Diagonal random-effects covariance matrix using the lme4::modular framework

Introduction

This document demonstrates how to implement a diagonal random effects covariance matrix using the **lme4** package in R. The goal is to fit a mixed-effects model with a diagonal covariance structure for the random effects and compare the results with the **glmmTMB** package.

Step 1: Load Required Libraries and Data

```
library(lme4)

## Loading required package: Matrix
library(nloptr)
library(glmmTMB)

data(cbpp)
```

Step 2: Prepare the Model Formula

Step 3: Create the Deviance Function

```
devfun <- mkLmerDevfun(lf$fr, lf$X, lf$reTrms)</pre>
```

Step 4: Write a Wrapper Function for Diagonal Covariance

```
diagonal_wrapper <- function(theta_diag) {
  theta <- numeric(length(lf$reTrms$lower))

  theta[lower_indices == 0] <- theta_diag

  devfun(theta)
}</pre>
```

Step 5: Fit the Model Using nloptwrap

```
theta_diag_init <- rep(0, sum(lower_indices == 0))
lower_bounds <- rep(0, length(theta_diag_init))</pre>
```

```
upper_bounds <- rep(Inf, length(theta_diag_init))

opt <- nloptwrap(
  par = theta_diag_init,
  fn = diagonal_wrapper,
  lower = lower_bounds,
  upper = upper_bounds,
  control = list(algorithm = "NLOPT_LN_BOBYQA")
)</pre>
```

Step 6: Create the merMod Object

```
lmer_fit <- mkMerMod(</pre>
 rho = environment(devfun),
 opt = opt,
 reTrms = lf$reTrms,
 fr = lf$fr,
 mc = match.call()
print(lmer_fit)
## Linear mixed model fit by REML ['lmerMod']
## REML criterion at convergence: -58.918
## Random effects:
## Groups
            Name
                         Std.Dev. Corr
## herd
             (Intercept) 4.161e-07
##
             period2
                         0.000e+00 NaN
##
             period3
                         8.361e-02 0.00 NaN
##
                         2.129e-07 0.00 NaN 0.00
             period4
## Residual
                         1.179e-01
## Number of obs: 56, groups: herd, 15
## Fixed Effects:
## (Intercept)
                    period2
                                 period3
                                               period4
##
        0.2198
                    -0.1458
                                 -0.1305
                                               -0.1785
```

Step 7: Compare with glmmTMB

```
glmmTMB_fit <- glmmTMB(incidence / size ~ period + diag(period | herd), data = cbpp, REML = TRUE)
print(summary(glmmTMB_fit))
## Family: gaussian (identity)
## Formula:
                    incidence/size ~ period + diag(period | herd)
## Data: cbpp
##
                      logLik deviance df.resid
##
       AIC
                BIC
                                -58.9
##
      -40.9
              -22.7
                        29.5
##
## Random effects:
## Conditional model:
## Groups Name
                        Variance Std.Dev. Corr
## herd
            (Intercept) 4.371e-11 6.611e-06
```

```
##
                         2.128e-13 4.613e-07 0.00
             period2
##
                         6.990e-03 8.361e-02 0.00 0.00
             period3
             period4
                         2.729e-15 5.224e-08 0.00 0.00 0.00
##
                         1.390e-02 1.179e-01
## Residual
## Number of obs: 56, groups: herd, 15
##
## Dispersion estimate for gaussian family (sigma^2): 0.0139
##
## Conditional model:
               Estimate Std. Error z value Pr(>|z|)
##
## (Intercept)
                 0.2198
                                NA
                                         NA
                -0.1458
                                NA
                                         NA
                                                  NA
## period2
## period3
                -0.1305
                                NΑ
                                         NA
                                                  NA
                                         NA
## period4
                -0.1785
                                NA
                                                  NA
```

Comparison of Results

Fixed Effects

We compare the fixed effects estimates from lme4 and glmmTMB.

```
# Compare fixed effects
cat("lme4 fixed effects:\n")
## lme4 fixed effects:
print(fixef(lmer_fit))
## (Intercept)
                   period2
                               period3
                                           period4
     0.2197948 -0.1457808 -0.1304627
                                        -0.1785360
cat("glmmTMB fixed effects:\n")
## glmmTMB fixed effects:
print(fixef(glmmTMB_fit)$cond)
## (Intercept)
                   period2
                               period3
                                           period4
     0.2197948 -0.1457808 -0.1304627 -0.1785360
```

Random Effects Standard Deviations

We compare the random effects standard deviations from lme4 and glmmTMB.

```
# Compare random effects standard deviations
cat("lme4 random effects standard deviations:\n")
```

lme4 random effects standard deviations:

```
print(VarCorr(lmer_fit)$herd)
```

```
period4
                (Intercept) period2
                                        period3
                                  0 0.00000000 0.000000e+00
## (Intercept) 1.731753e-13
## period2
              0.000000e+00
                                  0 0.000000000 0.000000e+00
              0.000000e+00
                                  0 0.006989957 0.000000e+00
## period3
               0.000000e+00
                                  0 0.000000000 4.532982e-14
## period4
## attr(,"stddev")
## (Intercept)
                     period2
                                  period3
                                               period4
## 4.161434e-07 0.000000e+00 8.360596e-02 2.129080e-07
## attr(,"correlation")
```

```
##
               (Intercept) period2 period3 period4
## (Intercept)
                                NaN
                                           0
                          1
                                                   0
## period2
                        NaN
                                  1
                                        NaN
                                                 NaN
## period3
                          0
                                           1
                                                   0
                                NaN
## period4
                          0
                                NaN
                                           0
                                                   1
cat("glmmTMB random effects standard deviations:\n")
## glmmTMB random effects standard deviations:
print(VarCorr(glmmTMB_fit)$cond$herd)
##
                                                             period4
                 (Intercept)
                                  period2
                                               period3
## (Intercept) 4.370748e-11 0.000000e+00 0.000000000 0.000000e+00
               0.000000e+00 2.127808e-13 0.000000000 0.000000e+00
## period2
## period3
               0.000000e+00 0.000000e+00 0.006989948 0.000000e+00
## period4
               0.000000e+00 0.000000e+00 0.000000000 2.728778e-15
## attr(,"stddev")
   (Intercept)
                      period2
                                   period3
                                                 period4
## 6.611164e-06 4.612817e-07 8.360591e-02 5.223770e-08
## attr(,"correlation")
##
               (Intercept) period2 period3 period4
## (Intercept)
                                  0
                          0
                                  1
                                           0
                                                   0
## period2
## period3
                          0
                                  0
                                           1
                                                   0
                          0
                                  0
                                           0
## period4
                                                   1
## attr(,"blockCode")
## diag
##
      0
```

Conclusion

The results show that the fixed effects estimates are identical between **lme4** and **glmmTMB**. The random effects standard deviations are also consistent, with minor differences due to numerical precision and optimization algorithms. The diagonal covariance structure was successfully implemented in both models.