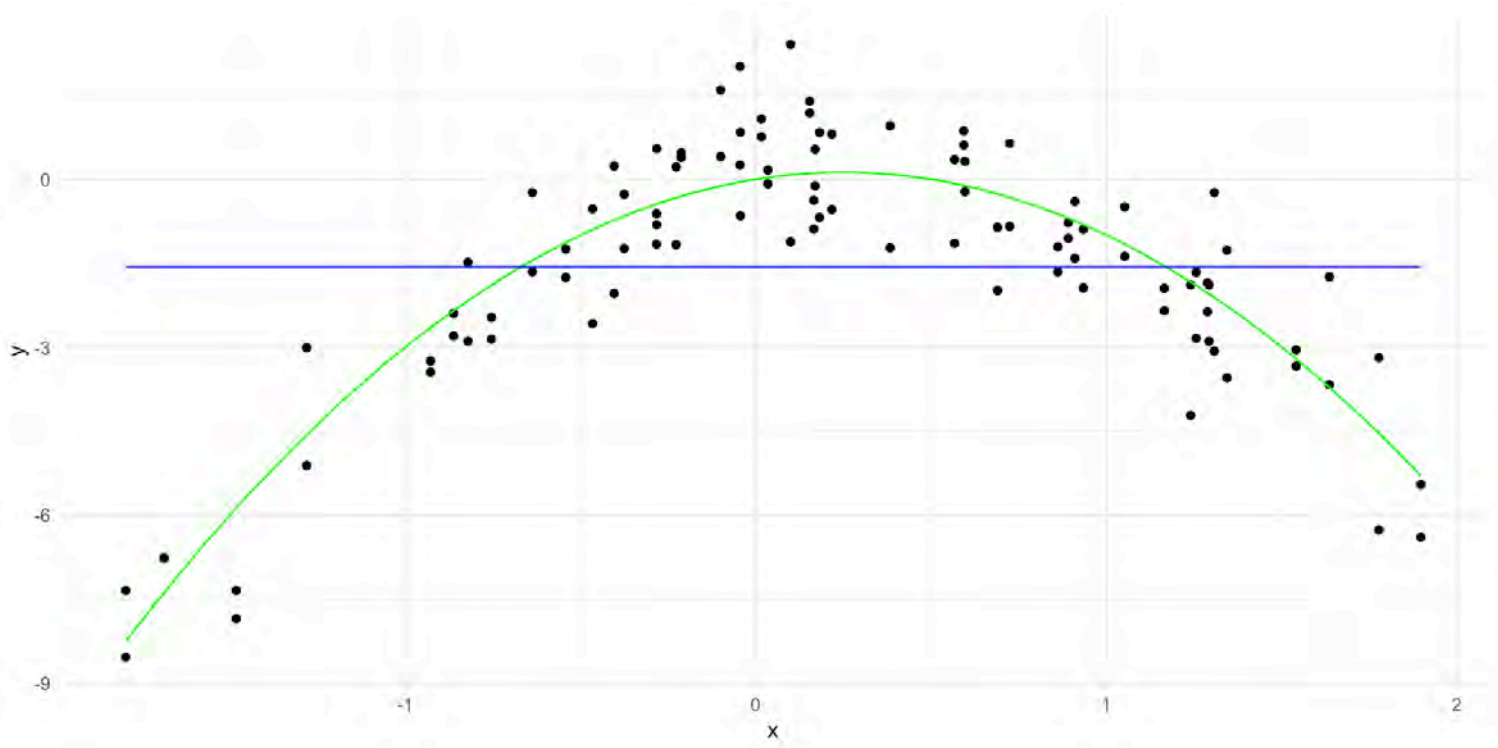
Lasso regression with $\lambda = 10$



$$\hat{y}(x) = -1.57 - 1.90 \times 10^{-16} x^2$$

The $\sum_{j=1}^{20} |\hat{\beta}_j|$ is 1.9e-16 and there is 1 non-zero coefficient.

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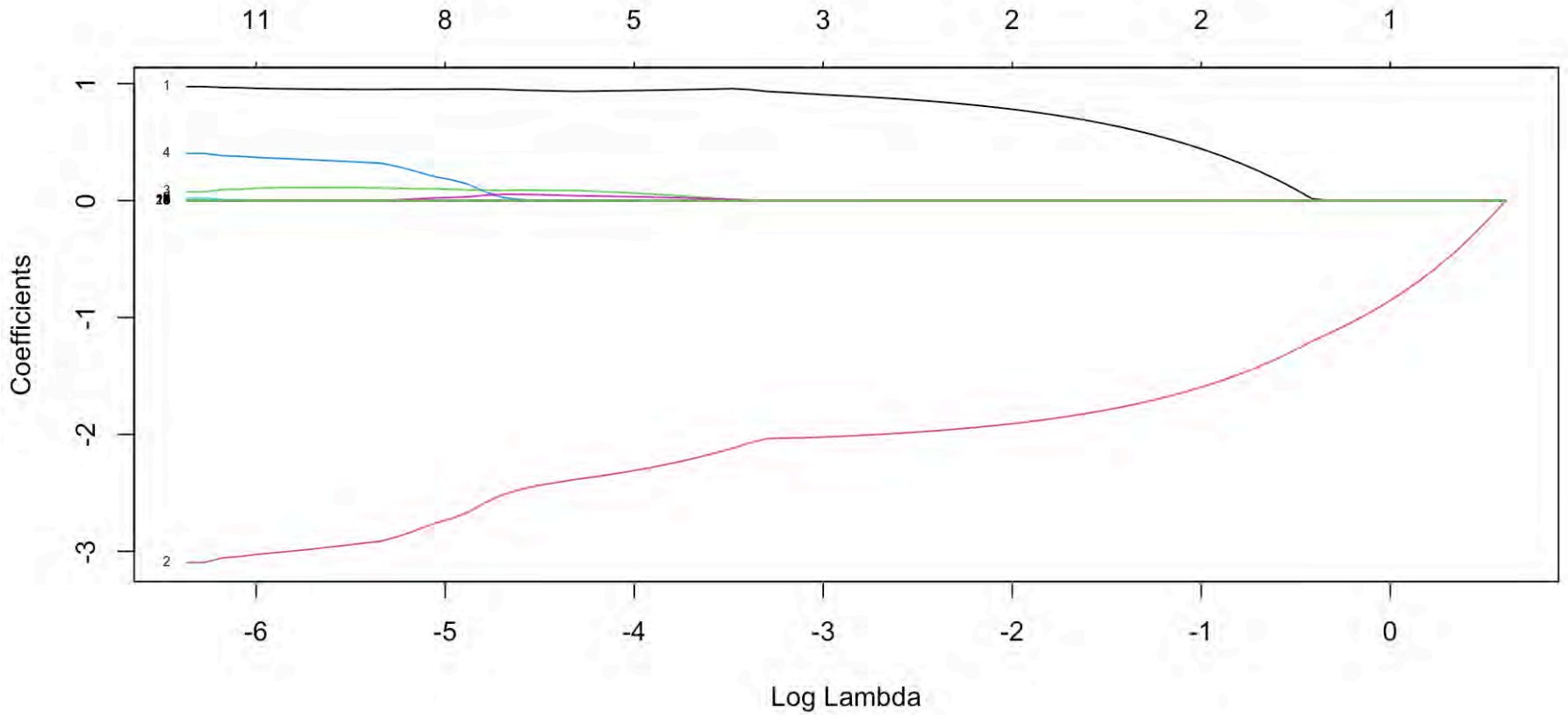
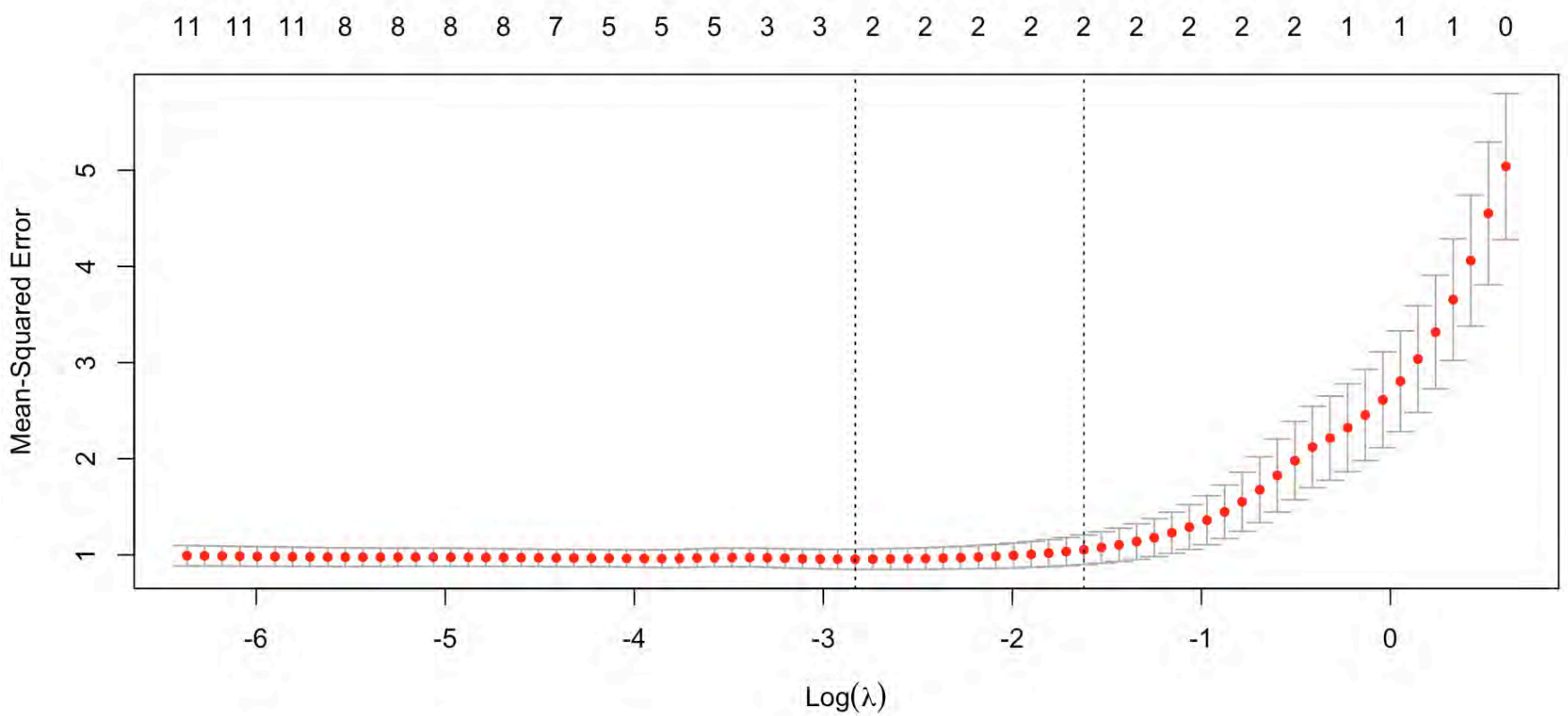
Regularisation path plots



Cross-validation errors



The λ which minimises the CV MSE is 0.0589482 ($\log(\lambda)$ is -2.8310954).

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Glassdoor preparation

```r
model_subrankings <- lm(overall_rating ~ work_life_balance + culture_values +
        career_opp + comp_benefits + senior_mgmt +
        recommend + ceo_approv, data = train_val)
summary(model_subrankings)
```

```
Call:
lm(formula = overall_rating ~ work_life_balance + culture_values +
    career_opp + comp_benefits + senior_mgmt + recommend + ceo_approv,
    data = train_val)

Residuals:
    Min      1Q  Median      3Q     Max
-4.0109 -0.3441 -0.0248  0.3595  3.4854

Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)        1.321466   0.032022  41.267  < 2e-16 ***
work_life_balance  0.068873   0.006287  10.954  < 2e-16 ***
culture_values     0.244629   0.007812  31.314  < 2e-16 ***
career_opp         0.175851   0.006339  27.741  < 2e-16 ***
comp_benefits      0.070892   0.006010  11.796  < 2e-16 ***
senior_mgmt        0.177644   0.007244  24.521  < 2e-16 ***
recommendPositive  0.121017   0.017635   6.862 7.19e-12 ***
recommendNegative -0.544801   0.025401 -21.448  < 2e-16 ***
ceo_approvPositive -0.020925   0.016648  -1.257  0.20884
ceo_approvMild     -0.047943   0.016599  -2.888  0.00388 **
```

```r
X <- model.matrix(overall_rating ~ work_life_balance + culture_values +
        career_opp + comp_benefits + senior_mgmt +
        recommend + ceo_approv, data = train_val)[,-1]
y <- train_val$overall_rating
```

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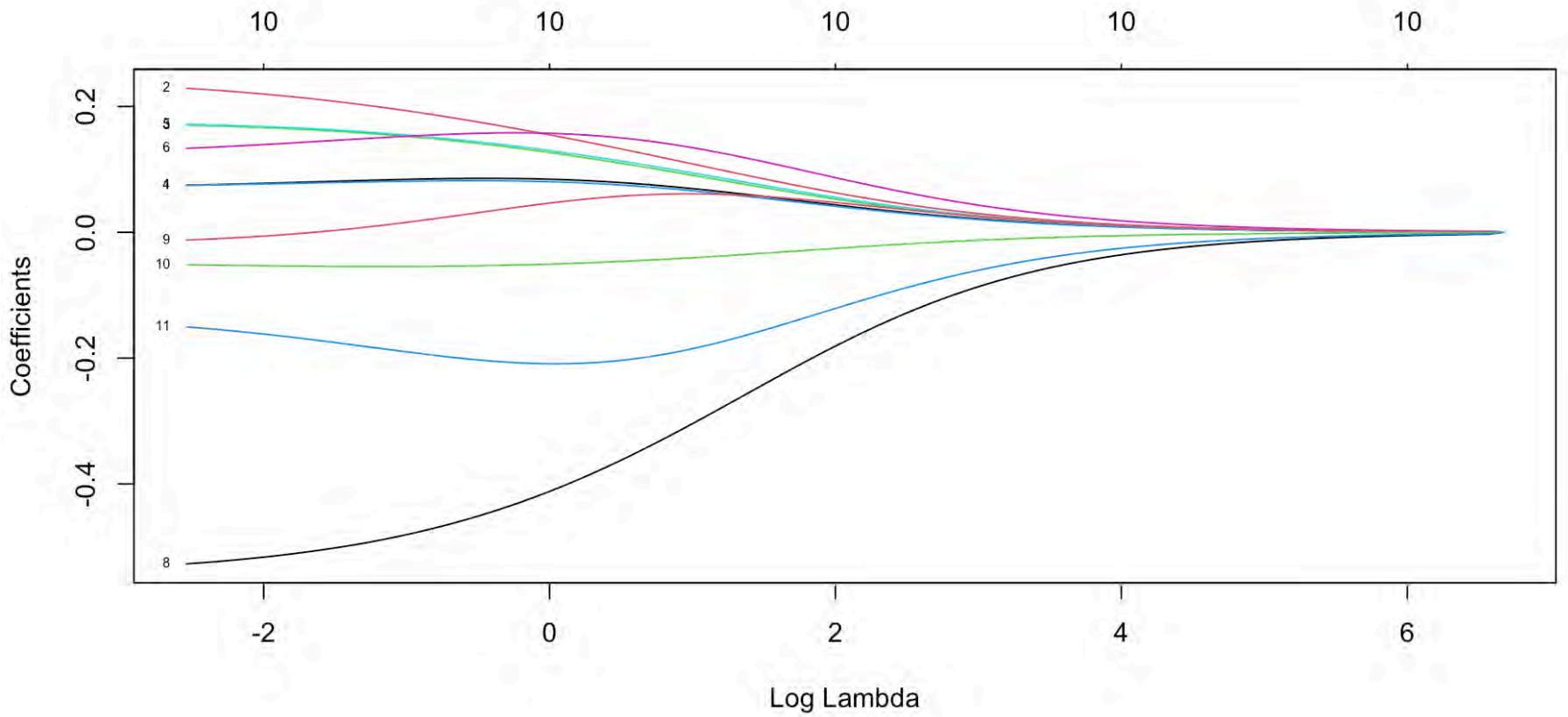
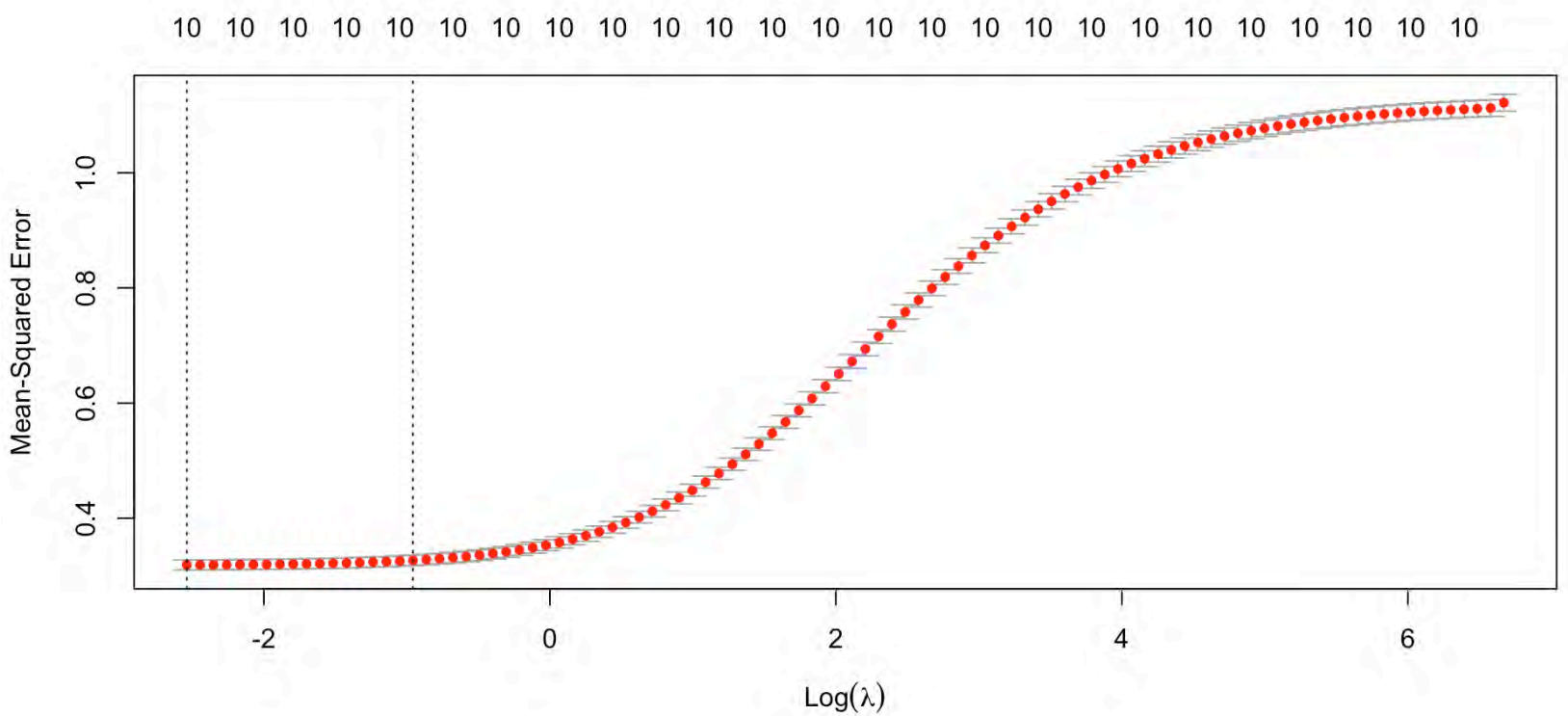
Glassdoor ridge regression

```
1 ridge <- glmnet(X, y, alpha = 0)
2 plot(ridge, xvar="lambda", label=TRUE)
```



Glassdoor ridge regression CV

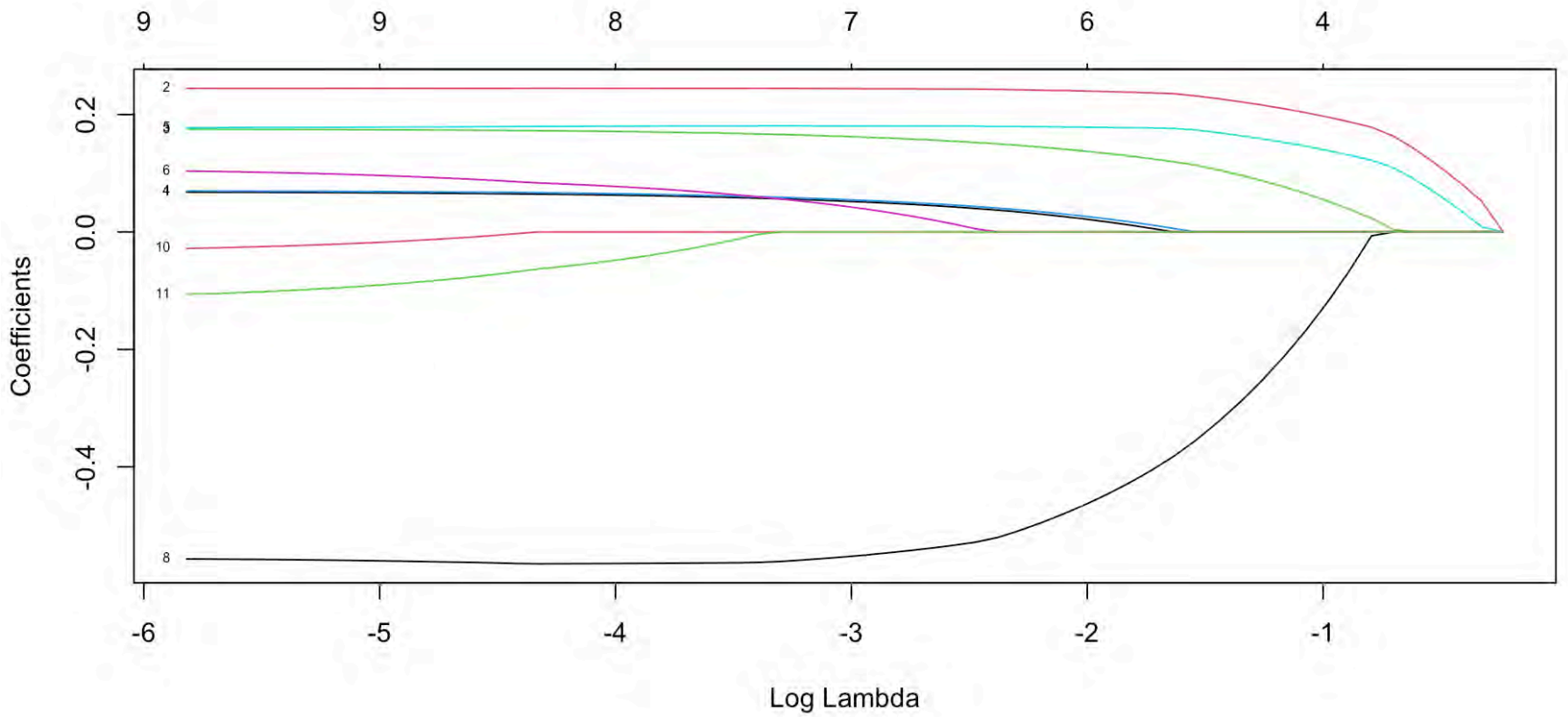
```r
cv_ridge <- cv.glmnet(X, y, alpha = 0)
plot(cv_ridge)
```



The λ which minimises the CV MSE is 0.0789461 ($\log(\lambda)$ is -2.5389899).

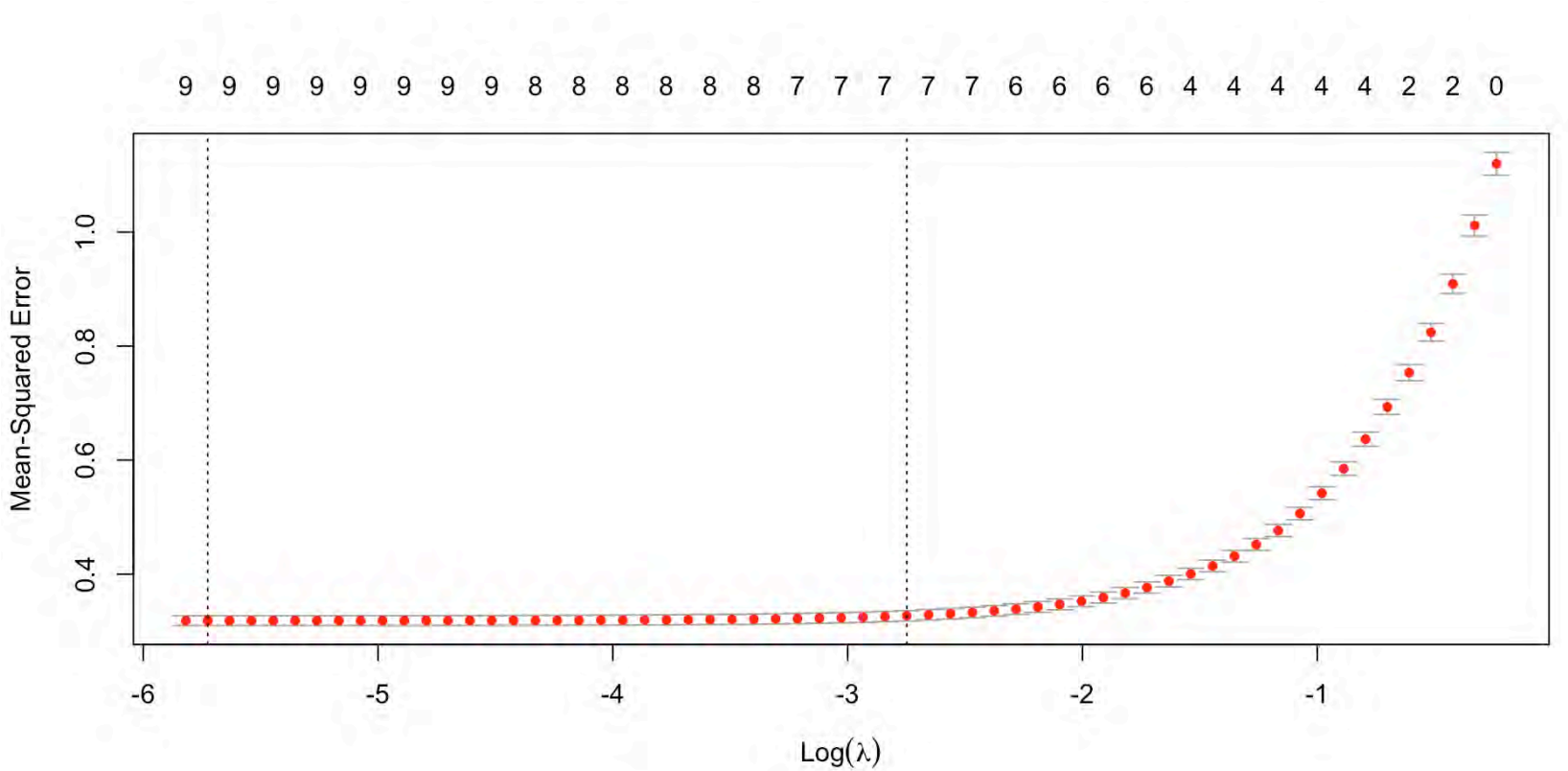
Glassdoor lasso regression

```
lasso <- glmnet(X, y, alpha = 1)
plot(lasso, xvar="lambda", label=TRUE)
```



Glassdoor lasso regression CV

```
cv_lasso <- cv.glmnet(X, y, alpha = 1)
plot(cv_lasso)
```



The λ which minimises the CV MSE is 0.0032621 ($\log(\lambda)$ is -5.7253955).

The "one standard error" model

> "lambda.min": the λ at which the smallest MSE is achieved.
>
> "lambda.1se": the largest λ at which the MSE is within one standard error of the smallest MSE (default).

```
coef(cv_lasso, s = "lambda.min")
```

```
12 x 1 sparse Matrix of class "dgCMatrix"
                            s1
(Intercept)          1.33348345
work_life_balance    0.06771192
culture_values       0.24444863
career_opp           0.17493054
comp_benefits        0.06970145
senior_mgmt          0.17788762
recommendPositive    0.10325936
recommendMild        .
recommendNegative   -0.55711640
ceo_approvPositive   .
ceo_approvMild      -0.02732177
ceo_approvNegative  -0.10528624
```

```
coef(cv_lasso, s = "lambda.1se")
```

```
12 x 1 sparse Matrix of class "dgCMatrix"
                            s1
(Intercept)          1.57364673
work_life_balance    0.04712771
culture_values       0.24371243
career_opp           0.15818381
comp_benefits        0.05006640
senior_mgmt          0.18033404
recommendPositive    0.02714509
recommendMild        .
recommendNegative   -0.54238656
ceo_approvPositive   .
ceo_approvMild       .
ceo_approvNegative   .
```

Source: Hastie et al. (2023), *An Introduction to* `glmnet`.

Gene expression data

```
1 df <- load_gene_data()
2 df
```

```
# A tibble: 99 × 4,405
      `8`   `18`    `20`   `21`   `22`    `26`    `27`    `28`   `29`   `30`
    <dbl>  <dbl>   <dbl>  <dbl>  <dbl>   <dbl>   <dbl>   <dbl>  <dbl>  <dbl>
 1  0.0164 -0.294 -0.166   0.423 -0.507 -0.559  -0.679  -0.123  -0.511 -0.837
 2 -0.435  -0.270  0.0251  0.474 -0.662 -0.678  -0.0576  0.396  -0.247 -0.705
 3 -0.327  -0.735 -0.0805  0.649 -0.786 -0.0397 -0.238  -0.851  -0.501 -0.820
 4  0.496  -0.389 -0.121  -0.227 -0.776  0.0559  0.0206 -0.683  -0.542 -0.995
 5  1.37   -0.192 -0.0716  0.265 -0.666 -0.342   0.180  -0.862  -0.386 -0.797
 6 -0.191  -0.232  0.547   0.287 -0.708 -0.250   0.355  -0.0872 -0.524 -0.890
 7  0.264  -0.424  0.259   1.98  -0.386  0.109   0.258  -0.749  -0.220 -0.789
 8 -0.537  -0.152  0.660   0.303 -0.778 -0.791  -0.0715 -0.517  -0.299 -0.866
 9  0.197  -0.292  0.173   2.17  -0.272 -0.819  -0.0359 -0.293  -0.232 -0.590
10  0.0915 -0.107  0.0381  2.44  -0.152  0.345   0.245   0.451  -0.103 -0.414
# ℹ 89 more rows
# ℹ 4,395 more variables: `32` <dbl>, `33` <dbl>, `35` <dbl>, `37` <dbl>,
#   `38` <dbl>, `39` <dbl>, `40` <dbl>, `42` <dbl>, `43` <dbl>, `44` <dbl>,
#   `45` <dbl>, `46` <dbl>, `49` <dbl>, `51` <dbl>, `53` <dbl>, `54` <dbl>,
#   `55` <dbl>, `56` <dbl>, `57` <dbl>, `59` <dbl>, `60` <dbl>, `61` <dbl>,
#   `63` <dbl>, `64` <dbl>, `65` <dbl>, `66` <dbl>, `67` <dbl>, `68` <dbl>,
#   `70` <dbl>, `71` <dbl>, `72` <dbl>, `73` <dbl>, `74` <dbl>, `101` <dbl>, …
```

Source: Sotiriou et al., *Breast cancer classification and prognosis based on gene expression profiles from a population-based study*, PNAS 100.18 (2003): 10393-10398.

Dataset information

> "Sotiriou et al. (2003) described a breast cancer study with 99 women divided into two groups according to their oestrogen receptor status. The ER+ group (65 women) are those women where the cancer has receptors for oestrogen, and the ER− group (34 women) are those without receptors. Out of 7650 variables there are 4404 measured in all 99 samples, and we use these variables for our analysis."

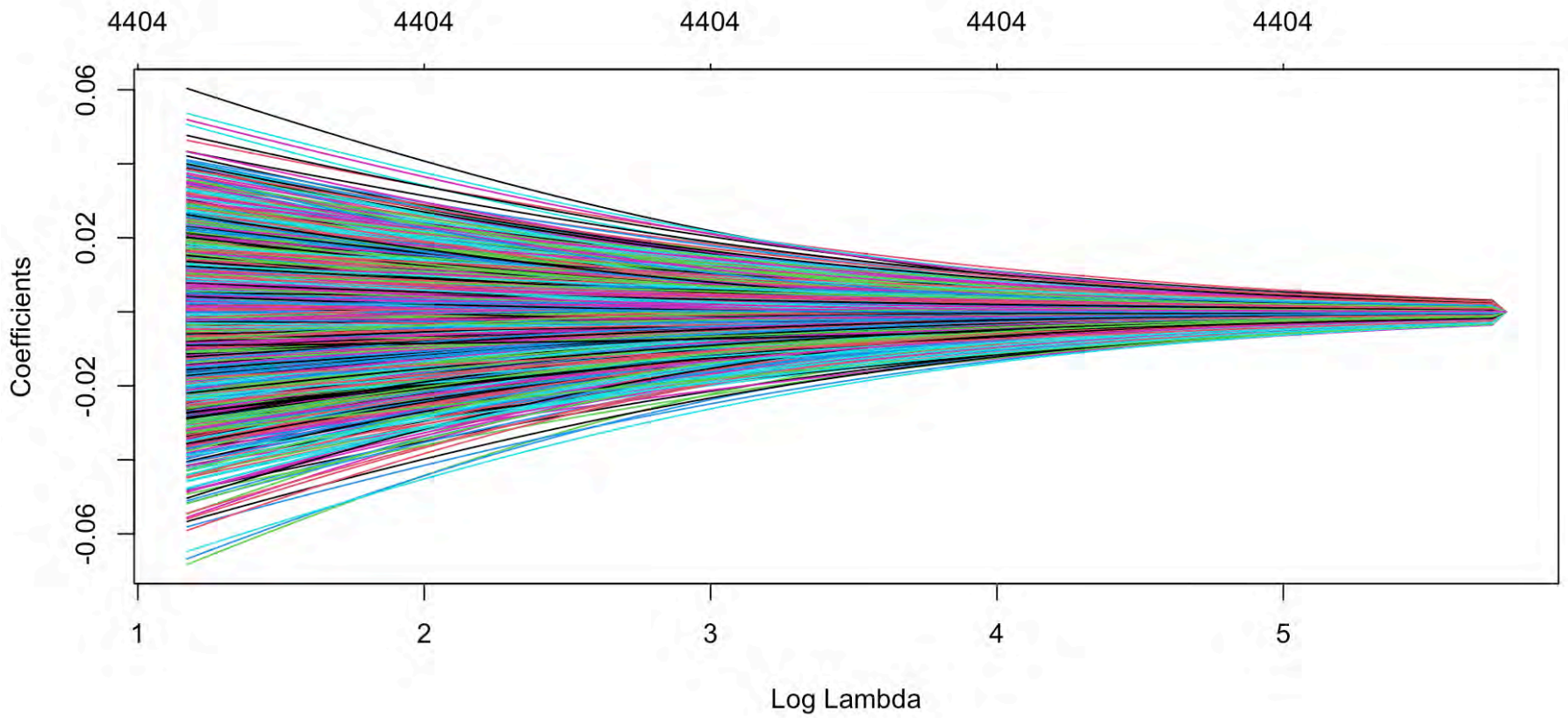
```r
# Split and convert to matrices for `glmnet`
set.seed(123)  # For reproducibility
test_index <- sample(1:nrow(df), 0.2 * nrow(df))
test <- df[test_index, ]
train_val <- df[-test_index, ]

# Prepare data for glmnet
X <- model.matrix(er ~ ., data = train_val)[, -1]
y <- train_val$er
X_test <- model.matrix(er ~ ., data = test)[, -1]
y_test <- test$er
```

Source: Bak, Britta Anker and Jens Ledet Jensen, *High dimensional classifiers in the imbalanced case*, Computational Statistics & Data Analysis 98 (2016): 46–59.

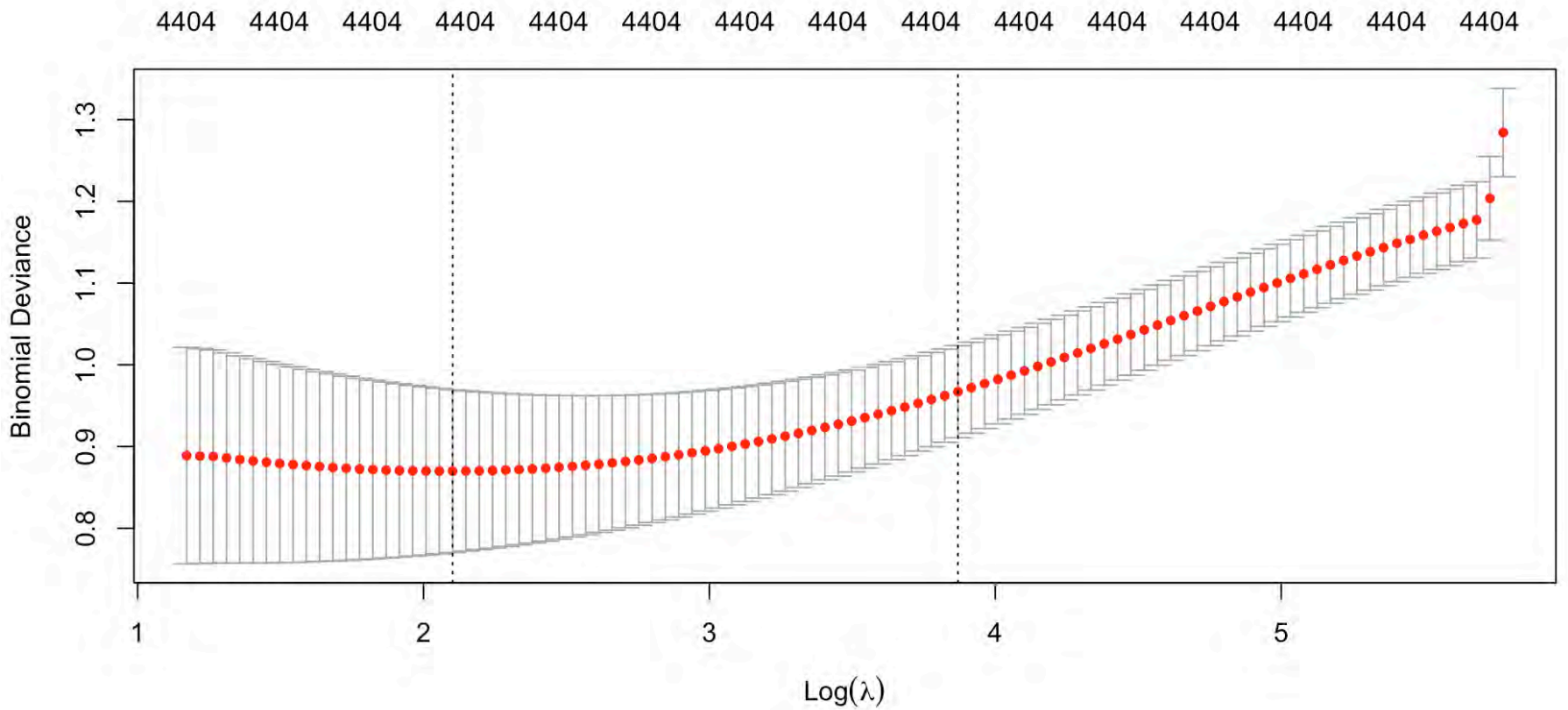
Ridge regression

```
1  ridge_model <- glmnet(X, y, family = "binomial", alpha = 0)
2  plot(ridge_model, xvar="lambda")
```



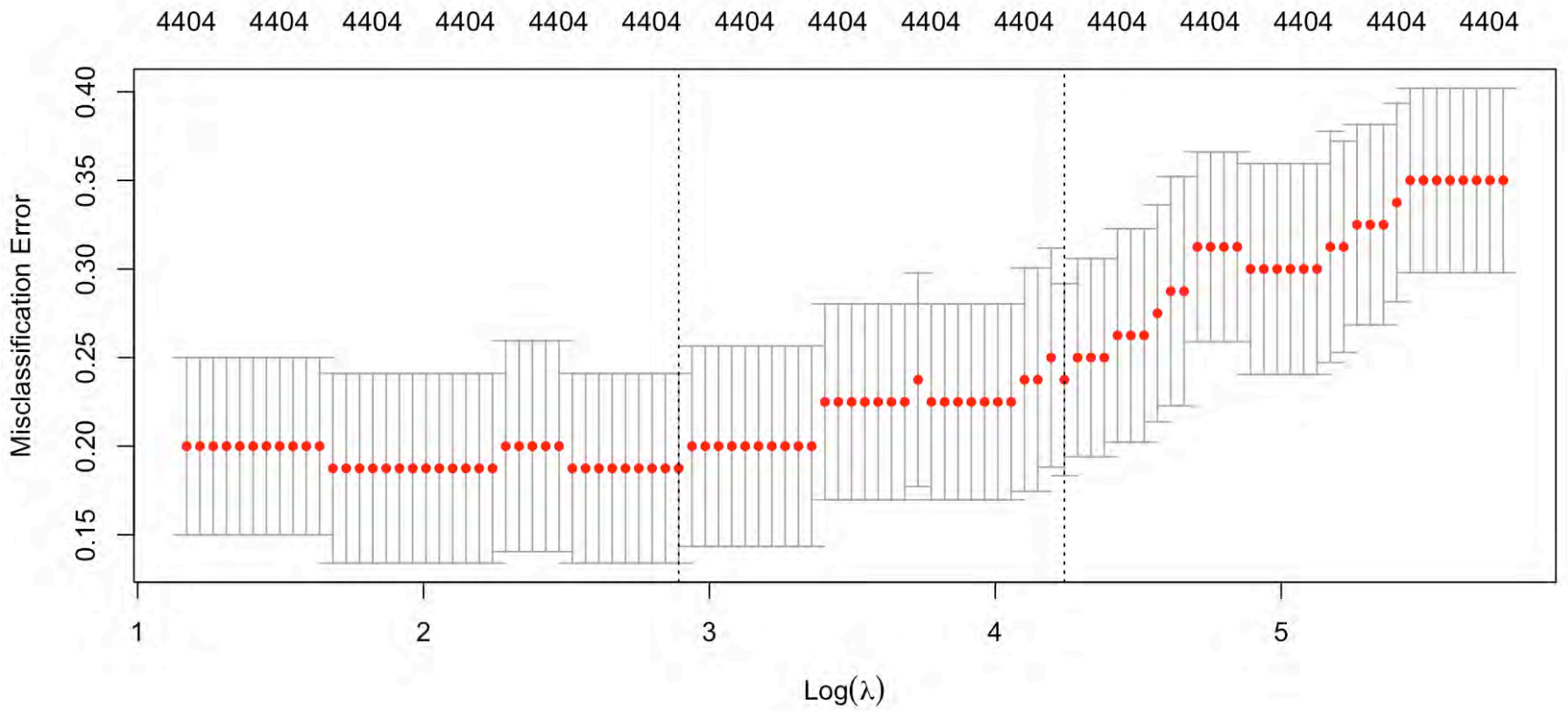
Ridge CV (Deviance)

```
1 cv_ridge <- cv.glmnet(X, y, family = "binomial", alpha = 0)
2 plot(cv_ridge)
```



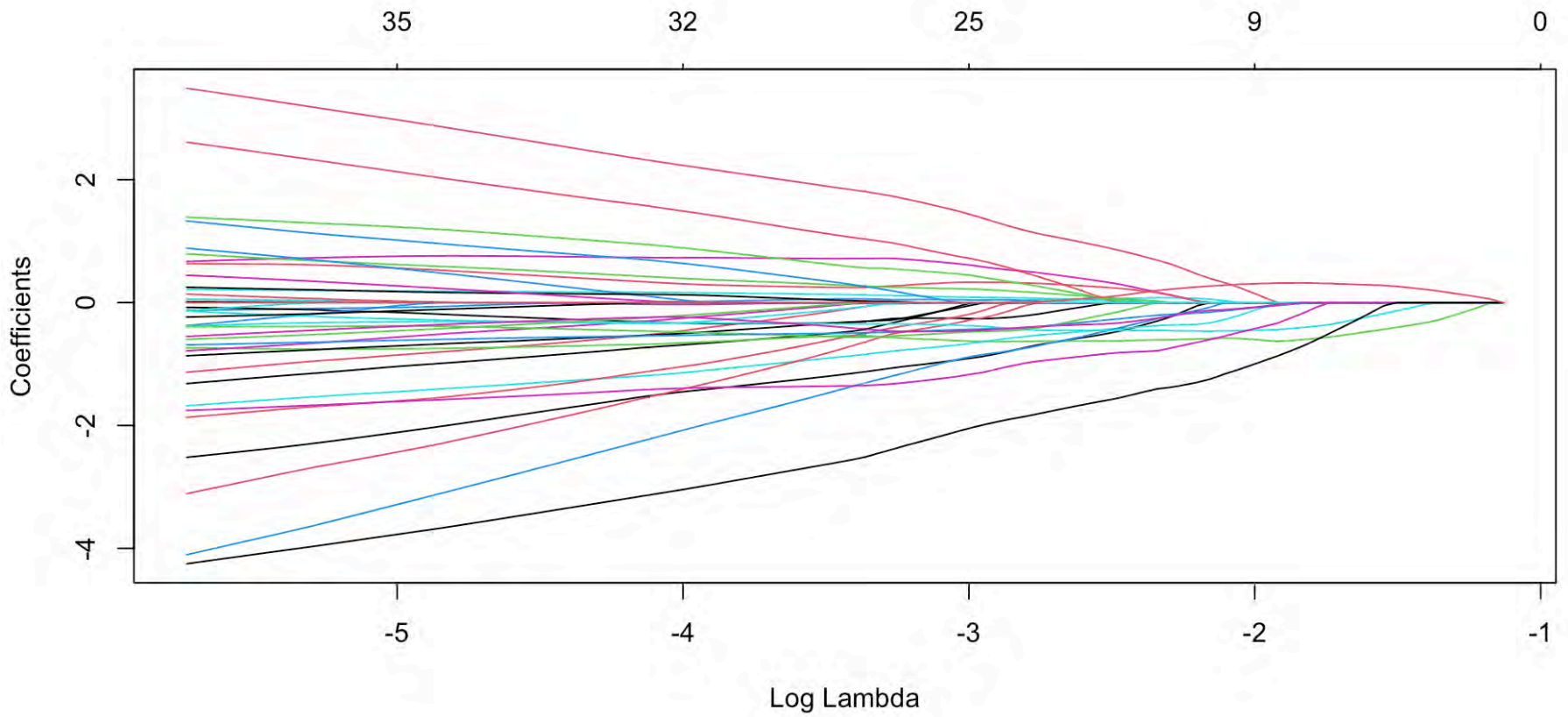
Ridge CV (Classification Error Rate)

```
cv_ridge <- cv.glmnet(X, y, family = "binomial", alpha = 0, type.measure = "class")
plot(cv_ridge)
```



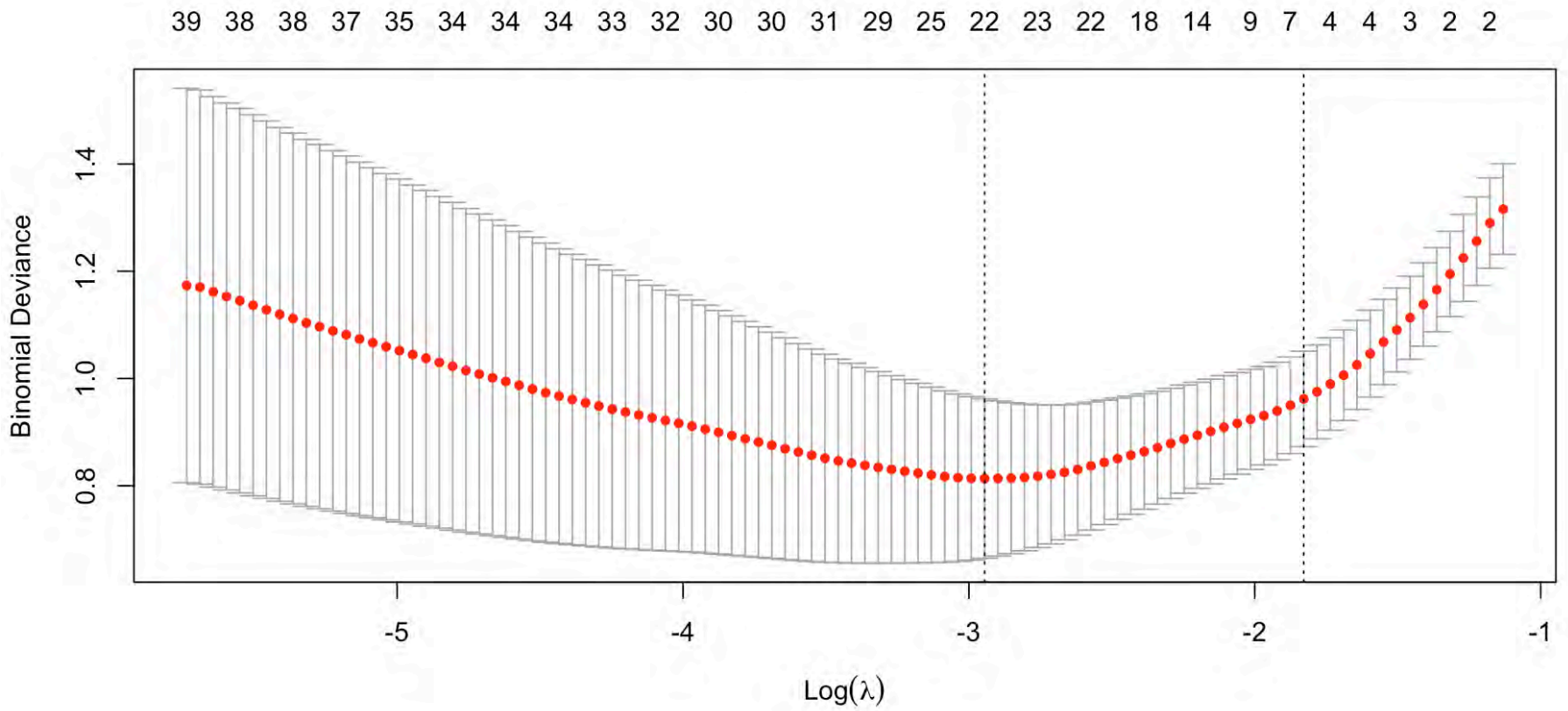
Lasso regression

```
1 lasso_model <- glmnet(X, y, family = "binomial", alpha = 1)
2 plot(lasso_model, xvar="lambda")
```



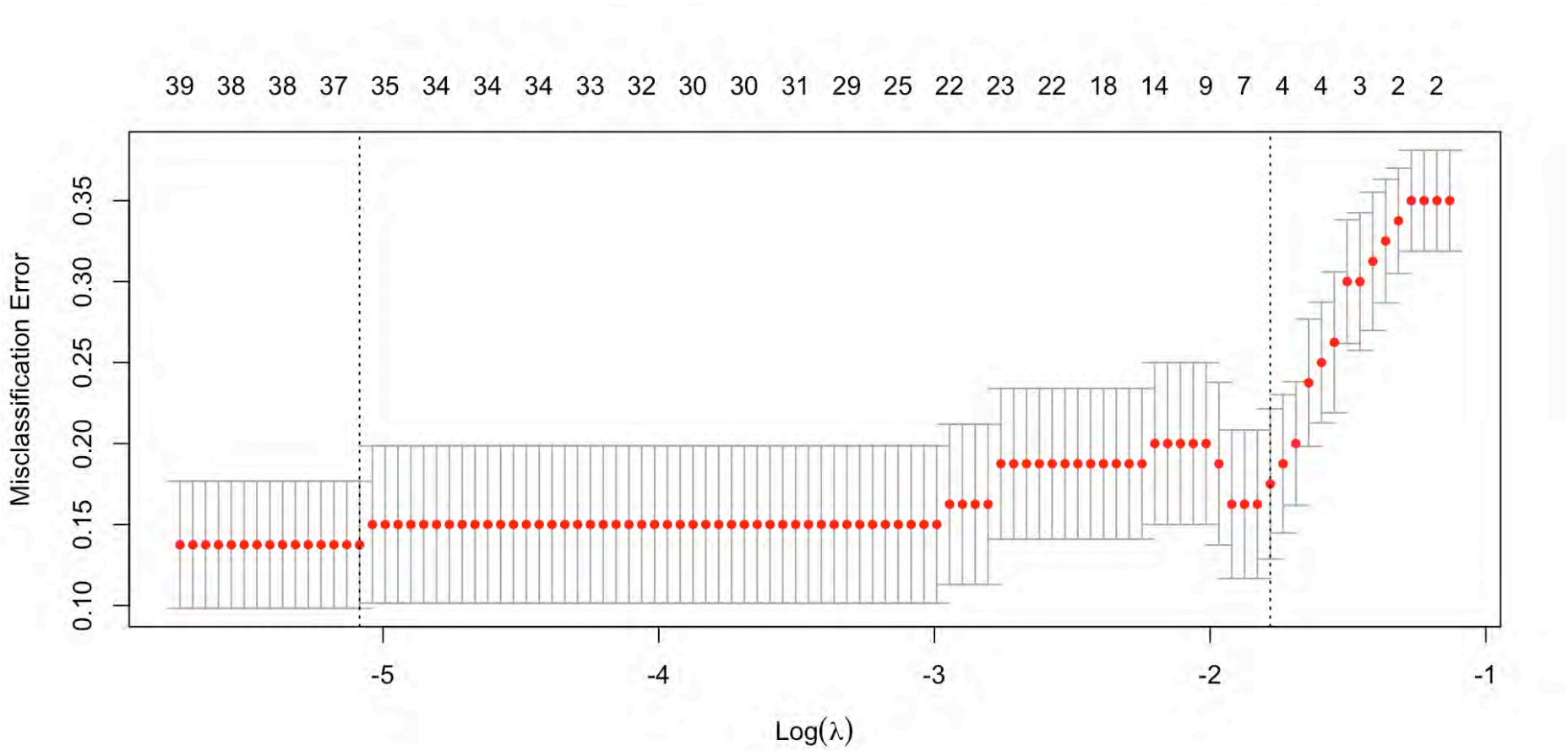
Lasso CV (Deviance)

```
1 cv_lasso <- cv.glmnet(X, y, family = "binomial", alpha = 1)
2 plot(cv_lasso)
```



Lasso CV (Classification Error Rate)

```
cv_lasso <- cv.glmnet(X, y, family = "binomial", alpha = 1, type.measure = "class")
plot(cv_lasso)
```



Select a winner & test it

```
(ridge_cv_error <- min(cv_ridge$cvm))
```

```
[1] 0.1875
```

```
(lasso_cv_error <- min(cv_lasso$cvm))
```

```
[1] 0.1375
```

```
sum(coef(cv_lasso, s = "lambda.min") != 0)
```

```
[1] 38
```

```
sum(coef(cv_lasso, s = "lambda.1se") != 0)
```

```
[1] 6
```

```
if (ridge_cv_error < lasso_cv_error) {
  best_model <- cv_ridge
  model_type <- "ridge"
} else {
  best_model <- cv_lasso
  model_type <- "lasso"
}

print(paste("Selected model type:", model_type))
```

```
[1] "Selected model type: lasso"
```

```
y_pred <- predict(best_model, X_test, type = "response", s = "lambda.min") > 0.5
test_accuracy <- mean(y_test == y_pred)
print(paste("Test set accuracy of the selected model:", test_accuracy))
```

```
[1] "Test set accuracy of the selected model: 0.842105263157895"
```

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Lecture Outline

- Linear Regression Recap
- Generalised Linear Models Recap
- Glassdoor Dataset
- Statistical Model Evaluation
- Validation Set Approach
- k-Fold Cross-Validation
- Leave-One-Out Cross-Validation
- Regularisation
- Regularisation Plots
- Regularisation Demos
- **Ridge and Lasso Intuition**

Alternate formulation

Ridge regression: minimise MSE subject to

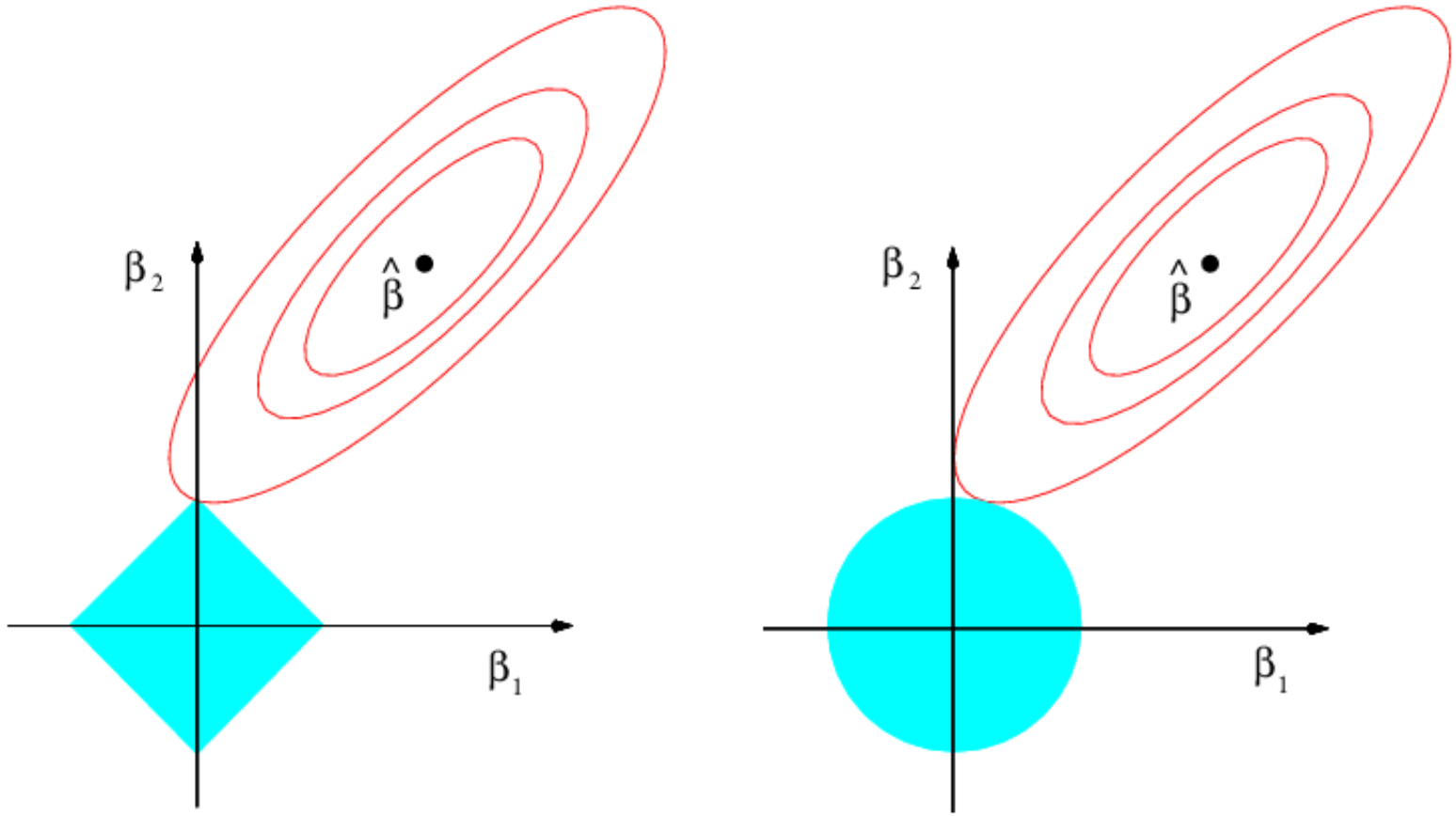
$$\sum_{j=1}^{n} \beta_j^2 \leq s$$

Lasso regression: minimise MSE subject to

$$\sum_{j=1}^{n} |\beta_j| \leq s$$

- Each method is assigns a "budget" to "spend" on the coefficient estimates
- The size of the "budget" is based on λ (ridge and lasso)
- This is like Lagrange multipliers (actually look up Karush–Kuhn–Tucker (KKT) conditions)

Ridge vs Lasso: Some intuition



Contours of training MSE against the constraint regions for ridge & lasso.

Lasso leads to a pointier solution space: more likely to set parameters to zero.

Source: James et al. (2021), *An Introduction to Statistical Learning, with applications in R*, Figure 6.7.

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Ridge regression - comments

- Almost all parameters are included, and coefficients are generally low: difficult to interpret model
- Far more efficient than best-subset: only one model for each λ needs to be computed, calculating for *all* λ is almost identical to least squares estimates
- Performs better than least-squares where the relationship is linear, but the estimate variance is high

When to use what?

> So when should you use elastic net regression, or ridge, lasso, or plain linear regression (i.e., without any regularization)? It is almost always preferable to have at least a little bit of regularization, so generally you should avoid plain linear regression. Ridge is a good default, but if you suspect that only a few features are useful, you should prefer lasso or elastic net because they tend to reduce the useless features' weights down to zero, as discussed earlier. In general, elastic net is preferred over lasso because lasso may behave erratically when the number of features is greater than the number of training instances or when several features are strongly correlated.

Source: Géron (2022), Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 3rd Edition, Chapter 4.