On the usage of the **pbkrtest** package

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`pbkrtest` version 0.3-7 as of 2013-10-01

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.

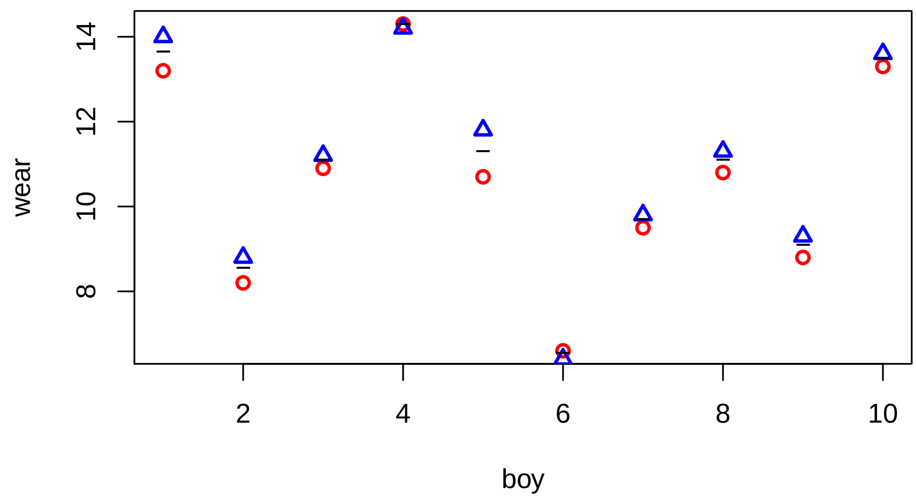
```
R> data(shoes, package="MASS")
R> shoes

$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: 0.14 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: 0.14 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: 0.06 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: 21.20 sec; samples: 500 extremes: 5;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
         stat df  p.value
LRT    8.1197  1 0.004379 **
PBtest 8.1197    0.011976 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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

```
Parametric bootstrap test; time: 21.20 sec; samples: 500 extremes: 5;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
           stat     df    ddf  p.value
PBtest   8.1197               0.011976 *
Gamma    8.1197               0.011056 *
Bartlett 6.2551 1.0000        0.012384 *
F        8.1197 1.0000 8.7093 0.019733 *
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: 21.40 sec; samples: 500 extremes: 26;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
         stat df p.value
LRT    5.1151  1 0.02372 *
PBtest 5.1151    0.05389 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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

```
Parametric bootstrap test; time: 21.40 sec; samples: 500 extremes: 26;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
           stat     df    ddf p.value
PBtest   5.1151               0.05389 .
Gamma    5.1151               0.05643 .
Bartlett 3.5738 1.0000        0.05870 .
F        5.1151 1.0000 6.6375 0.06022 .
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
```