

```

library(fda)
library(cluster)      #the 4 libraries used for data analysis and display
library(evd)
library(rgl)

```

```

#####
#####      Figure 3:      #####
#####

```

```

### Example of three kernels estimates (grey bolded curves) of a centered
Gaussian
### density (black bolded curve). The roughness of the estimates is
controlled by
### a smoothing parameter (bw). Each density is estimated on the same
dataset
### composed of 50 values of x randomly drawn from the Gaussian
distribution.

```

```

xabs=seq(-4, 4, 0.1)
n=length(xabs)
xmin=min(xabs)
xmax=max(xabs)
x=dnorm(xabs)
xx=rnorm(50)
xden1=density(xx,bw=0.3,from=xmin,to=xmax,n=n)
xden2=density(xx,bw=0.5,from=xmin,to=xmax,n=n)
xden3=density(xx,bw=1,from=xmin,to=xmax,n=n)
xest=cbind(x,xden1$y,xden2$y,xden3$y)
matplot(xabs,xest,col=c(1,rep("dark
grey",3)),lwd=c(2,1,1,1),type="l",lty=1,xlab="x",ylab="density")
rug(xx)
X11()

```

```

#####
#####      Figure 4:      #####
#####

```

```

### The six families of curves including the reference density for each
class
### (black bolded curves) and a sample of kernel density estimate. Each
random
### function in class Cj is estimated using 50 points randomly drawn from
the
### reference density fj.

```

```

gamma=3/5

dgumbel_inv=function(x,loc,sca){
  z=exp(-(-x-loc)/sca)
  res=1/sca*z*exp(-z)
  return(res)
}
par(mfcol=c(2,3))
#mar=c(2,1,1,1)
xabs=seq(-6,6,0.1)

```

```

xmin=min(xabs)
xmax=max(xabs)
n=length(xabs)
f1=dnorm(xabs,0,1.5)
f2=dnorm(xabs,0,3)
fa=dnorm(xabs,-1,0.5)
fb=dnorm(xabs,1,0.5)
f3=gamma*fa+(1-gamma)*fb
f4=gamma*fb+(1-gamma)*fa
f5=dgumbel(xabs,loc=-3,sca=1)
f6=dgumbel_inv(xabs,loc=-3,sca=1)
#####
##f1
xden=matrix(-99,n,10)
for(k in 1:10){
  x=rnorm(50,0,1.5)
  xden[,k]=density(x,from=xmin,to=xmax,n=n)$y
}

matplot(xabs,xden,type="l",lty=1,xlab="x",ylab="density
f1",ylim=c(0,0.5),col="dark grey")
lines(xabs,f1,col=1,lwd=2)
abline(v=0,lty=2)
text(-5,0.4,"C1",cex=2)
#####
##f2
xden=matrix(-99,n,10)
for(k in 1:10){
  x=rnorm(50,0,3)
  xden[,k]=density(x,from=xmin,to=xmax,n=n)$y
}

matplot(xabs,xden,type="l",lty=1,xlab="x",ylab="density
f2",ylim=c(0,0.5),col="dark grey")
lines(xabs,f2,col=1,lwd=2)
abline(v=0,lty=2)
text(-5,0.4,"C2",cex=2)
#####
##f3
xden=matrix(-99,n,10)
for(k in 1:10){
  xa=rnorm(3/5*50,-1,1/2)
  xb=rnorm(2/5*50,1,1/2)
  x=c(xa,xb)
  xden[,k]=density(x,from=xmin,to=xmax,n=n)$y
}

matplot(xabs,xden,type="l",lty=1,xlab="x",ylab="density
f3",ylim=c(0,0.5),col="dark grey")
lines(xabs,f3,col=1,lwd=2)
abline(v=0,lty=2)
text(-5,0.4,"C3",cex=2)
#####
##f4
xden=matrix(-99,n,10)
for(k in 1:10){
  xa=rnorm(2/5*50,-1,1/2)
  xb=rnorm(3/5*50,1,1/2)
  x=c(xa,xb)
  xden[,k]=density(x,from=xmin,to=xmax,n=n)$y
}

matplot(xabs,xden,type="l",lty=1,xlab="x",ylab="density
f4",ylim=c(0,0.5),col="dark grey")

```

```

lines(xabs, f4, col=1, lwd=2)
abline(v=0, lty=2)
text(-5, 0.4, "C4", cex=2)
#####
##f5
xden=matrix(-99, n, 10)
for(k in 1:10){
  x=rgumbel(50, loc=-3, sca=1)
  xden[,k]=density(x, from=xmin, to=xmax, n=n)$y
}
matplot(xabs, xden, type="l", lty=1, xlab="x", ylab="density
f5", ylim=c(0, 0.5), col="dark grey")
lines(xabs, f5, col=1, lwd=2)
abline(v=0, lty=2)
text(-5, 0.4, "C5", cex=2)
#####
##f6
xden=matrix(-99, n, 10)
for(k in 1:10){
  x=-rgumbel(50, loc=-3, sca=1)
  xden[,k]=density(x, from=xmin, to=xmax, n=n)$y
}
matplot(xabs, xden, type="l", lty=1, xlab="x", ylab="density
f6", ylim=c(0, 0.5), col="dark grey")
lines(xabs, f6, col=1, lwd=2)
abline(v=0, lty=2)
text(-5, 0.4, "C6", cex=2)
X11()

```

```

#####
#####      Figure 5:      #####
#####

```

```

### The research of the optimal number of clusters. First, the invariance
by
### orientation is not applied to compute the distance matrix. Then, the
### invariance by symmetry is taken into account for the computing.

```

```

s=100
nobs=100
n=600
ind<-c(rep(1,100), rep(2,100), rep(3,100), rep(4,100), rep(5,100), rep(6,100))
ind2<-c(rep(1,100), rep(1,100), rep(2,100), rep(3,100), rep(4,100), rep(4,100))

```

```

yy = list()
for(i in 1:n){
  if(ind[i]==1) yy[[i]] = c(rnorm(3*s/5, -1, 0.5), rnorm(2*s/5, 1, 0.5))
  if(ind[i]==2) yy[[i]] = c(rnorm(2*s/5, -1, 0.5), rnorm(3*s/5, 1, 0.5))
  if(ind[i]==3) yy[[i]] = rnorm(s, 0, 1.5)
  if(ind[i]==4) yy[[i]] = rnorm(s, 0, 3)
  if(ind[i]==5) yy[[i]] = rgumbel(s, -3, 1)
  if(ind[i]==6) yy[[i]] = rgumbel(s, -3, 1)
}

```

```

dens<-list()
xabs<-seq(-7, 7, length=nobs)
for(i in 1:n){
  dens[[i]]<-density(yy[[i]], from=-7, to=7, n=nobs, bw=bw.ucv(yy[[i]]))$y
}

```

```

yt=xt=vector()
  for ( i in seq(1,length(dens))) {
    xx1 <- seq(1,length(dens[[i]]),len=201)
    s1<-smooth.spline(dens[[i]])
    xt<-cbind(xt,predict(s1,xx1)$y)
    yt<-cbind(yt,xx1)
  }

basis=create.fourier.basis(c(0,1),21)
pop=data2fd(xt,basisobj=basis)
coefnorms=pop$coefs/matrix(rep(pop$coefs[1,],21),nrow=21,byrow=TRUE)
coefnorms[,ind==6]=coefnorms[,ind==6]*c(rep(c(1,-1),10),1)
popnorm=fd(coefnorms,basis)

par()
plot(popnorm,col=ind,xlab="support normalisé x",ylab="f(x)")

#functional acp
aa=pca.fd(popnorm,3)
plot3d(aa$scores[,1],aa$scores[,2],aa$scores[,3],col=ind,size=2,axes=F)
par(mfrow=c(1,3))
plot(aa$scores[,1],aa$scores[,2],col=ind)
plot(aa$scores[,2],aa$scores[,3],col=ind)
plot(aa$scores[,1],aa$scores[,3],col=ind)

#optimal number of groups with Silhouette plot
res=vector()
  for (k in 2:12) {
    kme=fanny(aa$scores,k)
    res[k]=summary(silhouette(kme))[[1]][4]
  }
par()
plot(2:12,res[-1],type="l", xlab="Number of groups", ylab="Silhouette
coefficient")
points(2:12,res[-1], pch=10, col="red", cex=2)
axis(side=1, 2:12, labels=FALSE)
title("Silhouette plot: Optimal number of groups without invariance by
orientation", font.main=3, adj=1)
X11()

#acp with distance invariant to orientation
dis=dist_inv2(coefnorms,21)
resmds=cmdscale(dis,3,eig=T)
afm=resmds$points
plot3d(afm[,1],afm[,2],afm[,3],col=ind,size=2,axes=F)

par(mfrow=c(1,3))
plot(afm[,1],afm[,2],col=ind)
plot(afm[,2],afm[,3],col=ind)
plot(afm[,1],afm[,3],col=ind)
X11()
#optimal number of groups with Silhouette plot
res=vector()
  for (k in 2:12) {
    kme=fanny(afm,k)
    res[k]=summary(silhouette(kme))[[1]][4]
  }

par()

```

```

plot(2:12,res[-1],type="l", xlab="Number of groups", ylab="Silhouette
coefficient")
points(2:12,res[-1], pch=10, col="red", cex=2)
axis(side=1, 2:12, labels=FALSE)
title("Silhouette plot: Optimal number of groups with invariance by
orientation", font.main=3, adj=1)

#test bagging
a=bagging(afm,ind2,4,30)
mean(a)

#####
#####      Figure 6:      #####
#####

### The first alteration experiment:  the alteration of the relative
abundance
### of class C1 to C6.

resultot=resultot3=vector()
resultot2=list()
tester=seq(from=0.05,to=0.165,length=50)
tester=tester[50:1]
pb <- winProgressBar(title = "progress bar", min = 0,max = 50, width = 300)
for(k in 1:50){
Sys.sleep(0.1)
setWinProgressBar(pb, k, title=paste( round(k/50*100, 0),"% done"))
nobs=600
n=100
s=100
spa=round(tester[k]*n)
spb=n-5*spa
ind<-c(rep(1,spa),rep(2,spa),rep(3,spb),rep(4,spa),rep(5,spa),rep(6,spa))
ind2<-c(rep(1,spa),rep(1,spa),rep(2,spb),rep(3,spa),rep(4,spa),rep(4,spa))
yy = list()
      for(i in 1:n){
        if(ind[i]==1) yy[[i]] = c(rnorm(3*s/5,-
1,0.5),rnorm(2*s/5,1,0.5))
        if(ind[i]==2) yy[[i]] = c(rnorm(2*s/5,-
1,0.5),rnorm(3*s/5,1,0.5))
        if(ind[i]==3) yy[[i]] = rnorm(s,0,1.5)
        if(ind[i]==4) yy[[i]] = rnorm(s,0,3)
        if(ind[i]==5) yy[[i]] = rgumbel(s,-3,1)
        if(ind[i]==6) yy[[i]] = rgumbel(s,-3,1)
      }
dens<-list()
xabs<-seq(-7,7,length=nobs)
      for(i in 1:n){
        dens[[i]]<-density(yy[[i]],from=-
7,to=7,n=nobs,bw=bw.nrd0(yy[[i]]))$y
      }
yt=xt=vector()
      for ( i in seq(1,length(dens))) {
        xx1 <- seq(1,length(dens[[i]]),len=201)
        s1<-smooth.spline(dens[[i]])
        xt<-cbind(xt,predict(s1,xx1)$y)
        yt<-cbind(yt,xx1)
      }
basis=create.fourier.basis(c(0,1),21)
pop=data2fd(xt,basisobj=basis)

```

```

coefnorms=pop$coefs/matrix(rep(pop$coefs[1,],21),nrow=21,byrow=TRUE)
coefnorms[,ind==6]=coefnorms[,ind==6]*c(rep(c(1,-1),10),1)
dis=dist_inv2(coefnorms,21)
resmds=cmdscale(dis,3,eig=T)
afm=resmds$points
newpar <- par()
par(mfrow=c(1,3))
plot(afm[,1],afm[,2],col=ind2)
plot(afm[,2],afm[,3],col=ind2)
plot(afm[,1],afm[,3],col=ind2)
par(newpar)

#clusplot(pam(afm,4,metric="euclidean")
#calcul of the optimal number of groups
#res2=vector()
# for (f in 2:10) {
# kme=pam(afm,f)
# res2[f]=summary(silhouette(kme))[[1]][4]
# }

tab=afm
flag=ind2
nbgrou=4 #which.max(res2) if we would like to consider the optimal number
of group
nbtir=200
nba1=round(2*(dim(tab)[1])/3)
sel=sort(sample(1:dim(tab)[1],nba1,replace=F))
sel2=setdiff(seq(1,dim(tab)[1]),sel)
a1= tab[sel,]
deucl<-function(x,y) {sqrt(sum((x-y)^2))}
txtot=vector()
for (d in seq(1,nbtir)){
tirage=sort(sample(1:nba1,nba1,replace=TRUE))
kme=pam(daisy(a1[tirage,]),nbgrou, diss =TRUE)
gp=by(tab[sel[tirage,],kme$cluster,list)
gpm=lapply(gp,mean)
gpmtab= t(matrix(unlist(gpm),ncol=nbgrou))
compare=flag[sel[tirage]]
tx=by(compare,kme$cluster,list)
txtab=lapply(tx,table)
txgrp=lapply(txtab,which.max)
txgp=as.numeric(lapply(txgrp,names))
la2= length(sel2)
a2=tab[sel2,]
test=flag[sel2]
res=vector()
for (n in seq(1,la2)){
qmin=vector()
qmin=apply(gpmtab,1,y=a2[n,],deucl)
res=c(res,is.element(test[n],unlist(txgp)[which.min(qmin)]))
}
tx1=mean(res[flag[sel2]==1])
tx2=mean(res[flag[sel2]==2])
tx3=mean(res[flag[sel2]==3])
tx4=mean(res[flag[sel2]==4])
txtot=cbind(txtot,c(tx1,tx2,tx3,tx4))
resultot=c(resultot,mean(txtot))
resultot3=c(resultot3,sd(txtot))
resultot2[[k]]=txtot
}
close(pb)

```

```

label=cbind(tester,tester,tester,tester,tester,(1-5*tester))
rownames(label)= 1:50
colnames(label)=c("C1","C2","C3","C4","C5","C6")
mp=barplot(t(label),legend= colnames(label), xlim = c(0, 70))
points(mp,resulttot,pch=20, col=1, cex=2)

#####
#####      Figure 9:      #####
#####

# The second sample alteration experiment: low noise vs strong noise

s=100
nobs=1000
n=6000
ind<-
c(rep(1,1000),rep(2,1000),rep(3,1000),rep(4,1000),rep(5,1000),rep(6,1000))
ind2<-
c(rep(1,1000),rep(1,1000),rep(2,1000),rep(3,1000),rep(4,1000),rep(4,1000))

yy = list()
for(i in 1:n){
  if(ind[i]==1) yy[[i]] = c(rnorm(3*s/5,-1,0.5),rnorm(2*s/5,1,0.5))
  if(ind[i]==2) yy[[i]] = c(rnorm(2*s/5,-1,0.5),rnorm(3*s/5,1,0.5))
  if(ind[i]==3) yy[[i]] = rnorm(s,0,3)
  if(ind[i]==4) yy[[i]] = rnorm(s,0,1.5)
  if(ind[i]==5) yy[[i]] = rgumbel(s,-3,1)
  if(ind[i]==6) yy[[i]] = rgumbel(s,-3,1)
}
dens<-list()
xabs<-seq(-7,7,length=nobs)
for(i in 1:n){
  dens[[i]]<-density(yy[[i]],from=-7,to=7,n=nobs,bw=0.0001)$y      #bw= 0.1
, 0.0001
}
yt=xt=vector()
for ( i in seq(1,length(dens))){
  xx1 <- seq(1,length(dens[[i]]),len=201)
  s1<-smooth.spline(dens[[i]])
  xt<-cbind(xt,predict(s1,xx1)$y)
  yt<-cbind(yt,xx1)
}

basis=create.fourier.basis(c(0,1),21)
pop=data2fd(xt,basisobj=basis)
coefnorms=pop$coefs/matrix(rep(pop$coefs[1,],21),nrow=21,byrow=TRUE)
coefnorms[,ind==6]=coefnorms[,ind==6]*c(rep(c(1,-1),10),1)
dis=dist_inv2(coefnorms,21)

resmds=cmdscale(dis,3,eig=T)
afm=resmds$points

par(mfrow=c(1,3))
plot(afm[,1],afm[,2],col=ind)
plot(afm[,2],afm[,3],col=ind)
plot(afm[,1],afm[,3],col=ind)

a=bagging(afm,ind2,4,30 )
mean(a)

```