Spatial modeling using the sommer package

Giovanny Covarrubias-Pazaran

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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 derect-inversion algorithms.

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

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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 sp12Db function which is a wrapper of the tpsmmb 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$C <- as.factor(DT$row)
### SPATS MODEL
###1.Spats <- Spats(response = "Y",</pre>
```

```
spatial = \sim 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:
# Genotypes (as fixed):
                              V
# Spatial:
                              ~PSANOVA(col, row, nseg = c(14, 21), degree = 3, pord = 2)
# Fixed:
                              ~1
# Random:
                              \sim R + C
#
                                 72
# Number of observations:
# Number of missing data:
                                 0
# Effective dimension:
                                17.09
# Deviance:
                                483.405
# Variance components:
                                               log10(lambda)
                   Variance
# R
                                 1.130e+01
                   1.277e+02
                                                      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
                                 1.997e+01
                   3.987e+02
# SOMMER MODEL
m1.sommer <- mmer(Y^{-1}+V+spl2Db(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2,2), what
                 random = {}^{\sim}R+C+spl2Db(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2,3)
                 data=DT, tolParConv = 1e-6, verbose = FALSE)
## Warning: fixed-effect model matrix is rank deficient so dropping 8 columns / coefficients
summary(m1.sommer)$varcomp
##
                 VarComp VarCompSE
                                       Zratio Constraint
              125.928235 89.77330 1.4027360
## R.Y-Y
                                                Positive
## C.Y-Y
              -7.789528 24.29529 -0.3206189
                                                Positive
## A:fC.Y-Y
                0.000000 19.09624 0.0000000 Positive
                0.000000 15.87659 0.0000000
## A:fR.Y-Y
                                                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)</pre>
\# DT\$fit \leftarrow 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 spl2Da 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 = {}^{\sim}R+C+spl2Da(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2
                  data=DT, tolParConv = 1e-6, verbose = FALSE)
summary(m1.sommer)$varcomp
##
                  VarComp VarCompSE
                                         Zratio Constraint
## R.Y-Y
               125.928235 89.77330
                                      1.4027360
                                                  Positive
## C.Y-Y
                -7.789528
                           24.29529 -0.3206189
                                                  Positive
## A:fC.Y-Y
                 0.000000
                           19.09624
                                      0.0000000
                                                  Positive
## A:fR.Y-Y
                 0.000000
                           15.87659
                                      0.0000000
                                                  Positive
## A:fC.R.Y-Y
                 0.000000
                            21.42763
                                      0.0000000
                                                  Positive
## A:C.fR.Y-Y
                82.177296
                            92.28630
                                      0.8904604
                                                  Positive
## A:fC.fR.Y-Y
                 0.000000
                            25.46390
                                      0.0000000
                                                  Positive
               405.900386
## units.Y-Y
                                     4.4859820
                           90.48195
                                                  Positive
# get the fitted values for the spatial kernel and plot
# ff <- fitted.mmer(m2.sommer)
# DT$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)))</pre>
head(DT2)
                                      V
                                                    MP R C trial
##
     row col
                      γ
## 1
           1
              91.79843 0.2
                               Victory B2
                                              Victory 1 1
       1
              61.85086
## 2
       2
           1
                          0
                               Victory B2
                                              Victory 2 1
## 3
       3
           1 120.55643 0.4 Marvellous B2 Marvellous 3 1
                                                               Α
## 4
           1 143.55323 0.6 Marvellous B2 Marvellous 4 1
                                                               Α
           1 149.01331 0.6 GoldenRain B2 GoldenRain 5 1
## 5
       5
                                                               Α
           1 106.56385 0.2 GoldenRain B2 GoldenRain 6 1
## 6
       6
                                                               Α
# SOMMER MODEL
m3.sommer \leftarrow mmer(Y~1+V)
                   random = ~vsr(dsr(trial),R)+vsr(dsr(trial),C)+
                     spl2Da(col,row, nsegments = c(14,21), degree = c(3,3), penaltyord = c(2,2), at.var
```

```
rcov = ~vsr(dsr(trial),units),
                  data=DT2, tolParConv = 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
               418.54730 901.30369 0.4643799
## B:all.Y-Y
                                                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)</pre>
# DT2\$fit \leftarrow as.matrix(Reduce("+", ff\$Zu[-c(1:4)]))
# lattice::levelplot(fit~row*col/trial,data=DT2)
```

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.