## Review of linear models

## 12 Sep 2024

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```
## it's nice to include packages at the top
## (and NOT automatically install them)
## try not to carry over packages you don't use
library(faux)
library(brglm2) ## for lizards data
library(ggplot2); theme_set(theme_bw())
## diagnostics
library(performance)
library(DHARMa)
## downstream model evaluation
library(broom)
library(dotwhisker)
library(emmeans)
library(effects)
library(marginaleffects)
library(parameters)
## library(ggeffects)
```

## Why linear models? (Lindeløv 2019)

#### Common statistical tests are linear models

See worked examples and more details at the accompanying notebook: https://lindeloev.github.io/tests-as-linear

	Common name Built-in function in R		Equivalent linear model in R Exact?		The linear model in words		
(×	y is independent of x P: One-sample t-test N: Wilcoxon signed-rank	t.test(y) wilcox.test(y)	Im(y ~ 1) Im(signed_rank(y) ~ 1)	for N >14	One number (intercept, i.e., the mean) predicts <b>y</b> (Same, but it predicts the <i>signed rank</i> of <b>y</b> .)	- <del>22</del>	
: Im(y ~ 1	P: Paired-sample t-test N: Wilcoxon matched pairs	t.test(y <sub>1</sub> , y <sub>2</sub> , paired=TRUE) wilcox.test(y <sub>1</sub> , y <sub>2</sub> , paired=TRUE)	$Im(y_2 - y_1 \sim 1)$ $Im(signed\_rank(y_2 - y_1) \sim 1)$	√ f <u>or N &gt;14</u>	One intercept predicts the pairwise y <sub>2</sub> -y <sub>1</sub> differences (Same, but it predicts the <i>signed rank</i> of y <sub>2</sub> -y <sub>1</sub> .)	<b>Z</b> →	
Multiple regression: Im(y ~ 1 + $x_1$ + $x_2$ +) Simple regression:	y ~ continuous x P: Pearson correlation N: Spearman correlation	cor.test(x, y, method='Pearson') cor.test(x, y, method='Spearman')	Im(y ~ 1 + x) Im(rank(y) ~ 1 + rank(x))	√ for N >10	One intercept plus <b>x</b> multiplied by a number (slope) predicts <b>y</b> .  - (Same, but with <i>ranked</i> <b>x</b> and <b>y</b> )	نعليبسر	
	y ~ discrete x P: Two-sample t-test P: Welch's t-test N: Mann-Whitney U	t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=TRUE) t.test(y <sub>1</sub> , y <sub>2</sub> , var.equal=FALSE) wilcox.test(y <sub>1</sub> , y <sub>2</sub> )	$\begin{split} & Im(y\sim 1+G_2)^A \\ & gls(y\sim 1+G_2, weights=^B)^A \\ & Im(signed\_rank(y)\sim 1+G_2)^A \end{split}$	√ √ for N >11	An intercept for group 1 (plus a difference if group 2) predicts y.  - (Same, but with one variance per group instead of one common.)  - (Same, but it predicts the signed rank of y.)	*	
	P: One-way ANOVA N: Kruskal-Wallis	aov(y ~ group) kruskal.test(y ~ group)	$\begin{split} & Im(y\sim 1+G_2+G_3++G_N)^A \\ & Im(rank(y)\sim 1+G_2+G_3++G_N)^A \end{split}$	√ for N >11	An intercept for <b>group 1</b> (plus a difference if group ≠ 1) predicts <b>y</b> .  - (Same, but it predicts the <i>rank</i> of <b>y</b> .)	i <sub>t</sub> t†	
	P: One-way ANCOVA	aov(y ~ group + x)	Im(y ~ 1 + $G_2$ + $G_3$ ++ $G_N$ + x) <sup>A</sup>	~	- (Same, but plus a slope on x.) Note: this is discrete AND continuous. ANCOVAs are ANOVAs with a continuous x.		
	P: Two-way ANOVA	aov(y ~ group * sex)	$\begin{split} & Im(y \sim 1 + G_2 + G_3 + \ldots + G_N + \\ & S_2 + S_3 + \ldots + S_K + \\ & G_2^* S_2 + G_3^* S_3 + \ldots + G_N^* S_K) \end{split}$	4	Interaction term: changing sex changes the $y \sim group$ parameters. Note: $G_{2x} = k3$ an $\frac{indicate}{i} (Op. C1)$ for each non-intercept levels of the group variable. Similarly for $S_{2x} = k7$ or sex. The first line (with $G$ ) is min effect of group, $k7$ is escond (with $S_1$ for sex and the third is the group $x$ sex interaction. For two levels (e.g. male/female), line $2$ would ps $S_1$ multiple with each $G_2$ .	[Coming]	
	Counts ~ discrete x N: Chi-square test	chisq.test(groupXsex_table)	Equivalent log-linear model glm(y ~ 1 + $G_2$ + $G_3$ + + $G_N$ + $G_2$ + $S_3$ + + $S_K$ + $G_2$ * $S_3$ + + $S_K$ + $S$	~	Interaction term: (Same as Two-way ANOVA.)  Note: Run gim using the following arguments: $z$ : $z$		
M	N: Goodness of fit	chisq.test(y)	glm(y ~ 1 + G <sub>2</sub> + G <sub>3</sub> ++ G <sub>N</sub> , family=) <sup>A</sup>	1	(Same as One-way ANOVA and see Chi-Square note.)	1W-ANOVA	

List of common parametric (P) non-parametric (N) tests and equivalent linear models. The notation y = 1 + x is R shorthand for  $y = 1 + b + a \cdot x$  which most of us learned in school. Models in similar colors are highly similar, but really, notice how similar they all are across colors! For non-parametric models, the linear models are reasonable approximations for non-small sample sizes (see "Exact" column and click links to see simulations). Other less accurate approximations exist, e.g., Wilcoxon for the sign test and Goodness-of-fit for the binomial test. The signed rank function is  $signed_t = tunction(x) sign(x) * tank (abs(x))$ . The variables (Gand S. are "dummy coded" indicator variables (either 0 or 1) exploiting the fact that when  $\Delta x = 1$  between categories the slope. Subscripts (e.g.,  $G_2$  or y.) indicate difference equations in data. Im requires long-format data for all non-continuous models. All of this is exposed in greater detail and worked examples at <a href="https://lindeloev.github.io/lests-as-linear">https://lindeloev.github.io/lests-as-linear</a>.



#### **Basics**

- assume  $\mathbf{v} \sim \text{Normal}(\mathbf{X}\beta, \sigma)^1$
- **X** is the *model matrix*, can be anything we want it to be
- the *Gauss-Markov theorem* (Wikipedia) makes weaker assumptions:  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \epsilon$ ; as long as  $\epsilon$  is mean-zero, homoscedastic with finite variance, and uncorrelated ... then the OLS solution

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$$

is the BLUE (or MVUE).

we'll embrace the assumptions (which are needed for inference!)

## Computation

- matrix decompositions (QR with pivoting; see here)
- big problems: biglm, speedglm, RcppEigen::fastLm

<sup>^</sup> See the note to the two-way ANOVA for explanation of the notation. 

B Same model, but with one variance per group:  $gls(value \sim 1 + G_{g_f}, weights = varIdent(form = ~1)group)$ , method="ML").

<sup>&</sup>lt;sup>1</sup>Notation-abuse warning ...

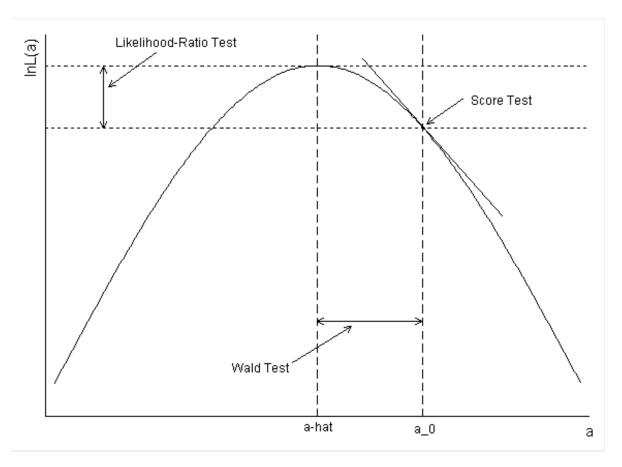
- optimized BLAS, kernel trick, etc.
- memory vs speed vs robustness ...
- -p vs. n vs. many-small-regressions vs. ...

#### Inference

- $\begin{array}{l} \bullet \ \, \sigma^2 \ \, (\text{residual variance}) \ \, \text{is RSS}/(n-p) \\ \bullet \ \, \text{The covariance matrix is } \Sigma = \sigma^2 (\mathbf{X}^\intercal \mathbf{X})^{-1}. \end{array}$
- Individual coefficients are *t*-distributed
- Linear combinations of coefficients (contrasts or predictions) are t-distributed with covariance matrix  $\mathbf{C}^{\top} \Sigma^{-1} \mathbf{C}$
- ullet Joint hypotheses on coefficients are F-distributed
- Wald and likelihood ratio test comparisons are equivalent (but need to be careful about marginality)

#### Wald vs LRT

- either approach can be used for tests of *single* parameters, *joint* tests of parameters, or confidence intervals
- Wald makes an additional assumption/approximation (quadratic log-likelihood surface)
  - this assumption is exact for linear models
- Wald may assume either known  $\sigma^2$  (Z,  $\chi^2$  tests) or estimated  $\hat{\sigma}^2$  (t, F tests)



From OARC stats, based on Fox 1977 Applied regression analysis

### **Model matrices**

- model definition converted to **X** before we start
- input variables vs predictor variables (Schielzeth (2010), Gelman and Hill (2006), CV)
  - transformations
  - encoding of categorical variables: **contrasts**
  - interactions
  - basis expansions (e.g. polynomials)

## Wilkinson-Rogers formulas

• Wilkinson and Rogers (1973), updated by Chambers and Hastie (1991, ch. 2)

• operators: +, \*, :, /, -, ^

• I()

#### **Contrasts**

#### treatment contrasts

• intercept = baseline, subsequent values are differences

 $\begin{array}{l} \bullet \ \left\{\beta_0 = \mu_0, \beta_i = \mu_i - \mu_0 \text{ for } i > 0\right\} \\ \bullet \ \text{equivalently: } \left\{\mu_0 = \beta_0, \mu_i = \beta_0 + \beta_i \text{ for } i > 0\right\} \end{array}$ 

• contrast matrix:

$$\mathbf{C}\beta = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 1 & 1 & 0 & \dots \\ 1 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \dots \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \dots \end{pmatrix} \quad .$$

Maybe easier to start from the **inverse** contrast matrix:  $\beta = \mathbf{C}^{-1}\mu$ .

 $C \leftarrow cbind(1, contr.treatment(3))$  ## R omits the intercept by default solve(C)

1 2 3

1 0 0

2 -1 1 0

3 -1 0 1

We have to specify the baseline level (contr.treatment uses first level of a factor; contr.SAS() uses the last level).

It's nice when contrasts are *orthogonal*, i.e. all rows are independent  $\to \mathbf{C}^\top \mathbf{C}$  is diagonal.

#### Sum-to-zero contrasts

• intercept is the (unweighted!) average rather than baseline value  $(\sum \mu_i/n)$ 

• other parameters are differences between mean of level i and intercept  $(\mu_i - \sum_i \mu_j/n)$ 

• **last** level is dropped

```
mfun <- function(C) MASS::fractions(solve(C))
(C <- cbind(1,contr.sum(3)))</pre>
```

## mfun(C)

#### **Helmert contrasts**

- Weird but orthogonal
- intercept, diff of first two levels, diff of level 3 from 1 & 2, ...

## (C <- cbind(1,contr.helmert(3)))</pre>

### mfun(C)

#### others

- MASS::contr.sdif() (successive-differences)
- contr.poly() (orthogonal polynomial contrasts)
- custom (e.g., "none" vs "symbiont effect" vs "crabs vs shrimp" vs "two-symbiont effect") (McKeon et al. (2012); data here)

```
none C S CS
intercept 1/4 1/4 1/4 1/4
avg_symb 1 -1/3 -1/3 -1/3
C.vs.S 0 1 -1 0
twosymb 0 1/2 1/2 -1
```

```
## contrast matrix
mfun(cc_inv)
```

```
intercept avg_symb C.vs.S twosymb
none 1 3/4 0 0
C 1 -1/4 1/2 1/3
S 1 -1/4 -1/2 1/3
CS 1 -1/4 0 -2/3
```

#### practical issues

- too many ways to set contrasts (options(), contrasts(f) <-, lm(..., contrasts =
   list(...))</pre>
- terrible naming conventions: you can get used to it or use the faux package
- OK to fit models and later use emmeans to recover desired contrasts (switching linear bases)

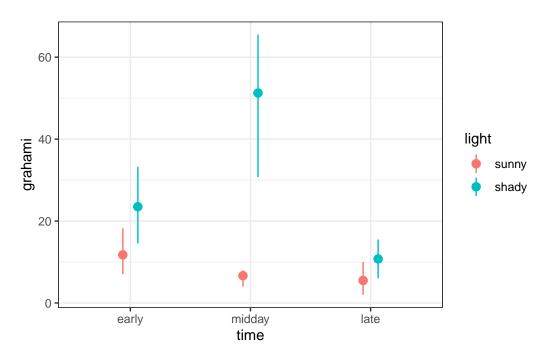
```
mtcars$fcyl <- factor(mtcars$cyl)</pre>
lm0 <- lm(mpg ~ fcyl, mtcars)</pre>
cn <- function(x) names(coef(x))</pre>
cn(lm0)
[1] "(Intercept)" "fcyl6"
                                 "fcyl8"
update(lm0, contrasts = list(fcyl = contr.sum(3))) |> cn()
[1] "(Intercept)" "fcyl1"
                                 "fcy12"
update(lm0, contrasts = list(fcyl = contr.helmert(3))) |> cn()
[1] "(Intercept)" "fcyl1"
                                 "fcy12"
using faux
update(lm0, data = transform(mtcars, fcyl = contr_code_sum(fcyl))) |> cn()
[1] "(Intercept)"
                        "fcyl.4-intercept" "fcyl.6-intercept"
update(lm0, data = transform(mtcars, fcyl = contr_code_helmert(fcyl))) |> cn()
```

#### Interactions

- differences in differences
- parameter values of main effects (and *p* values etc.) depend on contrasts/centering!
- overall model fit ( $R^2$ , predictions, etc.) is invariant

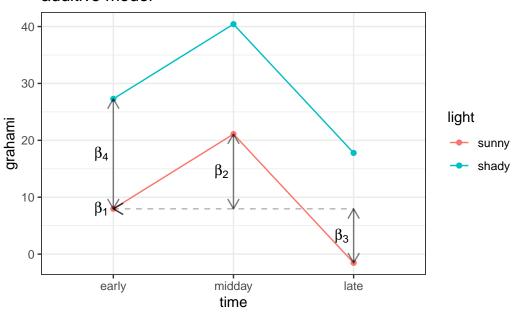
Lizard data (Schoener (1970), from the brglm2 package):

[1] "(Intercept)" "fcyl.6-4" "fcyl.8-4.6"



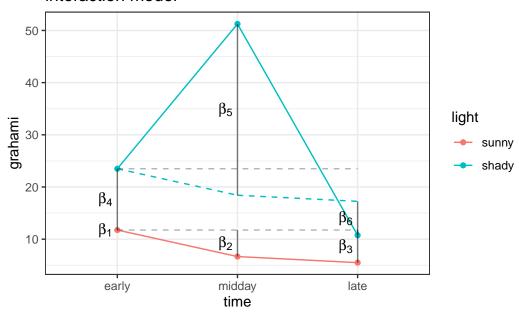
```
data("lizards", package = "brglm2")
lmTL1 <- lm(grahami~time+light,data=lizards)</pre>
pp <- with(lizards,expand.grid(time=levels(time),light=levels(light)))</pre>
pp$grahami <- predict(lmTL1,newdata=pp)</pre>
cc <- as.list(plyr::rename(coef(lmTL1),c(`(Intercept)`="int")))</pre>
labelpos <- with(cc,</pre>
  list(x=c(1,2,3,1), xend=c(1,2,3,1),
      y=c(int,int,int,int),
      yend=c(int,int+timemidday,int+timelate,int+lightshady)))
xpos < -0.1
ggplot(pp,aes(x=time,y=grahami,colour=light))+geom_point()+
  geom line(aes(group=light))+
  annotate("segment", x=labelpos$x, xend=labelpos$xend, y=labelpos$y,
           yend=labelpos$yend,alpha=0.5,
           arrow=arrow(length = unit(0.3, "cm"), ends="both"))+
  annotate("text", x=with(labelpos, (x+xend)/2)+xpos, y=with(labelpos, (y+yend)/2),
label=paste0("beta[",1:4,"]"),parse=TRUE)+
  annotate("segment", x=labelpos$x[1], xend=labelpos$x[3], y=labelpos$y[1],
           yend=labelpos$y[1],alpha=0.3,lty=2) +
    labs(title = "additive model")
```

#### additive model



```
lmTL2 <- lm(grahami~time*light,data=lizards)</pre>
gg_color_hue <- function(n) {
  hues = seq(15, 375, length=n+1)
  hcl(h=hues, l=65, c=100)[1:n]
}
pp2 <- pp
pp2$grahami <- predict(lmTL2,newdata=pp)</pre>
cc <- as.list(plyr::rename(coef(lmTL2),c(`(Intercept)`="int",</pre>
        `timemidday:lightshady`="midshady",`timelate:lightshady`="lateshady")))
labelpos <- with(cc,</pre>
  list(x=c(1,2,3,1,2,3), xend=c(1,2,3,1,2,3),
      y=c(int,int,int,int,int+lightshady+timemidday,int+lightshady+timelate),
      yend=c(int,int+timemidday,int+timelate,int+lightshady,
             int+timemidday+lightshady+midshady,int+timelate+lightshady+lateshady)))
xpos < -0.1
ggplot(pp2,aes(x=time,y=grahami,colour=light))+geom point()+
  geom_line(aes(group=light))+
  annotate("segment", x=1:2, xend=2:3,
           y=with(cc,c(int+lightshady,int+timemidday+lightshady)),
           yend=with(cc,c(int+timemidday+lightshady,int+timelate+lightshady)),
           colour=gg_color_hue(2)[2],lty=2)+
  annotate("segment", x=labelpos$x, xend=labelpos$xend, y=labelpos$y,
           yend=labelpos$yend,alpha=0.5) +
           ## arrow=arrow(length = unit(0.3, "cm"), ends="both"))+
```

#### interaction model



## Marginality

- Venables (1998)
- 'type (X) sums of squares'
- scaling and centering (Schielzeth 2010) alleviates many problems; sum-to-zero contrasts (weighted or unweighted?)

#### Making life easier with emmeans

- important to understand contrasts
- but easier to compute expected marginal means, contrasts via emmeans package
- contrasts expressed in terms of *group means*
- e.g.
- good documentation, vignettes

## Model interpretation, visualization, testing

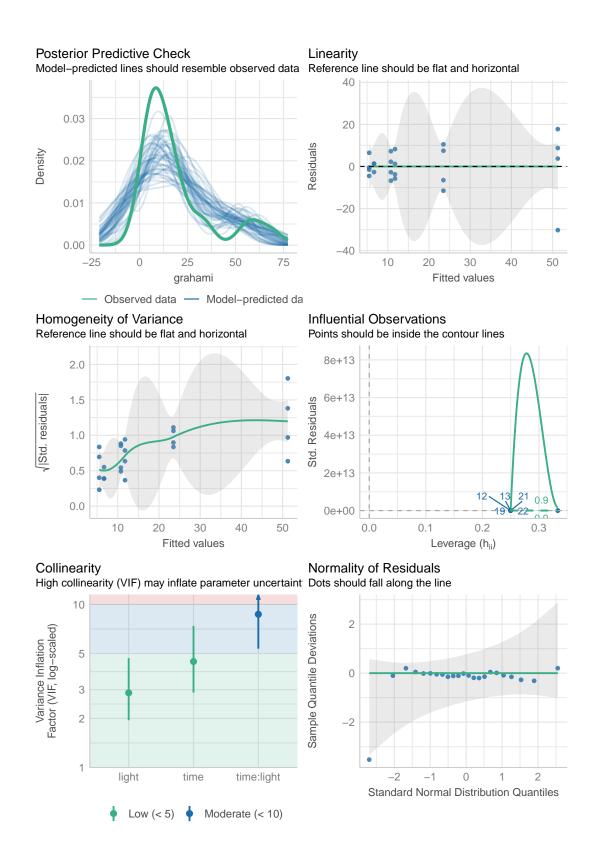
## **Diagnostics**

- linearity > heteroscedasticity, outliers > normality
- upstream problems can induce downstream problems first
- universal plots are universal, but less interpretable than problem-specific exploration (try to identify problematic predictors/groups/etc.)

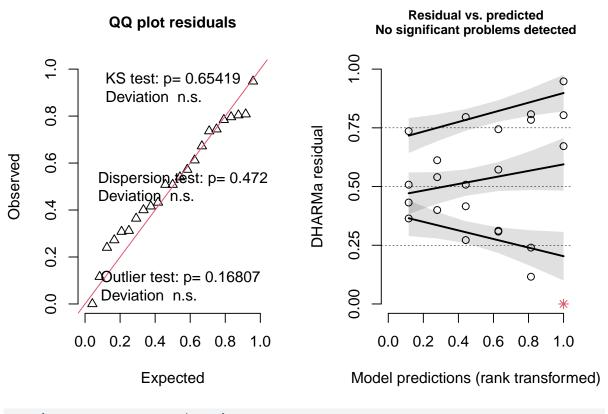
## **Graphical diagnostics**

```
    base R: stats::plot.lm()
    performance::check_model()
    DHARMa (simulateResiduals(., plot = TRUE))
    - (plotResiduals(simout, form = pred_var))
    broom::augment() + plot-your-own (ggplot2)
```

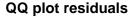
performance::check\_model(lmTL2)

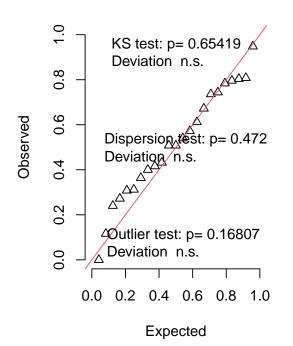


## DHARMa residual

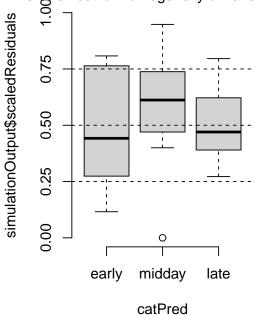


plot(ss, form = lizards\$time)





Within–group deviation from uniformity n.s. Levene Test for homogeneity of variance n.s.



## Solutions to problems

- **nonlinearity**: transformation, add covariates (??), add interactions, add polynomial terms etc.
- outliers: drop values (report both!), use robust regression
- heteroscedasticity: transformation, model dispersion explicitly, GLMs
- non-Normality: transformation, GLMs

#### **Transformation**

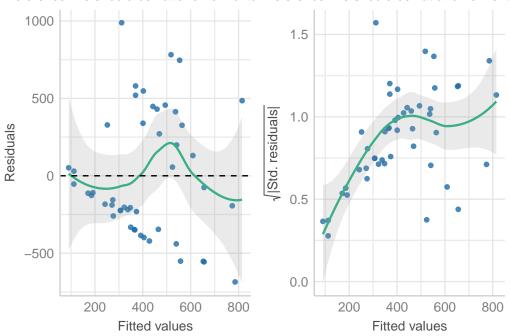
- May do too much at once (GLMs and GAMs allow more flexibility)
- Log-transformation is often interpretable and solves problems
- Transforming boundary values (e.g. log(0)) is problematic
- **Box-Cox transformations**:  $y \to \frac{y^{\lambda}-1}{\lambda}$  (include Jacobian term  $GM^{\lambda-1}$  in denominator to keep log-likelihood comparable)
  - flexible
  - in practice people often use 'round numbers':  $\lambda = 0$  (log), 1/2 (square root), etc.

- MASS::boxcox()
- hard to interpret!

## Example

```
library(faraway)
m1 <- lm(perm ~ area, rock)
performance::check_model(m1, check = c("linearity", "homogeneity", "outliers", "qq"))</pre>
```

Linearity Homogeneity of Variance
Reference line should be flat and horizontal Reference line should be flat and horizontal



Normality of Residuals

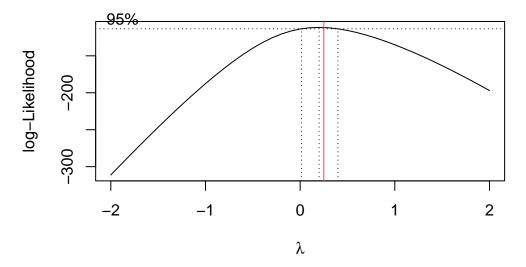
# Influential Observations Points should be inside the contour lines

Points should be inside the contour lines

Dots should fall along the line

Standard Normal Distribution Quantile

```
m <- MASS::boxcox(m1, interp = FALSE)
abline(v=1/4, col = 2)</pre>
```



```
m2 <- update(m1, perm^(1/4) ~ .)
performance::check_model(m2, check = c("linearity", "homogeneity", "outliers", "qq"))</pre>
```

Linearity Homogeneity of Variance Reference line should be flat and horizont Reference line should be flat and horizontal 2 √|Std. residuals| 1.0 Residuals 0 -10.5 -2 3.5 4.0 4.5 3.5 4.0 3.0 5.0 3.0 4.5 5.0 Fitted values Fitted values Influential Observations Normality of Residuals Points should be inside the contour lines Dots should fall along the line 4 Sample Quantile Deviations Std. Residuals 37 -40.00 0.05 0.10 0 Leverage (h<sub>ii</sub>) Standard Normal Distribution Quantiles

When we transform we have to add the logs of the Jacobian of the transform to the log-

likelihood, or subtract  $\sum \log(J_i)$  from the negative log-likelihood (Cranmer n.d.). For example, if we log-transform,

$$\begin{split} \sum \log(J(y_i)) &= \sum \log \left(\partial (\log(y_i))/\partial y\right) \\ &= \sum \log (1/y_i) \\ &= -\sum \log y_i. \end{split}$$

In this case  $\sum \log(J(y_i)) = \sum \log\left((1/4)P^{-3/4}\right) = -N\log 4 - 3/4\sum \log(P)$  . Check:

```
logJ <- -(nrow(rock)*log(4) + 3/4*sum(log(rock$perm)))
lm2 <- logLik(m2) + logJ
lm1 <- logLik(m1)
lm2-lm1</pre>
```

'log Lik.' 23.3844 (df=3)

```
## difference from Box-Cox sequence max(m$y)-m$y[m$x==1]
```

[1] 23.52213

#### Reminder about parameter scaling

- Schielzeth (2010), Gelman (2008)
- centering ensures no problems with marginality (analogous to sum-to-zero contrasts)
- scaling predictors gives coefficients equal units (analogous to Cohen's d)
- scaling response makes coefficients *standardized partial regression coefficients* (equal to partial correlation coefficients if predictors are independent)
- scaling by 2 SD makes coefficients equivalent to those from balanced binary predictors
- scaling inputs or scaling predictors?

#### What about correlated predictors?

- Can compute variance inflation factors (VIFs)
- Dropping correlated factors is dubious: Graham (2003), Dormann et al. (2012), Morrissey and Ruxton (2018), Vanhove (2021)

• perfect collinearity gets handled automatically by R's pivoting, but may want to change contrasts/model setup

#### summary(lmTL2)

#### Call:

lm(formula = grahami ~ time \* light, data = lizards)

#### Residuals:

Min 1Q Median 3Q Max -30.250 -4.125 1.250 6.875 17.750

#### Coefficients:

	${\tt Estimate}$	Std. Error	t value	Pr(> t )	
(Intercept)	11.750	5.375	2.186	0.04311	*
timemidday	-5.083	8.211	-0.619	0.54408	
timelate	-6.250	7.602	-0.822	0.42238	
lightshady	11.750	7.602	1.546	0.14061	
timemidday:lightshady	32.833	11.190	2.934	0.00927	**
timelate:lightshady	-6.500	10.751	-0.605	0.55343	

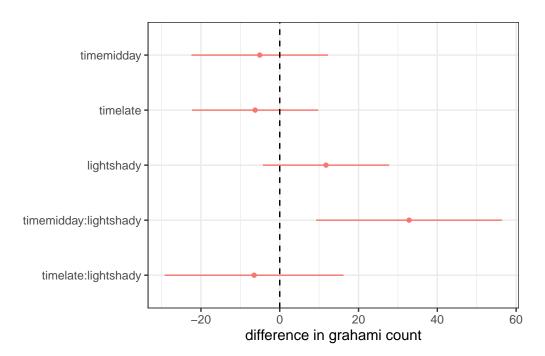
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10.75 on 17 degrees of freedom Multiple R-squared: 0.7504, Adjusted R-squared: 0.677 F-statistic: 10.22 on 5 and 17 DF, p-value: 0.0001179

#### broom::tidy(lmTL2)

#### # A tibble: 6 x 5 term estimate std.error statistic p.value <dbl> <dbl> <dbl> <chr> <dbl> 1 (Intercept) 11.8 5.38 2.19 0.0431 -0.619 0.544 2 timemidday -5.08 8.21 3 timelate -6.257.60 -0.822 0.422 4 lightshady 11.7 7.60 1.55 0.141 32.8 2.93 0.00927 5 timemidday:lightshady 11.2 -6.5 6 timelate:lightshady 10.8 -0.605 0.553

```
## automatically drop intercept; optional by_2sd argument
dotwhisker::dwplot(lmTL2) + geom_vline(xintercept = 0, lty = 2) +
    labs(x="difference in grahami count")
```



### Interpretation and testing

- Look at coefficient tables: summary() or coef(summary())
- model comparison: drop1(), anova(), car::Anova()
- coefficient *plots*: broom + ggplot2, dotwhisker

#### **Downstream methods**

- plot predictions with data
- partial residuals plots (e.g. remef package)
- prediction, effects plots
- uncertainty of predictions
- emmeans, marginal effects, effects, sjPlot ...

#### References

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