LS–means (least–squares means) and other linear estimates

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Contents

1 Introduction

1.1 Linear functions of parameters, contrasts

A linear function of a p–dimensional parameter vector β has the form

$$C = K\beta$$

where K is a $q \times p$ matrix. The corresponding linear estimate is $\hat{C} = K\hat{\beta}$. A linear hypothesis has the form $H_0 : K\beta = m$ for some q dimensional vector m.

1.2 Least-squares means (LS–means)

A special type of linear estimates is the so called least–squares means (or LS–means). Other names for these estimates include population means and marginal means. Consider an imaginary field experiment analyzed with model of the form

```
> lm( y ~ treat + block + year)
```

where `treat` is a treatment factor, `block` is a blocking factor and `year` is the year (a factor) where the experiment is repeated over several years. This model specifies the conditional mean $\mathbb{E}(Y|\texttt{treat}, \texttt{block}, \texttt{year})$. One may be interested in predictions of the form $\mathbb{E}(Y|\texttt{treat})$. This quantity can not formally be found from the model. However, it is tempting to average the fitted values of $\mathbb{E}(Y|\texttt{treat}, \texttt{block}, \texttt{year})$ across the levels of `block` and `year` and think of this average as $\mathbb{E}(Y|\texttt{treat})$. This average is precisely what is called the LS–means. If the experiment is balanced then this average is identical to the average of the observations when stratified according to `treat`.

An alternative is to think of `block` and `year` as random effects, for example:

```
> library(lme4)
> lmer( y ~ treat + (1|block) + (1|year))
```

In this case one would directly obtain $\mathbb{E}(Y|\texttt{treat})$ from the model. However, there are at least two reasons why one may be hesitant to consider such a random effects model.

- Suppose there are three blocks and the experiment is repeated over three consecutive years. This means that the random effects are likely to be estimated with a large uncertainty (the estimates will have only two degrees of freedom).
- Furthermore, treating `block` and `year` as random effects means they should in principle come from a large population of possible blocks and years. This may or may not be reasonable for the blocks, but it is certainly a dubious assumption for the years.

Below we describe `LSmeans` as implemented in the **doBy** package. Notice that the **lsmeans** package **?** also provides computations of LS–means, see `http://cran.r-project.org/web/packages/lsmeans/`.

2 LS–means for linear models

2.1 LS–means – a first example

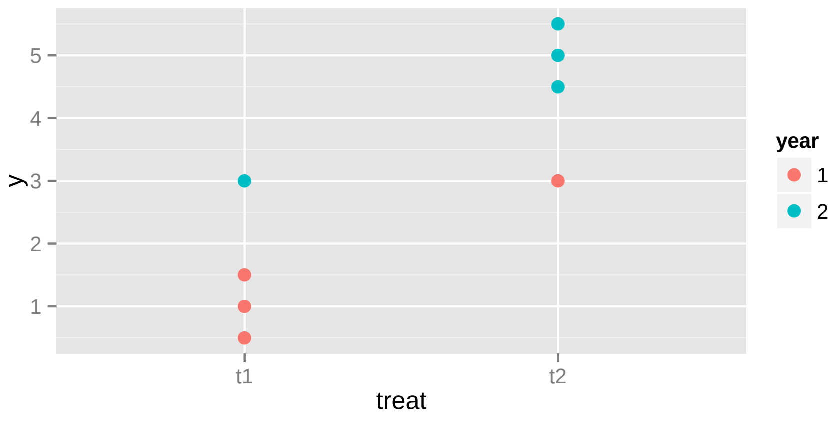
Consider these simulated data

```
> simdat

  treat year   y
1    t1    1 0.5
2    t1    1 1.0
3    t1    1 1.5
4    t2    1 3.0
```

```
5    t1    2 3.0
6    t2    2 4.5
7    t2    2 5.0
8    t2    2 5.5
```

shown in the figure below.

```
> library(ggplot2)
> qplot(treat, y, data=simdat, color=year, size=I(3))
```



The LS–means under an additive model for the factor `treat` is

```
> msim <- lm(y ~ treat + year, data=simdat)
> LSmeans( msim, effect="treat")
```

```
  estimate     se df t.stat   p.value   lwr   upr treat
1        2 0.2415  5  8.281 4.192e-04 1.379 2.621    t1
2        4 0.2415  5 16.562 1.465e-05 3.379 4.621    t2
```

whereas the population means are

```
> summaryBy(y~treat, data=simdat)
```

```
  treat y.mean
1    t1    1.5
2    t2    4.5
```

Had data been balanced (same number of observations for each combination of `treat` and `year`) the results would have been the same. An argument in favor of the LS–means is that these figures better represent what one would expect on in an "average year".

2.2 Example: Warpbreaks

```
> summary( warpbreaks )
```

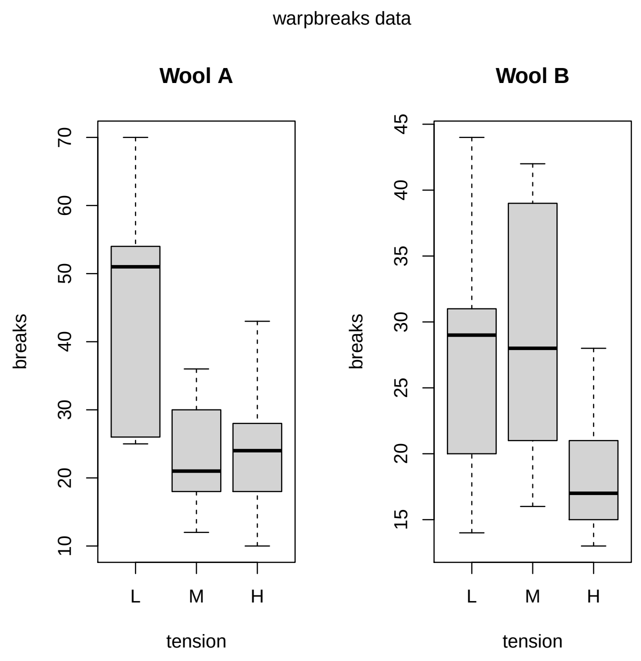
```
     breaks      wool   tension
 Min.   :10.0   A:27   L:18   
 1st Qu.:18.2   B:27   M:18   
 Median :26.0          H:18   
 Mean   :28.1                 
 3rd Qu.:34.0                 
 Max.   :70.0                 
```

```
> head( warpbreaks, 4 )
```

```
  breaks wool tension
1     26    A       L
2     30    A       L
3     54    A       L
4     25    A       L
```

```
> ftable(xtabs( ~ wool + tension, data=warpbreaks))
```

```
     tension L M H
wool
A            9 9 9
B            9 9 9
```



```
> (warp.lm <- lm(breaks ~ wool + tension, data=warpbreaks))
```

```
Call:
lm(formula = breaks ~ wool + tension, data = warpbreaks)

Coefficients:
(Intercept)        woolB     tensionM     tensionH
      39.28        -5.78       -10.00       -14.72
```

The fitted values are:

```
> uni <- unique(warpbreaks[,2:3])
> prd <- cbind(breaks=predict(warp.lm, newdata=uni), uni); prd
```

```
   breaks wool tension
1   39.28    A       L
10  29.28    A       M
19  24.56    A       H
28  33.50    B       L
37  23.50    B       M
46  18.78    B       H
```

2.3 The LS–means

We may be interested in making predictions of the number of breaks for each level of `tension` for *any* type or an *average* type of `wool`. The idea behind LS–means is to average the predictions above over the two wool types. These quantities are the `LSmeans` for the effect `tension`.

This is done with:

```
> LSmeans(warp.lm, effect="tension")

  estimate    se df t.stat   p.value   lwr   upr tension
1    36.39 2.738 50 13.289 4.948e-18 30.89 41.89       L
2    26.39 2.738 50  9.637 5.489e-13 20.89 31.89       M
3    21.67 2.738 50  7.913 2.269e-10 16.17 27.17       H
```

The term `LSmeans` comes from that these quantities are the same as the least squares main effects of `tension` when data is balanced:

```
> doBy::summaryBy(breaks ~ tension, data=warpbreaks)

  tension breaks.mean
1       L       36.39
2       M       26.39
3       H       21.67
```

When data is not balanced these quantities are in general not the same.

2.4 LS–means for models with interactions

Consider a model with interaction:

```
> warp.lm2 <- update(warp.lm, .~.+wool:tension)
> coef( summary( warp.lm2 ))

                 Estimate Std. Error t value  Pr(>|t|)
(Intercept)         44.56      3.647  12.218 2.426e-16
woolB              -16.33      5.157  -3.167 2.677e-03
tensionM           -20.56      5.157  -3.986 2.281e-04
tensionH           -20.00      5.157  -3.878 3.199e-04
woolB:tensionM      21.11      7.294   2.895 5.698e-03
woolB:tensionH      10.56      7.294   1.447 1.543e-01
```

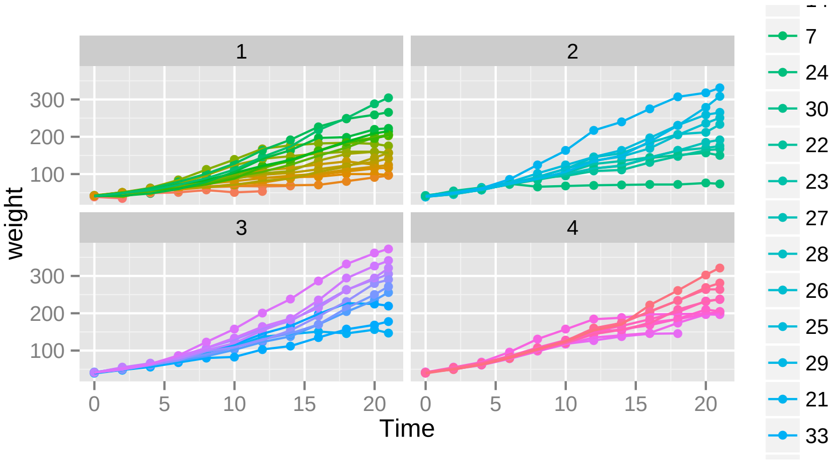
In this case the contrast matrix becomes:

```
> K2 <- LSmatrix(warp.lm2, effect="tension"); K2

     (Intercept) woolB tensionM tensionH woolB:tensionM woolB:tensionH
[1,]           1   0.5        0        0            0.0            0.0
[2,]           1   0.5        1        0            0.5            0.0
[3,]           1   0.5        0        1            0.0            0.5
```

```
> linest(warp.lm2, K=K2)

  estimate    se df t.stat   p.value   lwr   upr tension
1    36.39 2.579 48 14.112 1.055e-18 31.20 41.57       L
2    26.39 2.579 48 10.234 1.183e-13 21.20 31.57       M
3    21.67 2.579 48  8.402 5.468e-11 16.48 26.85       H
```

3 Using the at= argument

```
> library(ggplot2)
> ChickWeight$Diet <- factor(ChickWeight$Diet)
> qplot(Time, weight, data=ChickWeight, colour=Chick, facets=~Diet,
        geom=c("point","line"))
```



Consider random regression model:

```
> library(lme4)
> rr <- lmer(weight~Time*Diet + (0+Time|Chick), data=ChickWeight)
> coef(summary(rr))
            Estimate Std. Error t value
(Intercept)   33.218     1.7697 18.7701
Time           6.339     0.6103 10.3855
Diet2         -4.585     3.0047 -1.5258
Diet3        -14.968     3.0047 -4.9815
Diet4         -1.454     3.0177 -0.4818
Time:Diet2     2.271     1.0367  2.1902
Time:Diet3     5.084     1.0367  4.9043
Time:Diet4     3.217     1.0377  3.1004
```

The contrast matrix for `Diet` becomes:

```
> LSmatrix(rr, effect="Diet")
     (Intercept)  Time Diet2 Diet3 Diet4 Time:Diet2 Time:Diet3 Time:Diet4
[1,]           1 10.72     0     0     0       0.00       0.00       0.00
[2,]           1 10.72     1     0     0      10.72       0.00       0.00
[3,]           1 10.72     0     1     0       0.00      10.72       0.00
[4,]           1 10.72     0     0     1       0.00       0.00      10.72
```

The value of `Time` is by default taken to be the average of that variable. Hence the `LSmeans` is the predicted weight for each diet at that specific point of time. We can consider other points of time with

```
> K1 <- LSmatrix(rr, effect="Diet", at=list(Time=1)); K1
     (Intercept) Time Diet2 Diet3 Diet4 Time:Diet2 Time:Diet3 Time:Diet4
[1,]           1    1     0     0     0          0          0          0
[2,]           1    1     1     0     0          1          0          0
[3,]           1    1     0     1     0          0          1          0
[4,]           1    1     0     0     1          0          0          1
```

The `LSmeans` for the intercepts is the predictions at `Time=0`. The `LSmeans` for the slopes becomes

```
> K0 <- LSmatrix(rr, effect="Diet", at=list(Time=0))
> K1-K0
     (Intercept) Time Diet2 Diet3 Diet4 Time:Diet2 Time:Diet3 Time:Diet4
[1,]           0    1     0     0     0          0          0          0
[2,]           0    1     0     0     0          1          0          0
[3,]           0    1     0     0     0          0          1          0
[4,]           0    1     0     0     0          0          0          1
```

```
> LSmeans(rr, K=K1-K0)
```

```
8 x 8 Matrix of class "dpoMatrix"
            (Intercept)    Time   Diet2   Diet3   Diet4 Time:Diet2 Time:Diet3
(Intercept)      3.1320 -0.2296 -3.1320 -3.1320 -3.1320     0.2296     0.2296
Time            -0.2296  0.3725  0.2296  0.2296  0.2296    -0.3725    -0.3725
Diet2           -3.1320  0.2296  9.0283  3.1320  3.1320    -0.6195    -0.2296
Diet3           -3.1320  0.2296  3.1320  9.0283  3.1320    -0.2296    -0.6195
Diet4           -3.1320  0.2296  3.1320  3.1320  9.1067    -0.2296    -0.2296
Time:Diet2       0.2296 -0.3725 -0.6195 -0.2296 -0.2296     1.0747     0.3725
Time:Diet3       0.2296 -0.3725 -0.2296 -0.6195 -0.2296     0.3725     1.0747
Time:Diet4       0.2296 -0.3725 -0.2296 -0.2296 -0.6323     0.3725     0.3725
            Time:Diet4
(Intercept)     0.2296
Time           -0.3725
Diet2          -0.2296
Diet3          -0.2296
Diet4          -0.6323
Time:Diet2      0.3725
Time:Diet3      0.3725
Time:Diet4      1.0768
8 x 8 Matrix of class "dgeMatrix"
            (Intercept)    Time   Diet2   Diet3   Diet4 Time:Diet2 Time:Diet3
(Intercept)      3.1324 -0.2298 -3.1324 -3.1324 -3.1324     0.2298     0.2298
Time            -0.2298  0.3727  0.2298  0.2298  0.2298    -0.3727    -0.3727
Diet2           -3.1324  0.2298  9.0287  3.1324  3.1324    -0.6197    -0.2298
Diet3           -3.1324  0.2298  3.1324  9.0287  3.1324    -0.2298    -0.6197
Diet4           -3.1324  0.2298  3.1324  3.1324  9.1072    -0.2298    -0.2298
Time:Diet2       0.2298 -0.3727 -0.6197 -0.2298 -0.2298     1.0749     0.3727
Time:Diet3       0.2298 -0.3727 -0.2298 -0.6197 -0.2298     0.3727     1.0749
Time:Diet4       0.2298 -0.3727 -0.2298 -0.2298 -0.6325     0.3727     0.3727
            Time:Diet4
(Intercept)     0.2298
Time           -0.3727
Diet2          -0.2298
Diet3          -0.2298
Diet4          -0.6325
Time:Diet2      0.3727
Time:Diet3      0.3727
Time:Diet4      1.0770
     (Intercept) Time Diet2 Diet3 Diet4 Time:Diet2 Time:Diet3 Time:Diet4
[1,]           0    1     0     0     0          0          0          0
[2,]           0    1     0     0     0          1          0          0
[3,]           0    1     0     0     0          0          1          0
```

```
[4,]           0    1     0     0     0           0           0           1
  estimate     se    df t.stat   p.value   lwr    upr Diet Time
1    6.339 0.6105 49.86  10.38 4.632e-14 5.112  7.565    1    1
2    8.609 0.8380 48.28  10.27 9.705e-14 6.924 10.294    2    1
3   11.423 0.8380 48.28  13.63 3.588e-18 9.738 13.108    3    1
4    9.556 0.8392 48.56  11.39 2.584e-15 7.869 11.243    4    1
```

We can cook up our own function for comparing trends:

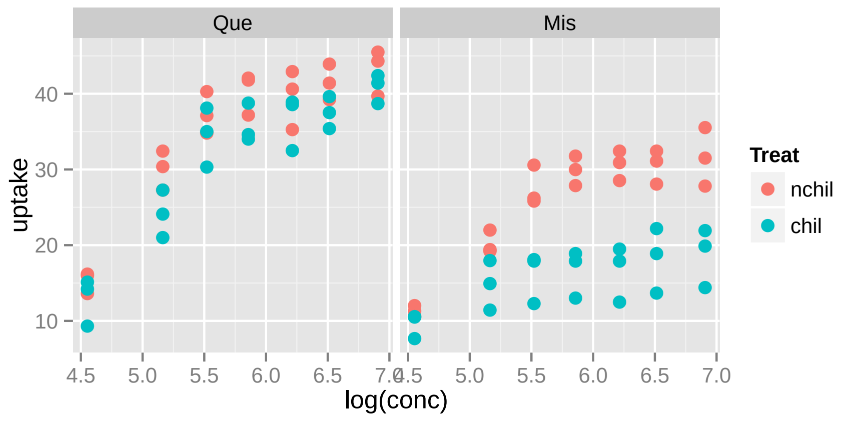
```
> LSmeans_trend <- function(object, effect, trend){

      K<-LSmatrix(object, effect=effect, at=as.list(setNames(1, trend))) -
          LSmatrix(object, effect=effect, at=as.list(setNames(0, trend)))
      LSmeans(object, K=K)
  }
> LSmeans_trend(rr, effect="Diet", trend="Time")
8 x 8 Matrix of class "dpoMatrix"
            (Intercept)    Time   Diet2   Diet3   Diet4 Time:Diet2 Time:Diet3
(Intercept)      3.1320 -0.2296 -3.1320 -3.1320 -3.1320     0.2296     0.2296
Time            -0.2296  0.3725  0.2296  0.2296  0.2296    -0.3725    -0.3725
Diet2           -3.1320  0.2296  9.0283  3.1320  3.1320    -0.6195    -0.2296
Diet3           -3.1320  0.2296  3.1320  9.0283  3.1320    -0.2296    -0.6195
Diet4           -3.1320  0.2296  3.1320  3.1320  9.1067    -0.2296    -0.2296
Time:Diet2       0.2296 -0.3725 -0.6195 -0.2296 -0.2296     1.0747     0.3725
Time:Diet3       0.2296 -0.3725 -0.2296 -0.6195 -0.2296     0.3725     1.0747
Time:Diet4       0.2296 -0.3725 -0.2296 -0.2296 -0.6323     0.3725     0.3725
            Time:Diet4
(Intercept)     0.2296
Time           -0.3725
Diet2          -0.2296
Diet3          -0.2296
Diet4          -0.6323
Time:Diet2      0.3725
Time:Diet3      0.3725
Time:Diet4      1.0768
8 x 8 Matrix of class "dgeMatrix"
            (Intercept)    Time   Diet2   Diet3   Diet4 Time:Diet2 Time:Diet3
(Intercept)      3.1324 -0.2298 -3.1324 -3.1324 -3.1324     0.2298     0.2298
Time            -0.2298  0.3727  0.2298  0.2298  0.2298    -0.3727    -0.3727
Diet2           -3.1324  0.2298  9.0287  3.1324  3.1324    -0.6197    -0.2298
Diet3           -3.1324  0.2298  3.1324  9.0287  3.1324    -0.2298    -0.6197
Diet4           -3.1324  0.2298  3.1324  3.1324  9.1072    -0.2298    -0.2298
Time:Diet2       0.2298 -0.3727 -0.6197 -0.2298 -0.2298     1.0749     0.3727
Time:Diet3       0.2298 -0.3727 -0.2298 -0.6197 -0.2298     0.3727     1.0749
Time:Diet4       0.2298 -0.3727 -0.2298 -0.2298 -0.6325     0.3727     0.3727
            Time:Diet4
(Intercept)     0.2298
Time           -0.3727
Diet2          -0.2298
Diet3          -0.2298
Diet4          -0.6325
Time:Diet2      0.3727
Time:Diet3      0.3727
```

```
Time:Diet4      1.0770
     (Intercept) Time Diet2 Diet3 Diet4 Time:Diet2 Time:Diet3 Time:Diet4
[1,]           0    1     0     0     0          0          0          0
[2,]           0    1     0     0     0          1          0          0
[3,]           0    1     0     0     0          0          1          0
[4,]           0    1     0     0     0          0          0          1
  estimate     se    df t.stat   p.value   lwr    upr Diet Time
1    6.339 0.6105 49.86  10.38 4.632e-14 5.112  7.565    1    1
2    8.609 0.8380 48.28  10.27 9.705e-14 6.924 10.294    2    1
3   11.423 0.8380 48.28  13.63 3.588e-18 9.738 13.108    3    1
4    9.556 0.8392 48.56  11.39 2.584e-15 7.869 11.243    4    1
```

4 Using (transformed) covariates

Consider the following subset of the CO2 dataset:

```
> data(CO2)
> CO2 <- transform(CO2, Treat=Treatment, Treatment=NULL)
> levels(CO2$Treat) <- c("nchil","chil")
> levels(CO2$Type) <- c("Que","Mis")
> ftable(xtabs( ~ Plant + Type + Treat, data=CO2), col.vars=2:3)
      Type    Que        Mis
      Treat nchil chil nchil chil
Plant
Qn1             7    0     0    0
Qn2             7    0     0    0
Qn3             7    0     0    0
Qc1             0    7     0    0
Qc3             0    7     0    0
Qc2             0    7     0    0
Mn3             0    0     7    0
Mn2             0    0     7    0
Mn1             0    0     7    0
Mc2             0    0     0    7
Mc3             0    0     0    7
Mc1             0    0     0    7
> qplot(x=log(conc), y=uptake, data=CO2, color=Treat, facets=~Type, size=I(3))
```



Below, the covariate `conc` is fixed at the average value:

```
> co2.lm1 <- lm(uptake ~ conc + Type + Treat, data=CO2)
> LSmeans(co2.lm1, effect="Treat")
```

```
  estimate     se df t.stat   p.value   lwr   upr Treat conc
1    30.64 0.9556 80  32.07 2.010e-47 28.74 32.54 nchil  435
2    23.78 0.9556 80  24.89 2.037e-39 21.88 25.69  chil  435
```

If we use `log(conc)` instead we will get an error when calculating LS–means:

```
> co2.lm <- lm(uptake ~ log(conc) + Type + Treat, data=CO2)
> LSmeans(co2.lm, effect="Treat")
```

In this case one can do

```
> co2.lm2 <- lm(uptake ~ log.conc + Type + Treat,
               data=transform(CO2, log.conc=log(conc)))
> LSmeans(co2.lm2, effect="Treat")
```

```
  estimate     se df t.stat   p.value   lwr   upr Treat log.conc
1    30.64 0.7611 80  40.26 7.169e-55 29.13 32.16 nchil    5.819
2    23.78 0.7611 80  31.25 1.366e-46 22.27 25.30  chil    5.819
```

This also highlights what is computed: The average of the log of `conc`; not the log of the average of `conc`.

In a similar spirit consider

```
> co2.lm3 <- lm(uptake ~ conc + I(conc^2) + Type + Treat, data=CO2)
> LSmeans(co2.lm3, effect="Treat")
```

```
  estimate     se df t.stat   p.value   lwr   upr Treat conc I(conc^2)
1    34.54 0.9816 79  35.19 4.926e-50 32.59 36.50 nchil  435    275754
2    27.68 0.9816 79  28.20 5.382e-43 25.73 29.64  chil  435    275754
```

Above `I(conc^2)` is the average of the squared values of `conc`; not the square of the average of `conc`, cfr. the following.

```
> co2.lm4 <- lm(uptake ~ conc + conc2 + Type + Treat, data=
                transform(CO2, conc2=conc^2))
> LSmeans(co2.lm4, effect="Treat")
```

```
  estimate     se df t.stat   p.value   lwr   upr Treat conc  conc2
1    30.64 0.7765 79  39.46 9.318e-54 29.10 32.19 nchil  435 275754
2    23.78 0.7765 79  30.63 1.356e-45 22.24 25.33  chil  435 275754
```

If we want to evaluate the LS–means at `conc=10` then we can do:

```
> LSmeans(co2.lm4, effect="Treat", at=list(conc=10, conc2=100))
```

```
  estimate    se df t.stat   p.value   lwr   upr Treat conc conc2
1   14.735 1.701 79  8.662 4.456e-13 11.35 18.12 nchil   10   100
2    7.876 1.701 79  4.630 1.417e-05  4.49 11.26  chil   10   100
```

5 Alternative models

5.1 Generalized linear models

We can calculate LS–means for e.g. a Poisson or a gamma model. Default is that the calculation is calculated on the scale of the linear predictor. However, if we think of LS–means as a prediction on the linear scale one may argue that it can also make sense to transform this prediction to the response scale:

```
> warp.poi <- glm(breaks ~ wool + tension, family=poisson, data=warpbreaks)
> LSmeans(warp.poi, effect="tension", type="link")
```

```
  estimate      se z.stat p.value   lwr   upr tension
1    3.589 0.03916  91.64       0 3.512 3.666       L
2    3.268 0.04596  71.10       0 3.178 3.358       M
3    3.070 0.05071  60.55       0 2.971 3.170       H
```

```
> LSmeans(warp.poi, effect="tension", type="response")
```

```
  estimate    se z.stat p.value   lwr   upr tension
1    36.20 1.418  91.64       0 33.52 39.08       L
2    26.25 1.206  71.10       0 23.99 28.72       M
3    21.55 1.093  60.55       0 19.51 23.80       H
```

```
> warp.qpoi <- glm(breaks ~ wool + tension, family=quasipoisson, data=warpbreaks)
> LSmeans(warp.qpoi, effect="tension", type="link")
```

```
  estimate      se z.stat    p.value   lwr   upr tension
1    3.589 0.08085  44.39  0.000e+00 3.431 3.747       L
2    3.268 0.09488  34.44 6.093e-260 3.082 3.454       M
3    3.070 0.10467  29.33 3.883e-189 2.865 3.276       H
```

```
> LSmeans(warp.qpoi, effect="tension", type="response")
```

```
  estimate    se z.stat    p.value   lwr   upr tension
1    36.20 2.926  44.39  0.000e+00 30.89 42.41       L
2    26.25 2.490  34.44 6.093e-260 21.80 31.61       M
3    21.55 2.256  29.33 3.883e-189 17.55 26.46       H
```

For comparison with the linear model, we use identity link

```
> warp.gam <- glm(breaks ~ wool + tension, family=Gamma(link=identity),
                  data=warpbreaks)
> LSmeans(warp.gam, effect="tension", type="link")
```

```
  estimate    se df t.stat   p.value   lwr   upr tension
1    35.66 3.222 50  11.07 4.766e-15 29.19 42.13       L
2    27.12 2.448 50  11.08 4.543e-15 22.21 32.04       M
3    21.53 1.944 50  11.08 4.629e-15 17.62 25.43       H
```

Notice that the linear estimates are practically the same as for the linear model, but the standard errors are smaller and hence the confidence intervals are narrower.

An alternative is to fit a quasi Poisson "model"

```
> warp.poi3 <- glm(breaks ~ wool + tension, family=quasipoisson(link=identity),
                   data=warpbreaks)
> LSmeans(warp.poi3, effect="tension")
```

```
  estimate    se z.stat   p.value   lwr   upr tension
1    36.00 2.950 12.204 2.965e-34 30.22 41.78       L
2    26.83 2.544 10.546 5.316e-26 21.84 31.81       M
3    21.62 2.281  9.475 2.657e-21 17.14 26.09       H
```

5.2 Linear mixed effects model

For the sake of illustration we treat `wool` as a random effect:

```
> library(lme4)
> warp.mm <- lmer(breaks ~ tension + (1|wool), data=warpbreaks)
> LSmeans(warp.mm, effect="tension")
3 x 3 Matrix of class "dpoMatrix"
            (Intercept) tensionM tensionH
(Intercept)      13.344   -7.498   -7.498
tensionM         -7.498   14.995    7.498
tensionH         -7.498    7.498   14.995
3 x 3 Matrix of class "dgeMatrix"
            (Intercept) tensionM tensionH
(Intercept)      13.344   -7.498   -7.498
tensionM         -7.498   14.995    7.498
tensionH         -7.498    7.498   14.995
     (Intercept) tensionM tensionH
[1,]           1        0        0
[2,]           1        1        0
[3,]           1        0        1
  estimate    se    df t.stat  p.value    lwr   upr tension
1    36.39 3.653 2.538  9.961 0.004230 23.471 49.31       L
2    26.39 3.653 2.538  7.224 0.009354 13.471 39.31       M
3    21.67 3.653 2.538  5.931 0.015093  8.749 34.58       H
```

Notice here that the estimates themselves are very similar to those above but the standard errors are much larger. This comes from that there that `wool` is treated as a random effect.

```
> VarCorr(warp.mm)

 Groups   Name        Std.Dev.
 wool     (Intercept)  3.42
 Residual             11.62
```

Notice that the degrees of freedom by default are adjusted using a Kenward–Roger approximation (provided that **pbkrtest** is installed). Unadjusted degrees of freedom are obtained with

```
> LSmeans(warp.mm, effect="tension", adjust.df=FALSE)

  estimate    se df t.stat   p.value   lwr   upr tension
1    36.39 3.653 49  9.961 2.288e-13 29.05 43.73       L
2    26.39 3.653 49  7.224 2.986e-09 19.05 33.73       M
3    21.67 3.653 49  5.931 2.986e-07 14.33 29.01       H
```

5.3 Generalized estimating equations

Lastly, for gee-type "models" we get

```
> library(geepack)
> warp.gee <- geeglm(breaks ~ tension, id=wool, family=poisson, data=warpbreaks)
> LSmeans(warp.gee, effect="tension")

  estimate      se z.stat    p.value   lwr   upr tension
1    3.594 0.15869  22.65 1.427e-113 3.283 3.905       L
2    3.273 0.06401  51.13  0.000e+00 3.147 3.398       M
3    3.076 0.09428  32.62 1.903e-233 2.891 3.261       H
```

```
> LSmeans(warp.gee, effect="tension", type="response")

  estimate    se z.stat   p.value   lwr   upr tension
1    36.39 5.775  22.65 1.427e-113 26.66 49.66       L
2    26.39 1.689  51.13  0.000e+00 23.28 29.92       M
3    21.67 2.043  32.62 1.903e-233 18.01 26.06       H
```

6 Miscellaneous

6.1 Under the hood

Under the hood, `LSmeans()` generates a contrast matrix

```
> K <- LSmatrix(warp.lm, effect="tension"); K

     (Intercept) woolB tensionM tensionH
[1,]           1   0.5        0        0
[2,]           1   0.5        1        0
[3,]           1   0.5        0        1
```

and passes this matrix onto `linest()`:

```
> linest( warp.lm, K=K )

  estimate    se df t.stat   p.value   lwr   upr tension
1    36.39 2.738 50 13.289 4.948e-18 30.89 41.89       L
2    26.39 2.738 50  9.637 5.489e-13 20.89 31.89       M
3    21.67 2.738 50  7.913 2.269e-10 16.17 27.17       H
```

6.2 Example: Non–estimable contrasts

Consider this highly unbalanced simulated dataset:

```
> head(dat.nst)

  AA BB CC        y
1  1  1  1 -0.06483
2  2  1  1 -0.31805
3  1  2  2 -0.85124
4  2  2  2 -0.37410
5  1  3  2  0.02159
6  2  3  2 -0.36949

> ftable(xtabs( ~ AA + BB + CC, data=dat.nst))

      CC 1 2 3 4
AA BB           
1  1     3 0 0 0
   2     0 1 1 1
   3     0 1 1 1
2  1     3 0 0 0
   2     0 1 1 1
   3     0 1 1 1
```

We have

```
> mod.nst  <- lm(y ~ AA + BB : CC, data=dat.nst)
> coef( mod.nst )
(Intercept)         AA2     BB1:CC1     BB2:CC1     BB3:CC1     BB1:CC2 
    -0.2118     -0.3513      0.1600          NA          NA          NA 
    BB2:CC2     BB3:CC2     BB1:CC3     BB2:CC3     BB3:CC3     BB1:CC4 
    -0.2252      0.2135          NA     -0.4421      1.1928          NA 
    BB2:CC4     BB3:CC4 
    -0.7133          NA 
```

In this case some of the `LSmeans` values are not estimable (see Section 6.3 for details):

```
> LSmeans(mod.nst, effect=c("BB", "CC"))
   estimate     se df  t.stat p.value     lwr    upr BB CC
1   -0.2274 0.3687 10 -0.6168  1.4489 -1.0489 0.5940  1  1
2        NA     NA NA      NA      NA      NA     NA  2  1
3        NA     NA NA      NA      NA      NA     NA  3  1
4        NA     NA NA      NA      NA      NA     NA  1  2
5   -0.6127 0.6386 10 -0.9595  1.6400 -2.0355 0.8101  2  2
6   -0.1739 0.6386 10 -0.2724  1.2091 -1.5968 1.2489  3  2
7        NA     NA NA      NA      NA      NA     NA  1  3
8   -0.8295 0.6386 10 -1.2990  1.7769 -2.2523 0.5933  2  3
9    0.8053 0.6386 10  1.2612  0.2359 -0.6175 2.2281  3  3
10       NA     NA NA      NA      NA      NA     NA  1  4
11  -1.1007 0.6386 10 -1.7237  1.8845 -2.5235 0.3221  2  4
12  -0.3874 0.6386 10 -0.6067  1.4424 -1.8102 1.0354  3  4
```

6.3 Handling non–estimability

The model matrix for the model in Section 6.2 does not have full column rank and therefore not all values are calculated by `LSmeans()`.

```
> X <- model.matrix( mod.nst ); as(X,"Matrix")
18 x 14 sparse Matrix of class "dgCMatrix"
                              
1  1 . 1 . . . . . . . . . . .
2  1 1 1 . . . . . . . . . . .
3  1 . . . . . 1 . . . . . . .
4  1 1 . . . . 1 . . . . . . .
5  1 . . . . . . 1 . . . . . .
6  1 1 . . . . . 1 . . . . . .
7  1 . 1 . . . . . . . . . . .
8  1 1 1 . . . . . . . . . . .
9  1 . . . . . . . . 1 . . . .
10 1 1 . . . . . . . 1 . . . .
11 1 . . . . . . . . . 1 . . .
12 1 1 . . . . . . . . 1 . . .
13 1 . 1 . . . . . . . . . . .
14 1 1 1 . . . . . . . . . . .
15 1 . . . . . . . . . . . 1 .
16 1 1 . . . . . . . . . . 1 .
17 1 . . . . . . . . . . . . 1
18 1 1 . . . . . . . . . . . 1
```

We consider a linear normal model, i.e. an n dimensional random vector $y = (y_i)$ for which $\mathbb{E}(y) = \mu = X\beta$ and $\mathbb{C}\text{ov}(y) = \sigma^2 I$ where X does not have full column rank We are interested in linear functions of β, say

$$c = k^\top \beta = \sum_j k_j \beta_j.$$

```
> K <- LSmatrix(mod.nst, effect="BB", at=list(CC=2));K
```

```
     (Intercept) AA2 BB1:CC1 BB2:CC1 BB3:CC1 BB1:CC2 BB2:CC2 BB3:CC2 BB1:CC3
[1,]           1 0.5       0       0       0       1       0       0       0
[2,]           1 0.5       0       0       0       0       1       0       0
[3,]           1 0.5       0       0       0       0       0       1       0
     BB2:CC3 BB3:CC3 BB1:CC4 BB2:CC4 BB3:CC4
[1,]       0       0       0       0       0
[2,]       0       0       0       0       0
[3,]       0       0       0       0       0
```

```
> LSmeans(mod.nst, K=K)
```

```
  estimate     se df  t.stat p.value    lwr    upr BB CC
1       NA     NA NA      NA      NA     NA     NA  1  2
2  -0.6127 0.6386 10 -0.9595   1.640 -2.035 0.8101  2  2
3  -0.1739 0.6386 10 -0.2724   1.209 -1.597 1.2489  3  2
```

A least squares estimate of β is

$$\hat{\beta} = G X^\top y$$

where G is a generalized inverse of $X^\top X$. Since the generalized inverse is not unique then neither is the estimate $\hat{\beta}$. One least squares estimate of β is

```
> XtXinv <- MASS::ginv(t(X)%*%X)
> bhat <- as.numeric(XtXinv %*% t(X) %*% dat.nst$y)
> zapsmall(bhat)
```

```
 [1] -0.1621 -0.3513  0.1103  0.0000  0.0000  0.0000 -0.2749  0.1638  0.0000
[10] -0.4918  1.1431  0.0000 -0.7630 -0.0497
```

Hence $\hat{c} = k^\top \hat{\beta}$ is in general not unique.

```
> K %*% bhat
```

```
        [,1]
[1,] -0.3377
[2,] -0.6127
[3,] -0.1739
```

However, for some values of k, the estimate $\hat{c}$ is unique (i.e. it does not depend on the choice of generalized inverse). Such linear functions are said to be estimable and can be described as follows:

All we specify with $\mu = X\beta$ is that μ is a vector in the linear subspace $L = C(X)$ where $C(X)$ denotes the column space of X. We can only learn about β through $X\beta$ so the only thing we can say something about is linear combinations $\rho^\top X\beta$. Hence we can only say something about $k^\top\beta$ if there exists ρ such that $k^\top\beta = \rho^\top X\beta$, i.e., if $k = X^\top\rho$, that is, if k is in the column space $C(X^\top)$ of $X^\top$. That is, if k is perpendicular to all vectors in the null space $N(X)$ of X. To check this, we find a basis B for $N(X)$. This can be done in many ways, for example via a singular value decomposition of X, i.e.

$$X = UDV^\top$$

A basis for $N(X)$ is given by those columns of V that corresponds to zeros on the diagonal of D.

```
> S<-svd(X)
> names(S)

[1] "d" "u" "v"

> B<-S$v[, S$d<1e-10, drop=FALSE ]; zapsmall(B) ## Basis for N(X)

         [,1]    [,2]    [,3]    [,4]    [,5] [,6]
 [1,]  0.3392 -0.0006  0.0997 -0.0043 -0.0023    0
 [2,]  0.0000  0.0000  0.0000  0.0000  0.0000    0
 [3,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
 [4,] -0.2727 -0.2494  0.9244 -0.0032 -0.0942    0
 [5,] -0.0727  0.9176  0.2509 -0.1669  0.2487    0
 [6,] -0.0019 -0.0951  0.0517  0.6615  0.7421    0
 [7,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
 [8,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
 [9,]  0.0001  0.2944  0.0193  0.7310 -0.6152    0
[10,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
[11,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
[12,]  0.0000  0.0000  0.0000  0.0000  0.0000   -1
[13,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0
[14,] -0.3392  0.0006 -0.0997  0.0043  0.0023    0

> zapsmall( rowSums(K%*%B) )

[1] 1.79 0.00 0.00
```

6.4 Pairwise comparisons

We will just mention that for certain other linear estimates, the matrix K can be generated automatically using `glht()` from the **multcomp** package. For example, pairwise comparisons of all levels of `tension` can be obtained with

```
> library("multcomp")
> g1 <- glht(warp.lm, mcp(tension="Tukey"))
> summary( g1 )

         Simultaneous Tests for General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts


Fit: lm(formula = breaks ~ wool + tension, data = warpbreaks)

Linear Hypotheses:
           Estimate Std. Error t value Pr(>|t|)
M - L == 0   -10.00       3.87   -2.58   0.0336 *
H - L == 0   -14.72       3.87   -3.80   0.0011 **
H - M == 0    -4.72       3.87   -1.22   0.4474
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)
```

The K matrix generated in this case is:

```
> K1 <- g1$linfct; K1
      (Intercept) woolB tensionM tensionH
M - L           0     0        1        0
H - L           0     0        0        1
H - M           0     0       -1        1
attr(,"type")
[1] "Tukey"
```