UNIVERSITAT DE BARCELONA

ARQUB R Scripts

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arqub
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Introduction

These R scripts are in-house code written to perform the usual analysis on archaeometric compositional data according to the procedure used in the ARQUB (GRACPE) research group at the Universitat de Barcelona.

These scripts produced Figures 3, 5 and 7 A in the paper by Ots, M. J., Buxeda i Garrigós, J., Madrid i Fernández, M., Cahiza, P. A., Small-scale pottery production and distribution in the southern confines of the Inca empire. An archaeometric insight to define the provincial style, submitted to *Archaeological and Anthropological Science* (December 2023).

These scripts need the installation of the following R libraries: **car** (Fox and Weisberg 2019), **compositions** (van den Boogaart *et al.* 2022), **devEMF** (Johnson 2020), **lattice** (Sarkar 2008), **latticeExtra** (Sarkar and Andrews 2019), **plotrix** (Lemon 2009) and **MASS** (Venables and Ripley 2002).

The author of these scripts is Jaume Buxeda i Garrigós https://github.com/jbuxeda/ARQUB.

The comments in the scripts are in Catalan. The scripts are in progress and are provided here without warranty of any kind, express or implied. In no event shall the author or copyright holder be liable for any claim, damages or other liability. If you find any problem or bug, please report it to the author, and he will try to fix it.

inicialCurt

Description

Calculates the variation matrix, the total variation and the information entropy and produces several graphs to summarise all this information.

Usage

```
xvar <- inicialCurt(x, talls = c(0.3, 0.5, 0.9), nom = "Dades", nonum = 0, idioma = 1)
```

Arguments

`x`	composition or dataset of compositions
`talls`	vertical dotted lines expressing different $tv/\tau_{.j}$ values in the compositional evenness graph. Components to the left of the dotted line are below those values. If only the value 0 is given, no dotted lines will be displayed
`nom`	gives the default title of "Data" (according to the selected language) for the compositional evenness graph. This default title can be changed to something relevant to the case study. If there is a title, it will automatically provide the number of cases (n). "NA" will exclude the title and the number of cases
`nonum`	indicates the columns with non-numeric variables that will be excluded. By default, it is 0, indicating that all variables should be used
`idioma`	by default: 1. Indicates the language of the compositional evenness graph and variation matrix: 1, Catalan; 2, Spanish; 3, English; 4, French

Details

Using the determined concentrations or the raw data, this script calculates the variation matrix as explained in the paper by Buxeda (1999), and it performs all possible bivariate graphics with the values $\tau_{.j}$ on the x-axis and the values τ_{ji} on the y-axis ($j = 1, \ldots, j-1, j+1, \ldots, S$) and their correlations. The script also performs the compositional evenness graph. The latter is automatically saved in emf and pdf formats in the current directory with the name "uniformitat" (uniformitat.emf and uniformitat.pdf). The script calculates the total variation (tv) as a measure of compositional variability in the dataset and the information entropy (H_2) (Shannon 1948) or Shannon index as a measure of evenness in contributing to the compositional variability for all retained components (Buxeda and Madrid 2017). It also calculates the percentage of the information entropy over the maximum attainable. The compositional evenness graph is inspired by the rank/abundance graph used in biodiversity studies (see, for example, Magurran 2004).

This script uses the script *evariationmatrix2* to calculate the variation matrix, the script *entropia02* to calculate the information entropy, and the script *etiqueteselements* to produce the components labels in the compositional evenness graph.

Value

A list of three with the following content:

`MVC`	the variation matrix as explained in the paper by Buxeda (1999)
`Probabilitat`	the probability used in the calculation of the information entropy and its percentage over the maximum attainable
`Entropia`	the entropy used in the calculation of the information entropy and its percentage over the maximum attainable

Author

For the scripts *inicialCurt*, *evariationmatrix2*, *entropia02*, and *etiqueteselements*:

Jaume Buxeda i Garrigós https://github.com/jbuxeda/ARQUB

Examples

```
Inkavar <- inicialCurt(Inka, nom = "CWA Provincial Inca Pottery", nonum = c(1:3),
                       idioma = 3)
Inkavar <- inicialCurt(Inka, nom = "CWA Provincial Inca Pottery", idioma = 3)
```

The latter will produce the Figure 3 of the paper. The first example assumes that the first three variables will not be used.

ACPacomp

Description

It performs a principal component analysis via the singular value decomposition of the double-centred clr-transformed data. It can produce biplots by groups and display their probabilistic ellipsoids.

Usage

```
xACPacomp <- ACPacomp(x, nom = "NA", grup = 0, llegenda = grup, ggrup = grup,
                      gllegenda = ggrup, titol1 = 0, titol2 = 0, idioma = 1,
                      paleta = 1, paleta0 = NA, color = "chocolate", cps = 3,
                      simbol = 0, simbol0 = NA, midall = 0.8, elli = T, pelli = 0.95,
                      nelli = 2, noelli = 0)
```

Arguments

`x`	composition or dataset of compositions
`nom`	is the title to use in the biplots. By default ("NA"), there is no title
`grup`	by default, it is 0 and then no groups are employed. The biplots only display the labels of the individuals. If there are groups, 0 must be changed for the column number where the group is expressed. Groups must be indicated by integer numbers, starting at 1 and continuing until the last one without empty numbers. This column must be a factor. If groups are indicated, the biplots are made twice, first with the labels of the individuals and then with symbols and colours indicating the group
`llegenda`	if there are groups, it indicates the column number with the labels of the groups. By default, the column number is the `grup` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each group in `x`. These labels will be used to produce the legend of the groups in the biplots
`ggrup`	if there are groups, we can use different symbols in the biplots. By default, `ggrup` is `grup`; therefore, the symbols may change for every group. However, we can have a different column for symbols to express a second factor other than group membership. Then, `ggrup` must be a column number where we express, by integer numbers starting at 1 and without empty numbers, this second factor
`gllegenda`	if there is a second factor, `gllegenda` can be used to indicate the column number with the labels for this second factor. By default, the column number is the `ggrup` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each level of this second factor in `x`. These labels will be used to produce the legend of the second factor in the biplots. In that case, the legend in the biplots will be doubled by group and by this second factor
`titol1`	by default (0), the legend of the biplot has no title. If the user wants a title for the legend, then the user can put the title here
`titol2`	if a second factor is used, the user can add a second title for the doubled legend here that will be used as the title of this second factor. By default (0), there is no title for this second factor

`idioma` by default: 1. Indicates the language used in labelling the biplots: 1, Catalan; 2, Spanish; 3, English; 4, French

`paleta` if there are groups, `paleta` indicates the colour palette to be used for the symbols. By default, the palette to be used is 1, a predefined palette by the ARQUB unit. The 15 colours in this palette are: gray75, grey9, cyan, red, goldenrod1, dodgerblue, darkgoldenrod4, chartreuse1, darkgreen, indianred1, blue, darkmagenta, maroon1, aquamarine, and lightpink (colours from R Color Chart: https://rstudio-pubs-static.s3.amazonaws.com/3486_79191ad32cf74955b4502b8530aad627.html). Palette 2 is another predefined palette by the ARQUB unit that contains 7 colours in a grey scale for a black and white palette: white, grey90, grey70, grey50, grey30, grey10, black (colours from R Color Chart). Palettes 3 to 7 are R predefined palettes: 3, rainbow; 4, heat.colors; 5, terrain.colors; 6, topo.colors; 7, cm.colors. The user can use a free palette, providing a value of 0

`paleta0` when the user chooses to use a free palette (`paleta` = 0), a vector of colour names must be provided here. By default, the palette in use is ARQUB, and then no custom palette is used (`paleta0` = NA)

`color` the colour of the bars in the bar chart with the per cent of variance explained by the first principal components. By default, it is chocolate, but it must be changed by the user giving the desired name

`cps` the number of the first principal components that will be displayed in all possible pairwise biplots. By default, there are 3

`simbol` in the colored biplots by group, indicates the symbol used to display the individuals. By default (`simbol` = 0), it is the point shape (`pch`) 21 (filled circle). A value different from 0 obliges the use of `simbol0`

`simbol0` if the user wants to use a different symbol or several symbols for groups or for a second factor, the user can provide a vector of point shapes with values between 21 and 25 (both included). The length of the vector must equal the number of groups in `grup` if only groups are displayed, or the number of levels in `ggrup` if a second factor is desired

`midall` refers to the size of the elements of the legend when present. By default, it is 0.8

`elli` is a logic argument that, when using groups (column `grup`), displays the probabilistic ellipsoids of the groups in the biplots with symbols, which is the option by default (`elli` = TRUE). To not display any ellipsoid, `elli` must be turned to FALSE

`pelli` is a value or a vector of values indicating the probability of the ellipsoids being displayed. By default, the probability ellipsoid for 0.95 will be displayed

`nelli` establishes the maximum number of individuals in a group not to display the probabilistic ellipsoids. By default, only groups with more than 2 individuals will be displayed

`noelli` is a vector with the number of groups (column `grup`) whose probabilistic ellipsoids will not be displayed regardless of the group's number of individuals. By default (`noelli` = 0), all groups will be used

Details

Using the **compositions** library (van den Boogaart *et al.* 2022), this script performs a principal component analysis in the Aitchison geometry (*i.e.*, clr-transform) of the simplex (van den Boogaart and Tolosana-Delgado 2013). The original library uses an acomp-dataset, *i.e.*, the composition or dataset of compositions transformed to a vector of class "acomp" representing one closed composition or a matrix of class "acomp" representing multiple closed compositions each in one row. This script uses the `x` composition or dataset of compositions (the determined concentrations or raw data) and transforms this into a class "acomp". Then, the R "princomp" command performs a singular value decomposition of the double-centred clr-transformed dataset.

The script performs the singular valued decomposition and displays a bar chart with up to the first 10 principal components' per cent variance explained. The plot is automatically saved in emf and pdf formats, in the current directory, named "BarplotVar" (BarplotVar.emf and BarplotVar.pdf). Then, for the number of desired components (`cps`), it produces all pairwise biplots of form and covariance using the labels of the individuals. These biplots are automatically saved in emf and pdf formats in the current directory named "EtBiplotForm12" (labelled form biplot for principal components 1 and 2) and "EtBiplotCov12" (labelled covariance biplot for principal components 1 and 2) (EtBiplotForm12.emf, EtBiplotForm12.pdf, EtBiplotCov12.emf, and EtBiplotCov12.pdf). In case groups are indicated (in column `grup`), it also produces all pairwise biplots of form and covariance using the desired palettes indicating group colour. The user can choose the desired symbols for all individuals or every group (using `simbol` and `simbol0`). Moreover, in those biplots, a second column (`ggrup`) might be used to choose symbols not for groups but for a second factor. Groups are differentiated by colour, and symbols indicate differences by the second factor. In addition, those plots can display probabilistic ellipsoids (using `elli`) expressing the desired probability (using `pelli`) for groups over a given number of individuals (using `nelli`) and excluding undesired groups (using `noelli`). These ellipses are drawn using the "dataEllipse" order in the **car** library (Fox and Weisberg 2019). In those colored biplots, a legend is automatically inserted using the legend text in column `llegenda`, for groups, and `gllegenda`, for a second factor. The legend might have a title for the groups (`titol1`) or two titles if a second factor is used (`titol2`). When producing each of these biplots, the program stops, and the cursor changes to a cross inside the plot when asking for the uppermost left corner of the legend box. Then, the user must locate this point with the mouse's left button and press it. The script moves to the next biplot. These biplots are automatically saved in emf and pdf formats in the current directory with the name "CoBiplotForm12" (colored form biplot for principal components 1 and 2) and "CoBiplotCov12" (colored covariance biplot for principal components 1 and 2) (CoBiplotForm12.emf, CoBiplotForm12.pdf, CoBiplotCov12.emf, and CoBiplotCov12.pdf).

Value

An object of type c("princomp.acomp","princomp") whose content is explained in the manual of the package **compositions** (van den Boogaart *et al.* 2022).

Author

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Examples

```
inka2ACPacomp01 <- ACPacomp(Inka21a7[ , -c(3:9)], nom = "Inka ?  Viluco pottery",
                      grup = 1, llegenda = 2, idioma = 3, paleta = 0,
                      paleta0 = c("navy", "dodgerblue", "thistle1", "chartreuse",
                      "red", "chocolate1", "yellow"))
inka2ACPacomp01 <- ACPacomp(Inka21a7[ , -c(3:9)], nom = "Inka ?  Viluco pottery",
                      grup = 1, llegenda = 2, idioma = 3, paleta = 0,
                      paleta0 = c("navy", "dodgerblue", "thistle1", "chartreuse",
                      "red", "chocolate1", "yellow"), simbol = 1,
                      simbol0 = c(21, 22, 23, 24, 25, 21, 25), midall = 0.8)
inka2ACPacomp01 <- ACPacomp(Inka21a7, grup = 1, llegenda = 2, ggrup = 3,
                      gllegenda = 4, nom = "Inka ?  Viluco pottery", idioma = 3,
                      paleta = 0, paleta0 = c("navy", "dodgerblue", "thistle1",
```

```
"chartreuse", "red", "chocolate1", "yellow"), simbol = 0,
simbol0 = c(21, 24, 25), midall = 0.8, nelli = 3, noelli = 7)
```

The latter will produce the form and covariance biplots in Figure 4 of the paper. Inka21a7 contains the determined concentrations of the retained components. The first column is a factor indicating group membership, and the second column indicates the label for each group in the legend. The third column contains a second factor with the type of material. The labels for this factor in the legend are in the fourth column. The doubled legend has no titles, but there is a title for the biplots. A probabilistic ellipsoid at 0.95 is displayed for groups with more than 3 individuals, excluding group 7, which corresponds to the ungrouped individuals. The palette is custom, and different symbols are used for different types of material. The first two examples assume that the columns 3 to 9 will not be used.

LDAclr

Description

It performs a linear discriminant analysis on clr-transformed data. It produces a biplot displaying the unstandardised coefficients, and can project a comparison group.

Usage

```
xclrLDAclr <- LDAclr(xclr, y = NA, pprevia = 0, grupx = 1, llegendax = grupx,
                     ggrupx = grupx, gllegendax = ggrupx, grupy = 1,
                     llegenday = grupy, ggrupy = grupy, gllegenday = ggrupy,
                     titol1 = 0, titol2 = 0, idioma = 1, paleta = 1, paleta0 = NA,
                     color = "chocolate", simbol = 0, simbol0 = NA, midall = 0.8,
                     nom = NA, lds = 3, colpf = "grey85", tex = 1, cexpunts = 1)
```

Arguments

`xclr`	a data frame of clr transformed composition or dataset of compositions that will be used for the linear discriminant analysis
`y`	a data frame of clr transformed composition or dataset of compositions to be classified or projected
`pprevia`	express the prior probability. By default, it is the proportion of each group (`pprevia` = 0). A value of 1 indicates the same probability for each group
`grupx`	indicates the group factor column of the `xclr` data frame. By default, it is the column 1. Groups must be indicated by integer numbers, starting at 1 and continuing until the last one without empty numbers. This column must be a factor
`llegendax`	indicates the column number with the labels of the groups for `xclr`. By default, the column number is the `grupx` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each group in `xclr`. These labels will be used to produce the legend of the groups in the biplot
`ggrupx`	by default, `ggrupx` is `grupx`, but the user can change the column number and use different symbols, and therefore the symbols may change for every group. However, we can have a different symbol column to express a second factor besides group membership. Then, `ggrupx` must be a column number where we express, by integer numbers starting at 1 and without empty numbers, this second factor
`gllegendax`	if there is a second factor, `gllegendax` can be used to indicate the column number with the labels for this second factor. By default, the column number is the `ggrupx` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each level of this second factor in `x`. These labels will be used to produce the legend of the second factor in the biplot. In that case, the legend in the biplot will be doubled by group and by this second factor

`grupy`	indicates the group factor column of the `y` data frame if it exists. By default, it is the column 1. Groups must be indicated by integer numbers, starting, if needed, after the last group of `grupx` and continuing until the last one without empty numbers. This column must be a factor
`llegenday`	indicates the column number with the labels of the groups for `y`. By default, the column number is the `grupy` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each group in `y`. These labels will also be used to produce the legend of the groups in the biplot
`ggrupy`	by default, `ggrupy` is `grupy`, but the user can change the column number and use different symbols, and therefore the symbols may change for every group. However, we can have a different symbol column to express a second factor besides group membership. Then, `ggrupy` must be a column number where we express, by integer numbers starting, if needed, after the last group of `ggrupx` and without empty numbers, this second factor
`gllegenday`	if there is a second factor, `gllegenday` can be used to indicate the column number with the labels for this second factor. By default, the column number is the `ggrupy` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each level of this second factor in `y`. These labels will also be used to produce the legend of the second factor in the biplot. In that case, the legend in the biplot will be doubled by group and by this second factor
`titol1`	by default (0), the legend of the biplot has no title. If the user wants a title for the legend, then the user can put the title here
`titol2`	if a second factor is used, the user can add a second title for the doubled legend here that will be used as the title of this second factor. By default (0), there is no title for this second factor
`idioma`	by default: 1. Indicates the language used in labelling the biplot: 1, Catalan; 2, Spanish; 3, English; 4, French
`paleta`	indicates the colour palette to be used for the symbols. By default, the palette to be used is 1, a predefined palette by the ARQUB unit. The 15 colours in this palette are: gray75, grey9, cyan, red, goldenrod1, dodgerblue, darkgoldenrod4, chartreuse1, darkgreen, indianred1, blue, darkmagenta, maroon1, aquamarine, and lightpink (colours from R Color Chart: https://rstudio-pubs-static.s3.amazonaws.com/3486_79191ad32cf74955b4502b8530aad627.html). Palette 2 is another predefined palette by the ARQUB unit that contains 7 colours in a grey scale for a black and white palette: white, grey90, grey70, grey50, grey30, grey10, black (colours from R Color Chart). Palettes 3 to 7 are R predefined palettes: 3, rainbow; 4, heat.colors; 5, terrain.colors; 6, topo.colors; 7, cm.colors. The user can use a free palette, providing a value of 0
`paleta0`	when the user chooses to use a free palette (`paleta` = 0), a vector of colour names must be provided here. By default, the palette in use is ARQUB, and then no custom palette is used (`paleta0` = NA)
`color`	the colour of the bars in the bar chart with the per cent of the between-group variances explained by the first linear discriminants. By default, it is chocolate, but it must be changed by the user giving the desired name

`simbol`	indicates the symbol used to display the individuals. By default (`simbol` = 0), it is the point shape (`pch`) 21 (filled circle). A value different from 0 obliges the use of `simbol0`
`simbol0`	if the user wants to use a different symbol or several symbols for groups or for a second factor, the user can provide a vector of point shapes with values between 21 and 25 (both included). The length of the vector must equal the number of groups in `grupx` if only groups are displayed, or the number of levels in `ggrupx` if a second factor is desired. If there is a second data frame `y`, the length of the vector must equal the number of groups in `grupx` and `grupy` if only groups are displayed, or the number of levels in `ggrupx` and `ggrupy` if a second factor is desired
`midall`	refers to the size of the elements of the legend when present. By default, it is 0.8
`nom`	is the title to use in the biplots. By default ("NA"), there is no title. If a title is specified, the script adds to the title the number of individuals in `xclr` (n)
`lds`	the number of the first linear discriminants that will be displayed in all possible pairwise biplots. By default, there are 3
`colpf`	is the color of the arrows of the unstandardised coefficients. By default it is grey85, but it must be changed by the user giving the desired name
`tex`	refers to the size of the labels of the unstandardised coefficients. By default, it is 1
`cexpunts`	refers to the size of symbols in the biplot. By default, it is 1

Details

Using the `xclr` data frame of clr transformed data, this script performs a linear discriminant analysis using the "lda" function in the **MASS** library and then classifies the individuals in `xclr` with the "predict" function of the same library (Venables and Ripley 2002). If there is a second data frame of clr transformed data `y` for comparison or projection, these individuals are also classified using the function "predict" and the previous linear discriminant analysis.

The script performs the linear discriminant analysis and displays a bar chart with up to the first 10 linear discriminants' per cent between-group variance explained. The plot is automatically saved in emf and pdf formats, in the current directory, named "BarplotVar" (BarplotVar.emf and BarplotVar.pdf). Then, it produces all pairwise biplots using the palettes and symbols established for the number of desired linear discriminants (`lds`). These biplots are automatically saved in emf and pdf formats in the current directory named "GraficDiscriminant12" (biplot for linear discriminants 1 and 2) (GraficDiscriminant12.emf and GraficDiscriminant12.pdf). In case a comparison data frame `y` is indicated, these individuals are projected in the biplot. The user can choose the desired symbols for all individuals or every group (using `simbol` and `simbol0`). Moreover, in those biplots, a second column (`ggrup`) might be used to choose symbols not for groups but for a second factor. Groups are differentiated by colour, and symbols indicate differences by the second factor. In addition, those plots display the unstandardised coefficients automatically scaled to fit the biplot. The display of the arrows and labels of coefficients are inspired by the function "lda.arrows" provided by the user Tyler (https://stackoverflow.com/questions/17232251/how-can-i-plot-a-biplot-for-lda-in-r). A legend is automatically inserted using the legend text in column `llegendax` and, if relevant, `llegenday`, for groups, and `gllegendax` and, if relevant, `gllegenday`, for a second factor. The legend might have a title for the groups (`titol1`) or two titles if a second factor is used (`titol2`). When producing each of these biplots, the program stops, and the cursor changes to a cross inside the plot when asking for the uppermost left corner of the legend box. Then, the user must locate this point with the mouse's left button and press it. The script moves to the next biplot.

Value

A list of 6 or 4 depending on the existence or not of a comparison data frame `y`.

`Coeficients_dels_discriminants_lineals`	the unstandardised coefficients of the linear discriminants
`Taula_Confusio_x`	the confusion matrix with the correct classifications and misclassifications for the individuals in the `xclr` data frame
`Fitxer_x_amb_Class`	the initial `xclr` data frame with a first column added indicating the group classification by "predict"
`Taula_Confusio_y`	the confusion matrix with the correct classifications and misclassifications for the individuals in the comparison or projection `y` data frame
`Fitxer_y_amb_Class`	the initial comparison or projection `y` data frame with a first column added indicating the group classification by "predict"
`Projeccions_LD`	the projections of the initial individuals in data frames `xclr` and `y` in the linear discriminants

Author

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Examples

```
Inka21a6clrLDAclr <-LDAclr(Inka21a6clr, grupx = 1, llegendax = 2, idioma = 1,
                      paleta = 0, paleta0 = c("navy", "dodgerblue", "thistle1",
                      "chartreuse", "red", "chocolate1"))
Inka21a6i7clrLDAclr <- ACPacomp(Inka21a6clr, y = Inka27clr, pprevia = 0, grupx = 1,
                      llegendax = 2, grupy = 1, llegenday = 2, ggrupx = 3,
                      gllegendax = 4, ggrupy = 3, gllegenday = 4, idioma = 3,
                      paleta = 0, paleta0 = c("navy", "dodgerblue", "thistle1",
                      "chartreuse", "red", "chocolate1", "yellow"), simbol = 1,
                      simbol0 = c(21, 24, 25), titol1 = "Group",
                      titol2 = "Type of material", tex = 0.7,
                      nom = "Linear discriminant analysis")
```

The latter will produce the linear discriminant biplots in Figure 4 of the paper. Inka21a6clr contains the clr transformed data of the retained components for the 6 defined groups. Inka27clr is the group for ungrouped individuals. In both data frames, the first column is a factor indicating group membership, and the second column indicates the label for each group in the legend. The third column contains a second factor with the type of material. The labels for this factor in the legend are in the fourth column. The doubled legend has one title for the groups and another for the type of material. There is also a title for the biplots. The palette is custom, and different symbols are used for different types of material. The labels of the unstandardised coefficients have a lower size than the default ones. The first example has no comparison data frame.

trianglescer

Description

It performs three different ternary phase diagrams relevant to ceramic analysis: the CaO-Al_2O_3-SiO_2 system, the ceramic triangle or (Fe_2O_3 + MgO + CaO)-Al_2O_3-SiO_2 system, and the CaO-MgO-SiO_2 system.

Usage

```
trianglescer(x, grup = 0, llegenda = grup, idioma = 1, color = "gray75", paleta = 1,
                    paleta0 = NA, ordenar = 1, encerclat = 1, mida = 0.8)
```

Arguments

`x`	composition or dataset of compositions. It must contain the concentrations, expressed in mass fraction per cent ($w\%$) of oxides, of MgO, Al_2O_3, SiO_2, CaO and Fe_2O_3
`grup`	by default is 0, meaning that the individuals are not classed in different groups. If there are groups, `grup` must provide the column number. Groups must be indicated by integer numbers, starting at 1 and continuing until the last one without empty numbers. This column must be a factor
`llegenda`	if there are groups, indicates the column number with the labels of the groups for `x`. By default, the column number is the `grup` column number. If another column is used, it must be defined as character. There is no need to put the group label on all individuals. The script will only use the label of the first individual of each group in `x`. These labels will be used to produce the legend of the groups in the ternary diagram
`idioma`	by default: 1. Indicates the language of the compositional evenness graph and variation matrix: 1, Catalan; 2, Spanish; 3, English; 4, French
`color`	if there are no groups, it indicates the colour of the symbol that displays every individual of `x`. By default, the colour is gray75, but it can be changed by introducing the name of the desired colour. If there are groups, a colour palette must be provided
`paleta`	if there are groups, `paleta` indicates the colour palette to be used for the symbols. By default, the palette to be used is 1, a predefined palette by the ARQUB unit. The 15 colours in this palette are: gray75, grey9, cyan, red, goldenrod1, dodgerblue, darkgoldenrod4, chartreuse1, darkgreen, indianred1, blue, darkmagenta, maroon1, aquamarine, and lightpink (colours from R Color Chart: https://rstudio-pubs-static.s3.amazonaws.com/3486_79191ad32cf74955b4502b8530aad627.html). Palette 2 is another predefined palette by the ARQUB unit that contains 7 colours in a grey scale for a black and white palette: white, grey90, grey70, grey50, grey30, grey10, black (colours from R Color Chart). Palettes 3 to 7 are R predefined palettes: 3, rainbow; 4, heat.colors; 5, terrain.colors; 6, topo.colors; 7, cm.colors. The user can use a free palette, providing a value of 0
`paleta0`	when the user chooses to use a free palette (`paleta` = 0), a vector of colour names must be provided here. By default, the palette in use is ARQUB, and then no custom palette is used (`paleta0` = NA)

`ordenar`	by default (1), the individuals are displayed in the order they appear in `x`. If the value is changed to 2, the individuals in `x` are ordered by group, and then they are displayed in this order
`encerclat`	by default: 1. Then, the script draws the symbol of point shape (`pch`) 21 (filled circle), with a grey circle, and the selected colours refer to the filling. If `encerclat` is changed to 2, then the symbol used is the solid circle (`pch`) 19, with the selected colour
`mida`	refers to the size of the symbols. By default, it is 0.8

Details

By using the concentrations of MgO, Al_2O_3, SiO_2, CaO and Fe_2O_3, expressed in mass fraction per cent ($w\%$) of oxides, this script performs three different ternary phase diagrams relevant to ceramic analysis: the CaO-Al_2O_3-SiO_2 system, the ceramic triangle or (Fe_2O_3 + MgO + CaO)-Al_2O_3-SiO_2 system, and the CaO-MgO-SiO_2 system. These systems enable a quick evaluation of the calcium and magnesium content of the ceramics under study. From a technical point of view, big differences are encountered among low calcareous (CaO <5%–6%), calcareous (5%–6% <CaO <15%–25%), and highly calcareous ceramics (CaO >15%–25%), but also according to the low (MgO <1%–1.5%), medium (1%–1.5% <MgO <4%–7%) or high (MgO >4%–7%) magnesium content.

In these ternary phase diagrams, individuals are displayed within their thermodynamic equilibrium triangles given by three mineralogical phases in the vertices of these triangles. Thermodynamic considerations suggest that these mineralogical phases should be the final ones at high temperatures. Nevertheless, these systems do not consider kinetics and represent a simplification of actual compositions. The relevant mineralogical phases in these ternary phase diagrams are åkermanite (Ak; $Ca_2Mg[Si_2O_7]$), anorthite (An; $Ca[Al_2Si_2O_8]$), diopside (Di; $CaMgSi_2O_6$), enstatite (En; $Mg_2Si_2O_6$), forsterite (Fo; Mg_2SiO_4), gehlenite (Gh; $Ca_2Al(Si,Al)_2O_7$), monticellite (Mtc; $CaMgSiO_4$), mullite (Mul; $Al_6[Si_2O_{13}]$), quartz (Qz; SiO_2), and wollastonite (Wo; $CaSiO_3$) (abbreviations according to Whitney and Evans 2010).

These ternary phase diagrams are automatically saved in emf and pdf formats in the current directory named "triangle1" (for the CaO-Al_2O_3-SiO_2 system) (triangle1.emf and triangle1.pdf), "triangle2" (for the ceramic triangle or (Fe_2O_3 + MgO + CaO)-Al_2O_3-SiO_2 system) (triangle2.emf and triangle2.pdf), and "triangle3" (for the CaO-MgO-SiO_2 system) (triangle3.emf and triangle3.pdf).

Value

This script does not provide any written output.

Author

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Examples

```
trianglescer(Inka21a7[ , -c(1:9)], idioma = 3, color = "red")
trianglescer(Inka21a7[ , -c(3:9)], idioma = 3, grup = 1, llegenda = 2, paleta = 0,
                      paleta0 = c("navy", "dodgerblue", "thistle1", "chartreuse",
                      "red", "chocolate1", "yellow"))
```

The latter will produce the ternary phase diagram in Figure 7, A of the paper. Inka21a7 is the data frame `x` with the determined concentrations. Columns 3 to 9 are not used. Group membership is in column 1, while legend labels are in column 2. The colours are a custom palette. In the first example, columns 1 to 9 are not used, and groups are not considered. The symbols are red.

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