Validation of VetResearchLMM

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1 Abstract

The engine of **VetResearchLMM** is checked in two ways: against every number the book prints for the data it gives in full, and against established R packages on unbalanced data. The book's numbers are reproduced (one printed value is truncated), and the likelihoods, variance components, Satterthwaite and Kenward-Roger degrees of freedom and least-squares means agree with **lme4**, **lmerTest**, **pbkrtest**, **nlme** and **emmeans**.

2 The published values

```
ref <-
  vlm_reference(
      source   = NULL
    , evaluate = TRUE
    , level    = 1
    )
c(values = nrow(ref), agree = sum(ref$agrees))
```

```
values  agree
   116     87
```

```
ref[agrees == FALSE, c("id", "value", "computed", "note")]
```

```
            id   value computed
 1: e2431_sire  3.6850 3.685537
 2:   e2511_b1 17.1300       NA
 3:   e2511_v1  1.2700       NA
 4:   e2511_b2  7.1500       NA
 5:   e2511_v2  0.8300       NA
 6:   e2511_b4  4.3500       NA
 7:   e2511_v4  0.7000       NA
 8:   e2511_b6 -3.1800       NA
 9:   e2511_v6  1.4000       NA
10:   e2521_m1 25.4500       NA
11:   e2521_m2 24.2800       NA
12:   e2521_m3 21.4800       NA
13:   e2521_m4 17.1300       NA
14:    e2521_v  1.2700       NA
15: e2531_est1 19.3100       NA
16: e2531_var1  1.0975       NA
17:  e2531_df1  6.2000       NA
18: e2531_var2  0.4780       NA
19:  e2531_df2  5.0000       NA
20: e2531_est3 21.4800       NA
21: e2531_var3  1.2720       NA
22:  e2531_df3  8.2000       NA
23: e2531_est4  4.3500       NA
24: e2531_var4  0.6980       NA
25:  e2531_df4 10.0000       NA
26:  e2541_var  0.1750       NA
27:     e261_F 31.2000       NA
28:   e261_ddf  7.1400       NA
29:     e261_p  0.0002       NA
            id   value computed
                                                                      note
 1: the book truncates 3.6855 (also given by lme4 and nlme) to 3.685
 2:
 3:
 4:
 5:
 6:
 7:
 8:
 9:
10:
11:
```

12:
13:
14:
15:
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21:
22:
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26:
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28:
29:

note

3 Against other packages

These checks run in the tests of the package (`tests/testthat/test-engine.R`) when the packages are installed.

```
d <- ex31
d$cell <- interaction(d$drug, d$dose, drop = TRUE)
fm <-
  vlm_fit(
      fixed    = PCV2 ~ drug + drug:dose
    , data     = ex31
    , random   = ~ drug:herd
    , repeated = NULL
    , method   = c("REML", "ML", "Type3")
    , ddfm     = "satterth"
    , type     = 3
    , class    = c("herd", "dose")
    , bound    = TRUE
    , control  = list()
    )
lt <- lmerTest::lmer(formula = PCV2 ~ 0 + cell + (1 | drug:herd), data =
 ↪  d)
ct <- lmerTest::contest(lt, rbind(c(0.5, -1, 0.5)), joint = TRUE)
data.frame(package = c("VetResearchLMM", "lmerTest"), F =
 ↪  c(fm$tests$F[1L], ct[["F value"]]),
           den_df = c(fm$tests$den_df[1L], ct[["DenDF"]]))
```

```
         package           F   den_df
1 VetResearchLMM 0.001544608 10.08194
2       lmerTest 0.001544636 10.08200
```

```
ar <-
  vlm_fit(
      fixed    = PCV ~ breed + breed:time
    , data     = ex33
    , random   = NULL
    , repeated = vlm_repeated(
          type    = c("vc", "cs", "ar1", "sp_pow", "un")[4]
        , subject = ~ animal_id:breed
        , order   = ~ time
        )
    , method   = c("REML", "ML", "Type3")
    , ddfm     = c("default", "contain", "residual", "betwithin",
 ↪  "satterth", "kr")
    , type     = 3
    , class    = NULL
    , bound    = TRUE
    , control  = list()
    )
ex33$sub <- interaction(ex33$animal_id, ex33$breed, drop = TRUE)
g <-
  nlme::gls(
      model       = PCV ~ breed + breed:time
    , data        = ex33
    , correlation = nlme::corExp(form = ~ time | sub)
    , method      = "REML"
    )
c(VetResearchLMM = -ar$fit$value[1L] / 2, nlme =
 ↪  as.numeric(stats::logLik(g)))
```

```
VetResearchLMM           nlme
     -414.6905       -414.6905
```

4 Differences from the book

- **Data.** Version 1.1.0 had three typing errors in `ex33` (two measurement days and a trailing space in an animal identifier); with them, the variances of Example 3.3 were 5.522 and 4.943 instead of the printed 5.478 and 4.965. Version 2.0.0 corrects them.
- **Containment degrees of freedom of random coefficient models.** For Model 3 of Example 3.3, SAS 6.12 (used by the book) gives the fixed effects 144 or 10 degrees of freedom by rules that later versions of SAS changed; the package follows the current containment rule (the random effect `time` per animal contains `breed*time`), which gives 10. The estimates and standard errors agree.

- **Information criteria.** SAS 6.12 printed the "larger is better" forms $\ell - d$ and $\ell - \frac{d}{2}\log(N - P)$; they are given next to the current forms.
- **Rounding.** The book rounds or truncates some numbers computed from rounded variance components (for example 1.0975 and 0.698 in Example 2.5.3.1); they are compared at the precision that the book's own computation supports.