

On the usage of the `pbkrtest` package

Søren Højsgaard and Ulrich Halekoh

`pbkrtest` version 0.4-5 as of 2016-01-20

Contents

1	Introduction	1
2	Kenward–Roger approach	3
3	Parametric bootstrap	4
A	Matrices for random effects	5

1 Introduction

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.

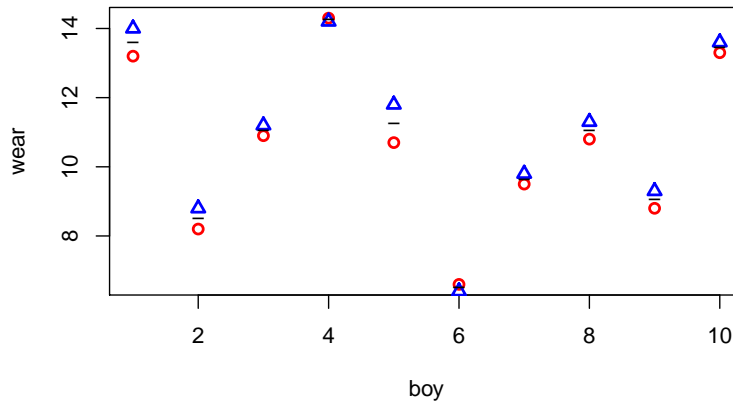
```
R> data(shoes, package="MASS")
R> shoes
```

```
$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: 0.10 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: 0.10 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: 0.04 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: 9.45 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: 9.45 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          0.006505 **
Bartlett 7.0830 1.0000      0.007782 **
F         8.1197 1.0000 15.664 0.011780 *
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: 9.99 sec; samples: 500 extremes: 17;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
      stat df p.value
LRT     5.1151 1 0.02372 *
PBtest  5.1151 0.03593 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R> summary( pb.i )

Parametric bootstrap test; time: 9.99 sec; samples: 500 extremes: 17;
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
      stat      df      ddf p.value
PBtest  5.1151          0.03593 *
Gamma    5.1151          0.03752 *
Bartlett 4.3033 1.0000      0.03804 *
F         5.1151 1.0000 12.601 0.04210 *
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

```