

Processing of Biological Data

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Exercise Sheet 1

Due: 16.05.2017 10:15

Submit your solutions on paper, hand-written or printed at the *beginning* of the lecture or in building E21, Room 3.03. Alternatively you may send an email with a single PDF attachment. If possible, please include source code listings. Additionally hand in all source code via mail to duy.nguyen@bioinformatik.uni-saarland.de.

Principal Component Analysis (PCA) and Data Imputation

Exercise 1.1: Principal Component Analysis (50 points)

- (a) Describe step-by-step the PCA technique on matrix \mathbf{X} (with \mathbf{I} observations and \mathbf{J} variables), from the pre-process until the transformed matrix is obtained (20 points).
- (b) In this section, we will apply the PCA technique to a toy dataset (“pca_toy.txt” in the supplement, with 50 observations and 4 variables: a , b , c and d) by using the built-in function `prcomp` in R. The documentation of `prcomp` can be found in: <https://stat.ethz.ch/R-manual/R-devel/library/stats/html/prcomp.html>
 - Plot the transformed data w.r.t. the first two principal components (PC1 and PC2) (10 points)
 - Which variables are the most important in PC1 and PC2? Why? (10 points)
- (c) Why do we need to standardize the data before doing PCA? (10 points)

Exercise 1.2: Data Imputation (50 points)

In this exercise, we will perform imputation based on a given data distribution. The main idea behind this method is to impute missing proteomics data which have expression below the detection limit (http://www.nature.com/nmeth/journal/v13/n9/fig_tab/nmeth.3901_SF3.html). Basically, the imputation can be broken down into the following steps:

1. Calculate the mean and standard deviation of the current data.
2. Derive the new mean and standard deviation for the missing data based on the current distribution. The new mean should be in the lower quantile of the distribution since we want to simulate the low expression data. The new standard deviation could be derived by taking a fraction of the current standard deviation.
3. Generate the new data based on the new mean and standard deviation from the previous step.
 - (a) The “ms_toy.txt” file contains an example of proteomics data with 6 samples (columns). Use any of the 6 samples and write a script to impute the missing data (which are indicated by “NA”) for the sample of your choice by following the steps mentioned above. (20 points)

Hint: in R, use function `qnorm` to derive the new mean and function `rnorm` to generate the data.
 - (b) Play around with different new means and standard deviations. Plot the distribution of the sample with the imputed data in a similar fashion as Fig. 1. What is the effect of different means and standard deviations? (20 points)

Hint: in R, use function `hist` and function `plot`

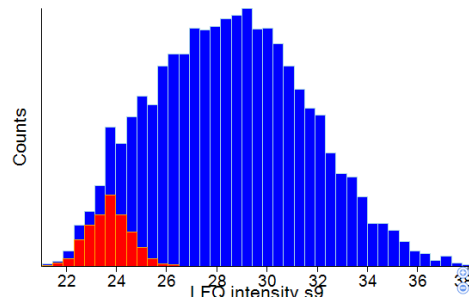


Figure 1: Sample Plot (blue is the overall distribution, red is the imputed data)

(c) What is the shortcoming of this method? (10 points)