Package ‘pca3d’

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Type Package
Title Three dimensional PCA plots
Version 0.3
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Author January Weiner
Maintainer January Weiner <january.weiner@gmail.com>
Description This package provides a function simplifying presentation of PCA models in a 3D interactive representation using rgl
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Imports rgl
NeedsCompilation no
Repository CRAN
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R topics documented:

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pca3d-package

Show a three- or two-dimensional plot of a prcomp object

Description

Show a three- two-dimensional plot of a prcomp object or a matrix, using different symbols and colors for groups of data
Usage

pca3d(pca, components = 1:3, col = "grey", title = NULL, new = FALSE,
axes.color = "grey", bg = "white", radius = NULL,
group = NULL, shape = "sphere", palette = NULL, fancy = FALSE,
biplot = FALSE, biplot.vars = 5,
show.scale = FALSE,
show.labels = FALSE, labels.col = "black", show.axes = TRUE,
show.axe.titles = TRUE, axe.titles = NULL,
show.plane = TRUE, show.shadows = FALSE,
show.centroids = FALSE, show.group.labels = FALSE, show.shapes = TRUE)

pca2d(pca, components = 1:2, col = "grey", title = NULL, new = FALSE,
axes.color = "black", bg = "white", radius = NULL,
group = NULL, shape = NULL, palette = NULL, fancy = FALSE,
biplot = FALSE, biplot.vars = 5,
show.scale = FALSE,
show.labels = FALSE, labels.col = "black", show.axes = TRUE,
show.axe.titles = TRUE, axe.titles = NULL,
show.plane = TRUE, show.shadows = FALSE,
show.centroids = FALSE, show.group.labels = FALSE, ...)

Arguments

pca
Either a prcomp object or a matrix with at least three columns

components
Vector of length 3 (pca3d) or 2 (pca2d) containing the components to be shown

col
Either a single value or a vector of length equal to number of rows, containing
color definitions for the plot points to be shown

title
Window title

new
Use TRUE to open a new window

axes.color
Axis color

This option has no effect in pca2d.

bg
Background color

palette
Specifies the color palette when colors are automatically assigned to the groups.
See Details.

fancy
set 'show.labels', 'show.shadows', 'show.centroids' and 'show.group.labels'
to TRUE.

radius
Scaling item for the size of points to be shown.
In pca2d, this corresponds to the cex parameter.

biplot
Specify whether to show a biplot (see section 'biplots' below)

biplot.vars
Specify which loading to show on the biplot (see section 'biplots' below)

group
either NULL or a factor of length equal to number of rows. Factor levels can be
used to automatically generate symbols and colors for the points shown
shape

Either a single value or a character vector describing the shapes to be used when drawing data points. Allowed shapes are: sphere, tetrahaedron and cube, and may be abbreviated.

In pca2d, the parameter is passed directly on to the pch option of the points() function.

details.show

TRUE for showing labels (taken from the coordinate matrix or the prcomp object). Alternatively, a vector with labels to be shown next to the data points.

details.labels.col

Single value or vector describing the colors of the labels.

details.show.scale

TRUE for showing a numeric scale at the edges of the plot.

This option has no effect in pca2d.

details.show.axes

TRUE to show the axes.

This option has no effect in pca2d.

details.show.axe.titles

If TRUE, show axe titles (PC 1, PC 2 etc.)

This option has no effect in pca2d.

details.axe.titles

A vector with two (pca2d) or three (pca3d) values containing the axe titles (corresponds to xlab and ylab in regular plot). If missing, but details.show.axe.titles is TRUE, axe titles will be generated automatically.

details.show.plane

If TRUE, show a grey horizontal plane at y = 0.

This option has no effect in pca2d.

details.show.shadows

If TRUE, show a "lollipop" representation of the points on the y = 0 plane: a vertical line joining the data point with the plane and a shadow.

In pca2d, for each sample at (x,y), a grey line is drawn from (x,y) to (x,0).

details.show.centroids

If TRUE and the group variable is defined, show cluster centroids (using appropriate group symbols) and lines from each data point to the corresponding centroid.

details.show.group.labels

Either TRUE/FALSE or a vector equal to the number of unique values in the group parameter. If set, labels for each of the defined group will be shown at the group’s centroid. If the value of the parameter is TRUE, then the group names will be taken from the group parameter. Otherwise, the values from this parameter will be used.

details.show.shapes

A TRUE/FALSE value indicating whether the different symbols (shapes) for the shown data points should be plotted (default TRUE).

... For pca2d, any further argument will be passed on to the points() function.

**Details**

pca3d shows a three dimensional representation of a PCA object or any other matrix. It uses the rgl package for rendering.

pca2d is the 2D counterpart. It creates a regular, two-dimensional plot on the standard graphic device. However, it takes exactly the same options as pca3d, such that it is easy to create 2D variants of the 3D graph.

Often, PCA visualisation requires using different symbols and colors for different groups of data. pca3d() and pca2d() aim at creating reasonable defaults, such that a simple call with two parameters
the pca object and the vector with group assignments of the samples – is sufficient for a basic
diagnosis.

Biplots

Value

The functions pca3d and pca2d both return a data frame containing the annotations of the symbols
used. This data frame contains the following columns:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>group</td>
<td>Group names</td>
</tr>
<tr>
<td>colors</td>
<td>associated colors</td>
</tr>
<tr>
<td>shapes</td>
<td>associated shapes</td>
</tr>
</tbody>
</table>

This comes in handy if you want to add a legend to your plot.

Biplots

If option ‘biplot’ is TRUE, a biplot showing both the PCA results (samples) and variables is
shown. This corresponds to the `biplot` function which works for the `prcomp` class objects. How-
ever, a biplot showing all variable loadings will be unreadable if the data is highly dimensional (for
example, gene expression data). Therefore, the option ‘biplot.vars’ specifies which variables are
shown on the biplot.

If ‘biplot.vars’ is a vector of length larger than one, it will be interpreted as a direct selection of
the variables to be shown; for example, for a `prcomp` object `pca`, the variable selection will happen
through `pca$rotation[biplot.vars,].`

If ‘biplot.vars’ is a single number, then for each of the components shown, a number of variables
equal to ‘biplot.vars’ with the highest absolute loadings will be shown on the biplot.

Author(s)

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Examples

data( metabo )
pca <- prcomp( metabo[-1], scale = TRUE )
pca3d( pca, group = metabo[,1] )
pca2d( pca, group = metabo[,1] )

# a bit more fancy:
# black background, white axes, # centroids
pca3d( pca, group = metabo[,1],
      fancy = TRUE, bg = "black",
      axes.color = "white", new = TRUE )
Description

Relative abundances of metabolites from serum samples of three groups of individuals.

Usage

data(metabo)

Format

A data frame with 136 observations on the following 425 variables.

- **group**: a factor with levels NEG POS TB
- **X1**: relative level of 1,5-anhydroglucitol (1,5-AG)
- **X2**: relative level of 10-heptadecenoate (17:1n7)
- **X3**: relative level of 10-nonadecenoate (19:1n9)
- **X4**: relative level of 10-undecenoate (11:1n1)
- **X5**: relative level of 1-arachidonoylglycerophosphocholine*
- **X6**: relative level of 1-arachidonoylglycerophosphoethanolamine*
- **X7**: relative level of 1-arachidonoylglycerophosphoinositol*
- **X8**: relative level of 1-docosahexaenoylglycerophosphocholine*
- **X9**: relative level of 1-docosapentaenoylglycerophosphocholine*
- **X10**: relative level of 1-eicosatrienoylglycerophosphocholine*
- **X11**: relative level of 1-heptadecanoylglycerophosphocholine
- **X12**: relative level of 1-linoleoylglycerophosphocholine
- **X13**: relative level of 1-linoleoylglycerophosphoethanolamine*
- **X14**: relative level of 1-myristoylglycerophosphocholine
- **X15**: relative level of 1-oleoylglycerophosphate
- **X16**: relative level of 1-oleoylglycerophosphocholine
- **X17**: relative level of 1-oleoylglycerophosphoethanolamine
- **X18**: relative level of 1-palmitoleoylglycerophosphocholine*
- **X19**: relative level of 1-palmitoylglycerol (1-monopalmitin)
- **X20**: relative level of 1-palmitoylglycerophosphocholine
- **X21**: relative level of 1-palmitoylglycerophosphoethanolamine
- **X22**: relative level of 1-palmitoylglycerophosphoinositol*
- **X23**: relative level of 1-stearoylglycerol (1-monostearin)
- **X24**: relative level of 1-stearoylglycerophosphocholine
X25 relative level of 1-stearoylglycerophosphoinositol
X26 relative level of 21-hydroxyprogrenolone disulfate
X27 relative level of 2-aminobutyrate
X28 relative level of 2-arachidonoylglycerophosphoethanolamine*
X29 relative level of 2-hydroxybutyrate (AHB)
X30 relative level of 2-hydroxyhippurate (salicylurate)
X31 relative level of 2-hydroxypalmitate
X32 relative level of 2-hydroxystearate
X33 relative level of 2-isopropylmalate
X34 relative level of 2-methylbutyrylcarnitine
X35 relative level of 2-palmitoylglycerophosphocholine*
X36 relative level of 2-stearoylglycerophosphocholine*
X37 relative level of 3-(4-hydroxyphenyl)lactate
X38 relative level of 3-(cystein-S-yl)acetaminophen*
X39 relative level of 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)
X40 relative level of 3-dehydrocarnitine*
X41 relative level of 3-hydroxybutyrate (BHBA)
X42 relative level of 3-hydroxydecanoate
X43 relative level of 3-hydroxykynurenine
X44 relative level of 3-indoxyl sulfate
X45 relative level of 3-methoxytyrosine
X46 relative level of 3-methyl-2-oxobutyrate
X47 relative level of 3-methyl-2-oxovalerate
X48 relative level of 3-methylhistidine
X49 relative level of 3-phenylpropionate (hydrocinnamate)
X50 relative level of 4-acetamidobutanoate
X51 relative level of 4-acetamidophenol
X52 relative level of 4-acetaminophen sulfate
X53 relative level of 4-androsten-3beta,17beta-diol disulfate 1*
X54 relative level of 4-androsten-3beta,17beta-diol disulfate 2*
X55 relative level of 4-ethylphenylsulfate
X56 relative level of 4-methyl-2-oxopentanoate
X57 relative level of 4-vinylphenol sulfate
X58 relative level of 5alpha-androstan-3alpha,17beta-diol monosulfate 1*
X59 relative level of 5alpha-androstan-3beta,17alpha-diol disulfate
X60 relative level of 5alpha-androstan-3beta,17beta-diol disulfate
X61 relative level of 5alpha-pregnan-3alpha,20beta-diol disulfate 1*
relative level of 5alpha-pregnan-3beta,20alpha-diol disulfate
relative level of 5alpha-pregnan-3beta,20alpha-diol monosulfate 2*
relative level of 5alpha-pregnan-3beta,20beta-diol monosulfate 1*
relative level of 5-dodecenoate (12:1n7)
relative level of 5-oxoproline
relative level of 7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)
relative level of acetylcarnitine
relative level of acetylphosphate
relative level of ADpSPEGDFXAEGGGVR*
relative level of adrenate (22:4n6)
relative level of ADSEGDFXAEGGGVR*
relative level of alanine
relative level of allantoin
relative level of alpha-hydroxyisovalerate
relative level of alpha-ketoglutarate
relative level of alpha-tocopherol
relative level of andro steroid monosulfate 1*
relative level of andro steroid monosulfate 2*
relative level of androsterone sulfate
relative level of arachidonate (20:4n6)
relative level of arginine
relative level of ascorbate (Vitamin C)
relative level of asparagine
relative level of aspartate
relative level of aspartylphenylalanine
relative level of beta-hydroxyisovalerate
relative level of betaine
relative level of bilirubin (E,E)*
relative level of bilirubin (E,Z or Z,E)*
relative level of bilirubin (Z,Z)
relative level of biliverdin
relative level of bradykinin, des-arg(9)
relative level of butyrylcarnitine
relative level of caffeine
relative level of caprate (10:0)
relative level of caproate (6:0)
relative level of caprylate (8:0)
X99  relative level of carnitine
X100  relative level of catechol sulfate
X101  relative level of C-glycosyltryptophan*
X102  relative level of chenodeoxycholate
X103  relative level of cholate
X104  relative level of cholesterol
X105  relative level of choline
X106  relative level of citrate
X107  relative level of citrulline
X108  relative level of cortisol
X109  relative level of cortisone
X110  relative level of cotinine
X111  relative level of creatine
X112  relative level of creatinine
X113  relative level of cysteine
X114  relative level of cysteine-glutathione disulfide
X115  relative level of cystine
X116  relative level of decanoylcarnitine
X117  relative level of dehydroisoandrosterone sulfate (DHEA-S)
X118  relative level of deoxycarnitine
X119  relative level of deoxycholate
X120  relative level of dihomo-linoleate (20:2n6)
X121  relative level of dihomo-linolenate (20:3n3 or n6)
X122  relative level of dimethylarginine (SDMA + ADMA)
X123  relative level of docosahexaenoate (DHA; 22:6n3)
X124  relative level of docosapentaenoate (n3 DPA; 22:5n3)
X125  relative level of DSGEGDFXAEGGGVR*
X126  relative level of eicosapentaenoate (EPA; 20:5n3)
X127  relative level of eicosenoate (20:1n9 or 11)
X128  relative level of epiandrosterone sulfate
X129  relative level of erythritol
X130  relative level of erythonate*
X132  relative level of fructose
X133  relative level of gamma-glutamylglutamate
X134  relative level of gamma-glutamylglutamine
X135  relative level of gamma-glutamylisoleucine*
X136  relative level of gamma-glutamylleucine
X137  relative level of gamma-glutamylmethionine*
X138  relative level of gamma-glutamylphenylalanine
X139  relative level of gamma-glutamyltyrosine
X140  relative level of gamma-tocopherol
X141  relative level of glucose
X142  relative level of glutamate
X143  relative level of glutamine
X144  relative level of glutaroyl carnitine
X145  relative level of glycerate
X146  relative level of glycerol
X147  relative level of glycerol 2-phosphate
X148  relative level of glycerol 3-phosphate (G3P)
X149  relative level of glycerophosphorylcholine (GPC)
X150  relative level of glycine
X151  relative level of glycochenodeoxycholate
X152  relative level of glycocholate
X153  relative level of glycocholenate sulfate*
X154  relative level of glycolate (hydroxyacetate)
X155  relative level of glycolithocholate sulfate*
X156  relative level of glycylvaline
X158  relative level of heme*
X159  relative level of heptanoate (7:0)
X160  relative level of hexadecanedioate
X161  relative level of hexanoylcarnitine
X162  relative level of hippurate
X163  relative level of histidine
X164  relative level of homostachydrine*
X165  relative level of HWESASXX*
X166  relative level of hydoxycholate
X167  relative level of hypoxanthine
X168  relative level of indoleacetate
X169  relative level of indolelactate
X170  relative level of indolepropionate
X171  relative level of inosine
X172  relative level of inositol 1-phosphate (I1P)
X173  relative level of isobutyrylcarnitine
X174  relative level of isoleucine
X175  relative level of isovalerate
X176  relative level of isovaleryl carnitine
X177  relative level of kynurenine
X178  relative level of lactate
X179  relative level of lathosterol
X180  relative level of laurate (12:0)
X181  relative level of laurycarnitine
X182  relative level of leucine
X183  relative level of leucyl leucine
X184  relative level of levulinate (4-oxovalerate)
X185  relative level of linoleate (18:2n6)
X186  relative level of linolenate [alpha or gamma; (18:3n3 or 6)]
X187  relative level of lysine
X188  relative level of malate
X189  relative level of maltose
X190  relative level of mannose
X191  relative level of margarate (17:0)
X192  relative level of mead acid (20:3n9)
X193  relative level of methionine
X194  relative level of myo-inositol
X195  relative level of myristate (14:0)
X196  relative level of myristoleate (14:1n5)
X197  relative level of N1-methyl adenosine
X198  relative level of N6-acetyl lysine
X199  relative level of N-acetylglycine
X200  relative level of N-acetylalanine
X201  relative level of N-acetylglutamate
X202  relative level of N-acetylmethionine
X203  relative level of N-acetylnearuminine
X204  relative level of N-acetylornithine
X205  relative level of N-acetyllthreonine
X206  relative level of nonadecanoate (19:0)
X207  relative level of octadecanediol
X208  relative level of octanoylearnitine
X209  relative level of oleate (18:1n9)
X210  relative level of ornithine
X211  relative level of p-acetamidophenyl glucuronide
X212  relative level of palmitate (16:0)
<table>
<thead>
<tr>
<th>Metabolite</th>
<th>Relative Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Palmitoleate (16:1n7)</td>
<td>X213</td>
</tr>
<tr>
<td>Pantothenate</td>
<td>X214</td>
</tr>
<tr>
<td>Paraxanthine</td>
<td>X215</td>
</tr>
<tr>
<td>p-Cresol Sulfate</td>
<td>X216</td>
</tr>
<tr>
<td>Pelargonate (9:0)</td>
<td>X217</td>
</tr>
<tr>
<td>Pentadecanoate (15:0)</td>
<td>X218</td>
</tr>
<tr>
<td>Phenol Sulfate</td>
<td>X219</td>
</tr>
<tr>
<td>Phenylacetate</td>
<td>X220</td>
</tr>
<tr>
<td>Phenylacetylglutamine</td>
<td>X221</td>
</tr>
<tr>
<td>Phenylalanine</td>
<td>X222</td>
</tr>
<tr>
<td>Phenyllactate (PLA)</td>
<td>X223</td>
</tr>
<tr>
<td>Phosphate</td>
<td>X224</td>
</tr>
<tr>
<td>Pipecolate</td>
<td>X225</td>
</tr>
<tr>
<td>Piperine</td>
<td>X226</td>
</tr>
<tr>
<td>Pregn Steroid Monosulfate*</td>
<td>X227</td>
</tr>
<tr>
<td>Pro-Hydroxy-Pro</td>
<td>X228</td>
</tr>
<tr>
<td>Proline</td>
<td>X229</td>
</tr>
<tr>
<td>Propionylcarnitine</td>
<td>X230</td>
</tr>
<tr>
<td>Pseudouridine</td>
<td>X231</td>
</tr>
<tr>
<td>Pyridoxate</td>
<td>X232</td>
</tr>
<tr>
<td>Pyroglutamine*</td>
<td>X233</td>
</tr>
<tr>
<td>Pyroglutamylglycine</td>
<td>X234</td>
</tr>
<tr>
<td>Pyrophosphate (PPI)</td>
<td>X235</td>
</tr>
<tr>
<td>Pyruvate</td>
<td>X236</td>
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<td>Quinate</td>
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<td>Ribose</td>
<td>X238</td>
</tr>
<tr>
<td>Salicylate</td>
<td>X239</td>
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<tr>
<td>Salicyluric Glucuronide*</td>
<td>X240</td>
</tr>
<tr>
<td>Scylo-Inositol</td>
<td>X241</td>
</tr>
<tr>
<td>Serotonin (5HT)</td>
<td>X242</td>
</tr>
<tr>
<td>Stachydrine</td>
<td>X243</td>
</tr>
<tr>
<td>Stearate (18:0)</td>
<td>X244</td>
</tr>
<tr>
<td>Stearidionate (18:4n3)</td>
<td>X245</td>
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<tr>
<td>Stearoyl Sphingomyelin</td>
<td>X246</td>
</tr>
<tr>
<td>Succinate</td>
<td>X247</td>
</tr>
<tr>
<td>Sucrose</td>
<td>X248</td>
</tr>
<tr>
<td>Relative Level of Salicylate</td>
<td>X239</td>
</tr>
</tbody>
</table>
X250  relative level of taurochenodeoxycholate
X251  relative level of taurocholate
X252  relative level of taurochenolate sulfate
X253  relative level of taurochenolate 3-sulfate
X254  relative level of theobromine
X255  relative level of theophylline
X256  relative level of threonate
X257  relative level of threonine
X258  relative level of threonylphenylalanine
X259  relative level of trans-4-hydroxyproline
X260  relative level of tryptophan
X261  relative level of tryptophan betaine
X262  relative level of tyrosine
X263  relative level of undecanoate (11:0)
X264  relative level of urate
X265  relative level of urea
X266  relative level of uridine
X267  relative level of valine
X268  relative level of xanthine
X269  relative level of xylitol
X270  relative level of unknown compound X - 01911_200
X271  relative level of unknown compound X - 02249_201
X272  relative level of unknown compound X - 02269_201
X273  relative level of unknown compound X - 03056_200
X274  relative level of unknown compound X - 06126_201
X275  relative level of unknown compound X - 07765_201
X276  relative level of unknown compound X - 09789_201
X277  relative level of unknown compound X - 10346_201
X278  relative level of unknown compound X - 10395
X279  relative level of unknown compound X - 10426
X280  relative level of unknown compound X - 10500
X281  relative level of unknown compound X - 10503
X282  relative level of unknown compound X - 10510
X283  relative level of unknown compound X - 10609
X284  relative level of unknown compound X - 10810
X285  relative level of unknown compound X - 11175
X286  relative level of unknown compound X - 11204
<table>
<thead>
<tr>
<th>Compound</th>
<th>Relative Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>X287</td>
<td>11261</td>
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<td>X289</td>
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**Details**

Serum samples from three groups of individuals were compared: tuberculin skin test negative (NEG), positive (POS) and clinical tuberculosis (TB).

**Source**

Examples

data(metabo)
## maybe str(metabo); plot(metabo) ...
pca <- prcomp( metabo[,1] )
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