

Functional principal components analysis of the bone shape data

We first construct matrices `landx` and `landy` containing the x and y coordinates of each of the 12 landmarks. These have been preprocessed so that the rows of `landx` corresponding to left femora are multiplied by -1 , corresponding to reflection of the left bones. The next stage is to do a procrustes rotation to fit the various bones together as closely as possible. We start by transforming to zero mean on both coordinates:

```
> landx <- sweep( landx, 1, apply(landx, 1, mean))
> landy <- sweep( landy, 1, apply(landy, 1, mean))
```

We create a $68 \times 12 \times 2$ array `landa` containing all the landmarks and then find the mean configuration corresponding to this matrix:

```
> landa <- array(c(landx,landy), dim=c(68,12,2),
  dimnames=list(dimnames(landx)[[1]],(1:12),c("x","y")))
> meanconfig <- apply(landa, c(2,3), mean)
```

Now we carry out a procrustes rotation on each set of landmarks in turn, allowing for a magnification effect:

```
> landb <- landa
> for ( j in (1:68)) landb[j,,] <- procrustes(landa[j,,],
  meanconfig, T, T, magnify=T)$rmat
> meanconfig <- apply(landb, c(2,3), mean)
```

If we iterate this twice we achieve convergence, but note that the argument `magnify` should be set to `F` after the first or second iteration, otherwise the configuration simply shrinks at each iteration. Now we make `landb` back into a matrix and perform pca.

```
> landbb <- matrix( landb, nrow=68)
> landb.pca <- prcomp(landbb)
```

The function `plotpc` then plots the curves.

```
> plotpc <- function(pc = landb.pca, meancon = meanconfig)
{
  oldpars <- par()
  par(mfrow = c(2, 2), pty = "s", mar = rep(0.1,4), lwd = 2)
  for(comp in (1:4)) {
    load <- pc$rotation[, comp]
    load <- matrix(load, ncol = 2)
    sd <- pc$sdev[comp]
    zz <- meancon + 3 * sd * load
    zz <- rbind(zz, zz[1, ])
    zzs1 <- spline(zz[, 1], n = 100, periodic = T)$y
    zzs2 <- spline(zz[, 2], n = 100, periodic = T)$y
    zz <- meancon - 3 * sd * load
    zz <- rbind(zz, zz[1, ])
    zzs3 <- spline(zz[, 1], n = 100, periodic = T)$y
    zzs4 <- spline(zz[, 2], n = 100, periodic = T)$y
    plot(zzs1, zzs2, type = "l", xlim = range(c(zzs1, zzs3))
         , ylim = range(c(zzs2, zzs4)), axes = F, xlab
         = "", ylab = "")
    box()
    lines(zzs3, zzs4, lty = 5, lwd = 2)
    text(150, 150, comp, cex = 2)
  }
  par(oldpars)
  invisible()
}
```

To get the rotated data, choose the matrix of principal component values and centre it at means:

```
> landb.rotx <- landb.pca$x
> landb.rotx <- sweep(landb.rotx, 2, apply(landb.rotx, 2, mean))
```

Now we can do a t test on each of the comparisons between eburnated and non-eburnated. Let `eb1` be a logical vector taking the value T for the eburnated bones. For the second component, for instance, we do

```
> t.test(landb.rotx[eb1, 2], landb.rotx[!eb1, 2])
```

```
Standard Two-Sample t-Test
data: landb.rotx[eb1, 2] and landb.rotx[!eb1, 2]
t = -3.0095, df = 66, p-value = 0.0037
alternative hypothesis: true difference in means is not equal
to 0
95 percent confidence interval:
 -23.707154 -4.796844
sample estimates:
mean of x mean of y
 -10.89859  3.353412
```

To carry out a pca using a varimax rotation, we have to use a vector version of the quadrimax procedure. See the separate document on quadrimax rotation for a discussion of this, and for the function `vectorquadrimax`. If you want to do this for a one dimensional function, use the Splus function `orthomax` instead, selecting the `rmat` component of the result.

```
> varmxpc.fun <-  
function(xdata = landb, ncomp = 5)  
{  
  # first make x into a matrix if it isn't already one  
  xd <- matrix(xdata, nrow = dim(xdata)[1])  
  # now do the pca of xd  
  pc <- prcomp(xd)  
  # now do the varimax rotation on the first ncomp components  
  rotation <- pc$rotation  
  zorth <- vectorquadrimax(rotation[, 1:ncomp])  
  # now replace the first ncomp columns of rotation  
  rotation[, 1:ncomp] <- zorth  
  # recalculate the scores  
  x <- xd %*% rotation  
  sdev <- sqrt(apply(x, 2, var))  
  return(sdev, rotation, x)  
}
```