

Spatial modeling using the sommer package

Giovanny Covarrubias-Pazaran

2021-10-07

The sommer package was developed to provide R users with a powerful and reliable multivariate mixed model solver for different genetic (in diploid and polyploid organisms) and non-genetic analyses. This package allows the user to estimate variance components in a mixed model with the advantages of specifying the variance-covariance structure of the random effects, specifying heterogeneous variances, and obtaining other parameters such as BLUPs, BLUEs, residuals, fitted values, variances for fixed and random effects, etc. The core algorithms of the package are coded in C++ using the Armadillo library to optimize dense matrix operations common in the direct-inversion algorithms.

This vignette is focused on showing the capabilities of sommer to fit spatial models using the two dimensional splines models.

SECTION 1: Introduction

- 1) Background in tensor products

SECTION 2: Spatial models

- 1) Two dimensional splines (multiple spatial components)
- 2) Two dimensional splines (single spatial component)
- 3) Spatial models in multiple trials at once

SECTION 1: Introduction

Backgrounds in tensor products

TBD

SECTION 2: Spatial models

1) Two dimensional splines (multiple spatial components)

In this example we show how to obtain the same results than using the SpATS package. This is achieved by using the `spl2Db` function which is a wrapper of the `tpsmb` function.

```
library(sommer)
data(DT_yatesoats)
DT <- DT_yatesoats
DT$row <- as.numeric(as.character(DT$row))
DT$col <- as.numeric(as.character(DT$col))
DT$R <- as.factor(DT$row)
DT$C <- as.factor(DT$col)

# SPATS MODEL
# m1.SpATS <- SpATS(response = "Y",
```

```

#           spatial = ~ PSANOVA(col, row, nseg = c(14,21), degree = 3, pord = 2),
#           genotype = "V", fixed = ~ 1,
#           random = ~ R + C, data = DT,
#           control = list(tolerance = 1e-04))
#
# summary(m1.SpATS, which = "variances")
#
# Spatial analysis of trials with splines
#
# Response:                Y
# Genotypes (as fixed):    V
# Spatial:                 ~PSANOVA(col, row, nseg = c(14, 21), degree = 3, pord = 2)
# Fixed:                   ~1
# Random:                  ~R + C
#
#
# Number of observations:   72
# Number of missing data:  0
# Effective dimension:     17.09
# Deviance:                483.405
#
# Variance components:
#           Variance          SD      log10(lambda)
# R          1.277e+02      1.130e+01      0.49450
# C          2.673e-05      5.170e-03      7.17366
# f(col)     4.018e-15      6.339e-08     16.99668
# f(row)     2.291e-10      1.514e-05     12.24059
# f(col):row  1.025e-04      1.012e-02      6.59013
# col:f(row)  8.789e+01      9.375e+00      0.65674
# f(col):f(row) 8.036e-04     2.835e-02      5.69565
#
# Residual    3.987e+02      1.997e+01
#
# SOMMER MODEL
m1.sommer <- mmer(Y~1+V+spl2Db(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2,2), wha
random = ~R+C+spl2Db(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2
data=DT, tolpar = 1e-6, verbose = FALSE)

```

fixed-effect model matrix is rank deficient so dropping 8 columns / coefficients

```
summary(m1.sommer)$varcomp
```

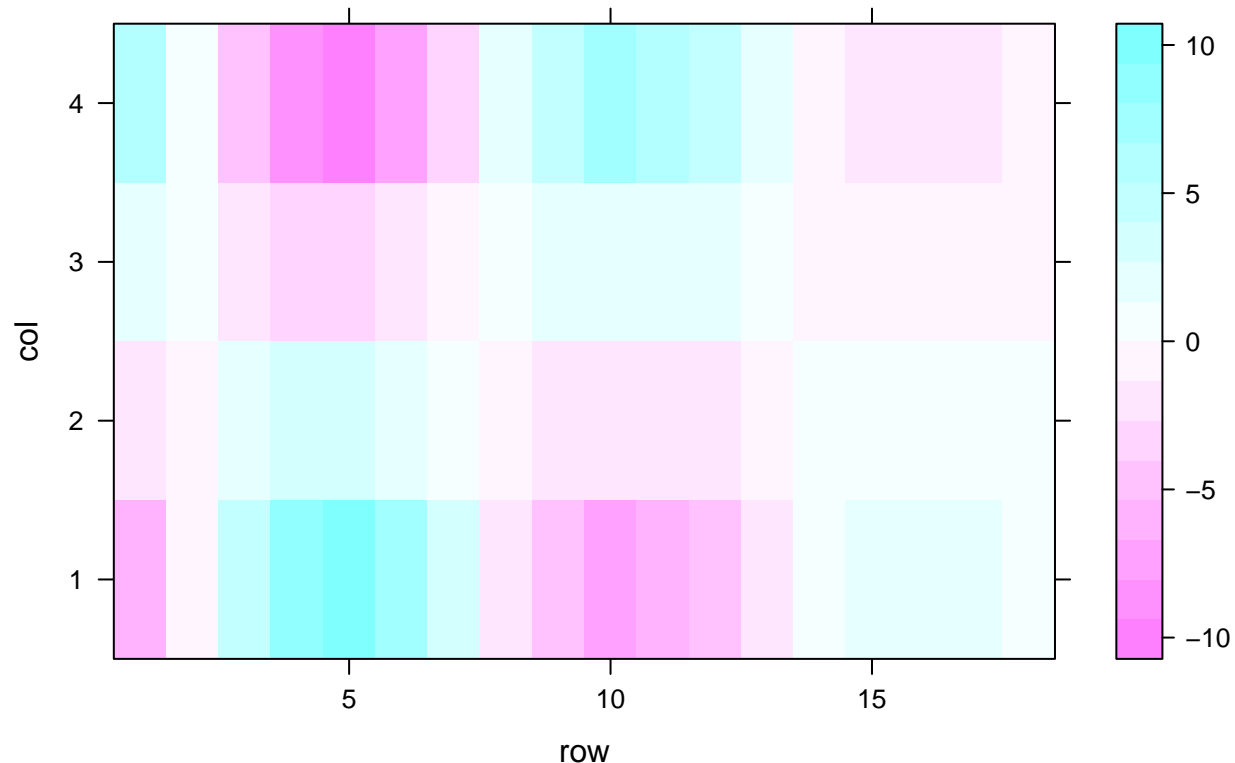
##	VarComp	VarCompSE	Zratio	Constraint
## R.Y-Y	125.928235	89.77330	1.4027360	Positive
## C.Y-Y	-7.789528	24.29529	-0.3206189	Positive
## A:fC.Y-Y	0.000000	19.09624	0.0000000	Positive
## A:fR.Y-Y	0.000000	15.87659	0.0000000	Positive
## A:fC.R.Y-Y	0.000000	21.42763	0.0000000	Positive
## A:C.fR.Y-Y	82.177296	92.28630	0.8904604	Positive
## A:fC.fR.Y-Y	0.000000	25.46390	0.0000000	Positive
## units.Y-Y	405.900386	90.48195	4.4859820	Positive

```

# get the fitted values for the spatial kernel and plot
ff <- fitted.mmer(m1.sommer)

```

```
## fixed-effect model matrix is rank deficient so dropping 8 columns / coefficients
## fixed-effect model matrix is rank deficient so dropping 8 columns / coefficients
DT$fit <- as.matrix(Reduce("+",ff$Zu[-c(1:2)]))
lattice::levelplot(fit~row*col,data=DT)
```



2) Two dimensional splines (single spatial component)

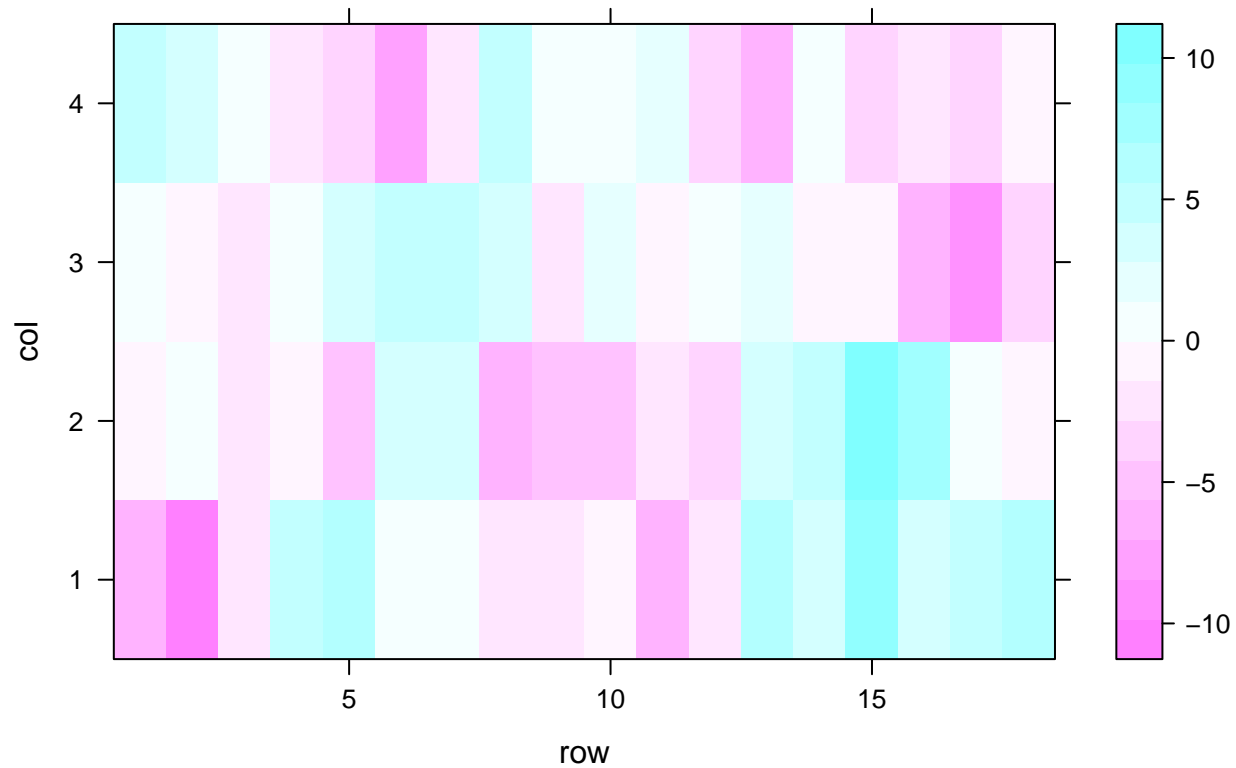
To reduce the computational burden of fitting multiple spatial kernels **sommer** provides a single spatial kernel method through the **sp12Da** function. This as will be shown, can produce similar results to the more flexible model. Use the one that fits better your needs.

```
# SOMMER MODEL
m2.sommer <- mmer(Y~1+V,
                  random = ~R+C+sp12Da(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2
                  data=DT, tolpar = 1e-6, verbose = FALSE)
summary(m1.sommer)$varcomp
```

##	VarComp	VarCompSE	Zratio	Constraint
## R.Y-Y	125.928235	89.77330	1.4027360	Positive
## C.Y-Y	-7.789528	24.29529	-0.3206189	Positive
## A:fC.Y-Y	0.000000	19.09624	0.0000000	Positive
## A:fR.Y-Y	0.000000	15.87659	0.0000000	Positive
## A:fC.R.Y-Y	0.000000	21.42763	0.0000000	Positive
## A:C.fR.Y-Y	82.177296	92.28630	0.8904604	Positive
## A:fC.fR.Y-Y	0.000000	25.46390	0.0000000	Positive
## units.Y-Y	405.900386	90.48195	4.4859820	Positive

```
# get the fitted values for the spatial kernel and plot
ff <- fitted.mmer(m2.sommer)
```

```
DT$fit <- as.matrix(Reduce("+",ff$Zu[-c(1:2)]))
lattice::levelplot(fit~row*col,data=DT)
```



3) Spatial models in multiple trials at once

Sometimes we want to fit heterogeneous variance components when e.g., have multiple trials or different locations. The spatial models can also be fitted that way using the `at.var` and `at.levels` arguments. The first argument expects a variable that will define the levels at which the variance components will be fitted. The second argument is a way for the user to specify the levels at which the spatial kernels should be fitted if the user doesn't want to fit it for all levels (e.g., trials or fields).

```
DT2 <- rbind(DT,DT)
DT2$Y <- DT2$Y + rnorm(length(DT2$Y))
DT2$trial <- c(rep("A",nrow(DT)),rep("B",nrow(DT)))
head(DT2)
```

##	row	col	Y	N	V	B	MP	R	C	fit	trial
## 1	1	1	91.79843	0.2	Victory	B2	Victory	1	1	-6.8551989	A
## 2	2	1	61.85086	0	Victory	B2	Victory	2	1	-9.8822858	A
## 3	3	1	120.55643	0.4	Marvellous	B2	Marvellous	3	1	-1.7663567	A
## 4	4	1	143.55323	0.6	Marvellous	B2	Marvellous	4	1	4.7259712	A
## 5	5	1	149.01331	0.6	GoldenRain	B2	GoldenRain	5	1	6.8147655	A
## 6	6	1	106.56385	0.2	GoldenRain	B2	GoldenRain	6	1	0.2831235	A

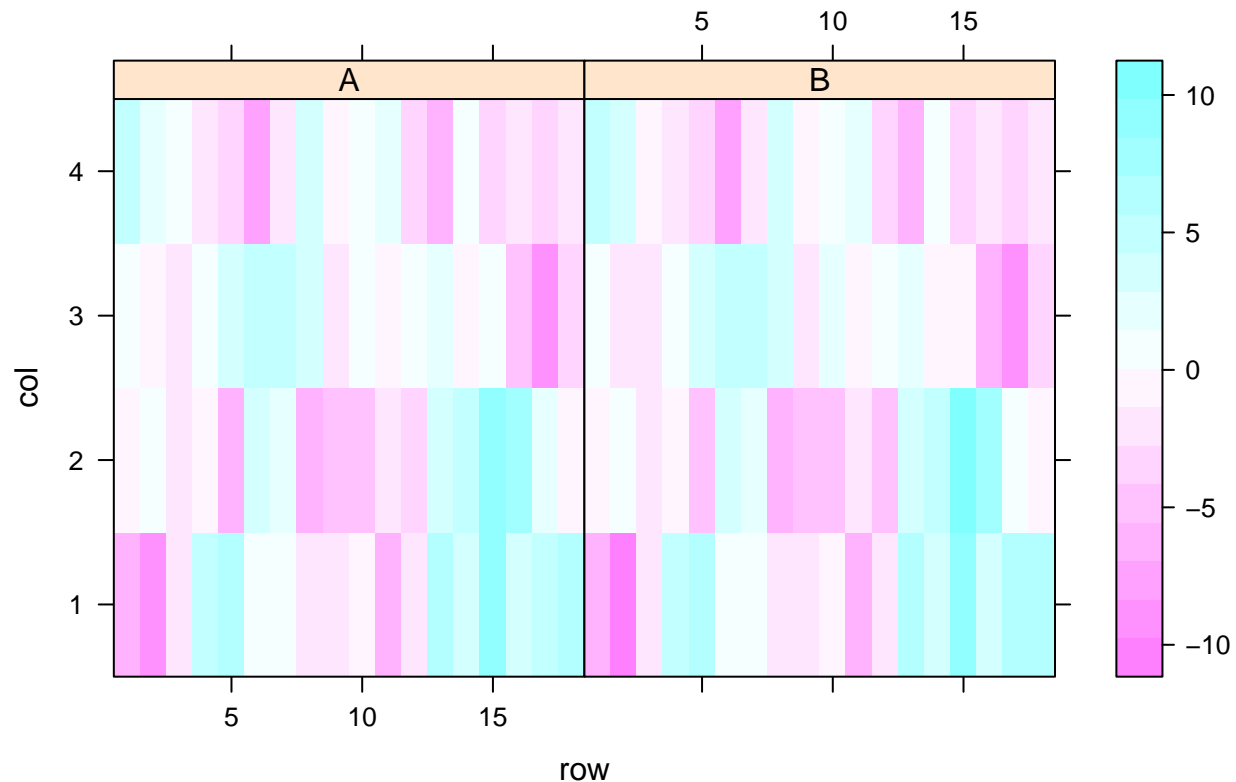
```
# SOMMER MODEL
```

```
m3.sommer <- mmer(Y~1+V,
  random = ~vs(ds(trial),R)+vs(ds(trial),C)+
    spl2Da(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2,2), at.var =
    rcov = ~vs(ds(trial),units),
```

```
data=DT2, tolpar = 1e-6, verbose = FALSE)
summary(m3.sommer)$varcomp
```

```
##          VarComp VarCompSE   Zratio Constraint
## A:R.Y-Y    107.48007  82.12826 1.3086855   Positive
## B:R.Y-Y     98.26652  80.47655 1.2210578   Positive
## A:C.Y-Y    144.95281 138.74448 1.0447465   Positive
## B:C.Y-Y    138.91292 134.98994 1.0290613   Positive
## A:all.Y-Y   403.81707 879.19318 0.4593041   Positive
## B:all.Y-Y   418.54730 901.30369 0.4643799   Positive
## A:units.Y-Y 385.64550 202.89149 1.9007475   Positive
## B:units.Y-Y 396.86541 208.15464 1.9065893   Positive
```

```
# get the fitted values for the spatial kernel and plot
ff <- fitted.mmer(m3.sommer)
DT2$fit <- as.matrix(Reduce("+",ff$Zu[-c(1:4)]))
lattice::levelplot(fit~row*col|trial,data=DT2)
```



Final remarks

Keep in mind that sommer uses a 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 experiments with dense covariance structures with low-replication (i.e. 2000 records from 1000 individuals replicated twice with a covariance structure of 1000x1000) 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 covariance structures or $n > p$ (i.e. 2000 records from 200 individuals replicated 10 times with covariance structure of 200x200) asreml or other MME-based algorithms will be much faster and we

recommend you to opt for those. When datasets are big, the installation of the OpenBLAS library can make sommer quite fast and sometimes faster than asreml given the capability of sommer to take advantage of the multi-processor architecture of some systems.

Literature

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

Covarrubias-Pazarán 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.