Translating lme4 models to sommer

Giovanny Covarrubias-Pazaran

2021-12-14

The sommer package was developed to provide R users a powerful and reliable multivariate mixed model solver. The package is focused on problems of the type p > n (more effects to estimate than observations) and its core algorithm is coded in C++ using the Armadillo library. This package allows the user to fit mixed models with the advantage of specifying the variance-covariance structure for the random effects, and specifying heterogeneous variances, and obtaining other parameters such as BLUPs, BLUEs, residuals, fitted values, variances for fixed and random effects, etc.

The purpose of this vignette is to show how to translate the syntax formula from lme4 models to sommer models. Feel free to remove the comment marks from the lme4 code so you can compare the results.

- 1) Random slopes with same intercept
- 2) Random slopes and random intercepts (without correlation)
- 3) Random slopes and random intercepts (with correlation)
- 4) Random slopes with a different intercept
- 5) Other models not available in lme4

1) Random slopes

This is the simplest model people use when a random effect is desired and the levels of the random effect are considered to have the same intercept.

```
# install.packages("lme4")
# library(lme4)
library(sommer)
data(DT_sleepstudy)
DT <- DT_sleepstudy
###########
## lme4
###########
# fm1 <- lmer(Reaction ~ Days + (1 | Subject), data=DT)
# summary(fm1) # or vc <- VarCorr(fm1); print(vc,comp=c("Variance"))</pre>
# Random effects:
# Groups Name
                        Variance Std.Dev.
# Subject (Intercept) 1378.2 37.12
                                 30.99
# Residual
                         960.5
# Number of obs: 180, groups: Subject, 18
###########
## sommer
###########
fm2 <- mmer(Reaction ~ Days,
            random= ~ Subject,
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

```
## VarComp VarCompSE Zratio Constraint
## Subject.Reaction-Reaction 1377.9758 505.0776 2.728246 Positive
## units.Reaction-Reaction 960.4705 107.0638 8.971013 Positive
```

2) Random slopes and random intercepts (without correlation)

This is the a model where you assume that the random effect has different intercepts based on the levels of another variable. In addition the | | in lme4 assumes that slopes and intercepts have no correlation.

```
###########
## lme4
###########
# fm1 <- lmer(Reaction ~ Days + (Days | | Subject), data=DT)
# summary(fm1) # or vc <- VarCorr(fm1); print(vc,comp=c("Variance"))</pre>
# Random effects:
# Groups
             Name
                         Variance Std. Dev.
# Subject
             (Intercept) 627.57 25.051
                                   5.988
# Subject.1 Days
                          35.86
# Residual
                         653.58
                                  25.565
# Number of obs: 180, groups: Subject, 18
##########
## sommer
###########
fm2 <- mmer(Reaction ~ Days,</pre>
            random= ~ Subject + vs(Days, Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

```
## Subject.Reaction-Reaction 627.54087 283.52939 2.213319 Positive ## Days:Subject.Reaction-Reaction 35.86008 14.53187 2.467686 Positive ## units.Reaction-Reaction 653.58305 76.72711 8.518281 Positive
```

Notice that Days is a numerical (not factor) variable.

3) Random slopes and random intercepts (with correlation)

This is the a model where you assume that the random effect has different intercepts based on the levels of another variable. In addition a single | in lme4 assumes that slopes and intercepts have a correlation to be estimated.

```
##########
## lme4
# fm1 <- lmer(Reaction ~ Days + (Days | Subject), data=DT)
# summary(fm1) # or # vc <- VarCorr(fm1); print(vc,comp=c("Variance"))</pre>
# Random effects:
# Groups
          Name
                        Variance Std. Dev. Corr
# Subject
           (Intercept) 612.10
                                 24.741
#
                         35.07
                                  5.922
                                          0.07
                        654.94
                                 25.592
# Number of obs: 180, groups: Subject, 18
###########
## sommer
```

```
###########
## no equivalence in sommer to find the correlation between the 2 vc
## this is the most similar which is equivalent to (intercept || slope)
fm2 <- mmer(Reaction ~ Days,</pre>
           random= ~ Subject + vs(Days, Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
##
                                    VarComp VarCompSE
                                                        Zratio Constraint
                                  627.54087 283.52939 2.213319
## Subject.Reaction-Reaction
                                                                  Positive
## Days:Subject.Reaction-Reaction 35.86008 14.53187 2.467686
                                                                  Positive
## units.Reaction-Reaction
                                  653.58305 76.72711 8.518281
                                                                 Positive
```

4) Random slopes with a different intercept

This is the a model where you assume that the random effect has different intercepts based on the levels of another variable but there's not a main effect. The 0 in the intercept in lme4 assumes that random slopes interact with an intercept but without a main effect.

```
###########
## lme4
###########
# fm1 <- lmer(Reaction ~ Days + (0 + Days | Subject), data=DT)
# summary(fm1) # or vc <- VarCorr(fm1); print(vc,comp=c("Variance"))</pre>
# Random effects:
# Groups
          Name Variance Std.Dev.
# Subject Days 52.71 7.26
# Residual
               842.03 29.02
# Number of obs: 180, groups: Subject, 18
##########
## sommer
###########
fm2 <- mmer(Reaction ~ Days,</pre>
           random= ~ vs(Days, Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
##
                                    VarComp VarCompSE
                                                        Zratio Constraint
## Days:Subject.Reaction-Reaction 52.70946 19.09984 2.759681
                                                                 Positive
```

4) Other models available in sommer but not in lme4

units.Reaction-Reaction

One of the strengths of sommer is the availability of other variance covariance structures. In this section we show 4 models available in sommer that are not available in lme4 and might be useful.

842.02736 93.84640 8.972399

Positive

VarComp VarCompSE Zratio Constraint

```
## 0:Subject.Reaction-Reaction 139.5473
                                          399.5095 0.3492967
                                                                Positive
## 1:Subject.Reaction-Reaction 196.8544
                                          411.8262 0.4780037
                                                                Positive
                                          365.3178 0.0000000
## 2:Subject.Reaction-Reaction
                                  0.0000
                                                                Positive
## 3:Subject.Reaction-Reaction 556.0773
                                          501.2665 1.1093445
                                                                Positive
## 4:Subject.Reaction-Reaction 855.2104
                                          581.8190 1.4698910
                                                                Positive
## 5:Subject.Reaction-Reaction 1699.4269
                                          820.4561 2.0713197
                                                                Positive
## 6:Subject.Reaction-Reaction 2910.8975 1175.7872 2.4757011
                                                                Positive
                                                                Positive
## 7:Subject.Reaction-Reaction 1539.6201 779.1437 1.9760413
## 8:Subject.Reaction-Reaction 2597.5337 1089.4522 2.3842568
                                                                Positive
## 9:Subject.Reaction-Reaction 3472.7108 1351.5702 2.5693899
                                                                Positive
## units.Reaction-Reaction
                                879.6958
                                          247.4680 3.5547862
                                                                Positive
## unstructured model
fm2 <- mmer(Reaction ~ Days,</pre>
            random= ~ vs(us(Daysf), Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

```
VarComp VarCompSE
                                                         Zratio Constraint
## 0:Subject.Reaction-Reaction
                                  402.6286
                                            572.0867 0.7037894
                                                                  Positive
## 1:0:Subject.Reaction-Reaction 1022.5098
                                            393.6922 2.5972314
                                                                  Unconstr
## 1:Subject.Reaction-Reaction
                                  417.6460
                                            521.3722 0.8010515
                                                                  Positive
## 2:0:Subject.Reaction-Reaction 540.3746
                                            287.1704 1.8817210
                                                                  Unconstr
## 2:1:Subject.Reaction-Reaction 828.5156
                                            325.7576 2.5433499
                                                                  Unconstr
## 2:Subject.Reaction-Reaction
                                    0.0000
                                            509.8962 0.0000000
                                                                  Positive
## 3:0:Subject.Reaction-Reaction 798.3750
                                            397.0884 2.0105726
                                                                  Unconstr
## 3:1:Subject.Reaction-Reaction 1137.3863
                                            443.9056 2.5622256
                                                                  Unconstr
## 3:2:Subject.Reaction-Reaction 1057.0708
                                            385.9026 2.7392162
                                                                  Unconstr
## 3:Subject.Reaction-Reaction
                                  760.2469
                                            436.7463 1.7407060
                                                                  Positive
## 4:0:Subject.Reaction-Reaction 757.8909
                                            411.2464 1.8429119
                                                                  Unconstr
## 4:1:Subject.Reaction-Reaction 1039.6832
                                            447.5192 2.3232148
                                                                  Unconstr
## 4:2:Subject.Reaction-Reaction 911.1369
                                            377.9651 2.4106377
                                                                  Unconstr
## 4:3:Subject.Reaction-Reaction 1590.6778
                                            566.5376 2.8077180
                                                                  Unconstr
## 4:Subject.Reaction-Reaction
                                  957.1797
                                            364.0599 2.6291817
                                                                  Positive
## 5:0:Subject.Reaction-Reaction 932.5247
                                            516.7169 1.8047110
                                                                  Unconstr
                                                                  Unconstr
## 5:1:Subject.Reaction-Reaction 1179.5219
                                            547.9498 2.1526095
## 5:2:Subject.Reaction-Reaction 859.1635
                                            440.5250 1.9503173
                                                                  Unconstr
## 5:3:Subject.Reaction-Reaction 1672.9989
                                            664.0846 2.5192556
                                                                  Unconstr
## 5:4:Subject.Reaction-Reaction 2003.0167
                                            738.6399 2.7117633
                                                                  Unconstr
## 5:Subject.Reaction-Reaction
                                 2067.9299
                                            553.3254 3.7372765
                                                                  Positive
## 6:0:Subject.Reaction-Reaction 666.1077
                                                                  Unconstr
                                            565.7589 1.1773702
## 6:1:Subject.Reaction-Reaction 850.9395
                                            583.6190 1.4580394
                                                                  Unconstr
                                                                  Unconstr
## 6:2:Subject.Reaction-Reaction 916.2375
                                            504.0273 1.8178333
## 6:3:Subject.Reaction-Reaction 1785.8432
                                            750.7274 2.3788171
                                                                  Unconstr
                                            822.0777 2.5271412
## 6:4:Subject.Reaction-Reaction 2077.5064
                                                                  Unconstr
## 6:5:Subject.Reaction-Reaction 2603.2823 1035.1406 2.5149070
                                                                  Unconstr
## 6:Subject.Reaction-Reaction
                                 3123.2005 1049.0352 2.9772123
                                                                  Positive
## 7:0:Subject.Reaction-Reaction 932.8190
                                            490.4744 1.9018709
                                                                  Unconstr
## 7:1:Subject.Reaction-Reaction 927.3416
                                            492.7764 1.8818709
                                                                  Unconstr
## 7:2:Subject.Reaction-Reaction 924.7079
                                            426.2387 2.1694602
                                                                  Unconstr
## 7:3:Subject.Reaction-Reaction 1282.8637
                                                                  Unconstr
                                            583.3415 2.1991642
## 7:4:Subject.Reaction-Reaction 1549.9053
                                            643.7083 2.4077757
                                                                  Unconstr
                                                                  Unconstr
## 7:5:Subject.Reaction-Reaction 1941.5523
                                            811.3286 2.3930529
## 7:6:Subject.Reaction-Reaction 2306.0261
                                            951.5128 2.4235367
                                                                  Unconstr
## 7:Subject.Reaction-Reaction
                                 1669.8274
                                            612.0081 2.7284398
                                                                  Positive
```

```
## 8:0:Subject.Reaction-Reaction 920.3110 576.8500 1.5954079
                                                                  Unconstr
## 8:1:Subject.Reaction-Reaction 1044.9313 592.5243 1.7635247
                                                                  Unconstr
## 8:2:Subject.Reaction-Reaction 831.4993 486.9625 1.7075221
                                                                  Unconstr
## 8:3:Subject.Reaction-Reaction 1607.0156
                                            717.6871 2.2391591
                                                                  Unconstr
## 8:4:Subject.Reaction-Reaction 2029.1022
                                            805.6724 2.5185201
                                                                  Unconstr
## 8:5:Subject.Reaction-Reaction 3058.1945 1093.4722 2.7967739
                                                                  Unconstr
## 8:6:Subject.Reaction-Reaction 2927.6051 1177.5589 2.4861644
                                                                  Unconstr
## 8:7:Subject.Reaction-Reaction 2433.2427
                                            957.7103 2.5406876
                                                                  Unconstr
## 8:Subject.Reaction-Reaction
                                 2947.1635
                                            844.8113 3.4885466
                                                                  Positive
## 9:0:Subject.Reaction-Reaction 1440.6886
                                            690.1726 2.0874323
                                                                  Unconstr
## 9:1:Subject.Reaction-Reaction 1514.9679
                                            703.4423 2.1536491
                                                                  Unconstr
## 9:2:Subject.Reaction-Reaction 967.8504
                                                                  Unconstr
                                            550.1628 1.7592073
## 9:3:Subject.Reaction-Reaction 1742.6866
                                            797.5934 2.1849310
                                                                  Unconstr
## 9:4:Subject.Reaction-Reaction 2198.3504 892.7701 2.4623924
                                                                  Unconstr
## 9:5:Subject.Reaction-Reaction 3236.8715 1196.2341 2.7058847
                                                                  Unconstr
## 9:6:Subject.Reaction-Reaction 2210.6321 1185.1233 1.8653182
                                                                  Unconstr
## 9:7:Subject.Reaction-Reaction 2399.5130 1027.8125 2.3345824
                                                                  Unconstr
## 9:8:Subject.Reaction-Reaction 3847.0132 1391.5584 2.7645359
                                                                  Unconstr
## 9:Subject.Reaction-Reaction
                                 3946.2369 1228.6678 3.2118013
                                                                  Positive
## units.Reaction-Reaction
                                  883.2477 577.9203 1.5283210
                                                                  Positive
## random regression (legendre polynomials)
fm2 <- mmer(Reaction ~ Days,</pre>
            random= ~ vs(leg(Days,1), Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
##
                                    VarComp VarCompSE
                                                          Zratio Constraint
## leg0:Subject.Reaction-Reaction 2817.4048 1011.23903 2.786092
                                                                   Positive
## leg1:Subject.Reaction-Reaction 473.4608
                                            199.53635 2.372805
                                                                   Positive
## units.Reaction-Reaction
                                   654.9433
                                              77.18822 8.485016
                                                                   Positive
## unstructured random regression (legendre)
fm2 <- mmer(Reaction ~ Days,</pre>
            random= ~ vs(us(leg(Days,1)), Subject),
            data=DT, tolparinv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
##
                                         VarComp
                                                  VarCompSE
                                                               Zratio Constraint
                                       2817.4056 1011.24156 2.786086
## leg0:Subject.Reaction-Reaction
                                                                        Positive
## leg1:leg0:Subject.Reaction-Reaction 869.9590
                                                  381.02481 2.283208
                                                                        Unconstr
## leg1:Subject.Reaction-Reaction
                                        473.4608
                                                  199.53612 2.372807
                                                                        Positive
## units.Reaction-Reaction
                                        654.9428
                                                   77.18763 8.485075
                                                                        Positive
```

Final remarks

Keep in mind that sommer uses the direct inversion (DI) algorithm which can be very slow for large datasets. The package is focused on problems of the type p > n (more random effect levels than observations) and models with dense covariance structures. For example, for an experiment with dense covariance structures with low-replication (i.e. 2000 records from 1000 individuals replicated twice with a covariance structure of 1000×1000), sommer will be faster than MME-based software. Also for genomic problems with large number of random effect levels, i.e. 300 individuals (n) with 100,000 genetic markers (p). For highly replicated trials with small number of individuals and covariance structures or n > p (i.e. 2000 records from 200 individuals replicated 10 times with covariance structure of 200×200), asrem1 or other MME-based algorithms will be much faster and we recommend you to opt for those software programs.

Literature

Covarrubias-Pazaran G. 2016. Genome assisted prediction of quantitative traits using the R package sommer. PLoS ONE 11(6):1-15.

Covarrubias-Pazaran G. 2018. Software update: Moving the R package sommer to multivariate mixed models for genome-assisted prediction. doi: https://doi.org/10.1101/354639

Bernardo Rex. 2010. Breeding for quantitative traits in plants. Second edition. Stemma Press. 390 pp.

Gilmour et al. 1995. Average Information REML: An efficient algorithm for variance parameter estimation in linear mixed models. Biometrics 51(4):1440-1450.

Henderson C.R. 1975. Best Linear Unbiased Estimation and Prediction under a Selection Model. Biometrics vol. 31(2):423-447.

Kang et al. 2008. Efficient control of population structure in model organism association mapping. Genetics 178:1709-1723.

Lee, D.-J., Durban, M., and Eilers, P.H.C. (2013). Efficient two-dimensional smoothing with P-spline ANOVA mixed models and nested bases. Computational Statistics and Data Analysis, 61, 22 - 37.

Lee et al. 2015. MTG2: An efficient algorithm for multivariate linear mixed model analysis based on genomic information. Cold Spring Harbor. doi: http://dx.doi.org/10.1101/027201.

Maier et al. 2015. Joint analysis of psychiatric disorders increases accuracy of risk prediction for schizophrenia, bipolar disorder, and major depressive disorder. Am J Hum Genet; 96(2):283-294.

Rodriguez-Alvarez, Maria Xose, et al. Correcting for spatial heterogeneity in plant breeding experiments with P-splines. Spatial Statistics 23 (2018): 52-71.

Searle. 1993. Applying the EM algorithm to calculating ML and REML estimates of variance components. Paper invited for the 1993 American Statistical Association Meeting, San Francisco.

Yu et al. 2006. A unified mixed-model method for association mapping that accounts for multiple levels of relatedness. Genetics 38:203-208.

Tunnicliffe W. 1989. On the use of marginal likelihood in time series model estimation. JRSS 51(1):15-27.