# Getting to do statistics in $\boldsymbol{\mathsf{R}}$

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Leibniz Institute for Zoo and Wildlife Research

IN THE FORSCHUNGSVERBUND BERLIN E.V.

# Getting started with $\boldsymbol{R}$

Some basic tests

Principal Component Analysis

Linear Models

# $\boldsymbol{R}$ provides many statistical tests out of the box

### E.g. the usual correlation tests:

#### Just the correlation coefficient:

```
cor(x = iris$Sepal.Length, y = iris$Sepal.Width, method = "pearson")
## [1] -0.1175698
```

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## [1] -0.1175698
```

#### Or the actual test:

```
cor.test(x = iris$Sepal.Length, y = iris$Sepal.Width, method = "pearson")
##
## Pearson's product-moment correlation
##
## data: iris$Sepal.Length and iris$Sepal.Width
## t = -1.4403, df = 148, p-value = 0.1519
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
## -0.27269325 0.0435i158
## sample estimates:
## cor
## -0.175698
```

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## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
## -0.27269325 0.04351158
## sample estimates:
## cor
## -0.1175698
```

Note: two other methods are available: "spearman" & "kendall".

Note: many (not all) tests allow for the use of both standard and formula-based syntax:

### E.g.

#### is synonymous to:

```
cor.test(x = iris$Sepal.Length, y = iris$Sepal.Width)
##
## Pearson's product-moment correlation
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```

### E.g. test(s) for comparing two unpaired groups:

### The t-test (parametric):

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### The t-test (parametric):

```
t.test(x = iris$Sepal.Length[iris$Species == "versicolor"],
    y = iris$Sepal.Length[iris$Species == "setosa"])

##

## Welch Two Sample t-test

## data: iris$Sepal.Length[iris$Species == "versicolor"] and iris$Sepal.Length[iris$Species == "setosa"]

## t = 10.521, df = 86.538, p-value < 2.2e-16

## alternative hypothesis: true difference in means is not equal to 0

## 95 percent confidence interval:

## 0.7542926 1.1057074

## sample estimates:

## mean of x mean of y

## 5.936 5.006</pre>
```

### The Mann-Whitney U test (non-parametric):

### E.g. test(s) for comparing two paired groups:

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#### The paired *t*-test (parametric):

#### The Wilcox-signed-rank test (non-parametric):

Note: if you forget to specify that the data are paired, it won't run the right test!

E.g. test(s) for comparing more than 2 unpaired groups:

### The Kurskal-Wallis test (non-parametric):

```
kruskal.test(formula = Petal.Length ~ Species, data = iris)
##
## Kruskal-Wallis rank sum test
##
## data: Petal.Length by Species
## Kruskal-Wallis chi-squared = 130.41, df = 2, p-value < 2.2e-16</pre>
```

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kruskal.test(formula = Petal.Length ~ Species, data = iris)
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## Kruskal-Wallis rank sum test
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## data: Petal.Length by Species
## Kruskal-Wallis chi-squared = 130.41, df = 2, p-value < 2.2e-16</pre>
```

#### The "test for equal means in a one-way layout" (parametric):

```
oneway.test(formula = Petal.Length ~ Species, data = iris)
##
## One-way analysis of means (not assuming equal variances)
##
## data: Petal.Length and Species
## F = 1828.1, num df = 2.000, denom df = 78.073, p-value < 2.2e-16</pre>
```

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```

Note: linear models allow for more sophisticated parametric alternatives (see later).

E.g. test(s) for comparing more than 2 paired groups:

#### The Quade test (non-parametric):

```
quade.test(y = as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")]))
##
## Quade test
##
## data: as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")])
## Quade F = 454.3, num df = 2, denom df = 298, p-value < 2.2e-16</pre>
```

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#### The Quade test (non-parametric):

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## Quade F = 454.3, num df = 2, denom df = 298, p-value < 2.2e-16</pre>
```

### The Friedman test (non-parametric):

```
friedman.test(y = as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")]))
##
## Friedman rank sum test
##
## data: as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")])
## Friedman chi-squared = 300, df = 2, p-value < 2.2e-16</pre>
```

E.g. test(s) for comparing more than 2 paired groups:

#### The Quade test (non-parametric):

```
quade.test(y = as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")]))
##
## Quade test
##
## data: as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")])
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### The Friedman test (non-parametric):

```
friedman.test(y = as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")]))
##
## Friedman rank sum test
##
## data: as.matrix(iris[, c("Petal.Length", "Sepal.Length", "Petal.Width")])
## Friedman chi-squared = 300, df = 2, p-value < 2.2e-16</pre>
```

Note: linear mixed-effects models allow for more sophisticated parametric alternatives.

E.g. test(s) for comparing variances between groups:

#### The F-test (parametric):

```
var.test(x = iris$Sepal.Length, y = iris$Petal.Length) ## max 2 groups, must be normaly distributed

##
## F test to compare two variances
## data: iris$Sepal.Length and iris$Petal.Length
## F = 0.22004, num df = 149, denom df = 149, p-value < 2.2e-16
## alternative hypothesis: true ratio of variances is not equal to 1
## 95 percent confidence interval:
## 0.1594015 0.3037352
## sample estimates:
## ratio of variances
## o.2200361</pre>
```

### E.g. test(s) for comparing variances between groups:

### The F-test (parametric):

### The Bartlett test (parametric):

```
bartlett.test(formula = Sepal.Length ~ Species, data = iris)
##
## Bartlett test of homogeneity of variances
##
## data: Sepal.Length by Species
## Bartlett's K-squared = 16.006, df = 2, p-value = 0.0003345
```

E.g. test(s) for comparing variances between groups (continues):

### The Fligner test (non-parametric):

```
fligner.test(formula = Sepal.Length - Species, data = iris)

##
## Fligner-Killeen test of homogeneity of variances
##
## data: Sepal.Length by Species
## Fligner-Killeen:med chi-squared = 11.618, df = 2, p-value = 0.003
```

E.g. test(s) for comparing variances between groups (continues):

### The Fligner test (non-parametric):

```
fligner.test(formula = Sepal.Length ~ Species, data = iris)
##
## Fligner-Killeen test of homogeneity of variances
##
## data: Sepal.Length by Species
## Fligner-Killeen:med chi-squared = 11.618, df = 2, p-value = 0.003
```

Note: also ansari.test() and mood.test() for rank-based two-sample test for a difference in scale parameters.

E.g. test(s) for comparing 2 distributions:

### The Kolmogorov-Smirnov test (non-parametric):

```
ks.test(x = iris$Sepal.Length, y = iris$Petal.Length)
## Warning in ks.test(x = iris$Sepal.Length, y = iris$Petal.Length): p-value will be approximate in the presence of ties
## Two-sample Kolmogorov-Smirnov test
## data: iris$Sepal.Length and iris$Petal.Length
## D = 0.56, p-value < 2.2e=16
## alternative hypothesis: two-sided</pre>
```

### E.g. test(s) for comparing 2 distributions:

### The Kolmogorov-Smirnov test (non-parametric):

```
ks.test(x = iris$Sepal.Length, y = iris$Petal.Length)
## Warning in ks.test(x = iris$Sepal.Length, y = iris$Petal.Length): p-value will be approximate in the presence of ties
## Two-sample Kolmogorov-Smirnov test
##
## data: iris$Sepal.Length and iris$Petal.Length
## D = 0.56, p-value < 2.2e-16
## alternative hypothesis: two-sided</pre>
```

### The Shapiro-Wilk Normality test (non-parametric):

```
set.seed(2L)
shapiro.test(x = rnorm(100))
##
## Shapiro-Wilk normality test
##
## data: rnorm(100)
## W = 0.97498, p-value = 0.05375
```

E.g. test(s) for comparing a binomial outcome to a probability (exact):

#### The exact binomial test:

```
binom.test(x = 8, n = 10, p = 0.5) ## 8 heads out of 10 coin throws -> is the coin biased?
##
## Exact binomial test
##
## data: 8 and 10
## number of successes = 8, number of trials = 10, p-value = 0.1094
## alternative hypothesis: true probability of success is not equal to 0.5
## 95 percent confidence interval:
## 0.439045 0.9747893
## sample estimates:
## probability of success
## ## 0.8
```

E.g. test(s) for comparing two independent proportions:

### The "test of equal proportions":

```
prop.test(x = cbind(success = c(8, 4), failure = c(2, 6))) ## 8 heads out of 10 for one coin, 4 out of 10 for the other, do they differ?
## Warning in prop.test(x = cbind(success = c(8, 4), failure = c(2, 6))): Chi-squared approximation may be incorrect
##
## 2-sample test for equality of proportions with continuity correction
##
## data: cbind(success = c(8, 4), failure = c(2, 6))
## X-squared = 1.875, df = 1, p-value = 0.1709
## alternative hypothesis: two.sided
## 95 percent confidence interval:
## -0.0919928 0.8919928
## sample estimates:
## prop 1 prop 2
## 0.8 0.4
```

### E.g. test(s) of independence:

#### The Fisher exact test:

```
## check WorldPhones before running the code!

fisher.test(WorldPhones, simulate.p.value = TRUE, B = 100) ## simulation needed as too large for exact test!

##

## Fisher's Exact Test for Count Data with simulated p-value (based on 100 replicates)

##

## data: WorldPhones

## p-value = 0.009901

## alternative hypothesis: two.sided
```

### E.g. test(s) of independence:

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##
## data: WorldPhones
## p-value = 0.009901
## alternative hypothesis: two.sided
```

### The Chi-squared test for independence:

```
chisq.test(WorldPhones)
##
## Pearson's Chi-squared test
##
## data: WorldPhones
## X-squared = 2194.4, df = 36, p-value < 2.2e-16</pre>
```

### E.g. test(s) of independence:

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```

Note: the McNemar test is also available when the same subjects are measured in two conditions (see ?mcnemar.test).

# Many more simple statistical tests are available in **R** packages

#### Some examples:

- coin provides permutation implementations of many tests.
- nsm3 provides tons of non-parametric tests.
- PMCMR provides post-hoc tests for non-parametric tests.
- nortest provides several tests for normality.

Note: this list is only a very small subset!!

### A note before we continue

R's original primary goal was to perform statistical analyses. So among the many thousands of packages many focus on statistical tools and by no means I will try to cover or even summarise this diversity.

I have chosen to only illustrate some of the tools I know and that I have used to show you how to do some statistics in  $\mathbf{R}$ .

Since time is limited, I will not for example illustrate any Bayesian methods, nor machine learning methods, although some good packages exist for that too!

# Getting started with **R**

Some basic tests

Principal Component Analysis

Linear Models

### PCA is a traditional method for dimentionality reduction:

<pre>head(USArrests) ## origin</pre>			original	coordinates	
##		Murder	Assault	UrbanPop	Rape
##	Alabama	13.2	236	58	21.2
##	Alaska	10.0	263	48	44.5
##	Arizona	8.1	294	80	31.0
##	Arkansas	8.8	190	50	19.5
##	${\tt California}$	9.0	276	91	40.6
##	Colorado	7.9	204	78	38.7

### PCA is a traditional method for dimentionality reduction:

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head(USArrests) ## original coordinates
             Murder Assault UrbanPop Rape
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            13.2
                        236
                                 58 21.2
## Alaska
               10.0
                        263
                                 48 44.5
## Arizona
             8.1
                        294
                            80 31.0
                            50 19.5
91 40.6
78 38 7
## Arkansas
                8.8
                        190
## California
                9.0
                        276
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                        204
                                 78 38.7
```

```
pca_US <- prcomp(- Murder + Assault + Rape, data = USArrests, scale. = TRUE) ## scaling is not the default (but should be)
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```

```
pca_US <- prcomp(- Murder + Assault + Rape, data = USArrests, scale. = TRUE) ## scaling is not the default (but should be)
```

```
head(pca_US$x) ## new coordinates

## PC1 PC3

## Alabama -1.1980278 0.8338118 -0.16217848

## Alabama -2.3087473 -1.5239622 0.03833574

## Arizona -1.5033307 -0.4983038 0.87822311

## Arkansas -0.1759894 0.3247326 0.07111174

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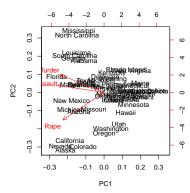
## California -2.0452386 -1.2725770 0.38153933

## Colorado -1.2634133 -1.4264063 -0.08369314
```

The first axis alone captures more than 78% of the total variation in the data:

### PCA without packages

The first axis alone captures more than 78% of the total variation in the data:



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### ade4 is a package with several multivariate tools, including the PCA:

```
library(ade4)
pca_US_ade4 <- dudi.pca(df = USArrests[, -3], scale = TRUE, scannf = FALSE)
summary(pca_US_ade4)
## Class: pca dudi
## Call: dudi.pca(df = USArrests[, -3], scale = TRUE, scannf = FALSE)
## Total inertia: 3
##
## Eigenvalues:
              Ax2
       Ax1
                      Ax3
   2.3586 0.4581 0.1834
## Projected inertia (%):
      Ax1
              Ax2
                      Ax3
   78.619 15.268 6.112
## Cumulative projected inertia (%):
      Ax1
           Ax1:2 Ax1:3
    78.62
            93.89 100.00
```

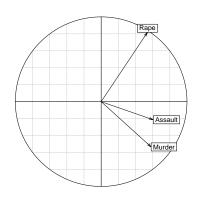
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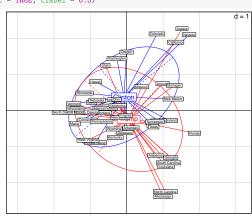
```
library(ade4)
pca US ade4 <- dudi.pca(df = USArrests[, -3], scale = TRUE, scannf = FALSE)
summary(pca_US_ade4)
## Class: pca dudi
## Call: dudi.pca(df = USArrests[, -3], scale = TRUE, scannf = FALSE)
## Total inertia: 3
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## Cumulative projected inertia (%):
           Ax1:2 Ax1:3
       Ax1
    78.62 93.89 100.00
```

#### Let us add voting data to this dataset:

#### The package allows a different kind of plot that is quite interesting:

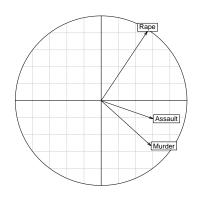
```
par(mfrow = c(1, 2))
s.corcircle(dfxy = pca_US_ade4$c1)
s.class(dfxy = pca_US_ade4$11, fac = USArrests$Vote, col = c("blue", "red"))
s.label(dfxy = pca_US_ade4$11, label = rownames(USArrests), add.plot = TRUE, clabel = 0.5)
```

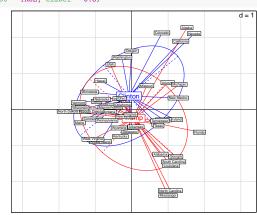




The package allows a different kind of plot that is quite interesting:

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par(mfrow = c(1, 2))
s.corcircle(dfxy = pca_US_ade4$c1)
s.class(dfxy = pca_US_ade4$11, fac = USArrests$Vote, col = c("blue", "red"))
s.label(dfxy = pca_US_ade4$11, label = rownames(USArrests), add.plot = TRUE, clabel = 0.5)
```





Note: using co & li instead of c1 & 11 would respect the relative contribution of each principal component according to the variance they capture.

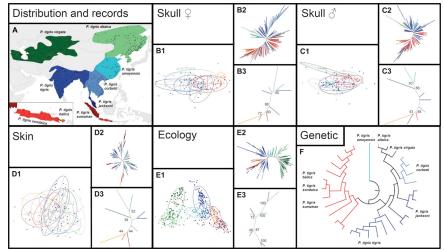
### Example of application of PCA: a revision of tiger taxonomy

RESEARCH ARTICLE | CONSERVATION ECOLOGY

# Planning tiger recovery: Understanding intraspecific variation for effective conservation

Andreas Wilting<sup>1,\*</sup>, Alexandre Courtiol<sup>1</sup>, Per Christiansen<sup>2</sup>, Jürgen Niedballa<sup>1</sup>, Anne K. Scharf<sup>1,†</sup>, Ludovic Orlando<sup>2</sup>, Niko Bal...
+ See all authors and affiliations

Science Advances 26 Jun 2015: Vol. 1, no. 5, e1400175 DOI: 10.1126/sciadv.1400175



# Getting started with $\boldsymbol{R}$

Some basic tests

Principal Component Analysis

3 Linear Models

# Getting started with ${\bf R}$

- Some basic tests
- Principal Component Analysis
- Linear Models
  - introduction
  - traditional linear model (LM)
  - generalised linear models (GLM)
  - mixed models (LMM & GLMM)

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

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In a linear model, the data-generating process is assumed to be a linear function: it is constructed from a set of terms by multiplying each term by a constant (a model parameter) and adding the results.

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

In a linear model, the data-generating process is assumed to be a linear function: it is constructed from a set of terms by multiplying each term by a constant (a model parameter) and adding the results.

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- linear mixed-effects models: LMM
- generalized linear mixed-effects models: GLMM
- general additive models & general additive mixed models: GAM & GAMM

Note: I have a 100 hours course on the topic (https://github.com/courtiol/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	stats*; spaMM	car; lmtest; visreg
GLM	stats*; spaMM; pscl	car; DHARMa; visreg
LMM	lme4; spaMM; glmmTMB	DHARMa; pbkrtest; visreg
GLMM	lme4; spaMM; glmmTMB	DHARMa; pbkrtest; visreg
GAM	mgcv	DHARMa; visreg
GAMM	mgcv	

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

<sup>\* =</sup> included in any R installation!

# Good books dealing with linear models in R



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

# Preparing data for (G)LM(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)
- data frames (i.e. object of class data.frame) and not tibbles (tbl)

# Preparing data for (G)LM(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)
- data frames (i.e. object of class data.frame) and not tibbles (tbl)

#### 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
             4.9
                        3.0
## 2
                                     1.4
                                                 0.2 setosa
## 3
             4.7
                        3.2
                                     1.3
                                                 0.2 setosa
            4.6
                        3.1
                                 1.5
## 4
                                                 0.2 setosa
             5.0
## 5
                        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 0.4 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 ...
anv(is.na(iris))
## [1] FALSE
```

# Getting started with R

- Some basic tests
- Principal Component Analysis
- Linear Models
  - introduction
  - traditional linear model (LM)
  - generalised linear models (GLM)
  - mixed models (LMM & GLMM)

Simple notation:

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

#### Simple notation:

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

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

#### Simple notation:

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

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

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

Matrix notation:

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

Matrix notation:

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

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

$$\widehat{S} = \widehat{Y} + \widehat{Y}$$

Matrix notation:

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

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

$$\widehat{S} = Y + \widehat{Y}$$

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

#### **R** formula notation:

mod <- lm(Petal.Length ~ Petal.Width, data = iris)</pre>

#### R formula notation:

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

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

#### R formula notation:

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

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width
model_frame <- model.frame(mod) ## the data used for the fit</pre>
model_frame[c(1:2, 51:52, 101:102), ]
      Petal.Length Petal.Width
## 1
             1.4
                          0.2
           1.4
## 2
                          0.2
## 51
            4.7
                         1.4
        4.5
## 52
                         1.5
              6.0
## 101
                          2.5
## 102
              5.1
                          1.9
```

#### R formula notation:

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

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
      Petal.Length Petal.Width
## 1
           1.4
                        0.2
         1.4
## 2
                        0.2
## 51
           4.7
                       1.4
       4.5
                  1.5
## 52
       6.0
## 101
                       2.5
## 102
             5.1
                       1.9
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102),] ## the model matrix
       (Intercept) Petal.Width
##
## 1
                          0.2
## 2
                          0.2
## 51
                        1.4
## 52
                        1.5
## 101
                          2.5
## 102
                          1.9
```

#### R formula notation:

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

```
formula(mod) ## the formula
## Petal.Length ~ Species
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
```

```
Petal.Length
                   Species
## 1
           1.4 setosa
## 2
            1.4
                   setosa
       4.7 versicolor
## 51
      4.5 versicolor
## 52
            6.0 virginica
## 101
## 102
             5.1 virginica
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Speciesversicolor Speciesvirginica
##
## 1
## 2
## 51
## 52
## 101
## 102
```

#### R formula notation:

## 52

## 101 ## 102

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width + Species
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
      Petal.Length Petal.Width
                                Species
## 1
             1.4
                         0.2
                                 setosa
## 2
              1.4
                         0.2
                                 setosa
              4.7 1.4 versicolor
## 51
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Petal.Width Speciesversicolor Speciesvirginica
##
## 1
                           0.2
## 2
                           0.2
                                                                 0
## 51
                           1.4
## 52
                           1.5
## 101
                           2.5
## 102
                           1.9
```

2.5 virginica

1.9 virginica

4.5 1.5 versicolor

6.0

5.1

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

#### 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
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
      Petal.Length Petal.Width
                                Species
##
## 1
              1.4
                          0.2
                                 setosa
## 2
              1.4
                          0.2
                                 setosa
              4.7
                         1.4 versicolor
## 51
              4.5
                         1.5 versicolor
## 52
              6.0
                          2.5 virginica
## 101
## 102
              5.1
                         1.9 virginica
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Petal.Width Speciesversicolor Speciesvirginica Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
##
## 1
                            0.2
                                                                                               0.0
                                                                                                                             0.0
## 2
                           0.2
                                                                                               0.0
                                                                                                                             0.0
## 51
                           1.4
                                                                                               1.4
                                                                                                                             0.0
## 52
                           1.5
                                                                                              1.5
                                                                                                                            0.0
## 101
                           2.5
                                                                                               0.0
                                                                                                                             2.5
## 102
                           1.9
                                                0
                                                                                              0.0
                                                                                                                            1.9
```

#### R formula notation:

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

```
formula(mod) ## the formula
## Petal.Length ~ Petal.Width * Species
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
##
      Petal.Length Petal.Width
                                Species
## 1
              1.4
                          0.2
                                 setosa
## 2
              1.4
                         0.2
                                 setosa
              4.7
                         1.4 versicolor
## 51
              4.5
                         1.5 versicolor
## 52
              6.0
                         2.5 virginica
## 101
## 102
              5.1
                         1.9 virginica
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Petal.Width Speciesversicolor Speciesvirginica Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
##
## 1
                           0.2
                                                                                              0.0
                                                                                                                            0.0
## 2
                           0.2
                                                                                              0.0
                                                                                                                            0.0
## 51
                           1.4
                                                                                              1.4
                                                                                                                            0.0
## 52
                           1.5
                                                                                              1.5
                                                                                                                            0.0
## 101
                           2.5
                                                                                              0.0
                                                                                                                            2.5
## 102
                           1.9
                                                0
                                                                                              0.0
                                                                                                                            1.9
```

#### R formula notation:

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

```
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
##
      Petal.Length Petal.Width
                              Species
## 1
             1.4
                        0.2
                               setosa
## 2
             1.4
                        0.2
                               setosa
             4.7
                       1.4 versicolor
## 51
        4.5 1.5 versicolor
## 52
             6.0
                        2.5 virginica
## 101
## 102
             5.1
                        1.9 virginica
```

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

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Petal.Width Petal.Width:Speciesversicolor Petal.Width:Speciesvirginica
##
## 1
                           0.2
                                                                                        0.0
## 2
                           0.2
                                                          0.0
                                                                                        0.0
## 51
                           1.4
                                                          1.4
                                                                                        0.0
## 52
                           1.5
                                                          1.5
                                                                                        0.0
## 101
                           2.5
                                                          0.0
                                                                                        2.5
## 102
                           1.9
                                                          0.0
                                                                                        1.9
```

#### R formula notation:

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

```
formula(mod) ## the formula
## Petal.Length ~ 1
model_frame <- model.frame(mod) ## the data used for the fit</pre>
model_frame[c(1:2, 51:52, 101:102), , drop = FALSE]
      Petal.Length
## 1
             1.4
           1.4
## 2
## 51
             4.7
           4.5
## 52
        6.0
## 101
## 102
              5.1
```

```
model.matrix(mod)[c(1:2, 51:52, 101:102), , drop = FALSE] ## the model matrix
       (Intercept)
##
## 1
## 2
## 51
## 52
## 101
## 102
```

#### R formula notation:

## 102

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

5.1

5.8

```
formula(mod) ## the formula
## Petal.Length ~ Sepal.Length + Sepal.Width + Petal.Width + Species
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), ]
      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
                              3.2
                                        1.4 versicolor
             4.7
                        7.0
## 51
                              3.2
                                        1.5 versicolor
             4.5
                         6.4
## 52
             6.0
                         6.3
                              3.3
                                              2.5 virginica
## 101
```

1.9 virginica

```
model.matrix(mod)[c(1:2, 51:52, 101:102), ] ## the model matrix
       (Intercept) Sepal.Length Sepal.Width Petal.Width Speciesversicolor Speciesvirginica
##
## 1
                                        3.5
                                                    0.2
                            5.1
                                                                                         0
## 2
                            4.9
                                        3.0
                                                    0.2
                                                                                         0
## 51
                            7.0
                                        3.2
                                                   1.4
## 52
                            6.4
                                        3.2
                                                  1.5
## 101
                            6.3
                                        3.3
                                                    2.5
## 102
                            5.8
                                        2.7
                                                    1.9
```

2.7

# 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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- your formula
- 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
## 51
## 101
```

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)

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
## 51
## 101
```

But other several alternative exist; e.g.:

```
mod2 <- lm(Petal.Length ~ Species, data = iris, contrasts = list(Species = "contr.sum"))</pre>
model.matrix(mod2)[c(1, 51, 101), ]
       (Intercept) Species1 Species2
## 1
## 51
## 101
```

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)

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
## 51
## 101
```

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
## 51
## 101
```

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

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)

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
## 51
## 101
```

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
## 51
## 101
```

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

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

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, you can use the function model.matrix() with a formula!

```
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
##
```

mod

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

## Simply printing the object provides you with the parameter estimates:

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

```
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
```

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

#### And thus the standard errors:

```
sqrt(diag(vcov(mod)))
##
         (Intercept)
                           Petal.Width Speciesversicolor Speciesvirginica
         0.06524192
                           0.15224171
                                                                0.28132455
##
                                              0.18094771
```

```
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
                     0.004256508 -0.005701674
                                                    0.003303912
                                                                      0.007295083
## (Intercept)
## 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
```

### And thus the standard errors:

```
sqrt(diag(vcov(mod)))
         (Intercept)
                           Petal.Width Speciesversicolor Speciesvirginica
                            0.15224171
##
          0.06524192
                                              0.18094771
                                                                0.28132455
```

### 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
```

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

#### And thus the standard errors:

```
sqrt(diag(vcov(mod)))
         (Intercept)
                           Petal.Width Speciesversicolor Speciesvirginica
          0.06524192
                            0.15224171
                                              0.18094771
                                                                0.28132455
```

### 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
```

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

# LM outputs: 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"
                                                          "rank"
                                                                          "fitted.values" "assign"
                                                                                                            "gr"
                                                                                                                             "df.residual"
                                         "effects"
   [9] "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!

# LM: 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
```

# LM: 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
```

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

```
methods(class = "lm")
   [1] add1
                                                                                                   cooks.distance deviance
                       alias
                                                                                    confint
                                                                                                                                  dfbeta
                                      anova
                                                      case.names
                                                                     coerce
## [10] dfbetas
                       drop1
                                      dummy.coef
                                                      effects
                                                                     extractAIC
                                                                                    family
                                                                                                   formula
                                                                                                                   hatvalues
                                                                                                                                  influence
## [19] initialize
                       kappa
                                      labels
                                                     logLik
                                                                    model.frame
                                                                                    model.matrix
                                                                                                   nobs
                                                                                                                   plot
                                                                                                                                  predict
## [28] print
                                                     residuals
                                                                                                                                  slotsFromS3
                       proj
                                      qr
                                                                    rstandard
                                                                                    rstudent
                                                                                                   show
                                                                                                                   simulate
## [37] summarv
                       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!

## LM tests: coefficients

## For LM, simply use summary():

```
summary(mod)
##
## Call:
## lm(formula = Petal.Length ~ Petal.Width + Species, data = iris)
## Residuals:
       Min
                 10 Median
                                  30
                                          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
```

# LM tests: predictors

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

Instead, better use the 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

## Response: Petal.Length

## 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
```

# LM tests: predictors

Don't use the default anova() function which performs 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 '**' 0.05 '.' 0.1 ' ' 1
```

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## Petal.Width 6.3892 1 44.775 4.409e-10 ***

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## Residuals 20.8334 146

## ---
## Signif. codes: 0 '***' 0.001 '**' 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!).

## LM tests: 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)
       146 20.83
       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!

# LM predictions: fitted values

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

```
fitted(mod)[1:39]
                                                         6
                                                                                               10
## 1.415139 1.415139 1.415139 1.415139 1.415139 1.415139 1.618882 1.517010 1.415139 1.415139 1.313268 1.415139 1.415139 1.415139 1.313268 1.313268 1.415139
                                      19
                                               20
                                                         21
                                                                            23
                                                                                     24
                                                                                               25
                                                                                                        26
## 1.618882 1.618882 1.517010 1.517010 1.517010 1.415139 1.618882 1.415139 1.720753 1.415139 1.415139 1.618882 1.415139 1.415139 1.415139
                                               35
                                                                  37
## 1.415139 1.618882 1.313268 1.415139 1.415139 1.415139 1.415139 1.313268 1.415139
```

# LM predictions: fitted values

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

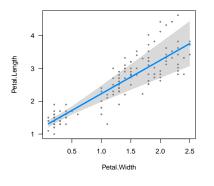
```
fitted(mod)[1:39]
                                              5
                                                        6
                                                                                           10
                                                                                                     11
                                                                                                              12
## 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 1.313268 1.415139
                                    19
                                                       21
                                                                         23
                                                                                           25
                                                                                                     26
                                              20
## 1.618882 1.618882 1.517010 1.517010 1.517010 1.415139 1.618882 1.415139 1.720753 1.415139 1.415139 1.618882 1.415139 1.415139 1.415139
                                              35
                                                                37
## 1.415139 1.618882 1.313268 1.415139 1.415139 1.415139 1.415139 1.313268 1.415139
```

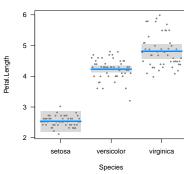
## As expected, observations are equal to the fitted values + residuals:

```
head(cbind("response" = model.response(model.frame(mod)),
           "fitted" = fitted(mod).
           "resid" = residuals(mod).
           "fitted + resid" = fitted(mod) + residuals(mod)))
              fitted
                             resid fitted + resid
    response
          1.4 1.415139 -0.01513927
                                              1.4
## 1
         1.4 1.415139 -0.01513927
                                              1.4
## 3
         1.3 1.415139 -0.11513927
                                              1.3
          1.5 1.415139 0.08486073
                                              1.5
## 4
## 5
          1.4 1.415139 -0.01513927
                                              1.4
         1.7 1.618882 0.08111841
                                              1.7
## 6
```

# LM predictions: fast and dirty plot

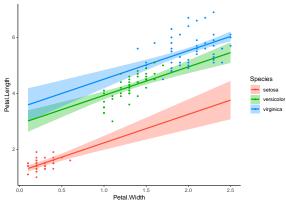
```
library(visreg)
par(mfrow = c(1, 2))
visreg(mod)
```





# LM predictions: fast & less dirty plot

```
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".

## LM predictions: 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(data.frame(Petal.Width = seq(min(.$Petal.Width), max(.$Petal.Width), length.out = 30))) %>%
                            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
```

# LM predictions: by "hand"

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

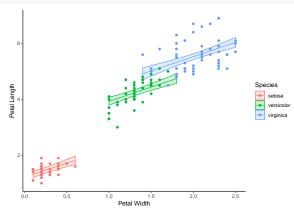
```
library(dplyr)
data for predictions <- iris %>%
                           group_by(Species) %>%
                           do(data.frame(Petal.Width = seq(min(.$Petal.Width), max(.$Petal.Width), length.out = 30))) %>%
                           data.frame()
                                                                       tail(data_for_predictions)
       head(data_for_predictions)
            Species Petal.Width
                                                                               Species Petal.Width
                                                                        ## 85 virginica
                                                                                          2.310345
       ## 1 setosa 0.1000000
                                                                        ## 86 virginica
                                                                                         2.348276
       ## 2 setosa 0.1172414
                                                                        ## 87 virginica
                                                                                         2.386207
       ## 3 setosa 0.1344828
                                                                       ## 88 virginica
                                                                                          2.424138
       ## 4 setosa 0.1517241
                                                                       ## 89 virginica
                                                                                         2.462069
       ## 5 setosa 0.1689655
       ## 6 setosa 0.1862069
                                                                       ## 90 virginica
                                                                                          2.500000
```

### 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
## 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
```

## LM predictions: 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()</pre>
```



# LM assumptions: generalities

### Model structure:

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

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- linearity
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- predictor variables have fixed values

### Errors:

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

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

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## Diagnostics:

- thinking
- other assumptions violated

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#### Solutions:

- ullet different model structure o change the formula
- transform one or several predictors (e.g. polynomials)  $\rightarrow$  function poly()
- transform the response (e.g. log and power transformation) → function powerTransform() in car (see later)

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- non-linear models → function nls or dedicated package (e.g. nlme)
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Quiz: can you express the following models as LM?

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

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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- change the experimental design
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none

## LM assumptions: lack of perfect multicollinearity

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#### Alternatives:

none

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

## LM assumptions: lack of perfect multicollinearity

### Example of perfect multicollinearity:

```
iris_silly <- iris
iris silly$Petal.Surface <- iris silly$Petal.Length*iris silly$Petal.Width
mod silly <- lm(Sepal.Width ~ log(Petal.Length) + log(Petal.Width) + log(Petal.Surface), data = iris_silly)
summary(mod_silly)
##
## Call:
## lm(formula = Sepal.Width ~ log(Petal.Length) + log(Petal.Width) +
      log(Petal.Surface), data = iris_silly)
## Residuals:
       Min
                 10 Median
                                   30
                                           Max
## -1.11386 -0.20803 0.03202 0.19723 1.03521
## Coefficients: (1 not defined because of singularities)
                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                       3.5978
                                  0.2609 13.790 <2e-16 ***
## log(Petal.Length)
                      -0.4520
                                  0.2031 -2.225
                                                 0.0276 *
## log(Petal.Width)
                       0.0543
                                  0.1220
                                           0.445
                                                   0.6568
## log(Petal.Surface)
                           NA
                                      NA
                                              NA
                                                       NA
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3813 on 147 degrees of freedom
## Multiple R-squared: 0.2448, Adjusted R-squared: 0.2345
## F-statistic: 23.83 on 2 and 147 DF, p-value: 1.089e-09
```

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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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#### Alternatives:

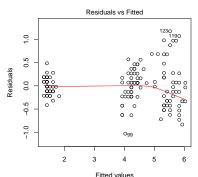
- multipurpose numerical approaches → function optim() or dedicated packages (e.g. nloptr, rjags, nimble, rstan)
- errors-in-variables models → not much directly but any procedure allowing for latent variables can handle that; packages (e.g. sem, lavaan, OpenMX)
- reduced major axis regression → dedicated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

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)



Im(Petal.Length ~ Petal.Width + Species)

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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
             0.1313867
                            1.734855 0.054
## Alternative hypothesis: rho != 0
```

Note: the alternative from the package 1mtest offer to rank the residuals according to a variable.

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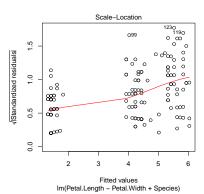
- ullet general additive models (GAM and GAMM) o dedicated package mgcv
- mixed models (LMM and GLMM) → dedicated packages (e.g. spaMM, lme4)

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

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plot(mod, which = 3)



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

### 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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##

## studentized Breusch-Pagan test
##

## data: mod
## BP = 28.571, df = 3, p-value = 2.755e-06
```

#### Solutions: modeling the heteroscedasticity

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

### 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
```

#### 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
```

#### Alternatives:

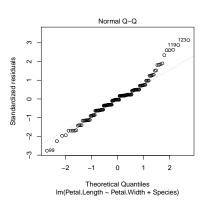
GLM (if stemming from an expected relationship between mean and variance) → function glm

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)



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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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- transformation or different model structure (see linearity)
- taking outliers out (mindfully!)

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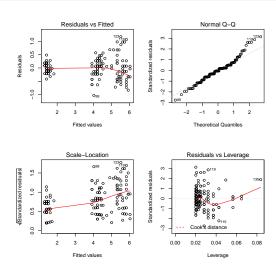
#### Alternatives:

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

# LM assumptions: simple glimpse

### You can check all assumptions about the erros at once:

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



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### 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.Spcsvrs dfb.Spcsvrg
                                                      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
      -0.039218 0.005750
                               0.00773
                                          0.002791 -0.04424 1.046 4.92e-04 0.0203
## 3
       0.028900 -0.004237
                              -0.00569
                                         -0.002056 0.03260 1.048 2.67e-04 0.0203
## 4
                               0.00102
                                          0.000367 -0.00582 1.049 8.51e-06 0.0203
## 5
      -0.005155 0.000756
       0.017579 0.013609
                              -0.02152
                                         -0.018998 0.03386 1.052 2.89e-04 0.0239
## 6
      -0.032568 -0.006861
                               0.01940
                                          0.015075 -0.04511 1.047 5.12e-04 0.0205
## 7
## 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
       0.075521 -0.029709
                                          0.015059 0.07734 1.045 1.50e-03 0.0235
## 10
                               0.00591
## 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
       0.035054 -0.013790
                               0.00275
## 13
                                          0.006990 0.03590 1.051 3.24e-04 0.0235
      -0.086276 0.033940
                              -0.00676
                                         -0.017203 -0.08835 1.043 1.96e-03 0.0235
## 14
## 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
      -0.069267 -0.053624
                               0.08480
                                          0.074856 -0.13343 1.032 4.46e-03 0.0239
## 17
      -0.032568 -0.006861
                                          0.015075 -0.04511 1.047 5.12e-04 0.0205
## 18
                               0.01940
       0.050956 0.010735
                              -0.03035
                                         -0.023587 0.07058 1.042 1.25e-03 0.0205
## 19
      -0.004733 -0.000997
                               0.00282
                                          0.002191 -0.00656 1.049 1.08e-05 0.0205
## 20
## 21
       0.097189 -0.014250
                                         -0.006916 0.10963 1.033 3.01e-03 0.0203
                              -0.01914
## 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
      -0.003221 -0.005781
                                          0.007085 -0.00986 1.060 2.45e-05 0.0305
## 24
                               0.00761
## 25
       0.166055 -0.024347
                              -0.03271
                                         -0.011816 0.18732 1.002 8.73e-03 0.0203
        0.062998 -0.009237
                                                    0.07106 1.042 1.27e-03 0.0203
## 26
                              -0.01241
                                         -0.004483
```

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

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                                                                   "Spcsvrg"
```

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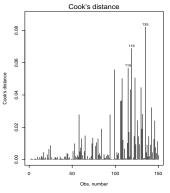
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- hat  $\rightarrow$  diagonal element of the hat matrix (the hat values); extent to which an observation is unusual in terms of X values (leverage)
- inf → some overall add hoc recipe to spot influential observations (not to be taken too seriously)

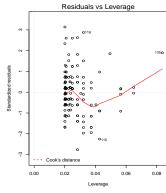
Note: for the df-betas, the name would change for another model as they use the abbreviated name of the estimates:

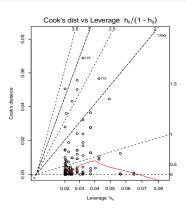
```
abbreviate(stats:::variable.names.lm(mod))
         (Intercept)
                           Petal.Width Speciesversicolor Speciesvirginica
                                 "Pt. W"
              "(In)"
                                                 "Spcsvrs"
                                                                   "Spcsvrg"
```

### There are also plotting possibilitites:

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



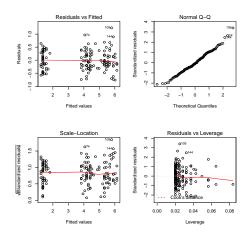




## LM assumptions: simple glimpse at residuals

### What would it look like if it was perfect?

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



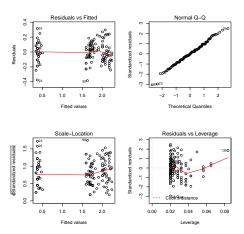
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# LM assumptions: fixing iris?

### Fixing attempt:

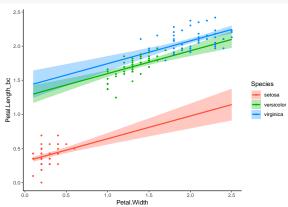
```
bc <- powerTransform(mod)
iris$Petal.Length_bc <- bcPower(iris$Petal.Length, lambda = bc$lambda)
mod_bc <- lm(Petal.Length_bc ~ Petal.Width + Species, data = iris)
par(mfrow = c(2, 2))
plot(mod_bc)</pre>
```



# LM assumptions: fixing iris?

### Plotting predictions:

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

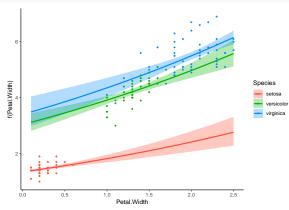


Note: that is not very useful because it is on the BoxCoxed scale!

# LM 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()
```



# Getting started with R

- Some basic tests
- Principal Component Analysis
- Linear Models
  - introduction
  - traditional linear model (LM)
  - generalised linear models (GLM)
  - mixed models (LMM & GLMM)

### GLM: what for?

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

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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)

### GLM: notation

### Definition:

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

with:

• 
$$\hat{\eta}_i = \hat{\beta}_0 + \hat{\beta}_1 \times x_{1,i} + \hat{\beta}_2 \times x_{2,i} + \dots + \hat{\beta}_p \times x_{p,i}$$

- $E(Y) = \mu = g^{-1}(\eta)$
- $Var(Y) = \phi V(\mu)$

#### Notation:

- $\eta$  the linear predictor
- g the link function ( $g^{-1}$  is sometimes called the mean function)
- V the variance function
- $\bullet$   $\phi$  is the dispersion parameter

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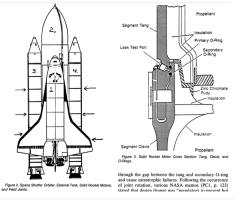
#### Notation:

- η the linear predictor
- g the link function ( $g^{-1}$  is sometimes called the mean function)
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This is identical to the LM if:

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

# The Challenger dataset



```
head(Challenger, n = 3L)
## oring_tot oring_dt temp psi flight
## 1 6 0 66 50 1
## 2 6 1 70 50 2
## 3 6 0 69 50 3
```

Note: we will study both the probability that one O-ring fails (binary event) or that at least one O-ring fails (binomial event) as a function of the temperature and the leak-check pressure.

### The VonBort dataset



```
head(VonBort, n = 3L)
    deaths year corps fisher
        0 1875
     0 1875 I
                  no
     0 1875 II yes
```

Note: we will compare the number of deaths caused by horse (or mule) kicks between the 14 corps of the Prussian army.

#### In R notation:

```
Challenger$issue <- Challenger$oring_dt > 0

mod_challenger_binar <- glm(issue ~ temp + psi, family = binomial(link = "logit"), data = Challenger)
```

#### In R notation:

```
Challenger\$issue <- Challenger\$oring_dt > 0

mod_challenger_binar <- glm(issue ~ temp + psi, family = binomial(link = "logit"), data = Challenger)

Challenger\$oring_ok <- Challenger\$oring_tot - Challenger\$oring_dt

mod_challenger_binom <- glm(cbind(oring_dt, oring_ok) ~ temp + psi, family = binomial(link = "logit"), data = Challenger)
```

#### In R notation:

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Challenger\$issue <- Challenger\$oring_dt > 0

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Challenger\$oring_ok <- Challenger\$oring_tot - Challenger\$oring_dt

mod_challenger_binom <- glm(cbind(oring_dt, oring_ok) ~ temp + psi, family = binomial(link = "logit"), data = Challenger)

mod_horsekick <- glm(deaths ~ corps, family = poisson(link = "log"), data = VonBort)
```

The family object contains all kinds of useful information required for the fitting procedure:

```
names(binomial(link = "logit"))
## [1] "family"
                  "link"
                              "linkfun"
                                         "linkinv"
                                                     "variance" "dev.resids" "aic"
                                                                                       "mu.eta"
                                                                                                   "initialize" "validmu"
## [11] "valideta" "simulate"
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```

#### The link function:

```
probs \leftarrow seq(0.1, 0.9, by = 0.1)
probs
## [1] 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
logits <- binomial(link = "logit")$linkfun(mu = probs)</pre>
logits
## [1] -2.1972246 -1.3862944 -0.8472979 -0.4054651 0.0000000 0.4054651 0.8472979 1.3862944 2.1972246
```

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```

#### The inverse link function:

```
binomial(link = "logit")$linkinv(eta = logits)
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```

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```
binomial(link = "logit")$linkinv(eta = logits)
## [1] 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
```

#### The variance function:

```
binomial(link = "logit")$variance(mu = probs)
## [1] 0.09 0.16 0.21 0.24 0.25 0.24 0.21 0.16 0.09
```

### The family object contains all kinds of useful information required for the fitting procedure:

```
names(binomial(link = "logit"))
## [1] "family"    "link"    "linkfun"    "variance"    "dev.resids" "aic"    "mu.eta"    "initialize" "validmu"
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```
binomial(link = "logit")$linkinv(eta = logits)
## [1] 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
```

#### The variance function:

```
binomial(link = "logit") $variance(mu = probs)
## [1] 0.09 0.16 0.21 0.24 0.25 0.24 0.21 0.16 0.09
```

Note: you can use these functions to better understand GLM or when you need them to process some outputs.

# GLM: outputs

```
mod_challenger_binar
##
## Call: glm(formula = issue ~ temp + psi, family = binomial(link = "logit"),
      data = Challenger)
##
## Coefficients:
## (Intercept) temp
                               psi
    21.843631 -0.350098
                              0.006007
##
## Degrees of Freedom: 22 Total (i.e. Null); 20 Residual
## Null Deviance:
                    26.4
## Residual Deviance: 14.03 AIC: 20.03
confint(mod_challenger_binar)
## Waiting for profiling to be done...
##
                   2.5 %
                          97.5 %
## (Intercept) 4.91856874 56.49606738
## temp
            -0.86018027 -0.11037072
## psi -0.01302771 0.02858975
```

# GLM: outputs

```
mod_challenger_binom
##
## Call: glm(formula = cbind(oring_dt, oring_ok) ~ temp + psi, family = binomial(link = "logit"),
      data = Challenger)
##
## Coefficients:
## (Intercept)
               temp
                                   psi
     7.772138 -0.169736
                              0.002585
##
## Degrees of Freedom: 22 Total (i.e. Null); 20 Residual
## Null Deviance:
                    20.71
## Residual Deviance: 9.431 AIC: 26.77
confint(mod_challenger_binom)
## Waiting for profiling to be done...
##
                   2.5 %
                             97.5 %
## (Intercept) -0.75786416 18.89655752
            -0.32094631 -0.05964840
## temp
## psi
            -0.01351725 0.02361973
```

## corpsIV

## corpsV

-1.5958865 0.1280845

-1.1704167 0.3841036

#### mod\_horsekick ## ## Call: glm(formula = deaths ~ corps, family = poisson(link = "log"), data = VonBort) ## ## Coefficients: ## (Intercept) corpsVIII corpsI corpsII corpsIII corpsIV corpsV corpsVI corpsVII corpsIX -2.231e-01 4.072e-09 -2.877e-01 -2.877e-01 -6.931e-01 -3.747e-01 6.062e-02 -2.877e-01 -8.267e-01 -2.076e-01 corpsX corpsXI corpsXIV corpsXV ## 4.463e-01 ## -6.454e-02 4.055e-01 -6.931e-01 ## Degrees of Freedom: 279 Total (i.e. Null); 266 Residual ## Null Deviance: 323.2 ## Residual Deviance: 297.1 AIC: 630.2 head(confint(mod\_horsekick)) ## Waiting for profiling to be done ... ## 2.5 % 97.5 % ## (Intercept) -0.7566949 0.2298300 ## corpsI -0.6999361 0.6999361 ## corpsII -1.0585453 0.4561131 ## corpsIII -1.0585453 0.4561131

# GLM: outputs

```
mod_horsekick
##
## Call: glm(formula = deaths ~ corps, family = poisson(link = "log"),
      data = VonBort)
##
## Coefficients:
                                                                                                          corpsVIII
## (Intercept)
                    corpsI
                                corpsII
                                            corpsIII
                                                         corpsIV
                                                                       corpsV
                                                                                   corpsVI
                                                                                               corpsVII
                                                                                                                         corpsIX
   -2.231e-01
                 4.072e-09
                             -2.877e-01
                                          -2.877e-01
                                                      -6.931e-01
                                                                   -3.747e-01
                                                                                 6.062e-02
                                                                                             -2.877e-01
                                                                                                          -8.267e-01
                                                                                                                      -2.076e-01
       corpsX
                corpsXI
                               corpsXIV
                                            corpsXV
## -6.454e-02
                4.463e-01
                              4.055e-01
                                          -6.931e-01
## Degrees of Freedom: 279 Total (i.e. Null); 266 Residual
## Null Deviance:
                     323.2
## Residual Deviance: 297.1 ATC: 630.2
head(confint(mod_horsekick))
## Waiting for profiling to be done ...
                   2.5 %
                         97.5 %
##
## (Intercept) -0.7566949 0.2298300
## corpsI
            -0.6999361 0.6999361
## corpsII -1.0585453 0.4561131
## corpsIII
           -1.0585453 0.4561131
## corpsIV
             -1.5958865 0.1280845
## corpsV
             -1.1704167 0.3841036
```

Note: but the interpretation of the parameters is very different since they are expressed on the scale of the linear

# GLM outputs: parameter estimates

There is no general receipe, it all depends on the link function used...

# GLM outputs: parameter estimates

There is no general receipe, it all depends on the link function used...

• For logistic regressions (link = "logit"; not for all binomial models), use odd-ratios:

```
exp(coef(mod_challenger_binar)["temp"])
## temp
## 0.7046192

1/exp(coef(mod_challenger_binar)["temp"])
## temp
## 1.419206
```

Every decrease by one degree increases the odd of failure for at least one O-ring by 1.4 time!

```
exp(coef(mod_challenger_binom)["temp"])
## temp
## 0.8438879

1/exp(coef(mod_challenger_binom)["temp"])
## temp
## 1.184992
```

Every decrease by one degree increases the odd of failure for exactly one O-ring by 1.2 time!

# GLM outputs: parameter estimates

There is no general receipe, it all depends on the link function used. . .

- For logistic regressions (link = "logit"; not for all binomial models), use odd-ratios.
- For Poisson regressions (link = "log"; not for all binomial models), use proportional increase:

```
exp(coef(mod_horsekick)["corpsXIV"])
## corpsXIV
        1.5
```

The army corp XIV received 1.5 times more kicks than the corp G (reference).

### GLM tests: the overall model

```
mod_challenger_binar_null <- glm(issue ~ 1, family = binomial(link = "logit"), data = Challenger)</pre>
anova(mod_challenger_binar, mod_challenger_binar_null, test = "LRT")
## Analysis of Deviance Table
## Model 1: issue ~ temp + psi
## Model 2: issue ~ 1
    Resid. Df Resid. Dev Df Deviance Pr(>Chi)
           20 14.033
           22 26.402 -2 -12.37 0.002061 **
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
mod_challenger_binar_null <- glm(issue ~ 1, family = binomial(link = "logit"), data = Challenger)</pre>
anova (mod_challenger_binar, mod_challenger_binar_null, test = "LRT")
## Analysis of Deviance Table
## Model 1: issue ~ temp + psi
## Model 2: issue ~ 1
    Resid. Df Resid. Dev Df Deviance Pr(>Chi)
            20
               14.033
## 1
            22 26.402 -2 -12.37 0.002061 **
## 2
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
mod_challenger_binom_null <- glm(cbind(oring_dt, oring_ok) ~ 1, family = binomial(link = "logit"), data = Challenger)</pre>
anova (mod challenger binom, mod challenger binom null, test = "LRT")
## Analysis of Deviance Table
##
## Model 1: cbind(oring dt, oring ok) ~ temp + psi
## Model 2: cbind(oring_dt, oring_ok) ~ 1
   Resid, Df Resid, Dev Df Deviance Pr(>Chi)
            20
                 9.4309
            22 20.7057 -2 -11.275 0.003562 **
## 2
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
mod_horsekick_null <- glm(deaths ~ 1, family = poisson(link = "log"), data = VonBort)</pre>
```

```
anova(mod_horsekick, mod_horsekick_null, test = "LRT")
## Analysis of Deviance Table
##
## Model 1: deaths - corps
## Model 2: deaths - 1
## Resid. Df Resid. Dev Df Deviance Pr(>Chi)
## 1 266 297.09
## 2 279 323.23 -13 -26.137 0.0163 *
## ---
## Simif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
GLM tests: predictors
```

```
Anova(mod_challenger_binar)
## Analysis of Deviance Table (Type II tests)
## Response: issue
       LR Chisq Df Pr(>Chisq)
## temp 11.3375 1 0.0007596 ***
## psi
        0.3929 1 0.5307798
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Anova(mod_challenger_binom)
## Analysis of Deviance Table (Type II tests)
##
## Response: cbind(oring_dt, oring_ok)
       LR Chisq Df Pr(>Chisq)
## temp 9.9508 1 0.001608 **
## psi
        0.0962 1 0.756451
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Anova(mod_horsekick)
## Analysis of Deviance Table (Type II tests)
##
## Response: deaths
        LR Chisq Df Pr(>Chisq)
## corps 26.137 13 0.0163 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

```
summary(mod_challenger_binar)
## Call:
## glm(formula = issue ~ temp + psi, family = binomial(link = "logit"),
      data = Challenger)
## Deviance Residuals:
       Min
                 1Q Median
                                    3Q
                                             Max
## -1.00837 -0.54507 -0.28098 0.02512 2.21488
##
## Coefficients:
              Estimate Std. Error z value Pr(>|z|)
## (Intercept) 21.843631 11.936459 1.830 0.0673 .
## temp -0.350098 0.172977 -2.024 0.0430 *
       0.006007 0.009749 0.616 0.5378
## psi
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
      Null deviance: 26.402 on 22 degrees of freedom
## Residual deviance: 14.033 on 20 degrees of freedom
## AIC: 20.033
##
## Number of Fisher Scoring iterations: 6
```

```
summary(mod_challenger_binar)
## Call:
## glm(formula = issue ~ temp + psi, family = binomial(link = "logit"),
      data = Challenger)
## Deviance Residuals:
       Min
                  10
                       Median
                                              Max
## -1.00837 -0.54507 -0.28098 0.02512
                                         2.21488
## Coefficients:
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) 21.843631 11.936459
                                  1.830
                                           0.0673 .
## temp -0.350098 0.172977 -2.024
                                           0.0430 *
       0.006007
                         0.009749 0.616
                                           0.5378
## psi
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
      Null deviance: 26,402 on 22 degrees of freedom
## Residual deviance: 14.033 on 20 degrees of freedom
## AIC: 20.033
##
## Number of Fisher Scoring iterations: 6
```

Note: these z-tests are asymptotic tests relying on normality of parameter estimates. They are not to be trusted with small dataset for GLM! There is no easy alternative, so better trust the likelihood ratio test of the overall predictor!

```
summary(mod_challenger_binom)
## Call:
## glm(formula = cbind(oring_dt, oring_ok) ~ temp + psi, family = binomial(link = "logit"),
      data = Challenger)
## Deviance Residuals:
      Min
                1Q Median
                                         Max
## -0.7331 -0.5350 -0.3749 -0.2175 1.6660
## Coefficients:
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) 7.772138 4.797582
                                   1.620 0.10523
## temp
        -0.169736 0.063915 -2.656 0.00792 **
               0.002585
                         0.008485 0.305 0.76065
## psi
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
      Null deviance: 20.7057 on 22 degrees of freedom
## Residual deviance: 9.4309 on 20 degrees of freedom
## ATC: 26.769
##
## Number of Fisher Scoring iterations: 6
```

Note: these z-tests are asymptotic tests relying on normality of parameter estimates. They are not to be trusted with small dataset for GLM! There is no easy alternative, so better trust the likelihood ratio test of the overall predictor!

```
summary(mod_horsekick)
## Call:
## glm(formula = deaths ~ corps, family = poisson(link = "log"),
      data = VonBort)
##
## Deviance Residuals:
      Min
               1Q Median
                                3Q
                                        Max
## -1.5811 -1.0955 -0.8367 0.5438
                                     2.0079
##
## Coefficients:
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -2.231e-01 2.500e-01 -0.893
                                           0.3721
## corpsI
            4.072e-09 3.535e-01 0.000
                                           1.0000
## corpsII -2.877e-01 3.819e-01 -0.753
                                           0.4512
## corpsIII -2.877e-01 3.819e-01 -0.753
                                           0.4512
## corpsIV
            -6.931e-01 4.330e-01 -1.601
                                           0.1094
## corpsV
           -3.747e-01 3.917e-01 -0.957
                                           0.3387
           6.062e-02 3.483e-01 0.174
## corpsVI
                                           0.8618
## corpsVII
            -2.877e-01 3.819e-01 -0.753
                                           0.4512
## corpsVIII
            -8.267e-01 4.532e-01 -1.824
                                           0.0681 .
## corpsIX
                                           0.5781
             -2.076e-01 3.734e-01 -0.556
## corpsX
            -6.454e-02 3.594e-01 -0.180
                                            0.8575
## corpsXI
            4.463e-01 3.202e-01 1.394
                                           0.1633
## corpsXIV 4.055e-01 3.227e-01 1.256
                                           0.2090
            -6.931e-01 4.330e-01 -1.601
                                           0.1094
## corpsXV
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for poisson family taken to be 1)
##
      Null deviance: 323.23 on 279 degrees of freedom
## Residual deviance: 297 09 on 266 degrees of freedom
```

### Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binar)
## 0.276382602 0.086048377 0.117868645 0.159403597 0.212056359 0.044656818 0.042581853 0.112793550 0.956455553 0.728863707 0.188189166
                                                            16
                                                                        17
## 0.013889951 0.398546225 0.988902144 0.398546225 0.038705137 0.188189166 0.004903474 0.027587785 0.009827446 0.038705137 0.027587785
## 0.939309297
```

## Fitted values are on the scale of probabilities:

```
## 1 2 3 4 5 6 7 8 9 10 11
## 0.276382602 0.086048377 0.117868645 0.159403597 0.212056359 0.044656818 0.042581853 0.112793550 0.956455553 0.728863707 0.188189166
## 12 13 14 15 16 17 18 19 20 21 22
## 0.013889951 0.398546225 0.988902144 0.398546225 0.038705137 0.188189166 0.004903474 0.027587785 0.009827446 0.038705137 0.027587785
## 23
## 0.939309297
```

```
predict(mod_challenger_binar, type = "link") ## the default!!!!!!!
## 1 2 3 4 5 6 7 8
                                                                                              10
## -0.9624767 -2.3628680 -2.0127701 -1.6626723 -1.3125745 -3.0630636 -3.1128120 -2.0625185 3.0894521 0.9888651 -1.4618197 -4.2626023
                                        17 18
                                                                 19
        13
                  14
                       15
                                16
                                                                           20
## -0.4115262 4.4898435 -0.4115262 -3.2123089 -1.4618197 -5.3128958 -3.5624067 -4.6127002 -3.2123089 -3.5624067 2.7393543
predict(mod_challenger_binar, type = "response") ## the useful one!!!!!!!!
                                                                                                      10
                              14
                                       15
                                                 16
                                                             17
                                                                        18
                                                                                  19
                                                                                            20
          12
                    13
                                                                                                       21
## 0.013889951 0.398546225 0.988902144 0.398546225 0.038705137 0.188189166 0.004903474 0.027587785 0.009827446 0.038705137 0.027587785
## 0.939309297
```

## 0.9999932

### Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binar)
                                           4
                                                      5
## 0.276382602 0.086048377 0.117868645 0.159403597 0.212056359 0.044656818 0.042581853 0.112793550 0.956455553 0.728863707 0.188189166
                                                     16
                                                                17
## 0.013889951 0.398546225 0.988902144 0.398546225 0.038705137 0.188189166 0.004903474 0.027587785 0.009827446 0.038705137 0.027587785
## 0.939309297
predict(mod_challenger_binar, type = "link") ## the default!!!!!!!
   1 2 3 4 5 6 7 8
                                                                                                  10
## -0.9624767 -2.3628680 -2.0127701 -1.6626723 -1.3125745 -3.0630636 -3.1128120 -2.0625185 3.0894521 0.9888651 -1.4618197 -4.2626023
                                          17
                                                          18
                                                                    19
         13
                   14
                        15
                                 16
## -0.4115262 4.4898435 -0.4115262 -3.2123089 -1.4618197 -5.3128958 -3.5624067 -4.6127002 -3.2123089 -3.5624067 2.7393543
predict(mod_challenger_binar, type = "response") ## the useful one!!!!!!!!
                                14
                                                    16
                                                                17
                                                                           18
                                                                                      19
          12
                     13
                                         15
                                                                                                20
## 0.013889951 0.398546225 0.988902144 0.398546225 0.038705137 0.188189166 0.004903474 0.027587785 0.009827446 0.038705137 0.027587785
## 0.939309297
predict(mod_challenger_binar, newdata = data.frame(temp = 31, psi = mean(Challenger$psi)), type = "response")
```

Note: the crash was almost inevitable (but we extrapolate)!

## Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binom)
## 0.035530620 0.018340627 0.021659999 0.025564480 0.030151101 0.013130540 0.012615879 0.020818071 0.200067319 0.082846346 0.026793507
                                                            16
                                                                        17
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
## 0.174277588
```

## 0.9480262

### Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binom)
                                            4
                                                       5
## 0.035530620 0.018340627 0.021659999 0.025564480 0.030151101 0.013130540 0.012615879 0.020818071 0.200067319 0.082846346 0.026793507
                                                      16
                                                                 17
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
## 0.174277588
predict(mod_challenger_binom, type = "link") ## the default!!!!!!!
                    2 3 4 5 6 7 8
                                                                                                    10
## -3.3011832 -3.9801257 -3.8103901 -3.6406545 -3.4709188 -4.3195969 -4.3601029 -3.8508960 -1.3858737 -2.4042874 -3.5924367 -4.9503217
                                 16 17 18
                                                                      19
         13
                              15
## -3.0832299 -0.7069312 -3.0832299 -4.4411148 -3.5924367 -5.4595285 -4.6108504 -5.1200573 -4.4411148 -4.6108504 -1.5556093
predict(mod_challenger_binom, type = "response") ## the useful one!!!!!!!!
                                14
                                           15
                                                     16
                                                                 17
                                                                            18
           12
                     13
                                                                                        19
                                                                                                   20
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
## 0.174277588
predict(mod_challenger_binom, newdata = data.frame(temp = 31, psi = mean(Challenger$psi)), type = "response")
```

Note: the crash was almost inevitable (but we extrapolate)!

#### Fitted values are on the scale of counts:

```
fitted(mod horsekick)[1:30]
                                                                   15
                                                                        16 17 18
                                     8
                                          9 10
                                                 11 12 13 14
                                                                                       19
## 0.80 0.80 0.60 0.60 0.40 0.55 0.85 0.60 0.35 0.65 0.75 1.25 1.20 0.40 0.80 0.80 0.60 0.60 0.40 0.55 0.85 0.60 0.35 0.65 0.75 1.25 1.20 0.
  29 30
## 0.80 0.80
```

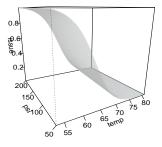
```
predict(mod_horsekick, type = "link")[1:30] ## the default!!!!!!!
                                 3
                                            4
                                                      5
                                                                 6
                                                                            7
                                                                                       8
                                                                                                            10
## -0.2231436 -0.2231435 -0.5108256 -0.5108256 -0.9162907 -0.5978370 -0.1625189 -0.5108256 -1.0498221 -0.4307829 -0.2876821 0.2231436
                                                     17
                                                                           19
                                15
                                           16
                                                                18
                                                                                      20
## 0.1823216 -0.9162907 -0.2231436 -0.2231435 -0.5108256 -0.5108256 -0.9162907 -0.5978370 -0.1625189 -0.5108256 -1.0498221 -0.4307829
## -0.2876821 0.2231436 0.1823216 -0.9162907 -0.2231436 -0.2231435
```

```
predict(mod_horsekick, type = "response")[1:30] ## the useful one!!!!!!!!
                    9 10 11 12 13 14 15 16 17
                                       18 19
                                            20
                                               21
## 29 30
## 0.80 0.80
```

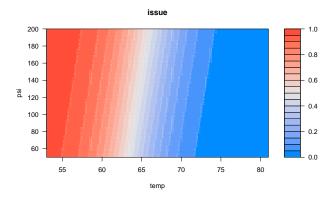
#### Try that:

```
visreg2d(mod_challenger_binar, xvar = "temp", yvar = "psi", plot.type = "rgl", scale = "response") ## I cannot do that easily inside a PDF.
```

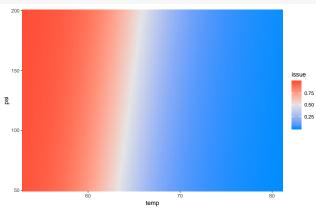
```
visreg2d(mod_challenger_binar, xvar = "temp", yvar = "psi", plot.type = "persp", scale = "response")
```

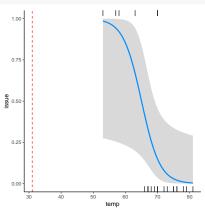


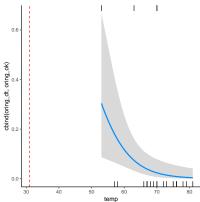
visreg2d(mod\_challenger\_binar, xvar = "temp", yvar = "psi", plot.type = "image", scale = "response")



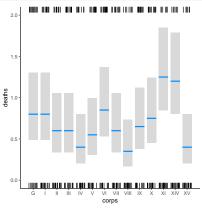
visreg2d(mod\_challenger\_binar, xvar = "temp", yvar = "psi", plot.type = "gg", scale = "response")







```
visreg(fit = mod_horsekick, gg = TRUE, scale = "response") +
 theme_classic() + ylim(min = 0, max = 2)
```



## GLM assumptions: generalities

### Model structure:

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

# GLM assumptions: generalities

### Model structure:

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

## Errors:

- independence (no serial autocorrelation)
- lack of overdispersion and underdispersion

## Other:

• no data separation or quasi-separation

Very difficult to diagnose...

You may try to:

- plot partial residuals using car
- compare prediction to GAM using mgcv
- overall goodness of fit test using DHARMa

Very difficult to diagnose...

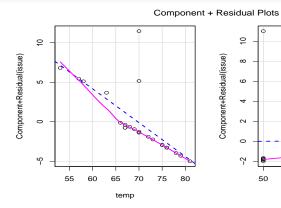
You may try to:

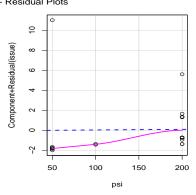
- plot partial residuals using car
- compare prediction to GAM using mgcv
- overall goodness of fit test using DHARMa

Note: same fix as for LM!

## Partial residual plots using car:

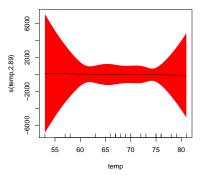
crPlots(mod\_challenger\_binar)





## General Additive Model fit using mgcv:

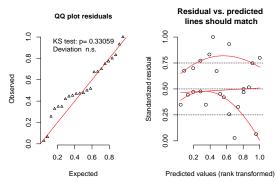
```
library(mgcv)
mod_challenger_binar_GAM <- gam(issue ~ s(temp) + psi, family = binomial(link = "logit"), data = Challenger)
plot(mod_challenger_binar_GAM, shade = TRUE, shade.col = "red") ## on the scale of the linear predictor!
```



```
library(DHARMa) ## package to create USEFUL residuals in GLM, GAM and GLMM
```

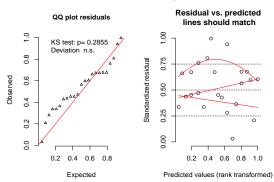
## Note that, since v0.1.6.2, DHARMa includes support for almmTMB, but there are still a few minor limitations associatd with this package. Please see https://qithub.com/florianhartiq/DHARMa/issues/16 for details, in particular if you use this for production. res mod challenger binar <- simulateResiduals(mod challenger binar) plot(res\_mod\_challenger\_binar)

### DHARMa scaled residual plots



```
res_mod_challenger_binom <- simulateResiduals(mod_challenger_binom)
plot(res_mod_challenger_binom)</pre>
```

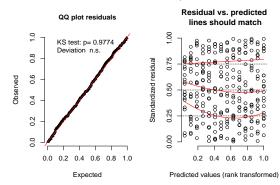
### DHARMa scaled residual plots



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res\_mod\_horsekick <- simulateResiduals(mod\_horsekick)
plot(res\_mod\_horsekick)</pre>

### DHARMa scaled residual plots

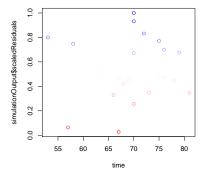


# GLM assumptions: multicollinearity & fixed-values

Same as for LM!

## GLM assumptions: lack for serial autocorrelation

```
testTemporalAutocorrelation(res_mod_challenger_binar, time = Challenger$temp)
```



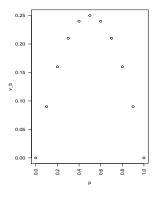
```
##
## Durbin-Watson test
##
## data: simulationOutput$scaledResiduals ~ 1
## DW = 2.4423, p-value = 0.2762
## alternative hypothesis: true autocorrelation is not 0
```

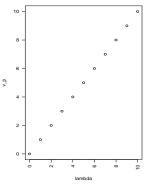
Note: this is best done for all predictors and according to predicted values!

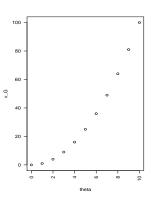
## GLM assumptions: correct amount of dispersion

## A GLM assumes a particular relationship between mean and variance:

```
p <- seq(0, 1, 0.1)
lambda <- 0:10
theta <- 0:10
v_b <- binomial()$variance(p)
v_p <- poisson()$variance(lambda)
v_G <- Gamma()$variance(theta)
par(mfrow = c(1, 3), las = 2)
plot(v_b - p); plot(v_p - lambda); plot(v_G - theta)</pre>
```







## GLM assumptions: correct amount of dispersion

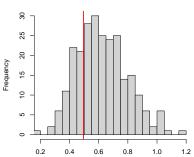
- Overdispersion = more variance than expected
  - $\bullet \ \ \mathsf{very} \ \mathsf{common} \ \to \ \mathsf{increases} \ \mathsf{false} \ \mathsf{positive}$
  - specially relevant for Poisson and Binomial
  - irrelevant for the binary case! (don't look for it)
  - Usual suspects:
    - lack of linearity
    - unobserved heterogeneity
    - zero-augmentation
- Underdispersion = less variance than expected
  - $\bullet$  rather rare  $\to$  increases false negative

## GLM assumptions: testing overdispersion

Usual recommended tests are quite poor (deviance / residual degree of freedom. . . ). A much better alternative: use DHARMa:

testDispersion(res\_mod\_challenger\_binom)

### DHARMa nonparametric dispersion test via sd of residuals fitted vs. simulated



Simulated values, red line = fitted model. p-value (two.sided) = 0.4

```
## DHARMa nonparametric dispersion test via sd of residuals fitted vs. simulated ## ## data: simulationOutput ## ratioObsSim = 0.79224, p-value = 0.464 ## alternative hypothesis: two.sided
```

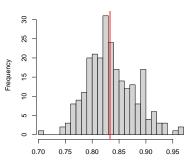
Alexandre Courtiol (IZW)

## GLM assumptions: testing overdispersion

Usual recommended tests are quite poor (deviance / residual degree of freedom...). A much better alternative: use DHARMa:

testDispersion(res\_mod\_horsekick)

# DHARMa nonparametric dispersion test via sd of residuals fitted vs. simulated



Simulated values, red line = fitted model. p-value (two.sided) = 0.5

```
##
## DHARMa nonparametric dispersion test via sd of residuals fitted vs. simulated
##
## data: simulationOutput
## ratioObsSim = 0.99726, p-value = 0.904
## alternative hypothesis: two.sided
```

## GLM assumptions: fixing overdispersion

### Potential solutions:

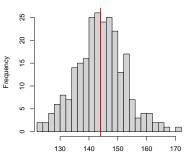
- fix linearity issues
- fix heterogeneity issues (if you have the data)
- model the overdispersion (e.g. using spaMM)
- try another probability distribution
  - $\bullet \ \, \text{Poisson overdispersed?} \to \text{quasipoisson overdispersed?} \to \text{Negative binomial or COMPoisson (e.g. using spaMM)}$
  - $\bullet$  Binomial overdispersed?  $\to$  quasibinomial or GLMM with random effect per observation

• there are specific solutions if the origin is zero-augmentation!!

## Do we have too many zeros?

```
testZeroInflation(res_mod_horsekick) ## again from DHARMa
```

### DHARMa zero-inflation test via comparison to expected zeros with simulation under H0 = fitted model



Simulated values, red line = fitted model. p-value (two.sided) =

```
## DHARMa zero-inflation test via comparison to expected zeros with simulation under HO = fitted model
##
## data: simulationOutput
## ratioObsSim = 0.99659, p-value = 1
## alternative hypothesis: two.sided
```

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Why could you have too many zeros (in GLM)?

It can occur when the response results from a 2 (or more) steps process

## Examples:

- detection issue (low counts are less detected, e.g. counting cells on microscope)
- biological (e.g. infection, then spread of microbes)

We have 2 main options if you have too many zeros:

- Fit an hurdle model:
  - binomial (or truncated count distribution) + truncated Poisson or truncated negative binomial
  - a single source of zeros (e.g. measuring device fails)
- Fit a zero-inflation model:
  - binomial (or truncated count distribution) + Poisson or negative binomial
  - two sources of zeros (e.g. number of viruses in individuals 0 for unexposed, 0 for exposed with strong immune system)

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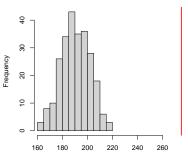
Note 1: If you are not sure where the zeros come from, try both!

Note 2: both solutions are implemented in the package pscl for GLM (and glmmTMB for mixed models).

```
library(pscl)
data("bioChemists", package = "pscl")
head(bioChemists)
                 mar kid5 phd ment
    art fem
      O Men Married
                        0 2.52
      O Women Single 0 2.05
      O Women Single 0 3.75
## 3
                                  6
## 4
     0 Men Married
                     1 1.18
## 5
    0 Women Single 0 3.75
## 6 0 Women Married 2 3.59
                                  2
mod bioch poiss <- glm(art ~ .. data = bioChemists, family = poisson(link = "log"))
res mod bioch poiss <- simulateResiduals(mod bioch poiss)
testOverdispersion(res_mod_bioch_poiss, plot = FALSE)
## plotSimulatedResiduals is deprecated, switch your code to using the testDispersion function
   DHARMa nonparametric dispersion test via sd of residuals fitted vs. simulated
## data: simulationOutput
## ratioObsSim = 1.414, p-value < 2.2e-16
## alternative hypothesis: two.sided
```

```
testZeroInflation(res_mod_bioch_poiss)
```

### DHARMa zero-inflation test via comparison to expected zeros with simulation under H0 = fitted model



Simulated values, red line = fitted model. p-value (two.sided) = (

```
DHARMa zero-inflation test via comparison to expected zeros with simulation under HO = fitted model
  data: simulationOutput
## ratioObsSim = 1.4391, p-value < 2.2e-16
## alternative hypothesis: two.sided
```

```
mod bioch zinfl <- zeroinfl(art ~ . | 1. data = bioChemists, dist = "poisson")
mod_bioch_zinfl ## mind that binomial model measures excess of _non-zero_
##
## Call:
## zeroinfl(formula = art ~ . | 1, data = bioChemists, dist = "poisson")
## Count model coefficients (poisson with log link):
## (Intercept) femWomen marMarried
                                               kid5
                                                             phd
                                                                        ment
     0.553995 -0.231609
                               0.131971
                                          -0.170474
                                                        0.002526
                                                                    0.021543
## Zero-inflation model coefficients (binomial with logit link):
## (Intercept)
     -1.681
mod bioch hurdle <- hurdle(art ~ . | 1, data = bioChemists, dist = "poisson")
mod_bioch_hurdle ## mind that binomial model measures excess of _zero_
##
## Call:
## hurdle(formula = art ~ . | 1, data = bioChemists, dist = "poisson")
## Count model coefficients (truncated poisson with log link):
## (Intercept) femWomen marMarried kid5
                                                             phd
                                                                        ment
      0.67114 -0.22858
                            0.09648
                                        -0.14219
                                                       -0.01273
                                                                     0.01875
## Zero hurdle model coefficients (binomial with logit link):
## (Intercept)
       0.8447
```

```
mod_bioch_zinfl2 <- zeroinfl(art ~ . | 1, data = bioChemists, dist = "negbin")
mod_bioch_zinfl2 ## mind that binomial model measures excess of _non-zero_
##
## Call:
## zeroinfl(formula = art ~ . | 1, data = bioChemists, dist = "negbin")
##
## Count model coefficients (negbin with log link):
## (Intercept) femWomen marMarried
                                               kid5
                                                            phd
                                                                        ment
       0.25615 -0.21642
                                0.15049 -0.17642
                                                         0.01527
                                                                     0.02908
## Theta = 2.2644
##
## Zero-inflation model coefficients (binomial with logit link):
## (Intercept)
## -11.95
mod bioch hurdle2 <- hurdle(art ~ . | 1, data = bioChemists, dist = "negbin")
mod_bioch_hurdle2 ## mind that binomial model measures excess of _zero_
##
## Call:
## hurdle(formula = art ~ . | 1, data = bioChemists, dist = "negbin")
## Count model coefficients (truncated negbin with log link):
## (Intercept) femWomen marMarried
                                               kid5
                                                             phd
                                                                        ment
     0.355125
               -0.244672
                              0.103417 -0.153260
                                                       -0.002933
                                                                    0.023738
## Theta = 1.8285
##
## Zero hurdle model coefficients (binomial with logit link):
## (Intercept)
##
       0.8447
```

```
library(lmtest)
lrtest(mod bioch zinfl, mod bioch zinfl2, mod bioch hurdle, mod bioch hurdle2)
## Warning in modelUpdate(objects[[i - 1]], objects[[i]]): original model was of class "zeroinfl", updated model is of class "hurdle"
## Warning in modelUpdate(objects[[i - 1]], objects[[i]]): original model was of class "zeroinfl", updated model is of class "hurdle"
## Likelihood ratio test
##
## Model 1: art ~ . | 1
## Model 2: art ~ . | 1
## Model 3: art ~ . | 1
## Model 4: art ~ . | 1
    #Df LogLik Df Chisa Pr(>Chisa)
## 1 7 -1620.8
## 2 8 -1561.0 1 119.65 < 2.2e-16 ***
## 3 7 -1639.4 -1 156.88 < 2.2e-16 ***
## 4
      8 -1586.7 1 105.43 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Note: the model mod\_bioch\_zinfl2 is clearly the best one.

### You can then evaluate then as usual:

```
lrtest(mod_bioch_zinfl2) ## test against null model
Anova(mod_bioch_zinfl2) ## test predictors
summary(mod_bioch_zinfl2) ## test parameter estimates (approximative)
```

## GLM assumptions: no separation

Separation occurs when a level or combination of levels for categorical predictor, or when a particular threshold along a continuous predictor, predicts the outcomes perfectly. It prevents the model to fit or lead to silly estimates and SF

```
set.seed(1L)
n <- 50
myxococcus <- data.frame(sporulation = rbinom(2*n, prob = c(rep(0, n), rep(0.75, n)), size = 1),
                  strain = factor(c(rep("sp1", n), rep("sp2", n))))
table(mvxococcus$sporulation, mvxococcus$strain)
       sp1 sp2
    0 50 13
    1 0 37
```

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table(mvxococcus$sporulation, mvxococcus$strain)
       sp1 sp2
     0 50 13
     1 0 37
mod <- glm(sporulation ~ strain, data = myxococcus, family = binomial(link = "log"))</pre>
summary(mod)
##
## Call:
## glm(formula = sporulation ~ strain, family = binomial(link = "log"),
       data = mvxococcus)
## Deviance Residuals:
        Min
                   10
                         Median
                                       30
                                                Max
  -1.64139 -0.00005 -0.00005 0.77602 0.77602
## Coefficients:
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -20.39
                           2291.90 -0.009
                                              0.993
## strainsp2
                  20.09
                                              0.993
                           2291.90
                                    0.009
## (Dispersion parameter for binomial family taken to be 1)
```

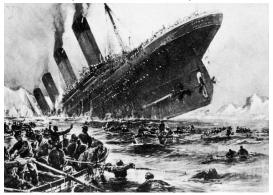
## GLM assumptions: fixing separation

## One possible way out is to use the package brglm2

```
library(brglm2)
mod2 <- glm(sporulation ~ strain, data = myxococcus, family = binomial(link = "log"), method = "brglmFit")
summary (mod2)
##
## Call:
## glm(formula = sporulation ~ strain, family = binomial(link = "log"),
      data = mvxococcus, method = "brglmFit")
##
## Deviance Residuals:
                10 Median
                                         Max
## -1.6474 -0.1411 -0.1411 0.7715 0.7715
##
## Coefficients:
              Estimate Std. Error z value Pr(>|z|)
## (Intercept) -4.615 1.414 -3.263 0.00110 **
## strainsp2 4.317 1.417 3.048 0.00231 **
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
      Null deviance: 131.795 on 99 degrees of freedom
## Residual deviance: 58.302 on 98 degrees of freedom
## AIC: 62.302
## Number of Fisher Scoring iterations: 3
```

## GLM: challenge

Try to understand what influenced survival (i.e. access to lifeboats) during the Titanic disaster.



### head(TitanicSurvival)

```
survived
                                                   age passengerClass
                                            sex
## Allen, Miss. Elisabeth Walton
                                     yes female 29.0000
## Allison, Master. Hudson Trevor
                                           male 0.9167
                                                                 1st
## Allison, Miss. Helen Loraine
                                    no female 2.0000
                                                                 1st
## Allison, Mr. Hudson Joshua Crei no male 30.0000
                                                                 1st
## Allison, Mrs. Hudson J C (Bessi
                                 no female 25.0000
                                                                 1st
                                     yes
## Anderson, Mr. Harry
                                           male 48.0000
                                                                  1st
```

# Getting started with R

- Some basic tests
- Principal Component Analysis
- Linear Models
  - introduction
  - traditional linear model (LM)
  - generalised linear models (GLM)
  - mixed models (LMM & GLMM)

Liner mixed-effects models (LMM) and generalised linear mixed-effects models (GLMM) are extensions from, respectivelly, LM and GLM for situations for which there is covariation between the errors.

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Mixed-effects models allow for:

- the study of other questions than LM (e.g. heritability)
- the fixing of assumption violations in LM (lack of dependence, some cases of overdispersion)
- the reduction of the uncertainty in estimates and predictions in cases where many parameters would have to be estimated at the cost of an additional hypothesis (the distribution of the random effects)

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The main sources of heterogeneity considered by mixed-effects models are:

- origin (in its widest sense)
- time
- space

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- origin (in its widest sense)
- time
- space

Note 1: how to perform predicitons, tests, checks of the assumptions... properly requires to first master (G)LM and is matter of current research; so it is beyond the context of this short introduction.

Note 2: for good packages, check lme4, spaMM & glmmTMB.

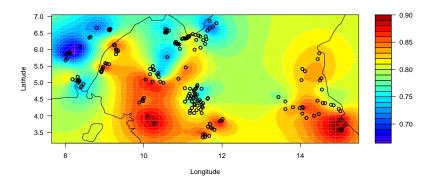
#### With mixed models, you can account for replicates! Example:

```
data("Oats", package = "nlme")
#coplot(yield ~ nitro | Variety + Block, data = Oats, type = "b")
library(spaMM)
mod_yield_spaMM <- fitme(yield ~ nitro + Variety + (1|Block), data = Oats)
mod vield spaMM
## formula: yield ~ nitro + Variety + (1 | Block)
## ML: Estimation of lambda and phi by ML.
      Estimation of fixed effects by ML.
## Family: gaussian ( link = identity )
  ----- Fixed effects (beta) ------
                   Estimate Cond. SE t-value
## (Intercept)
                     82.400 6.969 11.823
## nitro
                    73.667 7.889 9.338
## VarietvMarvellous
                            4.321 1.225
                      5.292
## VarietvVictorv
                     -6.875
                            4.321 -1.591
   ----- Random effects -----
## Family: gaussian ( link = identity )
            --- Variance parameters ('lambda'):
## lambda = var(u) for u ~ Gaussian;
     Block : 201.8
              --- Coefficients for log(lambda):
               Term Estimate Cond.SE
   Group
## Block (Intercept) 5.307 0.6035
## # of obs: 72; # of groups: Block, 6
   ----- Residual variance
## Coefficients for log(phi) ~ 1 :
              Estimate Cond. SE
## (Intercept) 5.412 0.1734
## Estimate of phi=residual var: 224.1
```

#### With mixed models, you can account for spatial and/or temporal autocorrelation!

#### Example:

```
data("Loaloa", package = "spaMM")
ndvi <- Loaloa[, c("maxNDVI", "latitude", "longitude")]
mod_ndvi_spaMM <- fitme(maxNDVI - 1 + Matern(1|longitude + latitude), data = ndvi, method = "REML")
filled.mapMM(mod_ndvi_spaMM, add.map = TRUE, plot.title = title(xlab = "Longitude", ylab = "Latitude"))</pre>
```



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With mixed models, you can estimate the effects of variable(s) that you cannot measure!

Example: the estimation of genetic additive effects and heritability.



#### **Journal of Animal Ecology**

Journal of Animal Ecology 2010, 79, 13-26

doi: 10.1111/j.1365-2656.2009.01639.x

SPECIAL 'HOW TO ... ' PAPER

An ecologist's guide to the animal model

Alastair J. Wilson1\*, Denis Réale2, Michelle N. Clements1, Michael M. Morrissey1, Erik Postma3, Craig A. Walling1, Loeske E. B. Kruuk1 and Daniel H. Nussey1

With mixed models, you can estimate the effects of variable(s) that you cannot measure!

Example: the estimation of genetic additive effects and heritability.

```
ID Dam Sire
## 1304 127 917
## 1305 117
            550
## 1306 95
## 1307 158 689
## 1308 131 1223
## 1309 144 1222
```

tail(Gryphon\$pedigree)

With mixed models, you can estimate the effects of variable(s) that you cannot measure!

Example: the estimation of genetic additive effects and heritability.

```
tail(Gryphon$pedigree)
         ID Dam Sire
## 1304 127
            917
## 1305 117
             550
## 1306 95
## 1307 158 689
## 1308 131 1223
## 1309 144 1222
```

```
library(nadiv)
## Loading required package: Matrix
A <- as(makeA(Gryphon$pedigree), "matrix")
colnames(A) <- rownames(A) <- Gryphon$pedigree$ID</pre>
A[1305:1309, 1296:1309]
             113 130 155 100 145 133 90
                                             110
                                                       127
                                                               117
                                                                                 131
                                                                       95 158
                                                                                        144
## 117 0.0000000
                                  0 0 0.0000000 0.0078125 1.00000 0.03125
                                                                           0 0.0000 0.0000
## 95 0.0000000 0
                                  0 0 0.0078125 0.0156250 0.03125 1.00000
                                                                           0 0.0000 0.0000
## 158 0.0078125 0 0
                                  0 0 0.0000000 0.0000000 0.00000 0.00000
                                                                           1 0.0000 0.0000
## 131 0.0000000 0
                                  0 0 0.0000000 0.0000000 0.00000 0.00000
                                                                           0 1.0000 0.0625
## 144 0.0000000
                                  0 0.0000000 0.0000000 0.00000 0.00000
                                                                            0 0.0625 1.0000
```

With mixed models, you can estimate the effects of variable(s) that you cannot measure! Example: the estimation of genetic additive effects and heritability.

```
mod_gryphon <- fitme(BWT ~ 1 + corrMatrix(1|ID), corrMatrix = A, data = Gryphon$data, method = "REML")
mod_gryphon
## formula: BWT ~ 1 + corrMatrix(1 | ID)
## REML: Estimation of corrPars, lambda and phi by REML.
       Estimation of fixed effects by ML.
## Estimation of lambda and phi by 'outer' REML, maximizing p_bv.
## Family: gaussian ( link = identity )
## ----- Fixed effects (beta) -----
             Estimate Cond. SE t-value
## (Intercept) 7.59 0.1391 54.57
  ----- Random effects -----
## Family: gaussian ( link = identity )
            --- Variance parameters ('lambda'):
## lambda = var(u) for u ~ Gaussian;
    ID : 3.395
## # of obs: 854; # of groups: ID, 854
   ----- Residual variance
## phi estimate was 3.82861
  ----- Likelihood values -----
                        logLik
## p_v(h) (marginal L): -2029.983
  p_beta,v(h) (ReL): -2031.037
```

With mixed models, you can estimate the effects of variable(s) that you cannot measure! Example: the estimation of genetic additive effects and heritability.

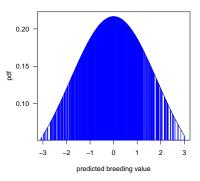
```
mod_gryphon <- fitme(BWT ~ 1 + corrMatrix(1|ID), corrMatrix = A, data = Gryphon$data, method = "REML")
mod_gryphon
## formula: BWT ~ 1 + corrMatrix(1 | ID)
## REML: Estimation of corrPars, lambda and phi by REML.
        Estimation of fixed effects by ML.
## Estimation of lambda and phi by 'outer' REML, maximizing p by.
## Family: gaussian ( link = identity )
## ----- Fixed effects (beta) -----
             Estimate Cond. SE t-value
## (Intercept) 7.59 0.1391 54.57
  ----- Random effects -----
## Family: gaussian ( link = identity )
           --- Variance parameters ('lambda'):
## lambda = var(u) for u ~ Gaussian:
     ID : 3.395
## # of obs: 854: # of groups: ID, 854
   ----- Residual variance
## phi estimate was 3.82861
  ----- Likelihood values ------
                        logLik
## p_v(h) (marginal L): -2029.983
  p_beta,v(h) (ReL): -2031.037
(h2 <- as.numeric(mod gryphon$lambda / (mod gryphon$lambda + mod gryphon$phi)))
## [1] 0.4700152
```

Note: the model is a little slow to fit ( $\sim$ 60 sec, but optimisations are possible)

With mixed models, you can estimate the effects of variable(s) that you cannot measure!

Example: the estimation of genetic additive effects and heritability.

```
curve(dnorm(x, sd = sqrt(as.numeric(mod_gryphon$lambda["ID"]))), from = -3, to = 3, las = 1,
     ylab = "pdf", xlab = "predicted breeding value")
BLUPs <- ranef(mod_gryphon)$"corrMatrix(1 | ID)"
points(dnorm(BLUPs, sd = sqrt(as.numeric(mod_gryphon$lambda["ID"]))) ~ BLUPs, col = "blue", type = "h", lwd = 0.1)
```



With mixed models, you can estimate the effects of variable(s) that you cannot measure!

Example: the estimation of genetic additive effects and heritability.

```
plot(BLUPs ~ scale(mod_gryphon$data$BWT), ylab = "Predicted breeding values", xlab = "Scaled phenotypic values")
```

