

Getting to fit models in R

Alexandre Courtiol

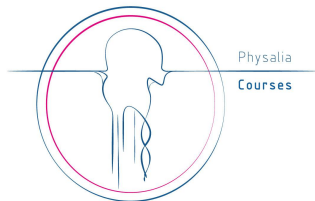
Leibniz Institute of Zoo and Wildlife Research

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and Wildlife Research**

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Getting started with R

- 1 Introduction
- 2 Linear Models
- 3 Generalised Linear Models
- 4 Mixed Models
- 5 General Additive (Mixed) Models

What is a linear model?

A statistical model represents, often in considerably idealized form, the data-generating process (https://en.wikipedia.org/wiki/Statistical_model).

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R allows to fit efficiently and easily all main kinds of linear models:

- classical linear models (t-test, correlation, linear regression, ANOVA, ANCOVA): LM
- generalized linear models (logistic regression, Poisson regression...): GLM
- linear mixed-effects models: LMM
- generalized linear mixed-effects models: GLMM
- general additive models & general additive mixed models: GAM & GAMM

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Note: I have a 100 hours course on the topic (<https://github.com/courtio1/LM2GLMM>) but it may be a bit terse without the bla bla...

Linear models in R

R is very rich in terms of capabilities to fit linear models due to an increasing number of dedicated packages!

For now, no other software seems to be remotely as good (prognostic: only Julia or Python may change that within a decade but I find it unlikely).

Linear models in R

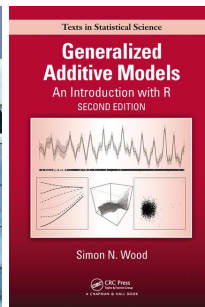
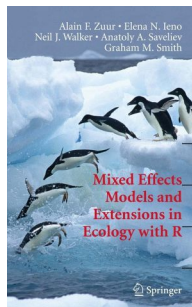
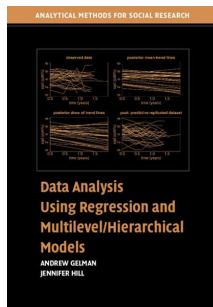
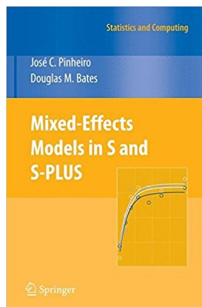
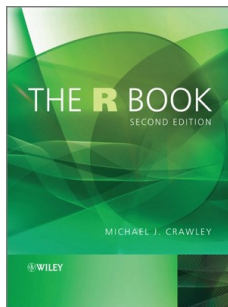
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Models	Packages for fitting	Helper packages
LM	none; spaMM	car; lmtest; visreg
GLM	none; spaMM	car; DHARMA; visreg
LMM	lme4; spaMM; glmmTMB	DHARMA; pbkrtest
GLMM	lme4; spaMM; glmmTMB	DHARMA; pbkrtest
GAM	mgcv	visreg
GAMM	mgcv	

Note: those are my personal favorite ones, but they are plenty more out there.

Good books dealing with linear models in R



Note: it is also useful to look at books not focussed on R!

Preparing data for (G)LM(M) & GA(M)

To maximize the chances of success prepare your data as follow:

- one row = one observation (if repeated measures, use several rows!)
- qualitative variables of class `factor` (check the levels, drop unused ones, set the reference properly)
- no NA (models can somewhat deal with them but it is a major source of headaches)

Preparing data for (G)LM(M) & GA(M)

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- qualitative variables of class factor (check the levels, drop unused ones, set the reference properly)
- no NA (models can somewhat deal with them but it is a major source of headaches)

Example of a good dataset:

```
head(iris)

##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1         5.1         3.5         1.4         0.2   setosa
## 2         4.9         3.0         1.4         0.2   setosa
## 3         4.7         3.2         1.3         0.2   setosa
## 4         4.6         3.1         1.5         0.2   setosa
## 5         5.0         3.6         1.4         0.2   setosa
## 6         5.4         3.9         1.7         0.4   setosa

str(iris)

## 'data.frame': 150 obs. of  5 variables:
##  $ Sepal.Length: num  5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
##  $ Sepal.Width : num  3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
##  $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
##  $ Petal.Width : num  0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
##  $ Species     : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...

any(is.na(iris))

## [1] FALSE
```

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Getting started with R

1 Introduction

2 Linear Models

- introduction & inputs
- outputs
- tests
- predictions
- assumptions

3 Generalised Linear Models

- introduction & inputs
- outputs
- tests
- predictions
- assumptions

4 Mixed Models

- introduction & inputs
- outputs
- tests
- predictions
- assumptions
- advanced MM

5 General Additive (Mixed) Models

The linear model: specifications

Simple notation:

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 \times x_{1,i} + \hat{\beta}_2 \times x_{2,i} + \cdots + \hat{\beta}_p \times x_{p,i} + \varepsilon_i$$

The linear model: specifications

Simple notation:

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$$y_i = \hat{y}_i + \varepsilon_i$$

The linear model: specifications

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$$y_i = \hat{y}_i + \varepsilon_i$$

- y_i = the observations to explain / response variable / dependent variable
- \hat{y}_i = the fitted values
- $x_{j,i}$ = constants derived from the predictors / explanatory variables / independent variables
- $\hat{\beta}_j$ = the (model parameter / regression coefficient) estimates
- ε_i = the residuals (i.e. the estimates for the error which is Gaussian with constant variance)

The linear model: specifications

Matrix notation:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,p} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,p} \\ 1 & x_{3,1} & x_{3,2} & \dots & x_{3,p} \\ \dots & \dots & \dots & \dots & \dots \\ 1 & x_{n,1} & x_{n,2} & \dots & x_{n,p} \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \dots \\ \hat{\beta}_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \dots \\ \varepsilon_n \end{bmatrix}$$

The linear model: specifications

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$$Y = X\hat{\beta} + \varepsilon = \hat{Y} + \varepsilon$$

$$\varepsilon = Y - \hat{Y}$$

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$$Y = X\hat{\beta} + \varepsilon = \hat{Y} + \varepsilon$$

$$\varepsilon = Y - \hat{Y}$$

- Y = the vector of observations
- \hat{Y} = the vector of fitted values
- X = a matrix called the design matrix (or the model matrix)
- ε = the vector of residuals

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod) ## the formula  
## Petal.Length ~ Petal.Width
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length Petal.Width  
## 1           1.4           0.2  
## 2           1.4           0.2  
## 3           1.3           0.2  
## 4           1.5           0.2  
## 5           1.4           0.2  
## 6           1.7           0.4
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length Petal.Width  
## 1           1.4           0.2  
## 2           1.4           0.2  
## 3           1.3           0.2  
## 4           1.5           0.2  
## 5           1.4           0.2  
## 6           1.7           0.4
```

```
head(model.response(model_frame))  ## the response variable  
##   1   2   3   4   5   6  
## 1.4 1.4 1.3 1.5 1.4 1.7
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit
##   Petal.Length Petal.Width
## 1           1.4          0.2
## 2           1.4          0.2
## 3           1.3          0.2
## 4           1.5          0.2
## 5           1.4          0.2
## 6           1.7          0.4
```

```
head(model.response(model_frame))  ## the response variable
##   1  2  3  4  5  6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod))  ## the model matrix
##   (Intercept) Petal.Width
## 1           1          0.2
## 2           1          0.2
## 3           1          0.2
## 4           1          0.2
## 5           1          0.2
## 6           1          0.4
```


The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Species, data = iris)
```

```
formula(mod)  ## the formula
## Petal.Length ~ Species
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit
##   Petal.Length Species
## 1          1.4   setosa
## 2          1.4   setosa
## 3          1.3   setosa
## 4          1.5   setosa
## 5          1.4   setosa
## 6          1.7   setosa
```

```
head(model.response(model_frame))  ## the response variable
##   1  2  3  4  5  6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod))  ## the model matrix
##   (Intercept) Speciesversicolor Speciesvirginica
## 1           1             0             0
## 2           1             0             0
## 3           1             0             0
## 4           1             0             0
## 5           1             0             0
## 6           1             0             0
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width + Species, data = iris)
```

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width + Species
```

```
head(model_frame <- model.frame(mod)) ## the data used for the fit
##   Petal.Length Petal.Width Species
## 1           1.4           0.2  setosa
## 2           1.4           0.2  setosa
## 3           1.3           0.2  setosa
## 4           1.5           0.2  setosa
## 5           1.4           0.2  setosa
## 6           1.7           0.4  setosa
```

```
head(model.response(model_frame)) ## the response variable
##   1  2  3  4  5  6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod)) ## the model matrix
##   (Intercept) Petal.Width Speciesversicolor Speciesvirginica
## 1           1           0.2                0                0
## 2           1           0.2                0                0
## 3           1           0.2                0                0
## 4           1           0.2                0                0
## 5           1           0.2                0                0
## 6           1           0.4                0                0
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width + Species + Petal.Width:Species, data = iris)
```

```
formula(mod) ## the formula
```

```
## Petal.Length ~ Petal.Width + Species + Petal.Width:Species
```

```
head(model_frame <- model.frame(mod)) ## the data used for the fit
```

```
##   Petal.Length Petal.Width Species
## 1           1.4           0.2  setosa
## 2           1.4           0.2  setosa
## 3           1.3           0.2  setosa
## 4           1.5           0.2  setosa
## 5           1.4           0.2  setosa
## 6           1.7           0.4  setosa
```

```
head(model.response(model_frame)) ## the response variable
```

```
##    1    2    3    4    5    6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod)) ## the model matrix
```

```
##   (Intercept) Petal.Width Speciesversicolor Speciesvirginica Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
## 1           1           0.2              0              0              0              0
## 2           1           0.2              0              0              0              0
## 3           1           0.2              0              0              0              0
## 4           1           0.2              0              0              0              0
## 5           1           0.2              0              0              0              0
## 6           1           0.4              0              0              0              0
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width*Species, data = iris)
```

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width * Species
```

```
head(model_frame <- model.frame(mod)) ## the data used for the fit
##   Petal.Length Petal.Width Species
## 1           1.4          0.2  setosa
## 2           1.4          0.2  setosa
## 3           1.3          0.2  setosa
## 4           1.5          0.2  setosa
## 5           1.4          0.2  setosa
## 6           1.7          0.4  setosa
```

```
head(model.response(model_frame)) ## the response variable
##   1  2  3  4  5  6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod)) ## the model matrix
##   (Intercept) Petal.Width Speciesversicolor Speciesvirginica Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
## 1           1           0.2              0              0              0              0
## 2           1           0.2              0              0              0              0
## 3           1           0.2              0              0              0              0
## 4           1           0.2              0              0              0              0
## 5           1           0.2              0              0              0              0
## 6           1           0.4              0              0              0              0
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width/Species, data = iris) ## dangerous
```

```
formula(mod) ## the formula
```

```
## Petal.Length ~ Petal.Width/Species
```

```
head(model_frame <- model.frame(mod)) ## the data used for the fit
```

```
##   Petal.Length Petal.Width Species
## 1           1.4           0.2  setosa
## 2           1.4           0.2  setosa
## 3           1.3           0.2  setosa
## 4           1.5           0.2  setosa
## 5           1.4           0.2  setosa
## 6           1.7           0.4  setosa
```

```
head(model.response(model_frame)) ## the response variable
```

```
##    1    2    3    4    5    6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod)) ## the model matrix
```

```
##   (Intercept) Petal.Width Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
## 1           1           0.2                                0                                0
## 2           1           0.2                                0                                0
## 3           1           0.2                                0                                0
## 4           1           0.2                                0                                0
## 5           1           0.2                                0                                0
## 6           1           0.4                                0                                0
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ 1, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ 1
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length  
## 1           1.4  
## 2           1.4  
## 3           1.3  
## 4           1.5  
## 5           1.4  
## 6           1.7
```

```
head(model.response(model_frame))  ## the response variable  
##   1  2  3  4  5  6  
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod))  ## the model matrix  
##   (Intercept)  
## 1           1  
## 2           1  
## 3           1  
## 4           1  
## 5           1  
## 6           1
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ ., data = iris)
```

```
formula(mod) ## the formula
```

```
## Petal.Length ~ Sepal.Length + Sepal.Width + Petal.Width + Species
```

```
head(model_frame <- model.frame(mod)) ## the data used for the fit
```

```
##   Petal.Length Sepal.Length Sepal.Width Petal.Width Species
## 1           1.4           5.1          3.5          0.2  setosa
## 2           1.4           4.9          3.0          0.2  setosa
## 3           1.3           4.7          3.2          0.2  setosa
## 4           1.5           4.6          3.1          0.2  setosa
## 5           1.4           5.0          3.6          0.2  setosa
## 6           1.7           5.4          3.9          0.4  setosa
```

```
head(model.response(model_frame)) ## the response variable
```

```
##   1  2  3  4  5  6
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod)) ## the model matrix
```

```
##   (Intercept) Sepal.Length Sepal.Width Petal.Width Speciesversicolor Speciesvirginica
## 1           1           5.1          3.5          0.2              0              0
## 2           1           4.9          3.0          0.2              0              0
## 3           1           4.7          3.2          0.2              0              0
## 4           1           4.6          3.1          0.2              0              0
## 5           1           5.0          3.6          0.2              0              0
## 6           1           5.4          3.9          0.4              0              0
```

The linear model: understanding the design matrix

It is most important to understand the design matrix because the interpretation of the parameters depend on it!

The design matrix depends on:

- your formula
- your data
- the contrasts (for qualitative variables)

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- the contrasts (for qualitative variables)

By default, each category is compared to the first one:

```
mod <- lm(Petal.Length ~ Species, data = iris)
model.matrix(mod)[c(1, 51, 101), ]
```

##	(Intercept)	Speciesversicolor	Speciesvirginica
## 1	1	0	0
## 51	1	1	0
## 101	1	0	1

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```

	(Intercept)	Speciesversicolor	Speciesvirginica
## 1	1	0	0
## 51	1	1	0
## 101	1	0	1

But other several alternative exist; e.g.:

```
mod2 <- lm(Petal.Length ~ Species, data = iris, contrasts = list(Species = "contr.sum"))
model.matrix(mod2)[c(1, 51, 101), ]
```

	(Intercept)	Species1	Species2
## 1	1	1	0
## 51	1	0	1
## 101	1	-1	-1

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```
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##      (Intercept) Speciesversicolor Speciesvirginica
## 1              1              0              0
## 51             1              1              0
## 101            1              0              1
```

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```
mod2 <- lm(Petal.Length ~ Species, data = iris, contrasts = list(Species = "contr.sum"))
model.matrix(mod2)[c(1, 51, 101), ]

##      (Intercept) Species1 Species2
## 1              1              1      0
## 51             1              0      1
## 101            1             -1     -1
```

Note 1: default contrats ("contr.treatment") are easy to interpret!

The linear model: understanding the design matrix

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- your data
- the contrasts (for qualitative variables)

By default, each category is compared to the first one:

```
mod <- lm(Petal.Length ~ Species, data = iris)
model.matrix(mod)[c(1, 51, 101), ]

##      (Intercept) Speciesversicolor Speciesvirginica
## 1              1              0              0
## 51             1              1              0
## 101            1              0              1
```

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mod2 <- lm(Petal.Length ~ Species, data = iris, contrasts = list(Species = "contr.sum"))
model.matrix(mod2)[c(1, 51, 101), ]

##      (Intercept) Species1 Species2
## 1              1              1              0
## 51             1              0              1
## 101            1             -1             -1
```

Note 1: default contrats ("contr.treatment") are easy to interpret!

Note 2: contrasts do not alter predicted values and thus likelihood, AIC. . .

The linear model: understanding the design matrix

Challenge: find out whether these different representations of gender are equivalent or not?

- "boy" vs "girl"
- "male" vs "female"
- 0 vs 1
- 1 vs 2
- TRUE vs FALSE

Note: no need to fit a model, use the function `model.matrix()` with a formula!

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5 General Additive (Mixed) Models

Parameter estimates

```
mod <- lm(Petal.Length ~ Petal.Width + Species, data = iris)
```

Simply printing the object provides you with the parameter estimates:

```
mod
##
## Call:
## lm(formula = Petal.Length ~ Petal.Width + Species, data = iris)
##
## Coefficients:
##      (Intercept)      Petal.Width Speciesversicolor Speciesvirginica
##           1.211           1.019           1.698           2.277
```

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##           1.211           1.019           1.698           2.277
```

If you need to work with them, use the specific extractor instead:

```
coefficients(mod) ## or coef(mod)
##      (Intercept)      Petal.Width Speciesversicolor Speciesvirginica
##           1.211397           1.018712           1.697791           2.276693
```


Parameter estimates

```
mod <- lm(Petal.Length ~ Petal.Width + Species, data = iris)
```

You can also easily extract the covariance matrix of the estimates:

```
vcov(mod)
```

##	(Intercept)	Petal.Width	Speciesversicolor	Speciesvirginica
## (Intercept)	0.004256508	-0.005701674	0.003303912	0.007295083
## Petal.Width	-0.005701674	0.023177537	-0.025031740	-0.041256016
## Speciesversicolor	0.003303912	-0.025031740	0.032742072	0.047410394
## Speciesvirginica	0.007295083	-0.041256016	0.047410394	0.079143501

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And thus the standard errors:

```
sqrt(diag(vcov(mod)))
```

##	(Intercept)	Petal.Width	Speciesversicolor	Speciesvirginica
##	0.06524192	0.15224171	0.18094771	0.28132455

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You can also get confidence intervals:

```
confint(mod)
```

##		2.5 %	97.5 %
## (Intercept)		1.0824564	1.340338
## Petal.Width		0.7178294	1.319594
## Speciesversicolor		1.3401762	2.055407
## Speciesvirginica		1.7206988	2.832688

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Note: that reveals that there are much more information in the object `mod` than it is being printed!

The model object

The fitted model object is in fact a big list of class "lm":

```
class(mod)
## [1] "lm"
typeof(mod)
## [1] "list"
names(mod)
## [1] "coefficients" "residuals" "effects" "rank" "fitted.values" "assign" "qr"
## [8] "df.residual" "contrasts" "xlevels" "call" "terms" "model"
```

So you can extract information from it; e.g.:

```
mod$df.residual
## [1] 146
```

but it is safer to use extractors if they are available!

Example of other outputs

There are quite a few extractors out there:

```
logLik(mod)
## 'log Lik.' -64.7851 (df=5)
AIC(mod)
## [1] 139.5702
```

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AIC(mod)
## [1] 139.5702
```

Here is how you can get the list of S3 methods for the class "lm":

```
methods(class = "lm")
## [1] add1          alias          anova          case.names    coerce        confint        cooks.distance
## [8] deviance      dfbeta        dfbetas       drop1         dummy.coef    effects       extractAIC
## [15] family        formula       hatvalues     influence     initialize    kappa         labels
## [22] logLik        model.frame   model.matrix  nobs         plot          predict       print
## [29] proj          qr            residuals     rstandard    rstudent     show          simulate
## [36] slotsFromS3   summary       variable.names vcov
## see '?methods' for accessing help and source code
```

Note: the list will change depending on the packages that are attached to the R session!

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Testing coefficients

For LM, simply use `summary()`:

```
summary(mod)

##
## Call:
## lm(formula = Petal.Length ~ Petal.Width + Species, data = iris)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.02977 -0.22241 -0.01514  0.18180  1.17449
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    1.21140    0.06524   18.568 < 2e-16 ***
## Petal.Width     1.01871    0.15224    6.691 4.41e-10 ***
## Speciesversicolor 1.69779    0.18095    9.383 < 2e-16 ***
## Speciesvirginica  2.27669    0.28132    8.093 2.08e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3777 on 146 degrees of freedom
## Multiple R-squared:  0.9551, Adjusted R-squared:  0.9542
## F-statistic: 1036 on 3 and 146 DF, p-value: < 2.2e-16
```

Testing predictors

Don't use the default `anova()` function which perform type-I analysis-of-variance:

```
anova(mod)
## Analysis of Variance Table
##
## Response: Petal.Length
##           Df Sum Sq Mean Sq  F value    Pr(>F)
## Petal.Width  1 430.48   430.48 3016.792 < 2.2e-16 ***
## Species      2  13.01     6.51   45.591 4.137e-16 ***
## Residuals    146  20.83     0.14
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Instead use the better function `Anova()` from the package `car` which performs type-II analysis-of-variance:

```
library(car)
Anova(mod)
## Anova Table (Type II tests)
##
## Response: Petal.Length
##           Sum Sq Df F value    Pr(>F)
## Petal.Width  6.3892  1  44.775 4.409e-10 ***
## Species     13.0113  2  45.591 4.137e-16 ***
## Residuals    20.8334 146
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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## Residuals    20.8334 146
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Note: p-values are the same no matter the order of the predictors in the formula for type-II (but not for type-I!).

Testing the overall model

Before looking at significance for estimates or predictor, always start by checking that your model fits the data better than a null model:

```
mod <- lm(Petal.Length ~ Petal.Width + Species, data = iris)
mod_null <- lm(Petal.Length ~ 1, data = iris)
anova(mod, mod_null)

## Analysis of Variance Table
##
## Model 1: Petal.Length ~ Petal.Width + Species
## Model 2: Petal.Length ~ 1
##   Res.Df    RSS Df Sum of Sq    F    Pr(>F)
## 1     146  20.83
## 2     149 464.33 -3    -443.49 1036 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Note 1: this was also given at the bottom of the summary table!

Note 2: here using `anova()` is perfectly fine!

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Fitted values

You can easily obtain the prediction for your observation (i.e. fitted values):

```
fitted(mod)[1:39]
```

```
##      1      2      3      4      5      6      7      8      9     10     11     12     13
## 1.415139 1.415139 1.415139 1.415139 1.415139 1.618882 1.517010 1.415139 1.415139 1.313268 1.415139 1.415139 1.313268
##      14     15     16     17     18     19     20     21     22     23     24     25     26
## 1.313268 1.415139 1.618882 1.618882 1.517010 1.517010 1.517010 1.415139 1.618882 1.415139 1.720753 1.415139 1.415139
##      27     28     29     30     31     32     33     34     35     36     37     38     39
## 1.618882 1.415139 1.415139 1.415139 1.415139 1.618882 1.313268 1.415139 1.415139 1.415139 1.415139 1.313268 1.415139
```

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##	1	2	3	4	5	6	7	8	9	10	11	12	13
##	1.415139	1.415139	1.415139	1.415139	1.415139	1.618882	1.517010	1.415139	1.415139	1.313268	1.415139	1.415139	1.313268
##	14	15	16	17	18	19	20	21	22	23	24	25	26
##	1.313268	1.415139	1.618882	1.618882	1.517010	1.517010	1.517010	1.415139	1.618882	1.415139	1.720753	1.415139	1.415139
##	27	28	29	30	31	32	33	34	35	36	37	38	39
##	1.618882	1.415139	1.415139	1.415139	1.415139	1.618882	1.313268	1.415139	1.415139	1.415139	1.415139	1.313268	1.415139

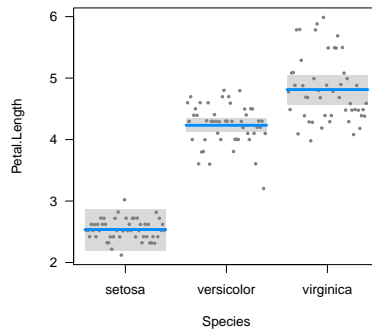
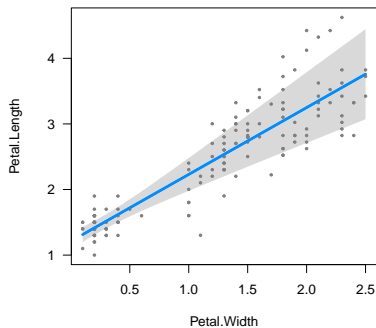
As expected, observations are equal to the fitted values + residuals:

```
head(cbind("response" = model.response(model.frame(mod)),
           "fitted" = fitted(mod),
           "resid" = residuals(mod),
           "fitted + resid" = fitted(mod) + residuals(mod)))
```

##	response	fitted	resid	fitted + resid
## 1	1.4	1.415139	-0.01513927	1.4
## 2	1.4	1.415139	-0.01513927	1.4
## 3	1.3	1.415139	-0.11513927	1.3
## 4	1.5	1.415139	0.08486073	1.5
## 5	1.4	1.415139	-0.01513927	1.4
## 6	1.7	1.618882	0.08111841	1.7

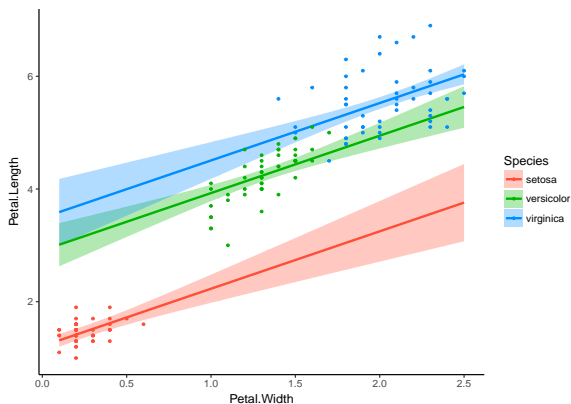
Plotting predictions: fast & dirty

```
library(visreg)
par(mfrow = c(1, 2))
visreg(mod)
```



Plotting predictions: fast & less dirty

```
library(visreg)
library(ggplot2)
visreg(fit = mod, xvar = "Petal.Width", by = "Species", overlay = TRUE, gg = TRUE) +
  theme_classic()
```



Note: if you have different quantitative predictors you can specify the value for the non focal predictor using the argument "cond".

Prediction by “hand”

The most difficult step is to create the data frame defining the predictor values:

```
library(dplyr)
data_for_predictions <- iris %>%
  group_by(Species) %>%
  do(tibble(Petal.Width = seq(min(.$Petal.Width), max(.$Petal.Width), length.out = 30))) %>%
  as.data.frame()
```

```
head(data_for_predictions)
```

##	Species	Petal.Width
## 1	setosa	0.1000000
## 2	setosa	0.1172414
## 3	setosa	0.1344828
## 4	setosa	0.1517241
## 5	setosa	0.1689655
## 6	setosa	0.1862069

```
tail(data_for_predictions)
```

##	Species	Petal.Width
## 85	virginica	2.310345
## 86	virginica	2.348276
## 87	virginica	2.386207
## 88	virginica	2.424138
## 89	virginica	2.462069
## 90	virginica	2.500000

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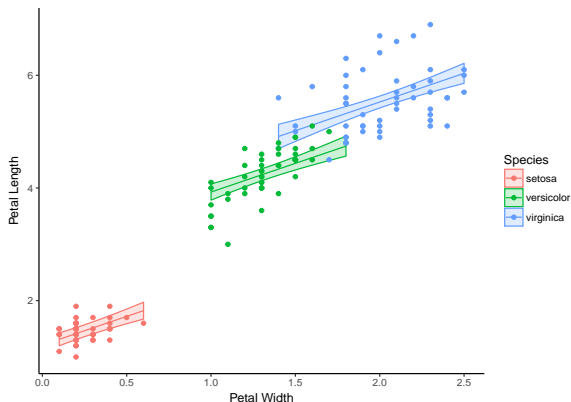
Then, it is easy:

```
pred_mod <- predict(object = mod, newdata = data_for_predictions, interval = "confidence") ## prediction intervals are also possible!
head(pred_mod)
```

```
##      fit      lwr      upr
## 1 1.313268 1.198914 1.427622
## 2 1.330832 1.218369 1.443296
## 3 1.348396 1.237613 1.459180
## 4 1.365960 1.256636 1.475284
## 5 1.383524 1.275430 1.491618
## 6 1.401088 1.293986 1.508190
```

Prediction by “hand”

```
data_for_plot <- cbind(pred_mod, data_for_predictions)
ggplot(data = data_for_plot, mapping = aes(x = Petal.Width, y = fit, colour = Species)) +
  geom_line() +
  geom_ribbon(mapping = aes(ymin = lwr, ymax = upr, fill = Species), alpha = 0.2) +
  geom_point(data = iris, mapping = aes(y = Petal.Length, x = Petal.Width, colour = Species)) +
  labs(x = "Petal Width", y = "Petal Length") +
  theme_classic()
```



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Assumptions behind linear models

Model structure:

- linearity
- lack of perfect multicollinearity (design matrix of full rank)
- predictor variables have fixed values

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Errors:

- independence (no serial autocorrelation)
- constant variance (homoscedasticity)
- normality

Assumptions: linearity

Departure from linearity can originate from a multitude of reasons and can create all kinds of problems.

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- thinking
- other assumptions violated

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- different model structure → change the formula
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- transform the response (e.g. log and power transformation) → function `powerTransform()` in `car` (see later)

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Alternatives:

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- general additive models → package `mgcv`

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Quiz: can you express the following models as LM?

- $y_i = \hat{\alpha} + \varepsilon_i$
- $y_i = x_i^{\hat{\beta}} + \varepsilon_i$
- $y_i = \hat{\alpha} + \hat{\beta}_1 x_i + \hat{\beta}_2 x_i^2 + \hat{\beta}_3 x_i^3 + \varepsilon_i$

Assumptions: lack of perfect multicollinearity

The number of parameters to be estimated must be equal to the rank of the design matrix.

Caused by having less data than parameters or when there is linear dependence between the column vectors of the design matrix. In such case, some parameters cannot be computed.

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Note: strong albeit imperfect collinearity is not great either; possible check correlation between estimates (\rightarrow `cov2cor(vcov(mod))`) and variance inflation factors (\rightarrow `vif(mod)`).

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The dependent variable are represented by fixed values.

The presence of measurement errors is the main cause of violation. Violation can trigger both estimates and tests to be biased.

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The dependent variable are represented by fixed values.

The presence of measurement errors is the main cause of violation. Violation can trigger both estimates and tests to be biased.

Diagnostics:

- thinking & replication

Solutions:

- often ignored in practice
- better measurements

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Alternatives:

- multipurpose numerical approaches → function `optim()` or dedicated packages (e.g. `nloptr`, `rjags`, `nimble`, `rstan`)
- errors-in-variables models → not much directly but any procedure allowing for latent variables can handle that; packages (e.g. `sem`, `lavaan`, `OpenMX`)
- reduced major axis regression → dedicated packages (e.g. `lmodel2`)

Assumptions: independence (no serial autocorrelation)

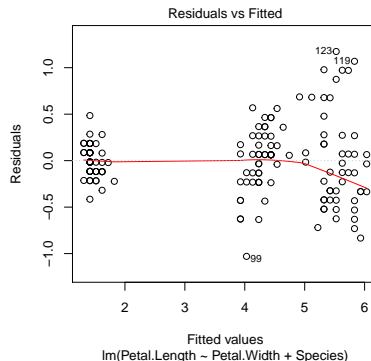
A lack of independence (serial autocorrelation) in the residuals can appear if there is a departure from linearity, if data have been sampled non-randomly (e.g. spatial or temporal series), or if there is an overarching structure (e.g. repeated measures within individuals, families, species, ...). Lack of independence increases the risk of false positive (sometimes a lot).

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Diagnostic by eye:

```
plot(mod, which = 1)
```



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Diagnostic by Durbin-Watson test:

```
durbinWatsonTest(mod) ## from package car (DW varies between 0 & 4, 2 is best, you wish for non-significant p-value)
## lag Autocorrelation D-W Statistic p-value
## 1 0.1313867 1.734855 0.076
## Alternative hypothesis: rho != 0
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Note: the alternative from the package `lmtest` offer to rank the residuals according to a variable.

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Alternatives:

- general additive models (GAM and GAMM) → dedicated package `mgcv`
- mixed models (LMM and GLMM) → dedicated packages (e.g. `spaMM`, `lme4`)

Assumptions: constant variance (homoscedasticity)

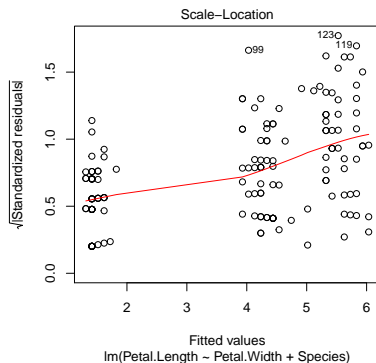
Heteros(c/k)edasticity can emerge when there is a mean - variance relationship, when there is non independence between observations, when reaction norm changes according to the treatment. It can create both false positives and false negative.

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Diagnostic by eye:

```
plot(mod, which = 3)
```



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Diagnostic by Breusch-Pagan test:

```
library(lmtest)
bptest(mod) ## BP = df is best, you wish for non-significant p-value
##
## studentized Breusch-Pagan test
##
## data: mod
## BP = 28.571, df = 3, p-value = 2.755e-06
```

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Solutions: modeling the heteroscedasticity

```
library(spaMM)
mod_heter_spaMM <- fitme(Petal.Length ~ Petal.Width + Species,
  resid.model = ~ Species,
  data = iris)
AIC(mod)
## [1] 139.5702
print(AIC(mod_heter_spaMM)) ## much better fit!
##      marginal AIC:
##      87.84896
```

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Alternatives:

- GLM (if stemming from an expected relationship between mean and variance) → function `glm`

Assumptions: normality

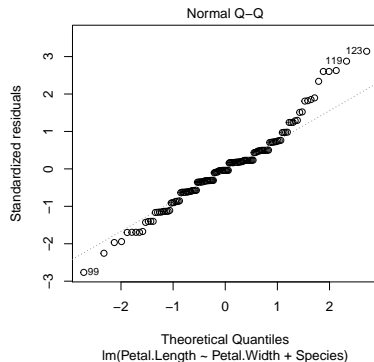
The distribution of residuals can be skewed, this is often caused by the presence of outliers, and/or when the process generating the data is very different from normal (e.g. Poisson, Binomial...).

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Diagnostic by eye:

```
plot(mod, which = 2)
```



Assumptions: normality

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Diagnostic by test (many test are possible):

```
shapiro.test(mod$residuals) ## stat = 1 when normal, you wish for non-significant p-value
##
## Shapiro-Wilk normality test
##
## data:  mod$residuals
## W = 0.96925, p-value = 0.001924
```

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- taking outliers out (mindfully!)

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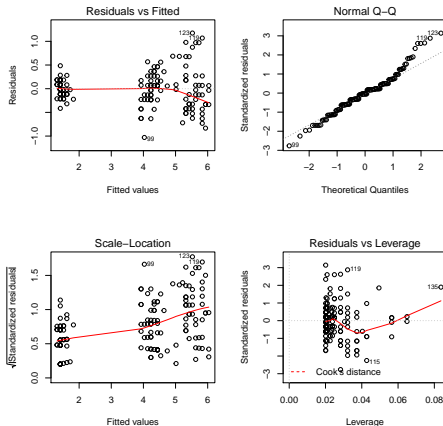
Alternatives:

- GLM (if stemming from the data generating process) → function `glm`

Assumptions: simple glimpse

You can check all assumptions about the errors at once:

```
par(mfrow = c(2, 2))  
plot(mod)
```



Assumptions: outliers

There is a powerful function in R:

```
influence.measures(mod)

## Influence measures of
##   lm(formula = Petal.Length ~ Petal.Width + Species, data = iris) :
##
##           dfb.1_   dfb.Pt.W dfb.Spccsvrs dfb.Spccsvrg   dffit cov.r   cook.d     hat inf
## 1  -0.005155  0.000756    0.00102    0.000367 -0.00582 1.049 8.51e-06 0.0203
## 2  -0.005155  0.000756    0.00102    0.000367 -0.00582 1.049 8.51e-06 0.0203
## 3  -0.039218  0.005750    0.00773    0.002791 -0.04424 1.046 4.92e-04 0.0203
## 4   0.028900 -0.004237   -0.00569   -0.002056  0.03260 1.048 2.67e-04 0.0203
## 5  -0.005155  0.000756    0.00102    0.000367 -0.00582 1.049 8.51e-06 0.0203
## 6   0.017579  0.013609   -0.02152   -0.018998  0.03386 1.052 2.89e-04 0.0239
## 7  -0.032568 -0.006861    0.01940    0.015075 -0.04511 1.047 5.12e-04 0.0205
## 8   0.028900 -0.004237   -0.00569   -0.002056  0.03260 1.048 2.67e-04 0.0203
## 9  -0.005155  0.000756    0.00102    0.000367 -0.00582 1.049 8.51e-06 0.0203
## 10  0.075521 -0.029709    0.00591    0.015059  0.07734 1.045 1.50e-03 0.0235
## 11  0.028900 -0.004237   -0.00569   -0.002056  0.03260 1.048 2.67e-04 0.0203
## 12  0.062998 -0.009237   -0.01241   -0.004483  0.07106 1.042 1.27e-03 0.0203
## 13  0.035054 -0.013790    0.00275    0.006990  0.03590 1.051 3.24e-04 0.0235
## 14 -0.086276  0.033940   -0.00676   -0.017203 -0.08835 1.043 1.96e-03 0.0235
## 15 -0.073339  0.010753    0.01445    0.005218 -0.08273 1.040 1.72e-03 0.0203
## 16 -0.025768 -0.019948    0.03155    0.027847 -0.04964 1.050 6.20e-04 0.0239
## 17 -0.069267 -0.053624    0.08480    0.074856 -0.13343 1.032 4.46e-03 0.0239
## 18 -0.032568 -0.006861    0.01940    0.015075 -0.04511 1.047 5.12e-04 0.0205
## 19  0.050956  0.010735   -0.03035   -0.023587  0.07058 1.042 1.25e-03 0.0205
## 20 -0.004733 -0.000997    0.00282    0.002191 -0.00656 1.049 1.08e-05 0.0205
## 21  0.097189 -0.014250   -0.01914   -0.006916  0.10963 1.033 3.01e-03 0.0203
## 22 -0.025768 -0.019948    0.03155    0.027847 -0.04964 1.050 6.20e-04 0.0239
## 23 -0.141957  0.020814    0.02796    0.010101 -0.16013 1.014 6.40e-03 0.0203
## 24 -0.003221 -0.005781    0.00761    0.007085 -0.00986 1.060 2.45e-05 0.0305
## 25  0.166055 -0.024347   -0.03271   -0.011816  0.18732 1.002 8.73e-03 0.0203
## 26  0.062998 -0.009237   -0.01241   -0.004483  0.07106 1.042 1.27e-03 0.0203
## 27  0.000000  0.000000    0.00000    0.000000  0.00000 1.000 0.00e+00 0.0000
```

Assumptions: outliers

Interpretation of the output from `influence.measures(mod)`:

- `dfb.1_` → extent to which the intercept changes if a given observation is dropped
- `dfb.Pt.W` → extent to which the slope for `Petal.Width` changes if a given observation is dropped
- `dfb.Spcsvrs` → extent to which the estimate for `versicolor` changes if a given observation is dropped
- `dfb.Spcsvrg` → extent to which the estimate for `virginica` changes if a given observation is dropped

Note: for the df-betas, the name would change for another model as they use the abbreviated name of the estimates:

```
abbreviate(stats::variable.names.lm(mod))
```

##	(Intercept)	Petal.Width	Speciesversicolor	Speciesvirginica
##	"(In)"	"Pt.W"	"Spcsvrs"	"Spcsvrg"

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- `inf` → some overall ad hoc recipe to spot influential observation (not to be taken too seriously)

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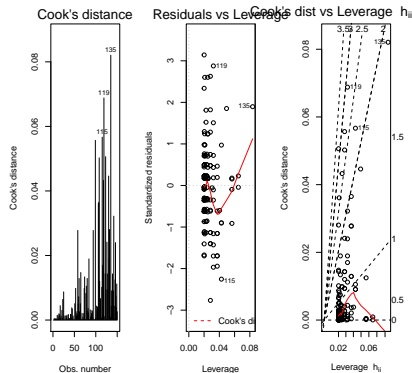
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Assumptions: outliers

There are also plotting possibilities:

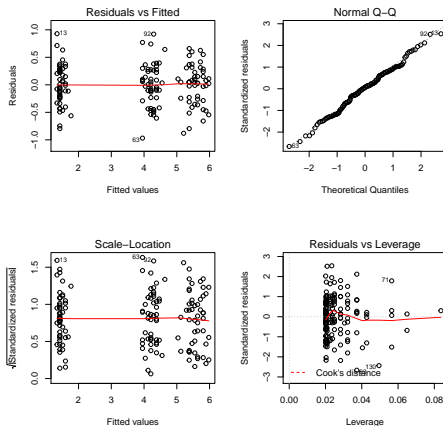
```
par(mfrow = c(1, 3))
plot(mod, which = 4:6)
```



Assumptions: simple glimpse at residuals

What would it look like if it was perfect?

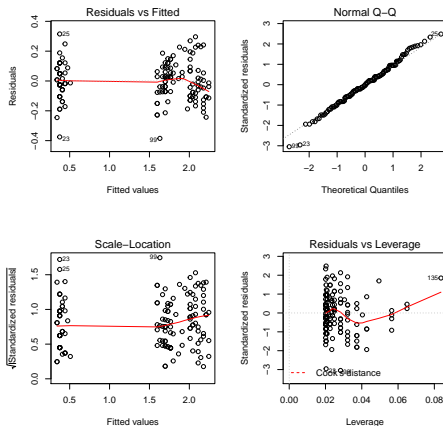
```
iris$Fake.Petal.Length <- simulate(object = mod)[, 1] ## redo it, it will change each time!
mod_perfect <- lm(Fake.Petal.Length ~ Petal.Width + Species, data = iris)
par(mfrow = c(2, 2))
plot(mod_perfect)
```



Assumptions: fixing iris

Fixing attempt:

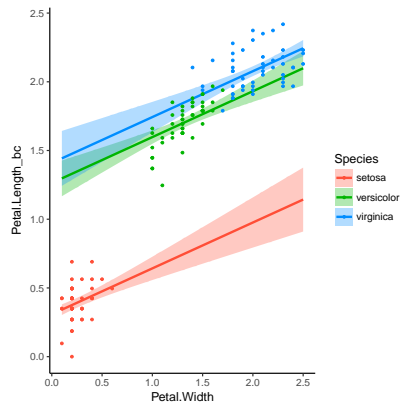
```
bc <- powerTransform(mod)
iris$Petal.Length_bc <- bcPower(iris$Petal.Length, lambda = bc$lambda)
mod_bc <- lm(Petal.Length_bc ~ Petal.Width + Species, data = iris)
par(mfrow = c(2, 2))
plot(mod_bc)
```



Assumptions: fixing iris

Plotting predictions:

```
visreg(fit = mod_bc, xvar = "Petal.Width", by = "Species", overlay = TRUE, gg = TRUE) +  
  theme_classic()
```

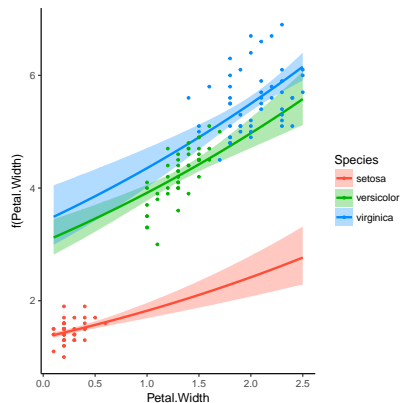


Note: that is not very useful because it is on the BoxCoxed scale!

Assumptions: fixing iris

Plotting predictions:

```
visreg(fit = mod_bc, xvar = "Petal.Width", by = "Species", overlay = TRUE, gg = TRUE,  
       trans = function(x) bcnPowerInverse(x, lambda = bc$lambda, gamma = 0), partial = TRUE) +  
       theme_classic()
```



Note: that is not very useful because it is on the BoxCoxed scale!

Getting started with R

- 1 Introduction
- 2 Linear Models
- 3 Generalised Linear Models**
- 4 Mixed Models
- 5 General Additive (Mixed) Models

Getting started with R

1 Introduction

2 Linear Models

- introduction & inputs
- outputs
- tests
- predictions
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5 General Additive (Mixed) Models

The generalised linear model: what for?

GLM are used for fitting data generating processes for which a relationship between mean and variance is expected.

The generalised linear model: what for?

GLM are used for fitting data generating processes for which a relationship between mean and variance is expected.

That includes the analysis of:

- binary events (probabilities)
- binomial events (probabilities)
- Poisson processes (counts)
- negative binomial processes (counts)
- variances (positive continuous)

The generalised linear model: specifications

Definition:

$$Y = g^{-1}(\hat{\eta}) + \varepsilon = g^{-1}(X\hat{\beta}) + \varepsilon$$

with:

- $\hat{\eta}_i = \hat{\beta}_0 + \hat{\beta}_1 \times x_{1,i} + \hat{\beta}_2 \times x_{2,i} + \dots + \hat{\beta}_p \times x_{p,i}$
- $E(Y) = \mu = g^{-1}(\eta)$
- $\text{Var}(Y) = \phi V(\mu)$

Notation:

- η the linear predictor
- g the link function (g^{-1} is sometimes called the mean function)
- V the variance function
- ϕ is the dispersion parameter

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- V the variance function
- ϕ is the dispersion parameter

This is identical to the LM if:

- $\mu = g^{-1}(\eta) = \eta$, thus if g is the identity function
- $\phi = \sigma^2$, thus if the dispersion parameter equals the error variance
- $V(\mu) = 1$, thus if the variance function is constant

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```


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```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
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```
formula(mod) ## the formula  
## Petal.Length ~ Petal.Width
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length Petal.Width  
## 1           1.4           0.2  
## 2           1.4           0.2  
## 3           1.3           0.2  
## 4           1.5           0.2  
## 5           1.4           0.2  
## 6           1.7           0.4
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length Petal.Width  
## 1           1.4           0.2  
## 2           1.4           0.2  
## 3           1.3           0.2  
## 4           1.5           0.2  
## 5           1.4           0.2  
## 6           1.7           0.4
```

```
head(model.response(model_frame))  ## the response variable  
##   1  2  3  4  5  6  
## 1.4 1.4 1.3 1.5 1.4 1.7
```

The linear model: specifications

R formula notation:

```
mod <- lm(Petal.Length ~ Petal.Width, data = iris)
```

```
formula(mod)  ## the formula  
## Petal.Length ~ Petal.Width
```

```
head(model_frame <- model.frame(mod))  ## the data used for the fit  
##   Petal.Length Petal.Width  
## 1           1.4          0.2  
## 2           1.4          0.2  
## 3           1.3          0.2  
## 4           1.5          0.2  
## 5           1.4          0.2  
## 6           1.7          0.4
```

```
head(model.response(model_frame))  ## the response variable  
##   1  2  3  4  5  6  
## 1.4 1.4 1.3 1.5 1.4 1.7
```

```
head(model.matrix(mod))  ## the model matrix  
##   (Intercept) Petal.Width  
## 1           1          0.2  
## 2           1          0.2  
## 3           1          0.2  
## 4           1          0.2  
## 5           1          0.2  
## 6           1          0.4
```

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