Redesign of lsmeans

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February 3, 2014

Introduction

Versions of lsmeans up through version 1.10 were based on a lot of "spaghetti code" that worked but was increasingly difficult to maintain. So starting with version 2.00, the package underwent a complete overhaul where the code is much more modular and extensible. These changes help make the package better prepared for future use.

Past users of lsmeans may use it in much the same ways as in the old version, but not entirely. And of course, that's the catch—especially when it comes to doing something later with an object created by the `lsmeans` function. The purpose of this document is to explain the changes that are being made before the package is released, so that users may be prepared for it.

Availability of old functionality

For a while, the lsmeans package will include a function `.old.lsmeans` which is the old version of `lsmeans` from version 1.10-4. Users should adapt to the new `lsmeans` function as quickly as possible. However, in a clutch, this old one may be used. We use it several tuimes in this diocument to illustrate the differences.

Changes that could break existing code that uses lsmeans

In a nutshell

If you have existing code that extracts or manipulates the result of `lsmeans` in its old manifestation (i.e. treats it as a list of `data.frames`s); or uses the arguments `cov.reduce`, `fac.reduce`, `conf`, `glhargs`, `lf`, or `mlf`, your code will break as-is. Details follow.

Returned objects

Probably the most problematic change for past users is that `lsmeans` used to return a list of `data.frame`s (except sometimes a `glht` object was thrown in). But now it returns a single object of a new class `lsmobj`, or a list thereof.

```
> library(lsmeans)
> ### OLD
> warp.lm <- lm(breaks ~ wool * tension, data = warpbreaks)
> warp.oldlsm <- .old.lsmeans(warp.lm, ~ tension | wool)
> class(warp.oldlsm)

[1] "lsm"  "list"

> class(warp.oldlsm[[1]])

[1] "data.frame.lsm" "data.frame"
```

```
> ### NEW
> warp.lsmobj <- lsmeans(warp.lm, ~ tension | wool)
> class(warp.lsmobj)

[1] "lsmobj"
```

Look at the results obtained the new way:

```
> warp.lsmobj

wool = A:
 tension   lsmean       SE df lower.CL upper.CL
 L       44.55556 3.646761 48 37.22325 51.88786
 M       24.00000 3.646761 48 16.66769 31.33231
 H       24.55556 3.646761 48 17.22325 31.88786

wool = B:
 tension   lsmean       SE df lower.CL upper.CL
 L       28.22222 3.646761 48 20.88992 35.55453
 M       28.77778 3.646761 48 21.44547 36.11008
 H       18.77778 3.646761 48 11.44547 26.11008

Confidence level used: 0.95
```

Unlike the old display (not shown), this one pays attention to the `| wool` part of the specification.

In the old version, users could access/manipulate the results by taking advantage of the fact that they inherited from `data.frame`:

```
> ### OLD
> warp.oldlsm[[1]]$lsmean

[1] 44.55556 24.00000 24.55556 28.22222 28.77778 18.77778

> Try <- function(expr) tryCatch(expr, error = function(e) cat("Oops!\n"))
> ### NEW
> Try(warp.lsmobj$lsmean)

Oops!
```

The `show` method for an `lsmobj` is `summary`, which indeed does produce an object that inherits from `data.frame`. So if you need to access values that you see, call `summary` first:

```
> ### NEW
> summary(warp.lsmobj)$lsmean

[1] 44.55556 24.00000 24.55556 28.22222 28.77778 18.77778
```

In casting to `data.frame`, note that the "by" variable (`wool` in this case) is included:

```
> as.data.frame(summary(warp.lsmobj))

  tension wool   lsmean       SE df lower.CL upper.CL
1       L    A 44.55556 3.646761 48 37.22325 51.88786
2       M    A 24.00000 3.646761 48 16.66769 31.33231
3       H    A 24.55556 3.646761 48 17.22325 31.88786
4       L    B 28.22222 3.646761 48 20.88992 35.55453
5       M    B 28.77778 3.646761 48 21.44547 36.11008
6       H    B 18.77778 3.646761 48 11.44547 26.11008
```

If there is also a contrast specification, then `lsmeans` does return a list (and not an extension thereof). But each element is of class `lsmobj`, not `data.frame`.

```
> ### NEW
> warp.l2 <- lsmeans(warp.lm, pairwise ~ tension)
> class(warp.l2)

[1] "list"

> sapply(warp.l2, class)

  lsmeans contrasts
 "lsmobj"  "lsmobj"
```

Changes to `cov.reduce` and `fac.reduce`

The `cov.reduce` and `fac.reduce` arguments to `lsmeans` required a second argument giving the name of the variable. This is awkward and, in the case of `fac.reduce`, doesn't even make sense if you think about it. But if you have existing code that uses these functions, you will have to change it.

In the new version, `cov.reduce` may be a function or a named list of functions of a single numeric variable. The default is `mean`. If it is a named list, then a covariate matching a name on the list is reduced using that function, and any mismatched covariates are reduced using `mean`. As before, `cov.reduce` may also be logical: `TRUE` is equivalent to `mean`, and `FALSE` is equivalent to `function(x) sort(unique(x))`.

`fac.reduce` must now be a function of one matrix argument. Its default is `function(X) apply(X, 2, mean)`. To override it (at least sensibly), you must provide a function that reduces the rows of the matrix into a single vector of the same length.

Arguments no longer provided

The `lsmeans` arguments `conf`, `glhargs`, `lf`, and `mlf` are no longer supported. The needs they serve are supported via `lsmobj` methods or slots.

Continuing with the `warp.lm` example and the returned object `warp.lsmobj`, the `conf` functionality is replaced by the `confint` method:

```
> confint(warp.lsmobj, level = .90)

wool = A:
 tension   lsmean       SE df lower.CL upper.CL
 L       44.55556 3.646761 48 38.43912 50.67199
 M       24.00000 3.646761 48 17.88356 30.11644
 H       24.55556 3.646761 48 18.43912 30.67199

wool = B:
 tension   lsmean       SE df lower.CL upper.CL
 L       28.22222 3.646761 48 22.10579 34.33866
 M       28.77778 3.646761 48 22.66134 34.89421
 H       18.77778 3.646761 48 12.66134 24.89421

Confidence level used: 0.9
```

The `glhargs` capability is replaced by a method for `glht` in the multcomp package:

```
> summary(glht(warp.lm, warp.lsmobj))

$`wool = A`

         Simultaneous Tests for General Linear Hypotheses
```

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

Linear Hypotheses:
       Estimate Std. Error t value Pr(>|t|)
L == 0   44.556      3.647  12.218   <1e-07 ***
M == 0   24.000      3.647   6.581   <1e-07 ***
H == 0   24.556      3.647   6.734   <1e-07 ***
---
Signif. codes:  0 Ś***Š 0.001 Ś**Š 0.01 Ś*Š 0.05 Ś.Š 0.1 Ś Š 1
(Adjusted p values reported -- single-step method)


$`wool = B`

         Simultaneous Tests for General Linear Hypotheses

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

Linear Hypotheses:
       Estimate Std. Error t value Pr(>|t|)
L == 0   28.222      3.647   7.739  < 1e-05 ***
M == 0   28.778      3.647   7.891  < 1e-05 ***
H == 0   18.778      3.647   5.149 1.36e-05 ***
---
Signif. codes:  0 Ś***Š 0.001 Ś**Š 0.01 Ś*Š 0.05 Ś.Š 0.1 Ś Š 1
(Adjusted p values reported -- single-step method)
```

In lieu of `lf`, simply access the `linfct` slot:

```
> warp.lsmobj@linfct

     (Intercept) woolB tensionM tensionH woolB:tensionM
[1,]           1     0        0        0              0
[2,]           1     0        1        0              0
[3,]           1     0        0        1              0
[4,]           1     1        0        0              0
[5,]           1     1        1        0              1
[6,]           1     1        0        1              0
     woolB:tensionH
[1,]              0
[2,]              0
[3,]              0
[4,]              0
[5,]              0
[6,]              1
```

The `mlm` argument was new and gave only rudementary support for multivariate responses. Now multivariate predictors cause `lsmeans` to create one or more additional factors that can be specified in the `lsmeans` specs. More on this later.

Corrections

A few bugs turned up in the course of disciovering that new results did not match old ones—and the new ones were right! Of cours, there could well be undiscovered new bugs.

Degrees of freedom

lsmeans uses the pbkrtest package to obtain degrees of freedom for models fitted using the lme4 package. These depend on both the adjusted and unadjusted covariance matrices, but it turns out that the old `lsmeans` supplied the adjusted one for both. This does not always make a difference:

```
> library(lme4)
> data(Oats, package = "nlme")
> Oats.lmer <- lmer(yield ~ factor(nitro) + Variety + (1|Block/Variety),
+     data = Oats, subset = -c(1,2,3,5,8,13,21,34,55))
> ### OLD
> .old.lsmeans(Oats.lmer, pairwise ~ Variety)

$`Variety lsmeans`
     Variety    lsmean       SE       df lower.CL upper.CL
 Golden Rain 105.24082 7.531769 8.458094 88.03491 122.4467
  Marvellous 108.46952 7.482684 8.277279 91.31451 125.6245
     Victory  96.93448 7.641696 8.793712 79.58575 114.2832

$`Variety pairwise differences`
                          estimate       SE       df  t.ratio
Golden Rain - Marvellous -3.228695 6.553864 9.509345 -0.49264
Golden Rain - Victory     8.306336 6.707951 9.617594  1.23828
Marvellous - Victory     11.535031 6.670503 9.637894  1.72926
                         p.value
Golden Rain - Marvellous 0.87645
Golden Rain - Victory    0.46005
Marvellous - Victory     0.24384
    p values are adjusted using the tukey method for 3 means

> ### NEW
> lsmeans(Oats.lmer, pairwise ~ Variety)

$lsmeans
 Variety        lsmean       SE   df lower.CL upper.CL
 Golden Rain 105.24082 7.531769 8.46 88.03692 122.4447
 Marvellous  108.46952 7.482684 8.28 91.31558 125.6234
 Victory      96.93448 7.641696 8.81 79.59000 114.2790

Confidence level used: 0.95

$contrasts
 contrast                  estimate       SE   df t.ratio p.value
 Golden Rain - Marvellous -3.228695 6.553864 9.56  -0.493  0.8764
 Golden Rain - Victory     8.306336 6.707951 9.80   1.238  0.4595
 Marvellous - Victory     11.535031 6.670503 9.80   1.729  0.2431

P value adjustment: tukey method for a family of 3 means
```

The discrepancies are not huge, but they are there. Without the `subset` that created unbalanced data, the results essentially agree.

Processing `at`

In models containing `factor` or `ordered` (like `Oats.lmer`), any `at` specification was ignored. The new version handles this correctly, including omitting inappropriate levels.

```
> ### OLD
> .old.lsmeans(Oats.lmer, ~ nitro, at = list(nitro = c(.1,.2,.3)))

$`nitro lsmeans`
 nitro    lsmean       SE       df  lower.CL  upper.CL
   0.0  78.89208 7.294425 7.775233  61.98609  95.79808
   0.2  97.03426 7.136318 7.182087  80.24589 113.82263
   0.4 114.19817 7.136234 7.183545  97.41067 130.98567
   0.6 124.06857 7.070283 6.953104 107.32712 140.81002

> ### NEW
> lsmeans(Oats.lmer, ~ nitro, at = list(nitro = c(.1,.2,.3)))

 nitro   lsmean       SE   df lower.CL upper.CL
   0.2 97.03426 7.136318 7.19 80.25017 113.8184

Confidence level used: 0.95
```

New object structure

The more recent vignettes for lsmeans have explained least-squares means as predictions on a "reference grid," or marginal averages thereof. By default, the reference grid consists of all combinations of factor levels, along with the averages of numeric predictors. But this can be changed by `at` or `cov.reduce`. The new design of lsmeans uses a reference-grid object explicitly. For example:

```
> (Oats.rg <- ref.grid(Oats.lmer))

'ref.grid' object with variables:
    nitro = 0.0, 0.2, 0.4, 0.6
    Variety = Golden Rain, Marvellous, Victory
    yield = response variable with mean 102.38

> Oats.quad <- update(Oats.lmer, yield ~ Variety + poly(nitro,2) + (1|Block/Variety))
> ref.grid(Oats.quad)

'ref.grid' object with variables:
    Variety = Golden Rain, Marvellous, Victory
    nitro = 0.31429
    yield = response variable with mean 102.38

> ref.grid(Oats.quad, at = list(nitro = c(.1,.2,.3)))

'ref.grid' object with variables:
    Variety = Golden Rain, Marvellous, Victory
    nitro = 0.1, 0.2, 0.3
    yield = response variable with mean 102.38
```

The `ref.grid` function calls two other functions, `recover.data` (to reproduce the dataset) and `lsm.basis` (to get the model matrix, coefficients, etc.), each of which has S3 methods for popular model objects like `lm`, `mlm`, `gls`, `lmer`, etc. This allows `ref.grid`'s capabilities to be easily extended to other model objects not yet supported. `ref.grid` serves as a constructor for an S4 object of class `ref.grid`, which encapsulates all the information needed to compute—and make inferences on—least-squares means, independently of the model object itself.

The `lsmeans` function now consists of S4 methods for a variety of signatures, one of which corresponds to the old version where `object` is a model object and `specs` is a formula. So, for example, we may call `lsmeans` with an existing `ref.grid`, and provide specifications in place of the old formula interface:

```
> (Oats.lsm <- lsmeans(Oats.rg, "nitro", by = "Variety"))

Variety = Golden Rain:
 nitro    lsmean       SE    df  lower.CL  upper.CL
   0.0  80.58463 8.194841 11.70  62.67900  98.49026
   0.2  98.72681 8.020181 10.87  81.04772 116.40590
   0.4 115.89072 8.098937 11.27  98.11661 133.66483
   0.6 125.76112 8.099519 11.21 107.97560 143.54664

Variety = Marvellous:
 nitro    lsmean       SE    df  lower.CL  upper.CL
   0.0  83.81333 8.152141 11.54  65.97316 101.65349
   0.2 101.95551 8.083595 11.19  84.20096 119.71005
   0.4 119.11941 8.005137 10.80 101.45952 136.77931
   0.6 128.98982 7.990096 10.71 111.34490 146.63473

Variety = Victory:
 nitro    lsmean       SE    df  lower.CL  upper.CL
   0.0  72.27830 8.376248 12.49  54.10738  90.44922
   0.2  90.42048 8.201327 11.58  72.47869 108.36226
   0.4 107.58438 8.200668 11.57  89.64360 125.52517
   0.6 117.45478 8.041848 10.91  99.73618 135.17339

Confidence level used: 0.95
```

Moreover, `lsmobj` is in fact an extension of `ref.grid`, and we can use it as such:

```
> str(Oats.lsm)

'ref.grid' object with variables:
    nitro = 0.0, 0.2, 0.4, 0.6
    Variety = Golden Rain, Marvellous, Victory

> (Oats.n <- lsmeans(Oats.lsm, "nitro"))

 nitro    lsmean       SE   df  lower.CL  upper.CL
   0.0  78.89208 7.294425 7.78  61.98918  95.79499
   0.2  97.03426 7.136318 7.19  80.25017 113.81836
   0.4 114.19817 7.136234 7.19  97.41441 130.98193
   0.6 124.06857 7.070283 6.95 107.32782 140.80933

Confidence level used: 0.95
```

Slots

The classes `ref.grid` and `lsmobj` are essentially identical in structure, with `lsmobj` being a minor extension with the same slots.

```
> slotNames(Oats.lsm)

 [1] "model.info" "roles"      "grid"       "levels"     "matlevs"
 [6] "linfct"     "bhat"       "nbasis"     "V"          "dffun"
[11] "dfargs"     "misc"
```

`model.info` has the call and terms. `roles` lists the names of predictors and responses. `grid` is a `data.frame` consisting of all combinations of the variables in the list `levels`. The rows of `grid` go in one-to-one correspondence with those of `linfct`, which contains the linear coefficients associated with each LS mean (or

reference-grid combination). `matlevs` has summary information for any matrices in the dataset. `bhat` holds the regression coefficients. `nbasis` holds information for determining non-estimability in rank-deficient situations. `V` is the covariance matrix for `bhat`. `ddfm` is a function to return the degrees of freedom for a linear function of `bhat`. It is passed the contents of the list `misc`, thus allowing for additional parameters. `misc` also is used for bookkeeping tasks such as remembering `by` variables, labels, `adjust` settings, etc.

New functions and methods

There are numerous methods for `lsmobj` objects. The `summary` method produces what you see in a listing, and is an extension of `data.frame` but it is printed with different formatting and with added messages about adjustments, confidence levels, etc. You can also display the results differently. For example:

```
> summary(Oats.lsm, by = "nitro")
```

(results not shown) will group the `Variety` means for each `nitro` rather than the way it is displayed above. There is also and `infer` argument for flagging whether confidence intervals and/or tests are displayed:

```
> summary(Oats.n, infer = c(TRUE,TRUE))

 nitro    lsmean       SE   df  lower.CL  upper.CL t.ratio p.value
   0.0  78.89208 7.294425 7.78  61.98918  95.79499  10.815  <.0001
   0.2  97.03426 7.136318 7.19  80.25017 113.81836  13.597  <.0001
   0.4 114.19817 7.136234 7.19  97.41441 130.98193  16.003  <.0001
   0.6 124.06857 7.070283 6.95 107.32782 140.80933  17.548  <.0001

Confidence level used: 0.95
```

Most other methods are S3 ones, as those are suitable to our needs and often extend existing S3 methods. The `glht` methodis illustrated earlier in this document. The `confint` and `test` methods are really courtesy methods for `summary` with argument `infer` set to `c(TRUE,FALSE)` and `c(FALSE,TRUE)` respectively.

An important method is `contrast`:

```
> (warp.con <- contrast(warp.lsmobj, method = "poly"))

wool = A:
 contrast    estimate       SE df t.ratio p.value
 linear    -20.000000 5.157299 48  -3.878  0.0003
 quadratic  21.111111 8.932705 48   2.363  0.0222

wool = B:
 contrast    estimate       SE df t.ratio p.value
 linear     -9.444444 5.157299 48  -1.831  0.0733
 quadratic -10.555556 8.932705 48  -1.182  0.2432
```

These methods all return new objects of class `lsmobj`. Hence they may be further analyzed or reanalyzed. For example, suppose we now want to compare the two linear and the two quadratic contrasts in the above:

```
> contrast(warp.con, "revpairwise", by = "contrast")

contrast = linear:
 contrast1  estimate        SE df t.ratio p.value
 B - A       10.55556  7.293523 48   1.447  0.1543

contrast = quadratic:
 contrast1  estimate        SE df t.ratio p.value
 B - A     -31.66667 12.632752 48  -2.507  0.0156
```

The `pairs` method is equivalent to `contrast` with `method = "pairwise"`. Closely related is the new `cld` method which produces a compact letter display for which pairwise comparisons are nonsignificant:

```
> cld(Oats.n, sort = FALSE)

 nitro    lsmean       SE   df  lower.CL  upper.CL .group
   0.0  78.89208 7.294425 7.78  61.98918  95.79499  1
   0.2  97.03426 7.136318 7.19  80.25017 113.81836   2
   0.4 114.19817 7.136234 7.19  97.41441 130.98193    3
   0.6 124.06857 7.070283 6.95 107.32782 140.80933    3

Confidence level used: 0.95
P value adjustment: tukey method for a family of 4 means
significance level used: alpha = 0.05
```

Finally, there is the `lstrends` function for estimating fitted trends of a covariate that interacts with a factor. Like the other methods, it returns an `lsmobj` object, subject to further analysis. To illustrate, the R-provided dataset `ChickWeight` has data on growth of chicks given different diets. We will fit a random-slopes model and compare the mean slope for each diet. In addition, we'll chose symbols for the display that mimic the grouping lines that some people use.

```
> chick.lmer <- lmer(weight ~ Time * Diet + (0 + Time | Chick), data = ChickWeight)
> chick.lst <- lstrends(chick.lmer, ~ Diet, var = "Time")
> cld(chick.lst, Letters = "|||||")

 Diet Time.trend        SE    df lower.CL  upper.CL .group
 1      6.338552 0.6105022 49.85 5.112234  7.564871  |
 2      8.609136 0.8380228 48.28 6.924433 10.293840  ||
 4      9.555825 0.8392650 48.56 7.868877 11.242774   |
 3     11.422871 0.8380228 48.28 9.738167 13.107575   |

Confidence level used: 0.95
P value adjustment: tukey method for a family of 4 means
significance level used: alpha = 0.05
```

Chicks fed with Diet 3 seem to grow faster than chicks with the other diets, and Diet 1 is the worst.

`lstrends` uses a difference quotient to do its work, and there is an optional argument `delta` that can be used to change its increment. It requires a model object—there is no `ref.grid` method for it. The `var` argument may imply a function call, i.e. `var=sqrt(Time)`, in which case the chain rule is applied.

Support for multivariate models

lsmeans now provides for models with multivariate responses, by way of defining factor levels that index the responses. Thus, linear functions of the multivariate response are available for inference. As an example, consider the package-provided dataset `MOats`, which is the same as `Oats` except that each observation is a whole plot with the yields for the four `nitro` levels as responses.

```
> head(MOats)

      Variety Block yield.1 yield.2 yield.3 yield.4
1     Victory     I     111     130     157     174
2 Golden Rain     I     117     114     161     141
3  Marvellous     I     105     140     118     156
4     Victory    II      61      91      97     100
5 Golden Rain    II      70     108     126     149
6  Marvellous    II      96     124     121     144
```

Let's fit a model and obtain the reference grid:

```
> MOats.mlm <- lm(yield ~ Block + Variety, data = MOats)
> (MOats.rg <- ref.grid(MOats.mlm, mult.levs = list(nitro = c(0,.2,.4,.6))))

'ref.grid' object with variables:
    Block = VI, V, III, IV, II, I
    Variety = Golden Rain, Marvellous, Victory
    nitro = multivariate response levels: 0.0, 0.2, 0.4, 0.6
    yield = multivariate response with means:
         79.389,  98.889, 114.222, 123.389
```

(The `mult.levs` argument gives a name and levels for later use; if it had been absent, the multivariate response would have been named `rep.meas`, with levels `1,2,3,4`.)

We may now use `nitro` just like we would in the univariate case:

```
> lsmeans(MOats.rg, ~ nitro)

 nitro    lsmean       SE df  lower.CL upper.CL
   0.0  79.38889 3.198862 10  72.26138  86.5164
   0.2  98.88889 3.811694 10  90.39591 107.3819
   0.4 114.22222 5.020268 10 103.03637 125.4081
   0.6 123.38889 4.216517 10 113.99390 132.7839

Confidence level used: 0.95

> lsmeans(MOats.rg, ~ Variety)

 Variety       lsmean       SE df lower.CL upper.CL
 Golden Rain 104.5000 5.005541 10 93.34696 115.6530
 Marvellous  109.7917 5.005541 10 98.63863 120.9447
 Victory      97.6250 5.005541 10 86.47196 108.7780

Confidence level used: 0.95
```

We can verify that the latter is exactly the same as if we had averaged the responses:

```
> MOats <- transform(MOats, avg.yield = apply(yield, 1, mean))
> lsmeans(lm(avg.yield ~ Block + Variety, data = MOats), ~ Variety)

 Variety       lsmean       SE df lower.CL upper.CL
 Golden Rain 104.5000 5.005541 10 93.34696 115.6530
 Marvellous  109.7917 5.005541 10 98.63863 120.9447
 Victory      97.6250 5.005541 10 86.47196 108.7780

Confidence level used: 0.95
```