On the usage of the pbkrtest package

Søren Højsgaard and Ulrich Halekoh

pbkrtest version 0.5.1 as of 2021-03-09

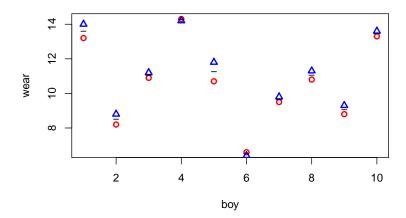
Contents

1	Introduction	1
2	Kenward–Roger approach	3
3	Parametric bootstrap	4
\mathbf{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:

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])</pre>
R> mat <- factor(c(rep("A", 10), rep("B",10)))</pre>
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
                    Α
          2
A2 8.2
                    Α
                b
A3 10.9
          3
                С
                    Α
A4 14.3
          4
                d
                    Α
A5 10.7
          5
                е
                    Α
                f
                    Α
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)</pre>
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)
      npar AIC BIC logLik deviance Chisq Df Pr(>Chisq)
lmm0.b 3 67.909 70.896 -30.955
                                   61.909
                                   53.817 8.092 1
                                                    0.004446 **
lmm1.b
         4 61.817 65.800 -26.909
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)
      npar AIC BIC logLik deviance Chisq 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
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) )</pre>
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; time: 0.18 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) )</pre>
large : wear ~ mat + (1 | boyf)
small : wear ~ (1 | boyf)
                        ddf F.scaling p.value
        stat ndf
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):

```
Bootstrap test; time: 4.42 sec; samples: 500; extremes: 1;
large : wear ~ mat + (1 | boyf)
wear ~ (1 | boyf)
           stat
                   df
                          ddf p.value
LRT
         8.1197 1.0000
                              0.004379 **
PBtest 8.1197
                              0.003992 **
Gamma
        8.1197
                              0.004411 **
Bartlett 7.9409 1.0000
                              0.004833 **
        8.1197 1.0000 90.806 0.005417 **
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
R> (pb.i<-PBmodcomp(lmm1.i, lmm0.i, nsim=500, cl=2))
Bootstrap test; time: 4.42 sec; samples: 500; extremes: 22;
large : wear ~ mat + (1 | boyf)
wear ~ (1 | boyf)
         stat df p.value
      5.1151 1 0.02372 *
LRT
PBtest 5.1151
                0.04591 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R> summary( pb.i )
Bootstrap test; time: 4.42 sec; samples: 500; extremes: 22;
large : wear ~ mat + (1 | boyf)
wear ~ (1 | boyf)
                         ddf p.value
           stat
                   df
I.R.T
         5.1151 1.0000
                            0.02372 *
PBtest
       5.1151
                             0.04591 *
Gamma
        5.1151
                             0.05198 .
Bartlett 4.2362 1.0000
                             0.03957 *
       5.1151 1.0000 11.64 0.04372 *
F
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</pre>
```

```
..$ :Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
 $ n.ggamma: int 2
R> round( SG$Sigma*10 )
10 x 10 sparse Matrix of class "dgCMatrix"
A1 53 52 . . . . . .
B1 52 53 . . . . . .
A2 . . 53 52 . .
B2 . . 52 53 . .
A3 . . . . 53 52 . . . .
B3 . . . . 52 53 . .
A4 . . . . . . . 53 52
B4 . . . . . . 52 53 . .
A5 . . . . . . . . . 53 52
      . . . . . . . . 52 53
R> SG$G
[[1]]
10 x 10 sparse Matrix of class "dgCMatrix"
A1 1 1 . . . . . . . .
B1 1 1 . . . . . . . .
A2 . . 1 1 . . . . . .
B2 . . 1 1 . . . . . .
A3 . . . . 1 1 . . . .
B3 . . . . 1 1 . . . .
A4 . . . . . . 1 1 . .
B4 . . . . . . 1 1 . .
A5 . . . . . . . . 1 1
B5 . . . . . . . 1 1
[[2]]
10 x 10 sparse Matrix of class "dgCMatrix"
 [1,] 1 . . . . . . . . .
 [2,] . 1 . . . . . . . .
 [3,] . . 1 . . . . . .
 [4,] . . . 1 . . . . .
 [5,] . . . 1 . . . .
 [6,] . . . . 1 . . .
 [7,] \ldots \ldots 1 \ldots
 [8,] . . . . . . 1 . .
 [9,] . . . . . . . 1 .
[10,] . . . . . . . . . 1
```