On the usage of the pbkrtest package

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Contents

1 Introduction

At the time of writing there are several versions of the lme4 package available. We will use the development version of the lme4 package from GitHub instead of the CRAN version at https://github.com/lme4/lme4. The reason is that the GitHub version is numerically more stable. The GitHub version of lme4 is installed by

```
R> library(devtools)
R> install_github("lme4", user = "lme4")
```

On Windows platforms, the above steps require that Rtools utilities (http://cran.r-project.org/bin/windows/Rtools/index.html) are installed.

The shoes data is a list of two vectors, giving the wear of shoes of materials A and B for one foot each of ten boys.

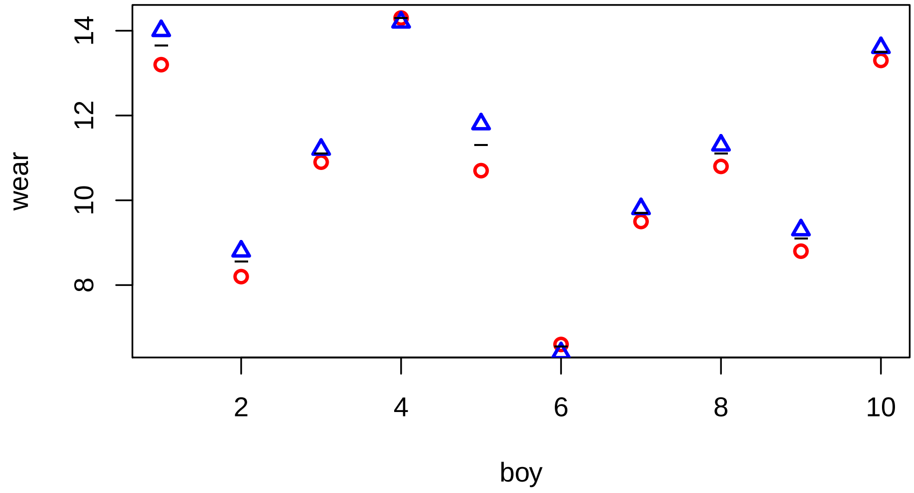
```
R> data(shoes, package="MASS")
R> shoes

$A
 [1] 13.2  8.2 10.9 14.3 10.7  6.6  9.5 10.8  8.8 13.3
```

```
$B
 [1] 14.0  8.8 11.2 14.2 11.8  6.4  9.8 11.3  9.3 13.6
```

A plot clearly reveals that boys wear their shoes differently.

```
R> plot(A~1, data=shoes, col='red',lwd=2, pch=1, ylab="wear", xlab="boy")
R> points(B~1, data=shoes, col='blue',lwd=2,pch=2)
R> points(I((A+B)/2)~1, data=shoes, pch='-', lwd=2)
```



One option for testing the effect of materials is to make a paired *t*–test. The following forms are equivalent:

```
R> r1<-t.test(shoes$A, shoes$B, paired=T)
R> r2<-t.test(shoes$A-shoes$B)
R> r1

        Paired t-test

data:  shoes$A and shoes$B
t = -3.3489, df = 9, p-value = 0.008539
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -0.6869539 -0.1330461
sample estimates:
mean of the differences
                  -0.41
```

To work with data in a mixed model setting we create a dataframe, and for later use we also create an imbalanced version of data:

```
R> boy <- rep(1:10,2)
R> boyf<- factor(letters[boy])
```

```
R> mat <- factor(c(rep("A", 10), rep("B",10)))
R> ## Balanced data:
R> shoe.b <- data.frame(wear=unlist(shoes), boy=boy, boyf=boyf, mat=mat)
R> head(shoe.b)

   wear boy boyf mat
A1 13.2   1    a   A
A2  8.2   2    b   A
A3 10.9   3    c   A
A4 14.3   4    d   A
A5 10.7   5    e   A
A6  6.6   6    f   A

R> ## Imbalanced data; delete (boy=1, mat=1) and (boy=2, mat=b)
R> shoe.i <-  shoe.b[-c(1,12),]
```

We fit models to the two datasets:

```
R> lmm1.b  <- lmer( wear ~ mat + (1|boyf), data=shoe.b )
R> lmm0.b  <- update( lmm1.b, .~. - mat)
R> lmm1.i  <- lmer( wear ~ mat + (1|boyf), data=shoe.i )
R> lmm0.i  <- update(lmm1.i, .~. - mat)
```

The asymptotic likelihood ratio test shows stronger significance than the t–test:

```
R> anova( lmm1.b, lmm0.b, test="Chisq" ) ## Balanced data

Data: shoe.b
Models:
lmm0.b: wear ~ (1 | boyf)
lmm1.b: wear ~ mat + (1 | boyf)
       Df    AIC    BIC  logLik deviance Chisq Chi Df Pr(>Chisq)
lmm0.b  3 67.909 70.896 -30.955   61.909
lmm1.b  4 61.817 65.800 -26.909   53.817 8.092      1   0.004446 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R> anova( lmm1.i, lmm0.i, test="Chisq" ) ## Imbalanced data

Data: shoe.i
Models:
lmm0.i: wear ~ (1 | boyf)
lmm1.i: wear ~ mat + (1 | boyf)
       Df    AIC    BIC  logLik deviance Chisq Chi Df Pr(>Chisq)
lmm0.i  3 63.869 66.540 -28.934   57.869
lmm1.i  4 60.777 64.339 -26.389   52.777 5.092      1    0.02404 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

2 Kenward–Roger approach

The Kenward–Roger approximation is exact for the balanced data in the sense that it produces the same result as the paired t–test.

```
R> ( kr.b<-KRmodcomp(lmm1.b, lmm0.b) )
```

```
F-test with Kenward-Roger approximation; computing time: 0.11 sec.
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
        stat    ndf    ddf F.scaling  p.value
Ftest 11.215  1.000  9.000         1 0.008539 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
R> summary( kr.b )
```

```
F-test with Kenward-Roger approximation; computing time: 0.11 sec.
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
         stat    ndf    ddf F.scaling  p.value
Ftest  11.215  1.000  9.000         1 0.008539 **
FtestU 11.215  1.000  9.000           0.008539 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Relevant information can be retrieved with

```
R> getKR(kr.b, "ddf")
```

```
[1] 9
```

For the imbalanced data we get

```
R> ( kr.i<-KRmodcomp(lmm1.i, lmm0.i) )
```

```
F-test with Kenward-Roger approximation; computing time: 0.07 sec.
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
        stat    ndf    ddf F.scaling p.value
Ftest 5.9893 1.0000 7.0219         1 0.04418 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Notice that this result is similar to but not identical to the paired t–test when the two relevant boys are removed:

```
R> shoes2 <- list(A=shoes$A[-(1:2)], B=shoes$B[-(1:2)])
R> t.test(shoes2$A, shoes2$B, paired=T)
```

```
        Paired t-test

data:  shoes2$A and shoes2$B
t = -2.3878, df = 7, p-value = 0.04832
```

```
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -0.671721705 -0.003278295
sample estimates:
mean of the differences
                -0.3375
```

3 Parametric bootstrap

Parametric bootstrap provides an alternative but many simulations are often needed to provide credible results (also many more than shown here; in this connection it can be useful to exploit that computings can be made en parallel, see the documentation):

```
R> ( pb.b <- PBmodcomp(lmm1.b, lmm0.b, nsim=500) )
```

```
Parametric bootstrap test; time: 14.71 sec; samples: 500 extremes: 3;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
         stat df   p.value
LRT    8.1197  1 0.004379 **
PBtest 8.1197    0.007984 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
R> summary( pb.b )
```

```
Parametric bootstrap test; time: 14.71 sec; samples: 500 extremes: 3;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
           stat     df    ddf   p.value
PBtest   8.1197               0.007984 **
Gamma    8.1197               0.009569 **
Bartlett 6.4309 1.0000        0.011215 *
F        8.1197 1.0000 9.6161 0.017918 *
LRT      8.1197 1.0000        0.004379 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

For the imbalanced data, the result is similar to the result from the paired t test.

```
R> ( pb.i<-PBmodcomp(lmm1.i, lmm0.i, nsim=500) )
```

```
Parametric bootstrap test; time: 15.50 sec; samples: 500 extremes: 18;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
         stat df p.value
LRT    5.1151  1 0.02372 *
PBtest 5.1151    0.03792 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
R> summary( pb.i )
```

```
Parametric bootstrap test; time: 15.50 sec; samples: 500 extremes: 18;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
           stat     df    ddf p.value
PBtest   5.1151               0.03792 *
Gamma    5.1151               0.04578 *
Bartlett 4.1799 1.0000        0.04091 *
F        5.1151 1.0000 10.939 0.04509 *
LRT      5.1151 1.0000        0.02372 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

A Matrices for random effects

The matrices involved in the random effects can be obtained with

```
R> shoe3 <- subset(shoe.b, boy<=5)
R> shoe3 <- shoe3[order(shoe3$boy), ]
R> lmm1  <- lmer( wear ~ mat + (1|boyf), data=shoe3 )
R> str( SG <- get_SigmaG( lmm1 ), max=2)
```

```
List of 3
 $ Sigma   :Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
 $ G       :List of 2
  ..$ :Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
  ..$ :Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
 $ n.ggamma: int 2
```

```
R> round( SG$Sigma*10 )
```

```
10 x 10 sparse Matrix of class "dgCMatrix"

 [1,] 53 52  .  .  .  .  .  .  .  .
 [2,] 52 53  .  .  .  .  .  .  .  .
 [3,]  .  . 53 52  .  .  .  .  .  .
 [4,]  .  . 52 53  .  .  .  .  .  .
 [5,]  .  .  .  . 53 52  .  .  .  .
 [6,]  .  .  .  . 52 53  .  .  .  .
 [7,]  .  .  .  .  .  . 53 52  .  .
 [8,]  .  .  .  .  .  . 52 53  .  .
 [9,]  .  .  .  .  .  .  .  . 53 52
[10,]  .  .  .  .  .  .  .  . 52 53
```

```
R> SG$G
```

```
[[1]]
10 x 10 sparse Matrix of class "dgCMatrix"
```

```
 [1,] 1 1 . . . . . . . .
 [2,] 1 1 . . . . . . . .
 [3,] . . 1 1 . . . . . .
 [4,] . . 1 1 . . . . . .
 [5,] . . . . 1 1 . . . .
 [6,] . . . . 1 1 . . . .
 [7,] . . . . . . 1 1 . .
 [8,] . . . . . . 1 1 . .
 [9,] . . . . . . . . 1 1
[10,] . . . . . . . . 1 1

[[2]]
10 x 10 sparse Matrix of class "dgCMatrix"

 [1,] 1 . . . . . . . . .
 [2,] . 1 . . . . . . . .
 [3,] . . 1 . . . . . . .
 [4,] . . . 1 . . . . . .
 [5,] . . . . 1 . . . . .
 [6,] . . . . . 1 . . . .
 [7,] . . . . . . 1 . . .
 [8,] . . . . . . . 1 . .
 [9,] . . . . . . . . 1 .
[10,] . . . . . . . . . 1
```