

Translating lme4 models to sommer

Giovanny Covarrubias-Pazaran

2023-04-02

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"))
# Random effects:
# Groups   Name      Variance Std.Dev.
# Subject (Intercept) 1378.2   37.12
# Residual              960.5   30.99
# 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

# fm2 <- mmec(Reaction ~ Days,
#             random= ~ Subject,
#             data=DT, tolParInv = 1e-6, verbose = FALSE)
# summary(fm2)$varcomp
```

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"))
# Random effects:
# Groups      Name          Variance Std.Dev.
# Subject     (Intercept) 627.57    25.051
# Subject.1 Days          35.86     5.988
# Residual                    653.58   25.565
# Number of obs: 180, groups: Subject, 18
#####
## sommer
#####
fm2 <- mmec(Reaction ~ Days,
            random= ~ Subject + vsr(Days, Subject),
            data=DT, tolParInv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

```
##                               VarComp VarCompSE   Zratio Constraint
## 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

# fm2 <- mmec(Reaction ~ Days,
#             random= ~ Subject + vsc(dsc(Days), isc(Subject)),
#             data=DT, tolParInv = 1e-6, verbose = FALSE)
# summary(fm2)$varcomp
```

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"))
# Random effects:
# Groups      Name                Variance Std.Dev. Corr
# Subject (Intercept) 612.10      24.741
# Days        35.07         5.922  0.07
# Residual      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,
            random= ~ Subject + vsr(Days, Subject),
            data=DT, tolParInv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

##		VarComp	VarCompSE	Zratio	Constraint
##	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

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"))
# 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,
            random= ~ vsr(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
##	units.Reaction-Reaction	842.02736	93.84640	8.972399	Positive

```
# fm2 <- mmec(Reaction ~ Days,
#             random= ~ vsr(dsc(Days), isc(Subject)),
#             data=DT, tolParInv = 1e-6, verbose = FALSE)
```

```
# summary(fm2)$varcomp
```

4) Other models available in sommer but not in lme4

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.

```
library(orthopolynom)
## diagonal model
fm2 <- mmer(Reaction ~ Days,
            random= ~ vsr(dsr(Daysf), Subject),
            data=DT, tolParInv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

##		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
##	2:Subject.Reaction-Reaction	0.0000	365.3178	0.0000000	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
##	7:Subject.Reaction-Reaction	1539.6201	779.1437	1.9760413	Positive
##	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,
            random= ~ vsr(usr(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
##	5:1:Subject.Reaction-Reaction	1179.5219	547.9498	2.1526095	Unconstr
##	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 565.7589 1.1773702 Unconstr
## 6:1:Subject.Reaction-Reaction 850.9395 583.6190 1.4580394 Unconstr
## 6:2:Subject.Reaction-Reaction 916.2375 504.0273 1.8178333 Unconstr
## 6:3:Subject.Reaction-Reaction 1785.8432 750.7274 2.3788171 Unconstr
## 6:4:Subject.Reaction-Reaction 2077.5064 822.0777 2.5271412 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 583.3415 2.1991642 Unconstr
## 7:4:Subject.Reaction-Reaction 1549.9053 643.7083 2.4077757 Unconstr
## 7:5:Subject.Reaction-Reaction 1941.5523 811.3286 2.3930529 Unconstr
## 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 550.1628 1.7592073 Unconstr
## 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,
            random= ~ vsr(log(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,
            random= ~ vsr(usr(log(Days,1)), Subject),
            data=DT, tolParInv = 1e-6, verbose = FALSE)
summary(fm2)$varcomp
```

```
##                               VarComp  VarCompSE  Zratio Constraint
```

```
## leg0:Subject.Reaction-Reaction      2817.4056 1011.24156 2.786086 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
```

```
# same can be done with the mmec function
```

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.

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