Review of linear models

23 Sep 2024

```r
## 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
Last updated: 02 April, 2019

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	Icon
Simple regression: lm(y ~ 1 + x)	**y is independent of x** P: One-sample t-test N: Wilcoxon signed-rank	t.test(y) wilcox.test(y)	lm(y ~ 1) lm(signed_rank(y) ~ 1)	✓ for N >14	One number (intercept, i.e., the mean) predicts **y**. - (Same, but it predicts the *signed rank* of **y**.)	
	P: Paired-sample t-test N: Wilcoxon matched pairs	t.test(y₁, y₂, paired=TRUE) wilcox.test(y₁, y₂, paired=TRUE)	lm(y₂ - y₁ ~ 1) lm(signed_rank(y₂ - y₁) ~ 1)	✓ for N >14	One intercept predicts the pairwise **y₂-y₁** differences. - (Same, but it predicts the *signed rank* of **y₂-y₁**.)	
	y ~ continuous x P: Pearson correlation N: Spearman correlation	cor.test(x, y, method='Pearson') cor.test(x, y, method='Spearman')	lm(y ~ 1 + x) lm(rank(y) ~ 1 + rank(x))	✓ for N >10	One intercept plus **x** multiplied by a number (slope) predicts **y**. - (Same, but with *ranked* **x** and **y**)	
	y ~ discrete x P: Two-sample t-test P: Welch's t-test N: Mann-Whitney U	t.test(y₁, y₂, var.equal=TRUE) t.test(y₁, y₂, var.equal=FALSE) wilcox.test(y₁, y₂)	lm(y ~ 1 + G₂)ᴬ gls(y ~ 1 + G₂, weights=…ᴮ)ᴬ lm(signed_rank(y) ~ 1 + G₂)ᴬ	✓ ✓ 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**.)	
Multiple regression: lm(y ~ 1 + x₁ + x₂ + …)	**P: One-way ANOVA** N: Kruskal-Wallis	aov(y ~ group) kruskal.test(y ~ group)	lm(y ~ 1 + G₂ + G₃ +…+ G_N)ᴬ lm(rank(y) ~ 1 + G₂ + G₃ +…+ G_N)ᴬ	✓ for N >11	An intercept for **group 1** (plus a difference if group ≠ 1) predicts **y**. - (Same, but it predicts the *rank* of **y**.)	
	P: One-way ANCOVA	aov(y ~ group + x)	lm(y ~ 1 + G₂ + G₃ +…+ G_N + x)ᴬ	✓	- (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)	lm(y ~ 1 + G₂ + G₃ + … + G_N + S₂ + S₃+ … + S_K + G₂*S₂+G₃*S₃+…+G_N*S_K)	✓	Interaction term: changing **sex** changes the **y ~ group** parameters. *Note: G₂ to K is an indicator (0 or 1) for each non-intercept levels of the **group** variable. Similarly for S₂ to K for sex. The first line (with Gᵢ) is main effect of group, the second (with Sᵢ) for sex and the third is the **group × sex** interaction. For two levels (e.g. male/female), line 2 would just be "S₂" and line 3 would be S₂ multiplied with each Gᵢ.*	[Coming]
	Counts ~ discrete x N: Chi-square test	chisq.test(groupXsex_table)	**Equivalent log-linear model** glm(y ~ 1 + G₂ + G₃ + … + G_N + S₂ + S₃+ … + S_K + G₂*S₂+G₃*S₃+…+G_N*S_K, family=…)ᴬ	✓	Interaction term: (Same as Two-way ANOVA.) *Note: Run glm using the following arguments: glm(model, family=poisson())* *As linear-model, the Chi-square test is log(y) = log(N) + log(αᵢ) + log(βⱼ) + log(αᵢβⱼ) where αᵢ and βⱼ are proportions. See more info in the accompanying notebook.*	Same as Two-way ANOVA
	N: Goodness of fit	chisq.test(y)	glm(y ~ 1 + G₂ + G₃ +…+ G_N, family=…)ᴬ	✓	(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·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_rank = function(x) sign(x) * rank(abs(x)). The variables Gᵢ and Sᵢ are "dummy coded" indicator variables (either 0 or 1) exploiting the fact that when Δx = 1 between categories the difference equals the slope. Subscripts (e.g., G₂ or y₁) indicate different columns in data. lm requires long-format data for all non-continuous models. All of this is exposed in greater detail and worked examples at https://lindeloev.github.io/tests-as-linear.

ᴬ See the note to the two-way ANOVA for explanation of the notation.
ᴮ Same model, but with one variance per group: gls(value ~ 1 + G₂, weights = varIdent(form = ~1|group), method="ML").

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Basics

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

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

  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`

---

[1]Notation-abuse warning …

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

Inference

- σ^2 (residual variance) is $\text{RSS}/(n - p)$
- The covariance matrix is $\Sigma = \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}$.
- Individual coefficients are t-distributed
- Linear combinations of coefficients (contrasts or predictions) are t-distributed with covariance matrix $\mathbf{C}^\top \Sigma^{-1} \mathbf{C}$
- 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 σ^2 (Z, χ^2 tests) or estimated $\hat{\sigma}^2$ (t, F tests)
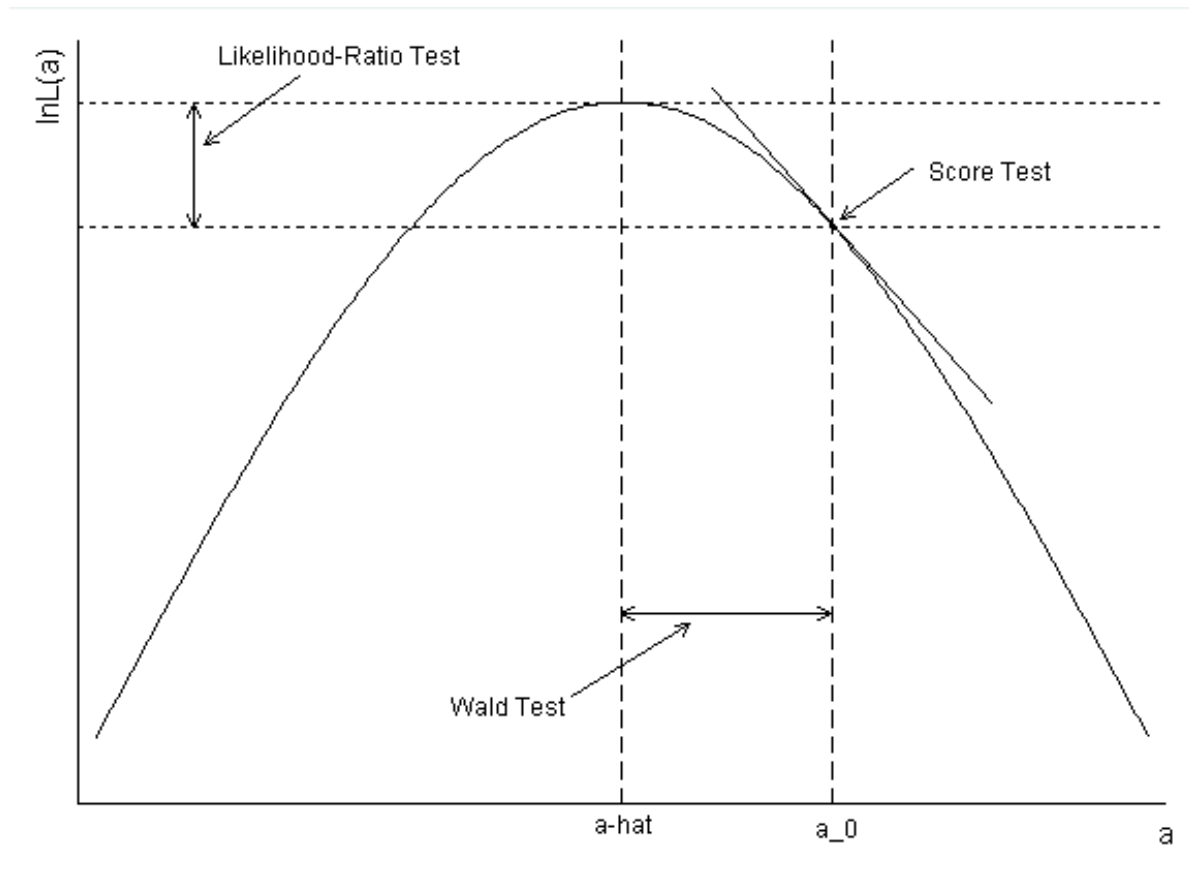
From OARC stats, based on Fox 1977 *Applied regression analysis*

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
- $\{\beta_0 = \mu_0, \beta_i = \mu_i - \mu_0 \text{ for } i > 0\}$
- equivalently: $\{\mu_0 = \beta_0, \mu_i = \beta_0 + \beta_i \text{ for } i > 0\}$
- **contrast matrix**:

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

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

```
C <- 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 $\rightarrow$ $\mathbf{C}^\top \mathbf{C}$ 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 $(\mu_i - \sum_j \mu_j / n)$
- **last** level is dropped

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

```
  [,1] [,2] [,3]
1    1    1    0
2    1    0    1
3    1   -1   -1
```

```r
mfun(C)
```

```
       1    2    3
[1,]  1/3  1/3  1/3
[2,]  2/3 -1/3 -1/3
[3,] -1/3  2/3 -1/3
```

Helmert contrasts

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

```r
(C <- cbind(1,contr.helmert(3)))
```

```
  [,1] [,2] [,3]
1    1   -1   -1
2    1    1   -1
3    1    0    2
```

```r
mfun(C)
```

```
       1    2    3
[1,]  1/3  1/3  1/3
[2,] -1/2  1/2    0
[3,] -1/6 -1/6  1/3
```

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)

```
cc_inv <- matrix(c(1/4,1/4,1/4,1/4,
                   1,-1/3,-1/3,-1/3,
                   0,1,-1,0,
                   0,1/2,1/2,-1),
                 byrow=TRUE,
                 nrow=4,
                 dimnames=list(c("intercept","avg_symb","C.vs.S","twosymb"),
                               c("none","C","S","CS")))
## inverse contrast matrix
MASS::fractions(cc_inv)
```

```
          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(...))`)
- 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)
lm0 <- lm(mpg ~ fcyl, mtcars)
cn <- function(x) names(coef(x))
cn(lm0)
```

```
[1] "(Intercept)" "fcyl6"        "fcyl8"
```

```
update(lm0, contrasts = list(fcyl = contr.sum(3))) |> cn()
```

```
[1] "(Intercept)" "fcyl1"        "fcyl2"
```

```
update(lm0, contrasts = list(fcyl = contr.helmert(3))) |> cn()
```

```
[1] "(Intercept)" "fcyl1"        "fcyl2"
```

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()
```

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

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):

```
data("lizards", package = "brglm2")
ggplot(lizards, aes(time, grahami, colour = light)) +
    stat_summary(fun.data = mean_cl_boot,
                 position = position_dodge(width = 0.25))
```
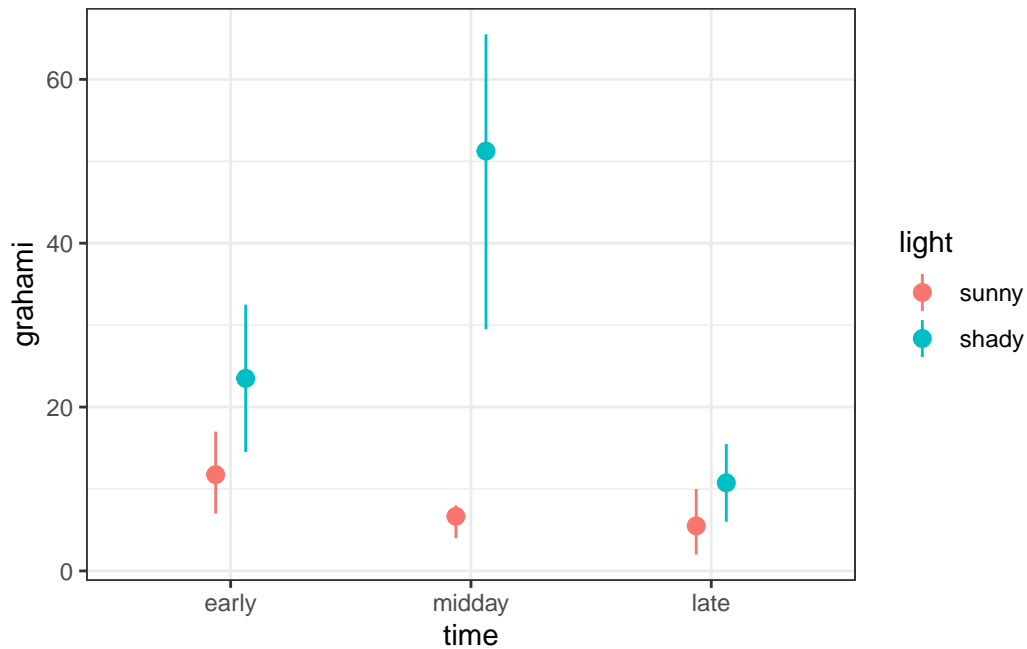
```
data("lizards", package = "brglm2")
lmTL1 <- lm(grahami~time+light,data=lizards)
pp <- with(lizards,expand.grid(time=levels(time),light=levels(light)))
pp$grahami <- predict(lmTL1,newdata=pp)
cc <- as.list(plyr::rename(coef(lmTL1),c(`(Intercept)`="int")))
labelpos <- with(cc,
  list(x=c(1,2,3,1),xend=c(1,2,3,1),
     y=c(int,int,int,int),
     yend=c(int,int+timemidday,int+timelate,int+lightshady)))
xpos <- -0.1
ggplot(pp,aes(x=time,y=grahami,colour=light))+geom_point()+
  geom_line(aes(group=light))+
  annotate("segment",x=labelpos$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")
```

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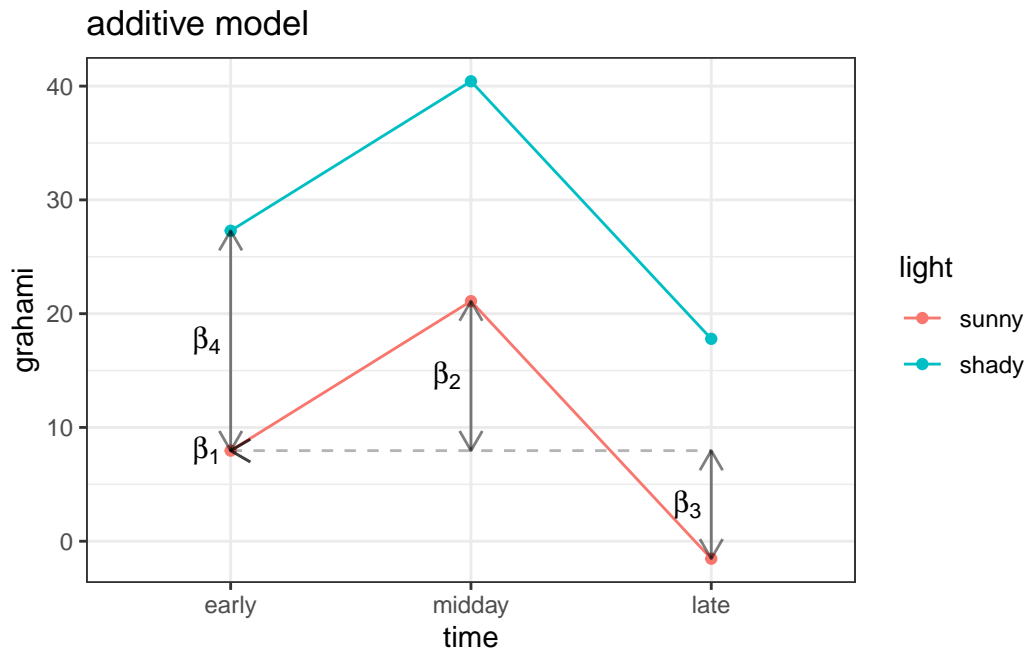
```
lmTL2 <- lm(grahami~time*light,data=lizards)
gg_color_hue <- function(n) {
  hues = seq(15, 375, length=n+1)
  hcl(h=hues, l=65, c=100)[1:n]
}
pp2 <- pp
pp2$grahami <- predict(lmTL2,newdata=pp)
cc <- as.list(plyr::rename(coef(lmTL2),c(`(Intercept)`="int",
        `timemidday:lightshady`="midshady",`timelate:lightshady`="lateshady")))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

```
    annotate("text",x=with(labelpos,(x+xend)/2)+xpos,y=with(labelpos,(y+yend)/2),
label=paste0("beta[",1:6,"]"),parse=TRUE)+
    annotate("segment",x=rep(labelpos$x[1],2),
                    xend=rep(labelpos$x[3],2),
                    y=labelpos$yend[c(1,4)],
             yend=labelpos$yend[c(1,4)],alpha=0.3,lty=2) +
     labs(title = "interaction model")
```
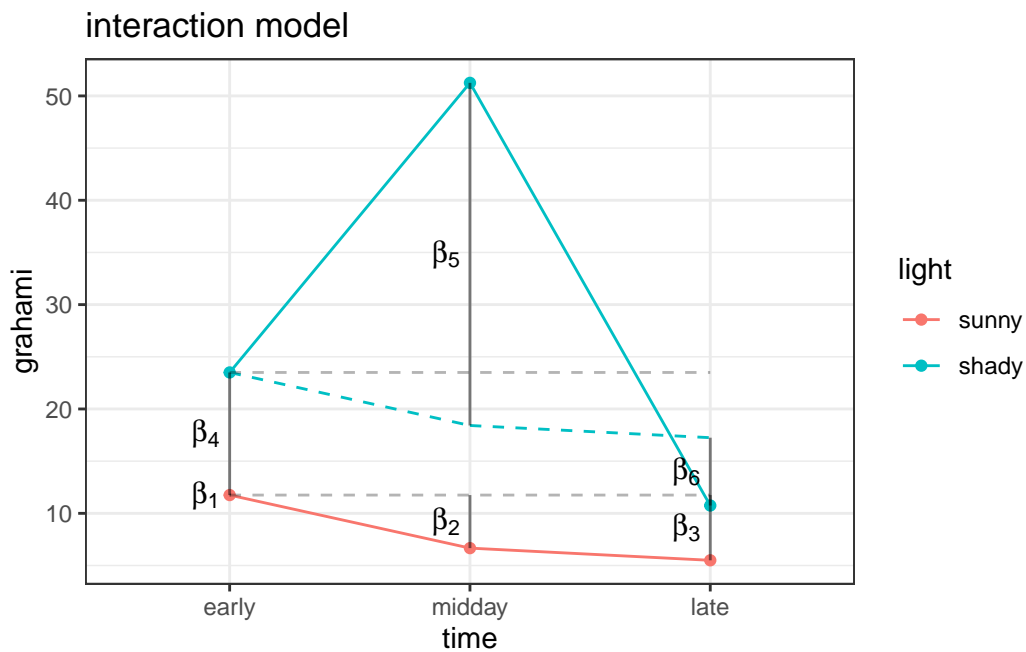

Marginality

- 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)
```

Posterior Predictive Check

Model–predicted lines should resemble observed data line
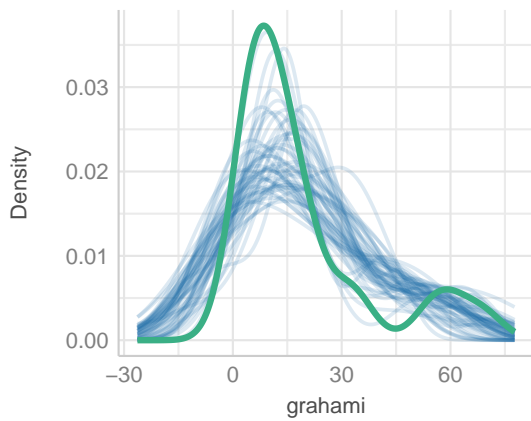
Linearity

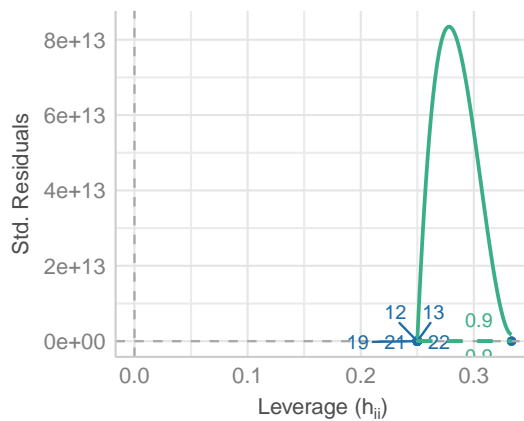Reference line should be flat and horizontal
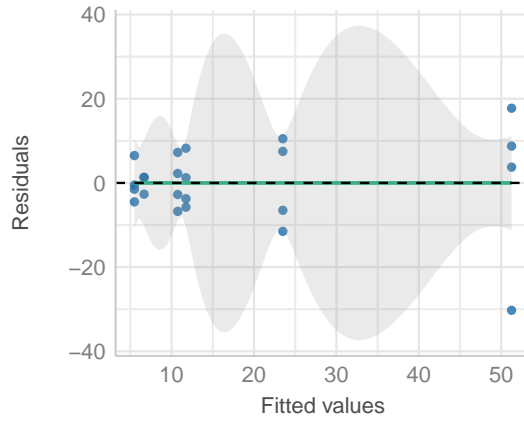
Homogeneity of Variance

Reference line should be flat and horizontal
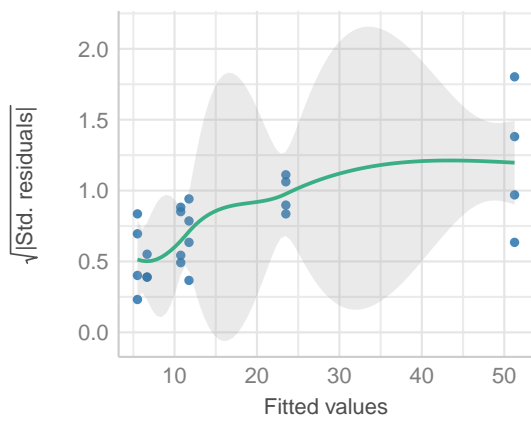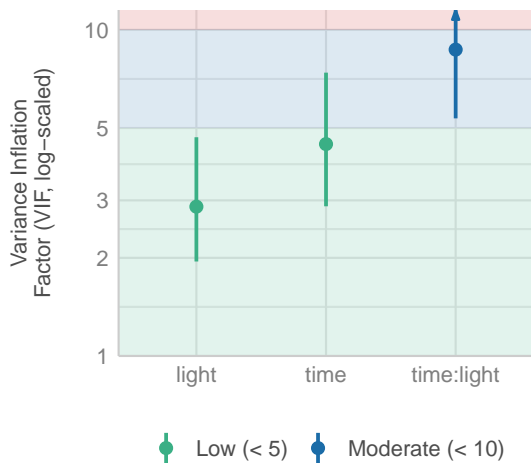

Influential Observations
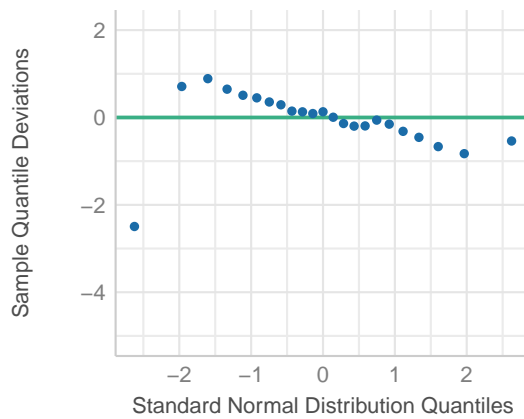
Points should be inside the contour lines

Collinearity

High collinearity (VIF) may inflate parameter uncertainty
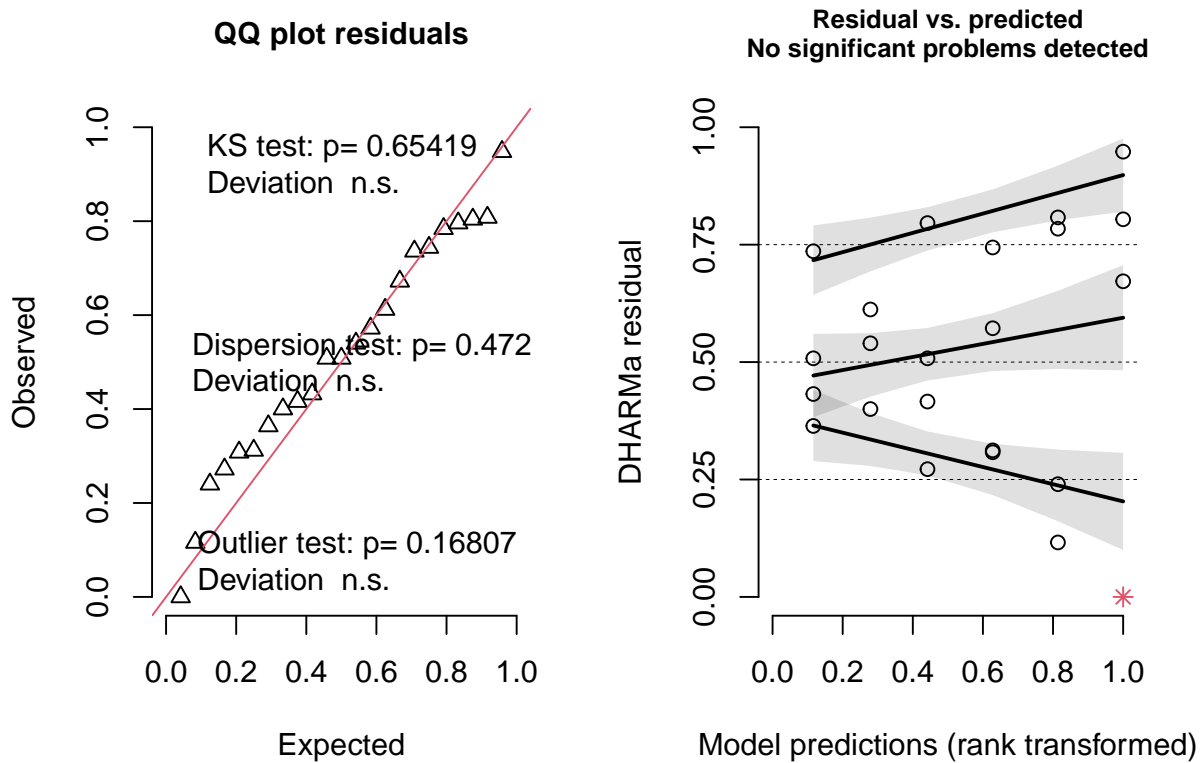

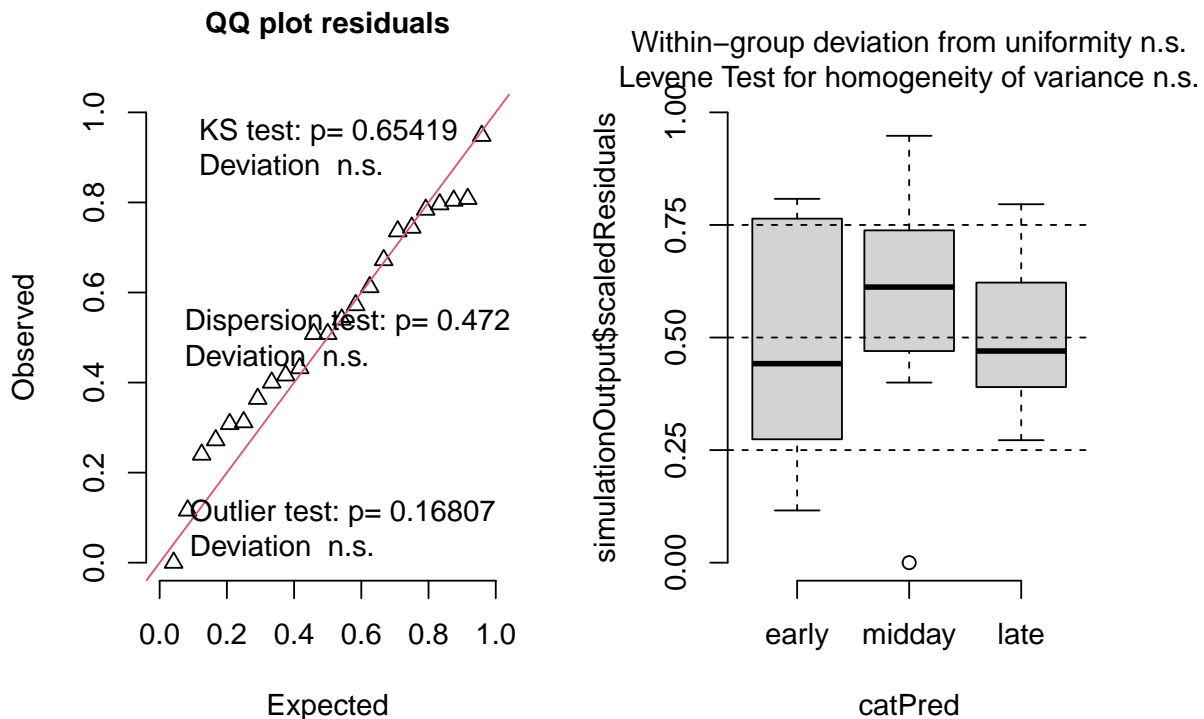## Normality of Residuals

Dots should fall along the line

```
ss <- simulateResiduals(lmTL2)
plot(ss)
```

DHARMa residual


```
plot(ss, form = lizards$time)
```

DHARMa residual

QQ plot residuals

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

KS test: p= 0.65419
Deviation n.s.

Dispersion test: p= 0.472
Deviation n.s.

Outlier test: p= 0.16807
Deviation n.s.

Observed

Expected

simulationOutput$scaledResiduals

early   midday   late

catPred

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**: $y \rightarrow \frac{y^\lambda - 1}{\lambda}$ (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.
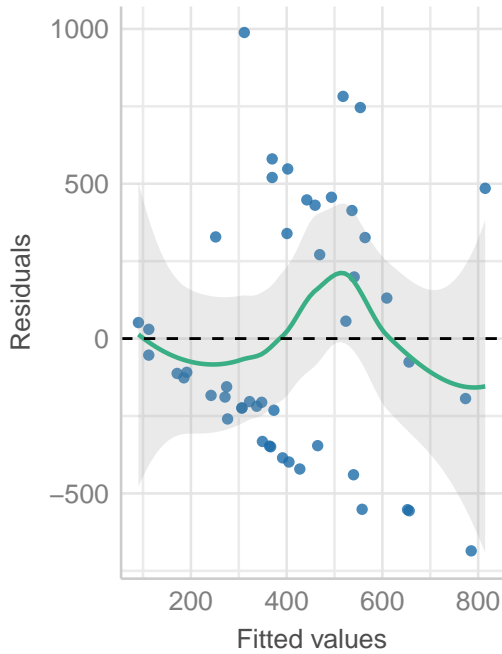
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– `MASS::boxcox()`
  – hard to interpret!

Example

```r
library(faraway)
m1 <- lm(perm ~ area, rock)
performance::check_model(m1, check = c("linearity", "homogeneity", "outliers", "qq"))
```
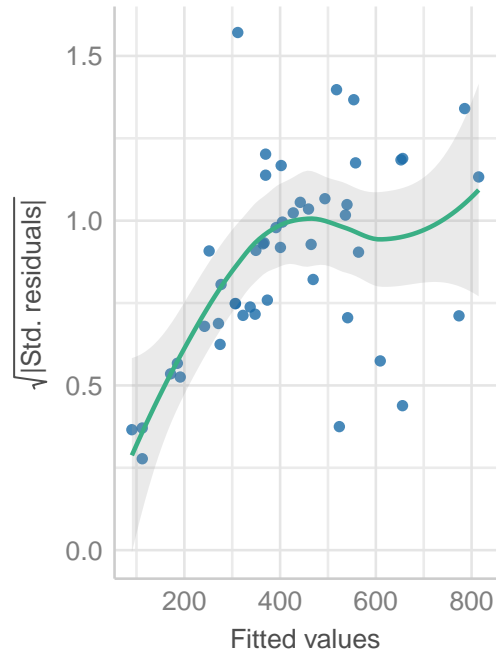
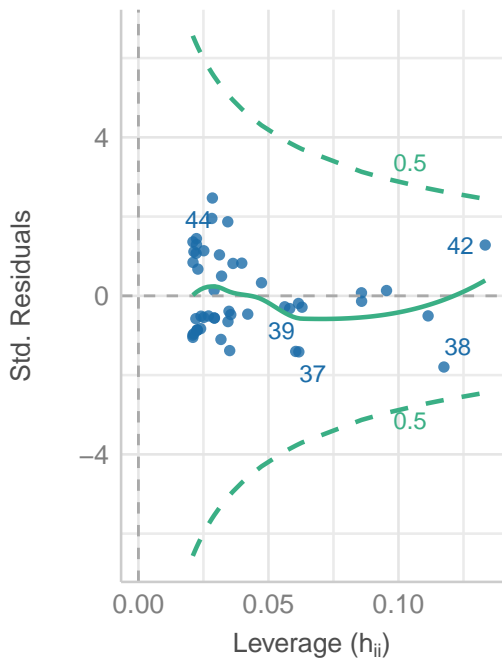## Linearity
Reference line should be flat and horizontal

Homogeneity of Variance
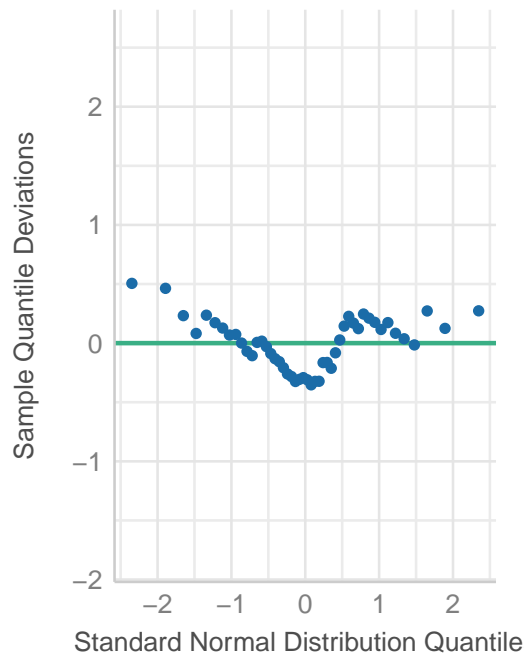Reference line should be flat and horizontal

Influential Observations
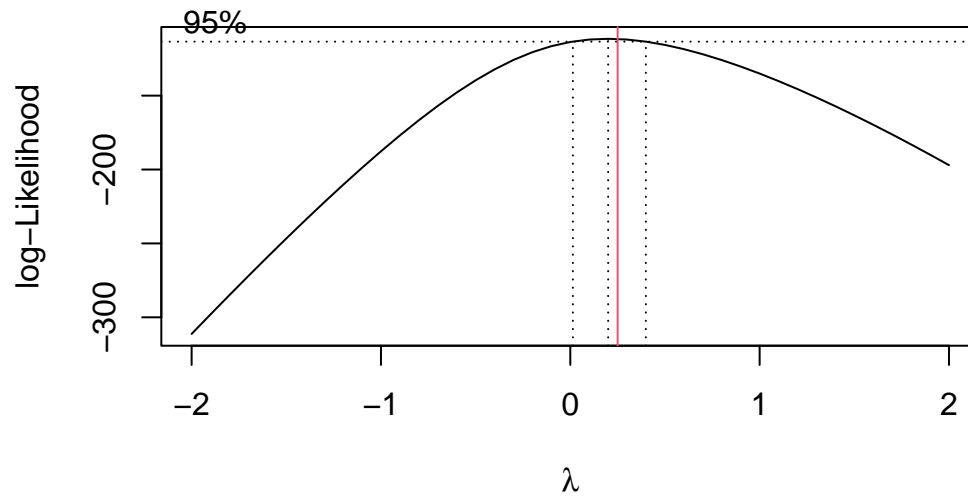Points should be inside the contour lines

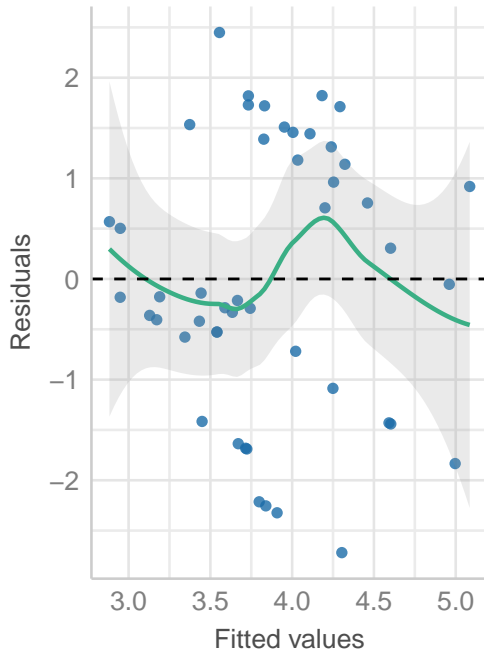## Normality of Residuals
Dots should fall along the line

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



```
m2 <- update(m1, perm^(1/4) ~ .)
performance::check_model(m2, check = c("linearity", "homogeneity", "outliers", "qq"))
```
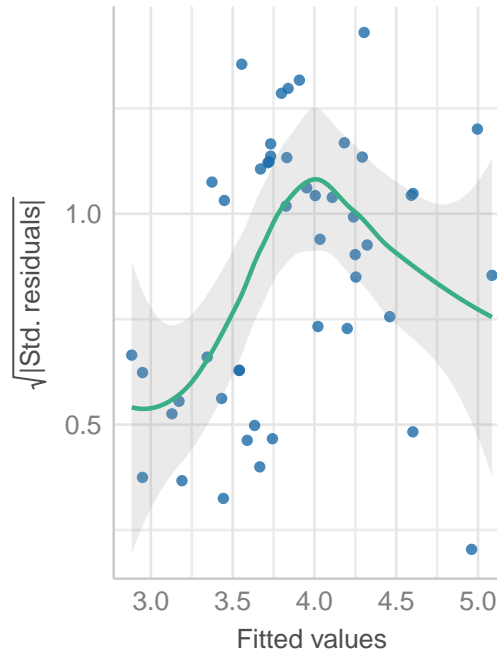
Linearity
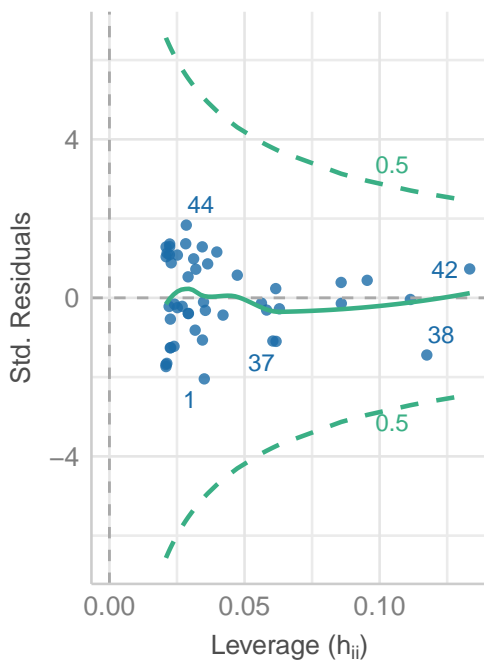Reference line should be flat and horizontal

Homogeneity of Variance
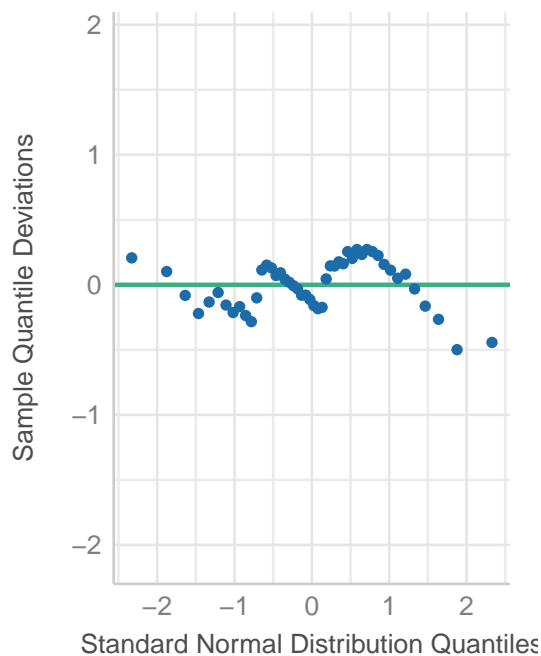Reference line should be flat and horizontal

Influential Observations
Points should be inside the contour lines

Normality of Residuals
Dots should fall along the line

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,

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

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
```

```
'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:
                       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 '**' 0.01 '*' 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
  <chr>                    <dbl>     <dbl>     <dbl>   <dbl>
1 (Intercept)              11.8       5.38     2.19  0.0431
2 timemidday               -5.08      8.21    -0.619 0.544
3 timelate                 -6.25      7.60    -0.822 0.422
4 lightshady               11.7       7.60     1.55  0.141
5 timemidday:lightshady    32.8      11.2      2.93  0.00927
6 timelate:lightshady      -6.5      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")
```
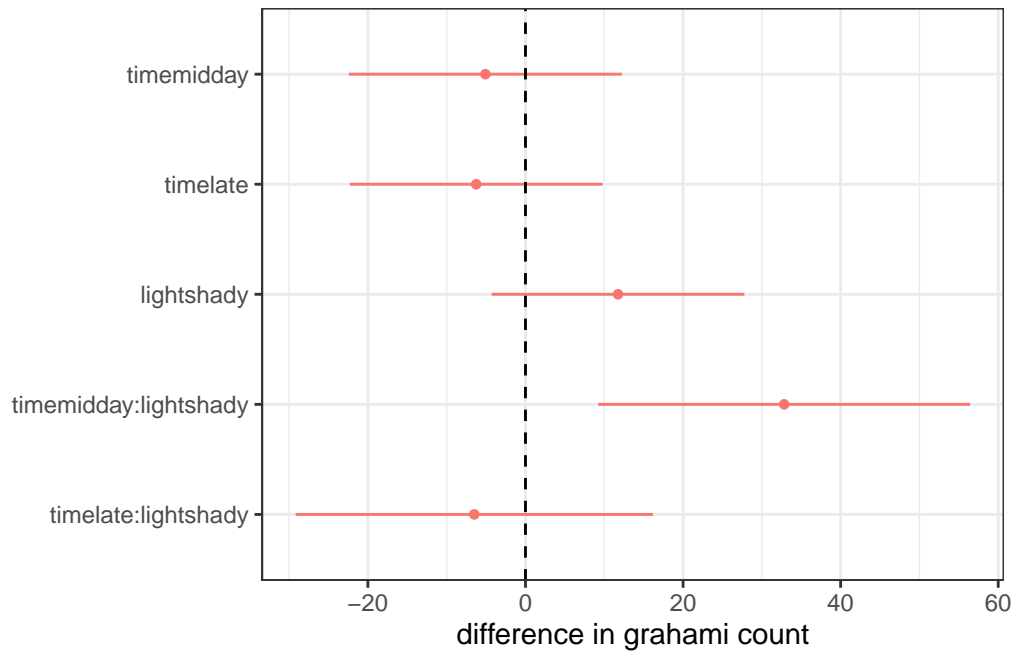

Interpretation and testing

- 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`, `marginaleffects`, `effects`, `sjPlot` ...

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