Review of linear models

25 Sep 2023

```
## 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)
```

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).

[1] Notation-abuse warning ...

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

Computation

- matrix decompositions (QR with pivoting; see here)
- big problems: `biglm`, `speedglm`, `RcppEigen::fastLm`
  - optimized BLAS, kernel trick, etc.
  - memory vs speed vs robustness ...
  - p vs. n vs. many-small-regressions vs. ...

Inference

- σ^2 (residual variance) is 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)

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**:

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

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

```
C <- 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

```
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
```

```
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, ...

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

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

```
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()
```

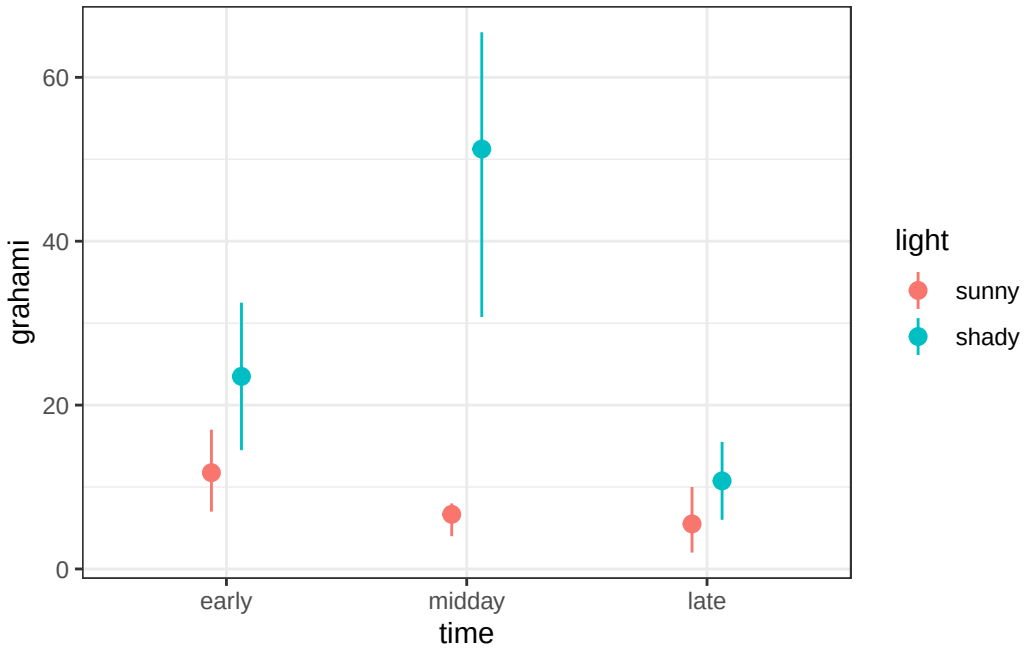
```
[1] "(Intercept)" "fcyl.6-4"    "fcyl.8-4.6"
```

Interactions

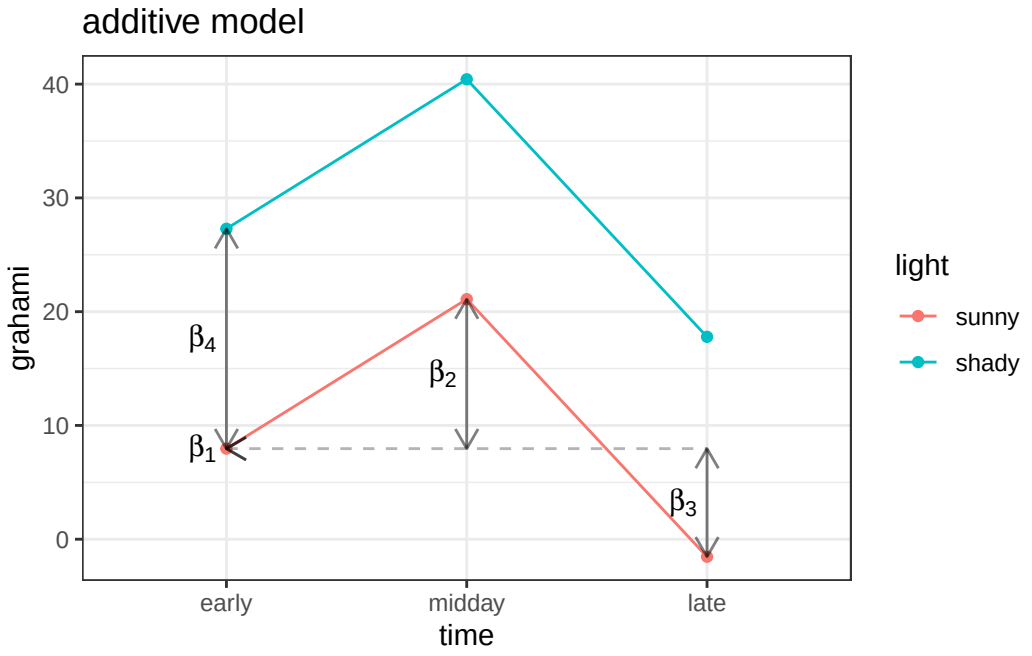
- differences in differences
- parameter values of main effects (and p values etc.) depend on contrasts/centering!
- overall model fit (R^2, predictions, etc.) is invariant

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))
```

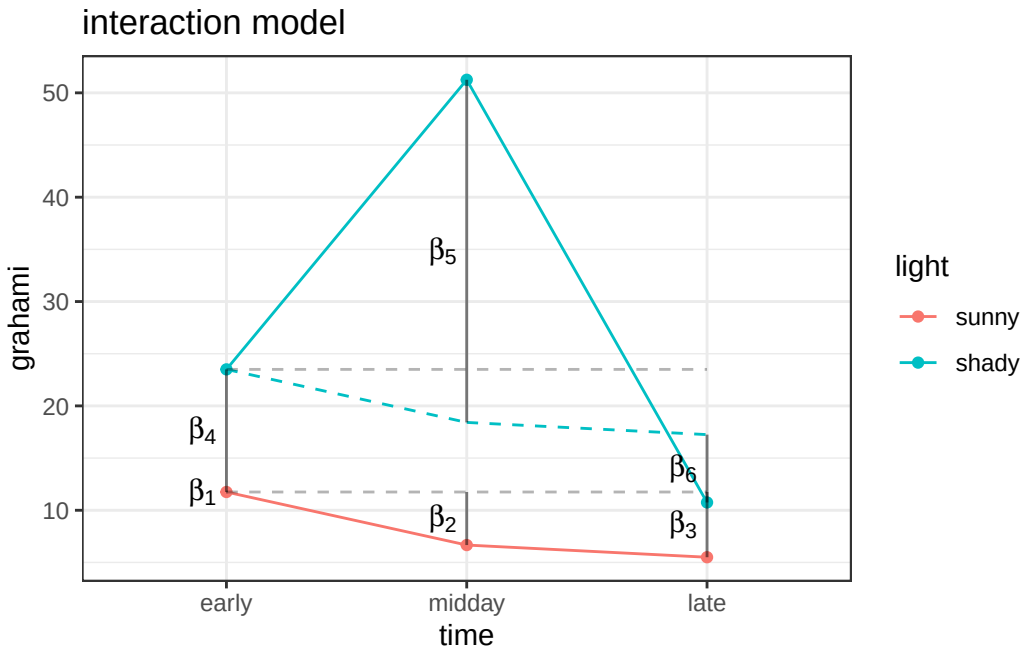



```
data("lizards", package = "brglm2")
lmTL1 <- lm(grahami~time+light,data=lizards)
pp <- with(lizards,expand.grid(time=levels(time),light=levels(light)))
pp$grahami <- predict(lmTL1,newdata=pp)
cc <- as.list(plyr::rename(coef(lmTL1),c(`(Intercept)`="int")))
labelpos <- with(cc,
  list(x=c(1,2,3,1),xend=c(1,2,3,1),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




```
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?)

Model interpretation, visualization, testing

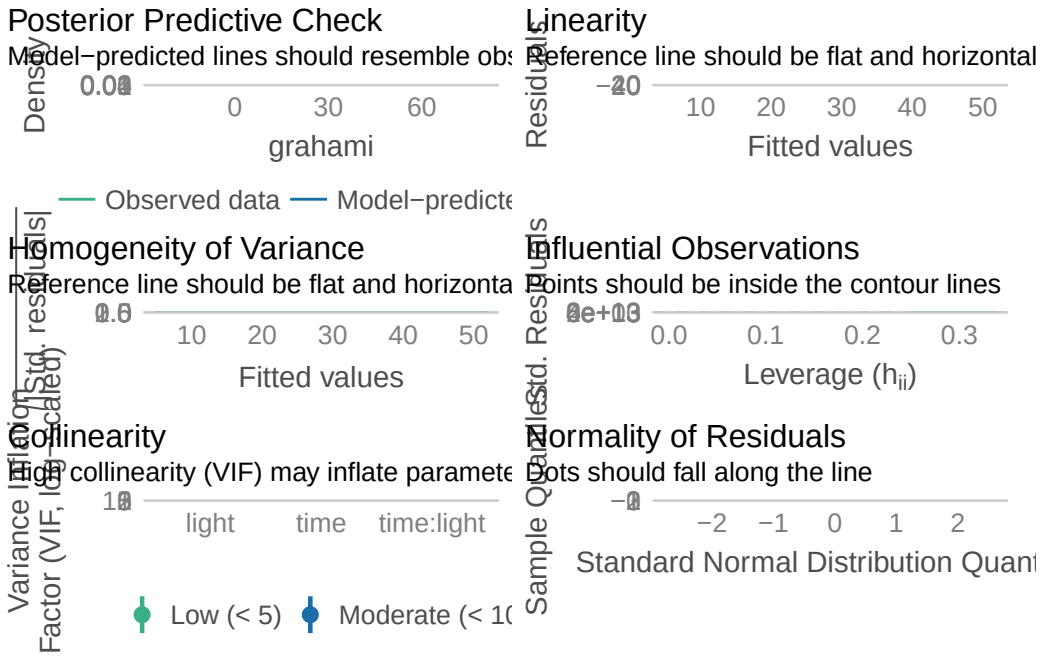
Diagnostics

- 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.)

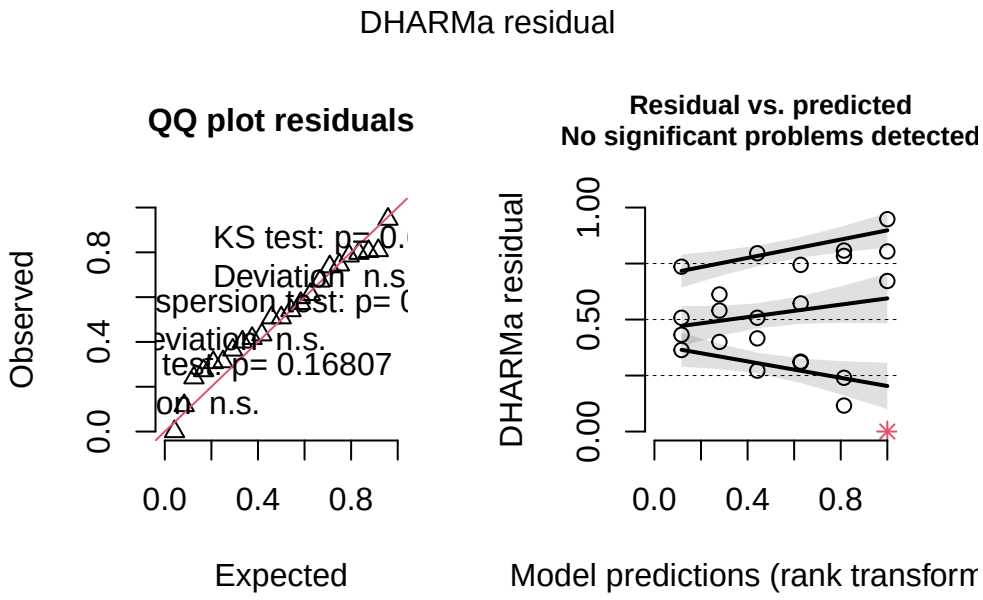
Graphical diagnostics

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

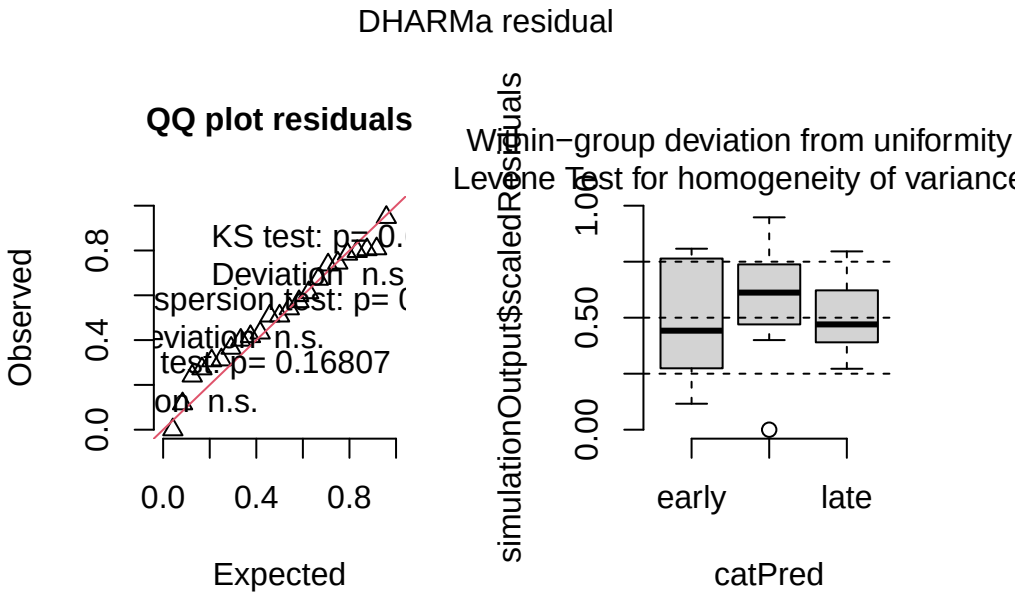
```
performance::check_model(lmTL2)
```



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




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



Solutions to problems

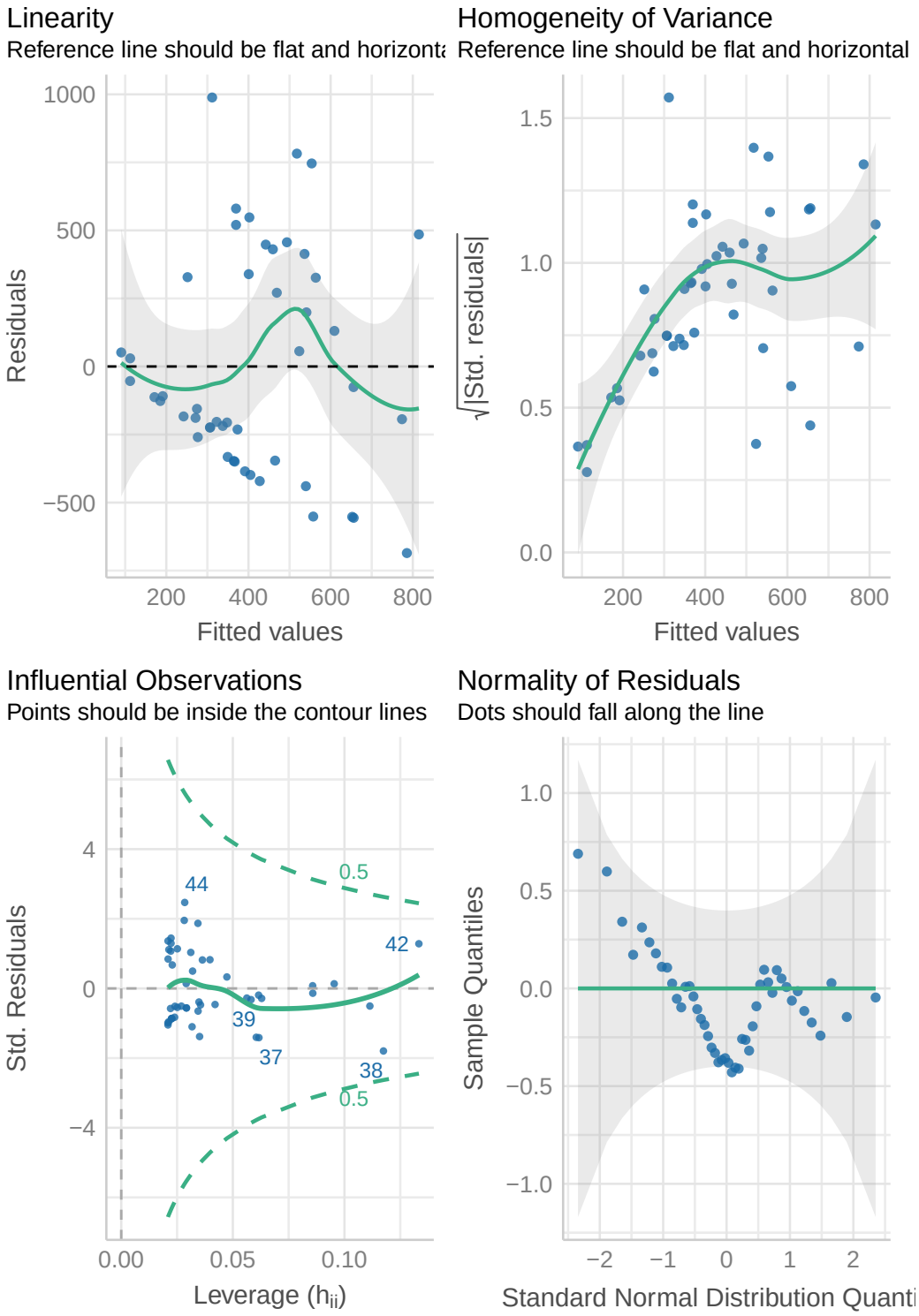
- **nonlinearity**: transformation, add covariates (??), add interactions, add polynomial terms etc.
- **outliers**: drop values (report both!), use robust regression
- **heteroscedasticity**: transformation, model dispersion explicitly, GLMs
- **non-Normality**: transformation, GLMs

Transformation

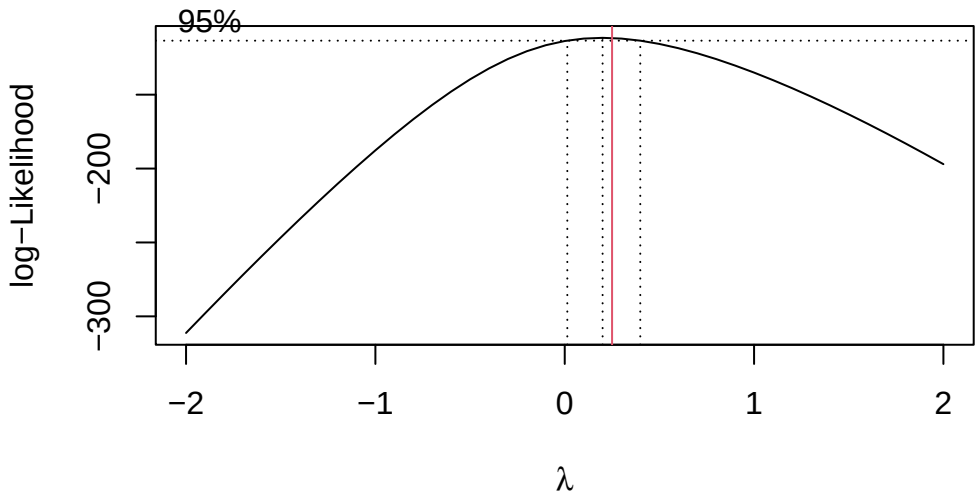
- May do too much at once (GLMs and GAMs allow more flexibility)
- Log-transformation is often interpretable and solves problems
- Transforming boundary values (e.g. $\log(0)$) is problematic
- **Box-Cox transformations**: $y \to \frac{y^\lambda - 1}{\lambda}$ (include Jacobian term $\mathrm{GM}^{\lambda-1}$ 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

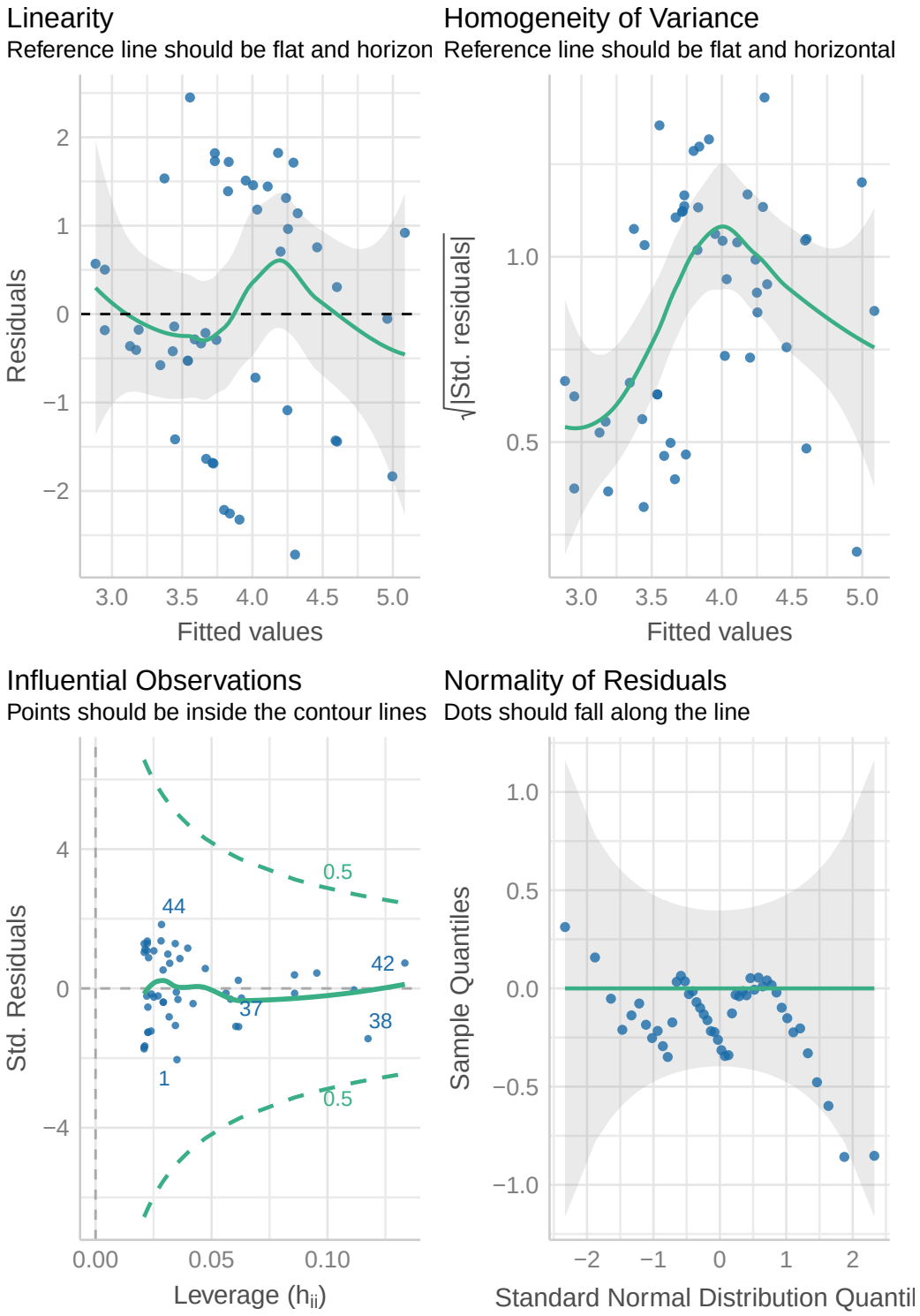
```
library(faraway)
m1 <- lm(perm ~ area, rock)
performance::check_model(m1, check = c("linearity", "homogeneity", "outliers", "qq"))
```


Linearity
Reference line should be flat and horizonta
Residuals
Fitted values
Homogeneity of Variance
Reference line should be flat and horizontal
√|Std. residuals|
Fitted values
Influential Observations
Points should be inside the contour lines
Std. Residuals
Leverage (h_ii)
Normality of Residuals
Dots should fall along the line
Sample Quantiles
Standard Normal Distribution Quanti

```
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 horizon
Residuals
Fitted values
Homogeneity of Variance
Reference line should be flat and horizontal
√|Std. residuals|
Fitted values
Influential Observations
Points should be inside the contour lines
Std. Residuals
Leverage (hii)
0.5
0.5
44
42
37
38
1
Normality of Residuals
Dots should fall along the line
Sample Quantiles
Standard Normal Distribution Quantil

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. e.g. if we log-transform, $\sum \log(J(y_i)) = \sum \log\left(\partial(\log(y_i))/\partial y\right) = \sum \log(1/y_i) = -\sum \log y_i$. In this case $\sum \log(J(y_i)) = \sum \log((1/4)P^(- 3/4)) = -N \log 4 - 3/4 \sum \log(P)$:

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)

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)
```

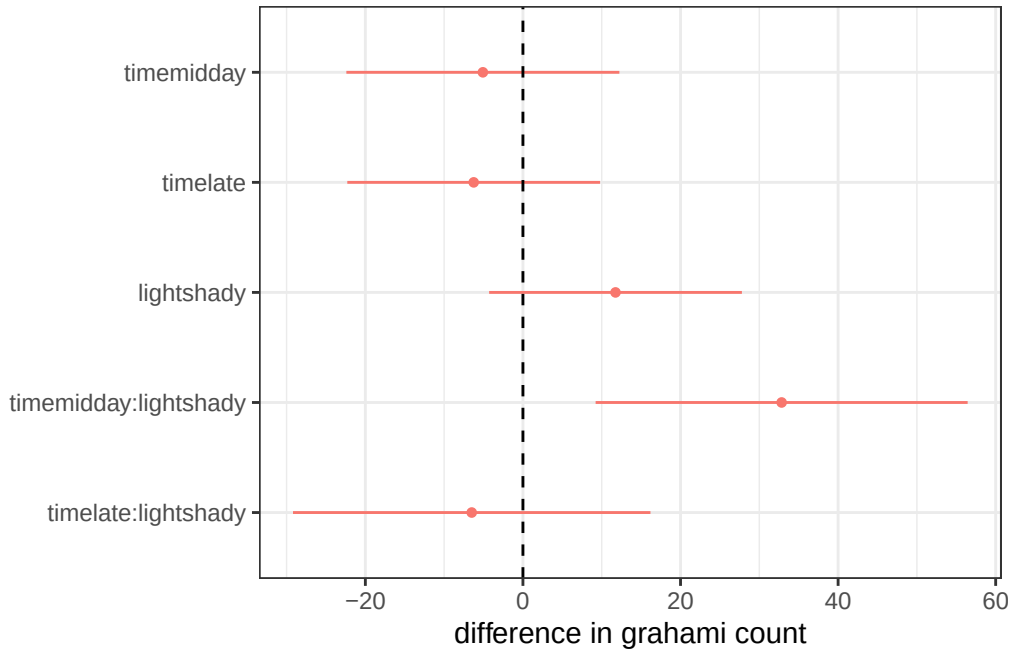
```
Call:
lm(formula = grahami ~ time * light, data = lizards)
```

```
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` ...

References

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