STAT 4/6C03: notes, week 2, part 2

Ben Bolker

September 20, 2013

Version: 2013-09-20 12:42:21

Design matrices and model parameterization (Friday)

Basics

Linear problem: $\boldsymbol{X}\boldsymbol{\beta}$ (solution)

What is $\boldsymbol{X}$? **Design matrix** or **parameterization**.

Setting up a parameterization is the same as setting up a hypothesis, unless your question is just "does this variable have some overall effect"?

[5] syntax (R version): (the response variable and tilde are implicit throughout, e.g. `y~f1`): see `?formula`

`f1`	1-way ANOVA (single categorical predictor)
`x1`	linear regression (single continuous predictor: implicit intercept term
`x1-1` or `x1+0`	regression through the origin (eliminate intercept) [dangerous]
`f1-1`	ANOVA, without intercepts (see below)
`x1+x2`	multiple regression
`f1+f2`	2-way ANOVA (additive model)
`f1*f2` ≡ `f1+f2+f1:f2`	2-way ANOVA (with interactions)
`f1:f2`	interaction model (equivalent to above, but parameterized differently
`(f1+f2)^2` ≡ `f1+f2+f1:f2`	crossing to a specified degree
`(f1+f2)^2-f1` ≡ `f2+f1:f2`	remove a term (example)
`I(x1^2)`	interpret as literal (arithmetic) operator rather than formula
`poly(x1,x2,n)`	n^{th} order orthogonal polynomial in `x1` and `x2`
`ns(x1,n)`	natural spline basis with n knots (requires `spline` package be loaded) [very handy but the `mgcv` package is more powerful for fitting GAMs]
`f1 %in% f2` ≡ `f2:f1`	nesting (rarely used)

- Wilkinson-Rogers notation has been extended in various, usually

sensible not always completely compatible, ways, across add-on packages

- The bar (|) is used as a grouping variable in various contexts (`lattice`: specify conditioning (subplots); `lme4`, `nlme`: specify grouping variables; `pscl`: separate models for binary and count models)
- The `:` shortcut for specifying an interaction works most of the time, but not always (sometimes R interprets it as a shortcut for the `seq` function): if it fails use `interaction()` instead

Continuous predictors

Correlation of slope, intercept: interpretation and numerical problem (especially with interactions). Solution: **centering**. [3]

Scaling variables also helps with interpretability, and numerics. `?scale`, `?sweep` in R.

- **Pro:** simple, sensible, prevents most common misinterpretations, allows interpretation of main effects
- **Con:** too simple (allows people to stop thinking)? Data set-specific. Alternatives to mean-centering and standard-deviation-scaling.

Categorical predictors: contrasts

Independent contrasts.

The *contrast matrix* determines what a given row of the design matrix (for level i of a categorical variable) looks like.

If we have a vector of predicted values $\bar{y}$, the contrast matrix is essentially defined as

$$\bar{y} = C\beta$$

Set contrasts in general via `options()` or per-factor via `contrasts()`, or within the model statement, e.g.

```
d <- data.frame(f=c("a","a","a","b","b","b"),y=c(1,1,1,3,3,3))
coef(lm(y~f,data=d))

## (Intercept)          fb
##           1           2

coef(lm(y~f,data=d,contrasts=list(f="contr.sum")))

## (Intercept)          f1
##           2          -1
```

Or:

```
contrasts(d$f) <- "contr.sum"
## or (dangerous)
options(contrasts=c("contr.sum","contr.poly"))
```

Reordering factors: `levels`, `reorder`, `relevel`

```
levels(relevel(d$f,"b"))

## [1] "b" "a"

levels(with(d,reorder(f,y,mean)))

## [1] "a" "b"
```

In general requesting a contrast for an n-level factor gets us only an $n \times (n-1)$ matrix: the first column is an implicit intercept (all-1) column.

Treatment contrasts (default: "dummy", "corner-point") First level of factor (often alphabetical!) is default. `contr.treatment` (default) vs. `contr.SAS` vs. `contr.treatment(n,base=b)`. Full contrast matrix is not orthogonal (i.e. $\boldsymbol{C}^T\boldsymbol{C}$ is not diagonal: we want $C_i^T C_j = 0$ whenever $i \neq j$).

```
(cc <- contr.treatment(4))

##   2 3 4
## 1 0 0 0
## 2 1 0 0
## 3 0 1 0
## 4 0 0 1
```

```
t(cc) %*% cc      ## orthogonal
cc <- cbind(1,cc) ## add intercept column
t(cc) %*% cc      ## NOT orthogonal
```

If we want to know the *meaning* of $\boldsymbol{\beta}$, it's easiest to invert:

$$\boldsymbol{\beta} = \boldsymbol{C}^{-1}\bar{\boldsymbol{y}}$$

```
solve(cc)
```

```
##    1 2 3 4
##    1 0 0 0
## 2 -1 1 0 0
## 3 -1 0 1 0
## 4 -1 0 0 1
```

Example (from [2])

```
ants <- data.frame(
    place=rep(c("field","forest"),c(6,4)),
    colonies=c(12, 9, 12, 10,
               9, 6, 4, 6, 7, 10))
```

```
mean(ants$colonies[ants$place=="field"])

## [1] 9.667

mean(ants$colonies[ants$place=="forest"])

## [1] 6.75

pr <- function(m) printCoefmat(coef(summary(m)),digits=3,signif.stars=FALSE)
pr(lm1 <- lm(colonies~place,data=ants))

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    9.667      0.958   10.09    8e-06
## placeforest   -2.917      1.515   -1.92     0.09
```

The `(Intercept)` row refers to β_1, which is the mean density in the "field" sites ("field" comes before "forest"). The `placeforest` row tells us we are looking at the effect of the `place` variable on the `forest` level, i.e. the difference between the "forest" and "field" sites. (The only ways we could know that "field" is the baseline site are (1) to remember, or look at `levels(ants$place)` or (2) to notice which level is *missing* from the list of parameter estimates.)

Helmert Orthogonal but less intuitive.

```
(cc <- cbind(1,contr.helmert(4)))

##   [,1] [,2] [,3] [,4]
## 1    1   -1   -1   -1
## 2    1    1   -1   -1
## 3    1    0    2   -1
## 4    1    0    0    3
```

```
t(cc) %*% cc  ## orthogonal
```

```
MASS::fractions(solve(cc))

##      1    2    3    4
## [1,]  1/4  1/4  1/4  1/4
## [2,] -1/2  1/2    0    0
## [3,] -1/6 -1/6  1/3    0
## [4,] -1/12 -1/12 -1/12  1/4
```

β_1=mean; β_2=contrast between levels 1 and 2; β_3=contrast between levels 1&2 and level 3; etc..

```
cfun <- function(contr) {
    pr(update(lm1,contrasts=list(place=contr)))
}
cfun("contr.helmert")

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    8.208      0.758   10.83  4.7e-06
## place1        -1.458      0.758   -1.92     0.09
```

Sum-to-zero What if I want to compare the values with the mean [3]

```
(cc <- cbind(1,contr.sum(4)))

##   [,1] [,2] [,3] [,4]
## 1    1    1    0    0
## 2    1    0    1    0
## 3    1    0    0    1
## 4    1   -1   -1   -1
```

```
t(cc) %*% cc  ## NOT orthogonal (??)
```

```
MASS::fractions(solve(cc))

##      1    2    3    4
## [1,]  1/4  1/4  1/4  1/4
## [2,]  3/4 -1/4 -1/4 -1/4
## [3,] -1/4  3/4 -1/4 -1/4
## [4,] -1/4 -1/4  3/4 -1/4
```

β_1=mean; β_2=level 1 vs levels 2–4; β_3=level 2 vs. levels 1,3, 4; β_4=level 3 vs. levels 1,2, 4

Note that we don't have level 4.

```
cfun("contr.sum")

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    8.208      0.758   10.83  4.7e-06
## place1         1.458      0.758    1.92     0.09
```

Same as Helmert contrasts in this example, except for the sign of `place1`.

No-intercept When we specify a formula with `-1` or `+0` (with default treatment contrasts) we get an identity matrix for the contrasts: each level has its own parameter.

```
pr(update(lm1,.~.-1))

##             Estimate Std. Error t value Pr(>|t|)
## placefield     9.667      0.958   10.09    8e-06
## placeforest    6.750      1.174    5.75  0.00043
```

Sometimes clearer (and we get confidence intervals etc. on the predictions for each level), but the hypotheses tested are rarely interesting (is the mean of each level equal to zero?)

More generally, if you want to compute the group means, you can

- Use the `predict` function:

```
predict(lm1,newdata=data.frame(place=c("field","forest")),interval="confidence")
```

- Use the `effects` package:

```
library("effects")
summary(allEffects(lm1))
```

- Use the `lsmeans` package:

```
library("lsmeans")
lsmeans(lm1,spec=~place)
```

Custom Can specify contrasts "by hand" ([1] gives an example too.)

Example:

```
cmat <- matrix(c(3,-1,-1,-1,
                 0,1,-1,0,
                 0,1,1,-2),
               nrow=4)
t(cmat) %*% cmat
```

[1] Crawley, M. J. (2002). *Statistical Computing: An Introduction to Data Analysis using S-PLUS*. John Wiley & Sons

```
##      [,1] [,2] [,3]
## [1,]   12    0    0
## [2,]    0    2    0
## [3,]    0    0    6
```

```
dimnames(cmat) <- list(c("none","C","S","CS"),
                c("symb","C.vs.S","twosymb"))
cc <- cbind(mean=1,cmat)
MASS::fractions(solve(cc))
```

```
##         none  C     S     CS
## mean     1/4   1/4   1/4   1/4
## symb     1/4 -1/12 -1/12 -1/12
## C.vs.S     0   1/2  -1/2     0
## twosymb    0   1/6   1/6  -1/3
```

How did we get here?

```
mm <- 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),
             nrow=4)
MASS::fractions(ss <- zapsmall(solve(t(mm))))
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1  3/4    0    0
## [2,]    1 -1/4  1/2  1/3
## [3,]    1 -1/4 -1/2  1/3
## [4,]    1 -1/4    0 -2/3
```

Forward difference:

```
(cc <- cbind(mean=1,MASS::contr.sdif(4)))
```

```
##   mean   2-1  3-2   4-3
## 1    1 -0.75 -0.5 -0.25
## 2    1  0.25 -0.5 -0.25
## 3    1  0.25  0.5 -0.25
## 4    1  0.25  0.5  0.75
```

```
MASS::fractions(solve(cc))
```

```
##      1   2   3   4
## mean 1/4 1/4 1/4 1/4
## 2-1   -1   1   0   0
```

```
## 3-2    0  -1   1   0
## 4-3    0   0  -1   1

## not orthogonal at all
```

Exercise. How would you modify this contrast so the intercept is the value of the first level, rather than the mean?

Interactions

Interactions as *differences in differences*

Interpretation problems/marginality principle: [4, 3]

```
head(d <- expand.grid(F=LETTERS[1:3],f=letters[1:3]))

##   F f
## 1 A a
## 2 B a
## 3 C a
## 4 A b
## 5 B b
## 6 C b

m0 <- model.matrix(~F*f,d)
ff <- solve(m0)
colnames(ff) <- apply(d,1,paste,collapse=".")
ff["FB",] ## contrast between (A,a) and (B,a)

## A.a B.a C.a A.b B.b C.b A.c B.c C.c
##  -1   1   0   0   0   0   0   0   0

ff["fb",] ## contrast between (A,a) and (A,b)

## A.a B.a C.a A.b B.b C.b A.c B.c C.c
##  -1   0   0   1   0   0   0   0   0
```

```
old.opts <- options(contrasts=c("contr.sum","contr.poly"))
m <- model.matrix(~F*f,d)
ff <- solve(m)*9
colnames(ff) <- apply(d,1,paste,collapse=".")
ff["F1",] ## contrast between (A,.) and (grand mean)

## A.a B.a C.a A.b B.b C.b A.c B.c C.c
##   2  -1  -1   2  -1  -1   2  -1  -1

ff["f1",] ## contrast between (a,.) and (grand mean)
```

```
## A.a B.a C.a A.b B.b C.b A.c B.c C.c
##   2   2   2  -1  -1  -1  -1  -1  -1
```

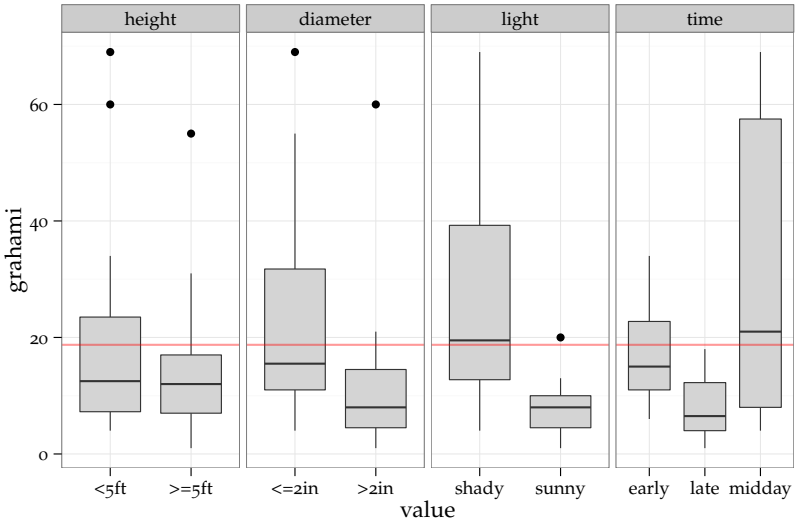
```
options(old.opts) ## reset
```

Exercise: How would you construct a version of `contr.sum` where the first, not the last, level is aliased/dropped?

Things get slightly more interesting/complicated when we have more than two levels of a categorical variable. I'll look at some data on lizard perching behaviour, from the `brglm` package (and before that from McCullagh and Nelder *Generalized Linear Models* 1989, ultimately from Schoener 1970 *Ecology* **51**:408-418). I'm going to ignore the fact that these data might best be fitted with generalized linear models.

```
lizards <- read.csv("lizards.csv")
```

A quick look at the data: response is number of *Anolis grahami* lizards found on perches in particular conditions.



For a moment we're going to just look at the `time` variable. If we leave the factors as is (alphabetical) then β_1="early", β_2="late"-"early", β_3="midday"-"early". At the very least, it probably makes sense to change the order of the levels:

```
lizards$time <- factor(lizards$time,levels=c("early","midday","late"))
```

All this does (since we haven't changed the baseline factor) is swap the definitions of β_2 and β_3.

In a linear model, we could also use so-called *sum-to-zero* contrasts:

```
pr(lm(grahami~time,data=lizards,contrasts=list(time=contr.sum)))

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    19.30       3.53    5.47  2.4e-05
## time1          -1.67       4.93   -0.34     0.74
## time2          12.85       5.10    2.52     0.02
```

Now the `(Intercept)` parameter is the overall mean: `time1` and `time2` are the deviations of the first ("early") and second ("midday") groups from the overall mean. (The names are useless: the `car` package offers a slightly better alternative called `contr.Sum`). There are other ways to change the contrasts (i.e., use the `contrasts()` function to change the contrasts for a particular variable permanently, or use `options(contrasts=c("contr.sum","contr.poly")))` to change the contrasts for *all* variables), but the way shown above may be the most transparent.

There are other options for contrasts such as `MASS::contr.sdif()`, which gives the successive differences between levels.

```
library("MASS")
pr(lm(grahami~time,data=lizards,contrasts=list(time=contr.sdif)))

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    19.30       3.53    5.47  2.4e-05
## time2-1        14.52       8.74    1.66    0.112
## time3-2       -24.02       8.74   -2.75    0.012
```

You might have particular contrasts in mind (e.g. "control" vs. all other treatments, then "low" vs "high" within treatments), in which case it is probably worth learning how to set contrasts. (We will talk about testing *all pairwise differences later*, when we discuss multiple comparisons. This approach is probably not as useful as it is common.)

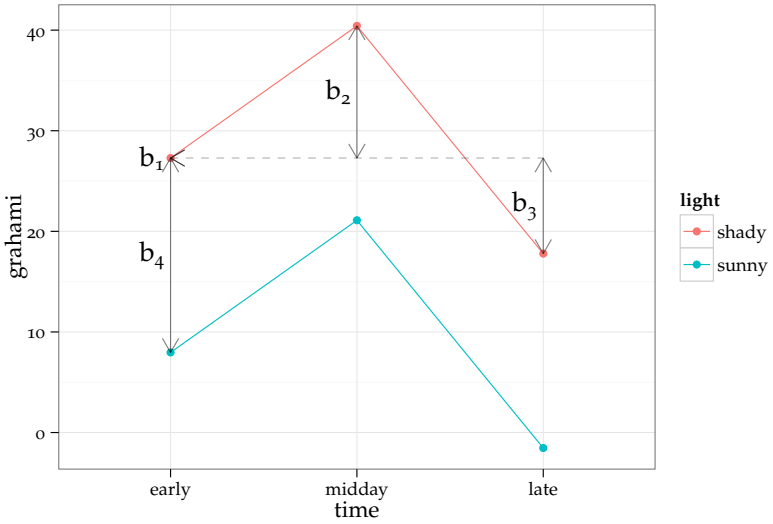
Multiple treatments and interactions

Additive model Let's consider the `light` variable in addition to `time`.

```
pr(lmTL1 <- lm(grahami~time+light,data=lizards))

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    27.29       5.63    4.85  0.00011
## timemidday     13.14       7.11    1.85  0.08010
## timelate       -9.50       6.85   -1.39  0.18174
## lightsunny    -19.32       5.73   -3.37  0.00321
```

Here's a graphical interpretation of the parameters:

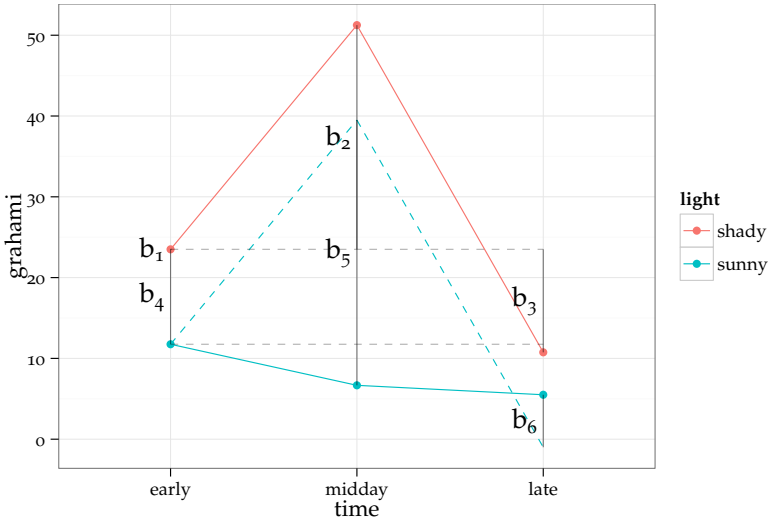


β_1 is the intercept ("early","sunny"); β_2 and β_3 are the differences from the baseline level ("early") of the *first* variable (`time`) in the *baseline* level of the other parameter(s) (`light`="shady"); β_4 is the difference from the baseline level ("sunny") of the *second* variable (`light`) in the *baseline* level of `time` ("early").

Now let's look at an interaction model:

```
pr(lmTL2 <- lm(grahami~time*light,data=lizards))

##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)              23.50       5.38    4.37  0.00042
## timemidday               27.75       7.60    3.65  0.00198
## timelate                -12.75       7.60   -1.68  0.11180
## lightsunny              -11.75       7.60   -1.55  0.14061
## timemidday:lightsunny   -32.83      11.19   -2.93  0.00927
## timelate:lightsunny       6.50      10.75    0.60  0.55343
```



Parameters β_1 to β_4 have the same meanings as before. Now we also have β_5 and β_6, labelled "timemidday:lightsunny" and "time-late:lightsunny", which describe the difference between the expected mean value of these treatment combinations based on the additive model (which are $\beta_1 + \beta_2 + \beta_4$ and $\beta_1 + \beta_3 + \beta_4$ respectively) and their actual values.

Now re-do this for sum-to-zero contrasts ... the fits are easy:

```
pr(lmTL1S <- update(lmTL1,contrasts=list(time=contr.sum,light=contr.sum)))

##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    18.84       2.87    6.57  2.7e-06
## time1          -1.21       4.01   -0.30   0.7654
## time2          11.93       4.15    2.87   0.0097
## light1          9.66       2.87    3.37   0.0032
```

```
pr(lmTL2S <- update(lmTL2,contrasts=list(time=contr.sum,light=contr.sum)))

##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    18.236      2.255    8.09  3.1e-07
## time1          -0.611      3.146   -0.19  0.84830
## time2          10.722      3.271    3.28  0.00444
## light1         10.264      2.255    4.55  0.00028
## time1:light1   -4.389      3.146   -1.39  0.18100
## time2:light1   12.028      3.271    3.68  0.00187
```

(The intercept doesn't stay exactly the same when we add the interaction because the data are unbalanced: try `with(lizards,table(light,time))`)

Other refs

- http://sas-and-r.blogspot.com/2010/10/example-89-contrasts.html
- see also: `gmodels::fit.contrast`, `rms::contrast.rms` for on-the-fly contrasts
- http://www.ats.ucla.edu/stat/r/library/contrast_coding.htm

References

[1] Crawley, M. J. (2002). *Statistical Computing: An Introduction to Data Analysis using S-PLUS*. John Wiley & Sons.

[2] Gotelli, N. J. and A. M. Ellison (2004). *A Primer of Ecological Statistics*. Sunderland, MA: Sinauer.

[3] Schielzeth, H. (2010). Simple means to improve the interpretability of regression coefficients. *Methods in Ecology and Evolution 1*, 103–113.

[4] Venables, W. N. (1998). Exegeses on linear models. 1998 International S-PLUS User Conference, Washington, DC.

[5] Wilkinson, G. N. and C. E. Rogers (1973). Symbolic description of factorial models for analysis of variance. *Applied Statistics 22*(3), 392–399.