Multivariate tools for compositional data analysis: the ToolsForCoDA package

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Abstract

Package **ToolsForCoDA** contains some functions for multivariate analysis with compositional data. It currently provides functions for doing compositional canonical correlation analysis. This analysis requires two data matrices of compositions, which can be adequately tranformed and used as entries in a specialized program for canonical correlation analysis, that is able to deal with singular covariance matrices. Some additional methods for the multivariate analysis of compositional data are planned to be included.

Keywords: log-ratio tranformation, canonical correlation analysis, generalized inverse.

1. Introduction

The **ToolsForCoDa** package provides some tools for the multivariate analysis of compositional data in the R environment (R Core Team 2014). The package is available from the Comprehensive R Archive Network (CRAN) at `http://CRAN.R-project.org/package=ToolsForCoDa`.

This vignette describes the first version 1.0.4 of the package, which mainly provides functions for doing canonical correlation analysis with compositional data. The package also includes a function for log-ratio principal component analysis, combined with the calculation of condition indices and condition numbers for subcompositions.

The remainder of this vignette shows an R example session showing how to perform a canonical analysis of compositions. Two examples will be given. The first example concerns a small artificial data set included in the package, where both the X and Y set are compositional. The second example concerns major oxides compositions of bentonites, where the X set is compositional and Y set is not.

2. An example session for a canonical analysis of compositions

The **ToolsForCoDa** package can be installed as usual via the command line or graphical user interfaces, e.g., the package can be installed and loaded by:

```
R> install.packages("ToolsForCoDa")
R> library("ToolsForCoDa")
```

The document describing the package (this document) can be consulted from inside R by typing:

```
R> vignette("ToolsForCoDa")
```

2.1. Canonical analysis of two compositions

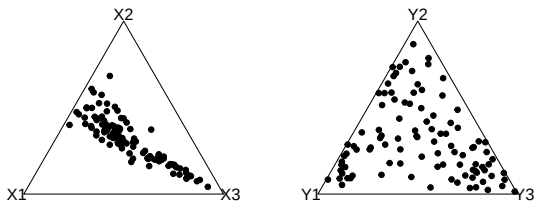
In the remainder we show how to perform the canonical analysis described in Section 3.1 of Graffelman et al. (2018).

We first load two artificial 3-part compositions.

```
R> library(HardyWeinberg) # needed for making some ternary diagrams
R> library(ToolsForCoDa)
R> data("Artificial")
R> Xsim.com <- Artificial$Xsim.com
R> Ysim.com <- Artificial$Ysim.com
R> colnames(Xsim.com) <- paste("X",1:3,sep="")
R> colnames(Ysim.com) <- paste("Y",1:3,sep="")
```

We make the ternary diagrams of the two sets of compositions (Figure 1)

```
R> opar <- par(mfrow=c(1,2),mar=c(3,3,2,0)+0.5,mgp=c(2,1,0),pty="s")
R> par(mfg=c(1,1))
R>   HWTernaryPlot(Xsim.com,n=100,region=0,hwcurve=FALSE,vbounds=FALSE)
R> par(mfg=c(1,2))
R>   HWTernaryPlot(Ysim.com,n=100,region=0,hwcurve=FALSE,vbounds=FALSE)
R> par(opar)
```



We do the centred log-ratio transformation

```
R> Xsub.clr <- clrmat(Xsim.com)
R> Ysub.clr <- clrmat(Ysim.com)
R> colnames(Xsub.clr) <- paste("X",1:3,sep="")
R> colnames(Ysub.clr) <- paste("Y",1:3,sep="")
```

We perform the canonical analysis:

```
R> res.cco <- canocov(Xsub.clr,Ysub.clr)
R> res.cco$ccor
```

```
          [,1]      [,2]         [,3]
[1,] 0.9438791 0.0000000 0.000000e+00
[2,] 0.0000000 0.1286852 0.000000e+00
[3,] 0.0000000 0.0000000 3.463766e-17
```

And we reproduce the results in Table 1. The canonical correlations are obtained as

```
R> round(diag(res.cco$ccor),digits=3)
```

```
[1] 0.944 0.129 0.000
```

The canonical weights of the X set and the Y set are obtained by:

```
R> res.cco$A
```

```
              [,1]      [,2]          [,3]
[1,]  0.0008130933  3.847198 -1.110223e-15
[2,] -0.7985815849 -3.446655  6.522560e-16
[3,]  0.7977684917 -0.400543  1.665335e-16
```

```
R> res.cco$B
```

```
           [,1]        [,2]          [,3]
[1,]  0.7624647 -0.05038131 -9.714451e-17
[2,] -0.7165761 -0.52116661  3.608225e-16
[3,] -0.0458886  0.57154792 -2.775558e-16
```

The canonical loadings of the X set and the Y set are obtained by

```
R> res.cco$Rxu

         [,1]       [,2]       [,3]
X1 -0.8857398  0.4641822 -0.9035794
X2 -0.9828511 -0.1844012 -0.4438392
X3  0.9940477 -0.1089461  0.6849272

R> res.cco$Ryv

         [,1]       [,2]       [,3]
Y1  0.8522677 -0.5231058  0.2439545
Y2 -0.6097840 -0.7925676  0.9387752
Y3 -0.3033098  0.9528920 -0.8183778
```

The adequacy coefficients of the X set and the Y set:

```
R> res.cco$fitXs

           [,1]       [,2]      [,3]
AdeX  0.9128873 0.08711271 0.4941914
cAdeX 0.9128873 1.00000000 1.4941914

R> res.cco$fitYs

           [,1]      [,2]      [,3]
AdeY  0.3967312 0.6032688 0.5368516
cAdeY 0.3967312 1.0000000 1.5368516
```

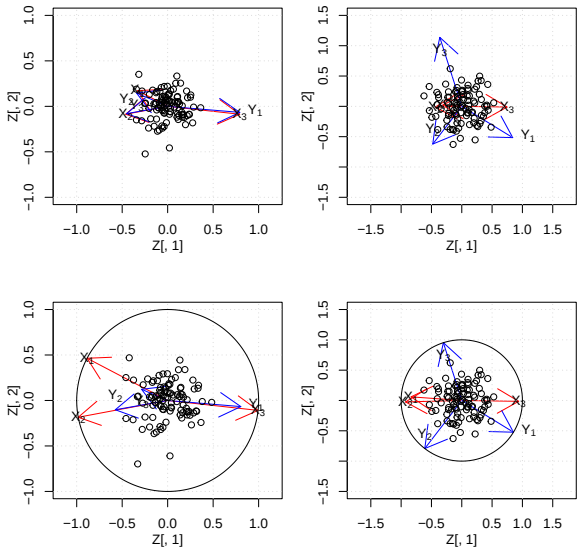
The redundancy coefficients of the X set and the Y set

```
R> res.cco$fitXp

           [,1]        [,2]       [,3]
RedX  0.8132984 0.001442577 0.06638809
cRedX 0.8132984 0.814740980 0.88112907

R> res.cco$fitYp

           [,1]        [,2]      [,3]
RedY  0.3534509 0.009990066 0.1440308
cRedY 0.3534509 0.363441013 0.5074718
```

Finally, we make the biplots given in Figure 2 of

```
R> opar <- par(mfrow=c(2,2),mar=c(3,3,2,0)+0.5,mgp=c(2,1,0))
R> par(mfg=c(1,1))
R> #
R> # Figure A
R> #
R> Z <- rbind(res.cco$Fs,res.cco$Gp)
R> plot(Z[,1],Z[,2],type="n",xlim=c(-1,1),ylim=c(-1,1),asp=1)
R> arrows(0,0,Z[1:3,1],Z[1:3,2],col="red")
R> arrows(0,0,Z[4:6,1],Z[4:6,2],col="blue")
R> text(res.cco$Fs[,1],res.cco$Fs[,2],
+      c(expression(X[1]),expression(X[2]),expression(X[3])))
R> text(res.cco$Gp[,1],res.cco$Gp[,2],
+      c(expression(Y[1]),expression(Y[2]),expression(Y[3])),pos=c(4,3,1))
R> grid()
R> fa <- 0.15
R> points(fa*res.cco$U[,1],fa*res.cco$U[,2])
R> par(mfg=c(1,2))
R> #
R> # Figure B
R> #
R>
R> Z <- rbind(res.cco$Fp,res.cco$Gs)
R> plot(Z[,1],Z[,2],type="n",xlim=c(-1.5,1.5),ylim=c(-1.5,1.5),asp=1)
R> arrows(0,0,Z[1:3,1],Z[1:3,2],col="red")
R> arrows(0,0,Z[4:6,1],Z[4:6,2],col="blue")
R> text(res.cco$Fp[,1],res.cco$Fp[,2],
+      c(expression(X[1]),expression(X[2]),expression(X[3])))
R> text(res.cco$Gs[,1],res.cco$Gs[,2],
+      c(expression(Y[1]),expression(Y[2]),expression(Y[3])),pos=c(4,3,1))
R> grid()
R> fa <- 0.25
R> points(fa*res.cco$V[,1],fa*res.cco$V[,2])
R> par(mfg=c(2,1))
R> #
R> # Standardizing the transformed data
R> #
R>
R> Xstan.clr <- scale(Xsub.clr)
R> Ystan.clr <- scale(Ysub.clr)
R> res.stan.cco <- canocov(Xstan.clr,Ystan.clr)
R> #
R> # Figure C
R> #
R>
R> Z <- rbind(res.stan.cco$Fs,res.stan.cco$Gp)
R> plot(Z[,1],Z[,2],type="n",xlim=c(-1,1),ylim=c(-1,1),asp=1)
R> arrows(0,0,Z[1:3,1],Z[1:3,2],col="red")
```

```
R> arrows(0,0,Z[4:6,1],Z[4:6,2],col="blue")
R> text(res.stan.cco$Fs[,1],res.stan.cco$Fs[,2],
+      c(expression(X[1]),expression(X[2]),expression(X[3])))
R> text(res.stan.cco$Gp[,1],res.stan.cco$Gp[,2],
+      c(expression(Y[1]),expression(Y[2]),expression(Y[3])),pos=c(4,3,1))
R> grid()
R> fa <- 0.2
R> points(fa*res.stan.cco$U[,1],fa*res.stan.cco$U[,2])
R> circle()
R> par(mfg=c(2,2))
R> #
R> # Figure D
R> #
R>
R> Z <- rbind(res.stan.cco$Fp,res.stan.cco$Gs)
R> plot(Z[,1],Z[,2],type="n",xlim=c(-1.5,1.5),ylim=c(-1.5,1.5),asp=1)
R> arrows(0,0,Z[1:3,1],Z[1:3,2],col="red")
R> arrows(0,0,Z[4:6,1],Z[4:6,2],col="blue")
R> text(res.stan.cco$Fp[,1],res.stan.cco$Fp[,2],
+      c(expression(X[1]),expression(X[2]),expression(X[3])))
R> text(res.stan.cco$Gs[,1],res.stan.cco$Gs[,2],
+      c(expression(Y[1]),expression(Y[2]),expression(Y[3])),pos=c(4,3,1))
R> grid()
R> fa <- 0.25
R> points(fa*res.stan.cco$V[,1],fa*res.stan.cco$V[,2])
R> circle()
R> par(opar)
```


Z[, 2]
Z[, 1]
Y1
Y2
Y3
X1
X2
X3

2.2. Canonical analysis of bentonites

In this subsection we treat the canonical analysis of bentonites. The X set concerns the concentrations of 9 major oxides, measured in 14 samples in the US (Cadrin, 1995). The first canonical analysis of this data set has been described by Reyment & Savazzi (1999), and is extended here with biplots. The Y set concerns two isotopes, δD and $\delta 18O$.

```
R> data("bentonites")
R> head(bentonites)
```

```
     Si    Al   Fe    Mn   Mg   Ca    K   Na   H2O  dD d18O
1 51.17 19.18 2.09 0.001 4.54 1.30 2.30 0.93  9.88  93 13.5
2 50.66 19.01 1.67 0.001 2.70 1.70 0.39 0.67  9.99  92 21.9
3 54.38 20.03 2.04 0.001 3.54 2.04 0.10 0.20 10.26  93 21.9
4 55.58 18.76 0.56 0.001 4.51 2.00 0.31 0.90  9.54 100 24.6
5 54.43 22.58 0.69 0.001 3.75 1.47 0.75 0.15  9.14 111 21.7
6 62.79 20.75 1.14 0.060 4.26 0.14 0.42 0.40  8.28 114 24.1
```

We clr-transform and column-center the major oxides, after deletion of MnO which is outlying and had many zeros, which were replaced with 0.001. We standardize the isotopes.

```
R> X <- bentonites[,1:9]
R> X <- X[,-4]
R> Y <- scale(bentonites[,10:11])
R> Xclr <- clrmat(X)
R> cco <- canocov(Xclr,Y)
```

The two canonical correlations are large:

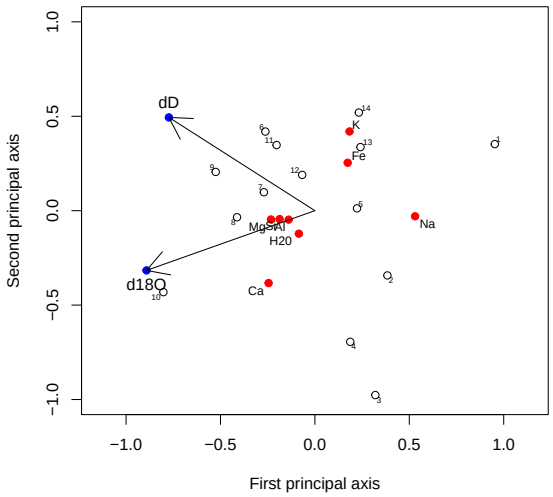
```
R> diag(cco$ccor)
```

```
[1] 0.9656383 0.8244852
```

We construct a biplot of the data:

```
R> plot(cco$Fs[,1],cco$Fs[,2],col="red",pch=19,xlab="First principal axis",
+      ylab="Second principal axis",xlim=c(-1,1),ylim=c(-1,1),asp=1)
R> textxy(cco$Fs[,1],cco$Fs[,2],colnames(X),cex=0.75)
R> points(cco$Gp[,1],cco$Gp[,2],col="blue",pch=19)
R> arrows(0,0,cco$Gp[,1],cco$Gp[,2])
R> text(cco$Gp[,1],cco$Gp[,2],colnames(Y),pos=c(3,1))
R> fa <- 0.45
R> points(fa*cco$U[,1],fa*cco$U[,2])
R> textxy(fa*cco$U[,1],fa*cco$U[,2],1:14)
```

We overplot the biplot with the canonical X-variates, which allows one to inspect the original samples (Graffelman (2005)). For plotting, the canonical variate is scaled with a convenient scaling factor (here 0.45). This factor does not affect the interpretation of the biplot, but gives the samples a convenient spread.


dD
d18O
K
Fe
Na
Mg
Al
H20
Ca
Second principal axis
First principal axis
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

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References

Graffelman J (2005). "Enriched biplots for canonical correlation analysis." *Journal of Applied Statistics*, **32**(2), 173–188.

Graffelman J, Pawlowsky-Glahn V, Egozcue J, Buccianti A (2018). "Exploration of geochemical data with compositional canonical biplots." *Journal of Geochemical Exploration*, **194**, 120–133. doi:10.1016/j.gexplo.2018.07.014.

R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. URL http://www.R-project.org/.

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