

PCA 3D: getting PCA plots quickly

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Abstract

The package `pca3d` quickly generates 2D and 3D graphics of PCA. The focus is on showing how samples are assigned to different groups or categories. Furthermore, a 2D counterpart facilitates producing publication-quality figures.

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Introduction

This package is actually a bunch of shortcuts to the RGL graphics library, which does the actual job. The idea is to have a few functions that can be quickly and reliably used to visualize and explore multivariate models, and then create a publication-ready figure. By default, `pca3d` can handle `prcomp`, `princomp` and matrix objects.

The provided data set, `metabo`, includes metabolic profiles for over 400 metabolites sampled from 136 tuberculosis (TB) patients and healthy volunteers, and has been described previously (Weiner 3rd et al. 2012). The samples fall into one of three groups: healthy, non-infected (“NEG”), healthy infected (“POS”) and individuals with active tuberculosis (TB).

First, we prepare the principal component analysis (PCA) object to work with. The data is contained in the data frame “`metabo`”; first column of the data set contains group assignments, and we need to remove it to work with the rest of the data set:

```
library(pca3d)
data(metabo)
pca <- prcomp(metabo[,-1], scale.=TRUE)
```

```
gr <- factor(metabo[,1])  
summary(gr)
```

```
## NEG POS TB  
## 46 46 44
```

When `pca3d` is called, the opened window is interactive and can be used to explore differences. Here, we call `pca3d()` and then save a screenshot (`snapshot`) to a file.

```
pca3d(pca, group=gr)  
snapshotPCA3d(file="first_plot.png")
```

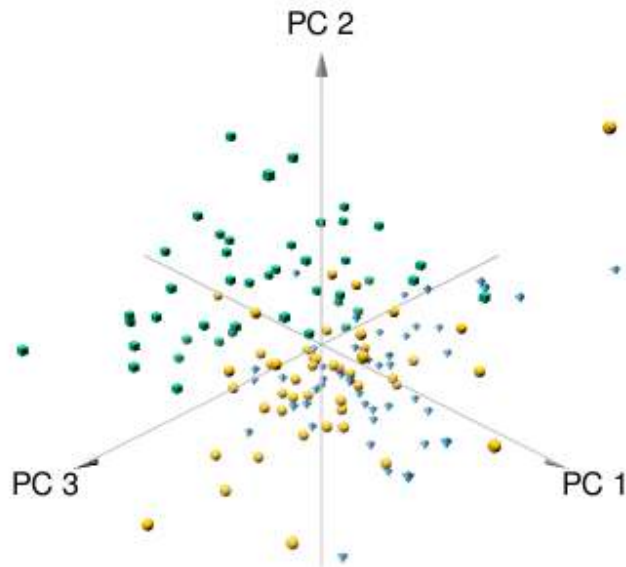
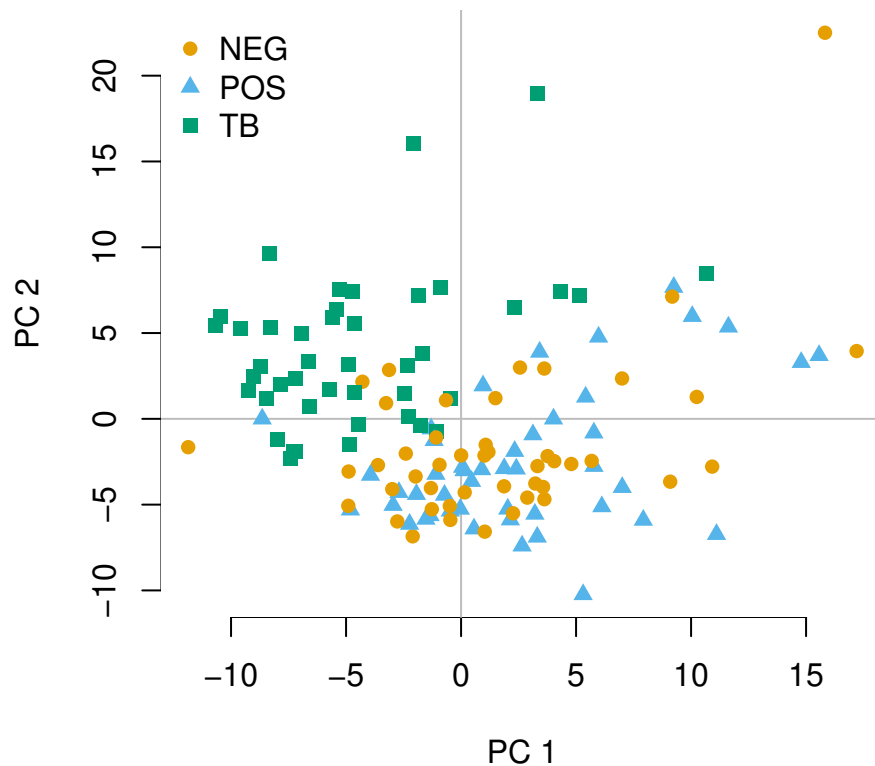


Figure 1: first_plot.png

There is a two-dimensional version of `pca3d`, called (of course) `pca2d`. Essentially, you can run exactly the

same command, and you should see a very similar output – just 2D, and not 3D. The idea is that you can fiddle around with the 3D version to explore your graphics and / or choose the components, and then use `pca2d` to create a figure for a publication.

```
pca2d(pca, group=gr, legend="topleft")
```



Both functions have several options for tweaking the visuals and adding bells and whistles.

Plotting options

Shapes, colors and palettes

The functions `pca3d` and `pca2d` try hard to guess the right values and there are many ways to specify the colors and shapes. Colors and shapes can be specified as follows:

- a single value; in that case, all drawn data points will have this associated value (e.g. the same color)
- a vector equal to the number of samples, specifying color / shape for each data point separately
- a named vector equal in length to the number of levels of the `group` option, that is, equal to the number of groups present in the data. In this case, the names of the vector must correspond to the levels of `group`.
- If color or shape are not specified, but `group` is not `NULL`, then shapes and colors will be attributed automatically to groups

Shapes / `pch`

Currently, there are four possible 3D shapes to choose from: tetrahedrons, cubes, spheres and octahedrons. The corresponding 2D `pch` values are 17, 15, 16 and 18, respectively. You can get the list of permissible shapes and their `pch` counterparts using the `listShapes` function.

`listShapes()`

```
##          Shape pch
## 1      sphere  16
## 2 tetrahedron  17
## 3         cube  15
## 4 octahedron  18
```

The shapes for 3D plots should be specified using these character values, or with an abbreviation (e.g. `t` for tetrahedrons).

For 2D plots, shapes can be specified using any valid numeric values of the `pch` parameter. However, shapes defined by their 3D names (tetrahedrons etc.) are also permissible.

Shape sizes

The parameter “radius” scales the symbols (much like `cex` for regular plots, or rather, exactly like `cex` for `pca2d`).

Colors and palettes

For 3D plots, colors and palette should not contain an alpha channel; that is, `#FF0000` is permissible, but `#FF000033` not.

Palette is a character vector with color names. A default, colorblind-friendly palette is predefined in the package (see the `defaultPalettePCA3D` function).

Ellipses / ellipsoids (option `show.ellipses`)

These option show a confidence interval (CI) ellipse (2D) or ellipsoid (3D). The option `ellipse.ci` corresponds to the level for which the CI is supposed to be drawn (default 0.95). A less conservative level (e.g. 0.75) will result in a morre narrow ellipse. For the 3D representation, it is worthwhile to remove the grey plane at $z=0$ with the `show.plane=FALSE` option.

```
pca3d(pca, group=gr, show.ellipses=TRUE,
      ellipse.ci=0.75, show.plane=FALSE)
snapshotPCA3d(file="ellipses.png")
```

Biplots

A biplot shows information on variable loadings, which helps to interpret a PCA. To see a biplot, use the `biplot` parameter. If `TRUE`, then variable loadings will be extracted from the `princomp` or `prcomp` object. If `biplot` is a matrix, then it is assumed to be a matrix of variable loadings.

The second option is `biplot.vars`, which describes how many variables are shown on the plot. The top N variables are selected based on their absolute loadings.

```
pca2d(pca, group=gr, biplot=TRUE, biplot.vars=3)
```

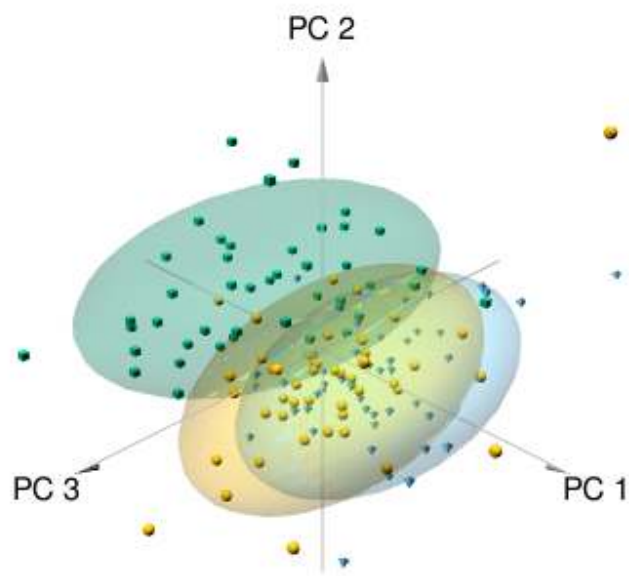
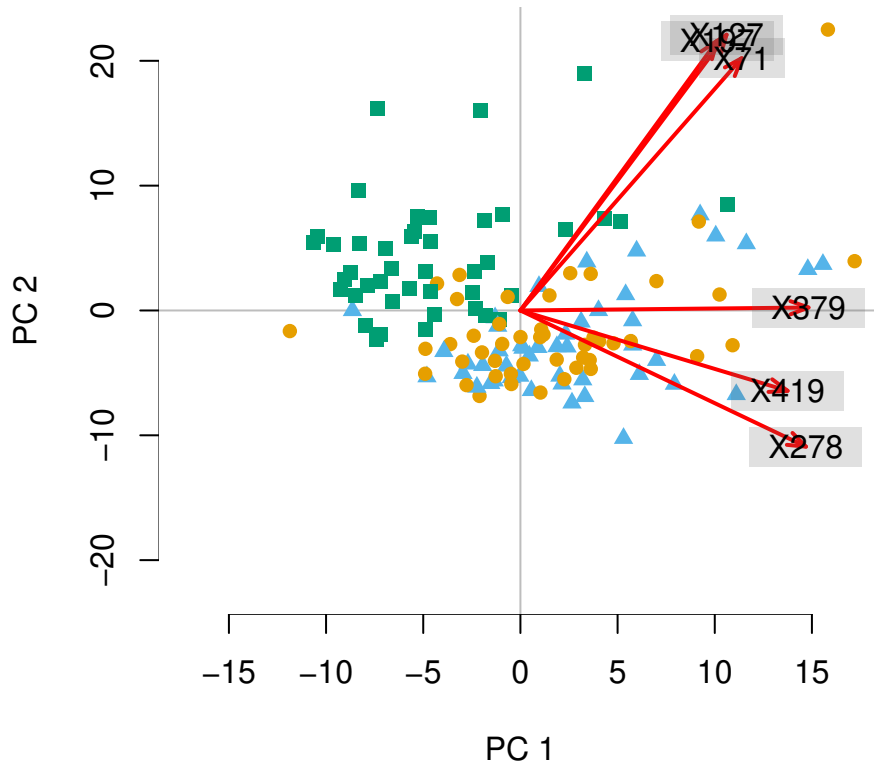


Figure 2: ellipses.png



Shadows (lollipops), centroids, labels, group labels

The options `show.shadows`, `show.centroids`, `show.labels` and `show.group.labels` determine about adding additional graphical information. You can set them all to “TRUE” with the `fancy=TRUE` option – mostly for demonstration purposes, because the plot is then hardly readable.

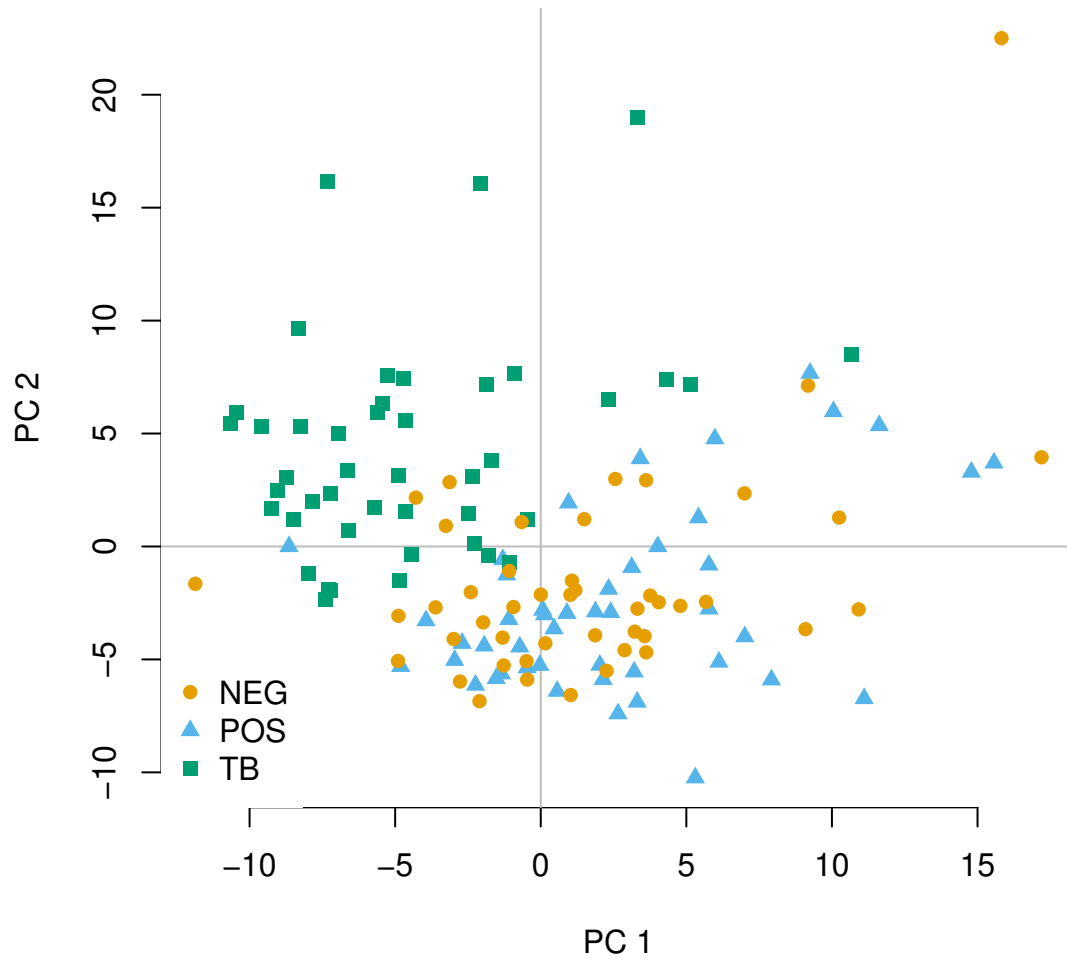
- **show.shadows** Draw a thin grey line from the point to the xy plane
- **show.centroids** Show a large symbol of the group at the average coordinates of samples in that group (centroids)
- **show.labels** Show text labels at each point
- **show.group.labels** Show group labels at the centroids

```
pca3d(pca, group=gr, fancy=TRUE)
snapshotPCA3d(file="fancy.png")
```

Legends

Both `pca3d` and `pca2d` will produce a legend if the option `legend` is not NULL. The argument to this option is anything acceptable by `xy.coords`. Typically, you will want something like “`topleft`” or “`bottomright`”.


```
pca2d(pca, group=gr, legend="bottomleft")
```



Return value

Both `pca2d` and `pca3d` return a data frame containing the assignments between groups, colors and shapes that can be used to plot a legend. Since shapes are character vectors, additionally a mapping to the 2D plotting “`pch`” parameter is provided. This can be used to draw a legend (however, it is more convenient to specify the `legend` option).

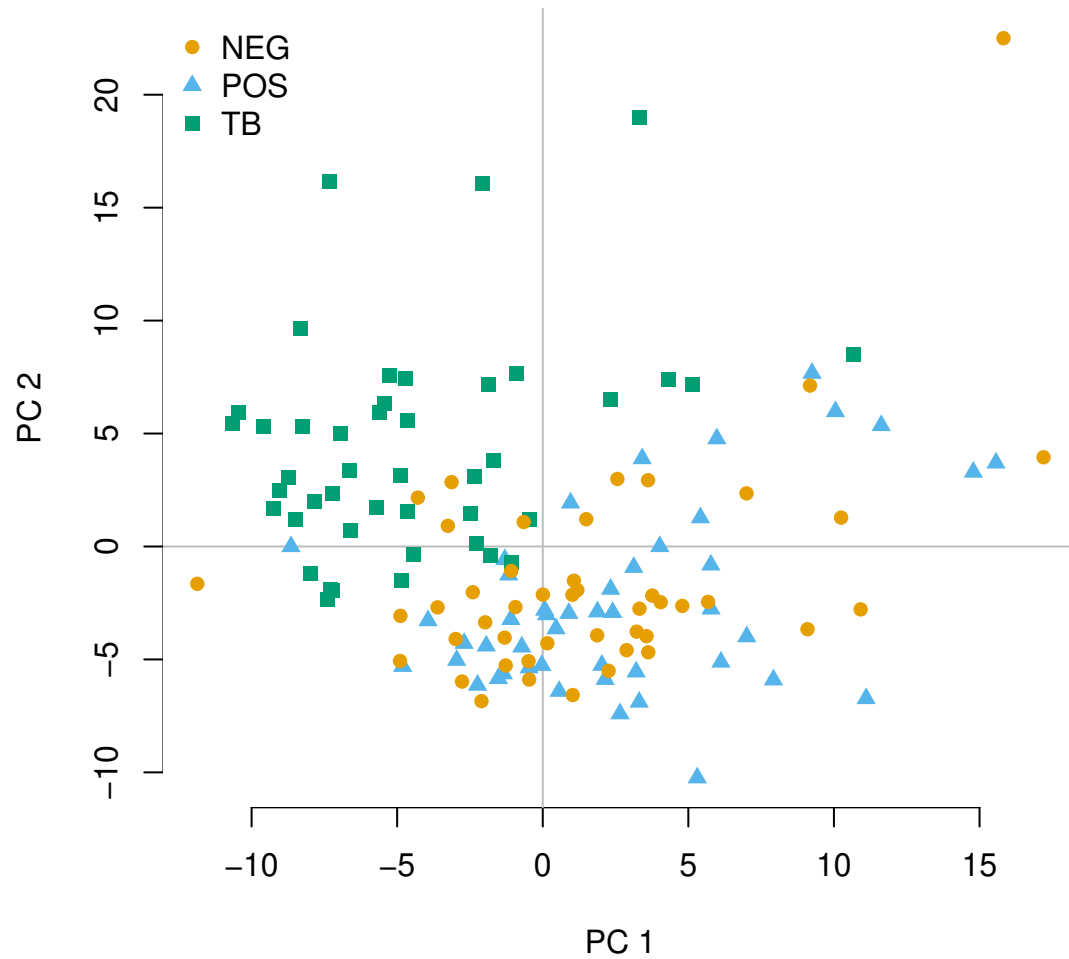
```
l <- pca2d(pca, group=gr)
```

```
l
```

```
##      groups colors      shapes pch
## NEG    NEG #E69F00    sphere  16
## POS    POS #56B4E9 tetrahedron 17
## TB     TB  #009E73     cube    15
```



```
legend("topleft", l$groups, col=l$colors, pch=l$pch, box.lty=0)
```



References

Weiner 3rd, January, Shreemanta K Parida, Jeroen Maertzdorf, Gillian F Black, Dirk Repsilber, Anna Telaar, Robert P Mohny, et al. 2012. "Biomarkers of Inflammation, Immunosuppression and Stress with Active Disease Are Revealed by Metabolomic Profiling of Tuberculosis Patients." *PloS One* 7 (7). Public Library of Science: e40221.