Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 6: *Mid-way evaluation and Machine Learning Intro*

November 2, 2021

by: Lau Møller Andersen

Study Café

how is it going?

Reminder:

Office hours

(If assignments are hard, why is no one coming?)

Python book in Stakbogladen

https://www.stakbogladen.dk/soegning.asp?phrase=9781783555130

Also available online at the Royal Library (thanks, Emil!)

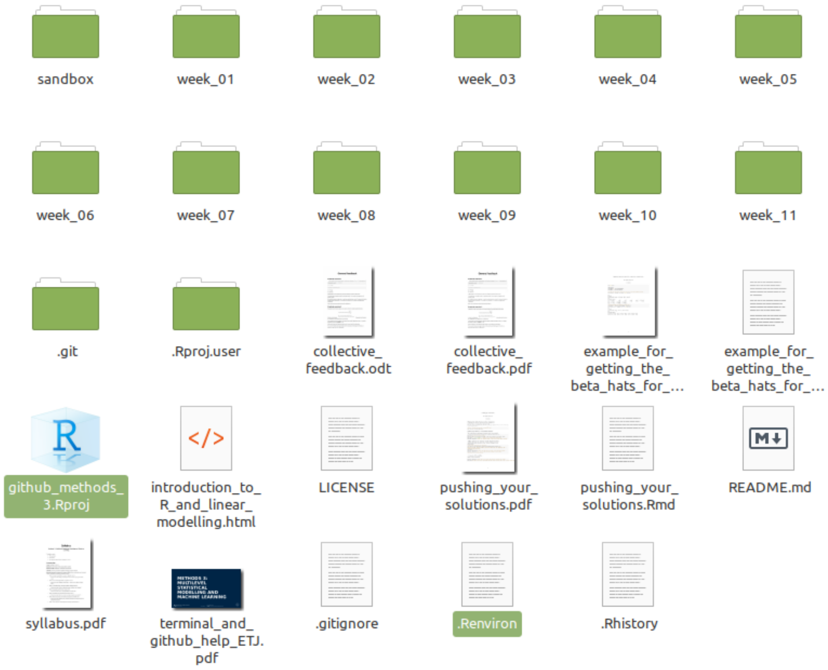
Practical exercise tomorrow

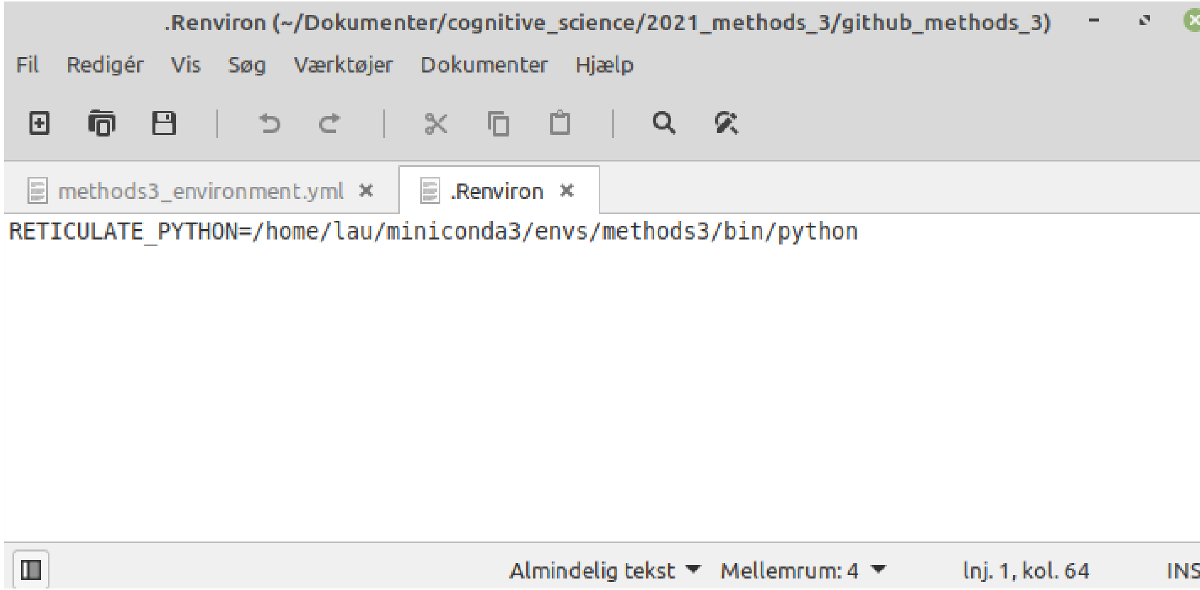
To make sure that *Python* runs within *R Markdown*, make sure you have the *reticulate* package installed `install.packages('reticulate')`
Also create a text file that is called *.Renviron* (remember the dot) placed in the folder where your *RProj* file is. It should have a single line: `RETICULATE_PYTHON=PATH` where `PATH` is the path to your *methods3* conda environment. Use the commands below to find the paths:

```
library(reticulate)
print(conda_list())
```

```
##           name                                              python
## 1   miniconda3                     /home/lau/miniconda3/bin/python
## 2     methods3       /home/lau/miniconda3/envs/methods3/bin/python
## 3          mne            /home/lau/miniconda3/envs/mne/bin/python
## 4     mne_0.17       /home/lau/miniconda3/envs/mne_0.17/bin/python
## 5 mne_func_sig   /home/lau/miniconda3/envs/mne_func_sig/bin/python
## 6       mnedev         /home/lau/miniconda3/envs/mnedev/bin/python
## 7     psychopy       /home/lau/miniconda3/envs/psychopy/bin/python
## 8    fslpython                /usr/local/fsl/fslpython/bin/python
## 9    fslpython /usr/local/fsl/fslpython/envs/fslpython/bin/python
```

Practical exercise tomorrow





NB! No spaces around equals sign!

Practical exercise tomorrow

Update environment

```
conda env create --force -f methods3_environment.yml
```

Overwrite old environment

Update environment (new packages have been added). Run this command from the folder *week_06*

Mid-way evaluation

Mid-way evaluation

1) Write something you liked about the course so far

2) Write something you did not like about the course so far

3) What would you change?

Next time: I’ll summarise the feedback on the three points and what I’ll change

Learning goals

Evaluating and comparing models

1) Learning tools for comparing models
    1) Variance explained
    2) Likelihood ratio tests
    3) Information criteria
2) Bridging to out-of-sample

Why are we modelling?

Remember Emil's slides from week 03

- To be able to understand the world

$$F = G\frac{m_1 m_2}{r^2}$$

EXPLANATION

- To be able to predict and manipulate the world

NASA/Bill Ingalls

PREDICTION

What constitutes a good model?

Remember Emil's slides from week 03

- Accurate estimation of the underlying parameters of the population distribution
- Generalisation to new data

EXPLANATION

PREDICTION

Within an **explanatory** framework, how can we assess whether we have done a good job?

quick recap of…

Variance explained

- Pros
  - R^2 is intuitive
- Cons
  - More complex models will always explain more variance
  - Hard to interpret in the case of collinearity
  - R^2 doesn't give us what we want

Doesn't tell us about the likelihood of this particular model to be true

Likelihood ratio

we now have a principles way of comparing models, which we didn't get from R2.

- Pros
  - Models can be compared in a principled way by reference to a theoretical distribution, χ^2. (In the single level case, *F* can be calculated)
- Cons
  - Models have to be nested in one another we can only compare models where one is a subset of the ot
  - Maximum likelihood fitting may be biased for complex models
  - Requires large sample sizes
  - Be careful if collinearity is high Text

Information criteria

also based on maximum likelihood fitting.

- Pros
  - Models can be compared even though one is not nested within the other (response data has to be the same though)
- Cons
  - Number of effective parameters not well defined for multilevel models
  - Maximum likelihood fitting may be biased for complex models

Did you learn? (it’s not easy)

Evaluating and comparing models

1) Learning tools for comparing models
    1) Variance explained
    2) Likelihood ratio tests
    3) Information criteria
2) Bridging to out-of-sample

Learning goals

Explanation and prediction

1) Understanding that fitting (explaining) often leads to overfitting

2) Learning methods to prevent overfitting by introducing *bias*

of our model fitting

3) Understanding how the error can be decomposed into *bias* and *variance*

To fit is to overfit

(Yarkoni and Westfall, 2017)

Overfitting: fitting sample-specific noise, which is thus not representative of the population

Text

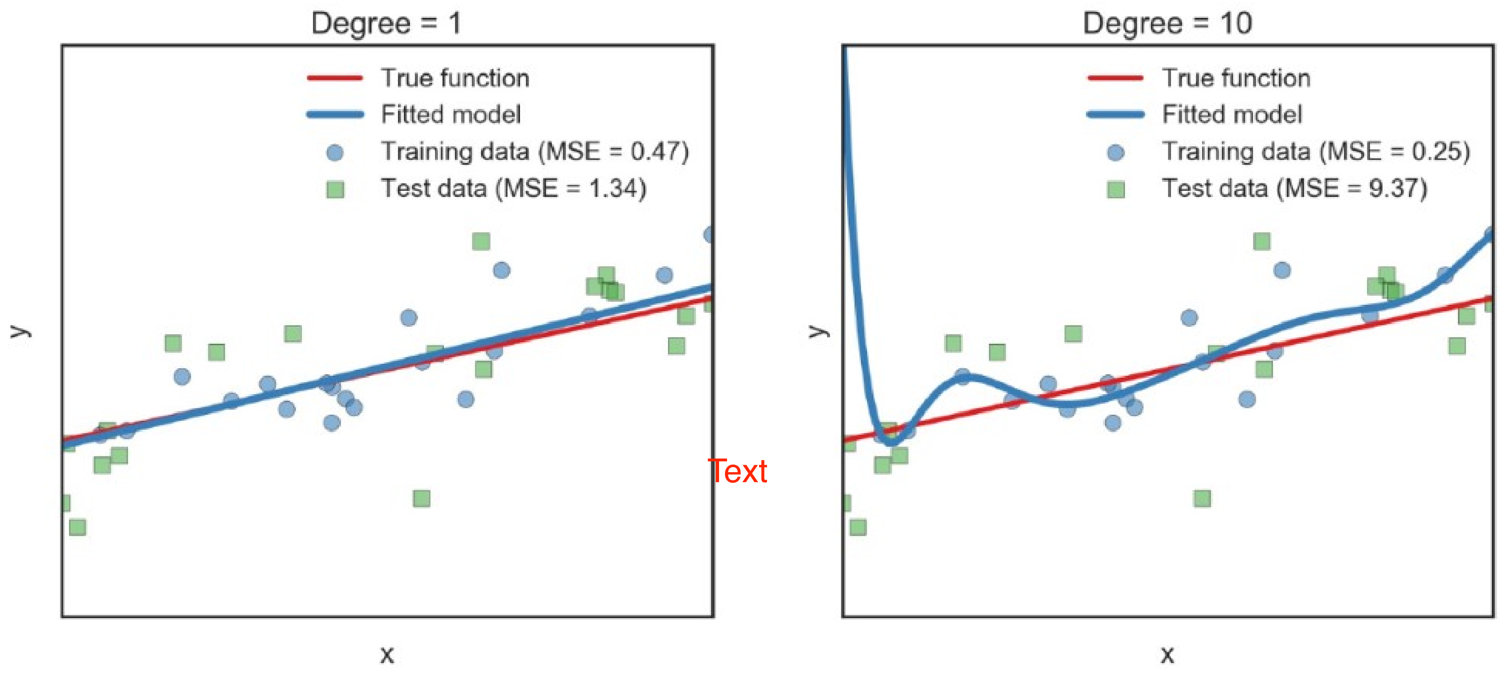
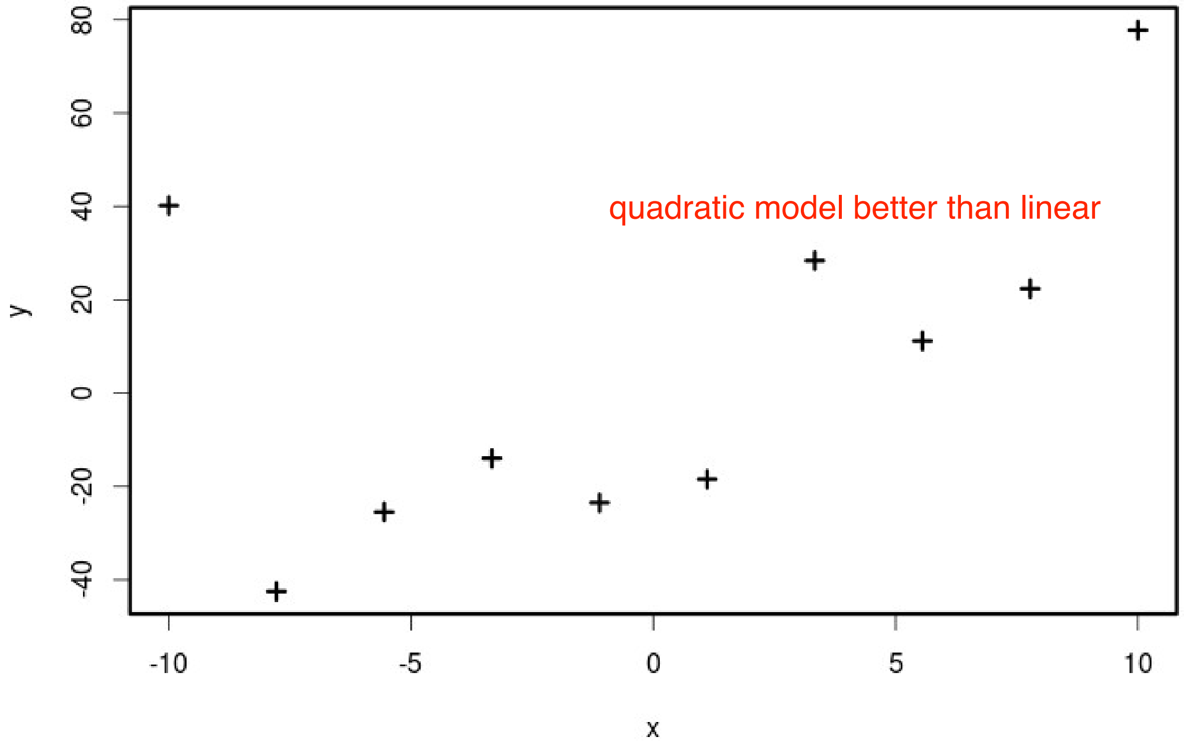


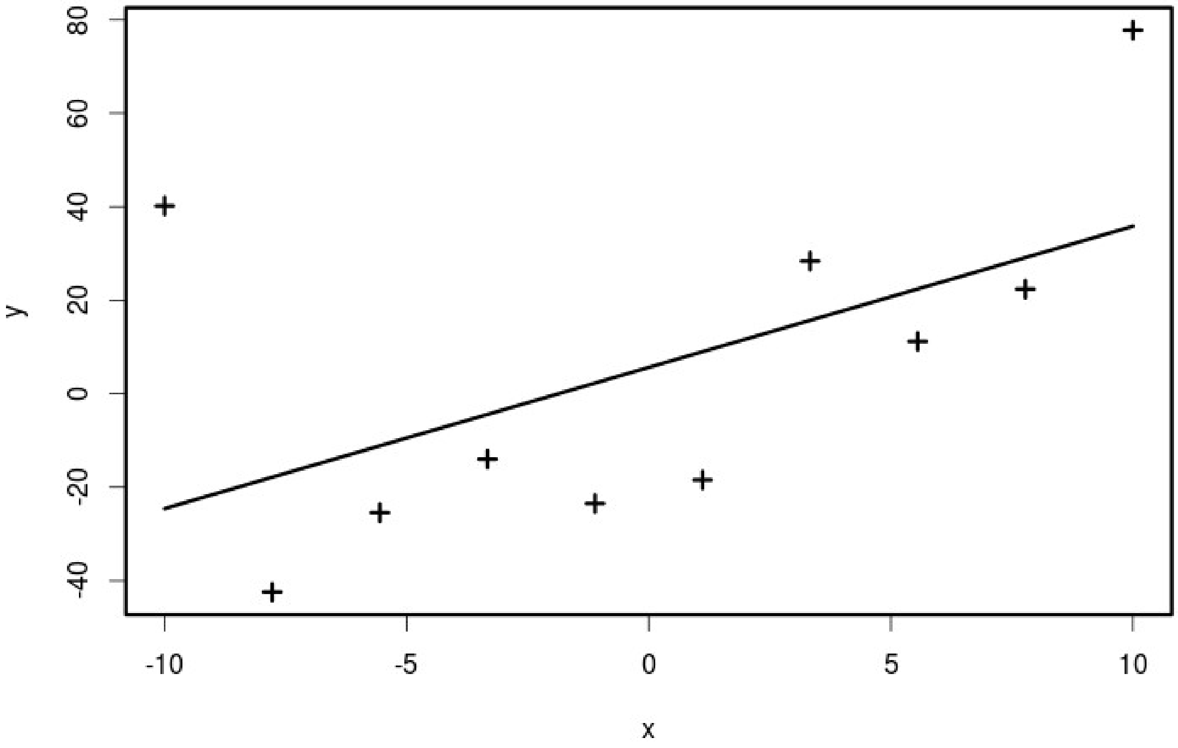
Fig. 1. Training and test error produced by fitting either a linear regression (left) or a 10th-order polynomial regression (right) when the true relationship in the population (red line) is linear. In both cases, the test data (green) deviate more from the model's predictions (blue line) than the training data (blue). However, the flexibility of the 10th-order polynomial model facilitates much greater overfitting, resulting in lower training error but much higher test error than the linear model. MSE = mean squared error.

(Yarkoni and Westfall, 2017)

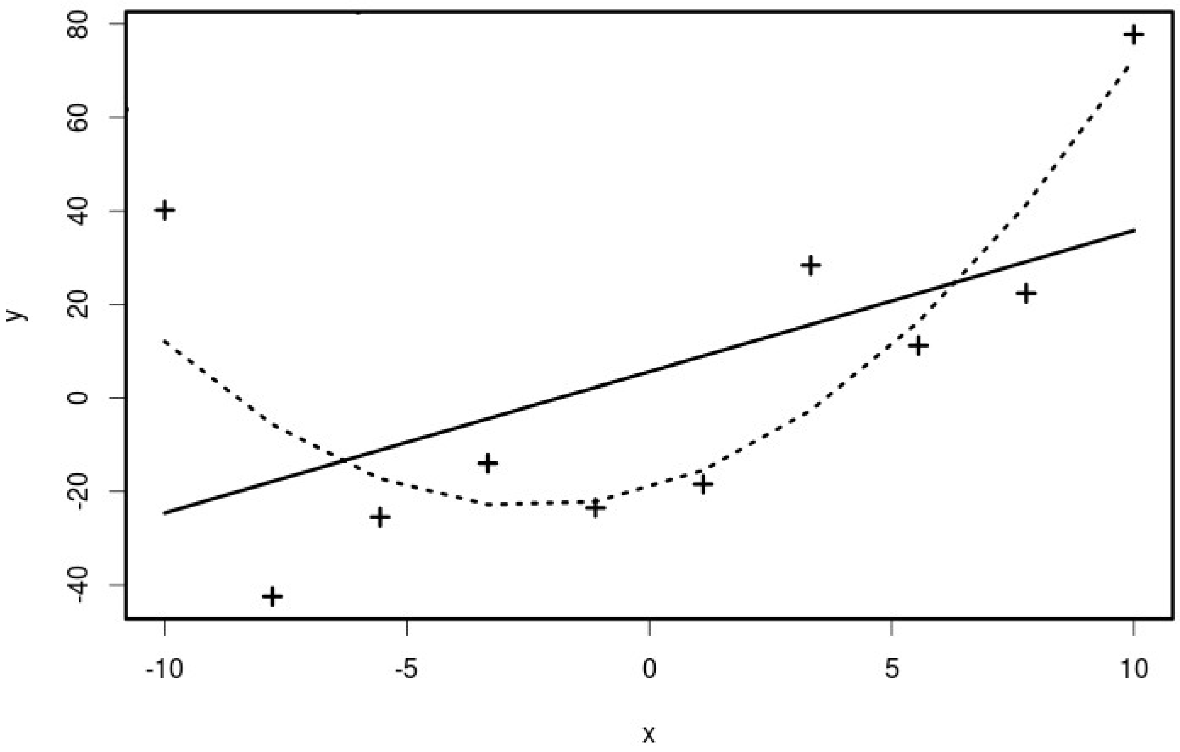
A sample of 10
linear or quadratic?



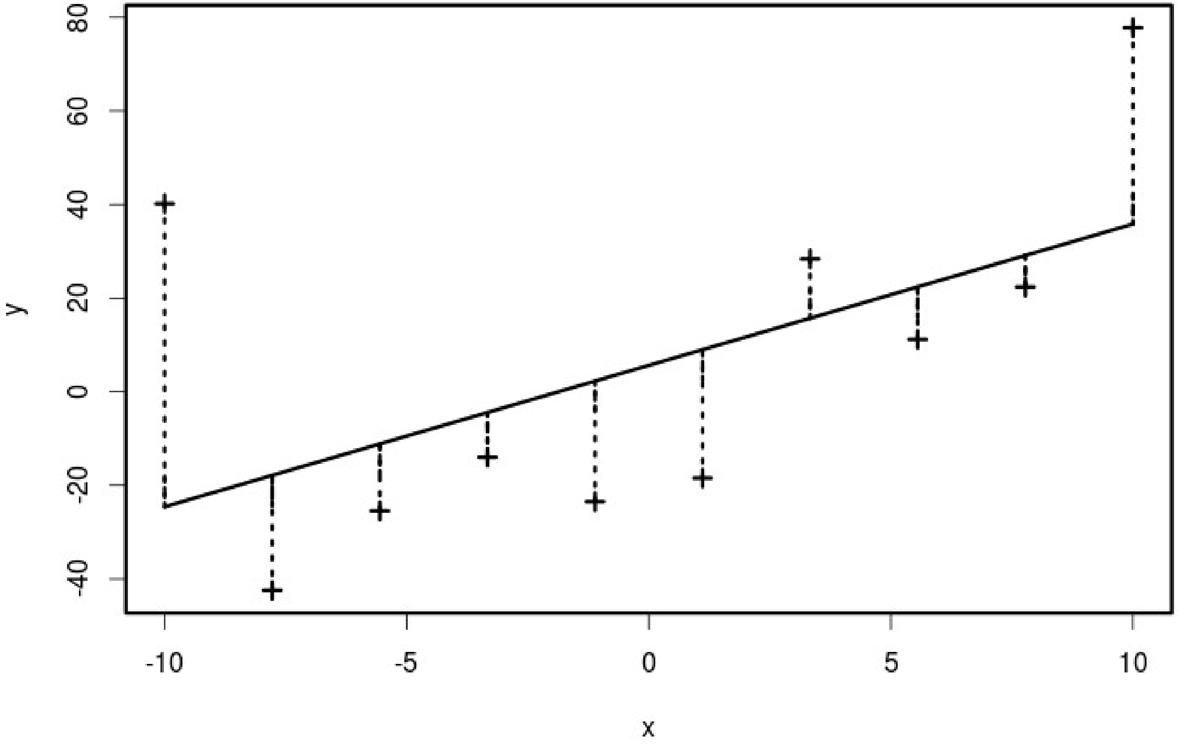
A sample of 10
linear or quadratic?



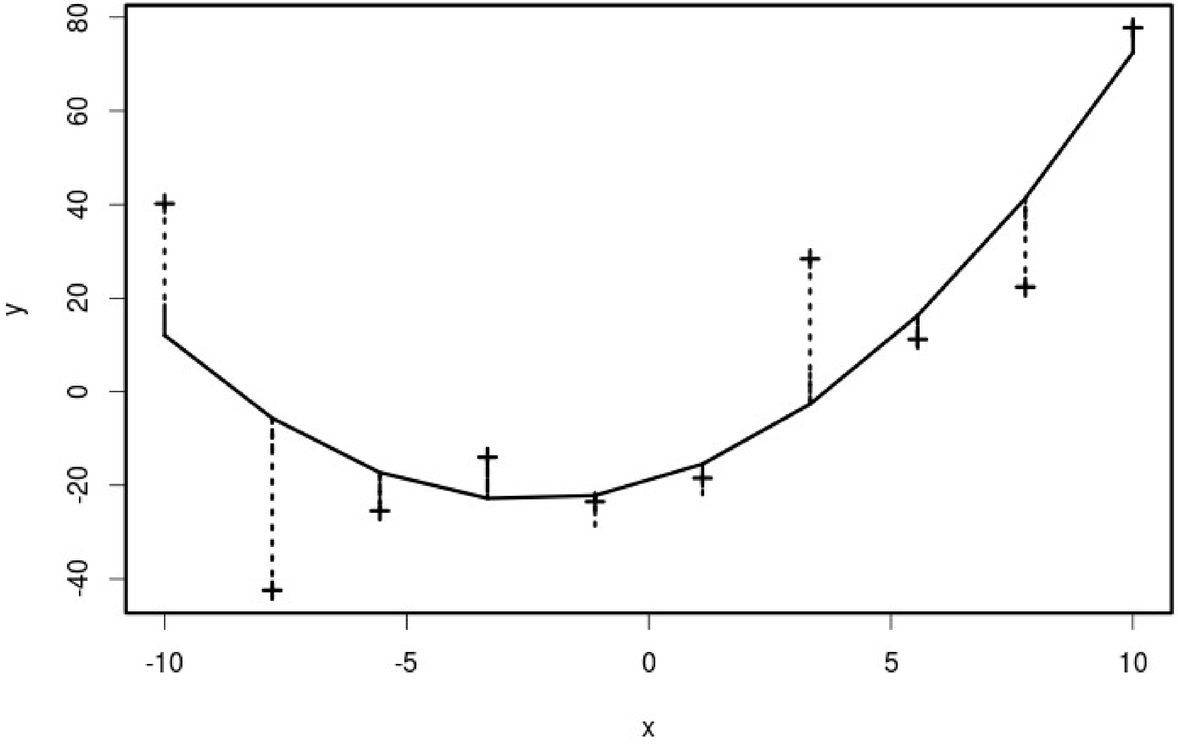
A sample of 10
linear or quadratic?



Residuals (linear)



Residuals (quadratic)



Quadratic:

$ax^2 + bx + c$

Linear:

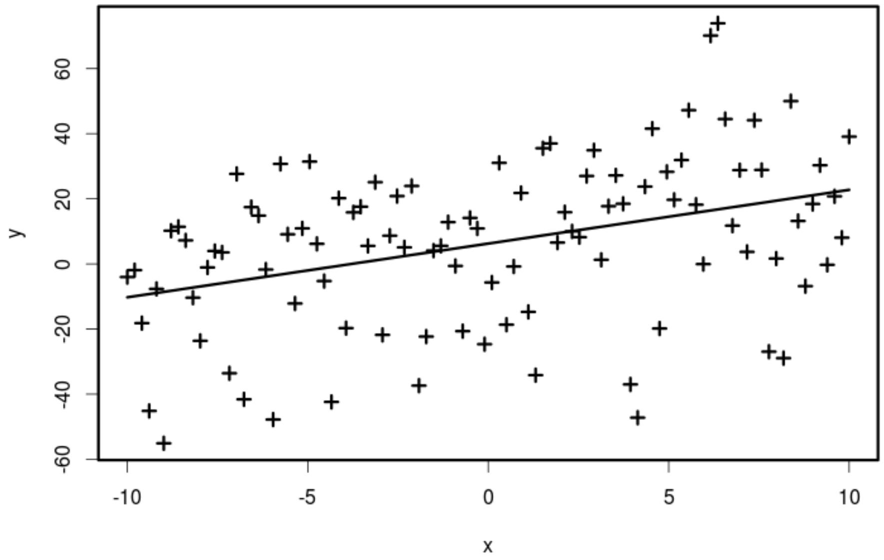
$bx + c$

Estimates

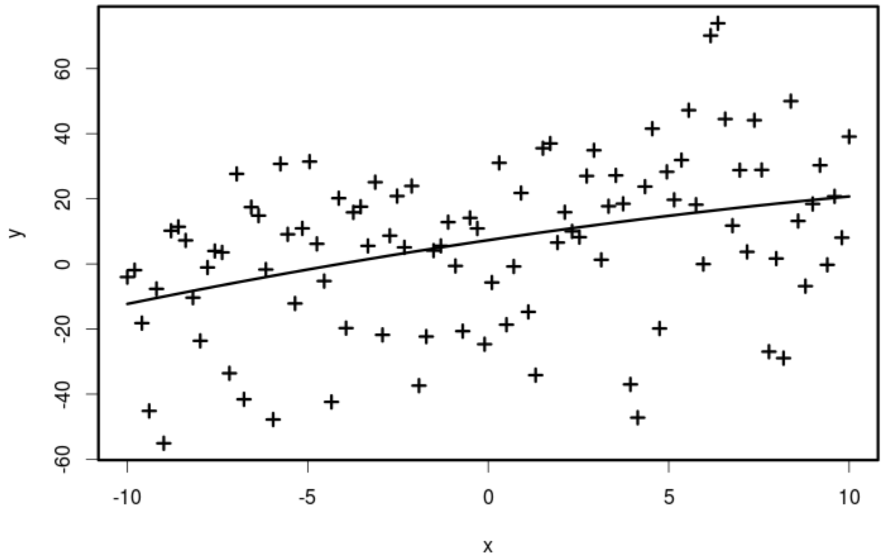
a = 0,6184; b = 3,0201

b = 3,020

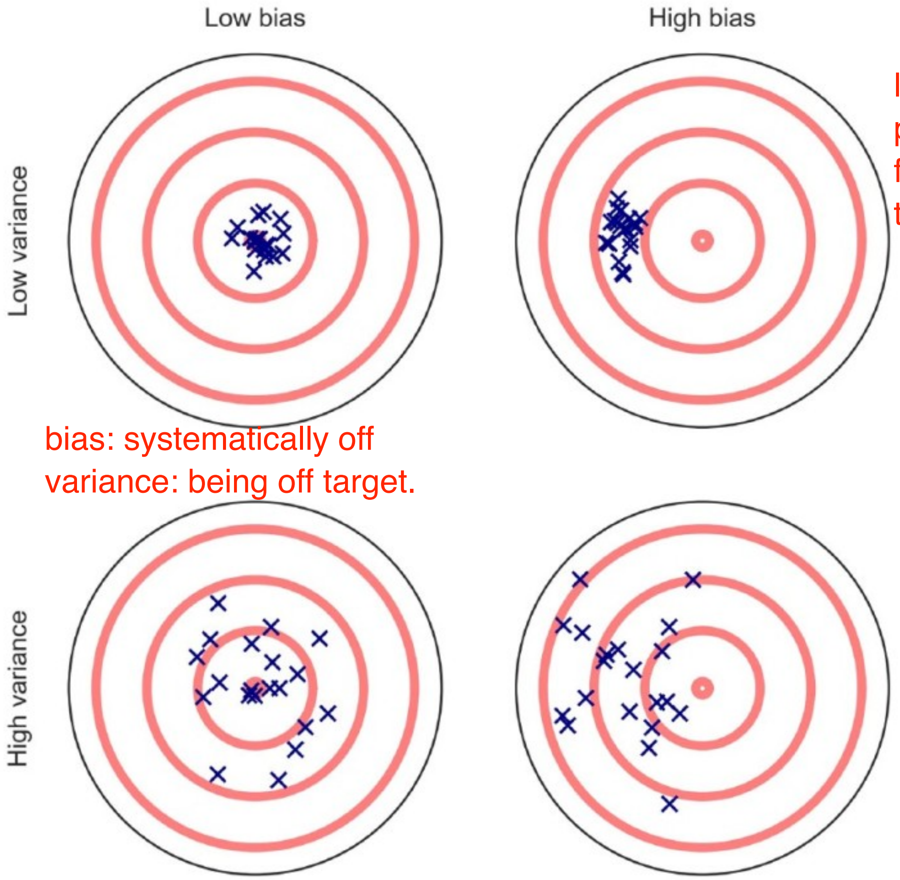
Now a sample of 100



b = 1,650



a = -0,03074 ≈ 0; b = 1,650



bias: systematically off
variance: being off target.

Fig. 2. An estimator's predictions can deviate from the desired outcome (or true scores) in two ways. First, the predictions may display a systematic tendency (or *bias*) to deviate from the central tendency of the true scores (compare right panels with left panels). Second, the predictions may show a high degree of *variance*, or imprecision (compare bottom panels with top panels).

(Yarkoni and Westfall, 2017)

Which two of these does our least-squares solution prefer?

least square solution will prefer where the distance from the true target is smallest

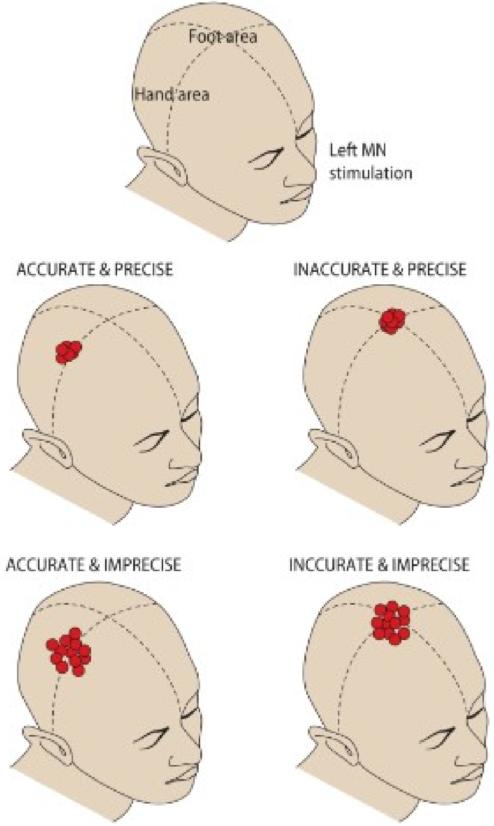
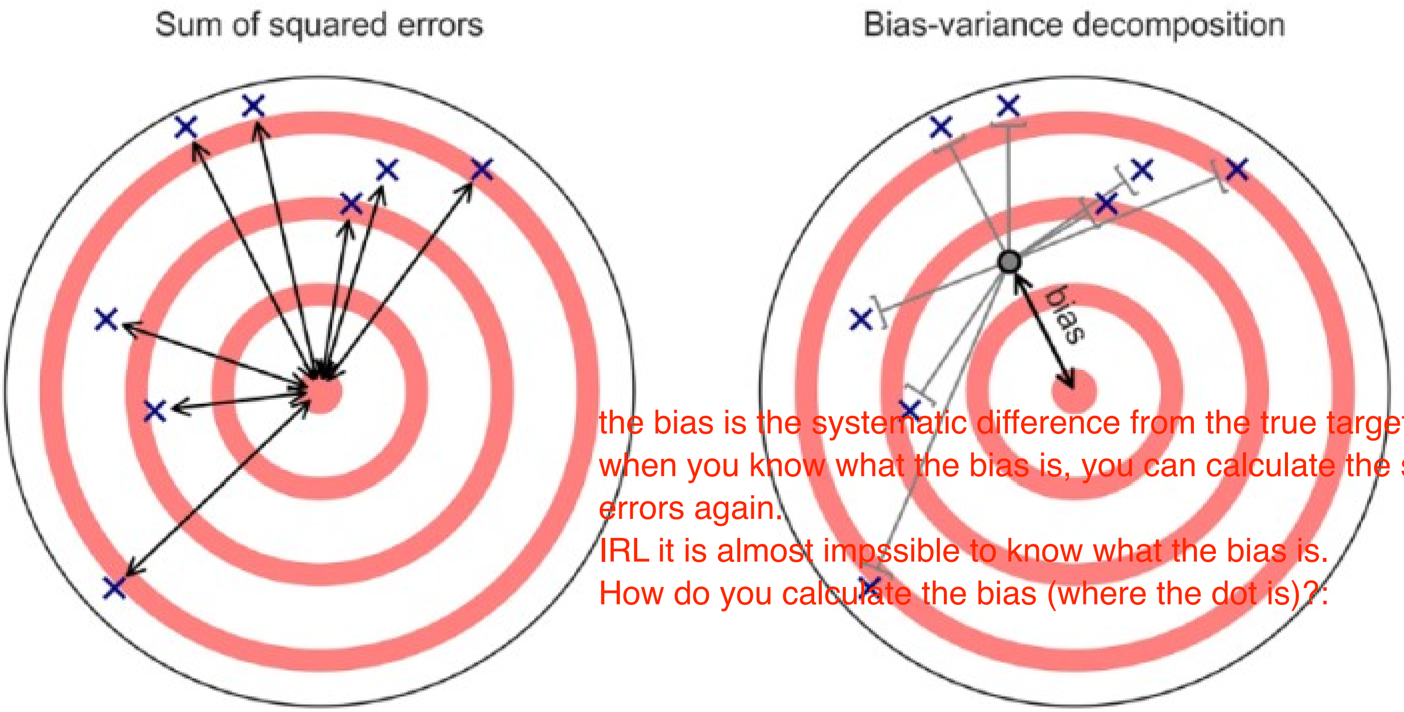


FIGURE 3.7. Accuracy versus precision. A schematic illustration of the differences between accuracy and precision of source localization. After left median-nerve stimulation, activations is expected in the right-hemisphere hand region of the primary somatosensory cortex. The foot area is shown at the top of the head. See text for further explanation.

(Hari and Puce, 2017)

(Yarkoni and Westfall, 2017)



the bias is the systematic difference from the true target.
when you know what the bias is, you can calculate the squared errors again.
IRL it is almost impssible to know what the bias is.
How do you calculate the bias (where the dot is)?:

Fig. 3. Schematic illustration of the bias-variance decomposition. (Left) Under the classical error model, prediction error is defined as the sum of squared differences between true scores and observed scores (black lines). (Right) The bias-variance decomposition partitions the total sum of squared errors into two separate components: a bias term that captures a model's systematic tendency to deviate from the true scores in a predictable way (black line) and a variance term that represents the deviations of the individual observations from the model's expected prediction (gray lines).

Bias variance decomposition

E=expection of the squared difference between the trrue value and the estimated value.

Expectation is the value it will take if you do it an infintie number of times.

The first term is our expection of the error. That can be decomposed into two: The square of the bias + the variance of the

$$E[(y_0 - \hat{f}(x_0))^2] = bias(\hat{f}(x_0))^2 + var(\hat{f}(x_0)) + \sigma^2$$

This formula is wrong! See the updated slides.

$$bias(\hat{f}(x_0)) = E[(y_0 \cancel{-} \hat{f}(x_0))^2]$$

actual formula:
bias(^f(x_0))=E[(^f(x_0)]-f(x_0)

is the *expected* squared error between the true value y_0 and its estimates based on fits $\hat{f}(x_0)$

If we introduce bias, we end up reducing variance.

We'll look more into this during tomorrow's exercise

Multilevel modelling as a *bias* introducer

“*For example, some readers may be surprised to learn that multilevel modeling approaches to analyzing clustered data—which have recently seen a dramatic increase in adoption in psychology—improve on ordinary least squares (OLS) approaches to estimating individual cluster effects by deliberately biasing (through “shrinking” or “pooling”) the cluster estimates toward the estimated population average*”

(Yarkoni and Westfall, 2017)

Introducing *bias*

“In a widely used form of penalized regression called lasso regression (Tibshirani, 1996, 2011), this leastsquares criterion is retained, but the overall cost function that the estimation seeks to minimize now includes an additional penalty term that is proportional to the sum of the absolute values of the coefficients.”

Text

(Yarkoni and Westfall, 2017)

Penalised regression

Why have small beta values?
because high beta values gotta
be right, and since we're not sure
that they are, we prefer them
to be a bit lower.

$$\text{RSS} = \sum (y_i - \hat{y}_i)^2 \,(\text{minimise to obtain least squares solution})$$

penalise the model for having too big beta hats.
taking the vertical values of beta hat and adding
them to the RSS, and that's what we're going to minimize.
We want to minimize the squares of errors, but still don't
want to have beta hats values too large.
In practice, we would just set the beta values to 0. Why?

$$\text{lasso regression}: \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j| \,(\text{minimise this sum})$$

lambda: A constant.

$$\text{ridge regression}: \text{RSS} + \lambda \sum_{j=1}^{p} (\beta_j^2) \,(\text{minimise this sum})$$

i : observations

p : predictor variables

λ : a constant

Penalised regression

If lambda goes to 0, the beta values increase.

$$\text{RSS} = \sum (y_i - \hat{y}_i)^2 (\text{minimise to obtain least squares solution})$$

$$\text{lasso regression}: \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j| (\text{minimise this sum})$$

$$\text{ridge regression}: \text{RSS} + \lambda \sum_{j=1}^{p} (\beta_j^2) (\text{minimise this sum})$$

i: observations
p: predictor variables
λ: a constant

Group discussion

In each case: what happens when?

1. λ increases?
2. λ decreases?
3. λ is 0?
4. λ goes towards infinity?

Penalised regression

$$\text{RSS} = \sum (y_i - \hat{y}_i)^2 (\text{minimise to obtain least squares solution })$$

We want to find the lambda that minimizes

$$\underset{\lambda}{\text{argmin}} = \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$\underset{\lambda}{\text{argmin}} = \text{RSS} + \lambda \sum_{j=1}^{p} (\beta_j^2)$$

i : observations

p : predictor variables

λ : a constant

How to choose λ?

```
##
## Call:
## lm(formula = hp ~ mpg + wt + drat + qsec, data = mtcars)
##
## Coefficients:
## (Intercept)          mpg           wt         drat         qsec
##     473.779       -2.877       26.037        4.819      -20.751
```

Text

What is λ equal to here?

```
sum.of.squares.total <- sum((y - mean(y))^2)
sum.of.squared.errors.lm <- sum(residuals(linear_model)^2)
print(r.squared.lm <- 1 - sum.of.squared.errors.lm/sum.of.squares.total)
```

```
## [1] 0.8072553
```

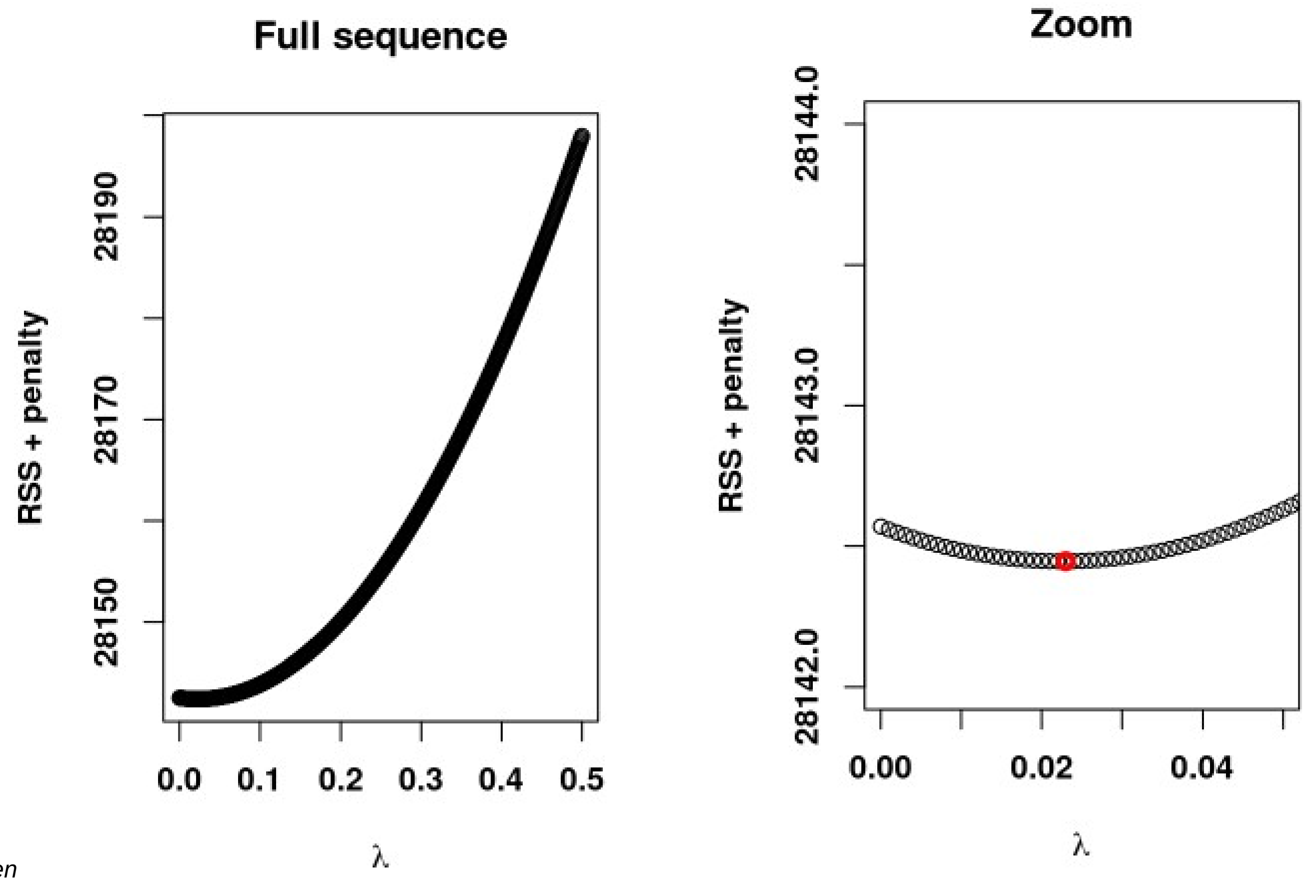
How to choose λ (lasso)?

Text

```
##
## Call:  glmnet(x = x, y = y, alpha = 1, lambda = c(0, 0.2, 2, 4, 20,
100))
##
##    Df   %Dev Lambda        lambda          RSS      penalty          sum
## 1   0 0.0000  100.0         100.0 145726.9      0.0          145726.9
## 2   2 0.6567   20.0      20.00000 50025.64218   14.05496 50039.69714
## 3   3 0.8004    4.0       4.00000 29082.92003   41.34363 29124.26366
## 4   3 0.8051    2.0       2.00000 28408.50683   44.99057 28453.49740
## 5   4 0.8072    0.2       0.20000 28097.60764   52.47741 28150.08505
## 6   4 0.8073    0.0       0.00000 28088.09951   54.46997 28142.56948
```

How to choose λ?

Text



What does λ do $_{\text{(ridge)}}$?

Text

$$\hat{\beta}_{ridge} = \left(X^T X + \lambda I \right)^{-1} X^T y$$

I: an identity matrix with p predictor variables

λ: a constant (small)

What is $X^T X$?

```r
head(X)
```

```
##                   (Intercept)  mpg    wt drat  qsec
## Mazda RX4                   1 21.0 2.620 3.90 16.46
## Mazda RX4 Wag               1 21.0 2.875 3.90 17.02
## Datsun 710                  1 22.8 2.320 3.85 18.61
## Hornet 4 Drive              1 21.4 3.215 3.08 19.44
## Hornet Sportabout           1 18.7 3.440 3.15 17.02
## Valiant                     1 18.1 3.460 2.76 20.22
```

```r
print(cov.X)
```

```
##            mpg        wt      drat      qsec
## mpg  14042.310 1909.7528 2380.2770 11614.745
## wt    1909.753  360.9011  358.7190  1828.095
## drat  2380.277  358.7190  422.7907  2056.914
## qsec 11614.745 1828.0946 2056.9140 10293.480
```

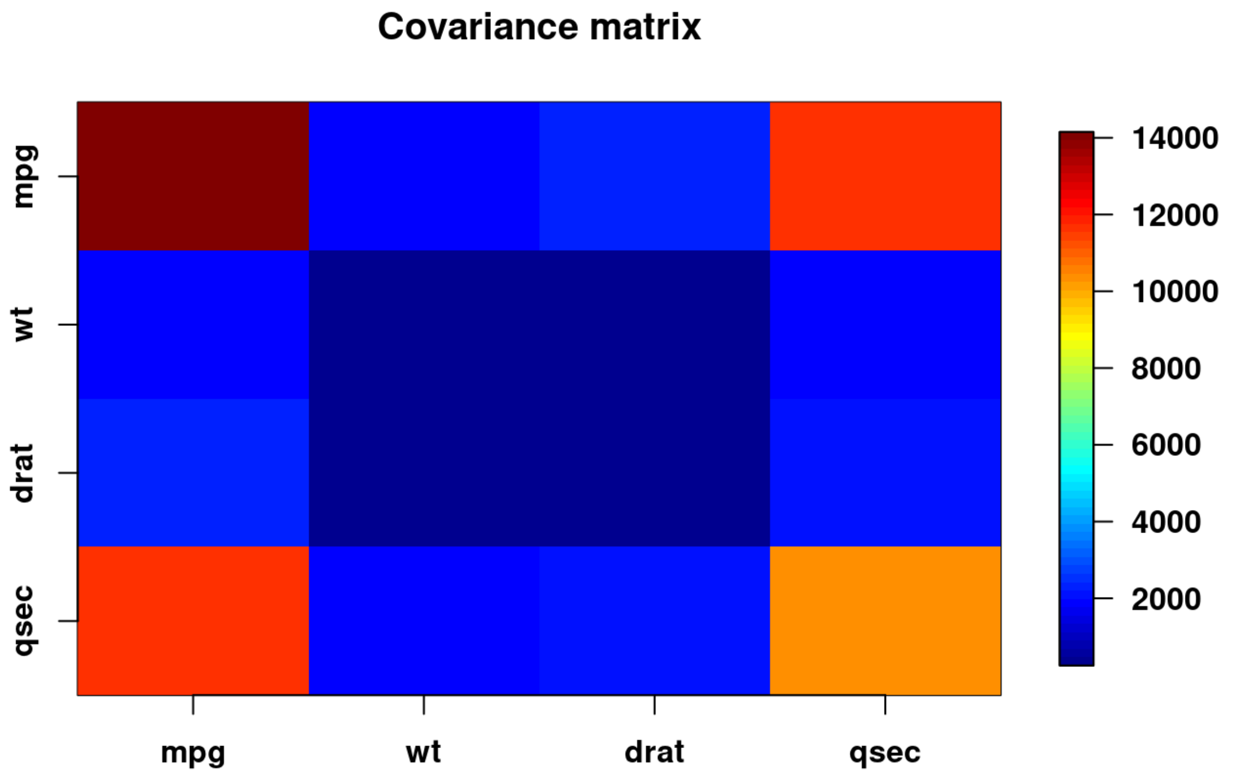
$$X_{COV} = X^T X$$

When multiplying these two matrices
we get a new matrice that's squared.
The diagonal is the variance

$$X_{COV} = X^T X$$

diagonal: Variance that each variable explains in isolation.
The other fields are the fileds in which the variables are co-explaining.

The fact that the off-diagonal > 0, indicates that there is **collinearity**



Collinearity can be bad

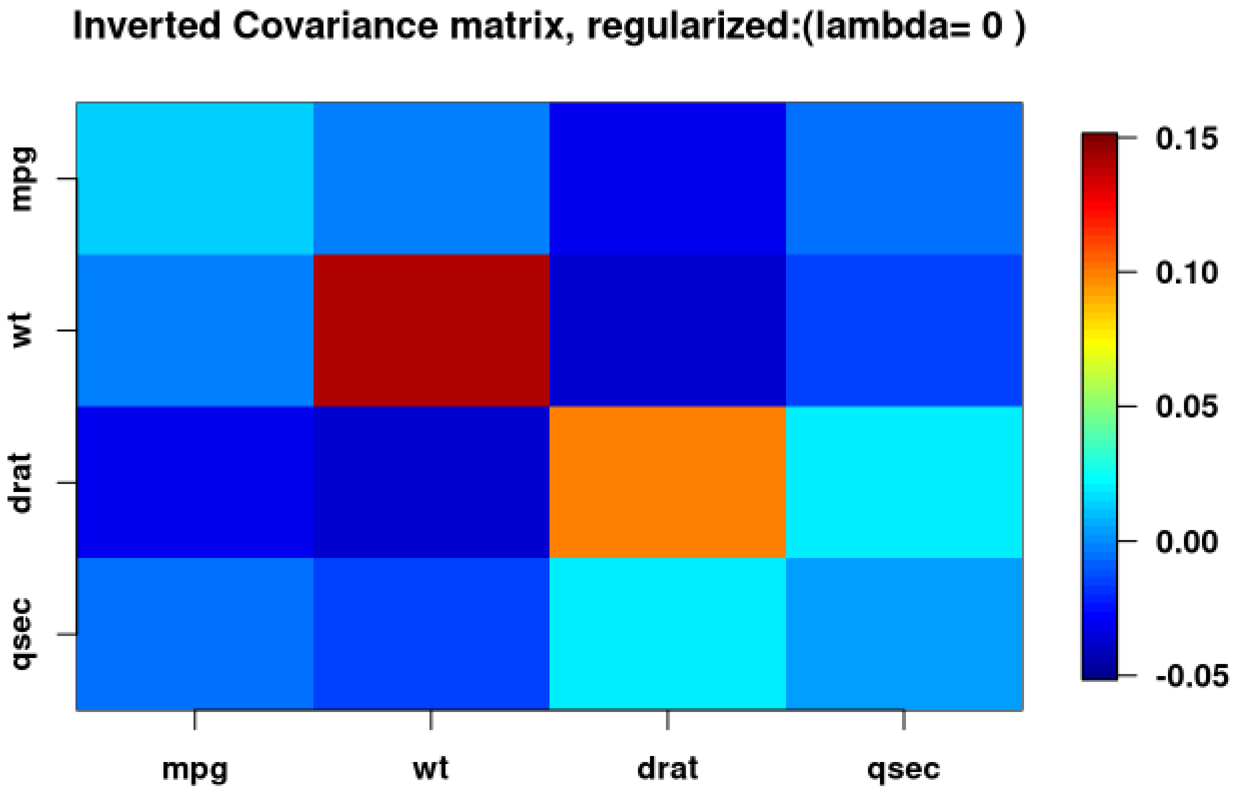
```
##
## Call:
## lm(formula = hp ~ mpg + wt + drat + qsec, data = mtcars)
##
## Coefficients:
## (Intercept)          mpg           wt         drat         qsec
##     473.779       -2.877       26.037        4.819      -20.751
```

Text

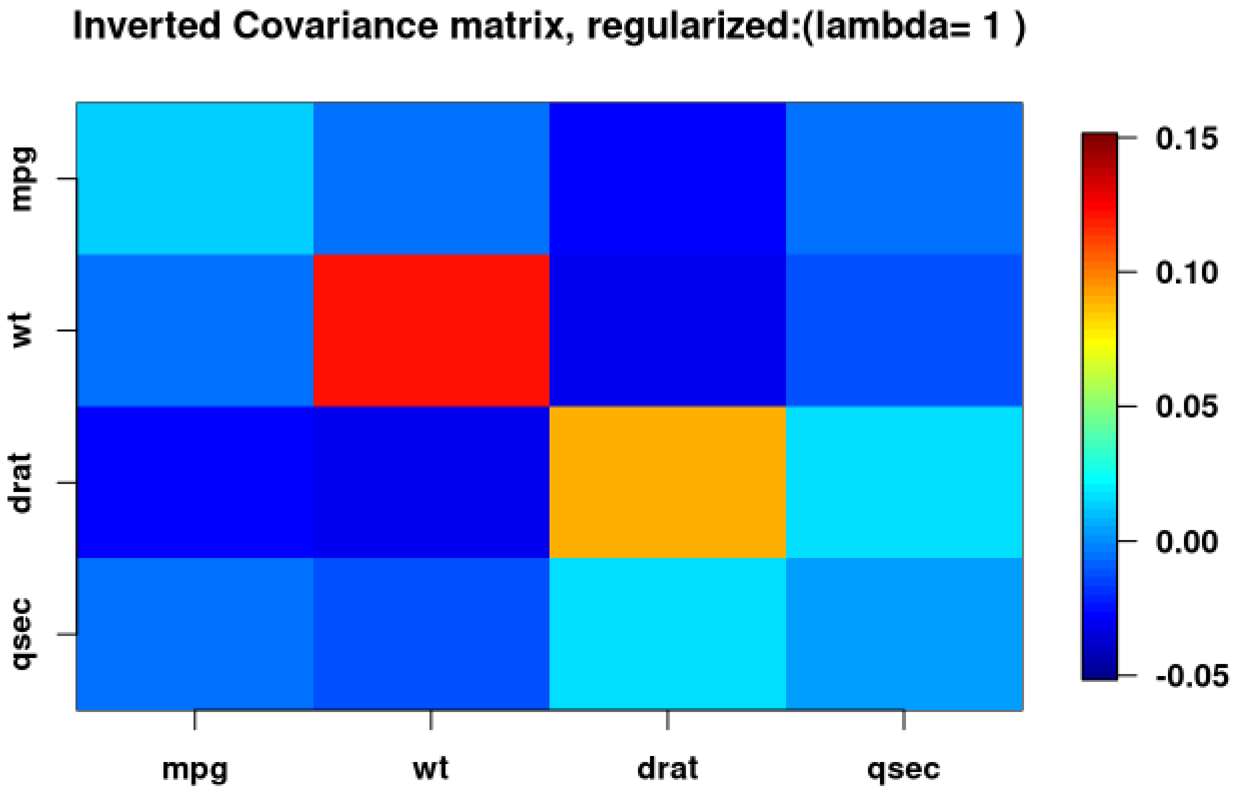
Assuming no collinearity, what is the interpretation of the coefficients?

With collinearity, is that interpretation possible?

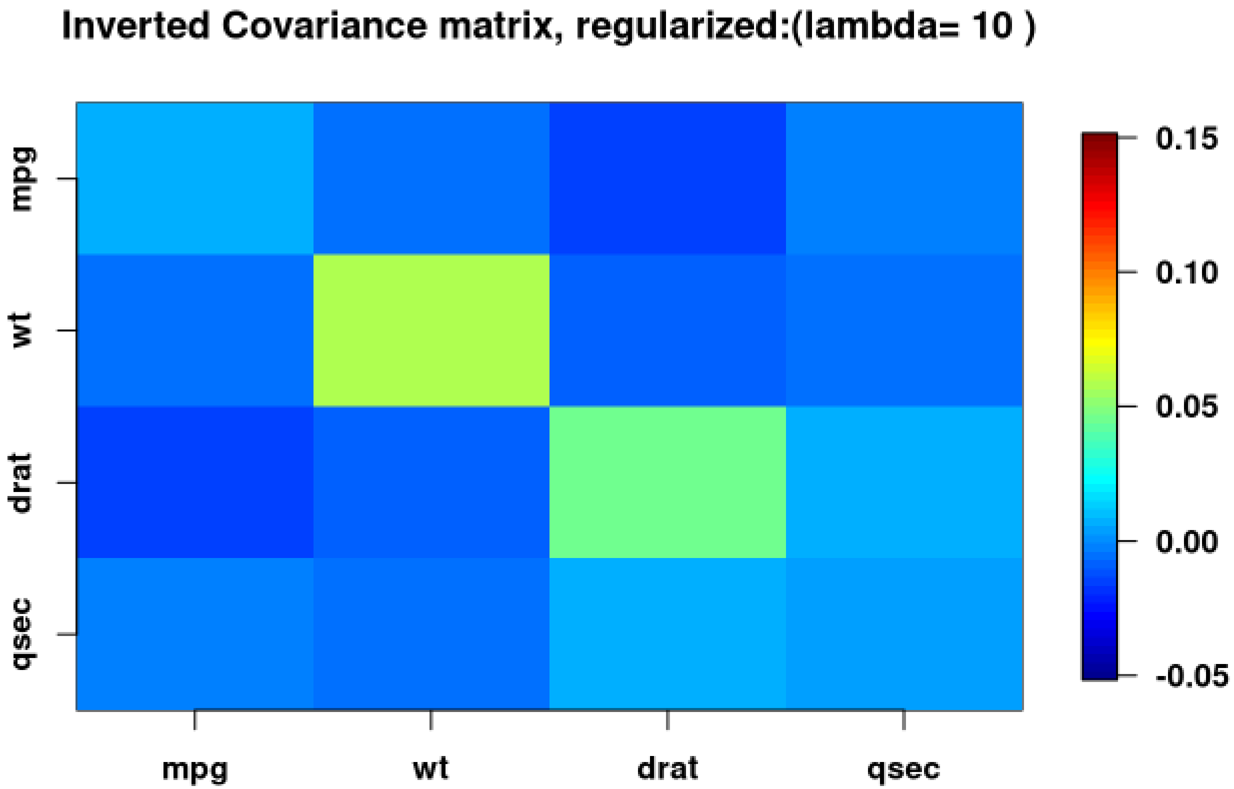
$$\hat{\beta}_{ridge} = \boxed{(X^T X + \lambda I)^{-1}} X^T y$$



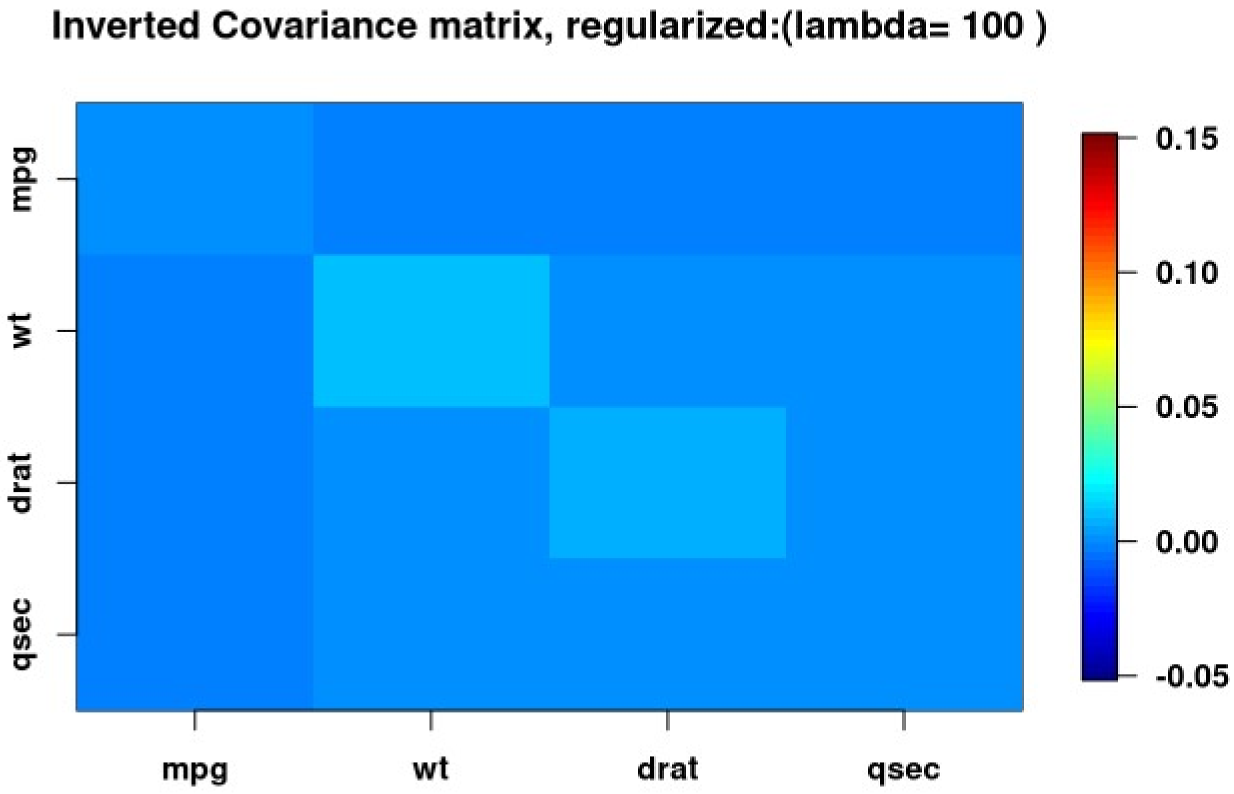
$$\hat{\beta}_{ridge} = \boxed{\left(X^T X + \lambda I\right)^{-1}} X^T y$$



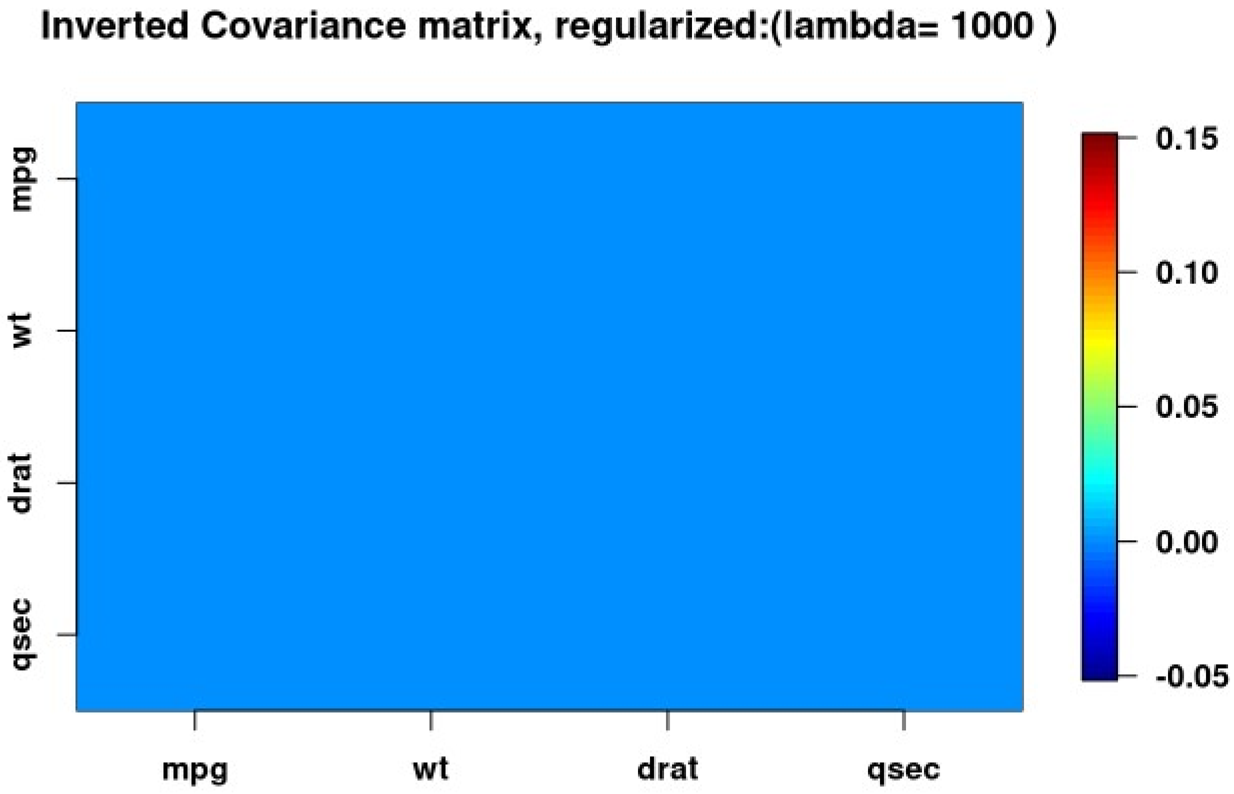
$$\hat{\beta}_{ridge} = \boxed{(X^T X + \lambda I)^{-1}} X^T y$$



$$\hat{\beta}_{ridge} = \boxed{\left(X^T X + \lambda I\right)^{-1}} X^T y$$



$$\hat{\beta}_{ridge} = \boxed{\left(X^T X + \lambda I \right)^{-1}} X^T y$$



So why is it called regularisation?

Two notes about the inverted matrix:

When increasing bias, we're moving away from the true parameters, but we're reducing colinirarity.

with increase of λ

1. Diagonal shrinks (bias is added)

2. Off-diagonal shrinks (collinearity is reduced, which improves the stability of the model)

In a stable model:

Feeding new data or adding new predictor variables will not change the parameter estimates a lot

We have succeeded in finding a λ making our model more stable (improved **in-sample** validity), but we haven’t found a λ that optimises predictive power – (**out-of-sample**)

Out-of-sample as validity check


```r
mtcars.1 <- mtcars[1:10, ]
```

Out-of-sample as validity check

```
Call:
lm(formula = hp ~ mpg + wt + drat + qsec, data = mtcars.1)

Coefficients:
(Intercept)          mpg           wt         drat         qsec
    414.541      -13.638       12.753       11.263       -5.042
```

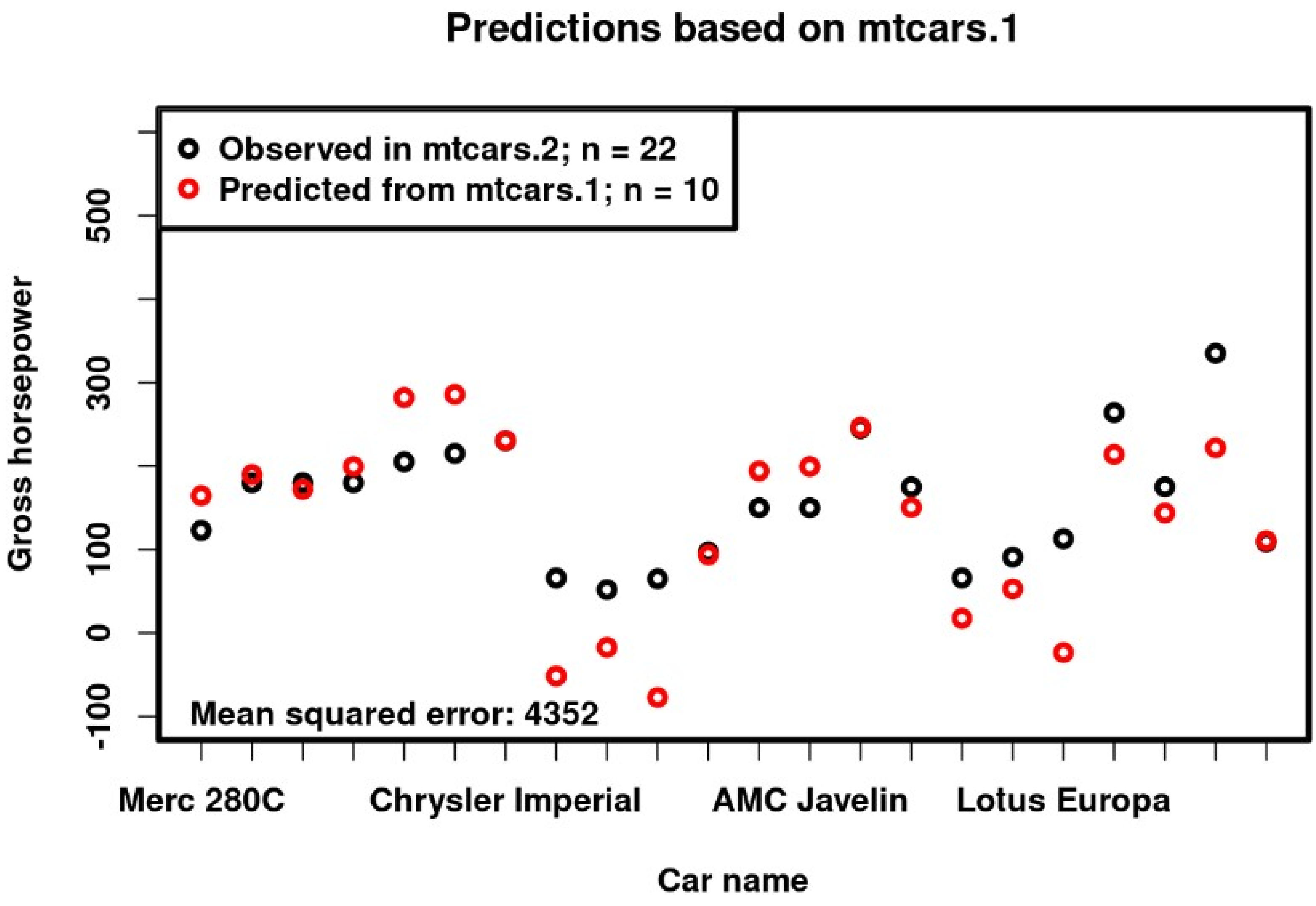
```
Call:
lm(formula = hp ~ mpg + wt + drat + qsec, data = mtcars)

Coefficients:
(Intercept)          mpg           wt         drat         qsec
    473.779       -2.877       26.037        4.819      -20.751
```

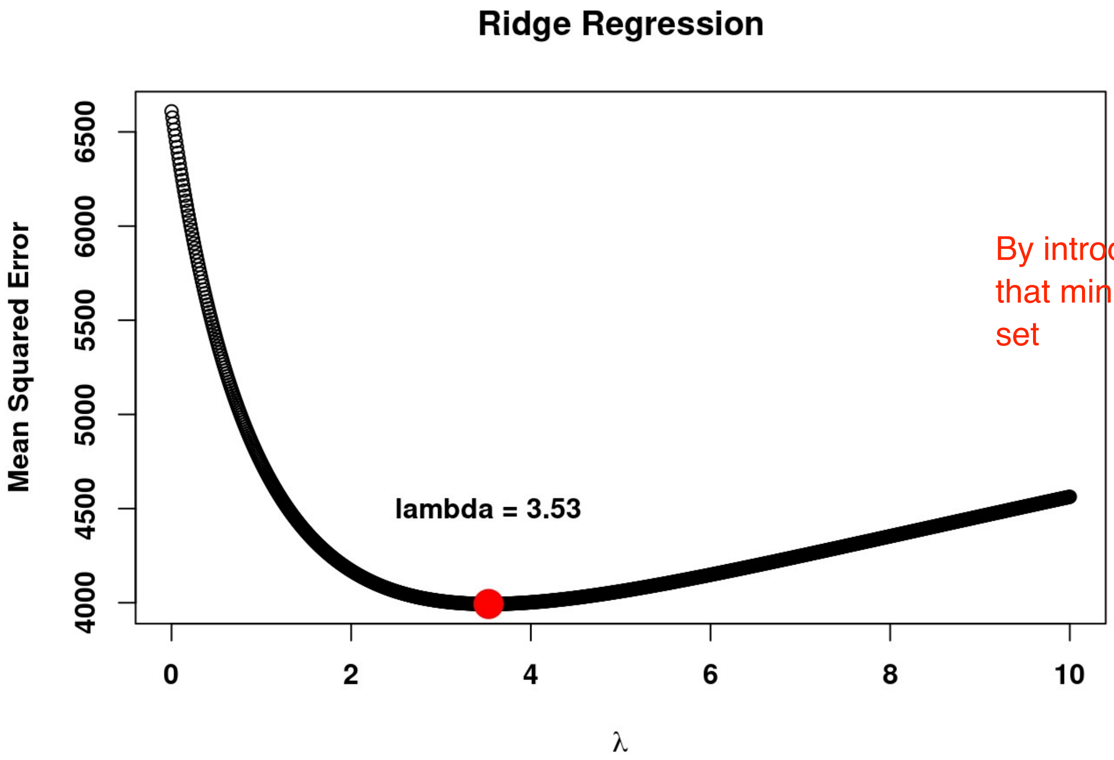
Suddenly, someone shows up with

Let's check our model

```
mtcars.2 <- mtcars[11:32, ]
```


Predictions based on mtcars.1
Observed in mtcars.2; n = 22
Predicted from mtcars.1; n = 10
Gross horsepower
-100
0
100
300
500
Mean squared error: 4352
Merc 280C
Chrysler Imperial
AMC Javelin
Lotus Europa
Car name

Finding optimal lambda



$$MSE = mean\left(\left(y - \hat{y}\right)^2\right)$$

By introducing bias with lambda = 3.54, we find that this is the one that minizmized the MSE in the first DF to predict the test (next) data set

Which dataset is the MSE calculated on?

```
Call:
lm(formula = hp ~ mpg + wt + drat + qsec + 0, data = mtcars.1)

Coefficients:
   mpg       wt     drat     qsec
-8.379   76.588   45.705   -5.850
```

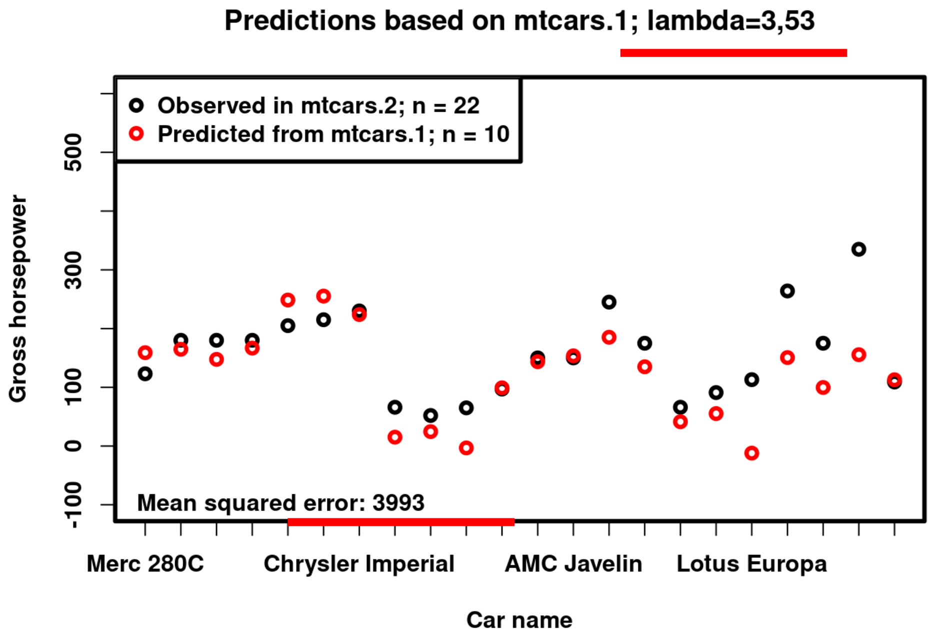
```
print(beta.hat.ridge <- ridge.regression(X, y, mtcars.1, min.lambda))
```

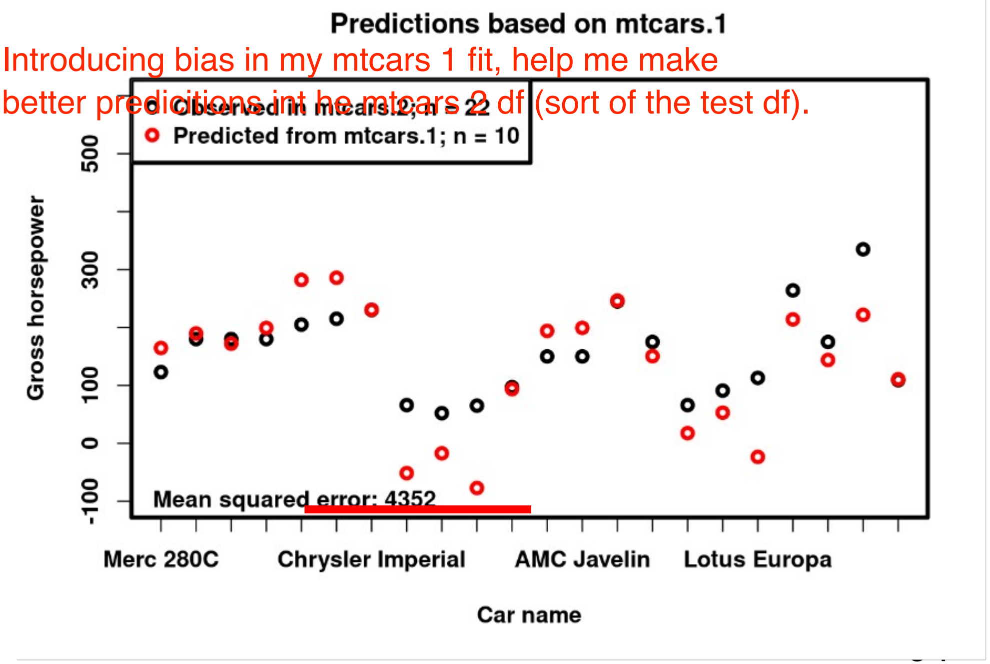
```
##              mpg     wt    drat    qsec
## [1,] -7.421887 33.637 22.0378 4.70691
```

What has happened to the coefficients?

Prediction on mtcars.2

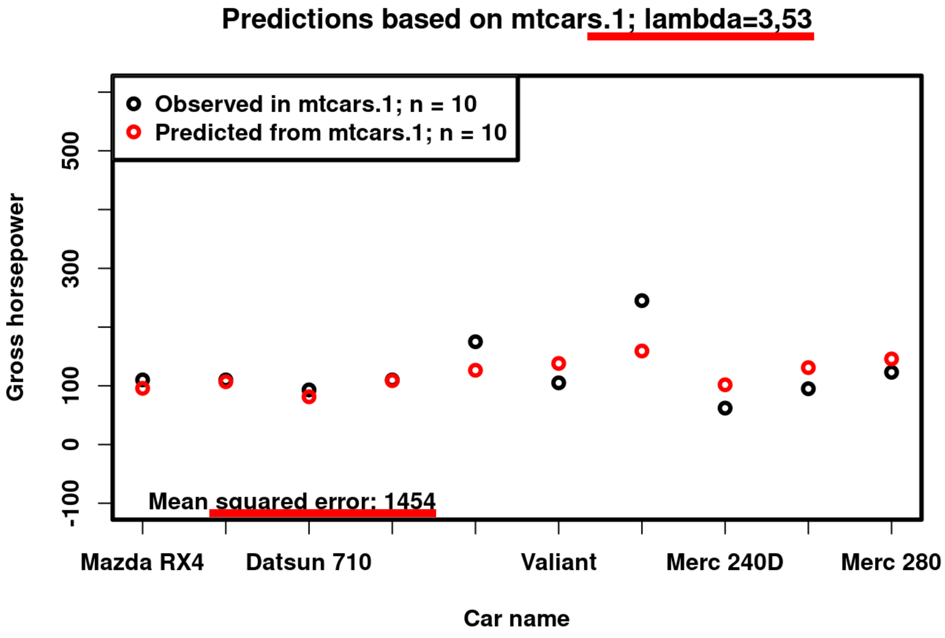
$$\lambda = 0$$



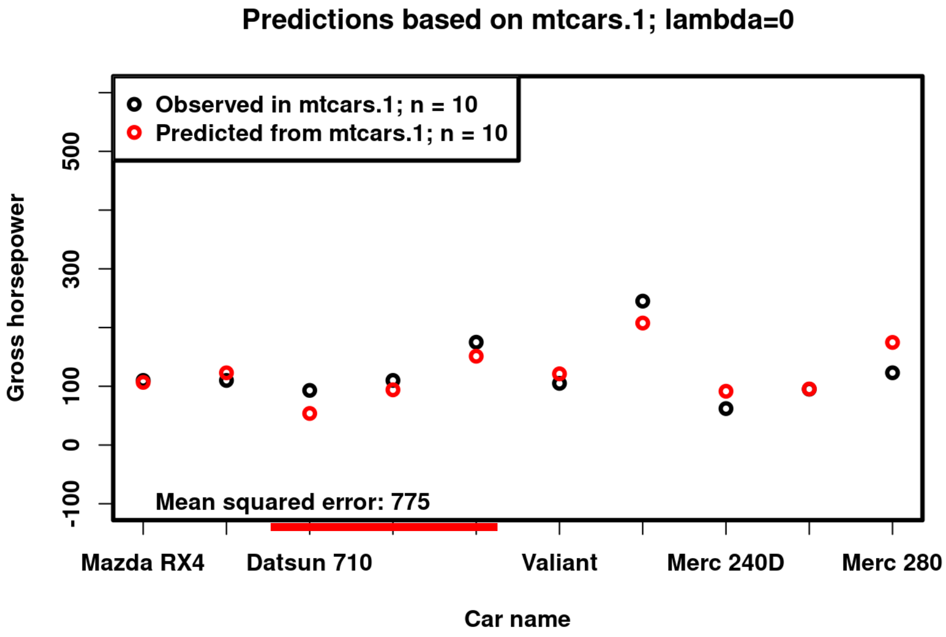


Introducing bias in my mtcars 1 fit, help me make better predicitions int he mtcars 2 df (sort of the test df).

“Prediction” on mtcars.1



$$\lambda = 0$$



Nomenclature

- mtcars.1 -> training set
- mtcars.2 -> test set
  - NB! Normally, we prefer that out training set is bigger than our test set

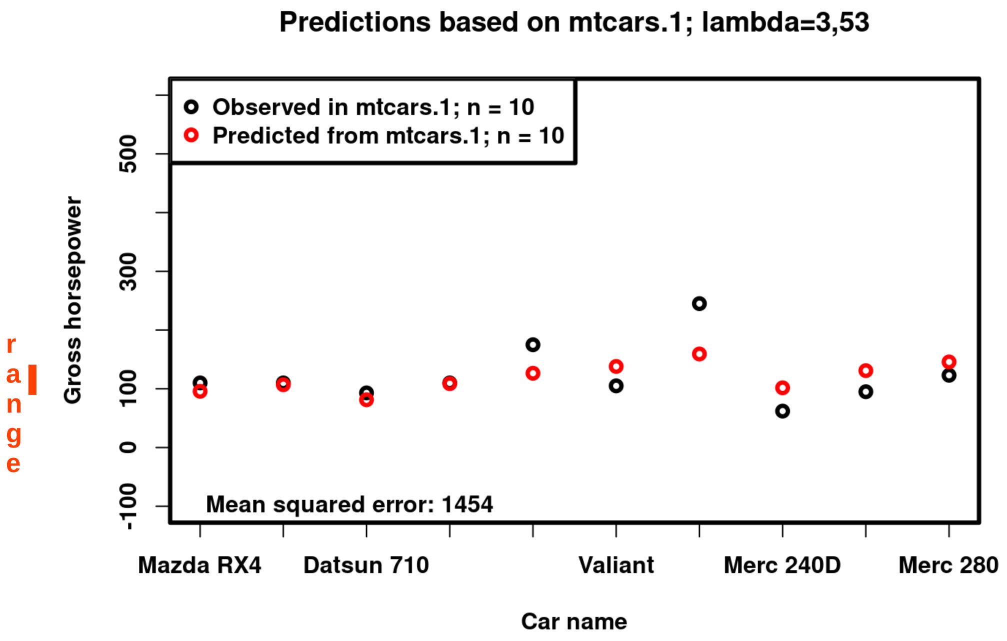
Text

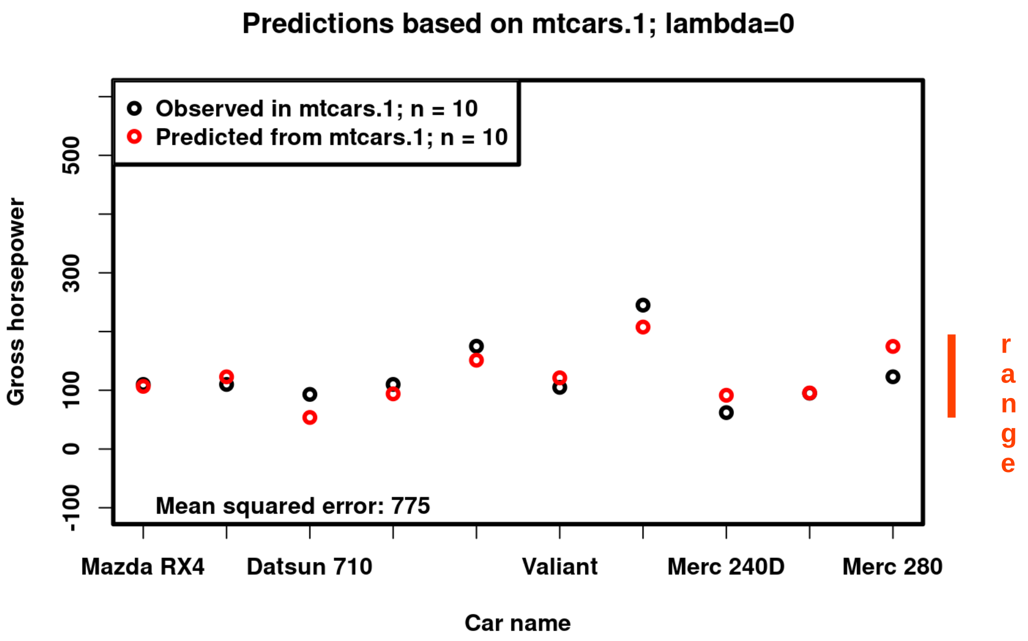
- By introducing *bias* in our training set, we at the same time reduce the *variance* of our training set, increasing the reliability of our predictions on a test set

"Testing" on training set

greater bias
lesser variance

smallest bias
greater variance (of $\hat{y}$)

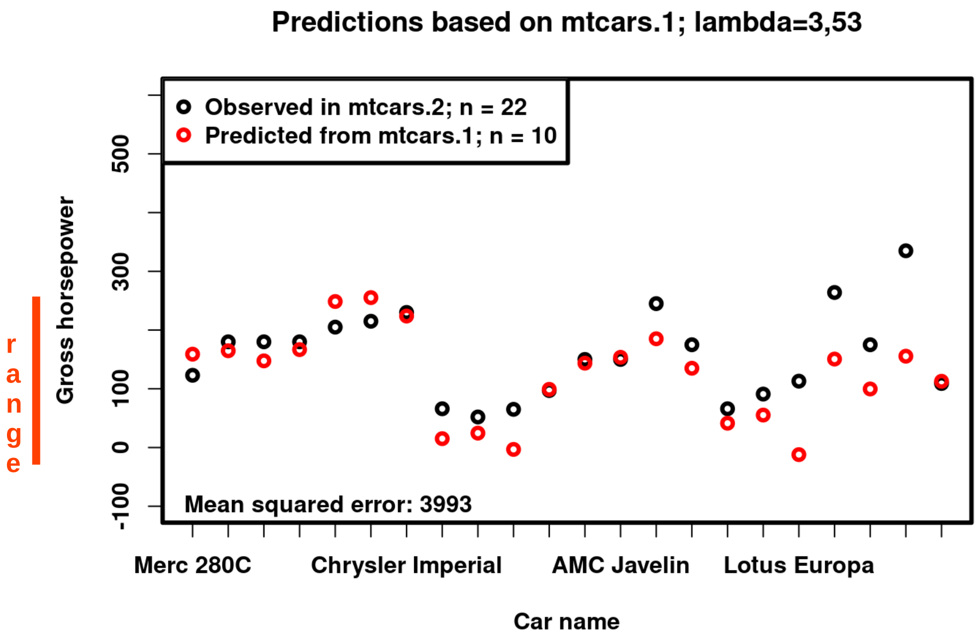


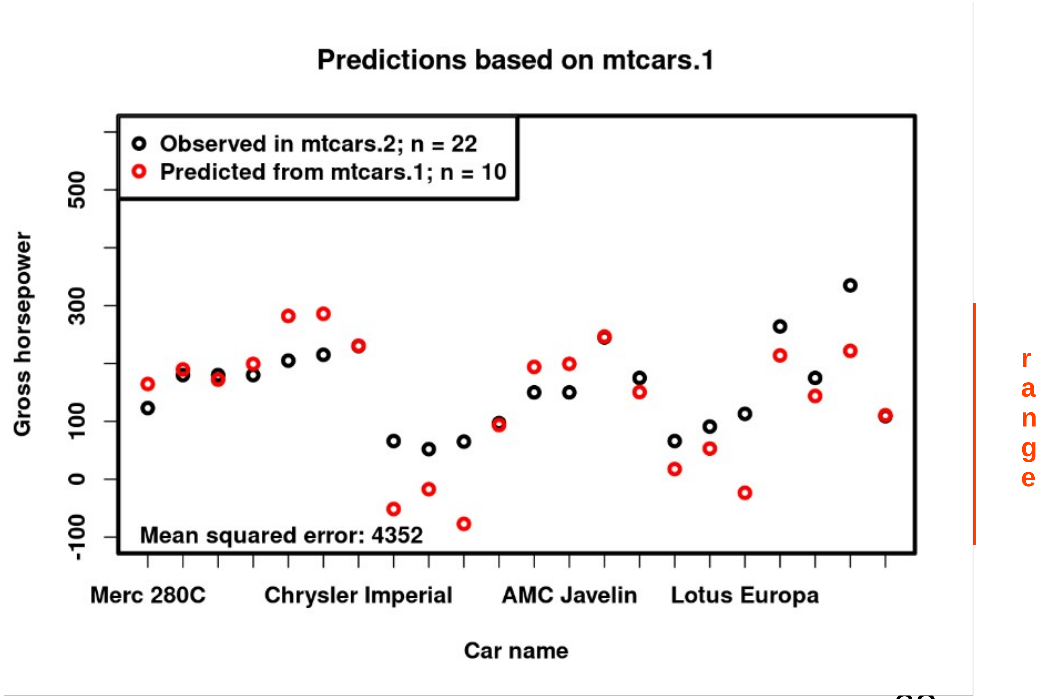


Optimal λ

lesser bias
lesser variance

more bias
greater variance (of $\hat{y}$)





Did you learn?

Explanation and prediction

1) Understanding that fitting (explaining) often leads to overfitting

2) Learning methods to prevent overfitting by introducing *bias*

3) Understanding that the error can be decomposed into *bias* and *variance*

Next time

- The Perceptron
- Adaline
- Linear regression

References

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