christophe.dutang@grenoble-inp.fr
olivier.francois@univ-grenoble-alpes.fr

▲ General guidelines for TPs

Each team shall upload its report on Teide before the deadline indicated at the course website. Please include the name of all members of the team on top of your report.

The report should contain graphical representations. For each graph, axis names should be provided as well as a legend when it is appropriate. Figures should be explained by a few sentences in the text. Answer to the questions in order and refer to the question number in your report. Computations and graphics have to be performed with R.

The report should be written using the Rmarkdown format. This is a file format that allows users to format documents containing text and R instructions. You should include all of the R instructions that you have used in the rmd document so that it may be possible to replicate your results. From your rmd file, you are asked to generate an html file for the final report. In Teide, you are asked to submit both the rmd and the html files. In the html file, you should limit the displayed R code to the most important instructions.

TP: Principal Component Analysis on breast cancer dataset

We are interested in detecting severe breast cancers. To this end, we use a datas coming from cytopathologic measures of tissue cell of women developping breast cancers, collected in Wolberg and Mangasarian (1990). *Multisurface method of pattern separation for medical diagnosis applied to breast cytology*, Proceedings of the National Academy of Sciences. BreastCancer contains 699 observations 9 explanatory variables and 1 response variable (the identification column is useless), see Table 1. All explanatory variables have been converted into 11 primitive numerical attributes with values ranging from 0 through 10.

This project aims to determine if cytological measures contain enough information to diagnose women for breast cancer. We use a PCA to reduce dimensions and study relationships between cytological measures and the cancer class: benign cancer, malignant cancer.

| Id Sample code number Cl.thickness Clump Thickness (ordered value) Cell.size Uniformity of Cell Size (ordered value) Cell.shape Uniformity of Cell Shape (ordered value) Marg.adhesion Marginal Adhesion (ordered value) Epith.c.size Single Epithelial Cell Size (ordered value) Bare.nuclei Bare Nuclei Bl.cromatin Bland Chromatin Normal.nucleoli Normal Nucleoli Mitoses Cl | Variable | Meaning |
|--|-----------------|---|
| Cell.size Uniformity of Cell Size (ordered value) Cell.shape Uniformity of Cell Shape (ordered value) Marg.adhesion Marginal Adhesion (ordered value) Epith.c.size Single Epithelial Cell Size (ordered value) Bare.nuclei Bare Nuclei Bl.cromatin Bland Chromatin Normal.nucleoli Mitoses Mitoses | Id | Sample code number |
| Cell.shapeUniformity of Cell Shape (ordered value)Marg.adhesionMarginal Adhesion (ordered value)Epith.c.sizeSingle Epithelial Cell Size (ordered value)Bare.nucleiBare NucleiBl.cromatinBland ChromatinNormal.nucleoliNormal NucleoliMitosesMitoses | Cl.thickness | Clump Thickness (ordered value) |
| Marg.adhesionMarginal Adhesion (ordered value)Epith.c.sizeSingle Epithelial Cell Size (ordered value)Bare.nucleiBare NucleiBl.cromatinBland ChromatinNormal.nucleoliNormal NucleoliMitosesMitoses | Cell.size | Uniformity of Cell Size (ordered value) |
| Epith.c.size Single Epithelial Cell Size (ordered value) Bare.nuclei Bare Nuclei Bl.cromatin Bland Chromatin Normal.nucleoli Normal Nucleoli Mitoses Mitoses | Cell.shape | Uniformity of Cell Shape (ordered value) |
| Bare.nuclei Bare Nuclei Bl.cromatin Bland Chromatin Normal.nucleoli Normal Nucleoli Mitoses Mitoses | Marg.adhesion | Marginal Adhesion (ordered value) |
| Bl.cromatin Bland Chromatin Normal.nucleoli Normal Nucleoli Mitoses Mitoses | Epith.c.size | Single Epithelial Cell Size (ordered value) |
| Normal.nucleoli Normal Nucleoli Mitoses Mitoses | Bare.nuclei | Bare Nuclei |
| Mitoses Mitoses | Bl.cromatin | Bland Chromatin |
| 1110000 | Normal.nucleoli | Normal Nucleoli |
| CI. | Mitoses | Mitoses |
| Class | Class | Class |

Table 1: Variable list for BreastCancer

Data preparation

1. Load the data and remove missing values using the code below.

- 2. Explore the dataset with a (short) descriptive and graphical analysis.
- 3. Emphasize the fact that using the log of explanatory variables is better. For the report, please carefully select the graphics displayed and comment them.

In the following, we work on X <- as.matrix(log(BreastCancer[, explvar])).

Principal component analysis using stats package

There are two functions in the core stats package to perform a PCA: prcomp() and princomp().

4. What are the differences between these two functions? what are the default behavior?

For the next two questions we check the outputs of the following code

```
> breast.prcomp <- prcomp(X, scale=FALSE)
> breast.princomp <- princomp(X, cor=FALSE)</pre>
```

- 5. We compute the spectral decomposition PDP^T using eigen() of the empirical covariance matrix V X.cov <- cov(X).
 - (a) Compute the eigenvalues of the covariance V and check you retrieve the explained variances of breast.prcomp\$sdev^ 2.
 - (b) Check the first eigenvector and the first axis breast.prcomp\$loadings[,1].
 - (c) Check the coordinates of observations (a matrix multiplication) against the output breast.princomp\$x (up to a sign).
- 6. We compute the singular value decomposition $U\Sigma V^T$.
 - (a) Center the observations X.s <- scale(X, center = TRUE, scale = FALSE) /sqrt(nrow(X) 1)
 - (b) Using svd(), check the explained variances against the output breast.prcomp\$sdev.
 - (c) Using svd(), check the right singular vectors against the output breast.prcomp\$rotation.

We now interpret the output breast.prcomp (the output of prcomp())

```
> breast.prcomp <- prcomp(X, scale=TRUE)</pre>
```

- 7. Interpret the values of explained variances. Use summary() and plot() on breast.prcomp
- 8. Interpret the components using biplot() and

```
> plot(., col=1+1*(BreastCancer$Class == "malignant"))
```

Principal component analysis using FactoMineR package

- 9. Redo the computation using the PCA() function of the FactoMineR package with scale.unit=FALSE. Use quali.sup argument to add the qualitative variable Class. Check your analysis of the previous question using summary(). Furthermore, dimdesc() provides further analysis of principal components.
- 10. Plot individuals in your plane(s) defined by your chosen principal components. Use habillage argument of plot() on the output of PCA() and comment.

```
> plot(., choix="ind", label="quali", habillage = .)
```

11. Retrieve the explanations of variable's contribution to principal components with plot() function.

```
> plot(., choix="var", habillage="cos2")
```