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!)

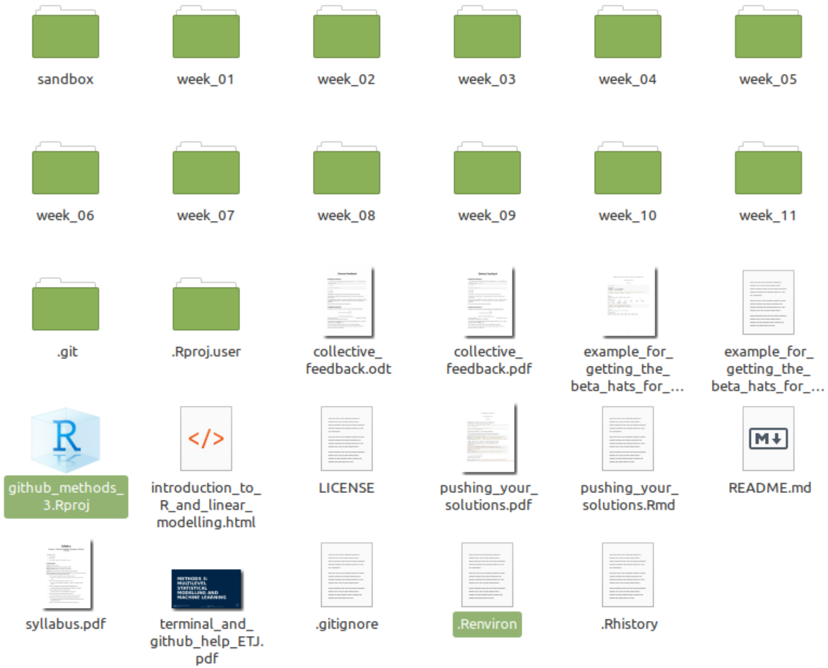
Practical exercise tomorrow

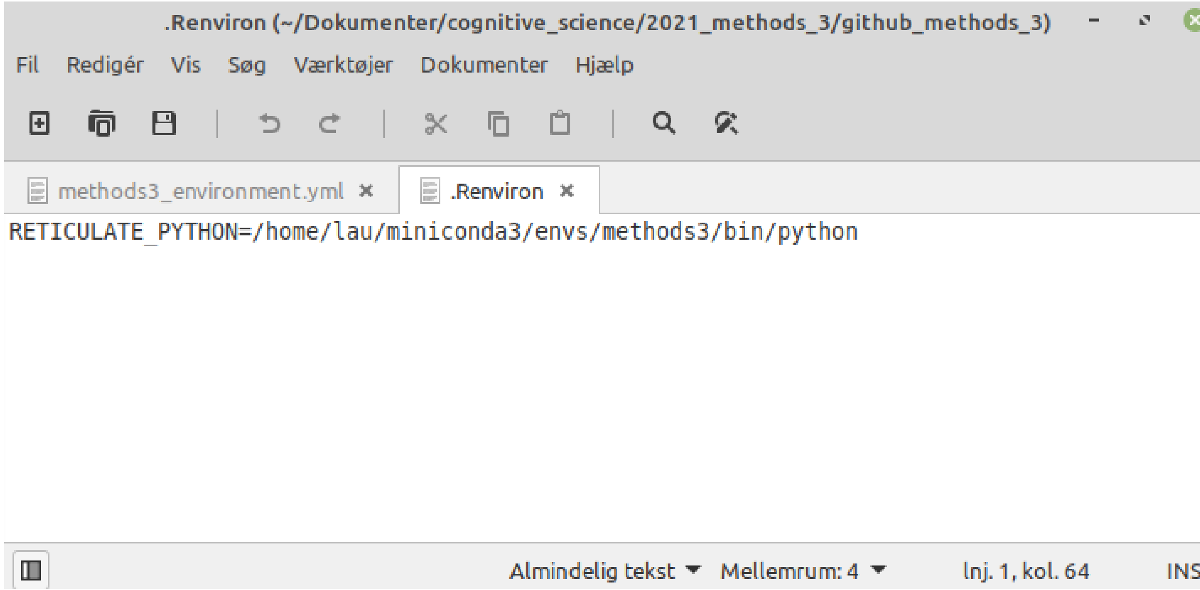
To make sure that *Python* runs within *R Markdown*, make sure you have the *reticulate* package installed `install.packages('reticulate')`
Also create a text file that is called *.Renviron* (remember the dot) placed in the folder where your *RProj* file is. It should have a single line: `RETICULATE_PYTHON=PATH`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

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

Likelihood ratio

- 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
  - Maximum likelihood fitting may be biased for complex models
  - Requires large sample sizes
  - Be careful if collinearity is high

Information criteria

- 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

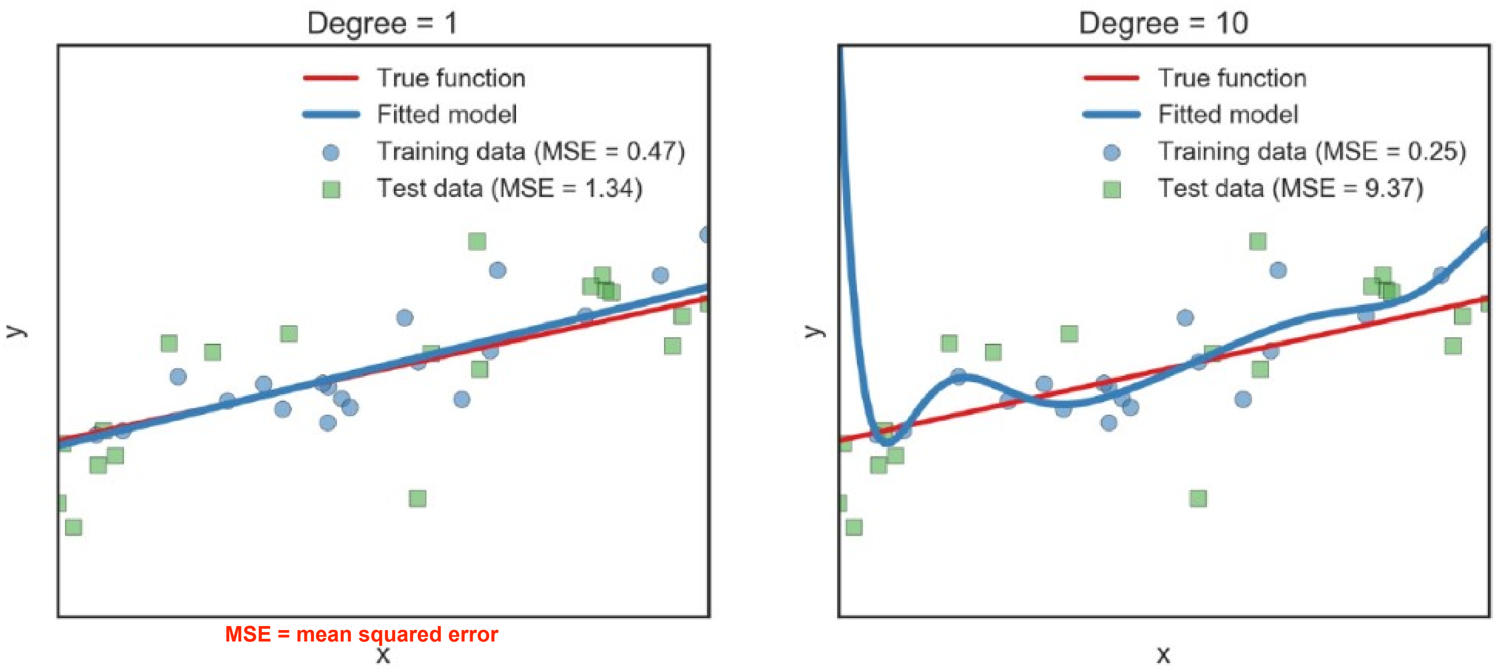
2) Learning methods to prevent overfitting by introducing *bias*

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



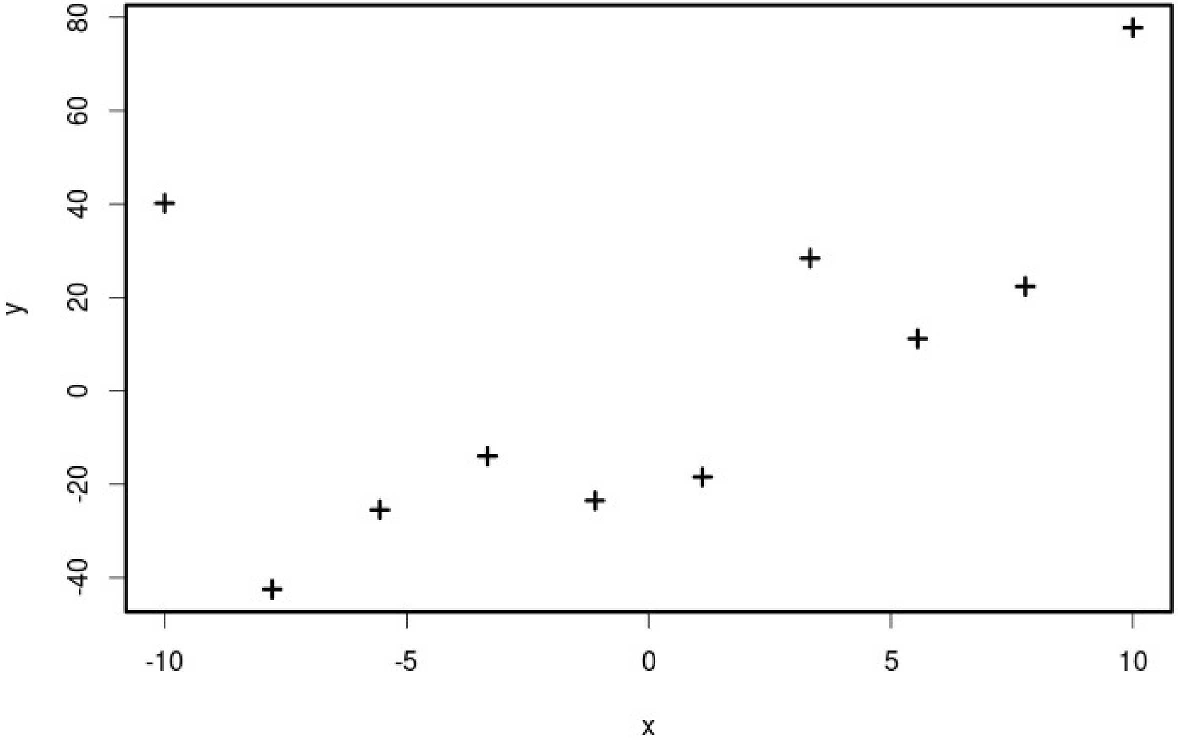
MSE = mean squared error

hvilket er the mean af RSS (residual sum og squares), så meanen af summen af residuals

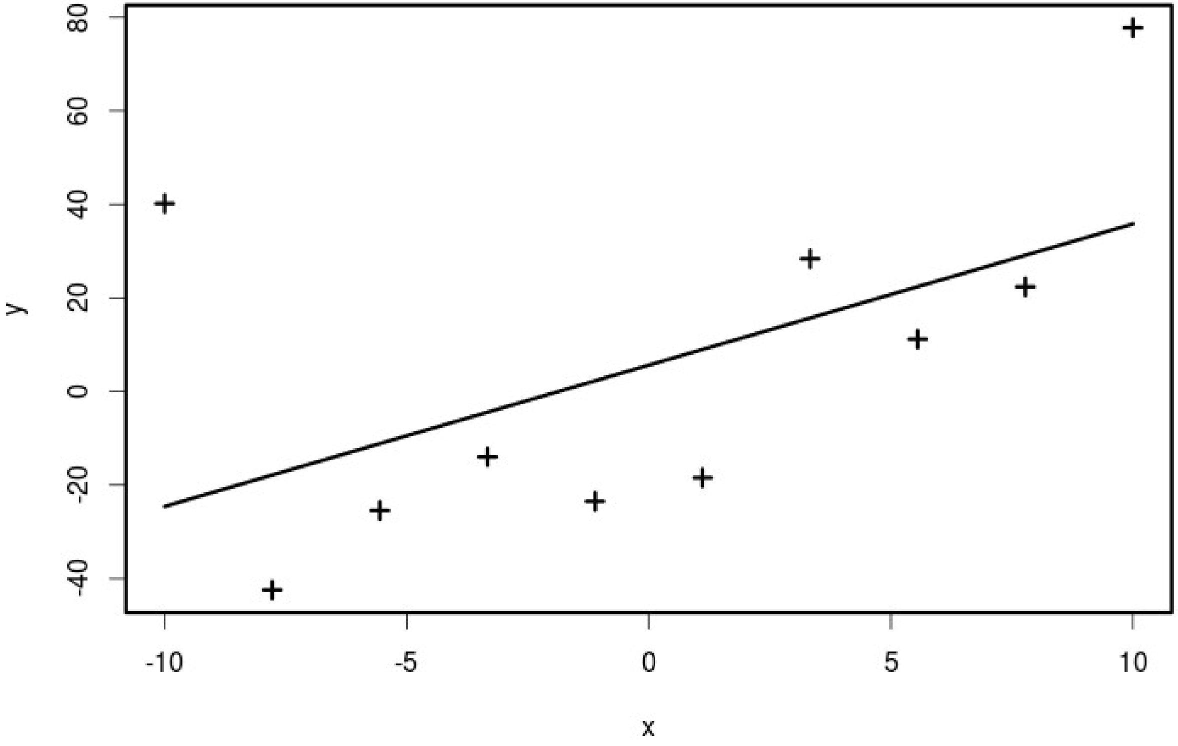
Fig. 1. Training and test error produced by fitting either a linear regression (left) or a 10th-order polynomial regression (right) when the true relationship in the population (red line) is linear. In both cases, the test data (green) deviate more from the model's predictions (blue line) than the training 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)

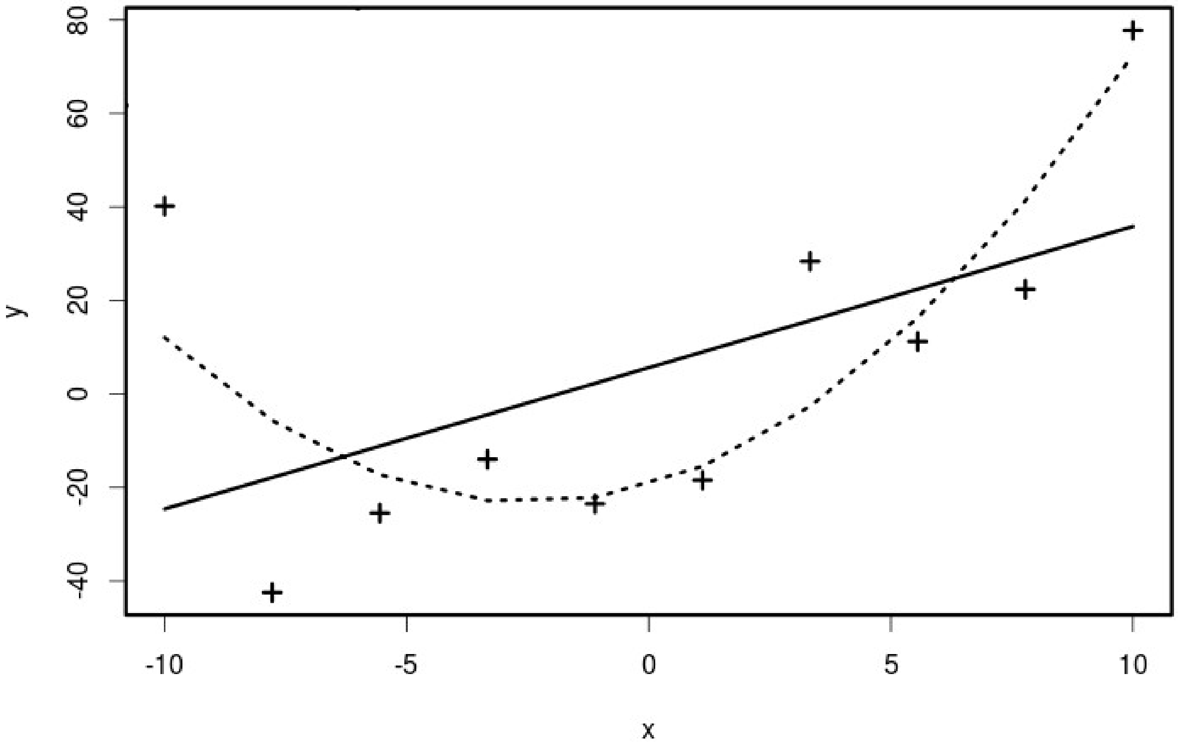
A sample of 10
linear or quadratic?



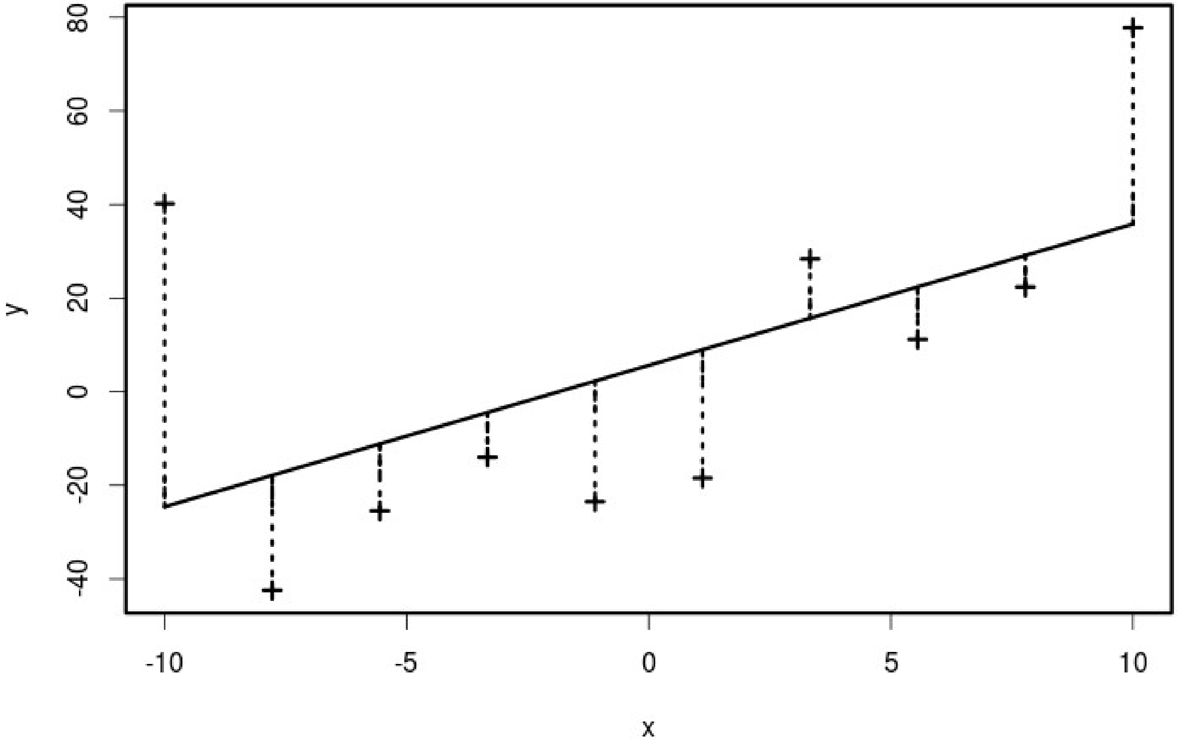
A sample of 10
linear or quadratic?



A sample of 10
linear or quadratic?

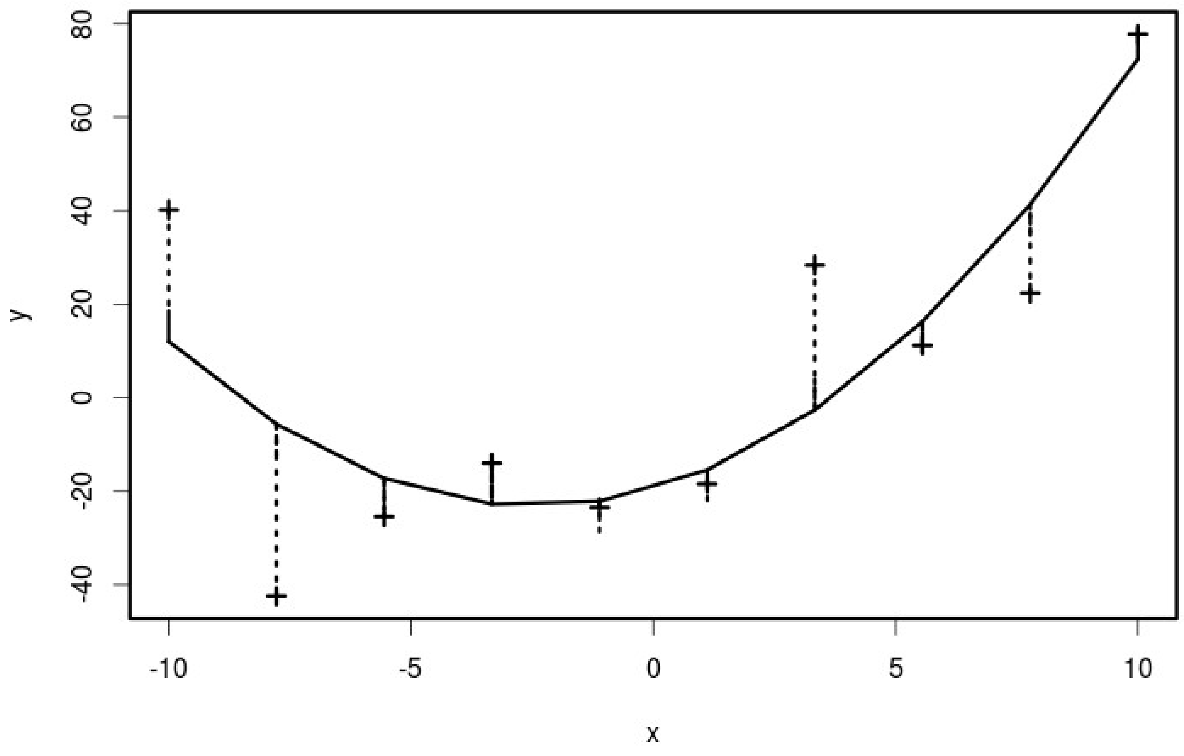


Residuals (linear)



Residuals (quadratic)

når den er quadratic har den en extra predictor (ectra predictor variable)



Quadratic:

$ax^2 + bx + c$

Linear:

$bx + c$

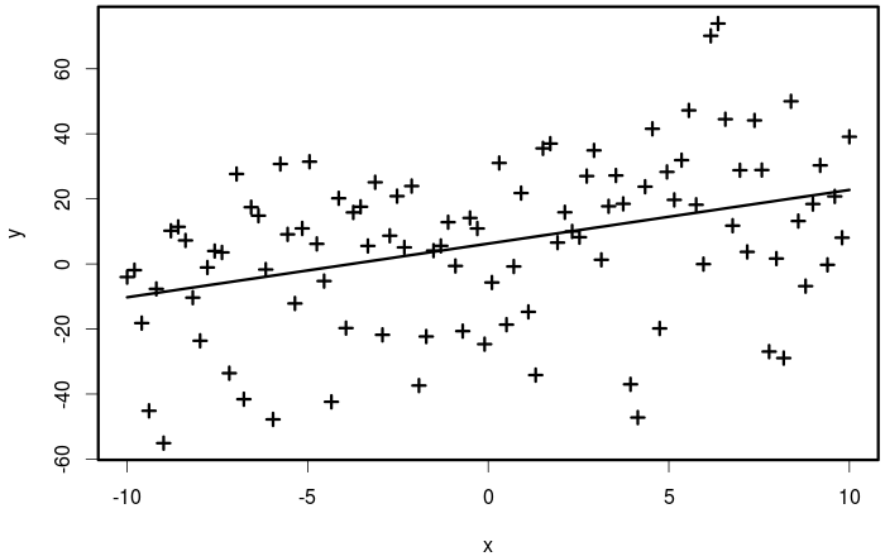
Estimates

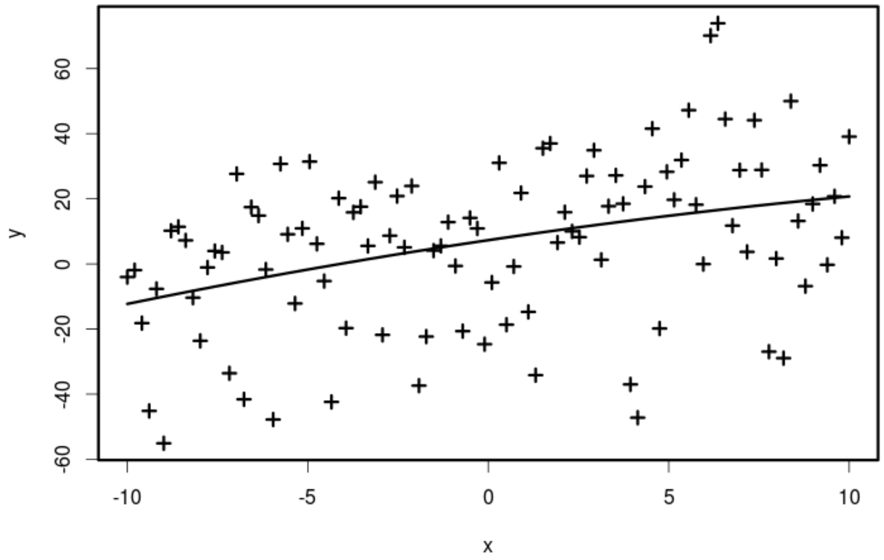
quadratic er bedre

a = 0,6184; b = 3,0201

b = 3,020

Now a sample of 100





b = 1,650

a = -0,03074 ≈ 0; b = 1,650

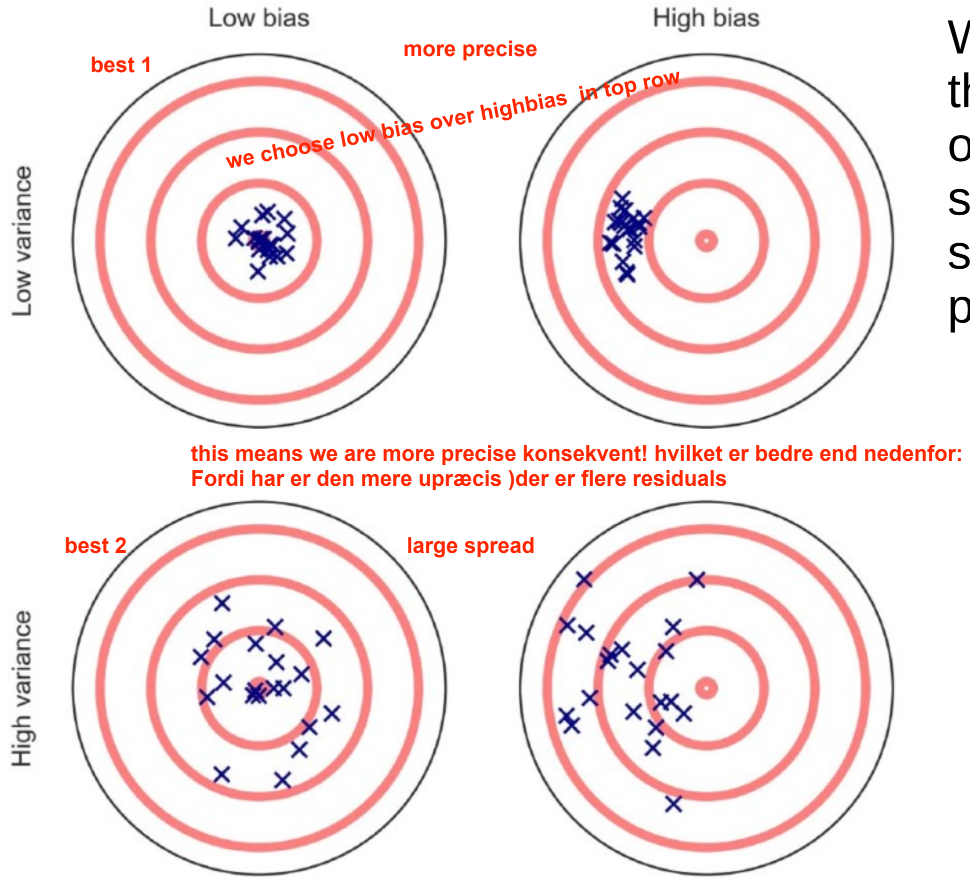


Fig. 2. An estimator's predictions can deviate from the desired outcome (or true scores) in two ways. First, the predictions may display a systematic tendency (or *bias*) to deviate from the central tendency of the true scores (compare right panels with left panels). Second, the predictions may show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

Text

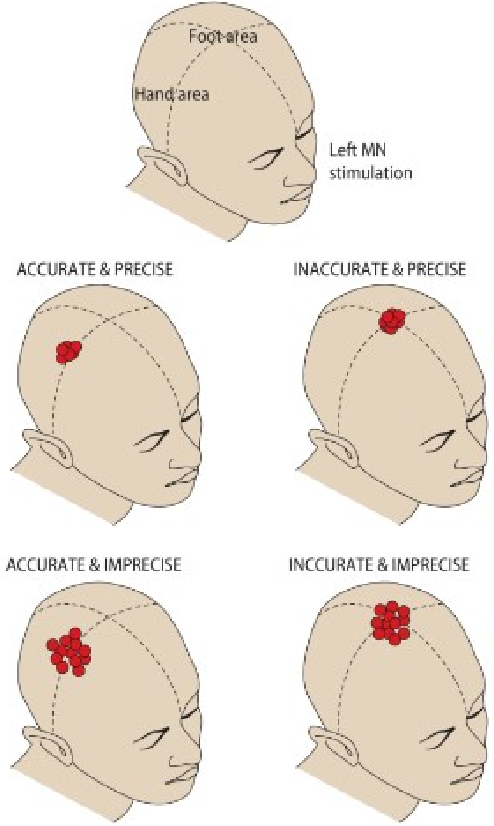
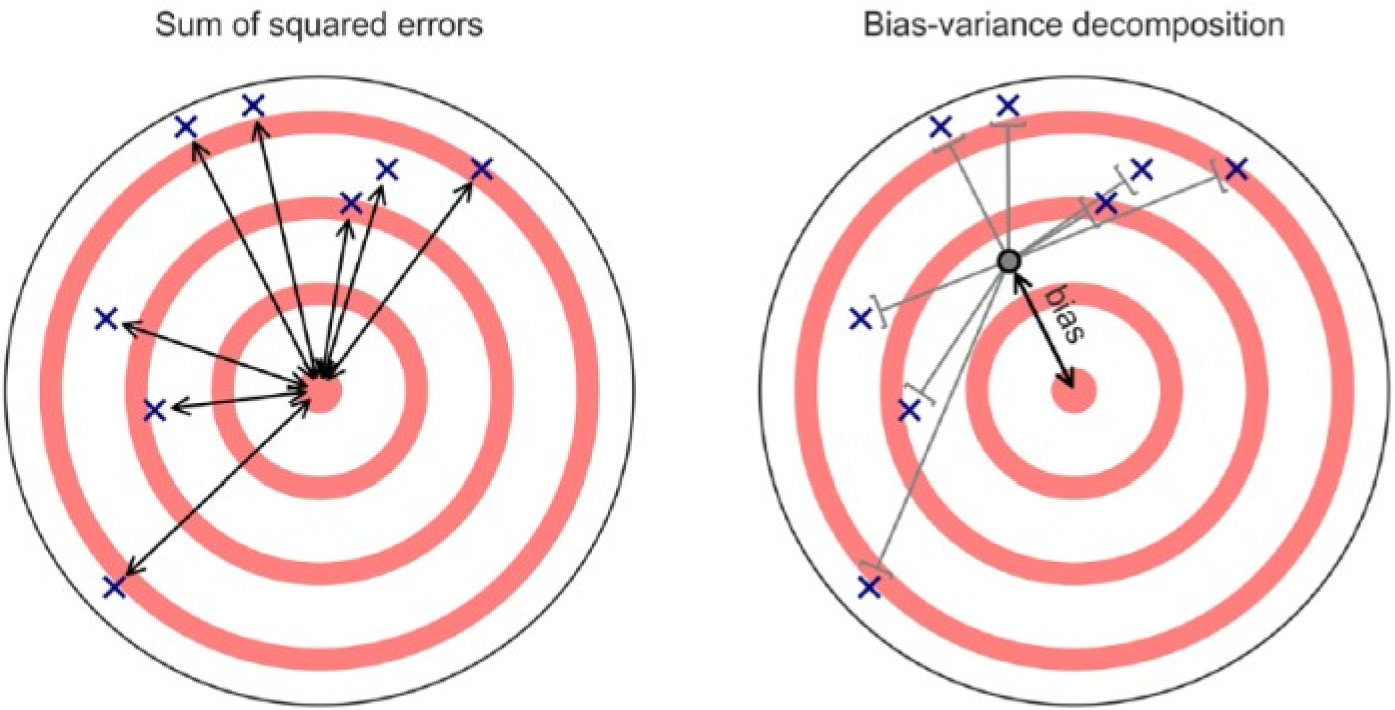


FIGURE 3.7. Accuracy versus precision. A schematic illustration of the differences between accuracy and precision of source localization. After left median-nerve stimulation, activations is expected in the right-hemisphere hand region of the primary somatosensory cortex. The foot area is shown at the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

(Hari and Puce, 2017)

(Yarkoni and Westfall, 2017)



its impossible to know the bias, because it comes form the true function (true estimates) which we never really know..

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

expectation of the error between true value and predicted value

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

what is expectation :
1) we have a popupation with true parameters (which we really dont know)
2) we dont know the bias, but we can estimate it
3) sample size 100
4) mx0 is one specific obsercation

bias (fhat)x0)) = E[fhat(x0)] - f (x0) —> the difference between the fitted values and the how much we
are off from the true function f(x0)

The only ting we know here is the true function, and with the true function we can calculate the bias (but in reality we never know the true function, but we have estimated paramters of the true function)..

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

this slide is not totally correct, lau will put new slides up for correction

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

Bias = difference between expected values of fits and the true value (parameters)

this is still stue tho

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.”

(Yarkoni and Westfall, 2017)

Penalised regression

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

vertical lines means absolute value

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

betas will be sat to 0 = will be shurnken

how can we ever set the betas to 0?
… setting a parameter (predictor) to 0 is just saying that it does not expalin anything

in a model with multiple predictors, when the vairables are correlated (e.g wt and mpg), then we can set some of them to 0

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

i : observations

p : predictor variables

λ : a constant

Penalised regression

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

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

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

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

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

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

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

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
```

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
```

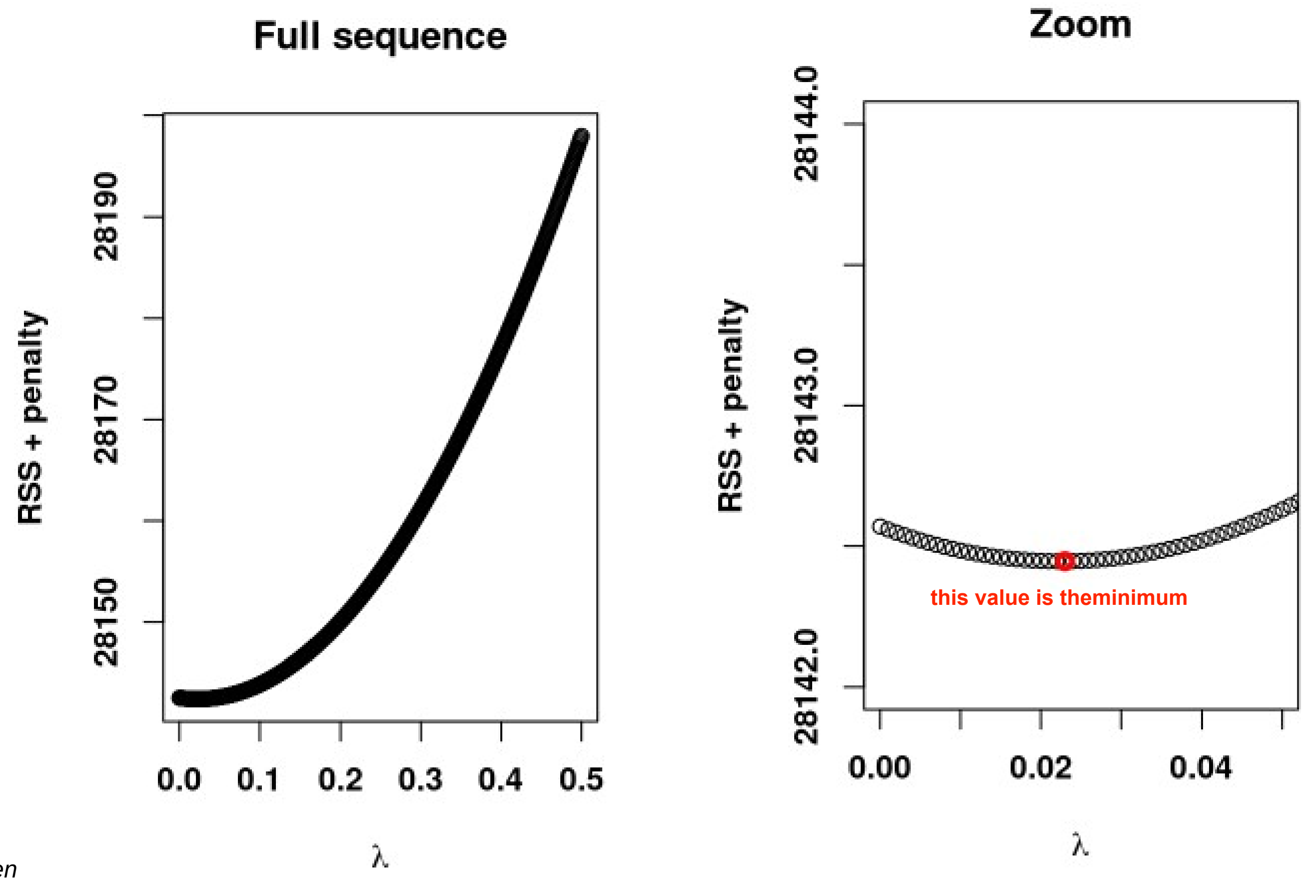
How to choose λ *(lasso)*?

```
##
## Call:  glmnet(x = x, y = y, alpha = 1, lambda = c(0, 0.2, 2, 4, 20,
100))
##
##    Df   %Dev Lambda
## 1   0 0.0000  100.0
## 2   2 0.6567   20.0
## 3   3 0.8004    4.0
## 4   3 0.8051    2.0
## 5   4 0.8072    0.2
## 6   4 0.8073    0.0
```

lambda	RSS	penalty	sum
100.0	145726.9	0.0	145726.9
20.00000	50025.64218	14.05496	50039.69714
4.00000	29082.92003	41.34363	29124.26366
2.00000	28408.50683	44.99057	28453.49740
0.20000	28097.60764	52.47741	28150.08505
0.00000	28088.09951	54.46997	28142.56948

something is wrong here too

How to choose λ?



What does λ do $_{\text{(ridge)}}$?

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

I : an identity matrix with p predictor variables

λ : a constant (small) lambda can only be positive

lambda is timed with our identity matrix

What is $X^T X$?

```r
head(X)
```

this is our X matrix

```
##                   (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
```

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

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

then we look at the covariated of the X matrix

```
##            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
```

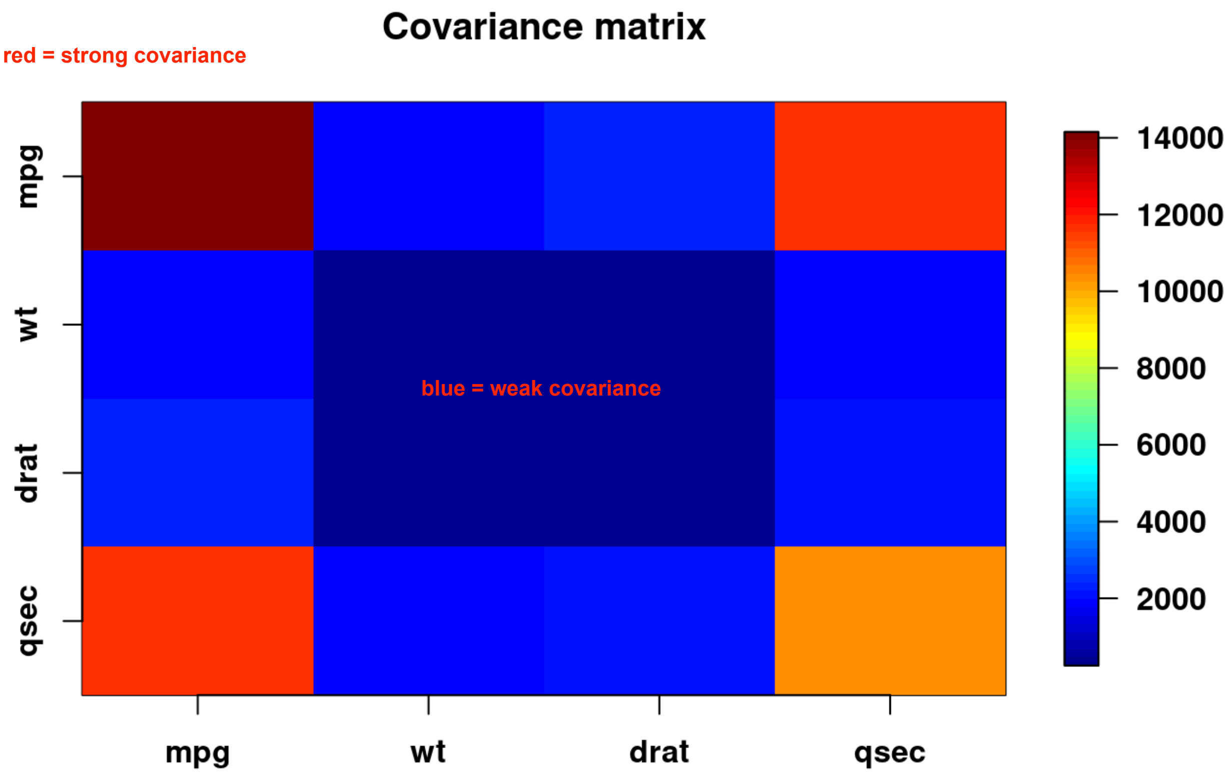
graphically

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

X cov = its a part of our least squares solution

in the ideal world, a covariance matrix would look like this

red = strong covariance



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

Collinearity can be bad

remember to give the correct order of predictors, cuz they have agency to impact in the way they are ordered

```
##
## 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
```

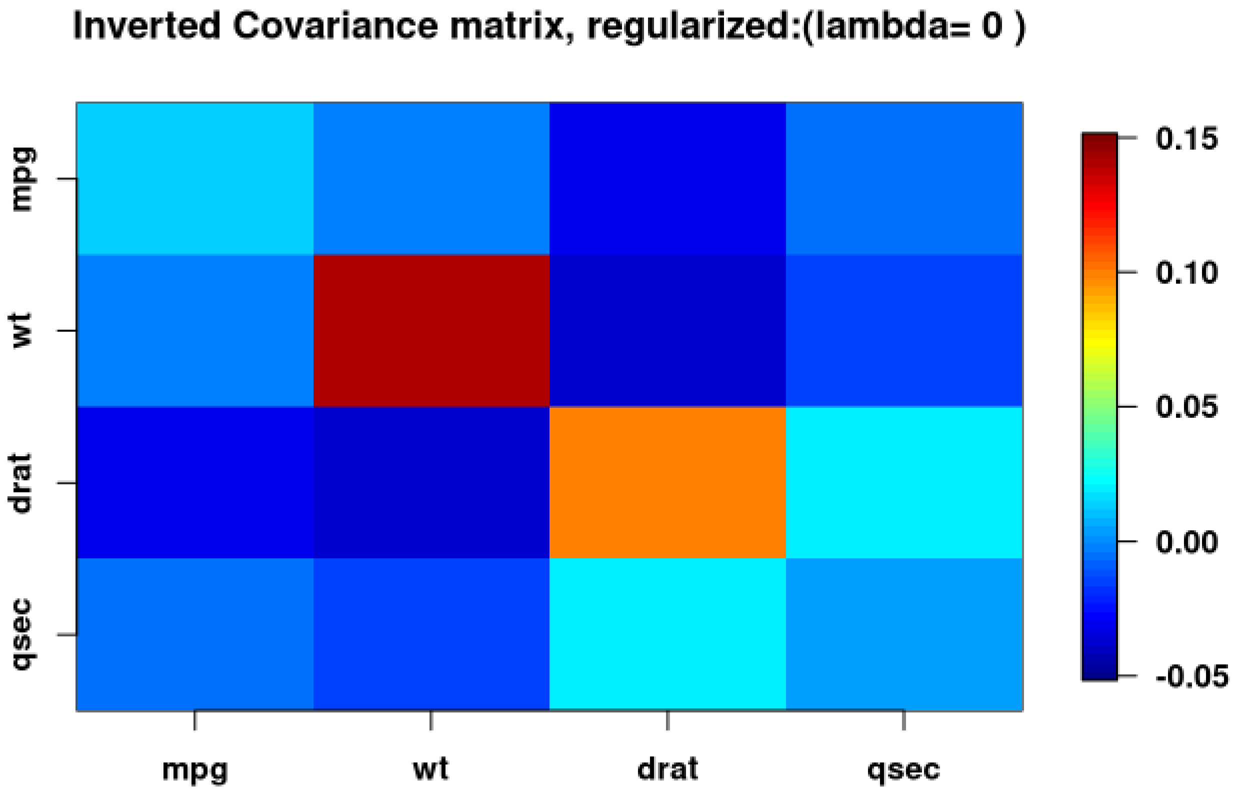
with colinarity being present, when we cant interpret the paramters below like we ususally do:

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

With collinearity, is that interpretation possible?

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

this is regularization = increasing lambda gives less colineaiity



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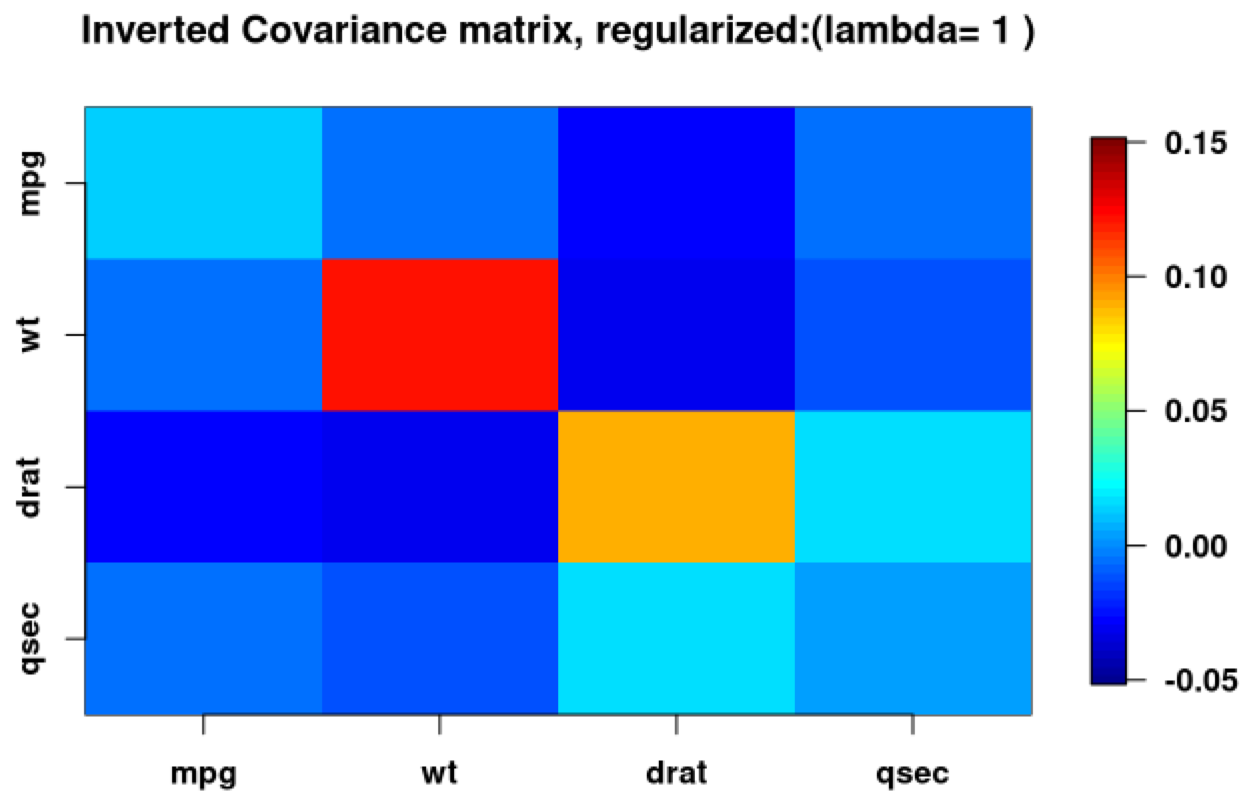

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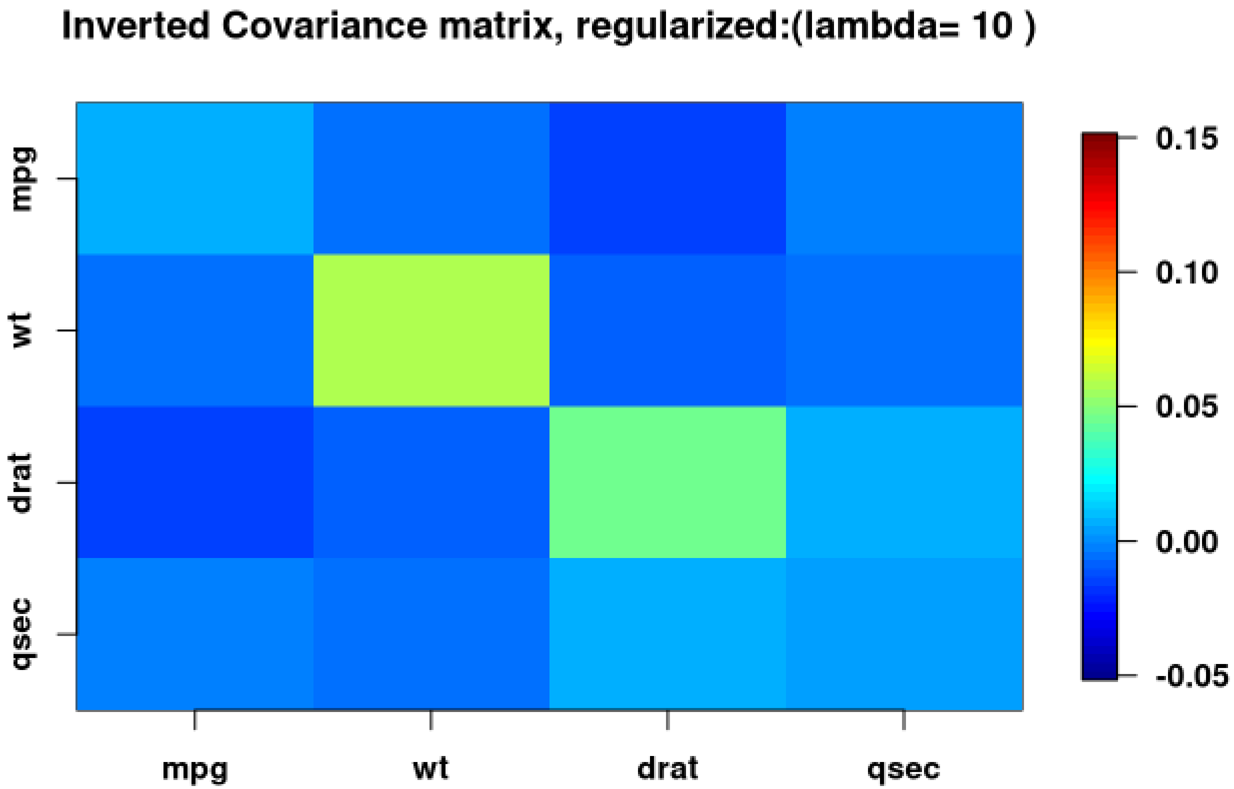

$$\hat{\beta}_{ridge} = \boxed{\left(X^T X + \lambda I\right)^{-1}} X^T y$$

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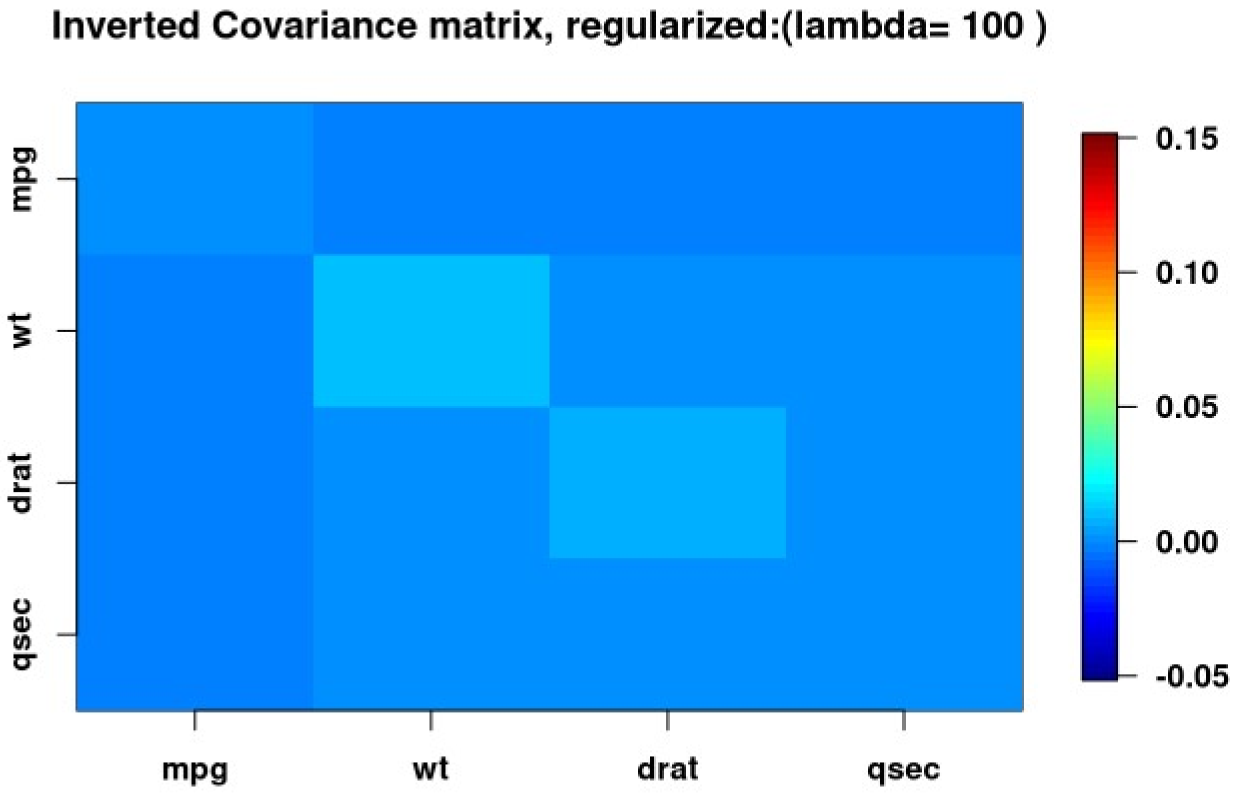

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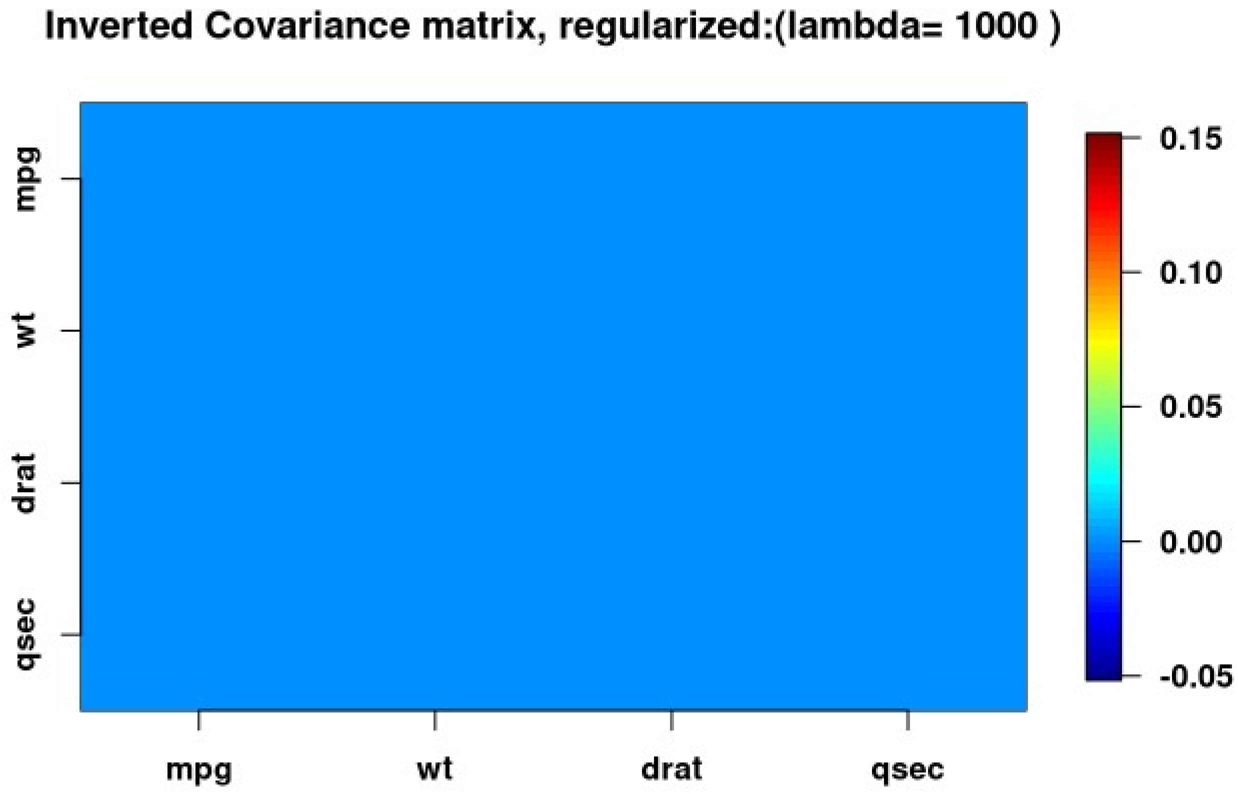


removing more and more variance

variance totally removed

So why is it called regularisation?

Two notes about the inverted matrix:

with increase of λ

we want low bias

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

less variance is present

its a trade offer= we give more bias but less variance

this is why we wanna find an optimal lambda

In a stable model:

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

so adding another parameter just exptains more noise, and if we keep on doing this,
we expalain more variance BUT we also start to fit noise (so we are moving torwards overfitting)

and that is why adding another predictor or adding data is not optimizing the model (it does to a certain extend) but
we cant just keep on adding predictos, then we will start to overfit:

ENTER LAMBDA!!!!!!!!!!!!!!!

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
```

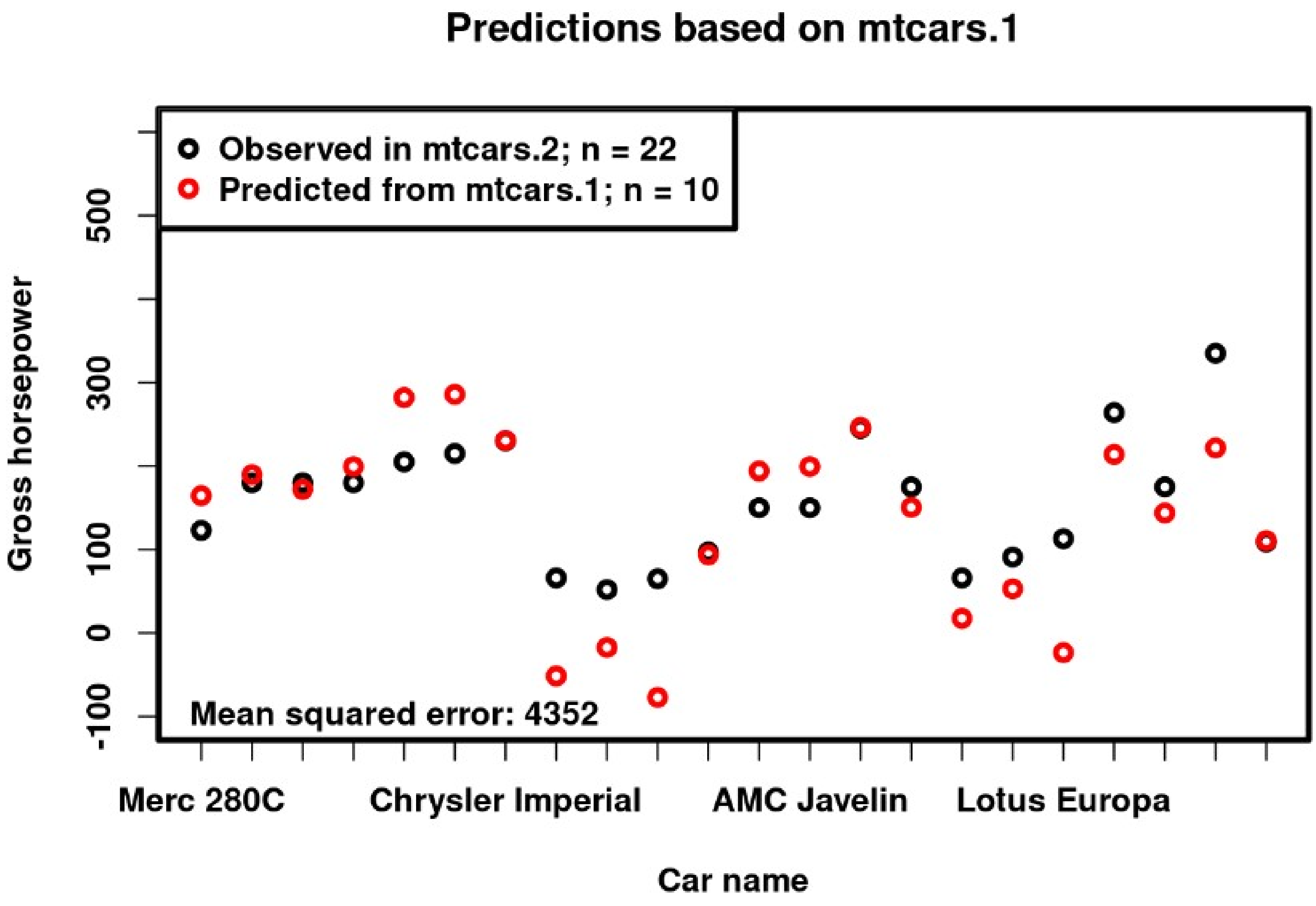
```
Call:
lm(formula = hp ~ mpg + wt + drat + qsec, data = mtcars)

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

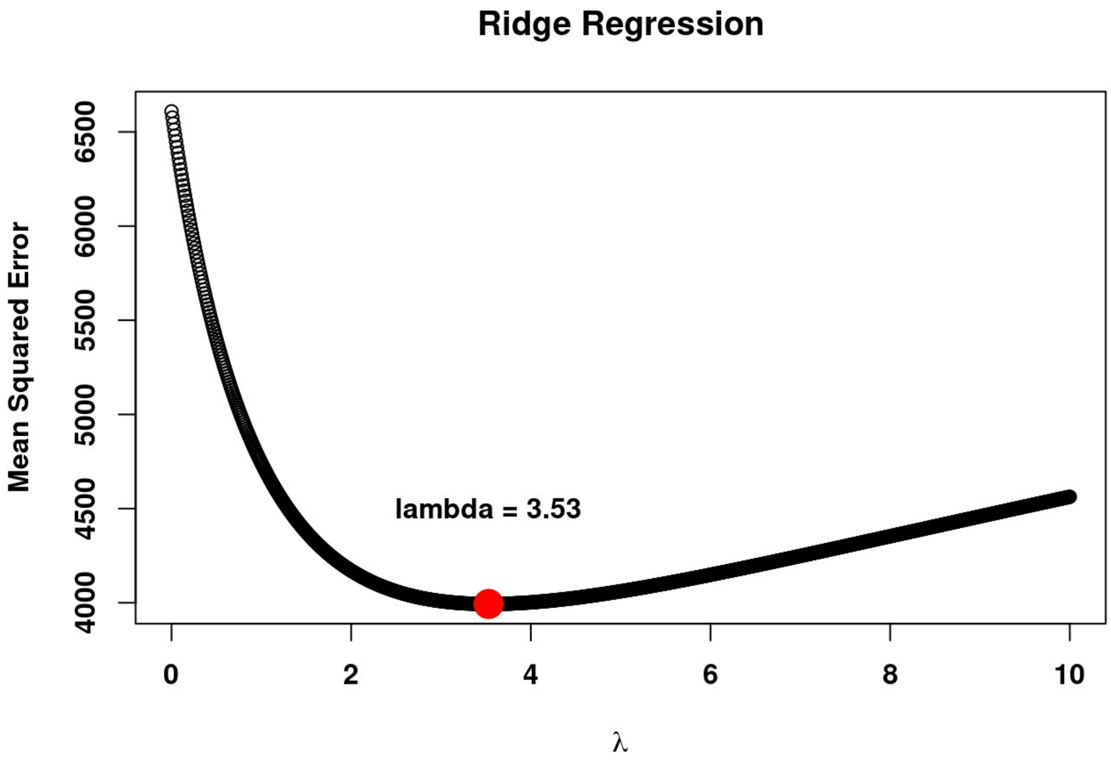
Suddenly, someone shows up with

Let's check our model

```r
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



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

Which dataset is the MSE calculated on?

by introducing bias with lambda, then we minimize the MSE the most!
we introduce bias to get better predictions

```
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
```

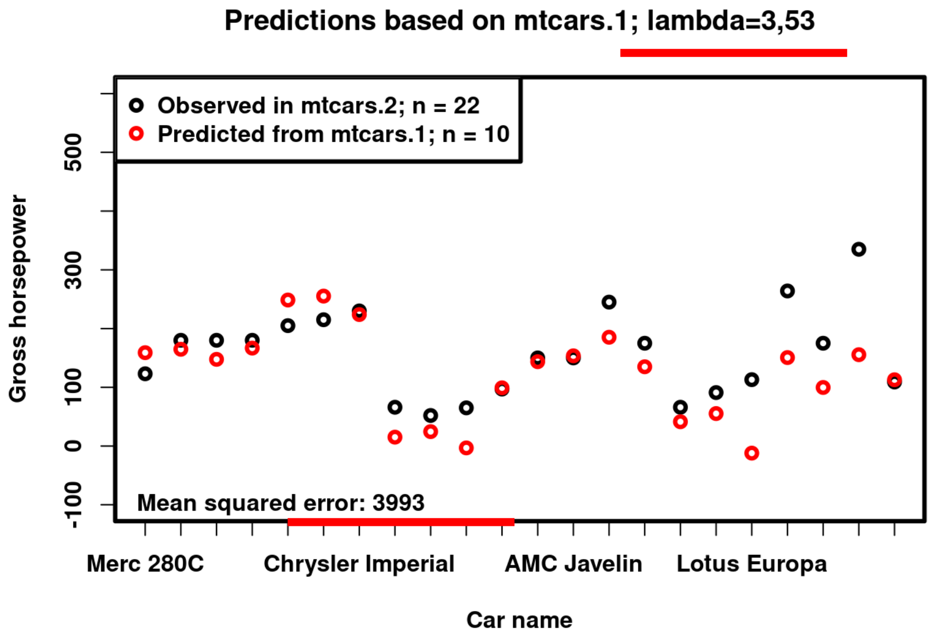
```
print(beta.hat.ridge <- ridge.regression(X, y, mtcars.1, min.lambda))
```

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

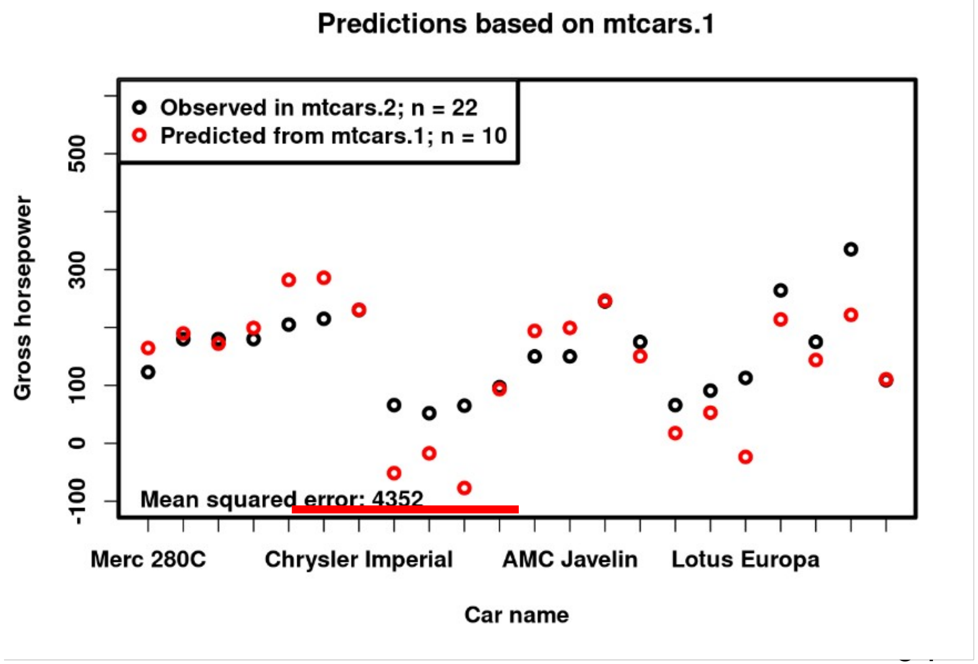
What has happened to the coefficients?

here lambda 3.53 is best cuz we predict mt wars 2 (test set)

Prediction on mtcars.2

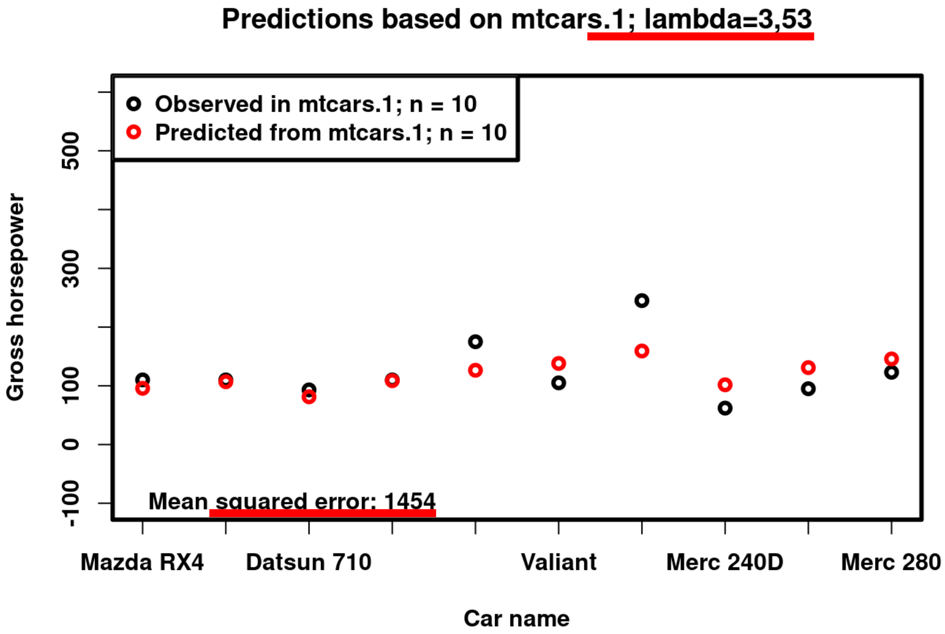


$$\lambda = 0$$

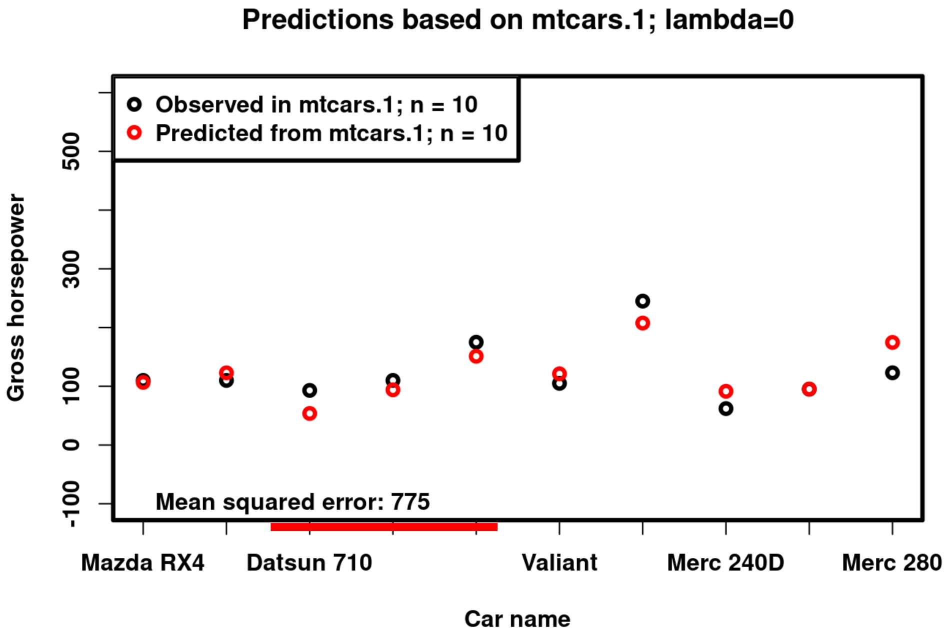


here a bambda of 0 is best when predicting the trainin set (mtcars 1)

“Prediction” on mtcars.1



$$\lambda = 0$$

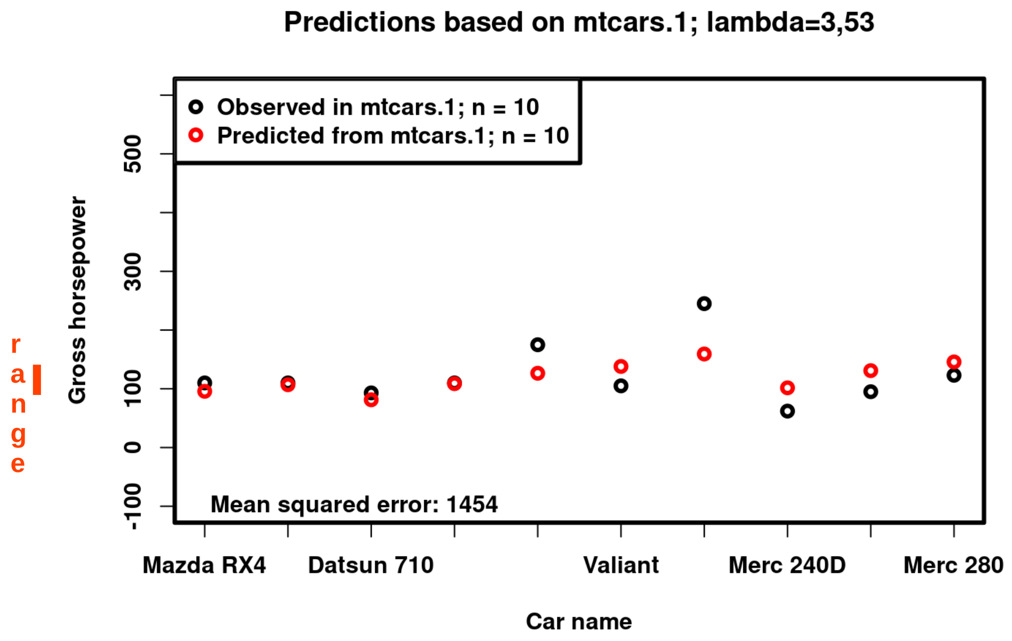


Nomenclature

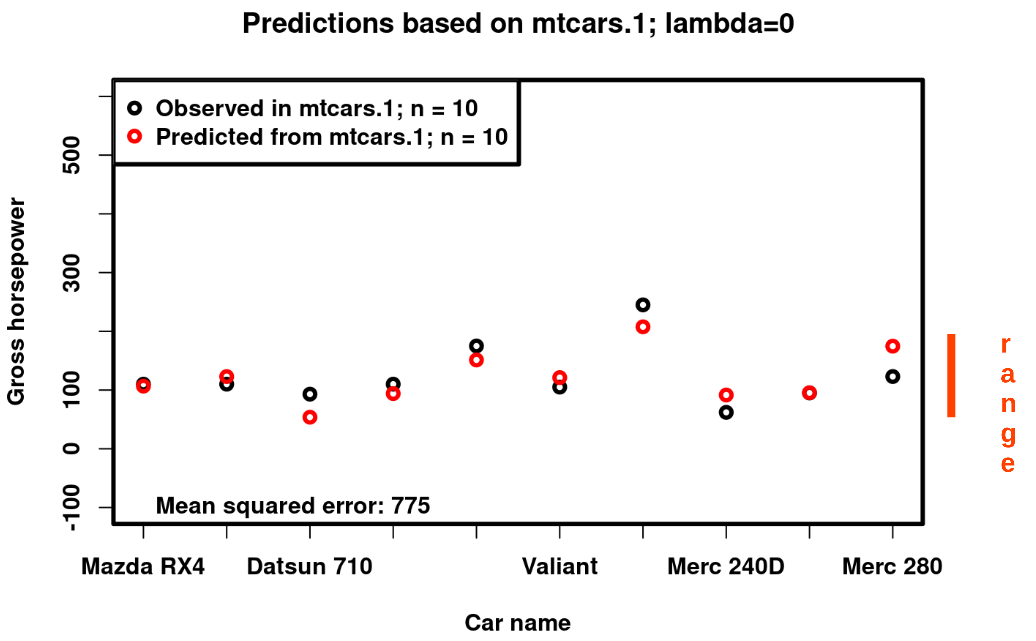
- mtcars.1 -> training set
- mtcars.2 -> test set
  - NB! Normally, we prefer that out training set is bigger than our test set
- By introducing *bias* in our training set, we at the same time reduce the *variance* of our training set, increasing the reliability of our predictions on a test set

“Testing” on training set

greater bias
lesser variance

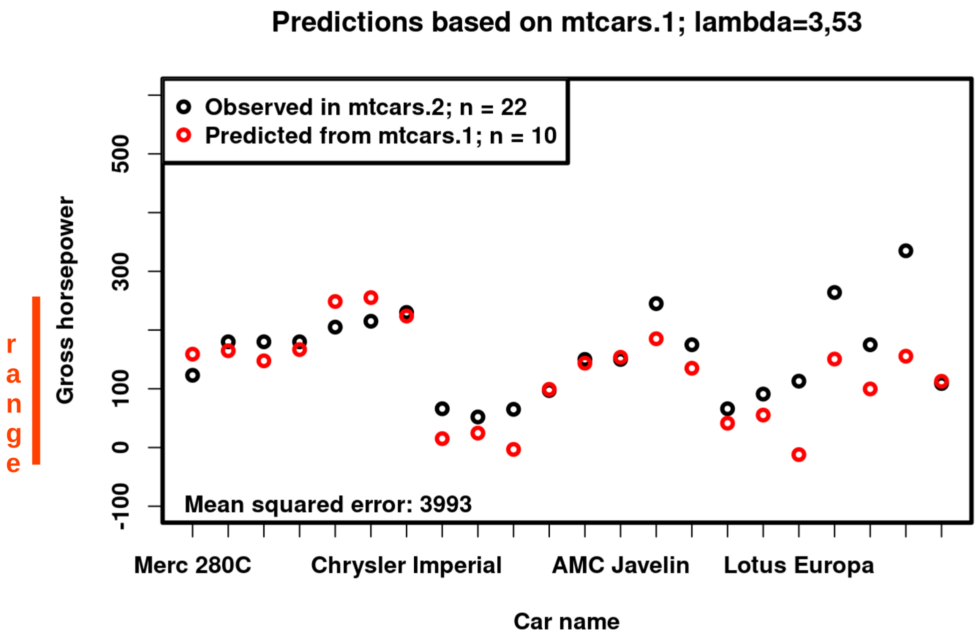


smallest bias
greater variance (of $\hat{y}$)

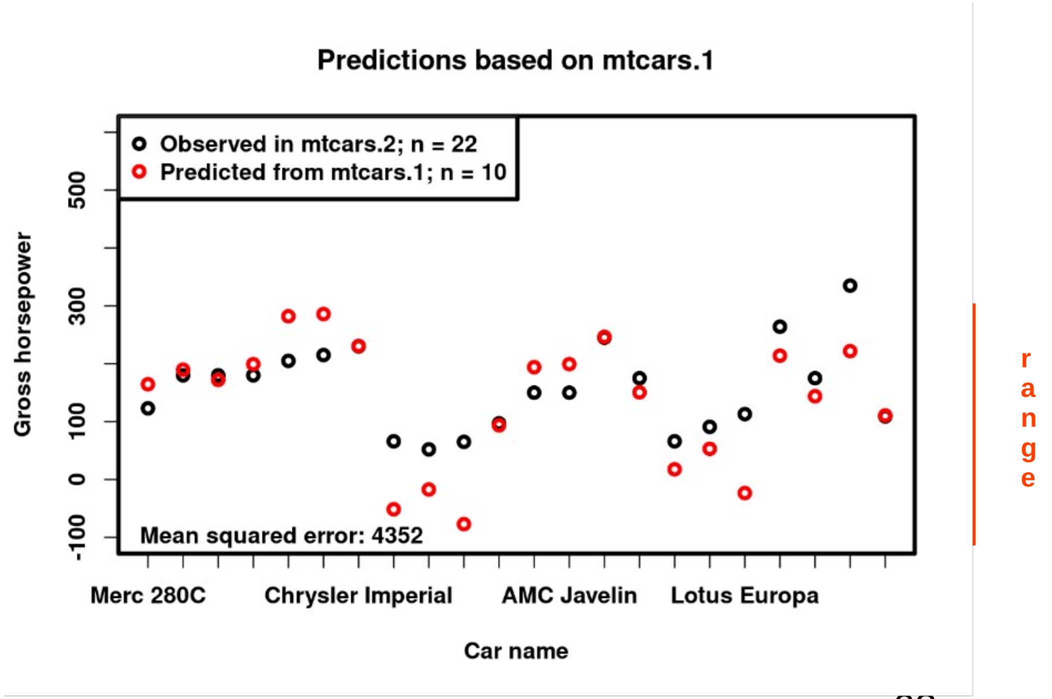


Optimal λ

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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