Fitting genotype by environment models in sommer

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The sommer package was developed to provide R users a powerful and reliable multivariate mixed model solver. The package is focused in 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 specify heterogeneous variances, and obtain 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 fit different genotype by environment (GxE) models using the sommer package:

- 1) Single environment model
- 2) Multienvironment model: Main effect model
- 3) Multienvironment model: Diagonal model (DG)
- 4) Multienvironment model: Compund symmetry model (CS)
- 5) Multienvironment model: Compund symmetry + diagonal model (CS+DG)
- 6) Multienvironment model: Unstructured model (US)
- 7) Multienvironment model: Random regression model (RR)
- 8) Multienvironment model: Other covariance structures for GxE

When the breeder decides to run a trial and apply selection in a single environment wheter because the amount of seed is a limitation or there's no availability for any location the breeder takes the risk of selecting material for a target population of environments (TPEs) and this environment tested not being representative of the larger TPE. Therefore, many breeding programs try to based their selection decision using multi-environment trial (MET) data. Although, models could be adjusted by adding additional information like spatial information, experimental design information, etc., in this tutorial we will focus mainly on the covariance structures for GxE and the incorporation of relationship matrices for the genotype effect.

1) Single environment model

A single environment model is the one that is fitted when the breeding program can only afford one location leaving out the possible information available from other environments. This will be used to further expand to GxE models.

```
##
         Multivariate Linear Mixed Model fit by REML
    *************** sommer 4.1 ************
         logLik
                   AIC
                          BIC Method Converge
## Value -78.80875 159.6175 162.8378
                                 NR
  ______
  Variance-Covariance components:
##
                  VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                   6.529
                           2.202 2.965
                                       Positive
  units.Yield-Yield
                  13.868
                           1.633 8.494
                                       Positive
##
  Fixed effects:
   Trait
            Effect Estimate Std.Error t.value
##
## 1 Yield (Intercept)
                     11.74
                            0.4876
## Groups and observations:
##
        Yield
## u:Name
## Use the '$' sign to access results and parameters
```

In this model the only term to be estimated is the one for the germplasm (here called Name). For the sake of example we have added a relationship matrices among the levels of the random effect Name. This is just a diagonal matrix with as many rows and columns as levels present in the random effect Name, but any other non-diagonal relationship matrix could be used.

2) MET: main effect model

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The main effect model assumes that GxE doesn't exist and that the main genotype effect plus the fixed effect for environment is enough to predict the genotype effect in all locations of interest.

```
ansMain <- mmer(Yield~Env,
           random= ~ vs(Name, Gu=A),
           rcov= ~ units,
           data=DT, verbose = FALSE)
summary(ansMain)
  ______
##
         Multivariate Linear Mixed Model fit by REML
  ****************** sommer 4.1 **************
  ______
##
         logLik
                   AIC
                          BIC Method Converge
## Value -32.59421 71.18842 80.84949
                                      TRUE
                                NR
  Variance-Covariance components:
##
                 VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                   4.856
                          1.5233 3.188
                                      Positive
  units.Yield-Yield
                   8.109
                          0.9615 8.434
                                      Positive
## Fixed effects:
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept) 16.385
                           0.5849
```

3) MET: diagonal model (DG)

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The diagonal model assumes that GxE exist and that the genotype variation is expressed differently at each location, therefore fitting a variance component for the genotype effect at each location. The main drawback is that assumes no covariance among locations, like if genotypes were independent (despite the fact that is the same genotypes). The fixed effect for environment plus the location-specific BLUP is used to predict the genotype effect in each locations of interest.

```
______
         Multivariate Linear Mixed Model fit by REML
  ************* sommer 4.1 ***********
                         BIC Method Converge
         logLik
                  AIC
## Value -21.04157 48.08315 57.74421
  _____
## Variance-Covariance components:
##
                      VarComp VarCompSE Zratio Constraint
## CA.2011: Name. Yield-Yield 17.493
                              6.1099
                                    2.863
## CA.2012:Name.Yield-Yield
                              1.7662 3.022
                       5.337
                                           Positive
## CA.2013:Name.Yield-Yield
                       7.884
                              2.5526 3.089
                                           Positive
## units.Yield-Yield
                       4.381
                              0.6493 6.747
                                           Positive
## Fixed effects:
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                   16.621
                            0.948 17.532
## 2 Yield EnvCA.2012
                   -5.958
                            1.045
                                 -5.699
## 3 Yield EnvCA.2013
                   -6.662
                            1.098 -6.067
## Groups and observations:
##
            Yield
## CA.2011:Name
               41
## CA.2012:Name
               41
## CA.2013:Name
## Use the '$' sign to access results and parameters
```

4) MET: compund symmetry model (CS)

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The compound symmetry model assumes that GxE exist and that a main genotype variance-covariance component is expressed across all location. In addition, it assumes that a main genotype by environment variance is expressed across all locations. The main drawback is that assumes same variance and covariance among locations. The fixed effect for environment plus the main effect BLUP plus genotype by environment effect is used to predict the genotype effect in each location of interest.

```
##
         Multivariate Linear Mixed Model fit by REML
  ******************* sommer 4.1 **************
  ______
##
         logLik
                   AIC
                           BIC Method Converge
  Value -20.14538 46.29075 55.95182
                                 NR
                                       TRUE
  ______
  Variance-Covariance components:
##
                     VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                       3.682
                               1.691
                                     2.177
## u:Env:Name.Yield-Yield
                       5.173
                               1.495
                                     3.460
                                           Positive
## units.Yield-Yield
                       4.366
                               0.647
                                    6.748
                                           Positive
  _____
## Fixed effects:
    Trait
             Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                    16.496
                            0.6855
                                   24.065
## 2 Yield EnvCA.2012
                    -5.777
                            0.7558
                                   -7.643
## 3 Yield EnvCA.2013
                    -6.380
                            0.7960
                                   -8.015
## Groups and observations:
##
           Yield
## u:Name
              41
## u:Env:Name
## Use the '$' sign to access results and parameters
```

5) MET: compund symmetry plus diagonal (CS+DIAG)

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The compound symmetry plus diagonal model is very similar to the CS model assuming that GxE exist and that a main genotype variance-covariance component is expressed across all location. In addition, it assumes that a location-specific genotype by environment variance is expressed in each location. The main drawback is that assumes same covariance among locations. The fixed effect for environment plus the main effect BLUP plus environment-specific genotype by environment effect is used to predict the genotype effect in each location of interest.

```
ansMain <- mmer(Yield~Env,
          random= ~ vs(Name, Gu=A) + vs(ds(Env), Name, Gu=A),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansMain)
##
        Multivariate Linear Mixed Model fit by REML
## ************** sommer 4.1 ***********
  _____
##
        logLik
                 AIC
                        BIC Method Converge
## Value -18.16164 42.32327 51.98434
## Variance-Covariance components:
##
                     VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                      2.965
                             1.5055 1.969
                                         Positive
## CA.2011:Name.Yield-Yield 10.424
                             4.4544 2.340
                                         Positive
## CA.2012:Name.Yield-Yield
                      2.658
                             1.8032 1.474
                                         Positive
## CA.2013:Name.Yield-Yield
                      5.702
                             2.5113 2.271
                                         Positive
## units.Yield-Yield
                      4.398
                             0.6517 6.748
                                         Positive
## Fixed effects:
   Trait
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                  16.511
                          0.8269 19.967
## 2 Yield EnvCA.2012
                  -5.809
                          0.8593
                                -6.760
## 3 Yield EnvCA.2013
                  -6.423
                          0.9358 -6.864
## Groups and observations:
##
            Yield
## u:Name
              41
## CA.2011:Name
              41
## CA.2012:Name
              41
## CA.2013:Name
## Use the '$' sign to access results and parameters
```

6) MET: unstructured model (US)

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The unstructured model is the most flexible model assuming that GxE exist and that a environment-specific variance exist in addition to as many covariances for each environment to environment combinations. The main drawback is that is difficult to make this models converge given the big number of variance components, the fact that some of this variance or covariance components are zero and the difficult to have good starting values. The fixed effect for environment plus the environment specific BLUP (adjusted by covariances) is used to predict the genotype effect in each location of interest.

```
## ****************** sommer 4.1 **************
  ______
##
          logLik
                    AIC
                            BIC Method Converge
## Value -14.20951 34.41901 44.08008
                                   NR.
                                         TRUE
  ______
  Variance-Covariance components:
                               VarComp VarCompSE Zratio Constraint
## CA.2011:Name.Yield-Yield
                                15.994
                                         5.381
                                               2.972
                                                      Positive
## CA.2012:CA.2011:Name.Yield-Yield
                                 6.172
                                         2.503
                                               2.465
                                                      Unconstr
## CA.2012:Name.Yield-Yield
                                 5.273
                                         1.750
                                               3.013
                                                      Positive
## CA.2013:CA.2011:Name.Yield-Yield
                                 6.366
                                         3.069
                                               2.074
                                                      Unconstr
## CA.2013:CA.2012:Name.Yield-Yield
                                 0.376
                                         1.535
                                               0.245
                                                      Unconstr
## CA.2013: Name. Yield-Yield
                                 7.689
                                         2.490
                                               3.088
                                                      Positive
                                               6.748
## units.Yield-Yield
                                 4.386
                                         0.650
                                                      Positive
## Fixed effects:
    Trait
             Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                     16.341
                              0.8141
## 2 Yield EnvCA.2012
                     -5.696
                              0.7406
                                     -7.692
## 3 Yield EnvCA.2013
                     -6.286
                              0.8202 - 7.664
## Groups and observations:
##
                    Yield
## CA.2011:Name
## CA.2012:CA.2011:Name
## CA.2012:Name
                       41
## CA.2013:CA.2011:Name
                       82
## CA.2013:CA.2012:Name
                       82
## CA.2013:Name
                       41
## Use the '$' sign to access results and parameters
# adjust variance BLUPs by adding covariances
# ansUS$U[1:6] <- unsBLUP(ansUS$U[1:6])
```

7) MET: random regression model

A multi environment model is the one that is fitted when the breeding program can afford more than one location. The random regression model assumes that the environment can be seen as a continuous variable and therefore a variance component for the intercept and a variance component for the slope can be fitted. The number of variance components will depend on the order of the Legendre polynomial fitted.

```
logLik
                  AIC BIC Method Converge
                              NR
## Value -27.70318 61.40636 71.06743
                                     TRUF.
## Variance-Covariance components:
                   VarComp VarCompSE Zratio Constraint
## leg0:Name.Yield-Yield 10.392
                           3.1473 3.302
                                        Positive
                           0.9792 2.123
## leg1:Name.Yield-Yield 2.079
                                       Positive
                    6.297
                           0.8442 7.459
## units.Yield-Yield
                                       Positive
## Fixed effects:
   Trait
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept) 16.541
                        0.6770 24.432
## 2 Yield EnvCA.2012 -5.832
                          0.6425 -9.078
## 3 Yield EnvCA.2013 -6.472
                          0.8239 - 7.854
## Groups and observations:
##
         Yield
## leg0:Name
            41
## leg1:Name
            41
## Use the '$' sign to access results and parameters
In addition, an unstructured, diagonal or other variance-covariance structure can be put on top of the
polynomial model:
library(orthopolynom)
DT$EnvN <- as.numeric(as.factor(DT$Env))</pre>
ansRR <- mmer(Yield~Env,
          random= ~ vs(us(leg(EnvN,1)),Name),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansRR)
         Multivariate Linear Mixed Model fit by REML
## ***************** sommer 4.1 ************
##
         logLik
                  AIC
                         BIC Method Converge
## Value -25.56967 57.13935 66.80042
                              NR
                                    TRUF.
## Variance-Covariance components:
##
                       VarComp VarCompSE Zratio Constraint
## leg0:Name.Yield-Yield
                       10.791 3.2745 3.295
                                           Positive
## leg1:leg0:Name.Yield-Yield -2.428
                               1.3699 -1.772
                                           Unconstr
## leg1:Name.Yield-Yield
                       2.286
                               1.0404 2.197
                                           Positive
## units.Yield-Yield
                        6.260
                               0.8421 7.434
                                           Positive
## Fixed effects:
            Effect Estimate Std.Error t.value
   Trait
## 1 Yield (Intercept) 16.501 0.7778 21.216
## 2 Yield EnvCA.2012 -5.791
                          0.6704 - 8.638
## 3 Yield EnvCA.2013 -6.476 0.8554 -7.570
## -----
## Groups and observations:
##
             Yield
```

8) Other GxE covariance structures

Although not very commonly used in GxE models, the autoregressive of order 1 (AR1) and other covariance structures could be used in the GxE modeling. Here we show how to do it (not recommending it).

```
##
       Multivariate Linear Mixed Model fit by REML
## ***************** sommer 4.1 *************
logLik
               AIC
                     BIC Method Converge
## Value -19.39067 44.78134 54.4424
                          NR.
                               TRUE.
## Variance-Covariance components:
##
                 VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                  2.225
                        1.7536 1.269
                                   Positive
## u:Env:Name.Yield-Yield
                  6.424
                        1.8293 3.512
                                   Positive
## units.Yield-Yield
                  4.334
                        0.6418 6.752
 _____
## Fixed effects:
   Trait
          Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                16.484
                       0.6735
## 2 Yield EnvCA.2012
                            -7.848
                -5.780
                       0.7365
## 3 Yield EnvCA.2013
                -6.372
                       0.7799
 _____
## Groups and observations:
##
         Yield
## u:Name
           41
          123
## u:Env:Name
## Use the '$' sign to access results and parameters
```

Final remarks

Keep in mind that sommer uses the direct inversion (DI) algorithms which can be very slow for large datasets. The package is focused in problems of the type p > n (more random effect levels than observations) and models with dense covariance structures. For example, for 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 number of individuals and covariance structures or n > p (i.e. 2000 records from 200 individuals replicated 10 times with covariance structure of 200x200) as reml or other MME-based algorithms will be much faster and we recommend you to opt for those software.

Literature

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