**Assignment Multivariate Component Analysis**

**(Data Science 2, BFVM19DATASC2**)

*October 24, 2022*

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**Read the instruction carefully!**

This assignment is to be made by the candidate in the form of a **single**, well-formatted (sectioned) **Jupyter notebook**, to be handed in through Blackboard before **Friday October 28th** **17:00**. Any material available may be used. The work handed in must be performed and written by the candidate, and in case of doubt, the candidate may be invited to an interview about the work.

For the assignment there are several datasets available in the assignment folder. These are described below. The assignment is to **perform meaningful, complete, and correct analyses of two or more datasets and present these properly**. Demonstrate (at least) three different methods. **PCA and/or FA** must be included, and **regression (MLR, PCR, or PLSR)** must be included. A third method may be selected as desired (PA, MDS, LDA, SGP, ...).

For each method write a section in the Jupyter notebook in which you:

- give the rationale for using the method for the data selected and state expectations (20%)

- justify the selections (rows/columns) and/or treatment of the data (15%)

- explain/justify the choices made in the application of the method (15%)

- plot the results in a clear and logical manner (20%)

- interpret and reflect on the results (30%)

It is allowed to make selections of columns or rows if deemed appropriate or required, e.g., due to memory constraints. Doing so will require justification of the approach and reflection on the consequences for the results.

It is allowed to chain methods, i.e., use the results from one method as input for another method.

For each method only one analysis will be considered for assessment. If multiple analyses are provided, the worst executed one will be selected for assessment.

Think, then implement. Good luck.

**Datasets:**

*The file* **contacts.dat.gz** *contains information about contacts during the simulated pulling of a protein. The experiment corresponds to AFM measurements, in which a protein is unfolded by pulling it, during which the force is measured. The unfolding is associated with the loss of contacts between atoms in the structure. The aim of the simulations is to provide a physical understanding of the process in the experiments. The first column contains the time (arbitrary units), the second column contains the position of the AFM tip, the third column contains the force exerted on the tip. The remaining columns correspond to contacts, in which a 1 indicates the contact is present and a 0 indicates the contact is not present.*

*The file* **clinical\_trajectories\_df.xlsx** *contains diagnostic data from patients with neurological disorders. For each patient, records are given of clinical symptoms with the year of diagnosis, as well as the condition, and the year and age of death. These data are part of an ongoing endeavor to classify and predict clinical trajectories of neurological conditions. (FA)*

*The file* **randompoisson.dat.gz** *contains 1000 by 10000 Poisson distributed random numbers with means per column taken from an exponential distribution. This can be considered simplified fictive/dummy count data, e.g., from genomics/transcriptomics, with 1000 observations in 10000 variables.*

*The file* **lysozyme\_rmsds.csv** *contains a distance matrix of a selection of lysozyme structures from the Protein DataBank (PDB). Lysozyme is one of the most used/studied proteins, with >5400 structures available in the database. Distances were determined as root-mean-square deviation (RMSD) after least-squares alignment using the CE align algorithm. (MDS)*