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 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, 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 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: Unstructured model (US)
- 6) Multienvironment model: Random regression model (RR)
- 7) Multienvironment model: Other covariance structures for GxE

When the breeder decides to run a trial and apply selection in a single environment (whether because the amount of seed is a limitation or there's no availability for a location) the breeder takes the risk of selecting material for a target population of environments (TPEs) using an environment that is not representative of the larger TPE. Therefore, many breeding programs try to base their selection decision on multi-environment trial (MET) data. 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 ***********
BIC Method Converge
##
       logLik AIC
## 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 24.07
## Groups and observations:
      Yield
##
## u:Name
## Use the '$' sign to access results and parameters
# or
Ai <- as(solve(A), Class="sparseMatrix")
ansSingle <- mmec(Yield~1,
        random= ~ vsc(isc(Name), Gu=Ai),
        rcov= ~ units,
         data=DT, verbose = FALSE)
summary(ansSingle)
Multivariate Linear Mixed Model fit by REML
## ************** sommer 4.1 ***********
       logLik AIC
##
                    BIC Method Converge
## Value -359.0037 720.0074 723.2278 AI TRUE
## Variance-Covariance components:
##
            VarComp VarCompSE Zratio Constraint
## Name:Ai:isc:isc 6.474
                 1.471 4.401
                             Positive
## units:isc:isc 13.868
                  1.776 7.807
                            Positive
## Fixed effects:
##
        Estimate Std.Error t.value
## Intercept) 11.74 0.4852 24.19
## Use the '$' 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 matrix 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

Name:Ai:isc:isc 4.849

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= ~ vsr(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
                         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:
   Trait
          Effect Estimate Std. Error t. value
## 1 Yield (Intercept) 16.385 0.5849 28.012
## 2 Yield EnvCA.2012 -5.688
                      0.5741 - 9.908
## 3 Yield EnvCA.2013 -6.218
                     0.6107 -10.182
## Groups and observations:
      Yield
## u:Name
        41
## Use the '$' sign to access results and parameters
# or
Ai <- as(solve(A), Class="sparseMatrix")
ansMain <- mmec(Yield~Env,
        random= ~ vsc(isc(Name), Gu=Ai),
        rcov= ~ units,
         data=DT, verbose = FALSE)
summary(ansMain)
Multivariate Linear Mixed Model fit by REML
## *************** sommer 4.1 ************
AIC
                     BIC Method Converge
       logLik
## Value -313.3008 632.6015 642.2626
                        ΑI
## Variance-Covariance components:
            VarComp VarCompSE Zratio Constraint
```

1.377 3.522 Positive

```
8.108
                     1.545 5.249
## units:isc:isc
                               Positive
 ______
## Fixed effects:
##
        Estimate Std.Error t.value
## Intercept
          16.386
                 0.5842 28.048
## CA.2012
          -5.689
                 0.5740 - 9.911
## CA.2013
          -6.219
                 0.6106 -10.186
## Use the '$' sign to access results and parameters
```

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 exists 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 this model assumes no covariance among locations, as 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
  ##
         logLik
                   AIC
                          BIC Method Converge
  Value -21.04157 48.08315 57.74421
                                NR.
                                      TRUE
  ##
  Variance-Covariance components:
                      VarComp VarCompSE Zratio Constraint
## CA.2011:Name.Yield-Yield 17.493
                               6.1099 2.863
                                            Positive
## CA.2012:Name.Yield-Yield
                        5.337
                               1.7662 3.022
                                            Positive
## CA.2013:Name.Yield-Yield
                        7.884
                               2.5526 3.089
                                            Positive
## units.Yield-Yield
                        4.381
                               0.6493 6.747
  ______
## Fixed effects:
    Trait
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                   16.621
                            0.948 17.532
                   -5.958
## 2 Yield EnvCA.2012
                            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
```

```
Ai <- as(solve(A), Class="sparseMatrix")
ansDG <- mmec(Yield~Env,
          random= ~ vsc(dsc(Env),isc(Name), Gu=Ai),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansDG)
##
          Multivariate Linear Mixed Model fit by REML
  _____
         logLik
                  AIC
                        BIC Method Converge
## Value -301.9224 609.8449 619.506
                               AΙ
                                    TRUE
## Variance-Covariance components:
                        VarComp VarCompSE Zratio Constraint
## Env:Name:Ai:CA.2011:CA.2011
                        15.792
                                 3.307
                                     4.775
                                            Positive
## Env:Name:Ai:CA.2012:CA.2012
                         5.192
                                 2.490 2.085
                                            Positive
## Env:Name:Ai:CA.2013:CA.2013
                         7.717
                                 2.732 2.825
                                            Positive
                         4.744
                                 1.697 2.796
## units:isc:isc
                                            Positive
## Fixed effects:
         Estimate Std.Error t.value
           16.622
                    0.911 18.245
## Intercept
## CA.2012
           -5.962
                    1.012
                        -5.888
## CA.2013
           -6.664
                    1.067 -6.249
## 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 exists 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 the model assumes the same variance and covariance among locations. The fixed effect for environment plus the main effect for BLUP plus genotype-by-environment effect is used to predict the genotype effect in each location of interest.

```
## -----
## Variance-Covariance components:
                  VarComp VarCompSE Zratio Constraint
## u:Name.Yield-Yield
                   3.682
                          1.691 2.177
                                     Positive
## u:Env:Name.Yield-Yield 5.173
                          1.495 3.460
## units.Yield-Yield
                   4.366
                          0.647 6.748 Positive
## Fixed effects:
           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
          123
## -----
## Use the '$' sign to access results and parameters
E <- diag(length(unique(DT$Env)));rownames(E) <- colnames(E) <- unique(DT$Env)
Ei <- solve(E)
Ai <- solve(A)
EAi <- kronecker(Ei, Ai, make.dimnames = TRUE)
Ei <- as(Ei, Class="sparseMatrix")</pre>
Ai <- as(Ai, Class="sparseMatrix")
EAi <- as(EAi, Class="sparseMatrix")</pre>
ansCS <- mmec(Yield~Env,
          random= ~ vsc(isc(Name), Gu=Ai) + vsc(isc(Env:Name), Gu=EAi),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansCS)
Multivariate Linear Mixed Model fit by REML
## ************** sommer 4.1 ***********
logLik
                AIC
                       BIC Method Converge
## Value -300.8632 607.7264 617.3875 AI
## Variance-Covariance components:
                 VarComp VarCompSE Zratio Constraint
##
## Name:Ai:isc:isc
                  3.703 1.699 2.180
## Env:Name:EAi:isc:isc 5.132
                         1.876 2.736
                                    Positive
## units:isc:isc
                  4.466
                         1.611 2.772
                                    Positive
## Fixed effects:
        Estimate Std.Error t.value
## Intercept 16.496 0.6863 24.035
          -5.777
## CA.2012
                 0.7564 -7.637
## CA.2013
         -6.380
                 0.7967 -8.008
## Use the '$' sign to access results and parameters
```

5) 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 exists and that an environment-specific variance exists in addition to as many covariances for each environment-to-environment combinations. The main drawback is that is difficult to make this models converge because of the large number of variance components, the fact that some of these variance or covariance components are zero, and the difficulty in choosing 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.

```
ansUS <- mmer(Yield~Env,
           random= ~ vsr(usr(Env), Name, Gu=A),
           rcov= ~ units,
           data=DT, verbose = FALSE)
summary(ansUS)
  ______
           Multivariate Linear Mixed Model fit by REML
  ______
##
                  AIC
                          BIC Method Converge
         logLik
## Value -14.20951 34.41901 44.08008
                                NR
  ______
## Variance-Covariance components:
##
                            VarComp VarCompSE Zratio Constraint
## CA.2011:Name.Yield-Yield
                             15.994
                                      5.381
                                           2.972
## 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
                              4.386
## units.Yield-Yield
                                      0.650
                                           6.748
                                                 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
                     41
## CA.2012:CA.2011:Name
                     82
## 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])
# or
Ai <- solve(A)
```

```
Ai <- as(Ai, Class="sparseMatrix")
ansUS <- mmec(Yield~Env,
          random= ~ vsc(usc(Env),isc(Name), Gu=Ai),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansUS)
##
         Multivariate Linear Mixed Model fit by REML
## ***************** sommer 4.1 **************
  _____
##
                         BIC Method Converge
         logLik
                  AIC
## Value -302.6944 611.3888 621.0499
 ______
## Variance-Covariance components:
##
                       VarComp VarCompSE Zratio Constraint
## Env:Name:Ai:CA.2011:CA.2011 14.002
                                3.1067 4.5071
                                            Positive
## Env:Name:Ai:CA.2011:CA.2012
                         4.951
                                1.7036 2.9059
                                            Unconstr
## Env:Name:Ai:CA.2012:CA.2012
                        4.394
                                2.0089 2.1874
                                            Positive
## Env:Name:Ai:CA.2011:CA.2013
                         6.145
                                2.1317 2.8828
                                            Unconstr
## Env:Name:Ai:CA.2012:CA.2013
                         0.604
                                0.6245 0.9672
                                            Unconstr
## Env:Name:Ai:CA.2013:CA.2013
                         7.946
                                2.5227 3.1497
                                            Positive
## units:isc:isc
                         2.663
                                1.0926 2.4371
                                            Positive
## Fixed effects:
         Estimate Std.Error t.value
## Intercept 16.341
                   0.7432 21.987
## CA.2012
           -5.685
                   0.6740 -8.435
## CA.2013
           -6.265
                   0.7418 -8.446
## Use the '$' sign to access results and parameters
```

6) 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.

```
library(orthopolynom)
DT$EnvN <- as.numeric(as.factor(DT$Env))</pre>
ansRR <- mmer(Yield~Env,
         random= ~ vsr(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 -27.70318 61.40636 71.06743
```

```
## Variance-Covariance components:
##
                  VarComp VarCompSE Zratio Constraint
## leg0:Name.Yield-Yield 10.392 3.1473 3.302 Positive
                          0.9792 2.123 Positive
## leg1:Name.Yield-Yield 2.079
## units.Yield-Yield
                    6.297
                          0.8442 7.459
                                      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
## Use the '$' sign to access results and parameters
# or
ansRR <- mmec(Yield~Env,
          random= ~ vsc(dsc(leg(EnvN,1)),isc(Name)),
          rcov= ~ units,
          data=DT, verbose = FALSE)
summary(ansRR)
        Multivariate Linear Mixed Model fit by REML
## *************** sommer 4.1 ************
AIC
                        BIC Method Converge
        logLik
## Value -308.4122 622.8243 632.4854 AI TRUE
## Variance-Covariance components:
                 VarComp VarCompSE Zratio Constraint
## EnvN:Name:leg0:leg0 10.276 2.278 4.511 Positive
                         1.403 1.487
## EnvN:Name:leg1:leg1 2.086
                                     Positive
## units:isc:isc
                  6.430
                         1.709 3.762
## Fixed effects:
        Estimate Std.Error t.value
## Intercept 16.542 0.6745 24.523
## CA.2012
          -5.833
                  0.6405 -9.107
## CA.2013
         -6.473 0.8217 -7.877
## -----
## Use the '$' 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= ~ vsr(usr(leg(EnvN,1)),Name),
          rcov= ~ units,
```

```
data=DT, verbose = FALSE)
summary(ansRR)
Multivariate Linear Mixed Model fit by REML
## ************** sommer 4.1 ***********
AIC
                     BIC Method Converge
        logLik
## Value -25.56967 57.13935 66.80042 NR
                               TRUF.
## Variance-Covariance components:
                   VarComp VarCompSE Zratio Constraint
                          3.2745 3.295
## leg0:Name.Yield-Yield
                    10.791
                                     Positive
## leg1:leg0:Name.Yield-Yield -2.428
                           1.3699 -1.772
                                     Unconstr
                         1.0404 2.197
## leg1:Name.Yield-Yield 2.286
                                     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
               -6.476
## 3 Yield EnvCA.2013
                       0.8554 - 7.570
## Groups and observations:
##
           Yield
## leg0:Name
             41
## leg1:leg0:Name
             82
## leg1:Name
             41
## Use the '$' sign to access results and parameters
# or
ansRR <- mmec(Yield~Env,
         random= ~ vsc(usc(leg(EnvN,1)),isc(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 -309.2045 624.409 634.0701 AI
                               TRUE
## Variance-Covariance components:
##
               VarComp VarCompSE Zratio Constraint
## EnvN:Name:leg0:leg0 10.5273 2.0637 5.1012
                                 Positive
## EnvN:Name:leg0:leg1 0.1493 0.1636 0.9126
                                 Unconstr
                     1.1742 1.7789
## EnvN:Name:leg1:leg1 2.0889
                                 Positive
## units:isc:isc
               7.2282
                      1.8573 3.8917
                                Positive
## Fixed effects:
```

7) 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).

```
E \leftarrow AR1(DT\$Env) \# can be AR1() or CS(), etc.
rownames(E) <- colnames(E) <- unique(DT$Env)</pre>
EA <- kronecker(E,A, make.dimnames = TRUE)
ansCS <- mmer(Yield~Env,
           random= ~ vsr(Name, Gu=A) + vsr(Env:Name, Gu=EA),
           rcov= ~ units,
           data=DT, verbose = FALSE)
summary(ansCS)
##
         Multivariate Linear Mixed Model fit by REML
## ***************** sommer 4.1 ************
  _____
##
                          BIC Method Converge
         logLik
                   AIC
## Value -19.39067 44.78134 54.4424
## =============
## 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
                                           Positive
## ============
## Fixed effects:
   Trait
            Effect Estimate Std.Error t.value
## 1 Yield (Intercept)
                   16.484
                            0.6735 24.474
## 2 Yield EnvCA.2012
                    -5.780
                            0.7365 - 7.848
## 3 Yield EnvCA.2013
                   -6.372
                            0.7799 -8.170
## Groups and observations:
##
           Yield
## u:Name
              41
```

Literature

u:Env:Name

Use the '\$' sign to access results and parameters

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