

Changes and FAQs for the sommer package

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2021-12-14

The sommer package was developed to provide R users with 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 specify the variance-covariance structure for the random effects, to specify heterogeneous variances, and to obtain other parameters such as BLUPs, BLUEs, residuals, fitted values, variances for fixed and random effects, etc.

Recently, I decided to code the main algorithm (Newton-Raphson & Average-Information) in C++ which encouraged me to refactor all the machinery including special functions and specification of the models. For a more in depth explanation of how the machinery works please read the “Quick start for the sommer package” vignette by typing `vignette('sommer.start')`. Here I will focus on just making a translation of the old specification to the new specification.

The purpose of this vignette is to first show the changes in syntax for `sommer` and frequently asked question.

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SECTION 1: The new syntax of sommer

1) The specification of multiresponse model

In past versions (depending how old your version) there was an argument called `MVM` which had to be set to `TRUE` if the user wanted to run a true multi-trait model since the specification

```
fixed= cbind(y1,y2)~x
```

would by default fit 2 univariate models in parallel. That is no longer the case, the `MVM` argument doesn't exist and if a model like the one above is specified it will run a true multi-trait model.

2) The specification of multivariate unknown covariance structures

In the previous versions when I introduced the multivariate solver I decided to follow the asreml syntax to specify the unknown covariance structure that needed to be estimated. For example, a diagonal model for the multitrait model, assuming a random effect called `re` looked something like this:

```
fixed= cbind(y1,y2)~x
random= ~ diag(trait):re
```

and an unstructured multitrait model was:

```
random= ~ us(trait):re
```

Although this was easier for users familiar with asreml, it put a lot of limitations on the way constraints for variance components were specified. The same model in the new versions looks like this:

```
random= ~ vs(re, Gtc=unsm(2))
```

where the `Gtc` argument helps us to indicate what type of structure this random effect represents. Here I specified an unstructured model with the function `unsm()` with a number 2 for 2 traits. The user can specify either `diag()` or `unsm()`, or any customized matrix with dimensions $t \times t$ (t being the number of traits) containing the number 0,1,2,3 that specify the constraint:

- 0: not to be estimated
- 1: estimated and constrained to be positive (i.e. variance component)
- 2: estimated and unconstrained (can be negative or positive, i.e. covariance component)
- 3: not to be estimated but fixed (value has to be provided in the `Gti` argument)

All these models fit a model with the following variance for `re`:

$$\text{var}(u) = T \otimes A$$

where:

$$\text{var}(\mathbf{u}) = \begin{bmatrix} \sigma_{g_{t1,t1}}^2 & \sigma_{g_{t1,t2}} \\ \sigma_{g_{t2,t1}} & \sigma_{g_{t2,t2}}^2 \end{bmatrix} \otimes A$$

By making this change now, the user has full control of the constraints applied to the estimation of variance components and can provide initial values easily using the `Gti` argument.

3) The specification of additional unknown covariance structures

If we focus for a moment on a univariate mixed model we can also have other unknown covariance structures specified.

$$\text{var}(u) = E \otimes \dots \otimes F \otimes A$$

where:

$$\text{var}(\mathbf{u}) = \begin{bmatrix} \sigma_{g_{e1,e1}}^2 & \sigma_{g_{e1,e2}} & \sigma_{g_{e1,e3}} \\ \sigma_{g_{e2,e1}} & \sigma_{g_{e2,e2}}^2 & \sigma_{g_{e2,e3}} \\ \sigma_{g_{e3,e1}} & \sigma_{g_{e3,e2}} & \sigma_{g_{e3,e3}}^2 \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} \sigma_{g_{f1,f1}}^2 & \sigma_{g_{f1,f2}} \\ \sigma_{g_{f2,f1}} & \sigma_{g_{f2,f2}}^2 \end{bmatrix} \otimes A$$

If we think about the multi trait model, this is very similar but with an additional kroneker product for the multivariate version:

$$\text{var}(u) = T \otimes E \otimes \dots \otimes F \otimes A$$

where:

$$\mathbf{var}(\mathbf{u}) = \begin{bmatrix} \sigma_{g_{t1,t1}}^2 & \sigma_{g_{t1,t2}} \\ \sigma_{g_{t2,t1}} & \sigma_{g_{t2,t2}}^2 \end{bmatrix} \otimes \begin{bmatrix} \sigma_{g_{e1,e1}}^2 & \sigma_{g_{e1,e2}} & \sigma_{g_{e1,e3}} \\ \sigma_{g_{e2,e1}} & \sigma_{g_{e2,e2}}^2 & \sigma_{g_{e2,e3}} \\ \sigma_{g_{e3,e1}} & \sigma_{g_{e3,e2}} & \sigma_{g_{e3,e3}}^2 \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} \sigma_{g_{f1,f1}}^2 & \sigma_{g_{f1,f2}} \\ \sigma_{g_{f2,f1}} & \sigma_{g_{f2,f2}}^2 \end{bmatrix} \otimes A$$

Getting back to the point—the additional unknown covariance structures besides the multi-trait (T) before were specified with asreml syntax. For example a univariate diagonal and unstructured model, assumed a random effect called `id` representing the treatments planted in different environments coded in a second random effect called `env`. The model used to look like:

```
fixed= y1~x
random= ~ diag(env):id or random= ~ us(env):id
```

and now it would be specified as:

```
fixed= y1~x
random= ~ vs(ds(env),id) or random= ~ vs(us(env),id)
```

where the `ds()` and `us()` functions specify diagonal and unstructured models respectively. Now `cs()` for a customized structure is available. The main gain from having changed the formulation is that the new specification through the `vs()` function allows for constructing more complex models. For example, assume individuals specified in a column called `id` tested in three environments in a column called `env` measured at two different time points specified in a column called `time`. We may want something more flexible than:

```
fixed= y1~x
random= ~ id
```

We could actually assume that individuals are correlated within the environments for the different time points but want to consider environments independent. The variance for such random effects is the following:

$$\mathbf{var}(\mathbf{u}) = \begin{bmatrix} \sigma_{g_{e1,e1}}^2 & \sigma_{g_{e1,e2}} & \sigma_{g_{e1,e3}} \\ \sigma_{g_{e2,e1}} & \sigma_{g_{e2,e2}}^2 & \sigma_{g_{e2,e3}} \\ \sigma_{g_{e3,e1}} & \sigma_{g_{e3,e2}} & \sigma_{g_{e3,e3}}^2 \end{bmatrix} \otimes \begin{bmatrix} \sigma_{g_{t1,t1}}^2 & \sigma_{g_{t1,t2}} \\ \sigma_{g_{t2,t1}} & \sigma_{g_{t2,t2}}^2 \end{bmatrix} \otimes A$$

which was not possible in previous versions of sommer and now can be specified as:

```
random= ~ vs(us(env),ds(time),id)
```

and the same logic can be extended to as many interacting factors as desired.

4) The specification of unknown covariance structures in the residuals

Previously, sommer was limited to only diagonal models in the residuals (unstructured available only for multi-trait before). Now all the same applications discussed for the random term also apply for the residual term. Just keep in mind that the residual term is always called `units`.

Previous versions:

```
random= ~ diag(trait):diag(env):units
random= ~ us(trait):diag(env):units # limit
```

New versions (>3.7):

```
random= ~ vs(ds(env),units, Gtc=mm) ## can be extended to more interacting factors
random= ~ vs(us(env),units, Gtc=mm) ## can be extended to more interacting factors
```

```
random= ~ vs(at(env),units, Gtc=mm) ## can be extended to more interacting factors
```

```
random= ~ vs(cs(env),units, Gtc=mm) ## can be extended to more interacting factors
```

where `mm` can be any matrix specifying the type of multi-trait model (constraints). For example we could use `unsm()` `diag()`, `uncm()` or any other customized matrix.

5) Special models

In previous versions the use of `asreml` formulation really limited the expansion of `sommer` to more sophisticated models. Now there are many more possible models.

Previous versions:

Overlay models Previous version: limited to 2 columns and only random and no covariance structures.

```
random= ~ x + and(y)
```

New versions (>3.7): in theory there are no limits. Can be extended to more interacting factors in the unknown covariance structures and can overlay as many columns as needed. Plus is fully functional with the multivariate models.

```
random=~ vs(..., overlay(x1,...,xn), Gtc=mm)
```

Random regression models Previous version: Not available before

New versions (>3.7): in theory no limits. Can be extended to more interacting factors in the unknown covariance structures and only requires the use of the `leg()` function. Plus is fully functional with the multivariate models.

```
random=~ vs(us(leg(v,1)),x)
```

```
random=~ vs(ds(leg(v,1)),x)
```

```
random=~ vs(leg(v,1),x)
```

GWAS models Previous version: Only univariate models available

New versions (>3.7): all the power of the `mmer()` function is available plus you can fit multivariate GWAS models. See details in the `sommer.start` vignettes.

Spatial models Previous version: It was called directly in the formula

```
random=~ spl2D(Row,Col,at=?)
```

New versions (>3.7): It has to be called within the `vs()` function but now it can be combined with all the unknown covariance structures available.

```
random=~ vs(...,spl2D(Row,Col,at=?), Gtc=mm) # being mm any multi-trait constraint-structure.
```

Customized random effects Previous version: It was provided in the grouping argument

```
random=~ grp(x),
```

```
grouping=list(x=Z)
```

New versions (>3.7): It has to be called within the `vs()` function but now it can be combined with all the unknown covariance structures available.

```
random=~vs(..., Z, Gtc=mm) # mm is any multi-trait constraint-structure.
```

SECTION 2: Frequently asked questions

1) I got an error similar to:

```
# iteration   LogLik      wall   cpu(sec)  restrained
#      1      -224.676  18:11:23    3         0
# Sistem is singular. Aborting the job. You could try a bigger tolparinv value.
```

This error indicates that your model is singular (phenotypic variance V matrix is not invertible) and therefore the model is stopped, throwing the error message and returning an empty list. You can try a simpler model or just modify the argument `tolparinv` in the `mmer()` function. The default is 1e-3, which means that it will try to invert V and if it fails it will try to add a small value to the diagonal of V of 1e-3 to make it invertible and try bigger and bigger numbers. If this fails then the program will return the empty list.

Sometimes the model becomes singular when you use variance covariance matrices (i.e. genomic relationship matrices) that are not full-rank. You can try to make it full-rank and try again.

2) My model runs very slow

Keep in mind that sommer uses 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 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 software.

3) Can I run both; rrBLUP for markers and GBLUP for individuals in sommer?

Both types of models can be fitted in sommer. The only thing that it changes is the random effect of interest; the marker matrix or the identifier for the individual. Here there is a complex example using multi-trait models but can be used with only one trait.

```
library(sommer)
## rrBLUP for makers
data(DT_cpdata)
DT <- DT_cpdata
GT <- GT_cpdata
MP <- MP_cpdata
mix.rrblup <- mmer(fixed=color~1,
                  random=~vs(GT,Gtc=unsm(1), buildGu = FALSE) + vs(Rowf,Gtc=diag(1)),
                  rcov=~vs(units,Gtc=unsm(1)), getPEV = FALSE,
                  data=DT, verbose = FALSE)
summary(mix.rrblup)
```

```
## =====
##           Multivariate Linear Mixed Model fit by REML
## ***** sommer 4.1 *****
## =====
```

```

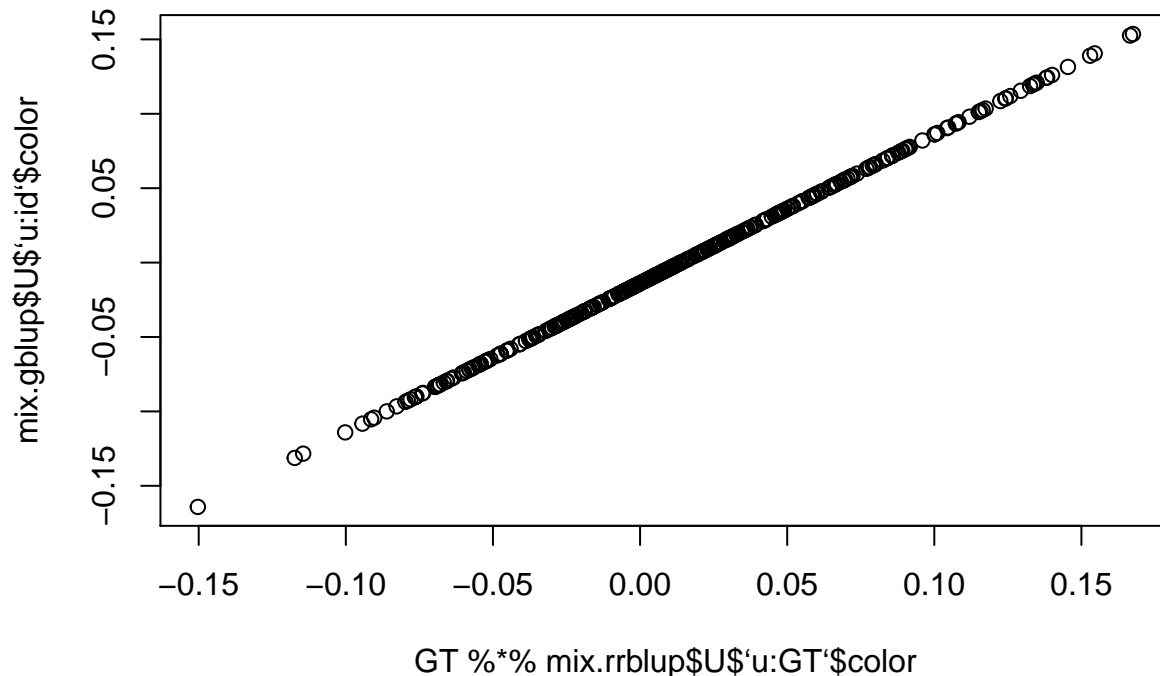
##          logLik      AIC      BIC Method Converge
## Value -108.1202 218.2403 222.132      NR      TRUE
## =====
## Variance-Covariance components:
##          VarComp VarCompSE Zratio Constraint
## u:GT.color-color  4.213e-06 8.581e-07  4.909  Positive
## u:Rowf.color-color 1.963e-04 1.355e-04  1.449  Positive
## u:units.color-color 2.612e-03 2.926e-04  8.928  Positive
## =====
## Fixed effects:
##   Trait      Effect Estimate Std.Error t.value
## 1 color (Intercept)  0.1692  0.03908  4.329
## =====
## Groups and observations:
##      color
## u:GT  2889
## u:Rowf  13
## =====
## Use the '$' sign to access results and parameters

## GBLUP for individuals
A <- A.mat(GT)
mix.gblup <- mmer(fixed=color~1,
                 random=~vs(id,Gu=A, Gtc=unsm(1)) + vs(Rowf,Gtc=diag(1)),
                 rcov=~vs(units,Gtc=unsm(1)),
                 data=DT, verbose = FALSE)
summary(mix.gblup)

## =====
##          Multivariate Linear Mixed Model fit by REML
## ***** sommer 4.1 *****
## =====
##          logLik      AIC      BIC Method Converge
## Value -108.1201 218.2403 222.1319      NR      TRUE
## =====
## Variance-Covariance components:
##          VarComp VarCompSE Zratio Constraint
## u:id.color-color  0.0049524 0.0010082  4.912  Positive
## u:Rowf.color-color 0.0001965 0.0001359  1.446  Positive
## u:units.color-color 0.0026123 0.0002926  8.928  Positive
## =====
## Fixed effects:
##   Trait      Effect Estimate Std.Error t.value
## 1 color (Intercept)  0.1831  0.004732  38.7
## =====
## Groups and observations:
##      color
## u:id  363
## u:Rowf  13
## =====
## Use the '$' sign to access results and parameters

## Equivalence
plot(GT%*%mix.rtblup$U$`u:GT`$color, mix.gblup$U$`u:id`$color)

```



Please notice that when specifying the marker matrix as a random effect we used the argument `buildGu=FALSE` to inform the `mmer()` function that a covariance matrix for the levels of the random effect shouldn't be built. Imagine a model with 100,000 markers, that would imply a relationship matrix of 100,000 x 100,000. If that matrix is a diagonal it would only compromise the speed and memory of the function. By setting `buildGu=FALSE` the `mmer()` solver will avoid the matrix multiplications using that huge diagonal matrix. If you want to specify a relationship matrix for the marker matrix then you cannot use that `buildGu` argument.

4) I am missing BLUPs for individuals even when I provided them in the relationship matrix

I got this good question in the past: “when I want to fit an animal model with the `sommer` package using an additive relationship matrix(A), this A matrix would contain parents. But the random effects only contains animals in the random effect but not including parents in the A matrix. How can I get the random effects for parents?”

Answer: The easy way to do it is to make sure that even if the parents don't show up in the dataset, you need to make sure that they are present in the levels of the column that contains the individuals (i.e. animal IDs), in addition they have to be provided in the relationship matrix and that's it. They should be returned in the blups.

```
library(sommer)

data(DT_cpdata)
DT <- DT_cpdata
GT <- GT_cpdata
MP <- MP_cpdata
#### create the variance-covariance matrix
A <- A.mat(GT) # additive relationship matrix
#### look at the data and fit the model
set.seed(12)
DT2 <- droplevels(DT[sample(1:nrow(DT),100),]) # we simulate a dataset with only 100 animals
nrow(DT2); length(levels(DT2$id))
```

```
## [1] 100
```

```
## [1] 100
# we fit a model with the reduced dataset where only 100 blups will be returned since only
# 100 levels exist in the "id" column
mix1 <- mmer(Yield~1,
             random=~vs(id,Gu=A)
               + Rowf + Colf,
             rcov=~units,
             data=DT2, verbose = FALSE)
```

```
## Adding additional levels of Gu in the model matrix of 'id'
```

```
summary(mix1)
```

```
## =====
##           Multivariate Linear Mixed Model fit by REML
## ***** sommer 4.1 *****
## =====
##           logLik      AIC      BIC Method Converge
## Value -47.00674 96.01348 98.61865      NR      TRUE
## =====
## Variance-Covariance components:
##           VarComp VarCompSE Zratio Constraint
## u:id.Yield-Yield 1531.7    1000.9 1.530  Positive
## Rowf.Yield-Yield  157.1     297.5 0.528  Positive
## Colf.Yield-Yield   0.0     396.4 0.000  Positive
## units.Yield-Yield 3358.4     883.6 3.801  Positive
## =====
## Fixed effects:
##   Trait      Effect Estimate Std.Error t.value
## 1 Yield (Intercept) 127.4      7.214 17.66
## =====
## Groups and observations:
##   Yield
## u:id  363
## Rowf  13
## Colf  35
## =====
## Use the '$' sign to access results and parameters
```

```
length(mix1$U$`u:id`$Yield) # only 100 levels
```

```
## [1] 363
# we add additional levels to the "id" column and also provide them in the relationship matrix
levels(DT2$id) <- c(levels(DT2$id), setdiff(levels(DT$id), levels(DT2$id)))
mix2 <- mmer(Yield~1,
             random=~vs(id,Gu=A)
               + Rowf + Colf,
             rcov=~units,
             data=DT2, verbose = FALSE)
```

```
summary(mix2)
```

```
## =====
##           Multivariate Linear Mixed Model fit by REML
## ***** sommer 4.1 *****
## =====
```



```
##           logLik      AIC      BIC Method Converge
## Value -47.00674 96.01348 98.61865      NR      TRUE
## =====
## Variance-Covariance components:
##           VarComp VarCompSE Zratio Constraint
## u:id.Yield-Yield 1531.7    1000.9 1.530    Positive
## Rowf.Yield-Yield 157.1     297.5 0.528    Positive
## Colf.Yield-Yield  0.0     396.4 0.000    Positive
## units.Yield-Yield 3358.4    883.6 3.801    Positive
## =====
## Fixed effects:
##   Trait      Effect Estimate Std.Error t.value
## 1 Yield (Intercept) 127.4     7.214 17.66
## =====
## Groups and observations:
##      Yield
## u:id  363
## Rowf  13
## Colf  35
## =====
## Use the '$' sign to access results and parameters
```

```
length(mix2$U$`u:id`$Yield) # now 363 levels
```

```
## [1] 363
```

As of 4.1.2 this shouldn't be a problem since internally the `mmer()` solver adds the missing levels, but we leave this for reference for people using older versions of sommer.

5) How can I use the `AR1()`, `CS()` and `ARMA()` functions

Sommer doesn't support the estimation of additional correlation components like AR1 in the way `asreml` does. Still, if the user knows the correlation value or can do an iterative approach to find the best value then these functions can be used to specify the variance covariance structure for a given random effect.

For example, in the `DT_cpdata` dataset we have a field with row and column coordinates. This allows fitting row and column as random effects:

```
library(sommer)
data(DT_cpdata)
DT <- DT_cpdata
mix1 <- mmer(Yield~1,
             random=~ Rowf + Colf,
             rcov=~units,
             data=DT, verbose = FALSE)
summary(mix1)$varcomp
```

```
##           VarComp VarCompSE   Zratio Constraint
## Rowf.Yield-Yield 832.2879 393.8951 2.112968    Positive
## Colf.Yield-Yield 153.9201 126.7582 1.214281    Positive
## units.Yield-Yield 3647.3486 290.4910 12.555804    Positive
```

If the user wants to relax the independence between rows and define an AR1 covariance structure among rows then the model could be fitted as:

```
library(sommer)
data(DT_cpdata)
```

```
DT <- DT_cpdata
mixAR1row <- mmer(Yield~1,
  random=~ vs(Rowf, Gu=AR1(Rowf, rho=0.3)) + Colf,
  rcov=~units,
  data=DT, verbose = FALSE)
summary(mixAR1row)$varcomp
```

```
##                VarComp VarCompSE   Zratio Constraint
## u:Rowf.Yield-Yield  791.8219  387.8695  2.041465   Positive
## Colf.Yield-Yield   154.5660  126.8094  1.218885   Positive
## units.Yield-Yield  3643.6027  290.1689 12.556834   Positive
```

The same could be done for the column random effect:

```
library(sommer)
data(DT_cpdata)
DT <- DT_cpdata
mixAR1col <- mmer(Yield~1,
  random=~ Rowf + vs(Colf, Gu=AR1(Colf, rho=0.3)),
  rcov=~units,
  data=DT, verbose = FALSE)
summary(mixAR1col)$varcomp
```

```
##                VarComp VarCompSE   Zratio Constraint
## Rowf.Yield-Yield   830.3623  392.8264  2.113815   Positive
## u:Colf.Yield-Yield  178.7490  134.2703  1.331262   Positive
## units.Yield-Yield  3624.6074  287.6072 12.602629   Positive
```

If on the other hand, you would like to model the presence of correlation in row and columns at the same time the model would look like this:

```
library(sommer)
data(DT_cpdata)
DT <- DT_cpdata
mixAR1rowcol <- mmer(Yield~1,
  random=~ vs(Rowf:Colf,
    Gu=kronecker(AR1(Rowf, rho=0.3),AR1(Colf, rho=0.3),make.dimnames = TRUE)
  ),
  rcov=~units,
  data=DT, verbose = FALSE)
summary(mixAR1rowcol)$varcomp
```

```
##                VarComp VarCompSE   Zratio Constraint
## u:Rowf:Colf.Yield-Yield 2474.339  730.1474 3.388821   Positive
## units.Yield-Yield     2025.584  622.1023 3.256030   Positive
```

Notice that if you specify a random effect that is the interaction between 2 random effects the covariance structure to be specified in the `Gu` argument has to be built using the `kronecker()` function. The same applies to the `ARMA()` and `CS()` functions. Please keep in mind that the correlation values (`rho` argument) is a fixed value not estimated by REML like `asreml` does but you can always follow an iterative approach.

6) Can I run GWAS in MET experiments with replicates?

Although the direct-inversion algorithm that `sommer` uses in the background is not the best choice to solve GWAS models for the $n > p$ scenario it is still possible to perform GWAS in MET models.

For example, assume a MET model that has 41 genetic lines with 1000 SNP markers, tested in 3 environments. The genetic term in a MET can be modeled as CS, DIAG or US covariance. The whole point of the GWAS function in sommer is to provide the name of the gTerm (random effect) that will match the marker data provided.

We first make up marker data for the MET data for example purposes

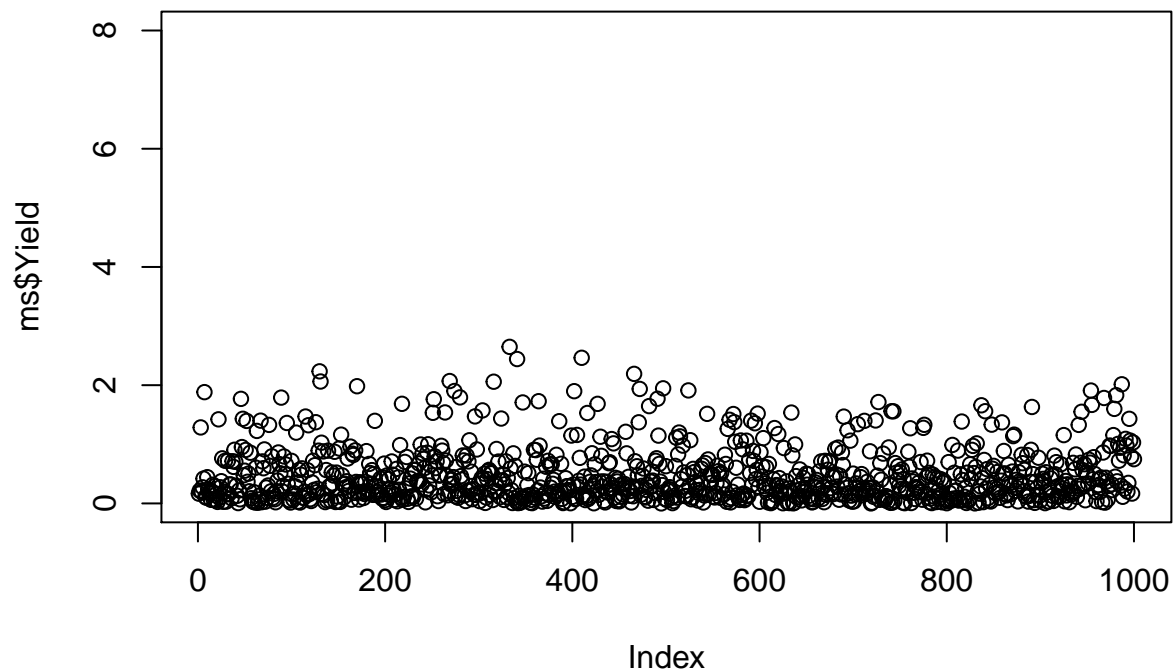
```
library(sommer)
data(DT_example)
DT <- DT_example
A <- A_example
M <- matrix(rep(0,41*1000),1000,41)
for (i in 1:41) {
  M[,i] <- ifelse(runif(1000)<0.5,-1,1)
}
tM <- t(M)
```

We then fit the MET model of the type compound symmetry (CS) and evaluate the GWAS for the main genetic term "Name":

```
## GWAS for main term in CS model
ansx <- GWAS(Yield~Env,
             random= ~ Name + Env:Name,
             rcov= ~ units,
             data=DT,
             M=tM,
             gTerm = "Name", verbose = FALSE)
```

```
## Performing GWAS evaluation
```

```
ms <- as.data.frame(ansx$scores)
plot(ms$Yield, ylim=c(0,8))
```



We could do the same but evaluate the GWAS considering the genetic term as the interaction term Env:Name

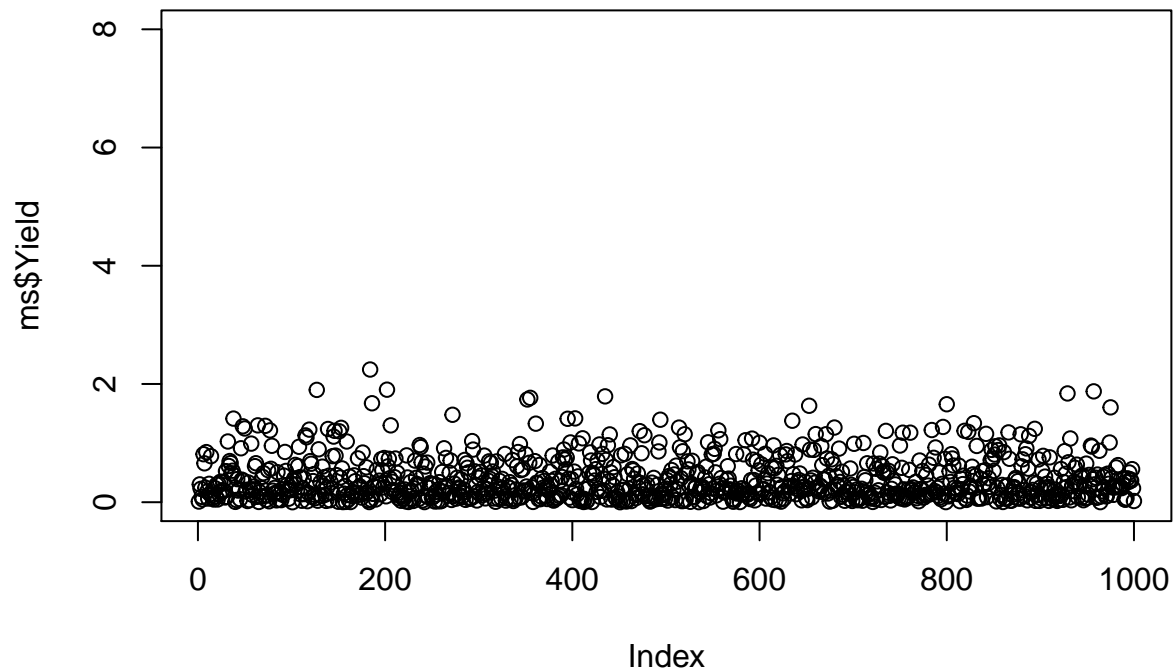
```
## GWAS for the interaction term in CS model
E <- matrix(1,nrow = length(unique(DT$Env)));E
```

```
##      [,1]
## [1,]  1
## [2,]  1
## [3,]  1
```

```
EtM <- kronecker(E,tM)
ansx <- GWAS(Yield~Env,
             random= ~ Name + Env:Name,
             rcov= ~ units,
             data=DT,
             M=EtM,
             gTerm = "Env:Name", verbose = FALSE)
```

```
## Performing GWAS evaluation
```

```
ms <- as.data.frame(ansx$scores)
plot(ms$Yield, ylim=c(0,8))
```



If the MET is a diagonal model, there is a variance component and BLUPs for each environment. Therefore we can evaluate the GWAS at any environment, here for example we evaluate the GWAS at the genetic term in the environment CA.2011.

```
## GWAS for the interaction term in DIAG model
E <- matrix(1,nrow = length(unique(DT$Env)));E
```

```
##      [,1]
## [1,]  1
## [2,]  1
## [3,]  1
```

```
EtM <- kronecker(E,tM)
ansx <- GWAS(Yield~Env,
```

```

random= ~Name + vs(ds(Env),Name),
rcov= ~ vs(ds(Env),units),
data=DT,
M=tM,
gTerm = "CA.2011:Name", verbose = FALSE )

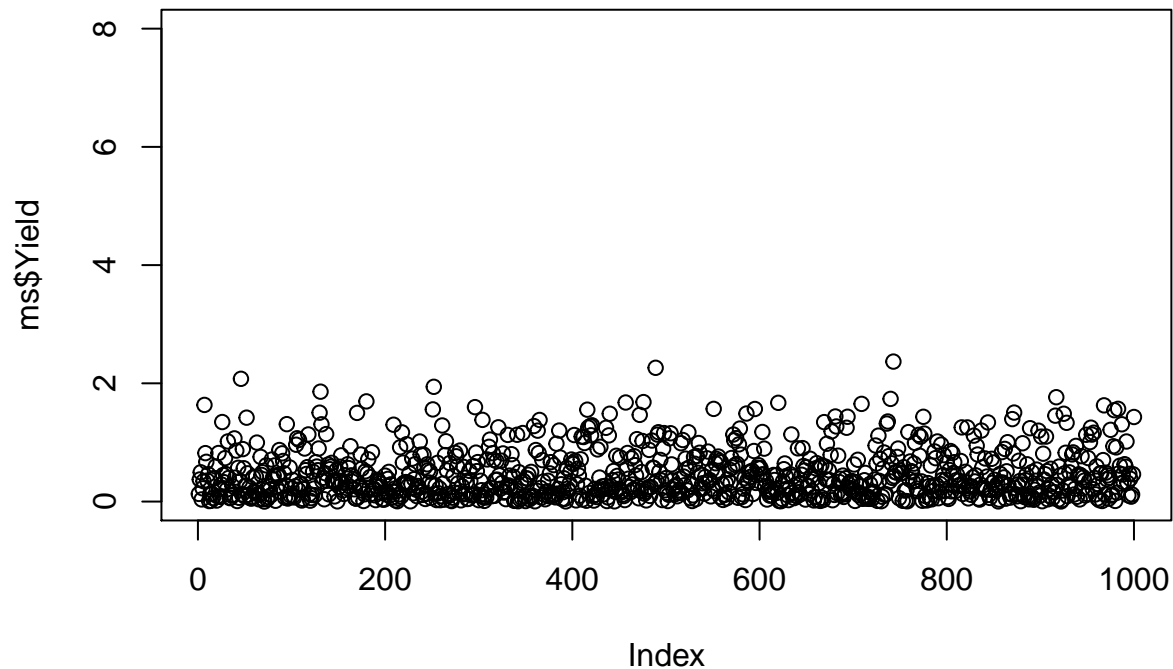
```

```
## Performing GWAS evaluation
```

```

ms <- as.data.frame(ansx$scores)
plot(ms$Yield, ylim=c(0,8))

```



If the MET is an unstructured model, there is a variance component and BLUPs for each environment and a covariance component among the different combinations of environments. Therefore we can evaluate the GWAS at any environment as before, here for example we evaluate the GWAS at the genetic term in the environment CA.2011. The difference with the previous model is that here we expect a greater accuracy in the environment CA.2011 since it has borrowed information from the other environments given the covariance fitted among environments.

```

## GWAS for main term in US model
ansx <- GWAS(Yield~Env,
  random= ~vs(us(Env),Name),
  rcov= ~ vs(us(Env),units),
  data=DT,
  M=tM,
  gTerm = "CA.2011:Name", verbose = FALSE)

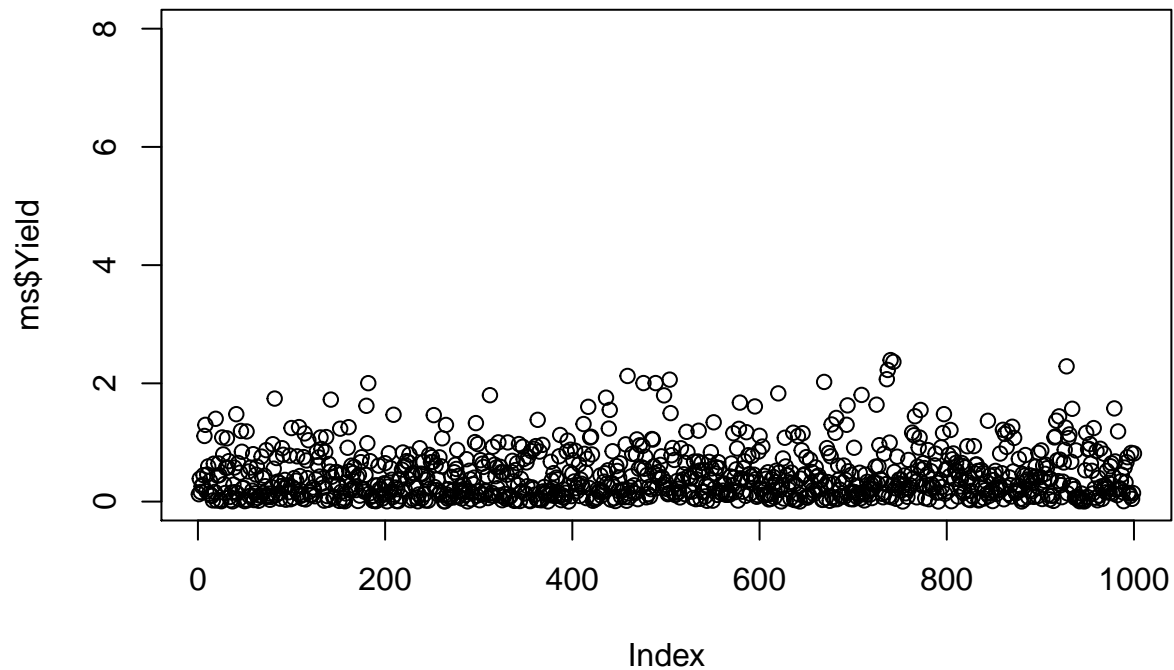
```

```
## Performing GWAS evaluation
```

```

ms <- as.data.frame(ansx$scores)
plot(ms$Yield, ylim=c(0,8))

```

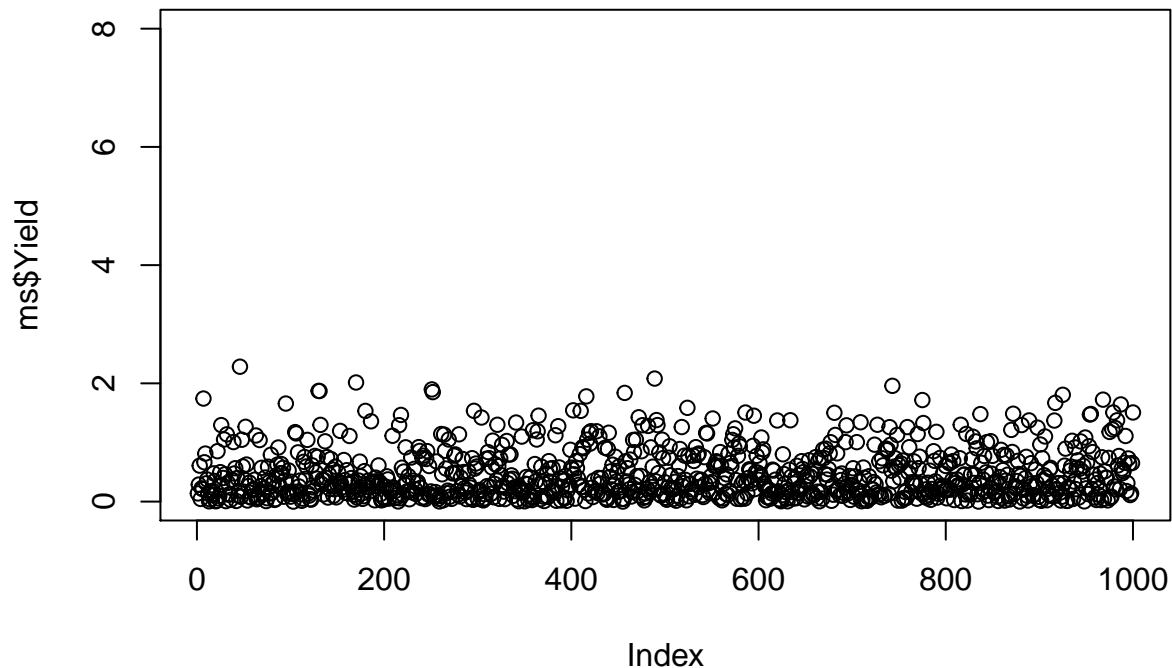


The same theory applies for the multitrait model:

```
## GWAS for main term in multitrait DIAG model
ansx <- GWAS(cbind(Weight,Yield)~Env,
             random= ~vs(ds(Env),Name, Gtc=unsm(2)),
             rcov= ~ vs(ds(Env),units, Gtc=diag(2)),
             data=DT,
             M=tM,
             gTerm = "CA.2011:Name", verbose = FALSE)
```

Performing GWAS evaluation

```
ms <- as.data.frame(ansx$scores)
plot(ms$Yield, ylim=c(0,8))
```



7) How can I constrain the value of specific random effects?

When using the `vs()` function three additional arguments help to control the following:

- `Gu`: matrix for covariances among levels for the `u.th` random effect
- `Gti`: matrix of initial values for the variance-covariance components
- `Gtc`: matrix of constraints for the variance-covariance components

Since each random effect can be seen as a multi-trait variance covariance structure, the univariate models are just an extension where the multi-trait variance covariance structure is a 1×1 matrix. When inspecting the results for the mixed models fitted by the `mmer()` function corresponding to the variance components stored in the `sigma` element, you will notice that each random effect contains a $t \times t$ matrix which corresponds to the multi-trait structure we referred to. For example:

```
data(DT_cpdata)
DT <- DT_cpdata
GT <- GT_cpdata
MP <- MP_cpdata
#### create the variance-covariance matrix
A <- A.mat(GT) # additive relationship matrix
#### look at the data and fit the model
mix1 <- mmer(Yield~1,
             random=~vs(id,Gu=A),
             rcov=~units,
             data=DT, verbose = FALSE)
mix1$sigma$`u:id`

##          Yield
## Yield 650.4145
```

Here the `sigma` element contains the random effects for `id` and `units` (error). Each of these contains a matrix of 1 by 1, but in a multi trait model would look like this:

```

data(DT_cpdata)
DT <- DT_cpdata
GT <- GT_cpdata
MP <- MP_cpdata
#### create the variance-covariance matrix
A <- A.mat(GT) # additive relationship matrix
#### look at the data and fit the model
mix2 <- mmer(cbind(Yield,color)~1,
             random=~vs(id,Gu=A, Gtc=unsm(2)),
             rcov=~vs(units,Gtc=diag(2)),
             data=DT, verbose = FALSE)
mix2$sigma$`u:id`

```

```

##           Yield      color
## Yield 634.6295932 0.471715518
## color  0.4717155 0.005126228

```

Notice that for 2 traits this becomes a 2 by 2 matrix. In order to put constraints in some of these random effect matrices you can use the `Gtc` argument as show above. For the `id` random effect we have specified that variance components should be estimated and be positive (diagonals with a 1), whereas covariance components should be estimated and unconstrained to be positive or negative (off-diagonals with a 2).

```
unsm(2)
```

```

##      [,1] [,2]
## [1,]    1    2
## [2,]    2    1

```

```
mix2$sigma$`u:id`
```

```

##           Yield      color
## Yield 634.6295932 0.471715518
## color  0.4717155 0.005126228

```

On the other hand, for the `units` (error) random effect we have specified in the `Gtc` argument that variance components should be estimated and be positive (diagonals), whereas covariance components should not be estimated (off-diagonals with a 0)

```
diag(2)
```

```

##      [,1] [,2]
## [1,]    1    0
## [2,]    0    1

```

```
mix2$sigma$`u:units`
```

```

##           Yield      color
## Yield 4009.336 0.000000000
## color   0.000 0.002563711

```

If the user would like to constrain a value to be fixed and not change through the estimation process of other random effects the user needs to provide the initial value (scaled with respect to the error variance) of those variance-covariance components in the `Gti` argument and use a matrix with the value 3 in the `Gtc` constraint matrix.

```

mm <- matrix(3,1,1) ## matrix to fix the var comp
initialVal <- mix1$sigma_scaled$`u:id`/2 # we want to fix the vc to be half of the previous univariate
mix3 <- mmer(Yield~1,

```



```

random=~vs(id, Gu=A, Gti=initialVal, Gtc=mm), # constrained
rcov=~vs(units), # unconstrained
data=DT, verbose = FALSE)

```

```

# analyze variance components
summary(mix1)$varcomp

```

```

##                VarComp VarCompSE   Zratio Constraint
## u:id.Yield-Yield  650.4145  325.5562  1.997856   Positive
## units.Yield-Yield 4031.0153  344.6051 11.697493   Positive

```

```
summary(mix3)$varcomp
```

```

##                VarComp VarCompSE   Zratio Constraint
## u:id.Yield-Yield   325.2072  259.0889  1.255196     Fixed
## u:units.Yield-Yield 4051.3786  352.4804 11.493912   Positive

```

8) How can I constrain two variance components to be equal?

Sometimes the built-in capacities of sommer are not flexible enough to do all what users want. One of those situations is to fix variance components to be equal. Let's simulate some multitrait data:

```

library("MASS") ## needed for mvrnorm
n <- 100
mu <- c(1,2)
Sigma <- matrix(c(10,5,5,10),2,2)
Y <- mvrnorm(n,mu,Sigma); colnames(Y) <- c("y1","y2")
## this simulates multivariate normal rvs
y <- as.vector(t(Y))
df1 <- data.frame(Y)
df2 <- data.frame(y)

```

Now lets assume that we want to fit a multitrait model with an unstructured error variance structure with the built-in capacity. That would be as easy as this:

```

mix1 <- mmmer(cbind(y1,y2)~1, rcov=~vs(units, Gtc=unsm(2)), data=df1, verbose = FALSE)
mix1$sigma

```

```

## $`u:units`
##          y1          y2
## y1 8.804435  5.324279
## y2 5.324279 10.806112

```

But now assume that you would like to constrain the variance of y1 and y2 to be equal. This requires the user to take a different approach. The user can build externally the multitrait matrices and fit them directly. Let's do this to recreate the exact same result as using the built-in capabilities:

```

X <- kronecker(rep(1,n),diag(1,2))
V1 <- matrix(c(1,0,0,0),2,2)
V2 <- matrix(c(0,0,0,1),2,2)
V3 <- matrix(c(0,1,1,0),2,2)
sig1 <- kronecker(diag(1,n),V1) # variance component 1
sig2 <- kronecker(diag(1,n),V2) # variance component 2
gam <- kronecker(diag(1,n),V3) # covariance component
# now fit the model

```

```
mix2 <- mmer(y~X-1, rcov = ~vs(sig1)+vs(sig2)+vs(gam), data=df2, verbose = FALSE)
mix2$sigmaVector
```

```
## u:sig1.y-y u:sig2.y-y u:gam.y-y
## 8.804453 10.806046 5.324242
```

Notice that we fitted a univariate model but we built the kernels and fitted those kernels one by one.

Now we will constrain the two variance components to be equal. This is done the following way:

```
sig <- sig1+sig2
mix3 <- mmer(y~X-1, rcov = ~vs(sig)+vs(gam), data=df2, iters=30, verbose = FALSE)
mix3$sigmaVector
```

```
## u:sig.y-y u:gam.y-y
## 9.805147 5.324050
```

Literature

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