Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 4: *Explanation and prediction*
October 5, 2021

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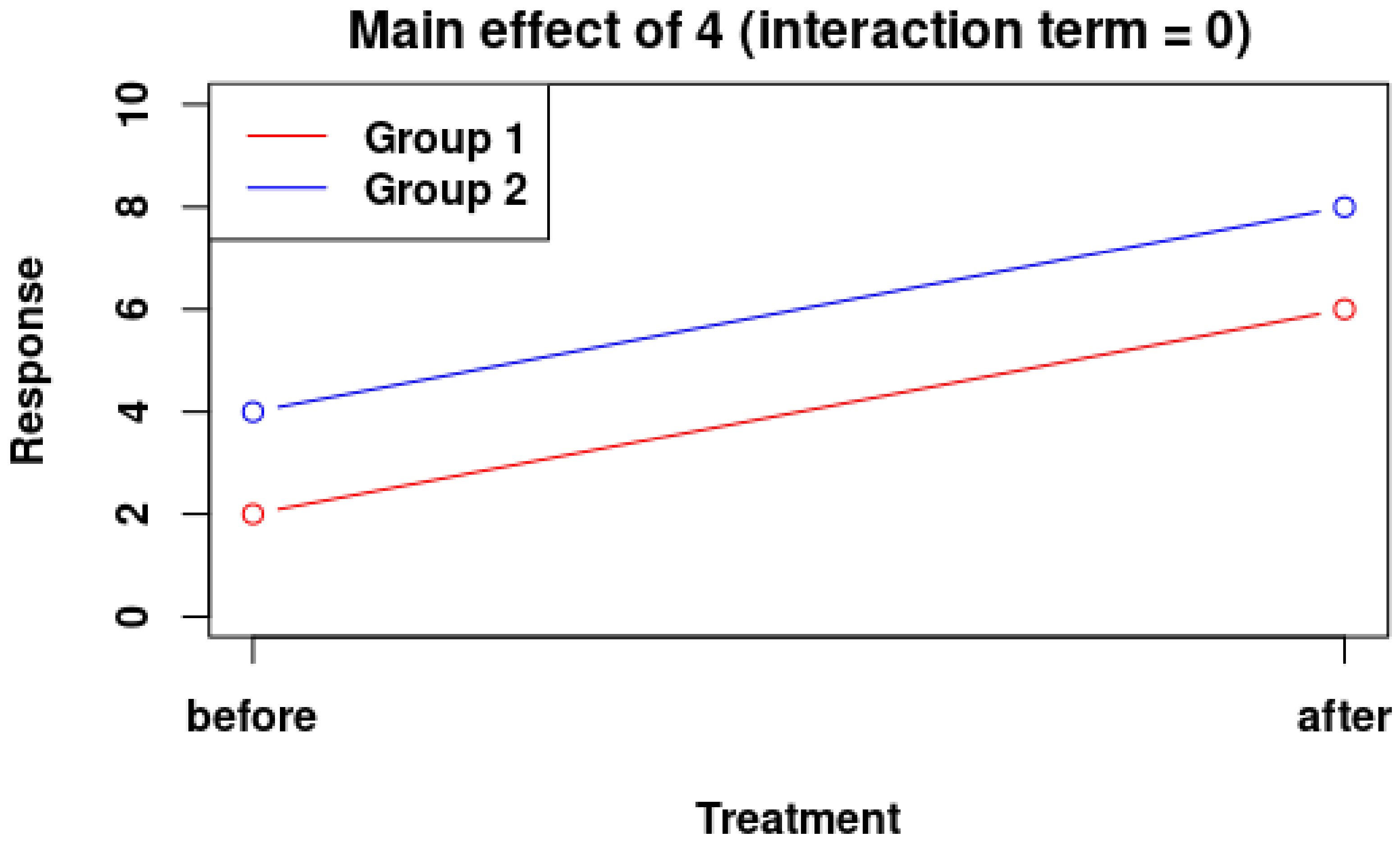
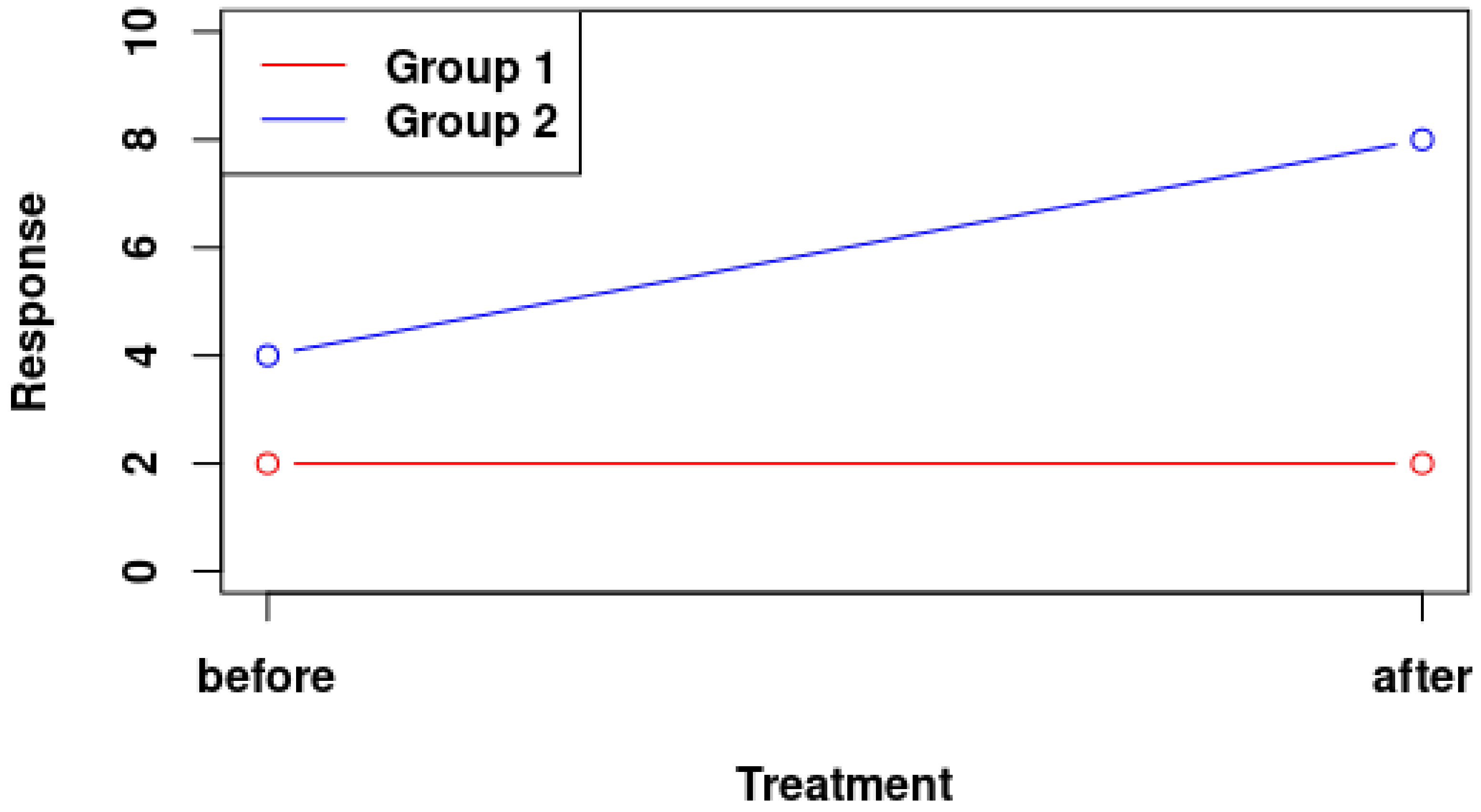
Questions since last time

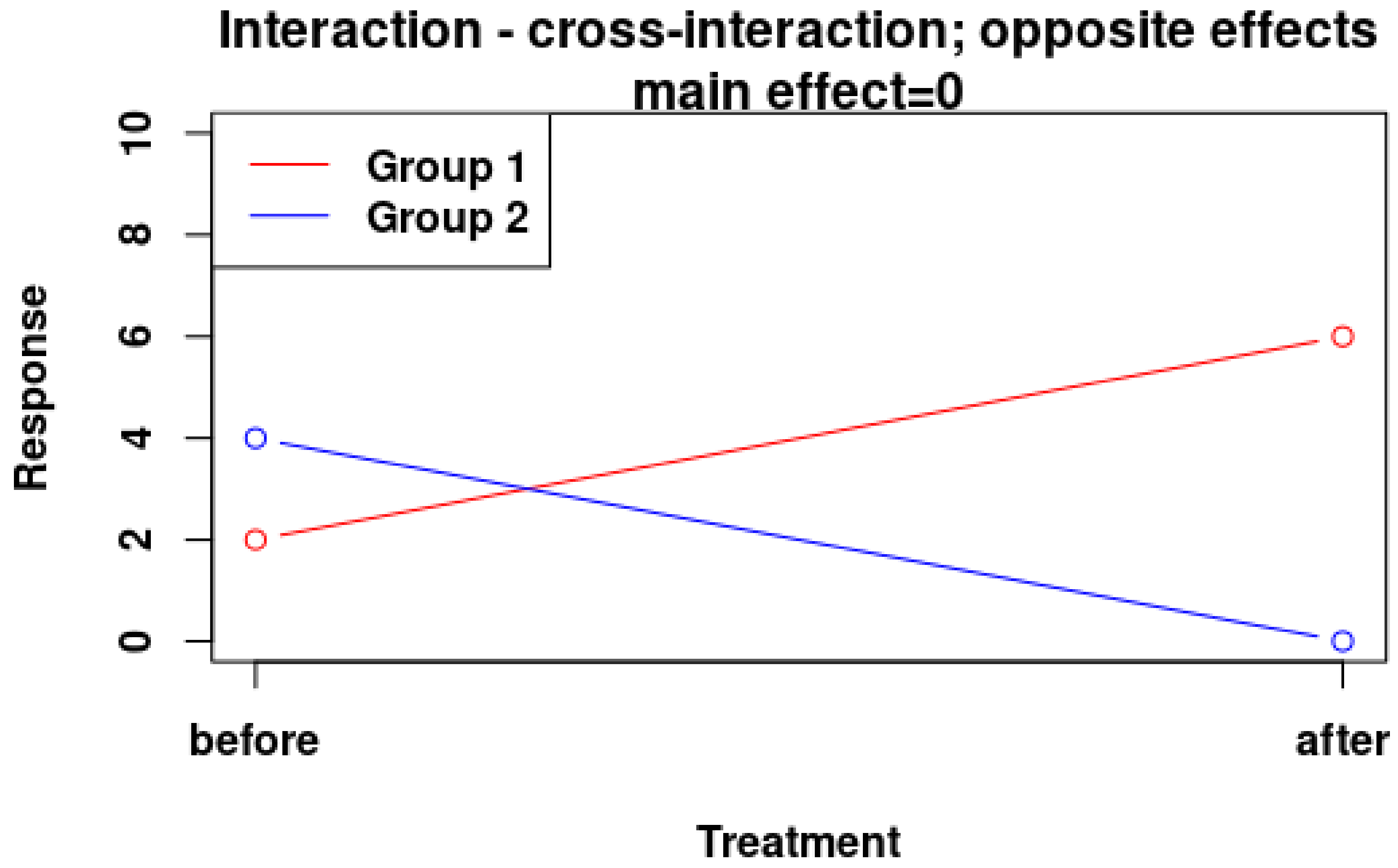
From CryptPad

Can you explain what it means that significance of main effects is uninterpretable in case of a significant interaction? In our case, the interaction wasn't significant. But what would we have done, had it in fact been significant?


Main effect of 4 (interaction term = 0)
Group 1
Group 2
Response
0
2
4
6
8
10
before
after
Treatment

Interaction - (main effect = 2, not interpretable)




Interaction - cross-interaction; opposite effects
main effect=0
Group 1
Group 2
Response
Treatment
before
after
0
2
4
6
8
10

More questions?

Learning goals

Generalized Linear Mixed Effects Models (GLMM)

1) Understanding that we can extend the scope of our multilevel modelling by using appropriate link functions and data distributions

2) Understanding the multilevel equivalent of the GLM

First some remarks on Exercises

- Assignments (those that go in the portfolio are marked in the syllabus)
- I’ll make an effort to write what I expect of you more succinctly
- Deadlines:
  - My suggestion: we move deadline to Wednesday (23.59)
- This week:
  - Practical exercise will be code review of each other’s assignments so far

At least four ingredients needed

1) A data vector: $y = (y_1, \ldots, y_n)$

2) Predictors: X and coefficients β, forming a linear predictor $X\beta$

3) A *link function* g: yielding a vector of transformed data $\hat{y} = g^{-1}(X\beta)$ that are used to model the data

4) A data distribution: $p(y \mid \hat{y})$

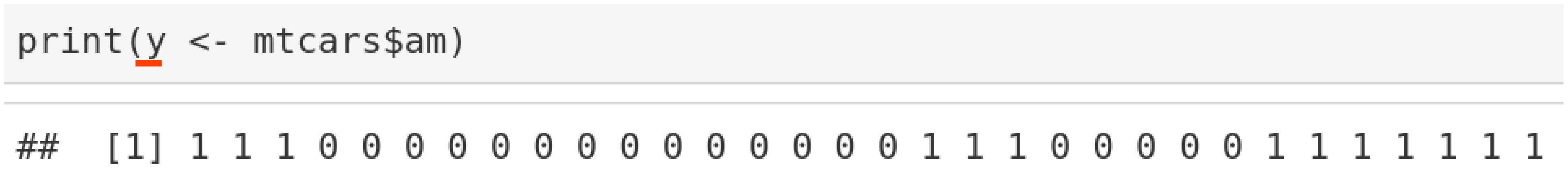
$(X\beta = \beta_0 + X_1\beta_1 + \ldots + X_k\beta_k)$

(Gelman and Hill, 2006, Chapter 6)

JEEP COMPASS VS NISSAN ROGUE SPORT VS SUBARU CROSSTREK
MOTOR TREND
DECEMBER 2017
EXCLUSIVE
FIRST TEST
MASERATI? NOPE, IT'S A KIA!
NEW & IMPROVED
ACCORD VS CAMRY
BEST-SELLER BATTLE ROYALE

Breaking all promises and going back to ***mtcars***

1) A data vector: $y = (y_1, \ldots, y_n)$



```
print(y <- mtcars$am)
```

```
##  [1] 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 0 0 0 0 1 1 1 1 1 1 1
```

2) Predictors: X and coefficients β, forming a linear predictor $X\beta$

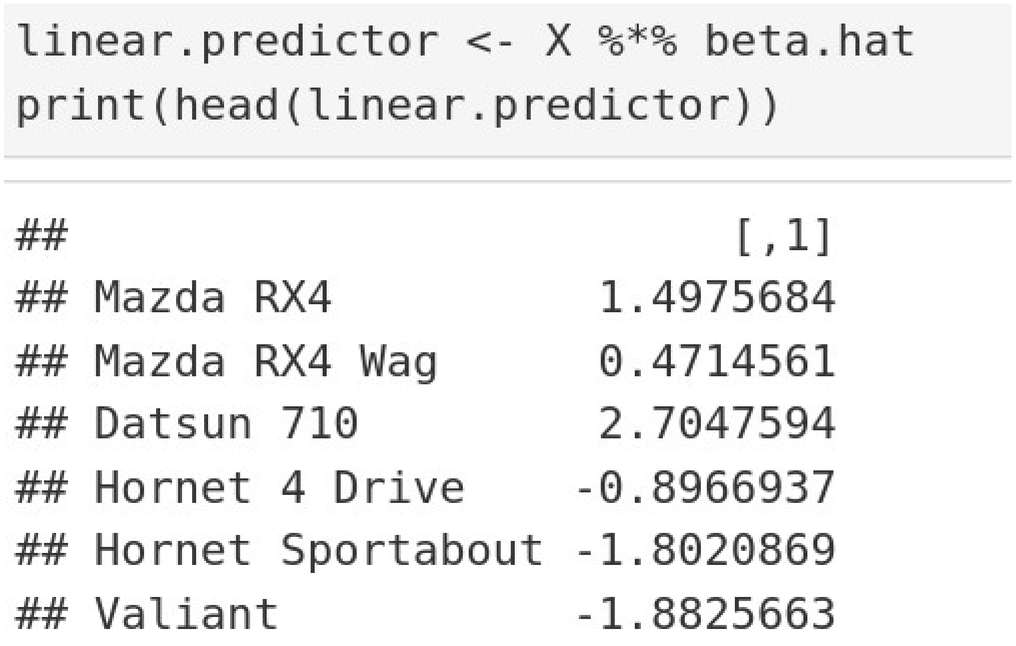
```r
logistic.model <- glm(am ~ wt + 1, data=mtcars, family='binomial')
X <- model.matrix(logistic.model)
print(head(X))
```

```
##                   (Intercept)    wt
## Mazda RX4                   1 2.620
## Mazda RX4 Wag               1 2.875
## Datsun 710                  1 2.320
## Hornet 4 Drive              1 3.215
## Hornet Sportabout           1 3.440
## Valiant                     1 3.460
```

```r
print(beta.hat <- logistic.model$coefficients)
```

```
## (Intercept)          wt
##    12.04037    -4.02397
```

2) Predictors: X and coefficients β, forming a linear predictor $X\beta$

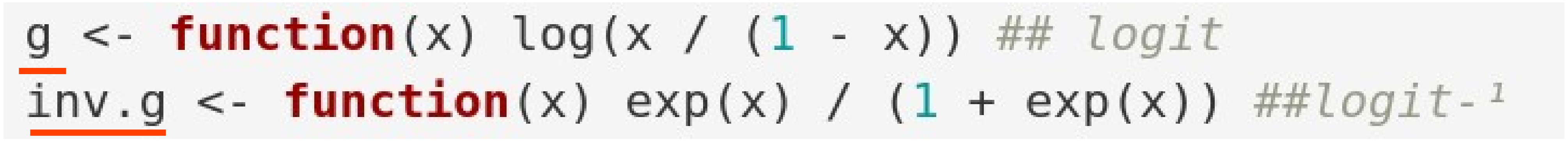


```r
linear.predictor <- X %*% beta.hat
print(head(linear.predictor))
```

```
##                         [,1]
## Mazda RX4          1.4975684
## Mazda RX4 Wag      0.4714561
## Datsun 710         2.7047594
## Hornet 4 Drive    -0.8966937
## Hornet Sportabout -1.8020869
## Valiant           -1.8825663
```

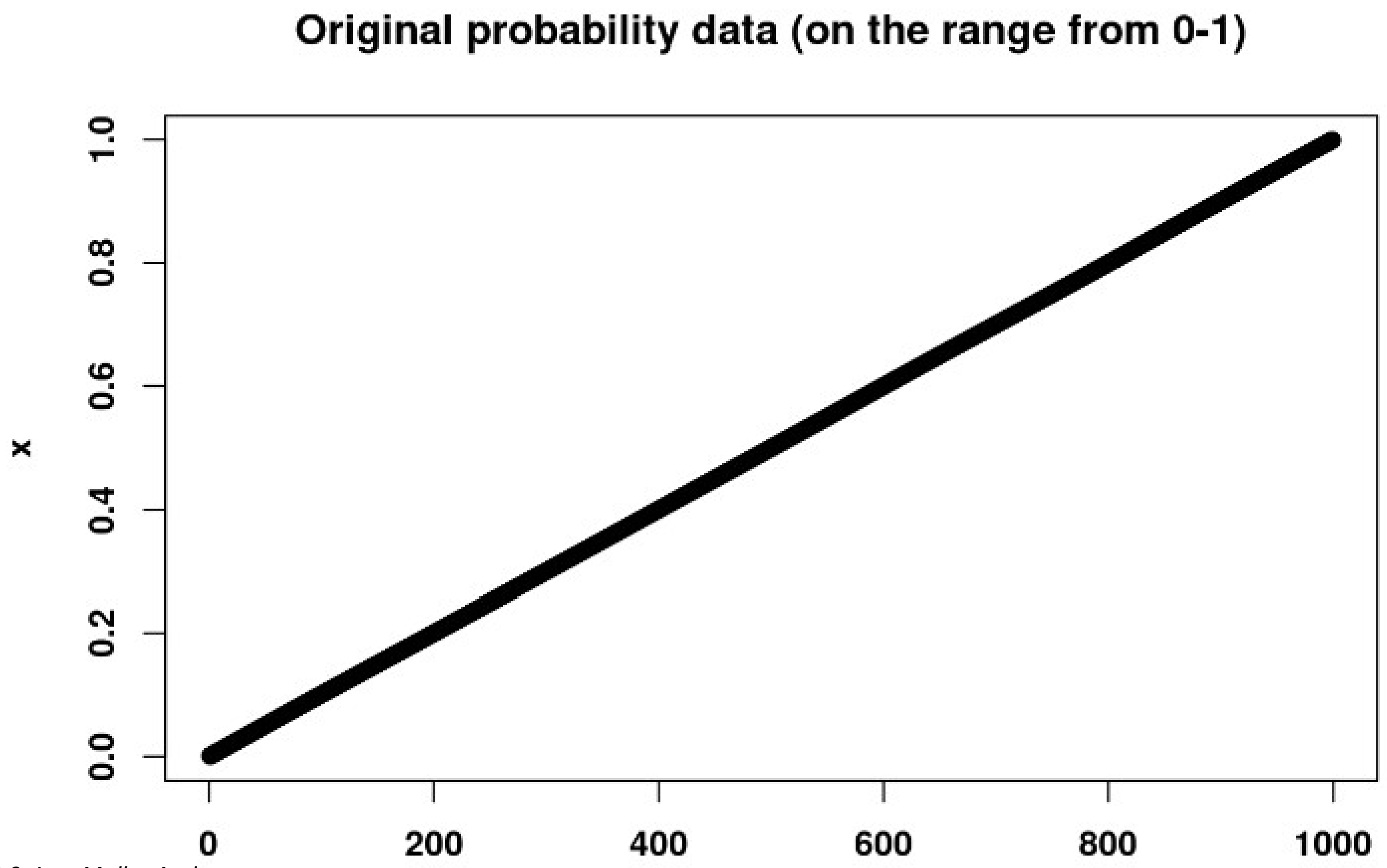
This lives on a continuous scale spanning all the real numbers

3) A *link function* g: yielding a vector of transformed data $\hat{y} = g^{-1}(X\beta)$ that are used to model the data

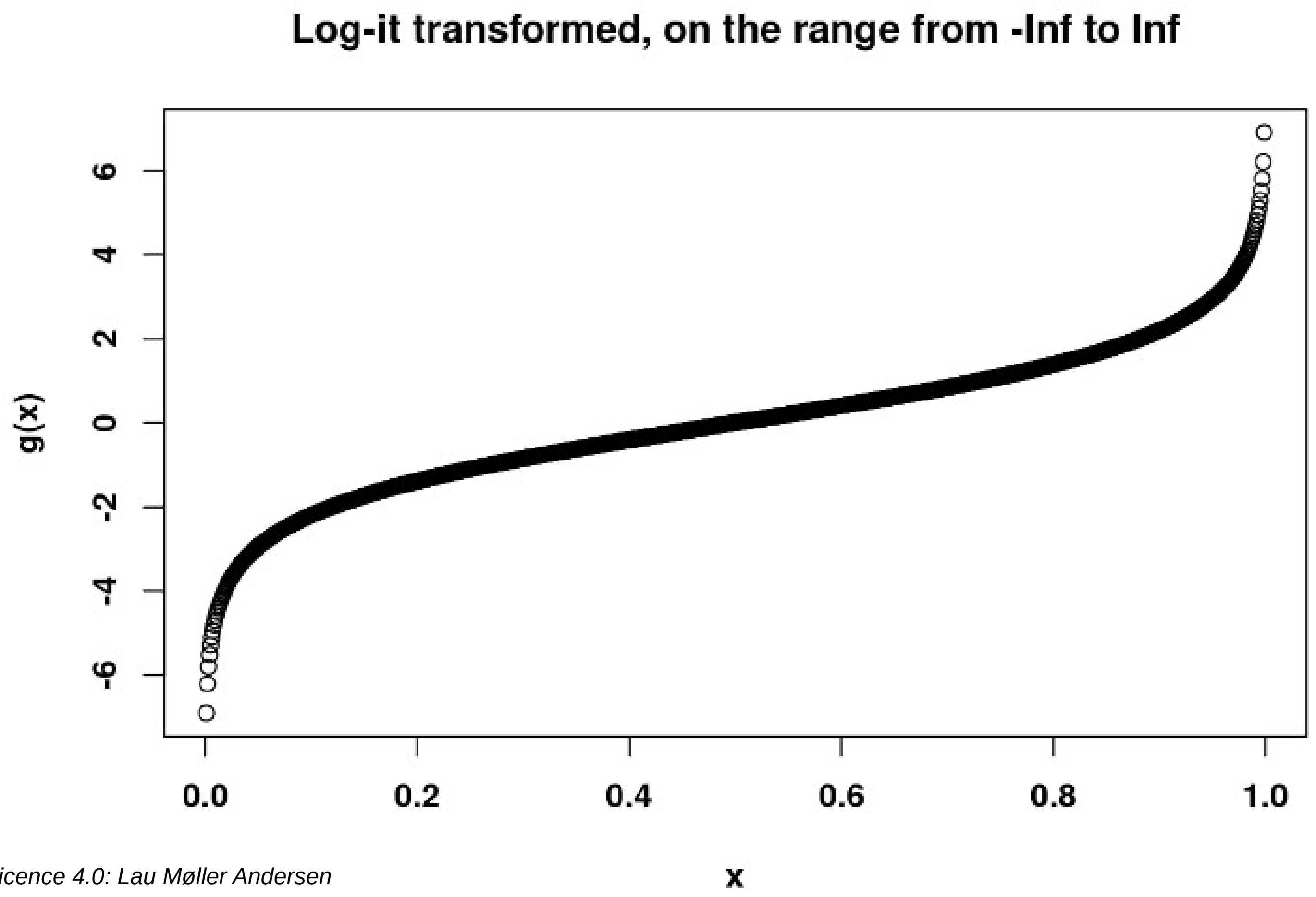


```
g <- function(x) log(x / (1 - x)) ## logit
inv.g <- function(x) exp(x) / (1 + exp(x)) ##logit-¹
```

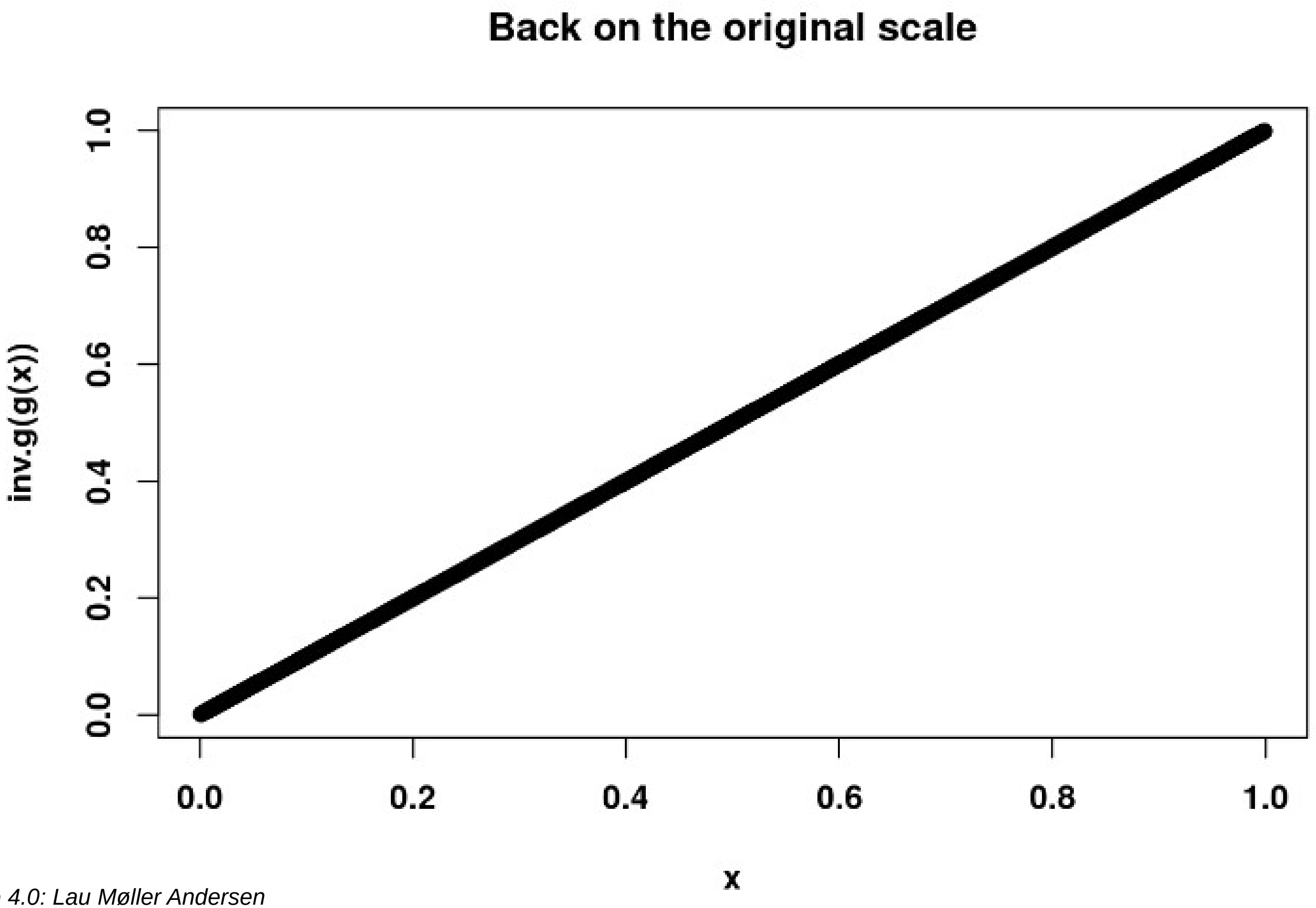
```r
x <- seq(0.001, 0.999, 0.001)
plot(x, main='Original probability data (on the range from 0-1)')
```



```r
plot(x, g(x), main='Log-it transformed, on the range from -Inf to Inf')
```



```r
plot(x, inv.g(g(x)), main='Back on the original scale')
```



These are the fitted values

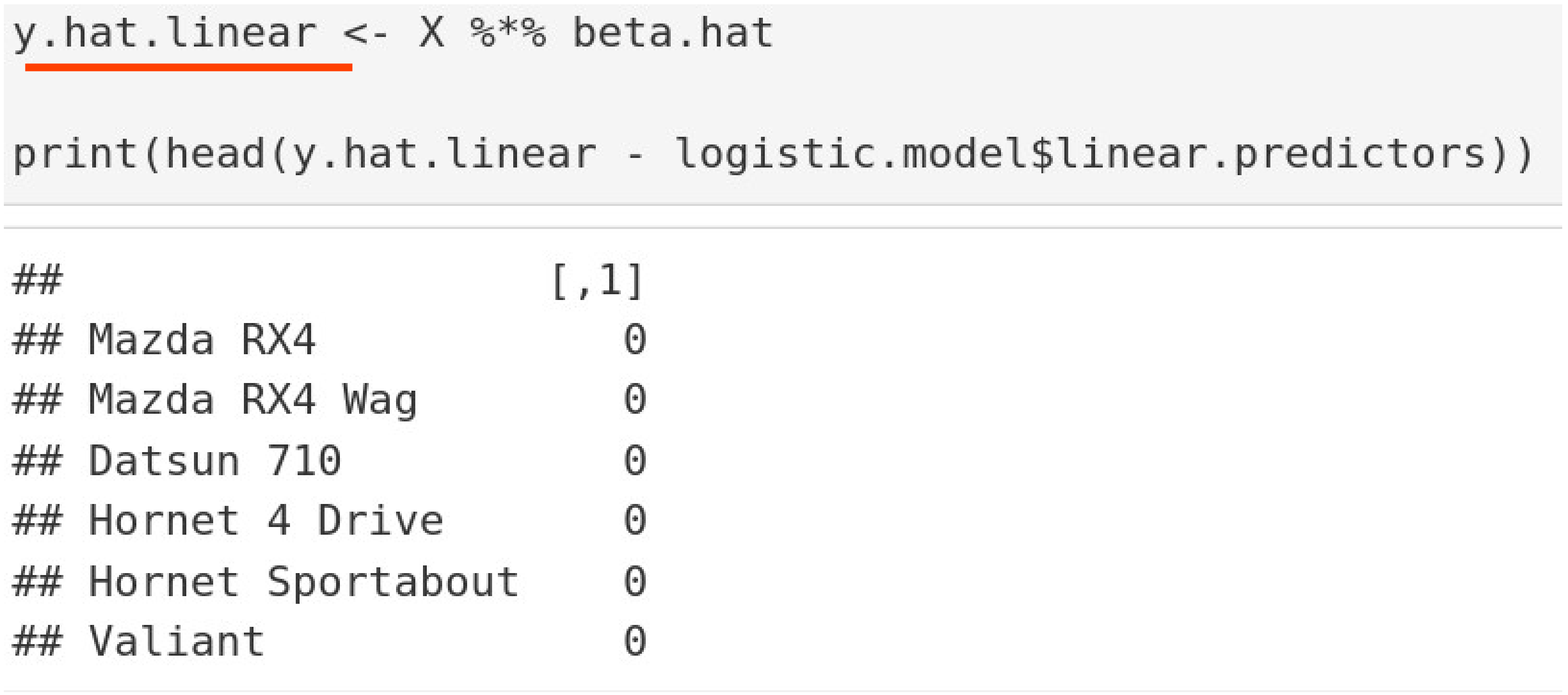
```
y.hat <- inv.g(X %*% beta.hat)
print(head(y.hat))
```

```
##                        [,1]
## Mazda RX4         0.8172115
## Mazda RX4 Wag     0.6157283
## Datsun 710        0.9373069
## Hornet 4 Drive    0.2897304
## Hornet Sportabout 0.1415972
## Valiant           0.1320944
```

```
print(head(y.hat - logistic.model$fitted.values))
```

```
##                   [,1]
## Mazda RX4            0
## Mazda RX4 Wag        0
## Datsun 710           0
## Hornet 4 Drive       0
## Hornet Sportabout    0
## Valiant              0
```

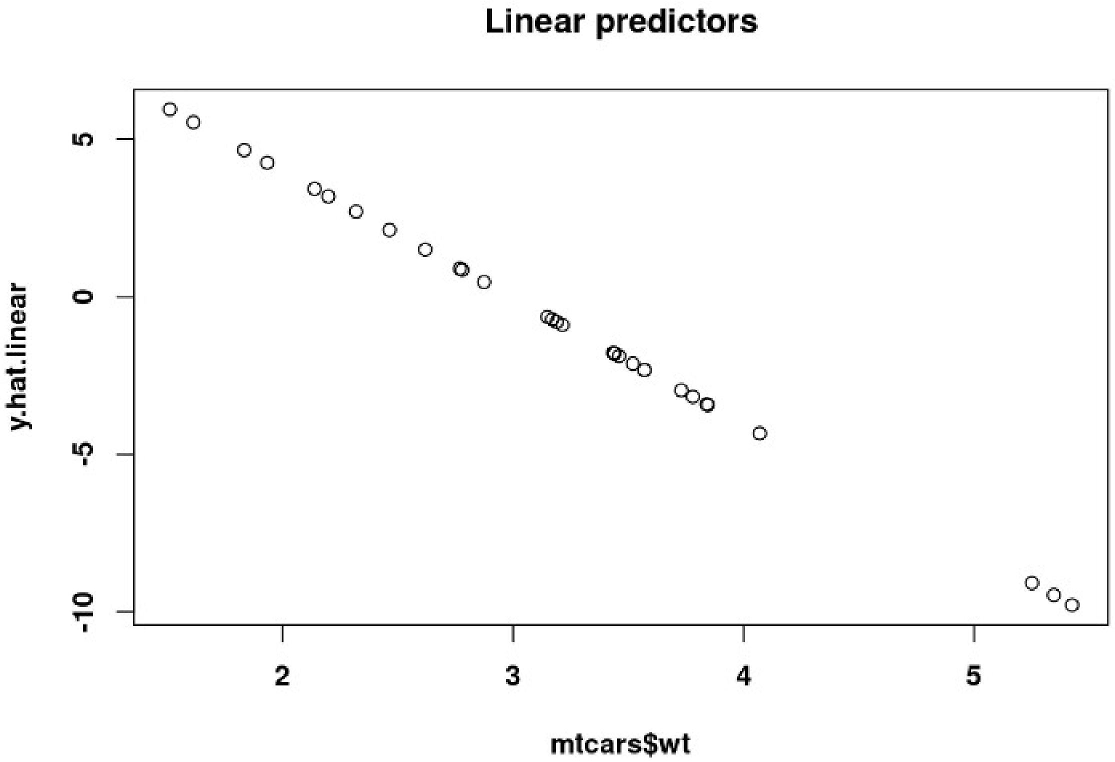
These are the linear predictors



```
y.hat.linear <- X %*% beta.hat

print(head(y.hat.linear - logistic.model$linear.predictors))
```

```
##                   [,1]
## Mazda RX4            0
## Mazda RX4 Wag        0
## Datsun 710           0
## Hornet 4 Drive       0
## Hornet Sportabout    0
## Valiant              0
```

Looks like a “normal” linear regression



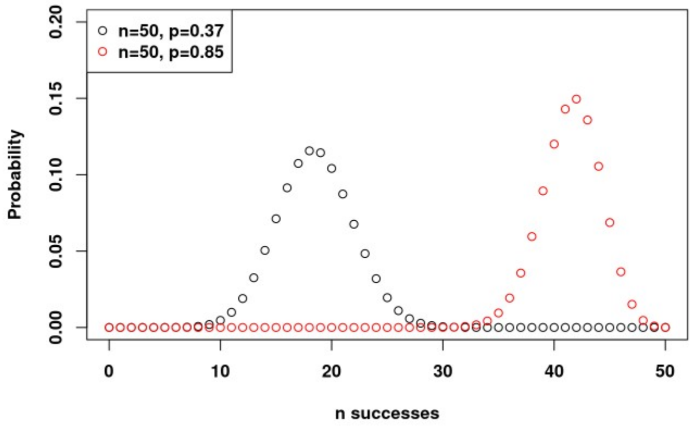
4) A data distribution: $p(y|\hat{y})$

Binomial distribution $B(n, p)$

Probability mass function (PMF): $\binom{n}{k} p^k q^{(n-k)}$

$n \in \{0,1,2,...\}$ - number of trials
$p \in [0,1]$ - success probability for each trial
$q = 1 - p$
$k \in \{0,1,...,n\}$ - number of successes

```
x <- 0:50
n <- 50
p <- 0.37
pmf <- dbinom(x=x, size=n, prob=p)

par(font.lab=2, font.axis=2)
plot(x, pmf, xlab='n successes', ylab='Probability', ylim=c(0, 0.2))

new.p <- 0.83
new.pmf <- dbinom(x=x, size=n, prob=new.p)
points(x, new.pmf, col='red')
legend('topleft', col=c('black', 'red'),
                         legend=c('n=50, p=0.37', 'n=50, p=0.85'), pch=1,
       text.font=2)
```



4) A data distribution: $p(y \mid \hat{y})$

But we are looking at the special case of n=1

$\Pr(y=1)=\hat{y}$

The $\textit{Bernoulli}$ distribution:

$$\mathbf{PMF_{Bernouilli}}=\boldsymbol{p^{k}q^{1-k}}$$

$0 \leq p \leq 1$

$q=1-p$

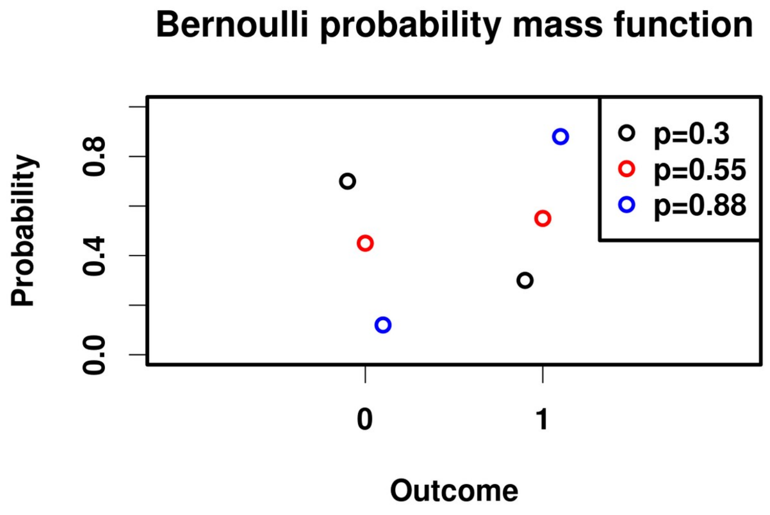
$k \in \{0,1\}$

$$\mathrm{PMF}_{\mathrm{Bernoulli}}=\binom{n}{k} p^{k} q^{(n-k)} (n=1 \text{ and } k \in \{0,1\})$$

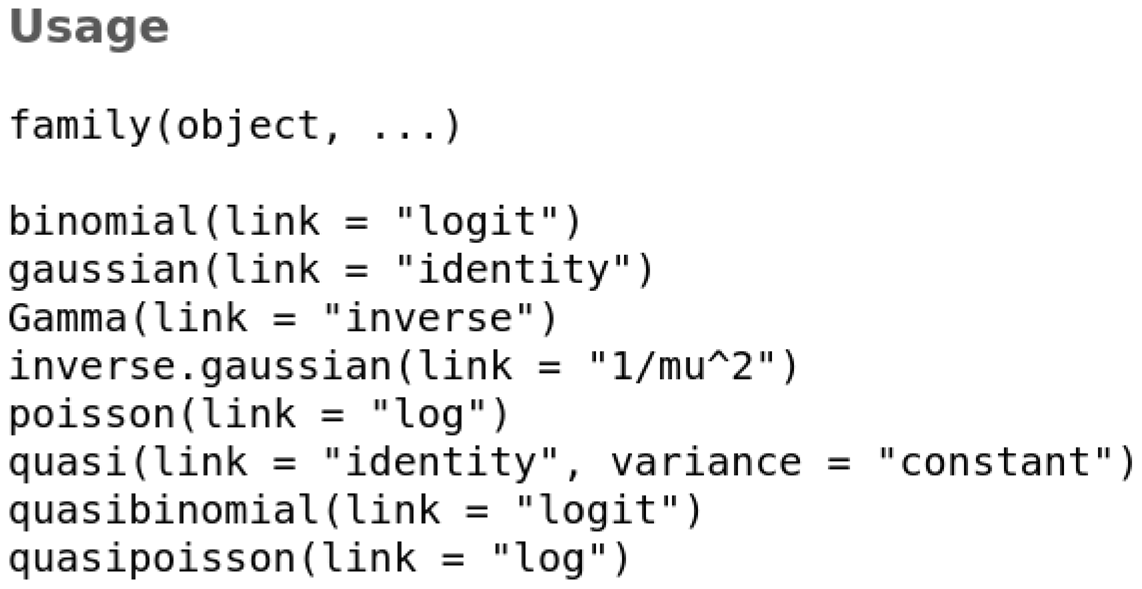
4) A data distribution: $p(y|\hat{y})$

$$\mathbf{PMF}_{\mathbf{Bernouilli}} = p^k q^{1-k}$$

```
dbernoul <- function(p, k) p^k * (1 - p)^(1 - k)

x <- c(0, 1)
pmf <- dbernoul(p=0.3, x)
par(font.lab=2, font.axis=2)
plot(x -0.1, pmf, xaxt='n', xlab='Outcome', ylab='Probability', ylim=c(0,
1),
     xlim=c(-1.1, 2.1), main='Bernoulli probability mass function')
axis(side=1, at=c(0, 1), labels=c(0, 1))

pmf <- dbernoul(p=0.55, x)
points(x, pmf, col='red')

pmf <- dbernoul(p=0.88, x)
points(x + 0.1, pmf, col='blue')

legend('topright', pch=1, col=c('black', 'red', 'blue'),
       legend=c('p=0.3', 'p=0.55', 'p=0.88'), text.font=2)
```



Some link functions



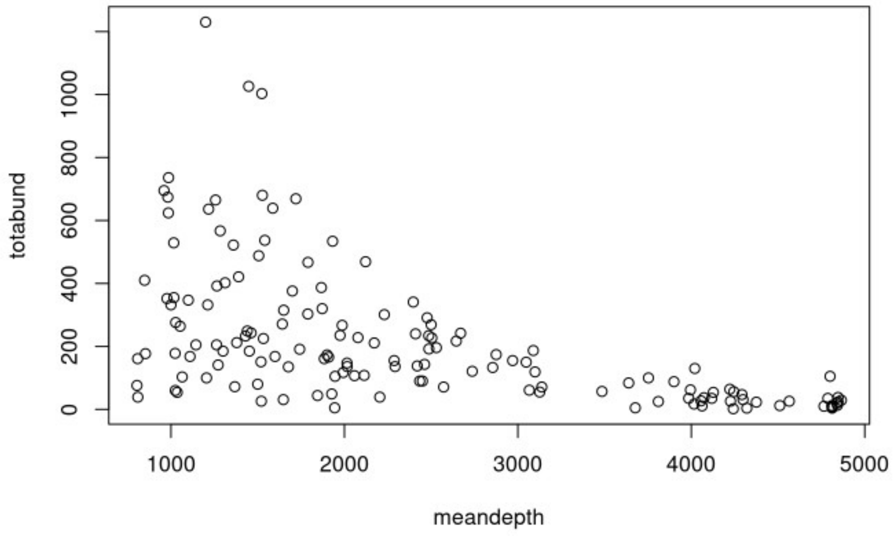
Usage

```
family(object, ...)

binomial(link = "logit")
gaussian(link = "identity")
Gamma(link = "inverse")
inverse.gaussian(link = "1/mu^2")
poisson(link = "log")
quasi(link = "identity", variance = "constant")
quasibinomial(link = "logit")
quasipoisson(link = "log")
```

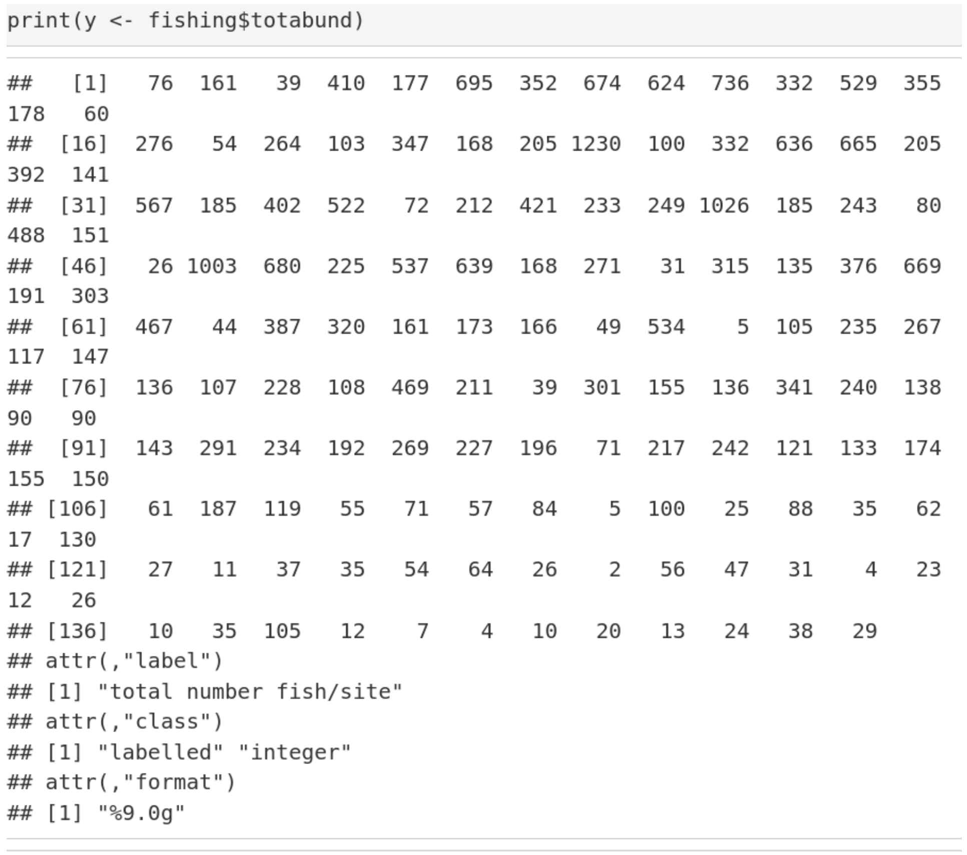
Have a look at Poisson as well

```
library(COUNT)
```

```
data(fishing)
plot(totabund ~ meandepth, data=fishing)
```



1) A data vector: $y = (y_1, \ldots, y_n)$



```
print(y <- fishing$totabund)
```

```
##   [1]   76  161   39  410  177  695  352  674  624  736  332  529  355
178   60
##  [16]  276   54  264  103  347  168  205 1230  100  332  636  665  205
392  141
##  [31]  567  185  402  522   72  212  421  233  249 1026  185  243   80
488  151
##  [46]   26 1003  680  225  537  639  168  271   31  315  135  376  669
191  303
##  [61]  467   44  387  320  161  173  166   49  534    5  105  235  267
117  147
##  [76]  136  107  228  108  469  211   39  301  155  136  341  240  138
90   90
##  [91]  143  291  234  192  269  227  196   71  217  242  121  133  174
155  150
## [106]   61  187  119   55   71   57   84    5  100   25   88   35   62
17  130
## [121]   27   11   37   35   54   64   26    2   56   47   31    4   23
12   26
## [136]   10   35  105   12    7    4   10   20   13   24   38   29
## attr(,"label")
## [1] "total number fish/site"
## attr(,"class")
## [1] "labelled" "integer"
## attr(,"format")
## [1] "%9.0g"
```

2) Predictors: X and coefficients β, forming a linear predictor $X\beta$

```
poisson.model <- glm(totabund ~ meandepth, data=fishing, family='poisson
')
X <- model.matrix(poisson.model)
print(head(X))
```

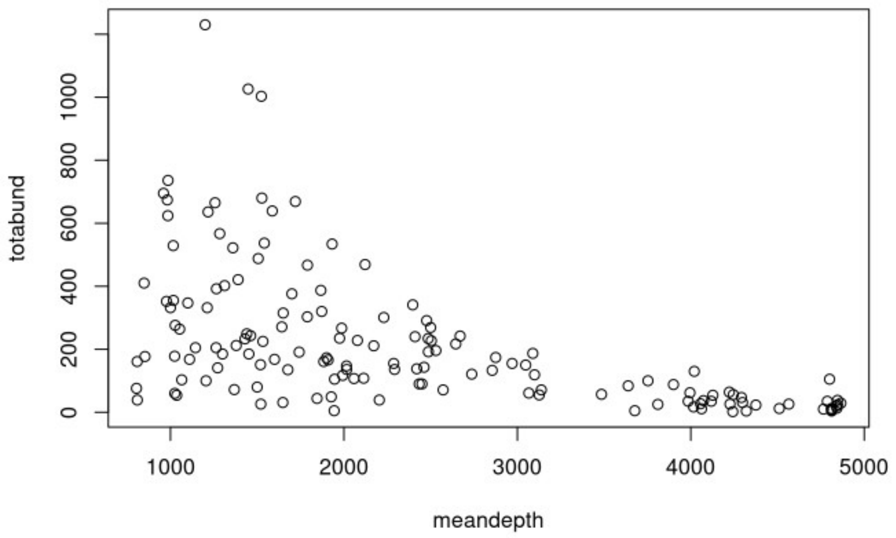
```
##   (Intercept) meandepth
## 1           1       804
## 2           1       808
## 3           1       809
## 4           1       848
## 5           1       853
## 6           1       960
```

```
print(beta.hat <- poisson.model$coefficients)
```

```
##   (Intercept)     meandepth
##  6.6465755329 -0.0006309148
```

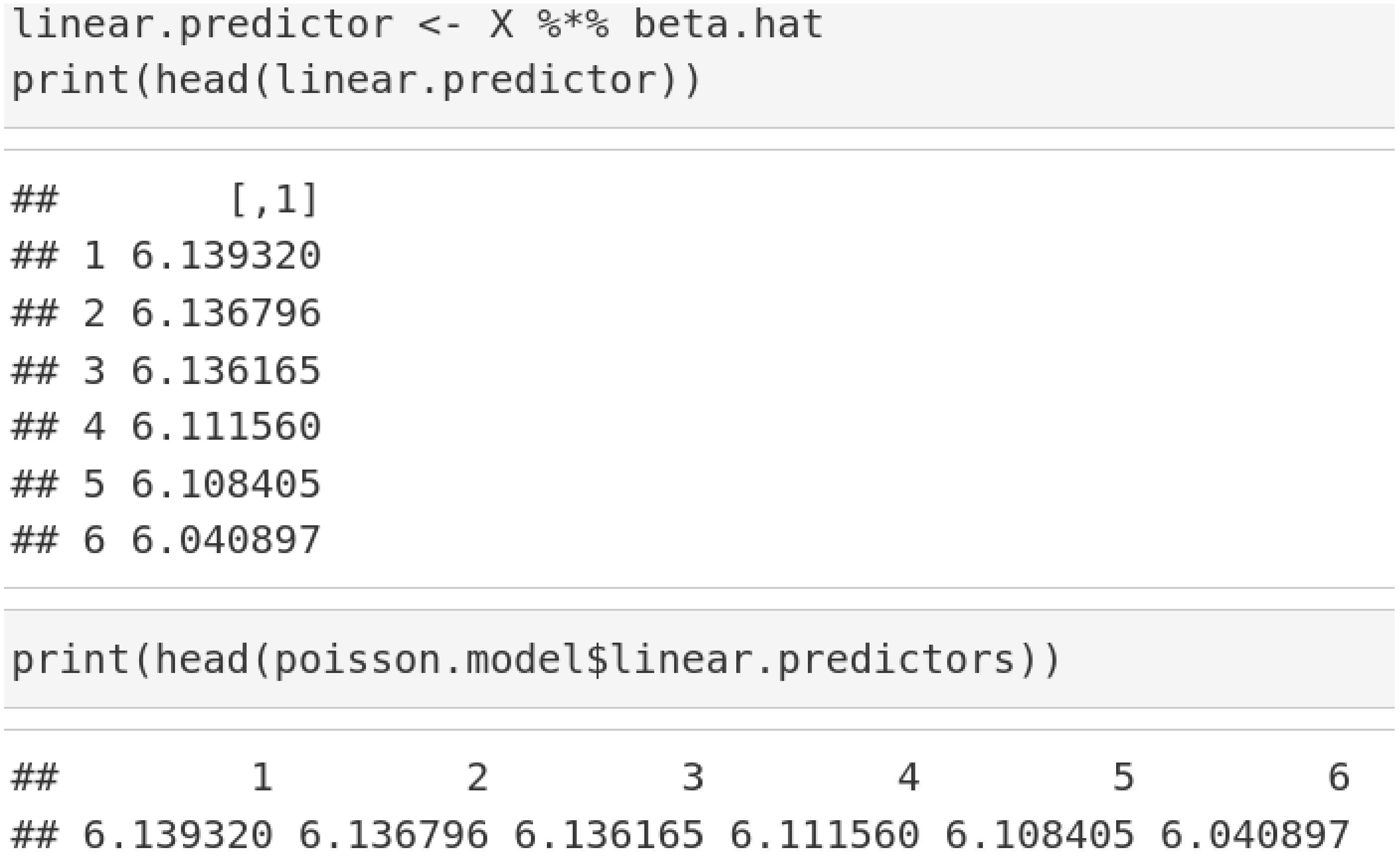
Data is not continuous...

```
data(fishing)
plot(totabund ~ meandepth, data=fishing)
```



... but the linear predictor is

$X\beta \in R_{>0}$



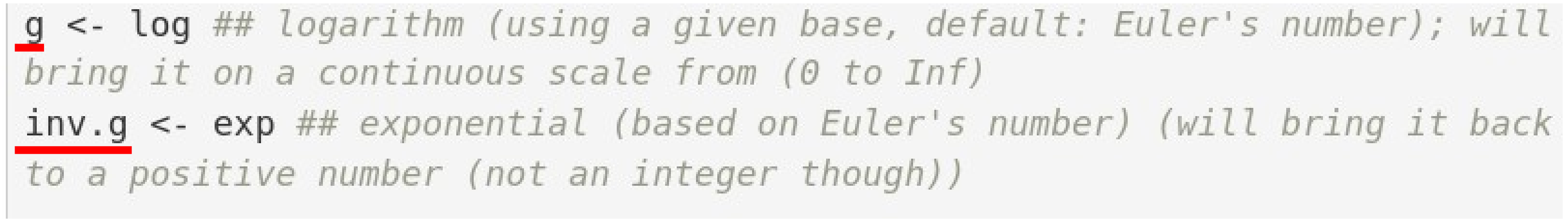
```
linear.predictor <- X %*% beta.hat
print(head(linear.predictor))
```

```
##       [,1]
## 1 6.139320
## 2 6.136796
## 3 6.136165
## 4 6.111560
## 5 6.108405
## 6 6.040897
```

```
print(head(poisson.model$linear.predictors))
```

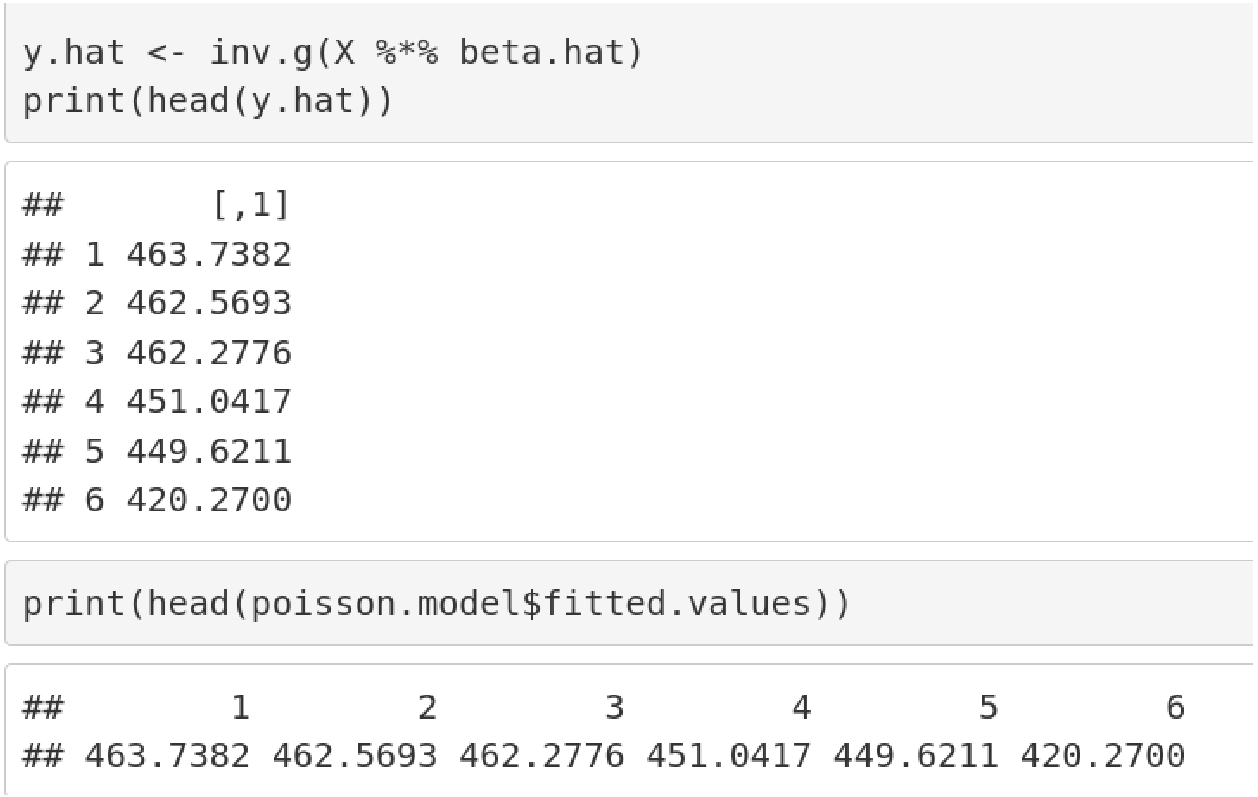
```
##        1        2        3        4        5        6
## 6.139320 6.136796 6.136165 6.111560 6.108405 6.040897
```

3) A *link function* g: yielding a vector of transformed data $\hat{y}=g^{-1}(X\beta)$ that are used to model the data



```
g <- log ## logarithm (using a given base, default: Euler's number); will
bring it on a continuous scale from (0 to Inf)
inv.g <- exp ## exponential (based on Euler's number) (will bring it back
to a positive number (not an integer though))
```

3) A *link function* g: yielding a vector of transformed data $\hat{y} = g^{-1}(X\beta)$ that are used to model the data



```
y.hat <- inv.g(X %*% beta.hat)
print(head(y.hat))
```

```
##       [,1]
## 1 463.7382
## 2 462.5693
## 3 462.2776
## 4 451.0417
## 5 449.6211
## 6 420.2700
```

```
print(head(poisson.model$fitted.values))
```

```
##        1        2        3        4        5        6
## 463.7382 462.5693 462.2776 451.0417 449.6211 420.2700
```

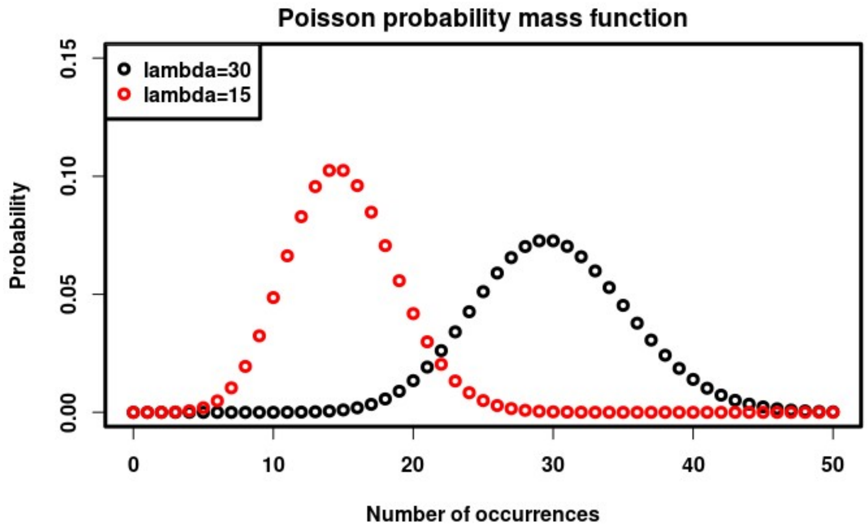
4) A data distribution: $p(y|\hat{y})$

$\boldsymbol{Poisson}(\boldsymbol{\lambda})$

$\lambda \in (0, \infty)$: the Expected value (rate)

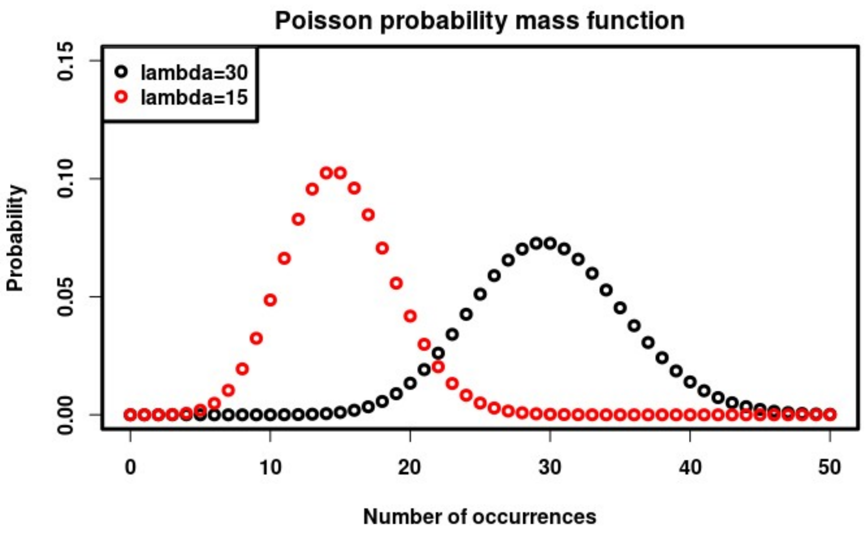
$k \in N_0$

$$PMF = \frac{\lambda^k e^{-\lambda}}{k!}$$



4) A data distribution: $p(y|\hat{y})$

```r
x <- 0:50 # counts, thus integers
lambda <- 30
pmf <- dpois(x, lambda)

par(font.lab=2, font.axis=2, cex=1, lwd=3)
plot(x, pmf, xlab='Number of occurrences', ylab='Probability',
     main='Poisson probability mass function', ylim=c(0, 0.15))

lambda <- 15
pmf <- dpois(x, lambda)
points(x, pmf, col='red')

legend('topleft',
       legend=c(expression(paste(lambda, '=', 30)),
                expression(paste(lambda, '=', 15))),
       pch=1, col=c('black', 'red'), text.font=2)
```

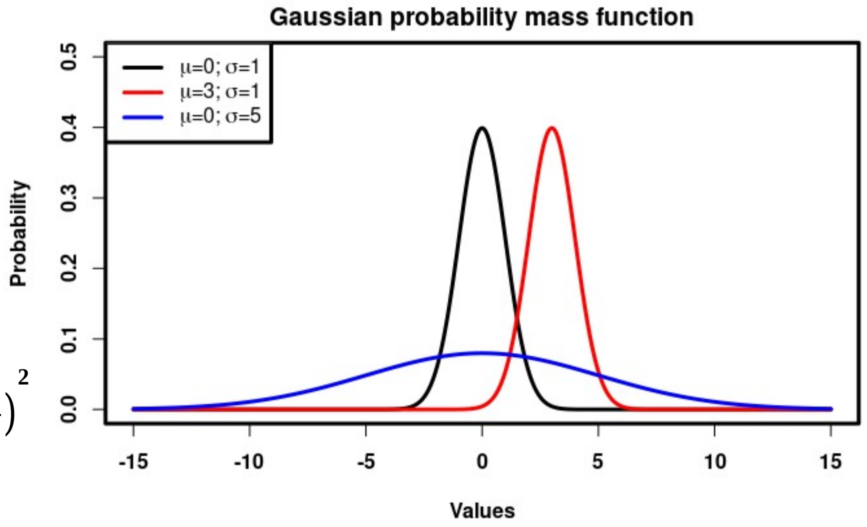


... the identity link

```r
g <- identity
inv.g <- identity ## identity-¹ = identity
```

$$N(\mu, \sigma^2)$$
$$\mu \in R$$
$$\sigma^2 \in R_{>0}$$
$$x \in R$$

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



Nomenclature

- General Linear Model (single level modelling)
  - $y = X\beta + \epsilon$
- Generalized Linear Model (single level modelling)
  - $y = X\beta + \epsilon$ – but now with link functions and other data distributions besides the Gaussian one
- General Linear Mixed Model (multilevel modelling)
  - $y = X\beta + Zu + \epsilon$
- Generalized Linear Mixed Model (multilevel modelling)
  - $y = X\beta + Zu + \epsilon$ – but now with link functions and other data distributions besides the Gaussian one

Specifying random (second-level) effects

```
(1 | subject) # intercept only
(slope | subject) # slope and intercept
(1 + slope | subject) # slope and intercept (explicit)
(0 + slope | subject) # slope only
(1 + slope || subject) # slope and intercept but force covariance to 0
```

The general linear mixed model (GLMM)

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u} + \boldsymbol{\epsilon}$$

$y : N \, x \, 1$ column vector

$X : N \, x \, p$ matrix of p predictor variables

$\beta :$ unknown $p \, x \, 1$ column vector of the first level regression coefficients

$Z : N \, x \, q$ design matrix for the q random effects

$u :$ unknown $q \, x \, 1$ column vector of the second-level effects

$\epsilon : N \, x \, 1$ column vector of the residuals

Sleep study

```
model <- lmer(Reaction ~ days_deprived + (days_deprived | Subject), data=
sleepstudy)
```

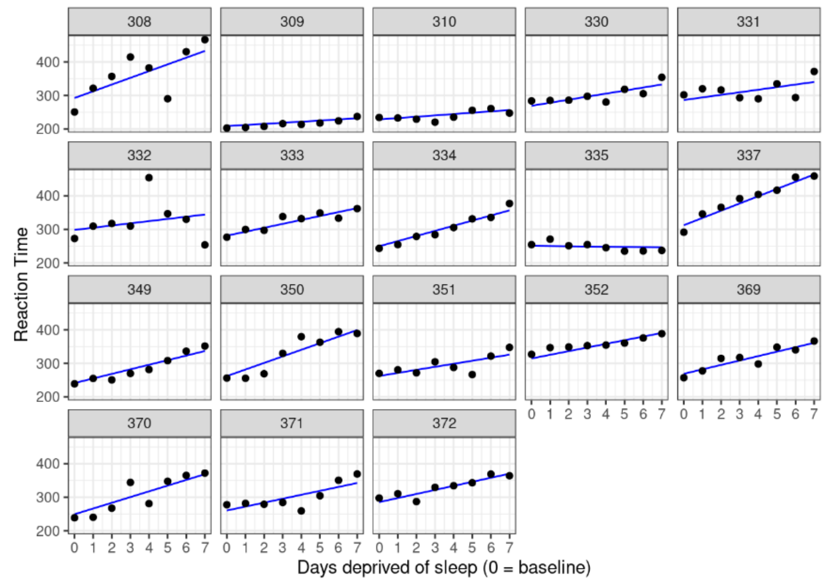
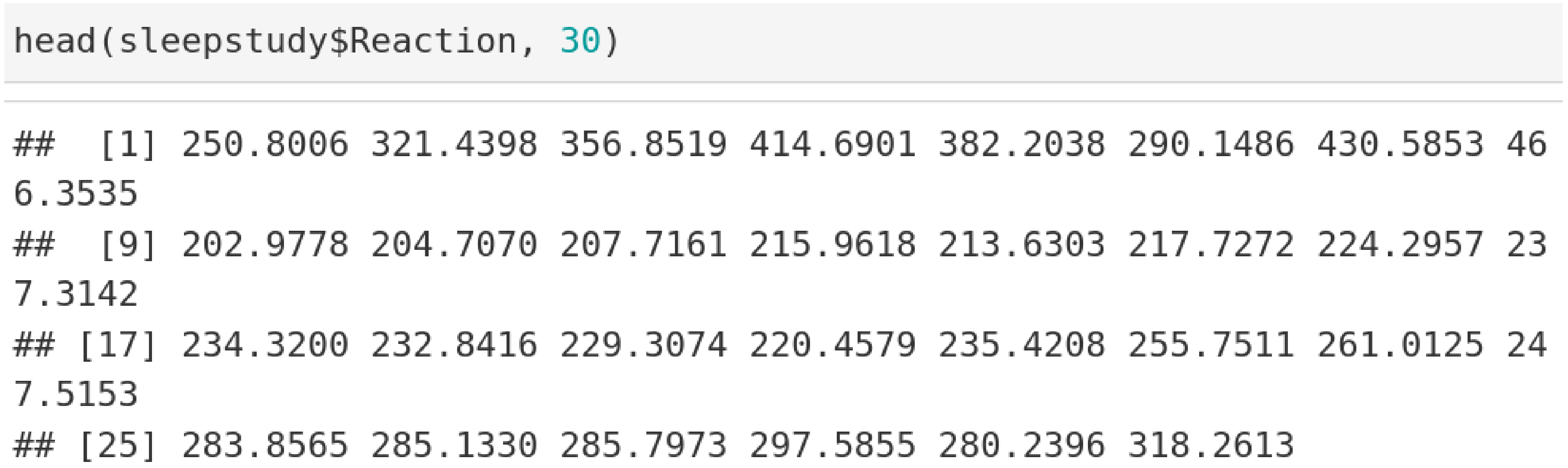


Figure 5.6: Data plotted against predictions from a partial pooling approach.

$$\boxed{y} = X\beta + Zu + \epsilon$$

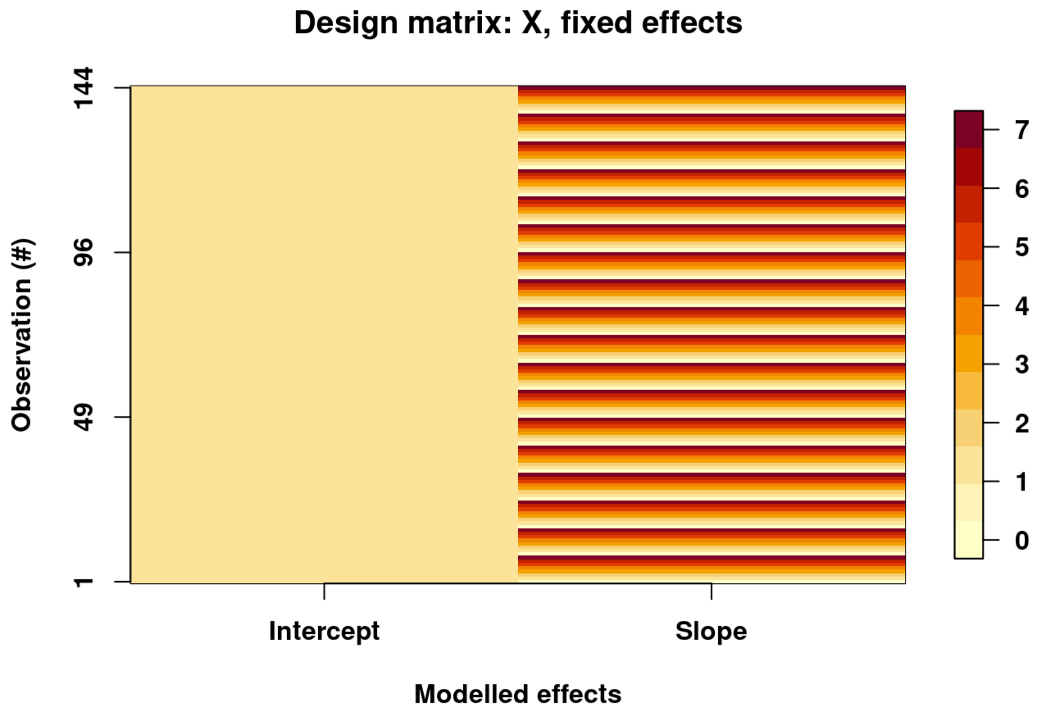
$y =$



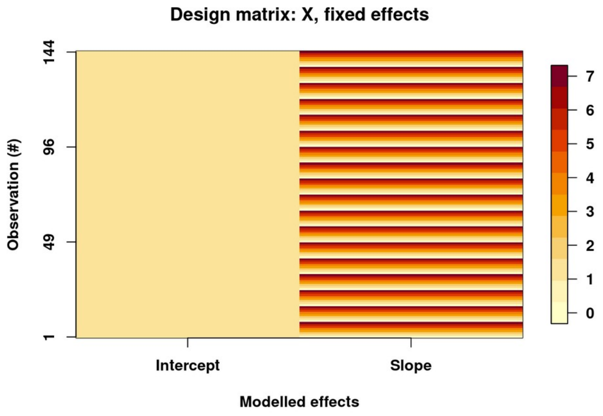
```
head(sleepstudy$Reaction, 30)
```

```
##  [1] 250.8006 321.4398 356.8519 414.6901 382.2038 290.1486 430.5853 46
6.3535
##  [9] 202.9778 204.7070 207.7161 215.9618 213.6303 217.7272 224.2957 23
7.3142
## [17] 234.3200 232.8416 229.3074 220.4579 235.4208 255.7511 261.0125 24
7.5153
## [25] 283.8565 285.1330 285.7973 297.5855 280.2396 318.2613
```

$$y = \boxed{X}\beta + Zu + \epsilon$$



$$y = X \boxed{\beta} + Zu + \epsilon$$



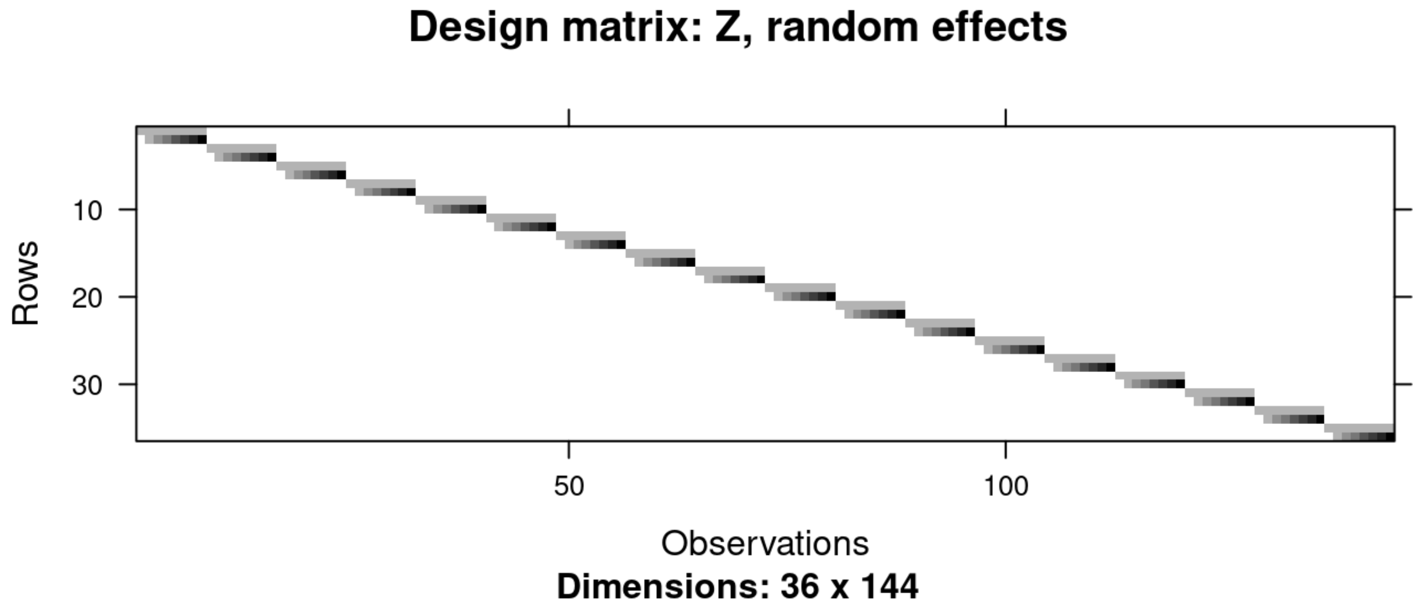
$$\hat{\beta} =$$

```
fixef(model)
```

```
##    (Intercept) days_deprived
##      267.96742      11.43543
```

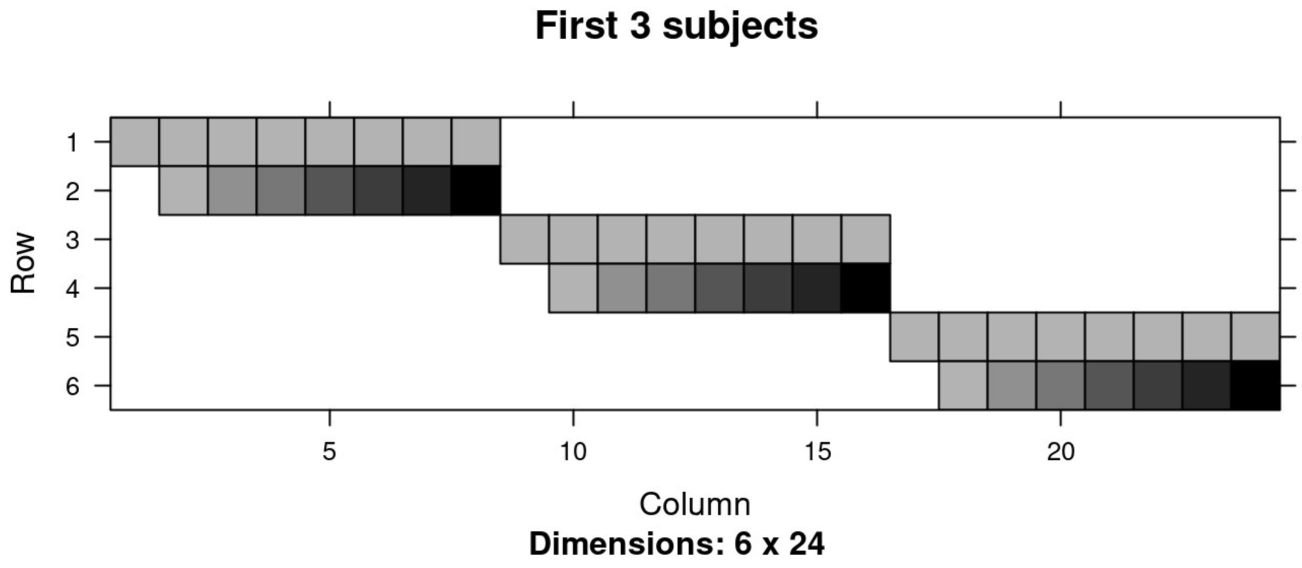
```
Xt <- t(getME(model, 'X'))
```

$$y = X\beta + \boxed{Z} u + \epsilon$$



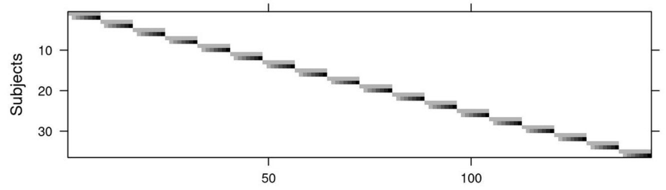
```r
Zt <- getME(model, 'Zt')
```

$$y = X\beta + \boxed{Z}u + \epsilon$$



$$y = X\beta + Z\boxed{u} + \epsilon$$

Design matrix: Z, random effects



Dimensions: 36 x 144

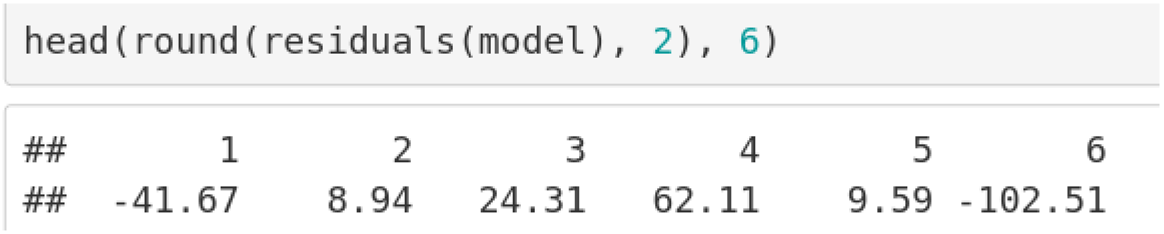
$$\hat{u} =$$

```
ranef(model)
```

```
## $Subject
##     (Intercept) days_deprived
## 308  24.4991541     8.6020120
## 309 -59.3707875    -8.1280623
## 310 -39.4754543    -7.4293973
## 330   1.3497667    -2.3845341
## 331  18.4565538    -3.7474999
## 332  30.5253684    -4.8933314
## 333  13.3677150     0.2889674
## 334 -18.1572414     3.8434349
## 335 -16.9742694   -12.0701072
## 337  44.5843235    10.1762260
## 349 -26.6826682     2.1944025
## 350  -5.9647975     8.1756325
## 351  -5.5710438    -2.3718429
## 352  46.6328765    -0.5612423
## 369   0.9617659     1.7384827
## 370 -18.5204352     5.6314774
## 371  -7.3428235     0.2728619
## 372  17.6819971     0.6625203
```

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u} + \boxed{\boldsymbol{\epsilon}}$$

$\boldsymbol{\epsilon} =$



```
head(round(residuals(model), 2), 6)
```

```
##       1       2       3       4       5       6
##  -41.67    8.94   24.31   62.11    9.59 -102.51
```

Bonus question:

Why do the random effects have a mean of 0?

Did you learn?

Generalized Linear Mixed Effects Models (GLMM)

1) Understanding that we can extend the scope of our multilevel modelling by using appropriate link functions and data distributions

2) Understanding the multilevel equivalent of the GLM

Learning goals (will not finish this today)

Explanation and prediction

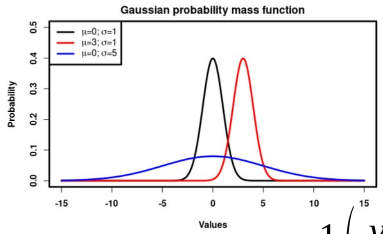
1) Understanding that fitting (explaining) often leads to overfitting

2) Learning methods to prevent overfitting, e.g. by introducing *bias* and using *cross-validation*

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

Maximum likelihood estimation

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



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

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

$$\textbf{Log-Likelihood function}: \log(L)$$

y: dependent variable
$X\beta$: linear predictor
$y - X\beta = \epsilon$: residuals
N: number of observations

We have so far been fitting *explanatory* models, i.e. by maximising log-likelihood

```
model <- lmer(Reaction ~ days_deprived + (days_deprived | Subject),
              data=sleepstudy)
model.ranint <- lmer(Reaction ~ days_deprived + (1 | Subject),
              data=sleepstudy)
```

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

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

```
print(ll.mr <- logLik(model.ranint))
```

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

```
exp(ll.m)
```

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

```
exp(ll.mr)
```

```
## 'log Lik.' 2.986092e-311 (df=4)
```

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

maximises the likelihood of

$$\boldsymbol{Y} = \boldsymbol{X} \boldsymbol{\beta} + \boldsymbol{\epsilon}$$

for which link function?

To fit is to overfit

(Yarkoni and Westfall, 2017)

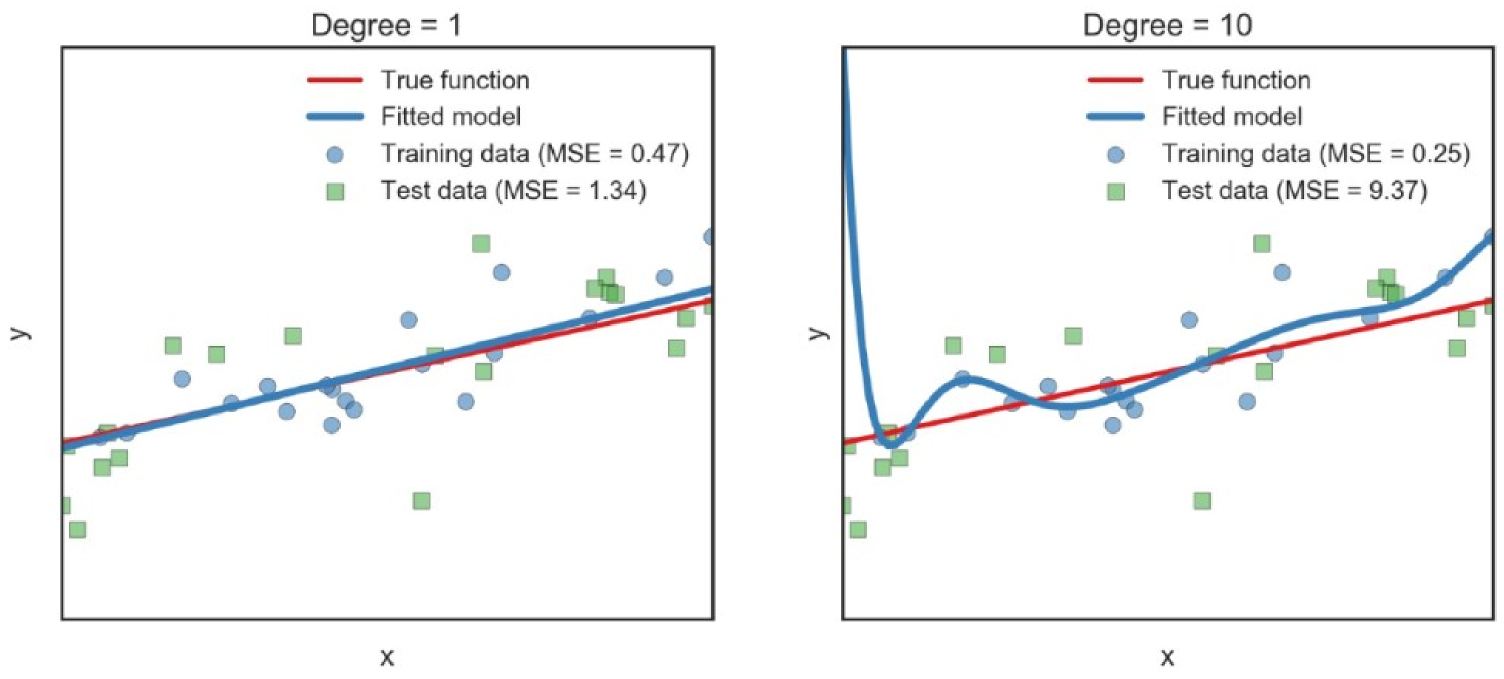
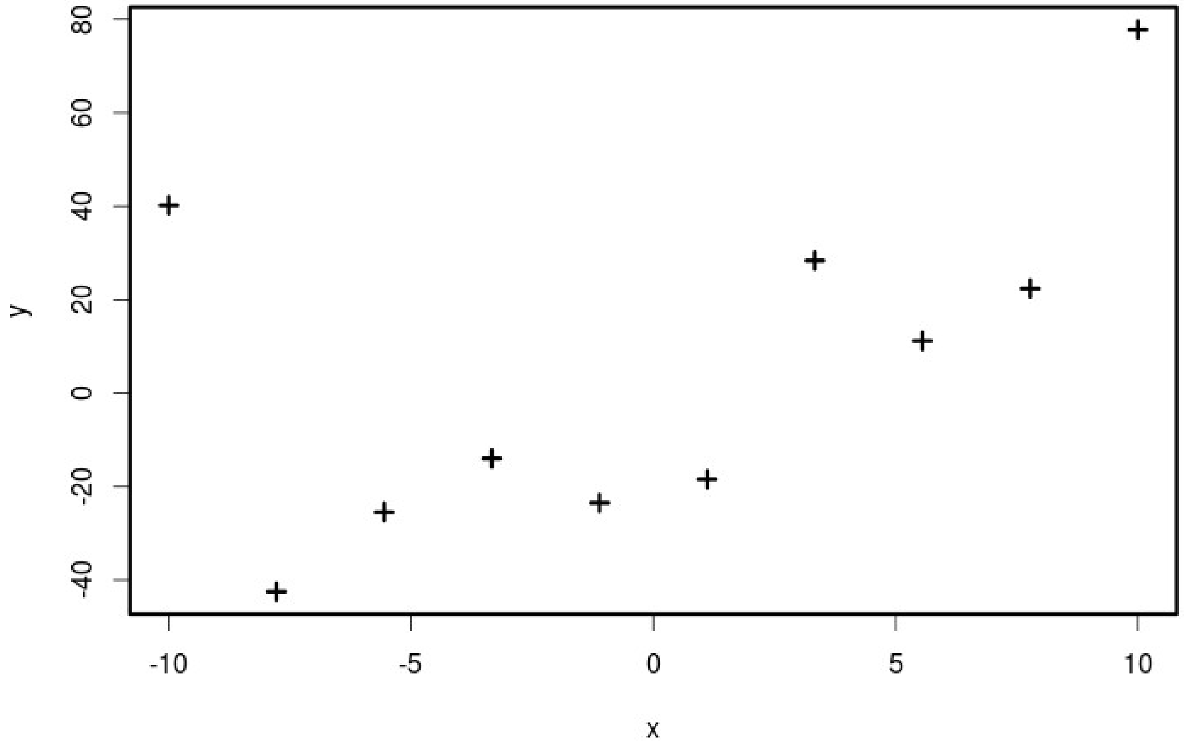


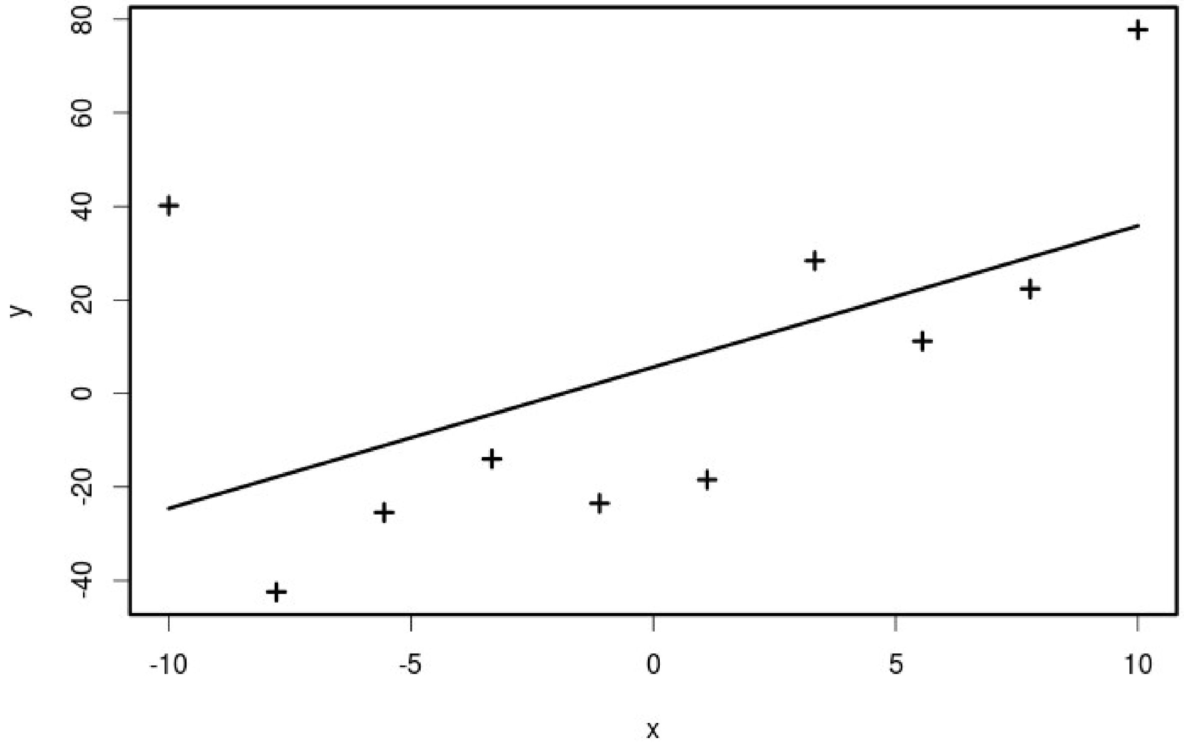
Fig. 1. Training and test error produced by fitting either a linear regression (left) or a 10th-order polynomial regression (right) when the true relationship in the population (red line) is linear. In both cases, the test data (green) deviate more from the model's predictions (blue line) than the training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

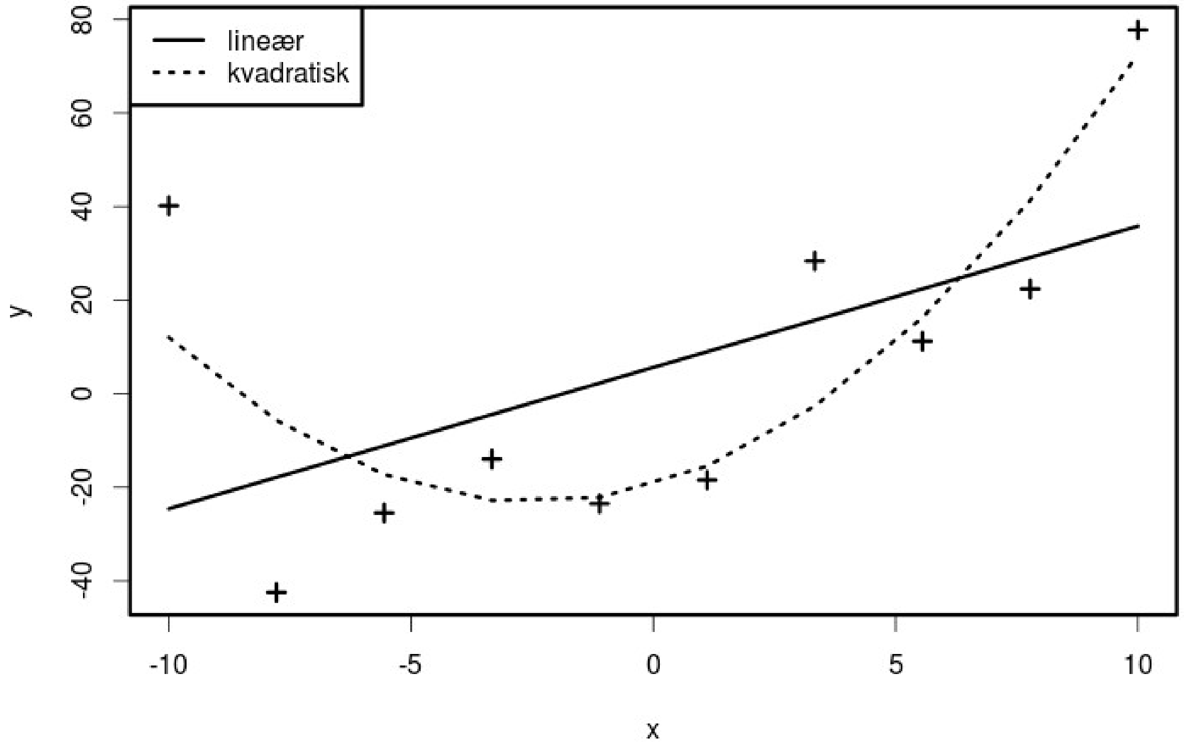
A sample of 10
linear or quadratic?



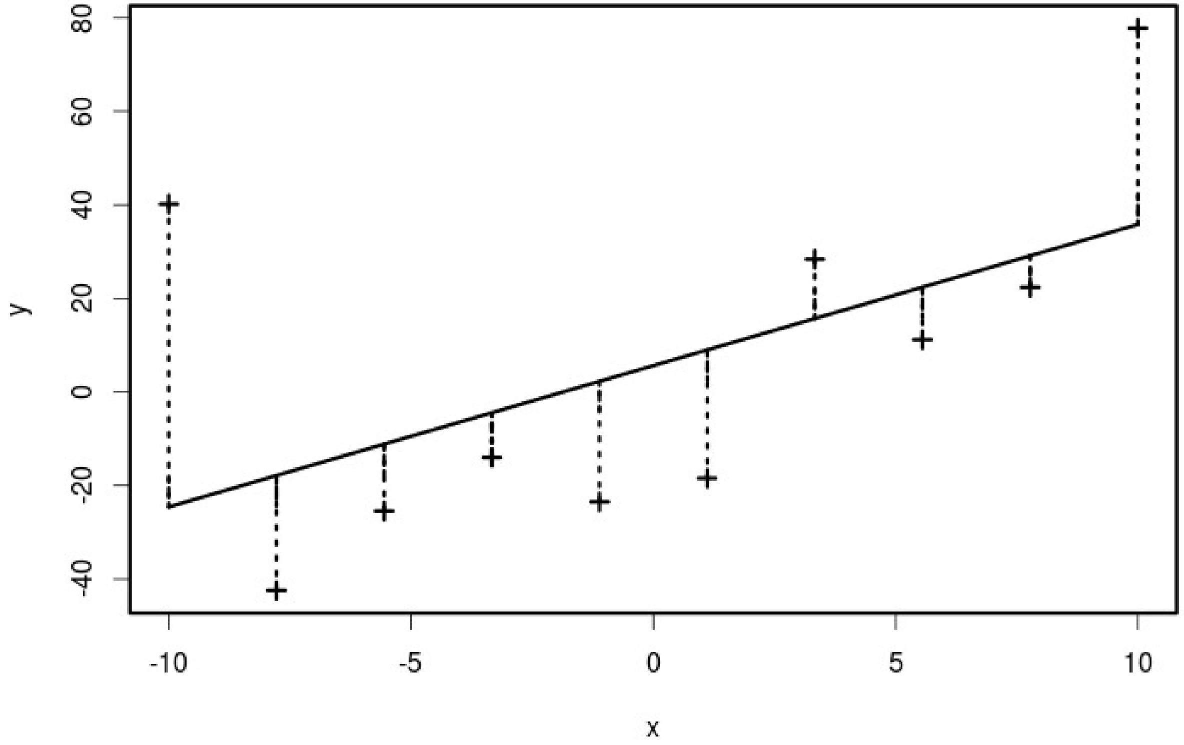
A sample of 10
linear or quadratic?



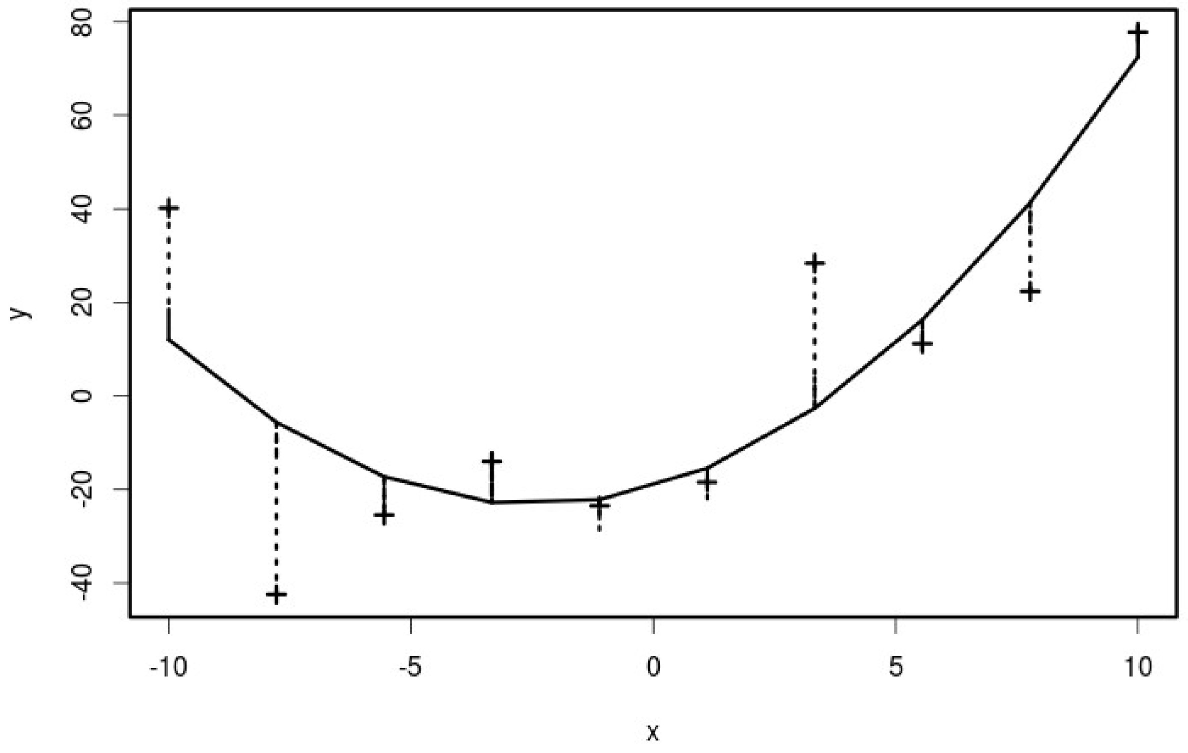
A sample of 10
linear or quadratic?



Residuals (linear)



Residuals (quadratic)



Quadratic:

$ax^2 + bx + c$

Linear:

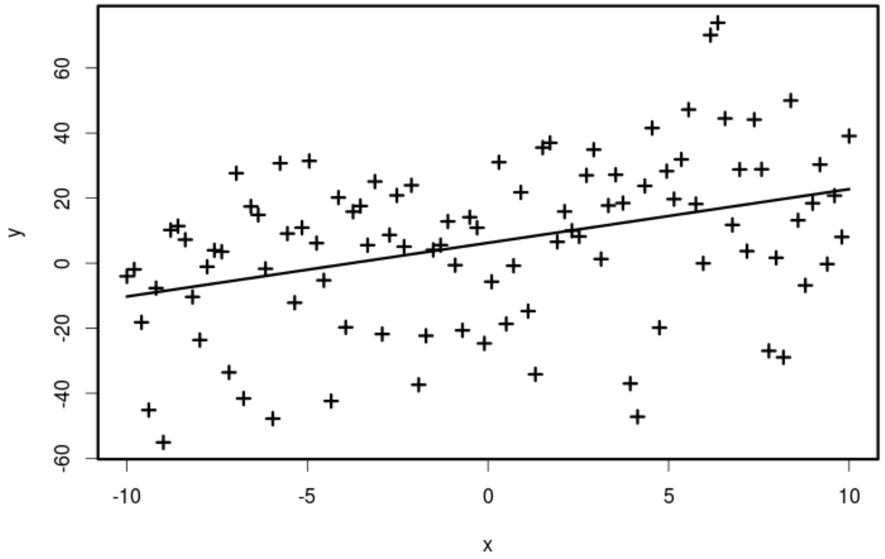
$bx + c$

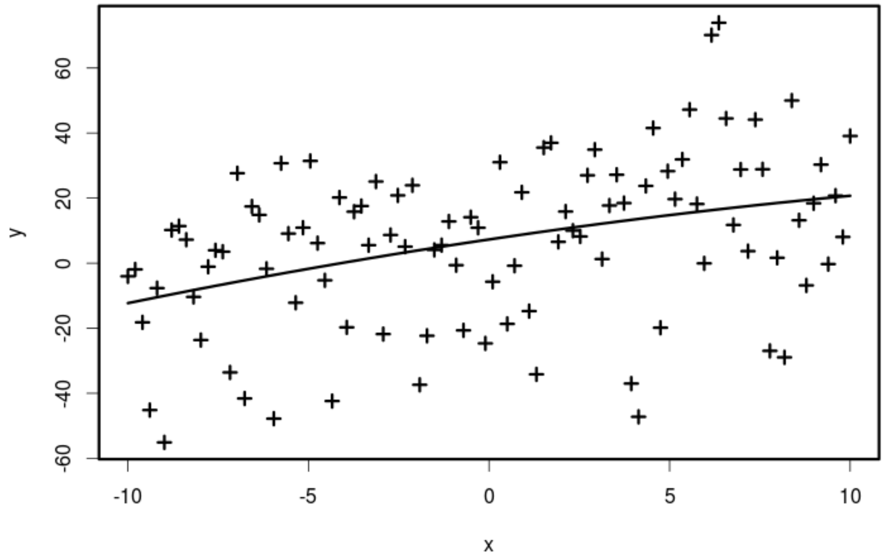
Estimates

a = 0,6184; $\boxed{b = 3,0201}$

$\boxed{b = 3,020}$

Now a sample of 100





b = 1,650

a = -0,03074 ≈ 0; b = 1,650

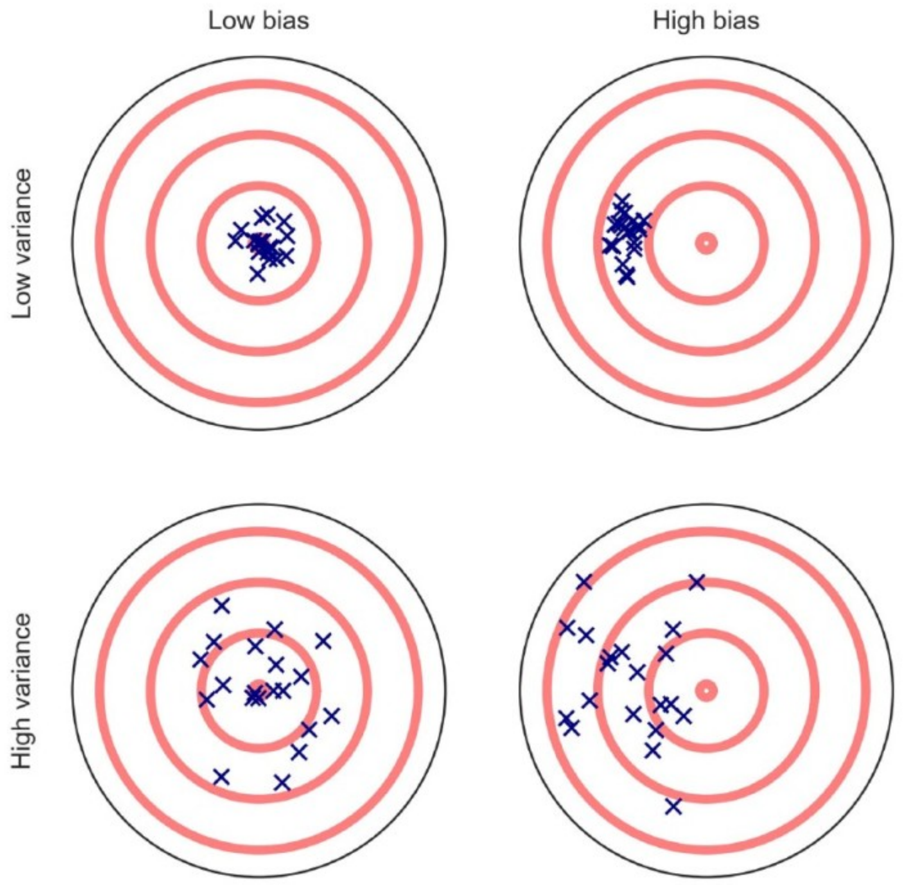


Fig. 2. An estimator's predictions can deviate from the desired outcome (or true scores) in two ways. First, the predictions may display a systematic tendency (or *bias*) to deviate from the central tendency of the true scores (compare right panels with left panels). Second, the predictions may show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

(Yarkoni and Westfall, 2017)

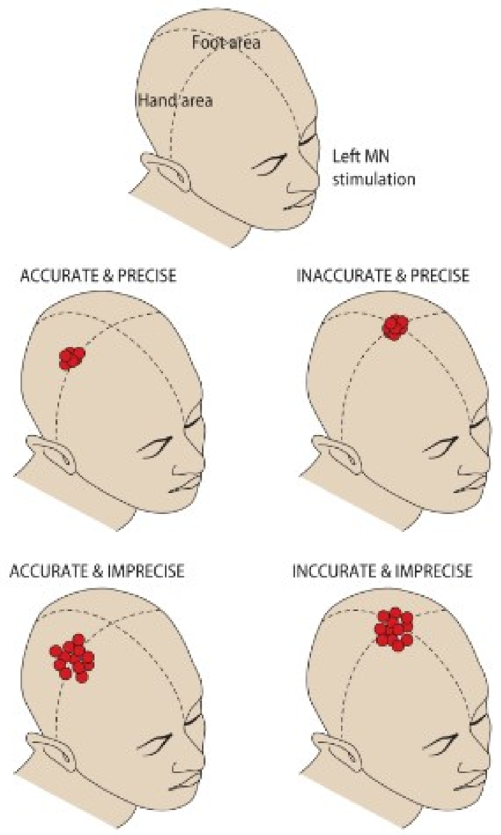


FIGURE 3.7. Accuracy versus precision. A schematic illustration of the differences between accuracy and precision of source localization. After left median-nerve stimulation, activations is expected in the right-hemisphere hand region of the primary somatosensory cortex. The foot area is shown at the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

(Hari and Puce, 2017)

(Yarkoni and Westfall, 2017)

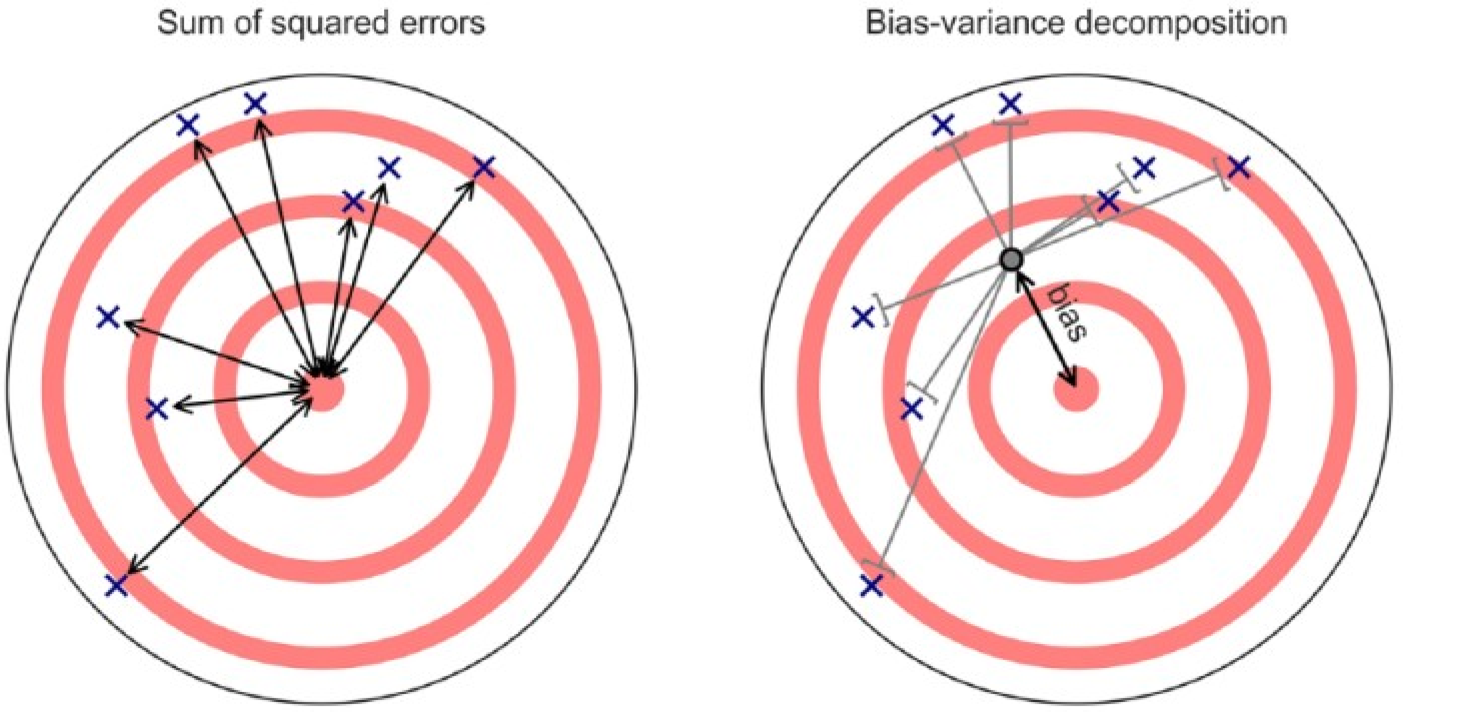


Fig. 3. Schematic illustration of the bias-variance decomposition. (Left) Under the classical error model, prediction error is defined as the sum of squared differences between true scores and observed scores (black lines). (Right) The bias-variance decomposition partitions the total sum of squared errors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

The benefit of large samples

(Yarkoni and Westfall, 2017)

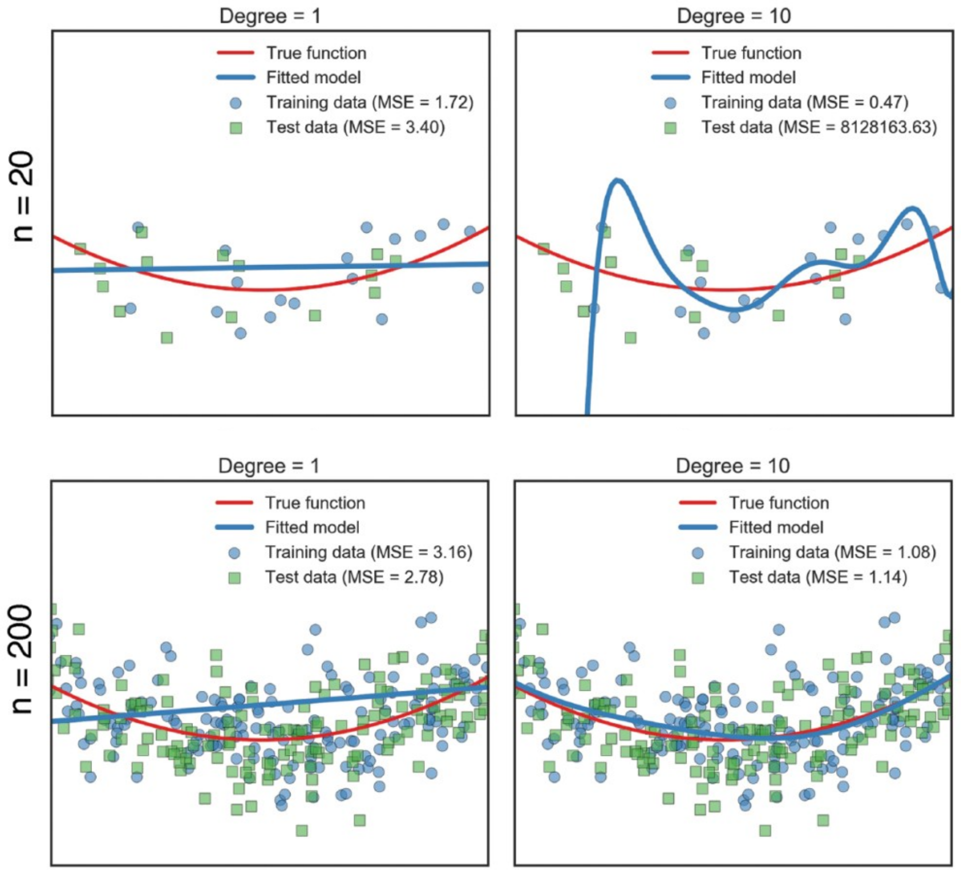


Fig. 4. Large samples guard against overfitting. See text for explanation.

References

- 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