emmeans: Estimated marginal means

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Estimated marginal means (EMMs, previously known as least-squares means in the context of traditional regression models) are derived by using a model to make predictions over a regular grid of predictor combinations (called a reference grid).

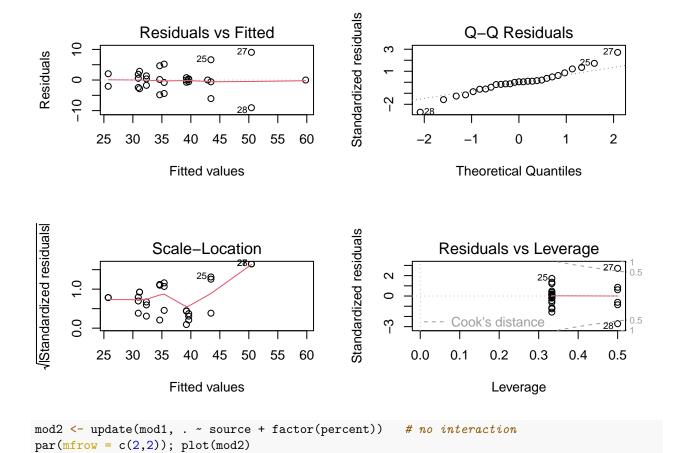
The pigs dataset

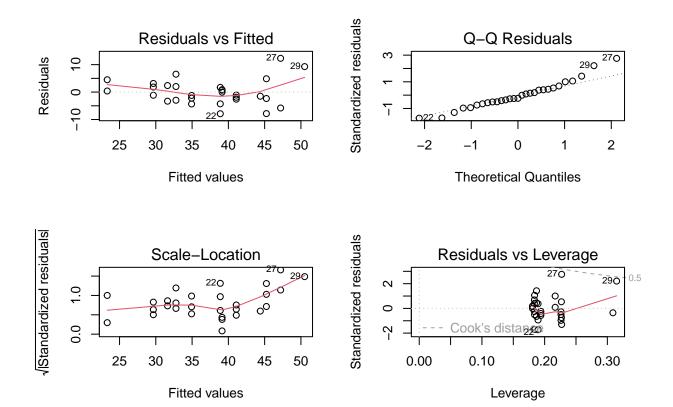
Initial model fitting

Consider the pigs dataset provided with the package (help("pigs") provides details). These data come from an experiment where pigs are given different percentages of protein (percent) from different sources (source) in their diet, and later we measured the concentration (conc) of leucine. The percent values are quantitative, but we chose those particular values deliberately, and (at least initially) we want separate estimates at each percent level; that is, we want to view percent as a factor, not a quantitative predictor.

As discussed, our first task is to come up with a good model. Doing so requires a lot of skill, and we don't want to labor too much over the details; you really need other references to deal with this aspect adequately. But we will briefly discuss five models and settle on one of them:

```
mod1 <- lm(conc ~ source * factor(percent), data = pigs)
par(mfrow = c(2,2)); plot(mod1)</pre>
```





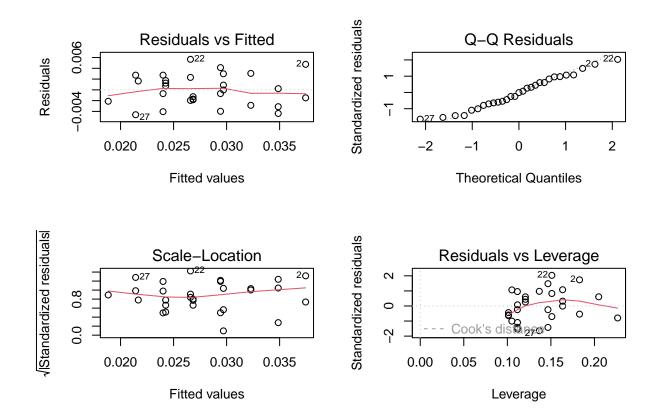
<pre>map_dfr(list(mod1, mod2), glance)</pre>	
r.squared adj.r.squared sigma statistic p.value df	logLik AIC BIC deviancedf.residual nobs
0.808381 6 .6843933 4.7160246.5198190.00034171	- 182.7661200.5409378.0950 17 29
0.699672 8 .6343843 5.07592610.71662 8 .00002075	78.38304 - 183.7977193.368&592.5957 23 29 84.89886

These models have R2 values of 0.808 and 0.700, and adjusted R2 values of 0.684 and 0.634. mod1 is preferable to mod2, suggesting we need the interaction term. However, a residual-vs-predicted plot of mod2 has a classic "horn" shape (curving and fanning out), indicating a situation where a response transformation might help better than including the interaction.

It turns out that an inverse transformation, (1/conc) really serves us well. (Perhaps this isn't too surprising, as concentrations are typically determined by titration, in which the actual measurements are volumes; and these are reciprocally related to concentrations, i.e., amounts per unit volume.)

So here are three more models:

```
mod3 <- update(mod1, inverse(conc) ~ .)
mod4 <- update(mod2, inverse(conc) ~ .)  # no interaction
mod5 <- update(mod4, . ~ source + percent)  # linear term for percent
par(mfrow = c(2,2)); plot(mod5)</pre>
```



r.squaredadj.r.squaredsigma statistic p.value df logLik AIC BIC deviance df.residualnobs 0.808381**6**.6843933 4.716024**6**.5198190.000341**7**1 182.7661200.5409378.0950000 17 29 78.38304 0.699672**8**.6343843 5.075926**5**0.71662**8**.00002075 183.7977193.3688592.5956760 23 29 84.89886 133.86797 29 0.817592**8**.6995647 0.003125**9**.9270990.000234**9**1 0.0001661 17 241.7359223.9611 0.7866456.7402641 0.00290656.960360.00000055 0.0001943 29 131.59563 23 249.1912239.6202 0.7487290.7185767 0.00302524.831410.00000013 129,22377 0.0002288 25 29

(Note: We could have used 1/conc as the response variable, but emmeans provides an equivalent inverse() function that will prove more advantageous later.) The residual plots for these models look a lot more like a random scatter of points (and that is good). The R2 values for these models are 0.818, 0.787, and 0.749, respectively; and the adjusted R2s are 0.700, 0.740, and 0.719. mod4 has the best adjusted R2 and will be our choice.

248.4475241.6111

Estimated marginal means

map dfr(list(mod1, mod2, mod3, mod4, mod5), glance)

```
(EMM.source <- emmeans(mod4, "source"))
                        SE df lower.CL upper.CL
##
   source emmean
## fish
           0.0337 0.000926 23 0.0318
                                        0.0356
           0.0257 0.000945 23
                                0.0237
                                         0.0276
## soy
## skim
           0.0229 0.000994 23 0.0208
                                        0.0249
## Results are averaged over the levels of: percent
## Results are given on the inverse (not the response) scale.
## Confidence level used: 0.95
(EMM.percent <- emmeans(mod4, "percent"))</pre>
## percent emmean
                         SE df lower.CL upper.CL
##
         9 0.0322 0.001032 23
                                 0.0301
                                          0.0344
##
         12 0.0270 0.000969 23
                                 0.0250
                                          0.0290
##
         15 0.0263 0.001104 23
                                 0.0240
                                          0.0286
##
         18 0.0241 0.001337 23
                                 0.0213
                                          0.0268
## Results are averaged over the levels of: source
## Results are given on the inverse (not the response) scale.
## Confidence level used: 0.95
Calling tidy() (from broom) on the object will put it into a beautiful data frame. we could make a plot.
```

percent	estimate	std.error	df	statistic	p.value
9	0.0322476	0.0010322	23	31.24043	0
12	0.0270034	0.0009688	23	27.87243	0
15	0.0262765	0.0011040	23	23.80154	0
18	0.0240784	0.0013370	23	18.00911	0

Comparison to ordinary means

tidy(EMM.percent)

Let's compare these with the ordinary marginal means (OMMs) on inverse(conc):

```
with(pigs, tapply(inverse(conc), source, mean))
## fish soy skim
## 0.03331687 0.02632333 0.02372024

Can I write the above ordinary means in Tidyverse/dplyr language?
pigs %>%
  mutate(conc = 1/conc) %>%
  summarize(mean = mean(conc), .by = source)
```

source	mean
fish	0.0333169
soy	0.0263233
skim	0.0237202

```
with(pigs, tapply(inverse(conc), percent, mean))
## 9 12 15 18
## 0.03146170 0.02700341 0.02602757 0.02659336
pigs %>%
   mutate(conc = 1/conc) %>%
   summarize(mean = mean(conc), .by = percent)
```

percent	mean
9	0.0314617
12	0.0270034
15	0.0260276
18	0.0265934

Both sets of OMMs are vaguely similar to the corresponding EMMs. However, please note that the EMMs for percent form a decreasing sequence, while the the OMMs decrease but then increase at the end.

The reference grid, and definition of EMMs

Estimated marginal means are defined as marginal means of model predictions over the grid comprising all factor combinations – called the reference grid. For the example at hand, the reference grid is

```
(RG <- expand.grid(source = levels(pigs$source), percent = unique(pigs$percent)))
```

source	percent
fish	9
soy	9
skim	9
fish	12
soy	12
skim	12
fish	15
soy	15
skim	15
fish	18
soy	18
skim	18

To get the EMMs, we first need to obtain predictions on this grid:

```
(preds <- matrix(predict(mod4, newdata = RG), nrow = 3))

##      [,1]      [,2]      [,3]      [,4]

## [1,] 0.03853514 0.03329091 0.03256404 0.03036586

## [2,] 0.03050486 0.02526063 0.02453376 0.02233558

## [3,] 0.02770292 0.02245869 0.02173182 0.01953364

then obtain the marginal means of these predictions:

apply(preds, 1, mean)  # row means -- for source</pre>
```

```
## [1] 0.03368899 0.02565870 0.02285677
```

```
apply(preds, 2, mean) # column means -- for percent
```

```
## [1] 0.03224764 0.02700341 0.02627654 0.02407836
```

These marginal averages match the EMMs obtained earlier via emmeans().

Now let's go back to the comparison with the ordinary marginal means. The source levels are represented by the columns of pred; and note that each row of pred is a decreasing set of values. So it is no wonder that the marginal means – the EMMs for source – are decreasing. That the OMMs for percent do not behave this way is due to the imbalance in sample sizes:

```
with(pigs, table(source, percent))
```

```
## percent
## source 9 12 15 18
## fish 2 3 2 3
## soy 3 3 3 1
## skim 3 3 2 1
```

This shows that the OMMs of the last column give most of the weight (3/5) to the first source, which tends to have higher inverse(conc), making the OMM for 18 percent higher than that for 15 percent, even though the reverse is true with every level of source. This kind of disconnect is an example of Simpson's paradox, in which a confounding factor can distort your findings. The EMMs are not subject to this paradox, but the OMMs are, when the sample sizes are correlated with the expected values.

In summary, we obtain a references grid of all factor combinations, obtain model predictions on that grid, and then the expected marginal means are estimated as equally-weighted marginal averages of those predictions. Those EMMs are not subject to confounding by other factors, such as might happen with ordinary marginal means of the data. Moreover, unlike OMMs, EMMs are based on a model that is fitted to the data.