R Codes Used for X2. MATI CASE STUDY--Chocolate Calcium Chew

|  |  |  |  |
| --- | --- | --- | --- |
| No. | Name | Purpose | Input of the codes |
| 1 | labfanout | Plot the T-I predicted group curves | x: original T-I data file (minus times in col 1)  a: vector containing the numbers of curves in each group  nn: codes of products (groups)  xtpt: x value where group level code annotated  xlab: x-axis label  ylab: y-axis label (attribute name)  title: title for plot |
| 2 | fdaparamf | Calculate parameters of the mean curve for one or multiple products for a specified attribute | x: original T-I data file (with times in col 1)  a: vector containing the numbers of curves in each group  nn: codes of products (groups) |
| 3 | w3datf | Format attribute dataset with 1 summary parameter for aov | Dataset for one attribute with 3 cols: assessor, sample and parameter value |
| 4 | fanpairstests | Perform the fanova.tests on all possible pairs | x: original T-I data file (with times in col 1)  a: vector containing the numbers of curves in each group  nn: codes of products (groups)  attlab: attribute name/label |

Examples are provided below using the *Identifying Flavor (chocolate)* attribute data for the four samples from the MATI case study.

R packages fda and fdANOVA are used for analysis and graphics.

STEP 1: Plot T-I and calculate parameters of the mean curve

1A) Plot the T-I mean group curves

> fanout <- labfanout(w3fa6[,2:35], c(9,8,8,9),w3fp,10, "Time (secs)", "Identifying Flavor", "Mean Curves of Products")

> fanout

A graph of a graph showing the amount of curves of products

Description automatically generated with medium confidence

1B) Calculate parameters of the mean curve

> fdaparamf(w3fa6[,1:10], c(9),w3fp[1])

Tmax Imax AUC

125 32 4.35 341.02

> fdaparamf(w3fa6, c(9,8,8,9),w3fp)

Tmax Imax AUC

125 32 4.35 341.02

416 29 4.51 355.14

576 36 5.13 425.96

923 34 5.23 419.51

STEP 2: Conduct FANOVA and pairwise comparisons

2A) Conduct FANOVA

> print(fanova.tests(x = w3fa6[,2:35], group.label =rep(w3fp, c(9,8,8,9)), test = "FB"))

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 2.558944 p-value = 0.003962729

2B) Conduct FANOVA Pairwise Comparison

> pairsout <- fanpairstests(w3fa6, a, w3fp, "Identifying Flavor")

[1] "PAIR 1 vs 2: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 0.3877509 p-value = 0.7750614

[1] "PAIR 1 vs 3: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 4.687485 p-value = 0.0009031749

[1] "PAIR 1 vs 4: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 3.621752 p-value = 0.006803869

[1] "PAIR 2 vs 3: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 3.336954 p-value = 0.02015006

[1] "PAIR 2 vs 4: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 2.75748 p-value = 0.03957529

[1] "PAIR 3 vs 4: "

Analysis of Variance for Functional Data

FB test - F-type test with bias-reduced method of estimation

Test statistic = 0.6095744 p-value = 0.6837033

[1] "Paired fanova.tests p-values for Identifying Flavor"

p1 p2 p-value

[1,] 1 2 0.7750613537

[2,] 1 3 0.0009031749

[3,] 1 4 0.0068038687

[4,] 2 3 0.0201500598

[5,] 2 4 0.0395752895

[6,] 3 4 0.6837033187

STEP 3: Conduct ANOVA and multiple comparisons for predicted parameters

3A. Conduct ANOVA

> x<-w3datf(f2Imax)

> y<-aov(ss~subj+samp,x)

> anova(y)

Analysis of Variance Table

Response: ss

Df Sum Sq Mean Sq F value Pr(>F)

subj 8 2.9920 0.37400 0.7437 0.65328

samp 3 5.6429 1.88098 3.7406 0.02599 \*

Residuals 22 11.0628 0.50285

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Signif. codes: 0 ‘\*\*\*’ 0.001 ‘\*\*’ 0.01 ‘\*’ 0.05 ‘.’ 0.1 ‘ ’ 1

> model.tables(y, type = "mean")[[1]]$samp

3B. Conduct Multiple Comparison Tests

> TukeyHSD(y,which="samp")

Tukey multiple comparisons of means

95% family-wise confidence level

Fit: aov(formula = ss ~ subj + samp, data = x)

$samp

diff lwr upr p adj

416-125 0.175398495 -0.78141895 1.1322159 0.9560683

576-125 0.877777662 -0.07903978 1.8345951 0.0798760

923-125 0.884777778 -0.04347149 1.8130270 0.0653971

576-416 0.702379167 -0.28217786 1.6869362 0.2252957

923-416 0.709379282 -0.24743816 1.6661967 0.1977596

923-576 0.007000116 -0.94981733 0.9638176 0.9999969

> f2Imax

subj samp Imax

1 1 125 5.0342

2 2 125 5.0342

3 6 125 5.1710

4 8 125 5.1710

5 9 125 4.1368

6 10 125 4.1368

7 11 125 4.0343

8 12 125 4.0343

9 13 125 3.1026

10 1 416 5.0342

11 2 416 5.1710

12 8 416 5.0684

13 9 416 3.1026

14 10 416 4.1368

15 11 416 5.0342

16 12 416 4.0336

17 13 416 5.0342

18 1 576 6.0342

19 2 576 5.1710

20 6 576 5.1710

21 8 576 5.0342

22 9 576 5.1710

23 10 576 6.2052

24 12 576 5.0342

25 13 576 5.1710

26 1 923 5.0337

27 2 923 5.1700

28 6 923 5.0342

29 8 923 5.0344

30 9 923 6.2052

31 10 923 6.2052

32 11 923 4.0344

33 12 923 5.0684

34 13 923 6.0327

Codes

> labfanout

function (xdat, a, nn, xtpt, xlab, ylab, title)

{

fanout <- plotFANOVA(x = xdat, group.label =as.character(rep(nn, a)),means=T,smooth=T)

#COLLECT VALUES AT TIME xtcode (ie t=8)

fanout$dataxtpt <- fanout$data[fanout$data[,"t"] == xtpt,]

group.means <- aggregate(fanout$dataxtpt$values1, fanout$dataxtpt[c("group.label")],mean)

p <- length(a) + 1

for (i in 1:(p - 1)) {

fanout <- fanout + ggplot2::annotate("text", xtpt, group.means[[2]][i],label=group.means[[1]][i])

}

#REMOVE LEGEND TITLE

fanout <- fanout + ggplot2::labs(color=NULL)

#REMOVE LEGEND

#fanout <- fanout + ggplot2::theme(legend.position="none")

#USE DEFAULT xlab and ylab

#fanout <- fanout + ggplot2::labs(x="time", y="value", title="Mean Curves of Products")

#USE ARGUMENT VALUES FOR LABELS

fanout <- fanout + ggplot2::labs(x=xlab, y=ylab, title=title)

fanout

}

> fdaparamf

function(x,a,nn){

#Estimation of mean curve parameters

k<-length(a)

para<-matrix(0,k,3)

dimnames(para)<-list(nn,c("Tmax","Imax","AUC"))

fdaparam0<-function(x){

#estimate parameters of curves

library(fda)

wfda0<-function (x)

{#for fda data

k1<-dim(x)[1]

p<-dim(x)[2]

bas<-create.bspline.basis(c(x[1,1],x[k1,1]),k1+2,4,x[,1])

fdpar<-fdPar(bas,2,lambda=10^0.01)

y.fd<-smooth.basis(x[,1],x[,2:p],fdpar)$fd

y.fd

}

s<-dim(x)[1]

ti<-x[,1]

xfd<-wfda0(x)

mxfd<-mean.fd(xfd)

ef<-function(t){eval.fd(t,mxfd)}

auc<-integrate(ef,x[1,1],x[s,1])[[1]]

names(auc)<-"AUC"

a<-cbind(seq(x[1,1],x[s,1]),eval.fd(seq(x[1,1],x[s,1]),mxfd))

res<-a[rev(sort.list(a[,2])),][1,]

names(res)<-c("time","Imax")

all<-round(c(res,auc),2)

all

}

for(i in 1:k){

x0<-cbind(x[,1],x[,(sum(a[0:(i-1)])+2):(sum(a[0:i])+1)])

para[i,]<-fdaparam0(x0)}

para

}

> w3datf

function(Imaxdat)

{

x <- Imaxdat

x <- x[x[, 2 + 1] != "NA",  ]

ss <- x[, 2 + 1]

samp <- x[, 2]

samp <- as.factor(samp)

subj <- x[, 1]

subj <- as.factor(subj)

x.dif <- data.frame(subj, samp, ss)

x.dif

}

> fanpairstests

function (x, a, nn, attlab)

{

library(fdANOVA)

fanpairs <- t(combn(c(1:length(nn)), 2))

fanpairs <- cbind(fanpairs, rep(0, nrow(fanpairs)))

colnames(fanpairs) <- c("p1", "p2", "p-value")

fa <- as.matrix(a)

fa <- cbind(fa, cumsum(fa[,1]))

fa <- cbind(fa, fa[,2]+1)

fa <- cbind(fa, fa[,3]- fa[,1]+1)

dimnames(fa)[[2]] <- c("a", "cuma", "end", "start")

for (i in 1:nrow(fanpairs)){

p1<- fanpairs[i,1]

p2<- fanpairs[i,2]

s1 <- fa[fanpairs[i,1], "start"]

e1 <- fa[fanpairs[i,1], "end"]

s2 <- fa[fanpairs[i,2], "start"]

e2 <- fa[fanpairs[i,2], "end"]

fanpairaovout <- fanova.tests(x[,c(s1:e1,s2:e2)], group.label =rep(nn[c(p1, p2)], a[c(p1,p2)]), test = "FB")

fanpairs[i,"p-value"] <- fanpairaovout[[1]][[2]]

cat()

print(paste("PAIR ", p1, " vs ", p2, ": ", sep="", collapse=""))

print(fanpairaovout)

cat()

}

print(paste("Paired fanova.tests p-values for ", attlab, sep="", collapse=""))

print(fanpairs)

cat()

fanpairs

}