Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 5: *Evaluating and comparing models*October 12, 2021

by: Lau Møller Andersen

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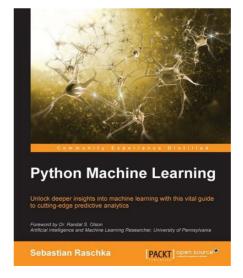


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Study Cafe

Python book in Stakbogladen

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



I still owe the answers to questions in the CryptPad Poisson and overdispersion, deviance in a logistic model, and the assumption of normality

Code review – pair programming

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
- To be able to predict and manipulate the world

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

EXPLANATION



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?

1) Variance explained?

R summary

```
##
## Call:
## lm(formula = mpg ~ wt, data = mtcars)
##
## Residuals:
## Min
          10 Median
                             30 Max
## -4.5432 -2.3647 -0.1252 1.4096 6.8727
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 37.2851 1.8776 19.858 < 2e-16 ***
## wt
     -5.3445 0.5591 -9.559 1.29e-10 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.046 on 30 degrees of freedom
## Multiple R-squared: 0.7528, Adjusted R-squared: 0.7446
## F-statistic: 91.38 on 1 and 30 DF, p-value: 1.294e-10
```

R² (coefficient of determination)

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \mu_{y})^{2}}$$

taking into account the number of parameters (p) and the number of observations (n).

number of p is BEYOND the constant term (intercept, what we call the mean)

R²; adjusted

lower than normal R^2 (penalized)

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \mu_{y})^{2}}$$

$$\bar{R}^2 = 1 - (1 - R^2) \frac{n - 1}{n - p - 1}$$

n: number of observations*p*: number of predictors beyond the constant term

```
37.285
                           -5.344
                                                                                  1.171
                                                              49.931
                                                                                                  -13.380
                                                                "R-squared: 0.819"
     "R-squared: 0.753"
                                                                "R-squared, adjusted: 0.807"
     "R-squared, adjusted: 0.745"
                                                           our explained variance increases (which is what we
                                                                  would expect due to physics...)
                                                           lm(formula = mpq \sim I(wt^4) + I(wt^3) + I(wt^2) + wt, data = mtcars)
  lm(formula = mpg \sim I(wt^3) + I(wt^2) + wt, data = mtcars)
                                                           Coefficients:
  Coefficients:
                                                           (Intercept)
                                                                          I(wt^4)
                                                                                     I(wt^3)
                                                                                                 I(wt^2)
                                                                                                                 wt
  (Intercept)
                I(wt^3)
                           I(wt^2)
                                                              14.4558
                                                                          -0.3863
                                                                                      5.2004
                                                                                                -23.7018
                                                                                                            36.6195
    48.40370
                0.04594
                           0.68938
                                     -11.82598
   "R-squared: 0.819"
                                                               "R-squared: 0.822"
   "R-squared, adjusted: 0.8"
                                                               "R-squared, adjusted: 0.796"
                                                                                                                 14
CC BY Licence 4.0: Lau Møller Andersen
```

Coefficients:

(Intercept)

 $lm(formula = mpg \sim I(wt^2) + wt, data = mtcars)$

wt

 $I(wt^2)$

Coefficients:

(Intercept)

lm(formula = mpg ~ wt, data = mtcars

wt

R² – mixed models

$$R_{GLMM}(m)^2 = \frac{\sigma_f^2}{\sigma_f^2 + \sigma_\alpha^2 + \sigma_\epsilon^2}$$
the fixed effects (how much does the group effects explain of the variance?)

$$R_{GLMM}(c)^{2} = \frac{\sigma_{f}^{2} + \sigma_{\alpha}^{2}}{\sigma_{f}^{2} + \sigma_{\alpha}^{2} + \sigma_{\epsilon}^{2}} \quad \text{combi of group and individual}$$

here u only have

 σ_f^2 : variance of the fixed effects σ_α^2 : variance of the random effects σ_ϵ^2 : unexplained variance

 \mathcal{O}_{ϵ} . Unlexplained variables 15

Variance explained

- Pros
 - R² is intuitive we get numbers and percentages which we can easily interpret!
- Cons
 - More complex models will always explain more variance
 - Hard to interpret in the case of collinearity
 - R² doesn't give us what we want

$$y_{i} = \beta_{0} + \beta_{1}X_{1i} + \beta_{2}X_{2i} + \varepsilon_{i}.$$

$$\hat{y}_{i} = 1.6 + 0.35X_{1i} + 0.62X_{2i}.$$

$$R^{2} = 0.750$$

Tempting interpretation: the parameter estimates are likely to be true, because R^2 is large

Correct interpretation:

"if one fits a model with the form of equation 1 in each new sample – each time estimating new values of b_0 , b_1 , and b_2 – what will be the average proportional reduction in the sum of squared errors?" (Yarkoni and Westfall 2017)

2) Likelihood ratios

Maximum likelihood estimation

$$\mathbf{PDF} = (2\pi\sigma^{2})^{-1/2}e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^{2} \int_{\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{2\pi} \int_{\frac{\pi}{$$

Conditional PDF
$$(y_i|X) = (2\pi\sigma^2)^{-1/2} e^{-\frac{1}{2}(\frac{y_i - x_i\beta}{\sigma_0})^2}$$

Likelihood function:
$$L(\sigma^2, \epsilon) = (2\pi\sigma^2)^{-N/2}e^{-\left(\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - x_i\beta)^2\right)}$$

Log-Likelihood function: $l(\sigma^2, \epsilon) = \log(L)$

y : dependent variable

 $X\beta$: linear predictor

 $y - X \beta = \epsilon$: residuals

N : number of observations

```
print(ll.m <- logLik(model))

## 'log Lik.' -702.0472 (df=6)

## 'log Lik.' -715.01 (df=4)

exp(ll.m)

## 'log Lik.' 1.272865e-305 (df=6)

## 'log Lik.' 2.986092e-311 (df=4)</pre>
```

Likelihood-ratio test

$$LR = -2(l(\theta_2) - l(\theta_1))$$

anova(model.ranint, model.ranslope.and.int)

```
## Data: sleepstudy
## Models:
## model.ranint: Reaction ~ days deprived + (1 | Subject)
## model.ranslope.and.int: Reaction ~ days deprived + (days deprived | Subject)
##
                        Df AIC
                                     BIC logLik deviance Chisq Chi Df
## model.ranint 4 1446.5 1458.4 -719.25
                                                 1438.5
## model.ranslope.and.int 6 1425.2 1443.0 -706.58
                                                  1413.2 25.332
##
                        Pr(>Chisq)
## model.ranint
## model.ranslope.and.int 3.156e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Likelihood-ratio test

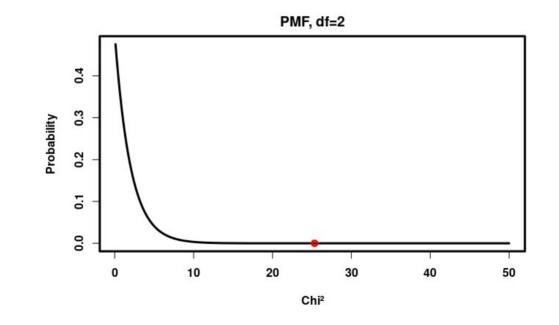
$$LR = -2(l(\theta_2) - l(\theta_1))$$

Chisq Chi Df

25.332 2

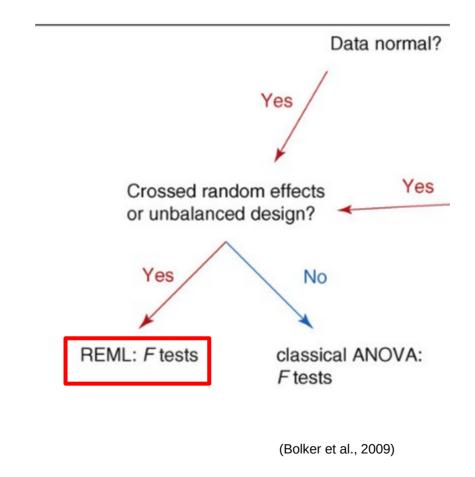
Pr(>Chisq)

3.156e-06



Regarding GLMMs

"The LR test is only adequate for testing fixed effects when both the ratio of the total sample size to the number of fixed-effect levels being tested and the number of random-effect levels (blocks) are large. We have found little guidance and no concrete rules of thumb in the literature [...]" (my highlights, Bolker et al., 2008)



Requires that degrees of freedom can be defined

24

$$F = \frac{\left(\frac{RSS_1 - RSS_2}{p_2 - p_1}\right)}{\left(\frac{RSS_2}{n - p_2}\right)} \xrightarrow{\text{difference in unexplained variance between "null" model and "target" model numerator degrees of freedom (difference in predictor variables)}$$

$$\xrightarrow{\text{unexplained variance by "target" model}}$$

$$\xrightarrow{\text{denominator degrees of freedom (degrees of freedom (degrees of freedom for observations)}}$$

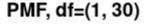
RSS: Residual sum of squares
p: number of predictor variables
n: number of observations

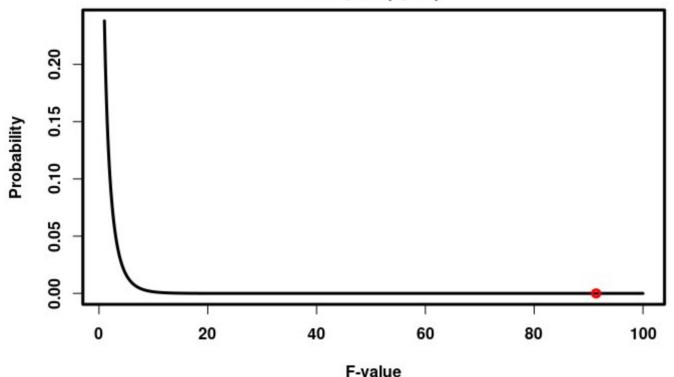
```
##
## Call:
                                                    Target model
## lm(formula = mpg ~ wt, data = mtcars)
##
## Residuals:
      Min
              10 Median
                          30
                                    Max
## -4.5432 -2.3647 -0.1252 1.4096 6.8727
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 37.2851 1.8776 19.858 < 2e-16 ***
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## F-statistic: 91.38 on 1 and 30 DF, p-value: 1.294e-10
```

```
Call:

lm(formula = mpg ~ 1, data = mtcars)

Null model
```





F-statistic: 91.38 on 1 and 30 DF, p-value: 1.294e-10

```
##
## Call:
## lm(formula = mpg \sim I(wt^2) + wt, data = mtcars)
##
## Residuals:
     Min
            10 Median 3Q
##
                               Max
## -3.483 -1.998 -0.773 1.462 6.238
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 49.9308 4.2113 11.856 1.21e-12 ***
## I(wt^2) 1.1711 0.3594 3.258 0.00286 **
## wt -13.3803 2.5140 -5.322 1.04e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.651 on 29 degrees of freedom
## Multiple R-squared: 0.8191, Adjusted R-squared: 0.8066
## F-statistic: 65.64 on 2 and 29 DF, p-value: 1.715e-11
```

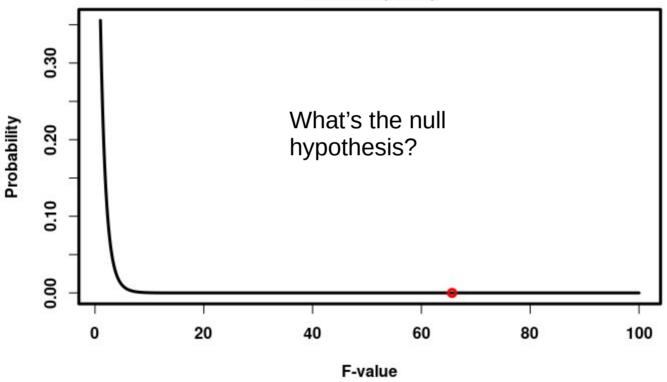
Target model

```
Call:
lm(formula = mpg ~ 1, data = mtcars)
```



Null model, (still!)

PMF, df=(2, 29)



F-statistic: 65.64 on 2 and 29 DF, p-value: 1.715e-11

What's the null hypothesis?

anova(model.1, model.2)

that the decrease in the highlighted blue is surprising

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

3) Information criteria

Information criteria

$$deviance = -2l(\hat{\theta})$$

 $AIC = deviance + 2k$

k : number of predictors

When we add k predictors that are pure noise, deviance is reduced by an amount corresponding to a χ^2 distribution with k degrees of freedom.

"On average, a predictor needs to reduce the deviance by 2 to in order to improve the fit to new data"

(Gelman and Hill, 2006)

(Gelman and Hill, 2006, p. 525)

How are the degrees of freedom calculated?

Hints: **Likelihood function**: $L(\sigma^2, \epsilon)$

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{i=1}^{N} (y_i - x_i \hat{\beta}_N)^2$$

How to estimate *k*?

With J parameters

- Complete pooling
 - all J parameters collapsed into 1 parameter, (k = 1)
- No pooling
 - each of the J parameters is estimated, (k = J)
- Partial pooling
 - the number of effective parameters may be estimated by sampling and the Deviance Information Criterion can be estimated (beyond this course)
 - the number of parameters, loosely speaking, depend on whether the parameters are estimated mostly by the group average or the individual's own average (k = ?)

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*

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \ \boldsymbol{X})^{-1} \ \boldsymbol{X}^T \ \boldsymbol{Y}$$

maximises the likelihood of

$$Y = X\beta + \epsilon$$

for which link function?

To fit is to overfit

(Yarkoni and Westfall, 2017)

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

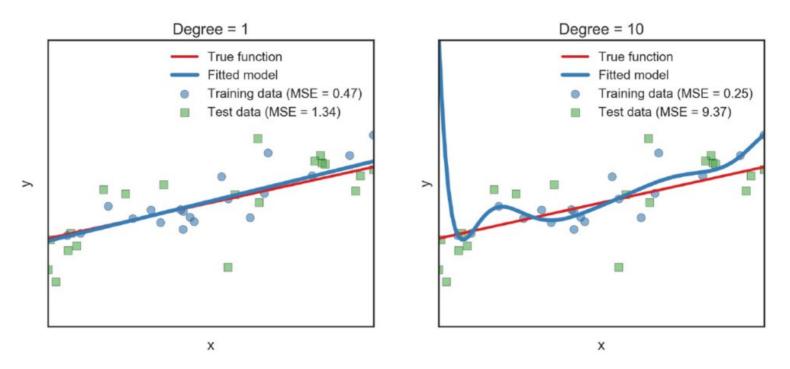
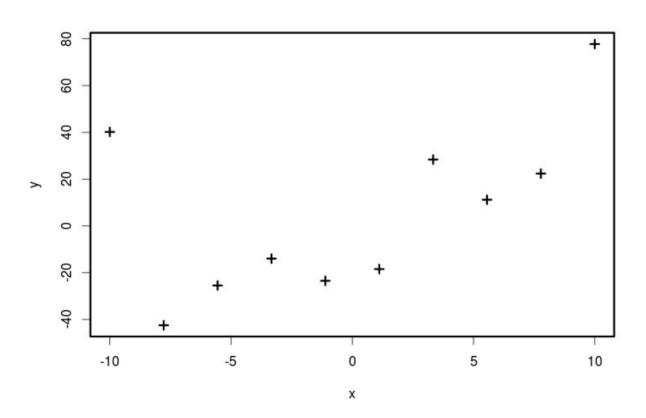


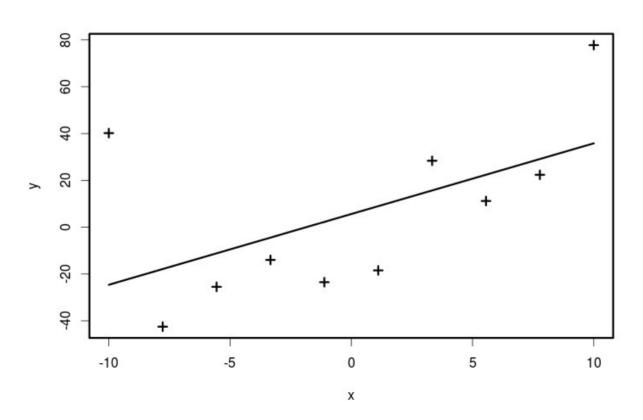
Fig. 1. Training and test error produced by fitting either a linear regression (left) or a 10th-order polynomial regression (right) when the true relationship in the population (red line) is linear. In both cases, the test data (green) deviate more from the model's predictions (blue line) than the training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

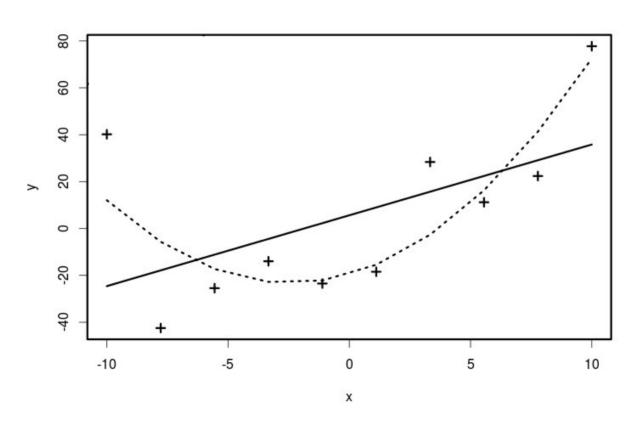
A sample of 10 linear or quadratic?



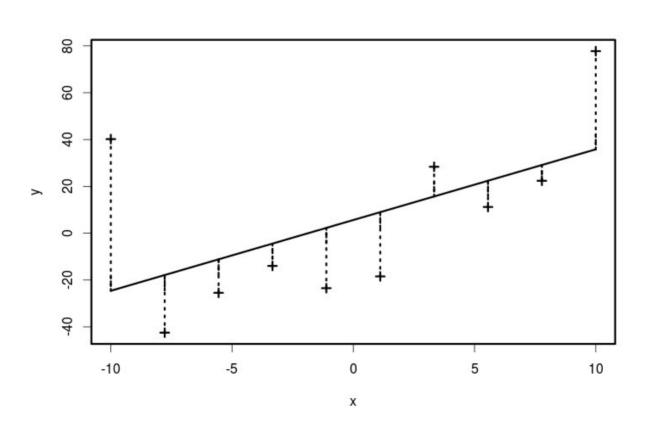
A sample of 10 linear or quadratic?



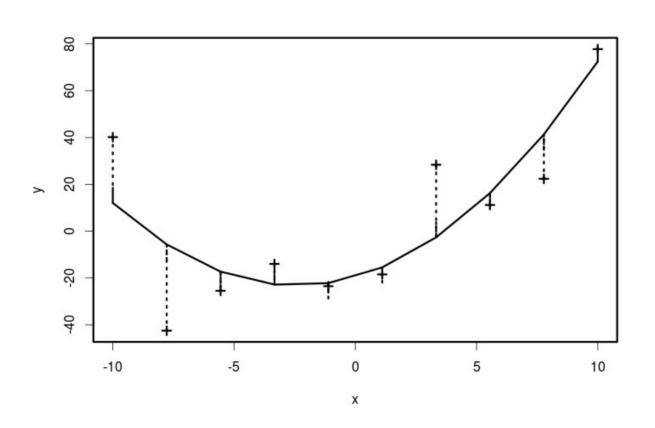
A sample of 10 linear or quadratic?



Residuals (linear)



Residuals (quadratic)



Quadratic:

 $ax^2 + bx + c$

Linear:

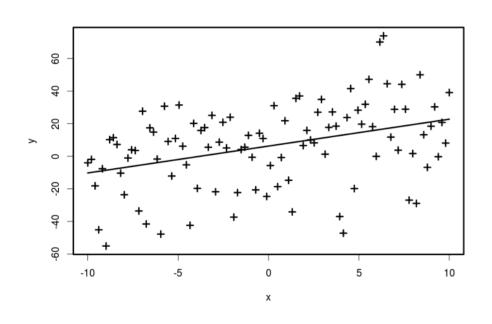
bx + c

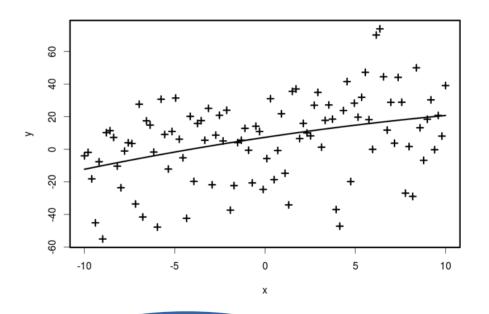
Estimates

$$a = 0.6184$$
; $b = 3.0201$

b = 3,020

Now a sample of 100





$$b = 1,650$$

$$a = -0.03074 \approx 0.5b = 1.650$$

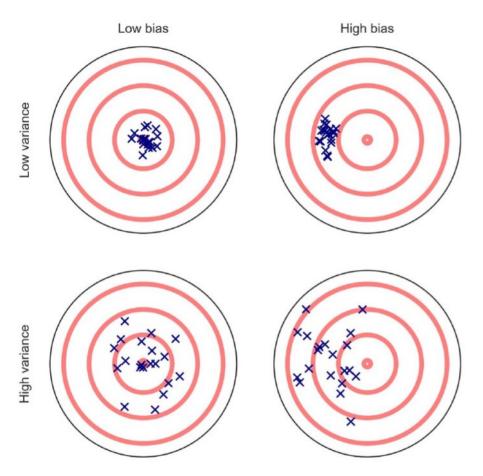


Fig. 2. An estimator's predictions can deviate from the desired outcome (or true scores) in two ways. First, the predictions may display a systematic tendency (or *bias*) to deviate from the central tendency of the true scores (compare right panels with left panels). Second, the predictions may show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

Which two of these does our leastsquares solution prefer?

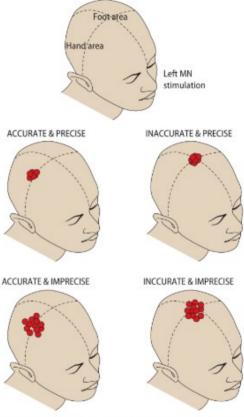


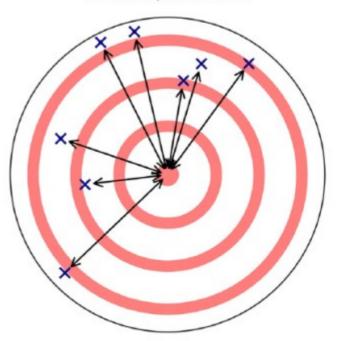
FIGURE 3.7. Accuracy versus precision. A schematic illustration of the differences between accuracy and precision of source localization. After left median-nerve stimulation, activations is expected in the right-hemisphere hand region of the primary somatosensory cortex. The foot area is shown at the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

(Yarkoni and Westfall, 2017)

(Yarkoni and Westfall, 2017)

Sum of squared errors

Bias-variance decomposition



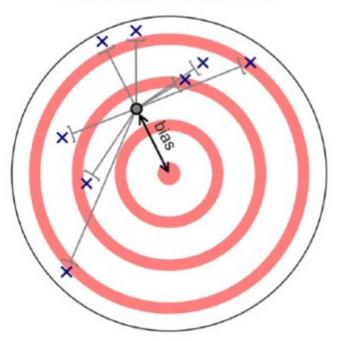


Fig. 3. Schematic illustration of the bias-variance decomposition. (Left) Under the classical error model, prediction error is defined as the sum of squared differences between true scores and observed scores (black lines). (Right) The bias-variance decomposition partitions the total sum of squared errors 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).

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

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

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

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

i:observations

p:predictor variables

 λ : a constant

Penalised regression

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

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

ridge regression : RSS +
$$\lambda \sum_{j=1}^{p} (\beta_{j}^{2})$$
 (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

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

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

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

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?

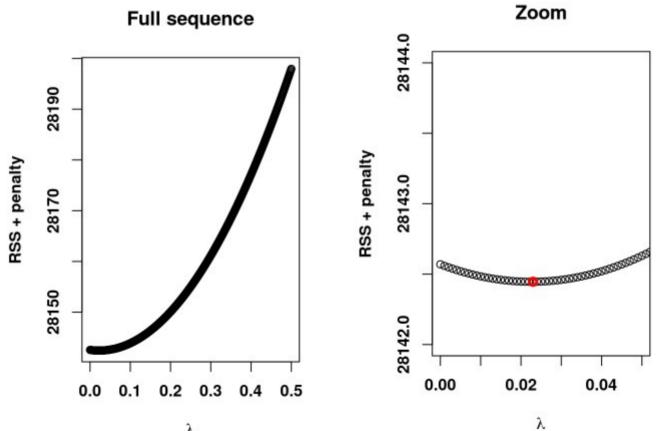
```
sum.of.squares.total <- sum((y - mean(y))^2)
sum.of.squared.errors.lm <- sum(residuals(linear_model)^2)
print(r.squared.lm <- 1 - sum.of.squared.errors.lm/sum.of.squares.total)</pre>
```

```
## [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))
##
                           lambda
                                          RSS
                                                  penalty
                                                                   sum
##
     Df
          %Dev Lambda
                                                            145726.9
                            100.0 145726.9
                                                 0.0
                100.0
      0.0000
## 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
                          2.00000 28408.50683
                                                  44.99057 28453.49740
##
               2.0
      3 0.8051
## 5
      4 0.8072
                  0.2
                          0.20000 28097.60764
                                                  52.47741 28150.08505
                          0.00000 28088.09951
                                                  54.46997 28142.56948
## 6
     4 0.8073
                  0.0
```

How to choose λ ?



What does λ do?

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

I : an identity matrix with p predictor variables λ : a constant

What is X^TX?

head(X)

print(cov.X)

$X_{COV} = X^T X$

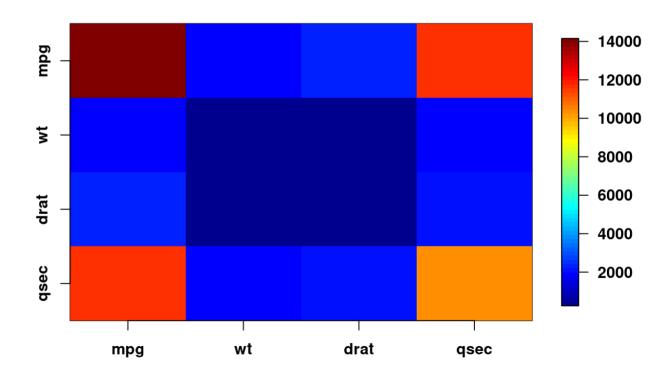
mpg wt drat qsec ## mpg 14042.310 1909.7528 2380.2770 11614.745 ## wt 1909.753 360.9011 358.7190 1828.095 ## drat 2380.277 358.7190 422.7907 2056.914

qsec 11614.745 1828.0946 2056.9140 10293.480

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

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

Covariance matrix



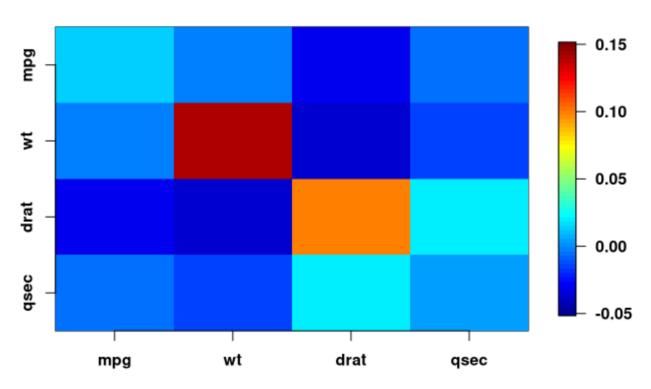
Collinearity can be bad

```
##
## 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
```

Assuming no collinearity, what is the interpretation of the coefficients? With collinearity, is that interpretation possible?

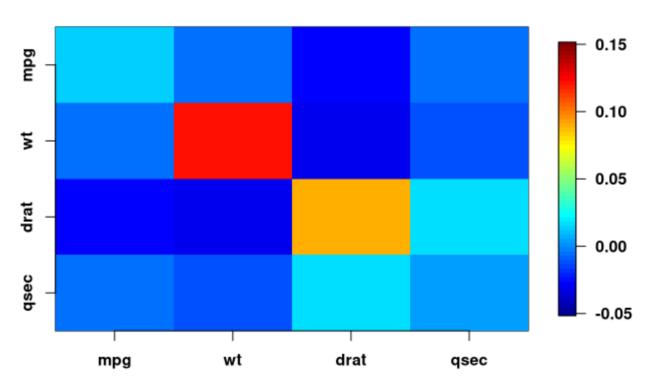
$$\hat{\beta_{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

Inverted Covariance matrix, regularized:(lambda= 0)



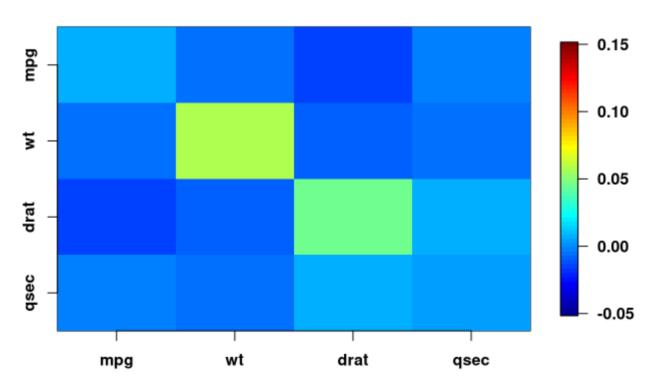
$$\hat{\beta_{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

Inverted Covariance matrix, regularized:(lambda= 1)



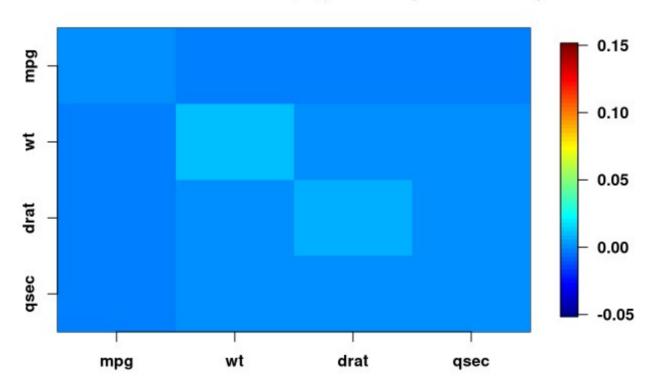
$$\hat{\beta_{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

Inverted Covariance matrix, regularized:(lambda= 10)



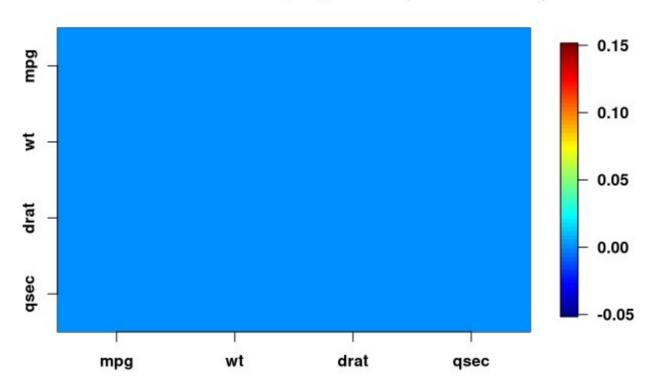
$$\hat{\beta_{ridge}} = (X^T X + \lambda I)^{-1} X^T y$$

Inverted Covariance matrix, regularized:(lambda= 100)



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

Inverted Covariance matrix, regularized:(lambda= 1000)



So why is it called regularisation?

Two notes about the inverted matrix:

with increase of λ

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

Stability of a 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) – week 6)

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 how the error can be decomposed into *bias* and *variance*

References

- Bolker, B.M., Brooks, M.E., Clark, C.J., Geange, S.W., Poulsen, J.R., Stevens, M.H.H., White, J.-S.S., 2009. Generalized linear mixed models: a practical guide for ecology and evolution. Trends in Ecology & Evolution 24, 127–135. https://doi.org/10.1016/j.tree.2008.10.008
- Gelman, A., Hill, J., 2006. Data Analysis Using Regression and Multilevel/Hierarchical Models. Cambridge University Press.
- Hari, R., Puce, A., 2017. MEG-EEG Primer. Oxford University Press, New York, NY, US.
- Yarkoni, T., Westfall, J., 2017. Choosing Prediction Over Explanation in Psychology: Lessons From Machine Learning. Perspect Psychol Sci 12, 1100–1122. https://doi.org/10.1177/1745691617693393