Problem Set 2: PCA

Stat 154, Fall 2017, Prof. Sanchez

Due date: Th Sep-21 (before midnight)

The purpose of this assignment is to perform an exhaustive Principal Component Analysis (PCA) from scratch in R. This means that you will have to perform PCA WITHOUT using any of the exisiting functions—or packages—for PCA (e.g. can't use `prcomp()` or `princomp()`). In other words, you must carry out all of the steps using either matrix operations or auxiliary functions such as `apply()`, `sweep()`, `scale()`, `crossprod()`, etc. You can use `eigen()` and/or `svd()`.

Use an R markdown (`.Rmd`) file to write your code and answers. You can *knit* the `Rmd` file as html or pdf. Please submit both your `Rmd` and knitted file to bCourses. Make sure to include your name, and your lab section. No late assignments will be accepted.

Data Set

In this problem, you will investigate the climates of different European countries using the data set `temperature.csv`, available in the `data/` folder of the github repository.

Monthly temperatures (in Celsius) were collected for the main European capitals and other major cities. In addition to the monthly temperatures, the average annual temperature and the thermal amplitude (difference between the maximum monthly average and the minimum monthly average of a city) were recorded for each city. The data set also includes two quantitative positioning variables (latitude and longitude) as well as one categorical variable: Area (with four categories north, south, east, and west).

You can download the file to your working directory (or any other location) with `download.file()`:

```
# download data to your working directory
repo <- 'https://raw.githubusercontent.com/ucb-stat154/'
file <- 'stat154-fall-2017/master/data/temperature.csv'

download.file(
  url = paste0(repo, file),
  destfile = 'temperature.csv'
)
```

Please get your own copy of the data file. This operation should not be part of the commands in your Rmd file. Otherwise, everytime you knit the Rmd file, you will be (unnecessarily) downloading the data file over and over.

Cities. We wish to understand the variability of monthly temperatures from one country to another in a multidimensional manner, that is, by taking into account the 12 months of the year simultaneously. Each country will be represented by the climate of its capital. The data of the other cities are not taken into account to avoid giving more weight to the countries for which several cities are listed. Thus, the capital will be regarded as **active individuals** while the other cities will be regarded as **supplementary individuals** (i.e. individuals which are not involved in the computation of the components).

Variables. We also wish to understand the relationship between the variables (i.e. the monthly temperatures)

Research Question. The main research question is: Can we summarize monthly precipitation with only a small number of components?

Exploratory Phase (not graded)

- Before computing PCA outputs, start with an Exploratory Data Analysis (EDA). Get descriptive statistics for each variable; produce visualizations for each variable, maybe some scatterplots.
- You don't need to report all the results, summaries, and plots that you obtain in this phase. However, you should carry out a comprehensive exploration to "get to know" the data better.
- Report two or three comprehensive graphs (e.g. maybe a `stars()` plot for the cities, a correlogram of the pairwise correlations, or a scatterplot matrix with `pairs()`).
- Report descriptions (e.g. summary statistics) that show an *interesting* pattern (something unique) of the variables that catch your attention.
- Tell the reader what things are eye-catching, why it is important to know the specific details that you found in the EDA.

1) Calculation of primary PCA outputs (30 pts)

As we saw in lecture, the primary outputs of a PCA can be obtained via various approaches. Perhaps the two most common approaches consist of using either a Singular Value Decomposition (SVD) or an Eigen-Value Decomposition (EVD) of some matrix.

Regardless of the approach you decide to use, please keep in mind the following specs:

- Work with standardized data: mean = 0, sample variance = 1.
- Active individuals: the first 23 rows are the active cities (country capitals);
- Active variables: the temperatures for all 12 months.
- Supplementary individuals: the rows 24 to 35 are supplementary cities.
- Supplementary variables: `Annual`, `Amplitude`, `Latitude`, `Longitude`, and `Area`.
- Show your computations (do NOT use `results = 'hide'` or `echo = FALSE` or `eval = FALSE` in any of the code chunks in your Rmd file).

a. Obtain the loadings and store them in a matrix, include row and column names. Display the first four loadings (10 pts).

b. Obtain the principal components and store them in a matrix, include row and column names. Display the first four PCs (10 pts).

c. Obtain the eigenvalues and store them in a vector. Display the entire vector, and compute their sum. (10 pts)

2) Choosing the number of dimensions to retain/examine (30 pts)

a. Make a summary table of the eigenvalues: eigenvalue in the first column (each eigenvalue represents the variance captured by each component); percentage of variance in the second column; and cumulative percentage in the third column. Comment on the table. (10 pts)

b. Create a scree-plot (with axis labels) of the eigenvalues. What do you see? How do you read/interpret this chart? (10 pts)

c. If you had to choose a number of dimensions (i.e. a number of PCs), how many would you choose and why? (10 pts)

3) Studying the cloud of individuals (30 pts)

a. Create a scatter plot of the cities on the 1st and 2nd PCs (10 pts).
  - In this plot, you should also project the supplementary cities.
  - Make sure to add a visual cue (e.g. size, font, shape) to differentiate between active and supplementary cities.
  - Color the cities according to the variable `Area`.
  - Comment on general patterns, as well as on particular patterns.

b. Compute the quality of individuals representation, that is, the squared cosines given by:

$$cos^2(i, k) = \frac{z_{ik}^2}{d^2(\mathbf{x_i}, \mathbf{g})}$$

where:

  - z_{ik} is the square value of the i-th individual on PC k
  - $\mathbf{x_i}$ represents the row-vector of the i-th individual
  - $\mathbf{g}$ is the centroid (i.e. average individual)

Store the squared cosines in a matrix or data frame, include row and column names. Display the first four columns. What cities are best represented on the first two PCs? What cities have the worst representation on the first two PCs? (10 pts).

c. Compute the contributions of the individuals to each extracted PC.

$$ctr(i, k) = \frac{m_i z_{ik}^2}{\lambda_k} \times 100$$

where:

- m_i is the mass or weight of individual i, in our case: $(\frac{1}{n-1})$
- z_{ik} is the value of k-th PC for individual i
- λ_k is the eigenvalue associated to k-th PC

Store the individuals contributions in a matrix or data frmae, include row and column names. Display the first four columns. Are there any influential cities on the first two PCs? (10 pts).

4) Studying the cloud of variables (30 pts)

a. Calculate the correlation of all quantitative variables (active and supplementary) with the principal components. Store the correlations in a matrix or data frame, include row and column names. Display the first four columns. (10 pts)

b. Make a Circle of Correlations plot between the PCs and all the quantitative variables (10 pts).

- For visualization purposes, include the circumference of a circle of radius one.
- Represent each variable in the plot as an arrow.
- Use color to distinguish between active and supplementary variables.
- Also include names of variables.

c. Based on the above parts (a) and (b), how are the active and supplementary variables related to the components? (10 pts)

5) Conclusions (10 pts)

Write summarizing conclusions for the performed PCA.