

Getting to do statistics in R

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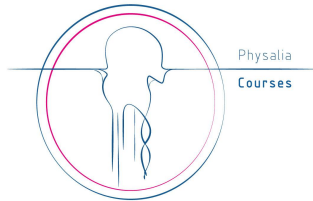
Leibniz Institute of Zoo and Wildlife Research

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**Leibniz Institute for Zoo
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Getting started with R

- 1 Some basic tests
- 2 Principal Component Analysis
- 3 Linear Models

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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Just the correlation coefficient:

```
cor(x = iris$Sepal.Length, y = iris$Sepal.Width, method = "pearson")
## [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 0.04351158
## sample estimates:
## cor
## -0.1175698
```

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```

Note: two other methods are available: “spearman” & “kendall”.

R provides many statistical tests out of the box

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

E.g.

```
cor.test(formula = ~ Sepal.Length + Sepal.Width, data = iris)

##
## Pearson's product-moment correlation
##
## data: Sepal.Length and 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 0.04351158
## sample estimates:
## cor
## -0.1175698
```

is synonymous to:

```
cor.test(x = iris$Sepal.Length, y = iris$Sepal.Width)

##
## 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
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```

R provides many statistical tests out of the box

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

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
```

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## mean of x mean of y
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```

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

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

##
## Wilcoxon rank sum test with continuity correction
##
## data: iris$Sepal.Length[iris$Species == "versicolor"] and iris$Sepal.Length[iris$Species == "setosa"]
## W = 2331.5, p-value = 8.346e-14
## alternative hypothesis: true location shift is not equal to 0
```


R provides many statistical tests out of the box

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

The paired *t*-test (parametric):

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

##
## Paired t-test
##
## data:  iris$Sepal.Length[iris$Species == "versicolor"] and iris$Petal.Length[iris$Species == "versicolor"]
## t = 34.006, df = 49, p-value < 2.2e-16
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  1.576957 1.775043
## sample estimates:
## mean of the differences
##                1.676
```

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##                1.676
```

The Wilcoxon-signed-rank test (non-parametric):

```
wilcox.test(x = iris$Sepal.Length[iris$Species == "versicolor"],
            y = iris$Petal.Length[iris$Species == "versicolor"], paired = TRUE)

##
## Wilcoxon signed rank test with continuity correction
##
## data:  iris$Sepal.Length[iris$Species == "versicolor"] and iris$Petal.Length[iris$Species == "versicolor"]
## V = 1275, p-value = 7.454e-10
## alternative hypothesis: true location shift is not equal to 0
```

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The paired *t*-test (parametric):

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t.test(x = iris$Sepal.Length[iris$Species == "versicolor"],
       y = iris$Petal.Length[iris$Species == "versicolor"], paired = TRUE)

##
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## V = 1275, p-value = 7.454e-10
## alternative hypothesis: true location shift is not equal to 0
```

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

R provides many statistical tests out of the box

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
```

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```
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##
##  Kruskal-Wallis rank sum test
##
## data:  Petal.Length by Species
## Kruskal-Wallis chi-squared = 130.41, df = 2, p-value < 2.2e-16
```

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
```

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## data:  Petal.Length and Species
## F = 1828.1, num df = 2.000, denom df = 78.073, p-value < 2.2e-16
```

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

R provides many statistical tests out of the box

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
```

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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
```

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
```


R provides many statistical tests out of the box

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
```

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
```

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

R provides many statistical tests out of the box

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 normally 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
##           0.2200361
```

R provides many statistical tests out of the box

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##  0.1594015 0.3037352
## sample estimates:
## ratio of variances
##          0.2200361
```

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
```

R provides many statistical tests out of the box

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
```

R provides many statistical tests out of the box

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.

R provides many statistical tests out of the box

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
```

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##
## data:  iris$Sepal.Length and iris$Petal.Length
## D = 0.56, p-value < 2.2e-16
## alternative hypothesis: two-sided
```

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
```

R provides many statistical tests out of the box

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:  
## 0.4439045 0.9747893  
## sample estimates:  
## probability of success  
## 0.8
```


R provides many statistical tests out of the box

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
```

R provides many statistical tests out of the box

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
```

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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
```

R provides many statistical tests out of the box

E.g. test(s) of independence:

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```

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
```

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 **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!

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PCA without packages

PCA is a traditional method for dimensionality reduction:

```
head(USArrests) ## 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
## California	9.0	276	91	40.6
## Colorado	7.9	204	78	38.7

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```
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	PC2	PC3
## Alabama	-1.1980278	0.8338118	-0.16217848
## Alaska	-2.3087473	-1.5239622	0.03833574
## Arizona	-1.5033307	-0.4983038	0.87822311
## Arkansas	-0.1759894	0.3247326	0.07111174
## California	-2.0452358	-1.2725770	0.38153933
## Colorado	-1.2634133	-1.4264063	-0.08369314

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	Murder	Assault	UrbanPop	Rape
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## Arizona	-1.5033307	-0.4983038	0.87822311
## Arkansas	-0.1759894	0.3247326	0.07111174
## California	-2.0452358	-1.2725770	0.38153933
## Colorado	-1.2634133	-1.4264063	-0.08369314

```
pca_US$rotation ## coefficients applied to original coordinate (after z-scoring them) to obtain the new coordinates by linear combination
```

	PC1	PC2	PC3
## Murder	-0.5826006	0.5339532	-0.6127565
## Assault	-0.6079818	0.2140236	0.7645600
## Rape	-0.5393836	-0.8179779	-0.1999436

PCA without packages

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

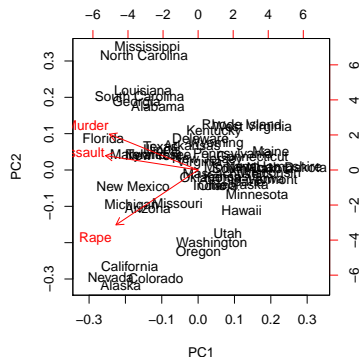
```
summary(pca_US)
## Importance of components:
##              PC1      PC2      PC3
## Standard deviation  1.5358 0.6768 0.42822
## Proportion of Variance 0.7862 0.1527 0.06112
## Cumulative Proportion 0.7862 0.9389 1.00000
```

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summary(pca_US)
## Importance of components:
##              PC1      PC2      PC3
## Standard deviation  1.5358 0.6768 0.42822
## Proportion of Variance 0.7862 0.1527 0.06112
## Cumulative Proportion 0.7862 0.9389 1.00000
```

```
biplot(x = pca_US)
```



PCA with ade4

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:
##      Ax1      Ax2      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
```

PCA with ade4

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)

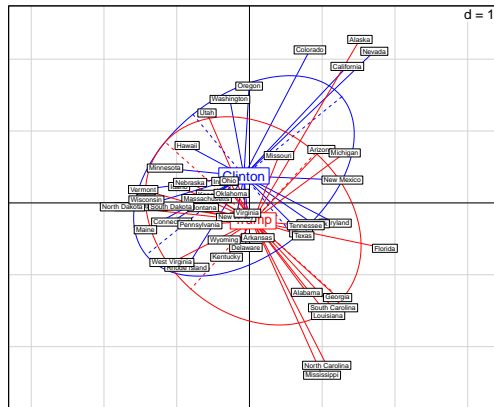
summary(pca_US_ade4)

## Class: pca dudi
## Call: dudi.pca(df = USArrests[, -3], scale = TRUE, scannf = FALSE)
##
## Total inertia: 3
##
## Eigenvalues:
##      Ax1      Ax2      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
```

Let us add voting data to this dataset:

```
USArrests$Vote <- rep("Trump", times = 50)
Clinton_state <- c("California", "Colorado", "Connecticut", "Delaware", "Hawaii", "Illinois", "Maine", "Maryland", "Massachusetts",
                  "Minnesota", "Nevada", "New Hampshire", "New Jersey", "New Mexico", "New York", "Oregon", "Rhode Island", "Vermont",
                  "Virginia", "Washington")
USArrests[Clinton_state, "Vote"] <- "Clinton"
USArrests$Vote <- factor(USArrests$Vote)
```

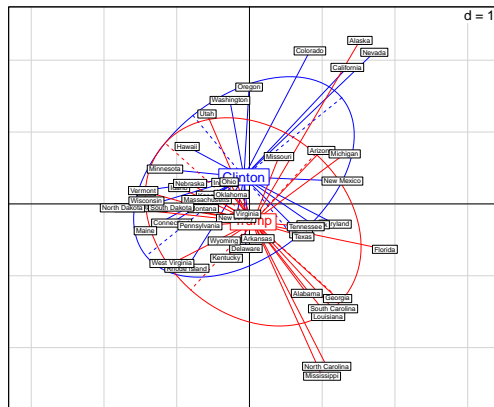
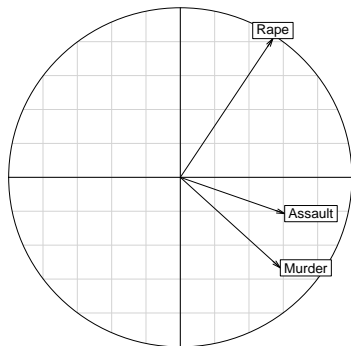
The package allows a different kind of plot that is quite interesting:



PCA with ade4

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

```
par(mfrow = c(1, 2))
s.corcircle(dfx = pca_US_ade4$c1)
s.class(dfx = pca_US_ade4$l1, fac = USArrests$Vote, col = c("blue", "red"))
s.label(dfx = pca_US_ade4$l1, label = rownames(USArrests), add.plot = TRUE, clabel = 0.5)
```



Note: using `co` & `li` instead of `c1` & `l1` would respect the relative contribution of each principal component according to the variance they capture.

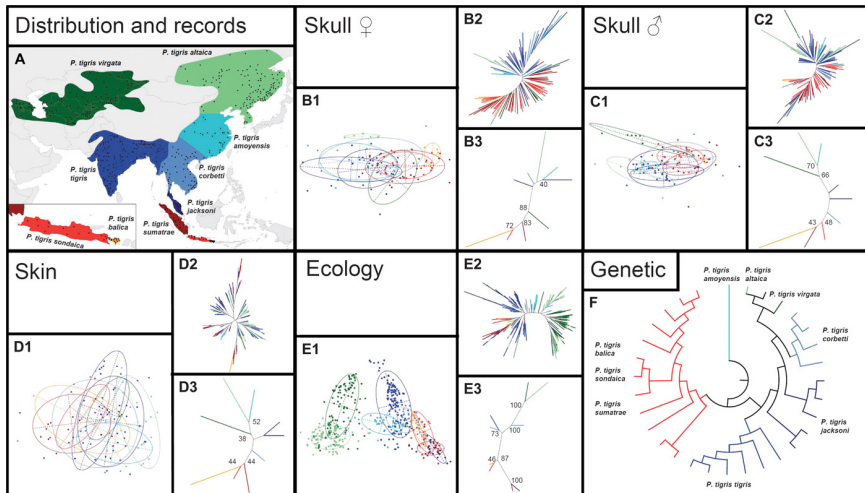
Example of application of PCA: a revision of tiger taxonomy

RESEARCH ARTICLE | CONSERVATION ECOLOGY

Planning tiger recovery: Understanding intraspecific variation for effective conservation

Andreas Wilting^{1,*}, Alexandre Courtiol¹, Per Christiansen², Jürgen Niedballa¹, Anne K. Scharf^{1,†}, Ludovic Orlando³, Niko Bal...

* See all authors and affiliations

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Getting started with R

- 1 Some basic tests
- 2 Principal Component Analysis
- 3 **Linear Models**

Getting started with R

1 Some basic tests

2 Principal Component Analysis

3 Linear Models

- introduction

- traditional linear model (LM)
- generalised linear models (GLM)
- mixed models (LMM & GLMM)

What is a linear model?

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

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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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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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- 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

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

Linear models in R

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

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

Linear models in R

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

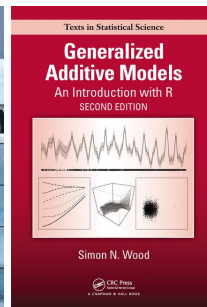
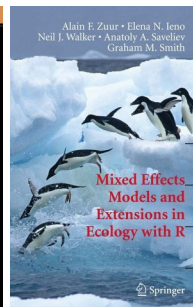
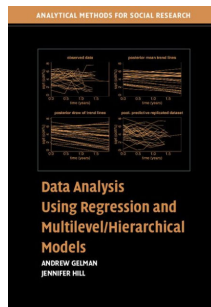
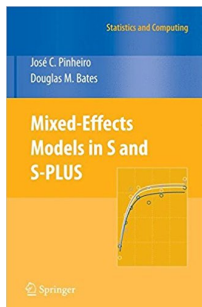
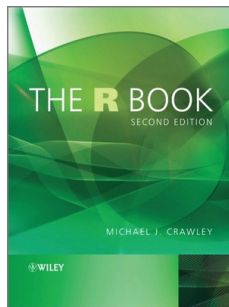
For now, no other software seems to be remotely as good (prognostic: only Julia or Python may change that within a decade but I find it unlikely).

Models	Packages for fitting	Helper packages
LM	stats*; spaMM	car; lmtest; visreg
GLM	stats*; spaMM; psc1	car; DHARMA; visreg
LMM	lme4; spaMM; glmmTMB	DHARMA; pbkrtest; visreg
GLMM	lme4; spaMM; glmmTMB	DHARMA; pbkrtest; visreg
GAM	mgcv	DHARMA; visreg
GAMM	mgcv	

* = included in any R installation!

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

Good books dealing with linear models in R



Note: it is also useful to look at books 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 (`tibble`)

Example of a good dataset:

```
head(iris)

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

str(iris)

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

any(is.na(iris))

## [1] FALSE
```

Getting started with R

1 Some basic tests

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3 Linear Models

- introduction
- **traditional linear model (LM)**
- generalised linear models (GLM)
- mixed models (LMM & GLMM)

LM: notation

Simple notation:

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

LM: notation

Simple notation:

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

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

LM: notation

Simple notation:

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

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

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

LM: notation

Matrix notation:

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

LM: notation

Matrix notation:

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

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

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

LM: notation

Matrix notation:

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

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

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

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

LM: specifications

R formula notation:

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

LM: specifications

R formula notation:

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

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

LM: specifications

R formula notation:

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

```
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  
## 2             1.4         0.2  
## 51            4.7         1.4  
## 52            4.5         1.5  
## 101           6.0         2.5  
## 102           5.1         1.9
```

LM: specifications

R formula notation:

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

```
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
## 2             1.4          0.2
## 51            4.7          1.4
## 52            4.5          1.5
## 101           6.0          2.5
## 102           5.1          1.9
```

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

##      (Intercept) Petal.Width
## 1             1          0.2
## 2             1          0.2
## 51            1          1.4
## 52            1          1.5
## 101           1          2.5
## 102           1          1.9
```


LM: specifications

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
## 51	4.7	versicolor
## 52	4.5	versicolor
## 101	6.0	virginica
## 102	5.1	virginica

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

	(Intercept)	Speciesversicolor	Speciesvirginica
## 1	1	0	0
## 2	1	0	0
## 51	1	1	0
## 52	1	1	0
## 101	1	0	1
## 102	1	0	1

LM: specifications

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
## 51	4.7	1.4	versicolor
## 52	4.5	1.5	versicolor
## 101	6.0	2.5	virginica
## 102	5.1	1.9	virginica

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

	(Intercept)	Petal.Width	Speciesversicolor	Speciesvirginica
## 1	1	0.2	0	0
## 2	1	0.2	0	0
## 51	1	1.4	1	0
## 52	1	1.5	1	0
## 101	1	2.5	0	1
## 102	1	1.9	0	1

LM: specifications

R formula notation:

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

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

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

```
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
## 51	4.7	1.4	versicolor
## 52	4.5	1.5	versicolor
## 101	6.0	2.5	virginica
## 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	1	0.2	0	0	0.0	0.0
## 2	1	0.2	0	0	0.0	0.0
## 51	1	1.4	1	0	1.4	0.0
## 52	1	1.5	1	0	1.5	0.0
## 101	1	2.5	0	1	0.0	2.5
## 102	1	1.9	0	1	0.0	1.9

LM: specifications

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
## 51	4.7	1.4	versicolor
## 52	4.5	1.5	versicolor
## 101	6.0	2.5	virginica
## 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	1	0.2	0	0	0.0	0.0
## 2	1	0.2	0	0	0.0	0.0
## 51	1	1.4	1	0	1.4	0.0
## 52	1	1.5	1	0	1.5	0.0
## 101	1	2.5	0	1	0.0	2.5
## 102	1	1.9	0	1	0.0	1.9

LM: specifications

R formula notation:

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

```
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
## 51	4.7	1.4	versicolor
## 52	4.5	1.5	versicolor
## 101	6.0	2.5	virginica
## 102	5.1	1.9	virginica

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

##	(Intercept)	Petal.Width	Petal.Width:Speciesversicolor	Petal.Width:Speciesvirginica
## 1	1	0.2	0.0	0.0
## 2	1	0.2	0.0	0.0
## 51	1	1.4	1.4	0.0
## 52	1	1.5	1.5	0.0
## 101	1	2.5	0.0	2.5
## 102	1	1.9	0.0	1.9

LM: specifications

R formula notation:

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

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

```
model_frame <- model.frame(mod) ## the data used for the fit
model_frame[c(1:2, 51:52, 101:102), , drop = FALSE]

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

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

##      (Intercept)
## 1             1
## 2             1
## 51            1
## 52            1
## 101           1
## 102           1
```

LM: specifications

R formula notation:

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

```
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
## 51	4.7	7.0	3.2	1.4	versicolor
## 52	4.5	6.4	3.2	1.5	versicolor
## 101	6.0	6.3	3.3	2.5	virginica
## 102	5.1	5.8	2.7	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	1	5.1	3.5	0.2	0	0
## 2	1	4.9	3.0	0.2	0	0
## 51	1	7.0	3.2	1.4	1	0
## 52	1	6.4	3.2	1.5	1	0
## 101	1	6.3	3.3	2.5	0	1
## 102	1	5.8	2.7	1.9	0	1

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)

Understanding the design matrix

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- your formula
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- the contrasts (for qualitative variables)

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

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

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

Understanding the design matrix

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

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- your data
- the contrasts (for qualitative variables)

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model.matrix(mod2)[c(1, 51, 101), ]
```

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## 1	1	1	0
## 51	1	0	1
## 101	1	-1	-1

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

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

Understanding the design matrix

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

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

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

LM outputs: parameter estimates

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

Simply printing the object provides you with the parameter estimates:

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

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

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

LM outputs: parameter estimates

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

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

```
vcov(mod)
```

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

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And thus the standard errors:

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

##	(Intercept)	Petal.Width	Speciesversicolor	Speciesvirginica
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You can also get confidence intervals:

```
confint(mod)
```

	2.5 %	97.5 %
## (Intercept)	1.0824564	1.340338
## Petal.Width	0.7178294	1.319594
## Speciesversicolor	1.3401762	2.055407
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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" "effects" "rank" "fitted.values" "assign" "qr" "df.residual"
## [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
```

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```

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

```
methods(class = "lm")
## [1] add1          alias          anova          case.names    coerce        confint        cooks.distance deviance      dfbeta
## [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         proj          qr            residuals    rstandard    rstudent      show         simulate     slotsFromS3
## [37] summary       variable.names vcov
## see '?methods' for accessing help and source code
```

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

LM tests: coefficients

For LM, simply use `summary()`:

```
summary(mod)

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

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 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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

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)
## 1      146  20.83
## 2      149 464.33 -3    -443.49 1036 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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

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

LM predictions: fitted values

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

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

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

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```

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

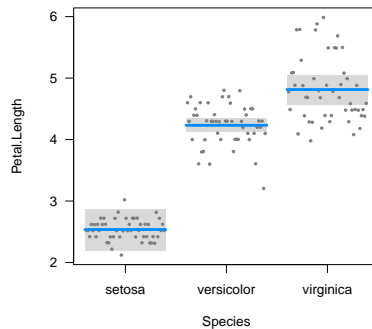
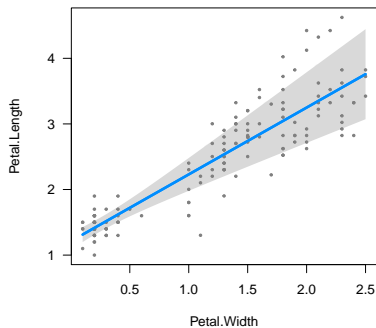
As expected, observations are equal to the fitted values + residuals:

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

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

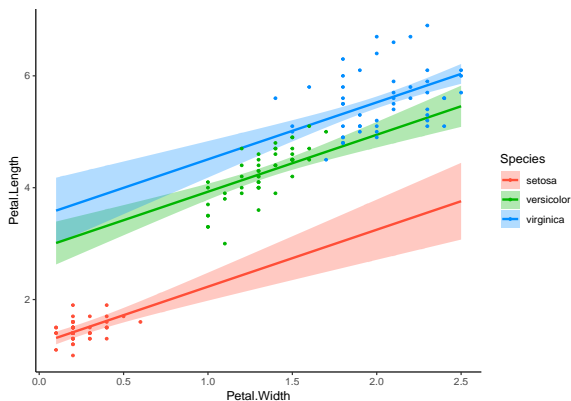
LM predictions: fast and dirty plot

```
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

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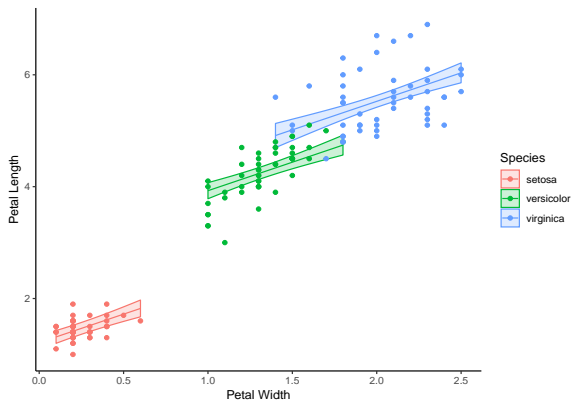
Then, it is easy:

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

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


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()
```



LM assumptions: generalities

Model structure:

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

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Errors:

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

LM assumptions: linearity

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

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

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- non-linear models → function `nls` or dedicated package (e.g. `nlme`)
- general additive models → package `mgcv`

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Quiz: can you express the following models as LM?

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

LM assumptions: lack of perfect multicollinearity

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

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

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Diagnostics:

- plot the predictors against each other → `function pairs()`
- `findLinearCombos` from the package `caret`

Solutions:

- change design matrix (change parameterization or drop redundant effects) → argument `formula`
- change the experimental design
- collect more data

LM assumptions: lack of perfect multicollinearity

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

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

Diagnostics:

- plot the predictors against each other \rightarrow function `pairs()`
- `findLinearCombos` from the package `caret`

Solutions:

- change design matrix (change parameterization or drop redundant effects) \rightarrow argument `formula`
- change the experimental design
- collect more data

Alternatives:

- none

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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	1Q	Median	3Q	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
```

LM assumptions: predictor variables have fixed values

The dependent variable are represented by fixed values.

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

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- better measurements

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Diagnostics:

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Solutions:

- often ignored in practice
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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`)

LM assumptions: independence (no serial autocorrelation)

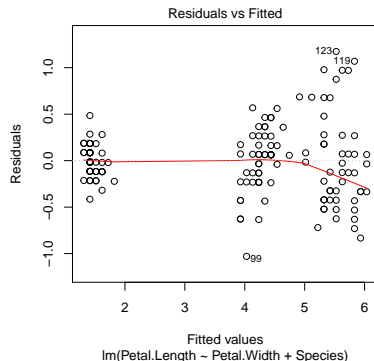
A lack of independence (serial autocorrelation) in the residuals can appear if there is a departure from linearity, if data have been sampled non-randomly (e.g. spatial or temporal series), or if there is an overarching structure (e.g. repeated measures within individuals, families, species, ...). Lack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

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Diagnostic by eye:

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



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Diagnostic by Durbin-Watson test:

```
durbinWatsonTest(mod) ## from package car (DW varies between 0 & 4, 2 is best, you wish for non-significant p-value)
## lag Autocorrelation D-W Statistic p-value
## 1 0.1313867 1.734855 0.054
## Alternative hypothesis: rho != 0
```

Note: the alternative from the package `lmtest` offer to rank the residuals according to a variable.

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Alternatives:

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

LM assumptions: constant variance (homoscedasticity)

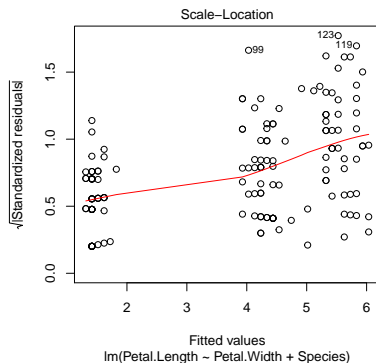
Heteros(c/k)edasticity can emerge when there is a mean - variance relationship, when there is non independence between observations, when reaction norm changes according to the treatment. It can create both false positives and false negative.

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Diagnostic by eye:

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



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Diagnostic by Breusch-Pagan test:

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

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

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Alternatives:

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

LM assumptions: normality

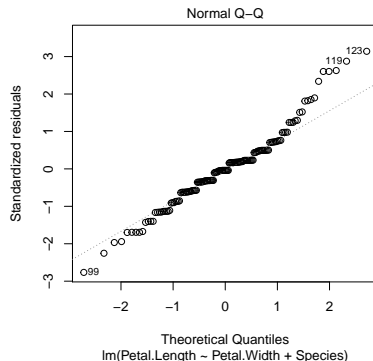
The distribution of residuals can be skewed, this is often caused by the presence of outliers, and/or when the process generating the data is very different from normal (e.g. Poisson, Binomial...).

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Diagnostic by eye:

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



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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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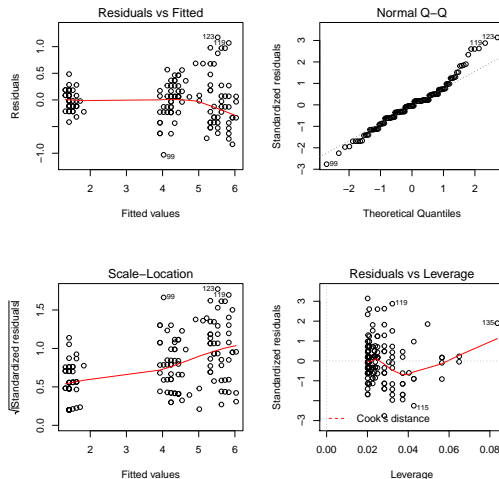
Alternatives:

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

LM assumptions: simple glimpse

You can check all assumptions about the errors at once:

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



LM assumptions: outliers

There is a powerful function in R:

```
influence.measures(mod)

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

LM assumptions: outliers

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

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

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

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

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

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- `cook.d` → F statistics comparing simultaneously the changes in all estimates when the observation is dropped or not

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- `hat` → 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)

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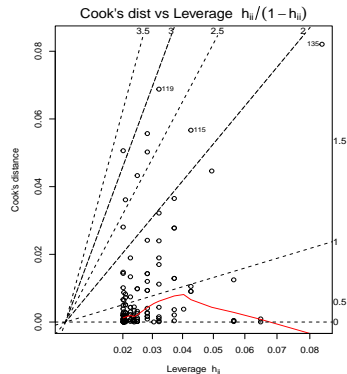
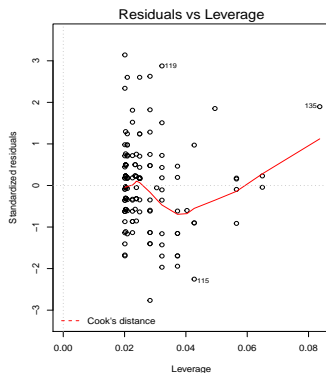
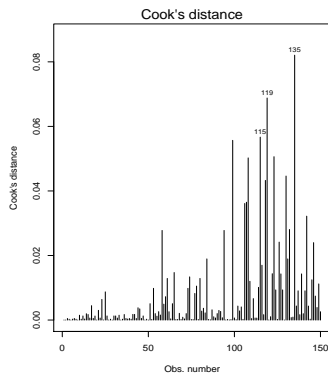
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```

LM assumptions: outliers

There are also plotting possibilities:

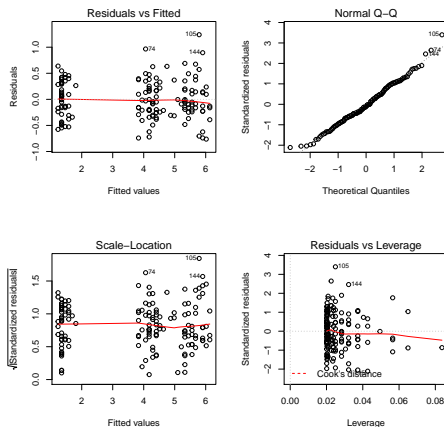
```
par(mfrow = c(1, 3))
plot(mod, which = 4:6)
```



LM assumptions: simple glimpse at residuals

What would it look like if it was perfect?

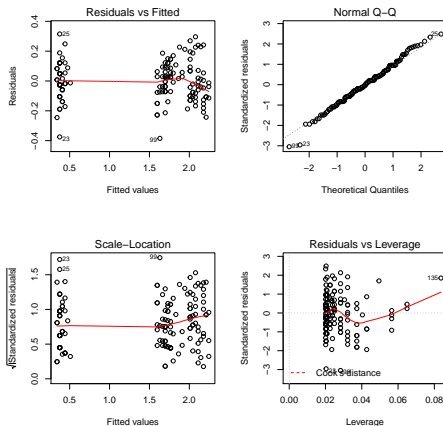
```
iris$Fake.Petal.Length <- simulate(object = mod)[, 1] ## if you rerun that, it will change each time!
mod_perfect <- lm(Fake.Petal.Length ~ Petal.Width + Species, data = iris)
par(mfrow = c(2, 2))
plot(mod_perfect)
```



LM assumptions: fixing iris?

Fixing attempt:

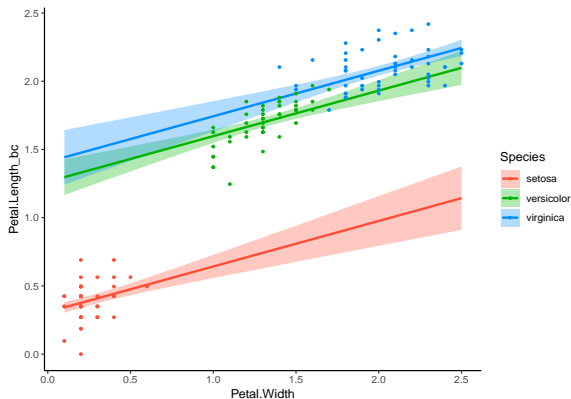
```
bc <- powerTransform(mod)
iris$Petal.Length_bc <- bcPower(iris$Petal.Length, lambda = bc$lambda)
mod_bc <- lm(Petal.Length_bc ~ Petal.Width + Species, data = iris)
par(mfrow = c(2, 2))
plot(mod_bc)
```



LM assumptions: fixing iris?

Plotting predictions:

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

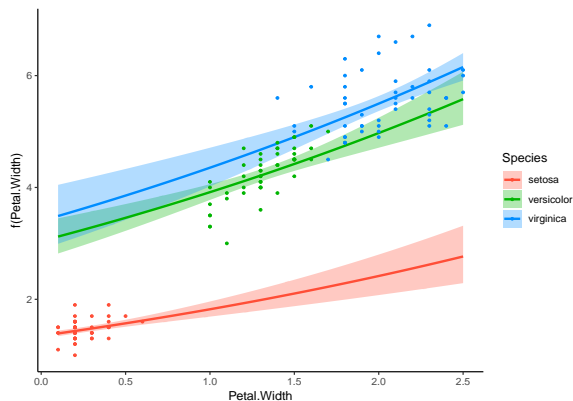


Note: that is not very useful because it is on the BoxCoxed scale!

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

1 Some basic tests

2 Principal Component Analysis

3 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.

GLM: what for?

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

That includes the analysis of:

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

GLM: notation

Definition:

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

with:

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

Notation:

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

GLM: notation

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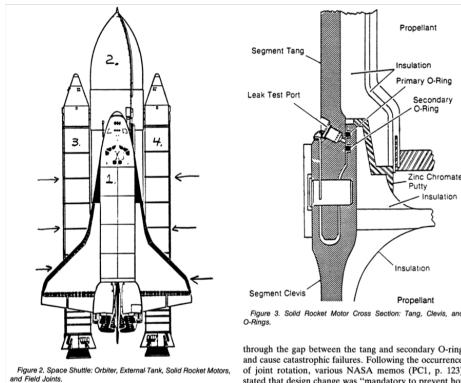
Notation:

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

This is identical to the LM if:

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

The 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
## 1      0 1875     G     no
## 2      0 1875     I     no
## 3      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.

GLM: specifications

In R notation:

```
Challenger$issue <- Challenger$oring_dt > 0  
  
mod_challenger_binar <- glm(issue ~ temp + psi, family = binomial(link = "logit"), data = Challenger)
```

GLM: specifications

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)
```

GLM: specifications

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)
```

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


GLM: specifications

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"
```

GLM: specifications

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

The link function:

```
probs <- 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)
logits
## [1] -2.1972246 -1.3862944 -0.8472979 -0.4054651  0.0000000  0.4054651  0.8472979  1.3862944  2.1972246
```

GLM: specifications

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```
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## [1] "family"      "link"         "linkfun"      "linkinv"      "variance"     "dev.resids"  "aic"          "mu.eta"       "initialize"   "validmu"
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```

The inverse link function:

```
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
```

GLM: specifications

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

```
names(binomial(link = "logit"))
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## [11] "valideta"    "simulate"
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```

The inverse link function:

```
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
```

GLM: specifications

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"
```

The link function:

```
probs <- 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)
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:

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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
## temp        -0.32094631 -0.05964840
## psi         -0.01351725  0.02361973
```

GLM: outputs

```
mod_horsekick
##
## Call:  glm(formula = deaths ~ corps, family = poisson(link = "log"),
##       data = VonBort)
##
## Coefficients:
## (Intercept)      corpsI      corpsII      corpsIII      corpsIV      corpsV      corpsVI      corpsVII      corpsVIII      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  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
## corpsIV     -1.5958865  0.1280845
## corpsV      -1.1704167  0.3841036
```


GLM: outputs

```
mod_horsekick
##
## Call:  glm(formula = deaths ~ corps, family = poisson(link = "log"),
##       data = VonBort)
##
## Coefficients:
## (Intercept)      corpsI      corpsII      corpsIII      corpsIV      corpsV      corpsVI      corpsVII      corpsVIII      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  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
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## 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 predictor!!

GLM outputs: parameter estimates

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

GLM outputs: parameter estimates

There is no general recipe, 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 recipe, 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)
```

```
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)
```

```
## 1         20      14.033
```

```
## 2         22      26.402 -2    -12.37 0.002061 **
```

```
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

GLM tests: the overall model

```
mod_challenger_binar_null <- glm(issue ~ 1, family = binomial(link = "logit"), data = Challenger)
```

```
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)
```

```
## 1         20      14.033
```

```
## 2         22      26.402 -2    -12.37 0.002061 **
```

```
## ---
```

```
## 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)
```

```
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)
```

```
## 1         20       9.4309
```

```
## 2         22      20.7057 -2    -11.275 0.003562 **
```

```
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

GLM tests: the overall model

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

```
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 *  
## ---  
## Signif. 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 '**' 0.01 '*' 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 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```


GLM tests: coefficients

```
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 *
## psi          0.006007   0.009749   0.616   0.5378
## ---
## 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
```

GLM tests: coefficients

```
summary(mod_challenger_binar)

##
## Call:
## glm(formula = issue ~ temp + psi, family = binomial(link = "logit"),
##      data = Challenger)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
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## 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 *
## psi          0.006007   0.009749   0.616   0.5378
## ---
## 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!

GLM tests: coefficients

```
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       3Q      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 **
## psi          0.002585   0.008485   0.305  0.76065
## ---
## 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
## AIC: 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!

GLM tests: coefficients

```
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
## corpsVI       6.062e-02  3.483e-01   0.174   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      -2.076e-01  3.734e-01  -0.556   0.5781
## 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
## corpsXV      -6.931e-01  4.330e-01  -1.601   0.1094
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 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
```

GLM: predictions

Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binar)
```

```
##           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
```

GLM: predictions

Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binar)
```

```
##           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           9           10          11          12
## -0.9624767 -2.3628680 -2.0127701 -1.6626723 -1.3125745 -3.0630636 -3.1128120 -2.0625185  3.0894521  0.9888651 -1.4618197 -4.2626023
##           13           14           15           16           17           18           19           20           21           22           23
## -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!!!!!!!!!!
```

```
##           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, newdata = data.frame(temp = 31, psi = mean(Challenger$psi)), type = "response")
```

```
##           1
## 0.9999932
```

GLM: predictions

Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binar)
```

```
##           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           9           10          11          12
## -0.9624767 -2.3628680 -2.0127701 -1.6626723 -1.3125745 -3.0630636 -3.1128120 -2.0625185  3.0894521  0.9888651 -1.4618197 -4.2626023
##           13           14           15           16           17           18           19           20           21           22           23
## -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!!!!!!!
```

```
##           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, newdata = data.frame(temp = 31, psi = mean(Challenger$psi)), type = "response")
```

```
##           1
## 0.9999932
```

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

GLM: predictions

Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binom)
```

```
##           1           2           3           4           5           6           7           8           9          10          11
## 0.035530620 0.018340627 0.021659999 0.025564480 0.030151101 0.013130540 0.012615879 0.020818071 0.200067319 0.082846346 0.026793507
##           12           13           14           15           16           17           18           19           20           21           22
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
##           23
## 0.174277588
```


GLM: predictions

Fitted values are on the scale of probabilities:

```
fitted(mod_challenger_binom)
```

```
##           1           2           3           4           5           6           7           8           9           10          11
## 0.035530620 0.018340627 0.021659999 0.025564480 0.030151101 0.013130540 0.012615879 0.020818071 0.200067319 0.082846346 0.026793507
##           12           13           14           15           16           17           18           19           20           21           22
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
##           23
## 0.174277588
```

```
predict(mod_challenger_binom, type = "link") ## the default!!!!!!!!!!
```

```
##           1           2           3           4           5           6           7           8           9           10          11          12
## -3.3011832 -3.9801257 -3.8103901 -3.6406545 -3.4709188 -4.3195969 -4.3601029 -3.8508960 -1.3858737 -2.4042874 -3.5924367 -4.9503217
##           13           14           15           16           17           18           19           20           21           22           23
## -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!!!!!!!!!!
```

```
##           1           2           3           4           5           6           7           8           9           10          11
## 0.035530620 0.018340627 0.021659999 0.025564480 0.030151101 0.013130540 0.012615879 0.020818071 0.200067319 0.082846346 0.026793507
##           12           13           14           15           16           17           18           19           20           21           22
## 0.007031341 0.043804332 0.330277287 0.043804332 0.011645578 0.026793507 0.004237529 0.009845462 0.005940184 0.011645578 0.009845462
##           23
## 0.174277588
```

```
predict(mod_challenger_binom, newdata = data.frame(temp = 31, psi = mean(Challenger$psi)), type = "response")
```

```
##           1
## 0.9480262
```

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

GLM: predictions

Fitted values are on the scale of counts:

```
fitted(mod_horsekick)[1:30]
```

```
##      1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18     19     20     21     22     23     24     25     26     27
## 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!!!!!!!
```

```
##           1           2           3           4           5           6           7           8           9           10           11           12
## -0.2231436 -0.2231435 -0.5108256 -0.5108256 -0.9162907 -0.5978370 -0.1625189 -0.5108256 -1.0498221 -0.4307829 -0.2876821 0.2231436
##           13           14           15           16           17           18           19           20           21           22           23           24
## 0.1823216 -0.9162907 -0.2231436 -0.2231435 -0.5108256 -0.5108256 -0.9162907 -0.5978370 -0.1625189 -0.5108256 -1.0498221 -0.4307829
##           25           26           27           28           29           30
## -0.2876821 0.2231436 0.1823216 -0.9162907 -0.2231436 -0.2231435
```

```
predict(mod_horsekick, type = "response")[1:30] ## the useful one!!!!!!!
```

```
##      1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18     19     20     21     22     23     24     25     26     27
## 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
```

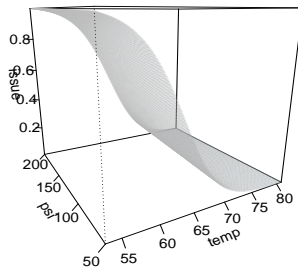
GLM: predictions

Try that:

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

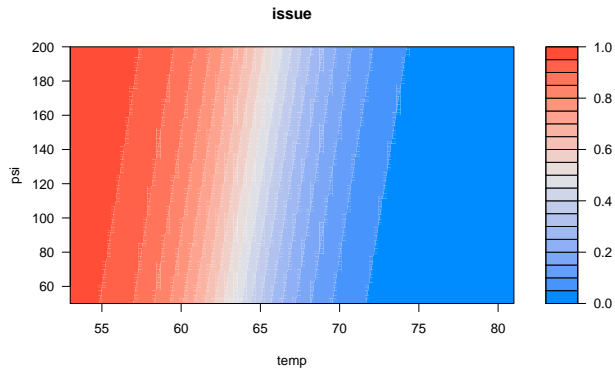
GLM: predictions

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



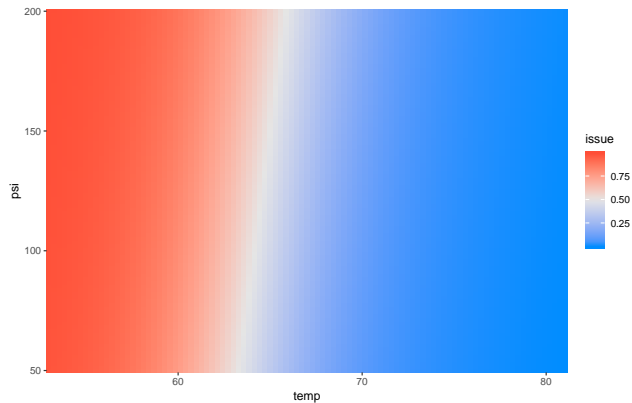
GLM: predictions

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



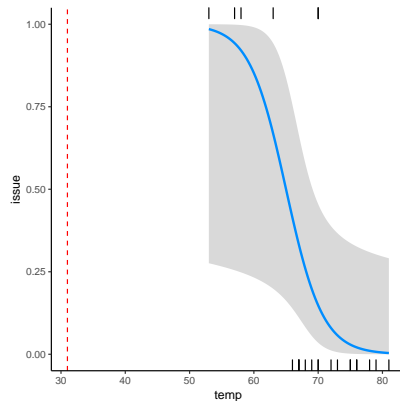
GLM: predictions

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



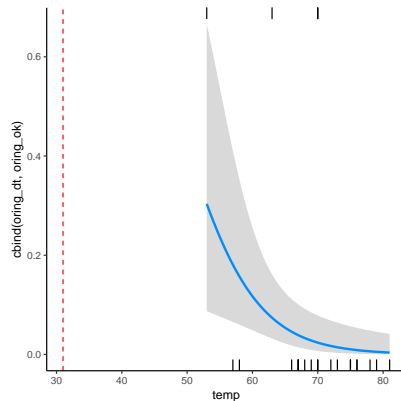
GLM: predictions

```
visreg(fit = mod_challenger_binar, xvar = "temp",  
       cond = list(psi = mean(Challenger$psi)),  
       gg = TRUE, scale = "response") +  
  geom_vline(xintercept = 31, colour = "red", lty = 2) +  
  theme_classic()
```



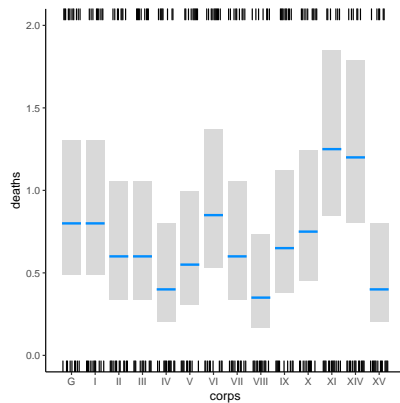
GLM: predictions

```
visreg(fit = mod_challenger_binom, xvar = "temp",  
       cond = list(psi = mean(Challenger$psi)),  
       gg = TRUE, scale = "response") +  
  geom_vline(xintercept = 31, colour = "red", lty = 2) +  
  theme_classic()
```



GLM: predictions

```
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

GLM assumptions: linearity

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`

GLM assumptions: linearity

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`

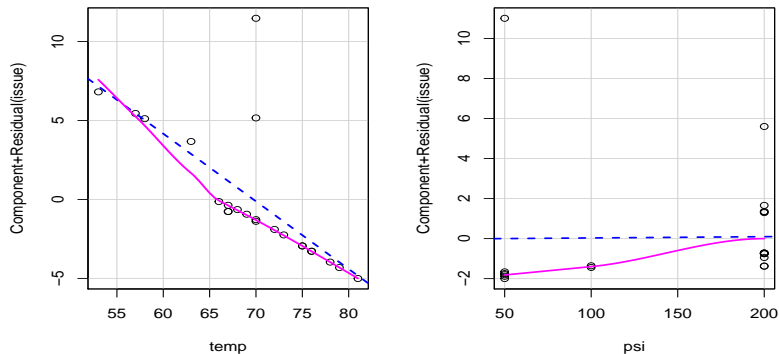
Note: same fix as for LM!

GLM assumptions: linearity

Partial residual plots using car:

```
crPlots(mod_challenger_binar)
```

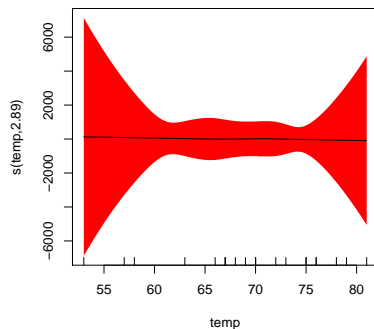
Component + Residual Plots



GLM assumptions: linearity

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!
```



GLM assumptions: linearity

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

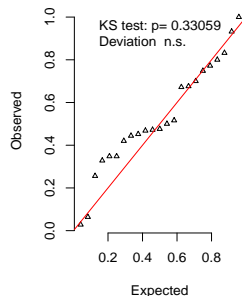
Note that, since v0.1.6.2, DHARMA includes support for glmmTMB, but there are still a few minor limitations associated with this package. Please see <https://github.com/florianhartig/DHARMA/issues/16> for details, in particular if you use this for production.

```
res_mod_challenger_binar <- simulateResiduals(mod_challenger_binar)
```

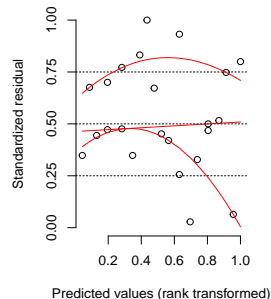
```
plot(res_mod_challenger_binar)
```

DHARMA scaled residual plots

QQ plot residuals



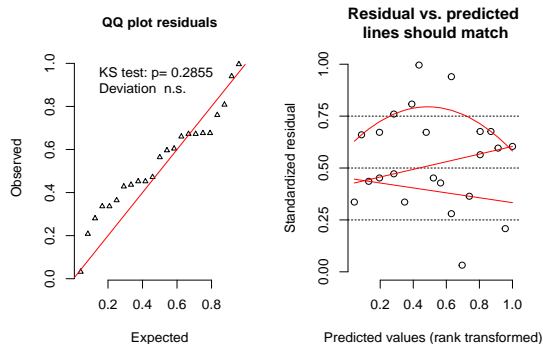
Residual vs. predicted
lines should match



GLM assumptions: linearity

```
res_mod_challenger_binom <- simulateResiduals(mod_challenger_binom)  
plot(res_mod_challenger_binom)
```

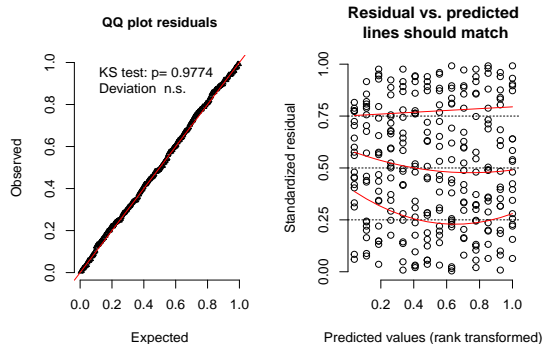
DHARMa scaled residual plots



GLM assumptions: linearity

```
res_mod_horsekick <- simulateResiduals(mod_horsekick)
plot(res_mod_horsekick)
```

DHARMa scaled residual plots

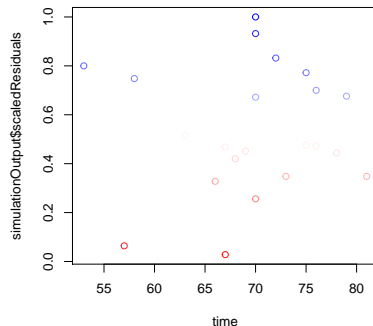


GLM assumptions: multicollinearity & fixed-values

Same as for LM!

GLM assumptions: lack for serial autocorrelation

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



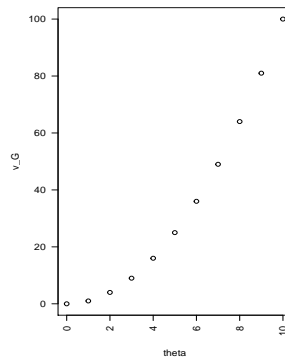
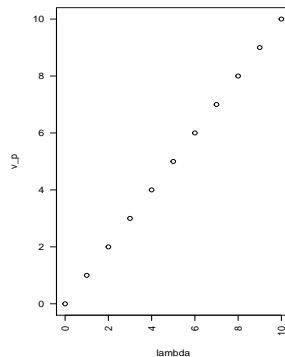
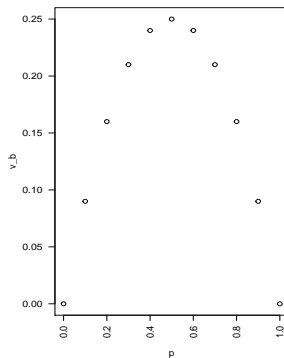
```
##
## Durbin-Watson test
##
## data: simulationOutput$scaledResiduals ~ 1
## DW = 2.4423, p-value = 0.2762
## alternative hypothesis: true autocorrelation is not 0
```

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)
```



GLM assumptions: correct amount of dispersion

- Overdispersion = more variance than expected
 - very common → increases false 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
 - rather rare → increases false negative

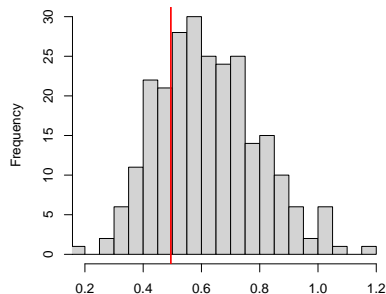
GLM assumptions: testing overdispersion

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
```

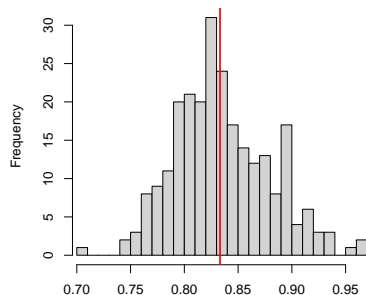
GLM assumptions: testing overdispersion

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) = 0.904

```
##
## 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:

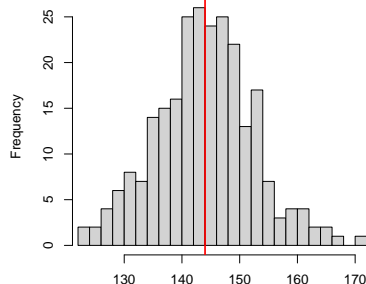
- fix linearity issues
- fix heterogeneity issues (if you have the data)
- model the overdispersion (e.g. using `spaMM`)
- try another probability distribution
 - Poisson overdispersed? → quasipoisson overdispersed? → Negative binomial or COMPoisson (e.g. using `spaMM`)
 - Binomial overdispersed? → quasibinomial or GLMM with random effect per observation
- there are specific solutions if the origin is zero-augmentation!!

GLM assumptions: the right amount of zeros

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 H_0 = fitted model



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

```
##
## DHARMA zero-inflation test via comparison to expected zeros with simulation under  $H_0$  = fitted model
##
## data: simulationOutput
## ratioObsSim = 0.99659, p-value = 1
## alternative hypothesis: two.sided
```

GLM assumptions: the right amount of zeros

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)

GLM assumptions: the right amount of zeros

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)

GLM assumptions: the right amount of zeros

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)

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).

Example of zero-inflation

```
library(psc1)
data("bioChemists", package = "psc1")
head(bioChemists)
```

```
##   art   fem   mar kid5  phd ment
## 1    0   Men Married    0 2.52    7
## 2    0 Women Single    0 2.05    6
## 3    0 Women Single    0 3.75    6
## 4    0   Men Married    1 1.18    3
## 5    0 Women Single    0 3.75   26
## 6    0 Women Married    2 3.59    2
```

```
mod_bioc_h_poiss <- glm(art ~ ., data = bioChemists, family = poisson(link = "log"))
```

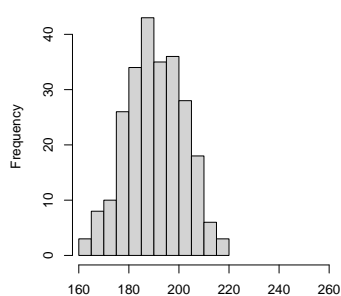
```
res_mod_bioc_h_poiss <- simulateResiduals(mod_bioc_h_poiss)
testOverdispersion(res_mod_bioc_h_poiss, plot = FALSE)

## 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
```

Example of zero-inflation

```
testZeroInflation(res_mod_bioch_pois)
```

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) = 1

```
##
## DHARMA zero-inflation test via comparison to expected zeros with simulation under H0 = fitted model
##
## data: simulationOutput
## ratioObsSim = 1.4391, p-value < 2.2e-16
## alternative hypothesis: two.sided
```

Example of zero-inflation

```
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
```


Example of zero-inflation

```
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
```

Example of zero-inflation

```
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  Chisq Pr(>Chisq)
## 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 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Note: the model `mod_bioch_zinfl2` is clearly the best one.

Example of zero-inflation

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 SE.

```
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(myxococcus$sporulation, myxococcus$strain)

##
##      sp1 sp2
##  0    50  13
##  1     0  37
```

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table(myxococcus$sporulation, myxococcus$strain)

##
##      sp1 sp2
##    0  50  13
##    1   0  37
```

```
mod <- glm(sporulation ~ strain, data = myxococcus, family = binomial(link = "log"))
summary(mod)

##
## Call:
## glm(formula = sporulation ~ strain, family = binomial(link = "log"),
##      data = myxococcus)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      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    2291.90   0.009   0.993
##
## (Dispersion parameter for binomial family taken to be 1)
##
```

GLM assumptions: fixing separation

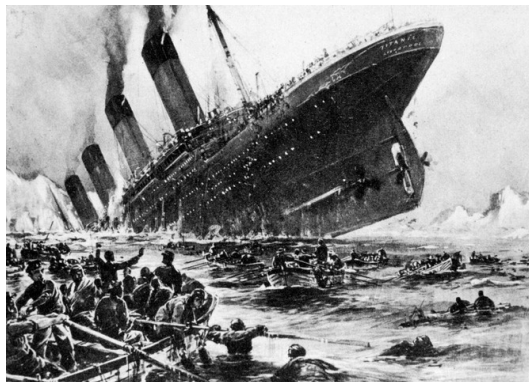
One possible way out is to use the package `brglm2`

```
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 = myxococcus, method = "brglmFit")
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      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    sex    age passengerClass
## Allen, Miss. Elisabeth Walton      yes female 29.0000          1st
## Allison, Master. Hudson Trevor      yes  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
## Anderson, Mr. Harry                 yes   male 48.0000          1st
```

Getting started with R

1 Some basic tests

2 Principal Component Analysis

3 Linear Models

- introduction
- traditional linear model (LM)
- generalised linear models (GLM)
- **mixed models (LMM & GLMM)**

(G)LMM: introduction

Linear mixed-effects models (LMM) and generalised linear mixed-effects models (GLMM) are extensions from, respectively, LM and GLMM for situation for which there is covariation between the errors.

(G)LMM: introduction

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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)

(G)LMM: introduction

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

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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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Note 1: how to perform predicitions, 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`.

(G)LMM: showcase

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_yield_spaMM

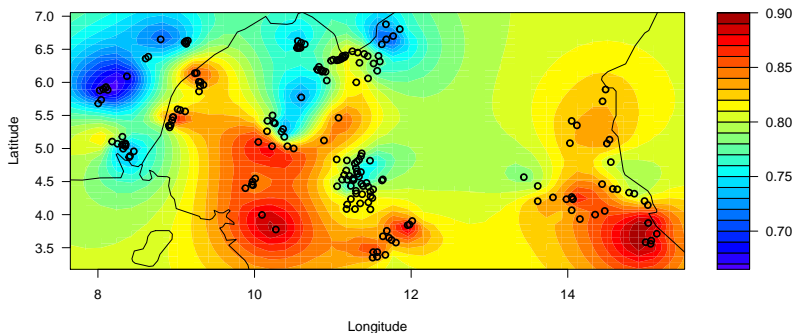
## formula: yield ~ nitro + Variety + (1 | Block)
## ML: Estimation of lambda and phi by ML.
##      Estimation of fixed effects by ML.
## Family: gaussian ( link = identity )
## ----- Fixed effects (beta) -----
##              Estimate Cond. SE t-value
## (Intercept)      82.400    6.969  11.823
## nitro            73.667    7.889   9.338
## VarietyMarvellous  5.292    4.321   1.225
## VarietyVictory    -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):
## Group      Term Estimate Cond.SE
## 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
## ----- Likelihood values -----
```

(G)LMM: showcase

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"))
```



(G)LMM: showcase

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. Wilson^{1*}, Denis Réale², Michelle N. Clements¹, Michael M. Morrissey¹,
Erik Postma³, Craig A. Walling¹, Loeske E. B. Kruuk¹ and Daniel H. Nussey¹



(G)LMM: showcase

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  NA
## 1305 117  550  NA
## 1306  95   29  NA
## 1307 158  689  NA
## 1308 131 1223  NA
## 1309 144 1222  NA
```


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```
tail(Gryphon$pedigree)
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## 1304 127  917  NA
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## 1306  95   29  NA
## 1307 158  689  NA
## 1308 131 1223  NA
## 1309 144 1222  NA
```

```
library(nadiv)
```

```
## Loading required package: Matrix
```

```
A <- as(makeA(Gryphon$pedigree), "matrix")
```

```
colnames(A) <- rownames(A) <- Gryphon$pedigree$ID
```

```
A[1305:1309, 1296:1309]
```

```
##      113 130 155 100 145 133 90      110      127      117      95 158      131      144
## 117 0.0000000 0 0 0 0 0 0 0.0000000 0.0078125 1.00000 0.03125 0 0.0000 0.0000
## 95 0.0000000 0 0 0 0 0 0 0.0078125 0.0156250 0.03125 1.00000 0 0.0000 0.0000
## 158 0.0078125 0 0 0 0 0 0 0.0000000 0.0000000 0.00000 0.00000 1 0.0000 0.0000
## 131 0.0000000 0 0 0 0 0 0 0.0000000 0.0000000 0.00000 0.00000 0 1.0000 0.0625
## 144 0.0000000 0 0 0 0 0 0 0.0000000 0.0000000 0.00000 0.00000 0 0.0625 1.0000
```

(G)LMM: showcase

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
```

(G)LMM: showcase

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")
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```

```
## formula: BWT ~ 1 + corrMatrix(1 | ID)
## REML: Estimation of corrPars, lambda and phi by REML.
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## Estimation of lambda and phi by 'outer' REML, maximizing p_bv.
## Family: gaussian ( link = identity )
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##      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
```

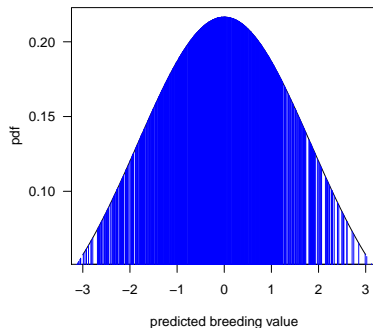
Note: the model is a little slow to fit...

(G)LMM: showcase

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)
```



(G)LMM: showcase

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")
```

