Bioinformatics III

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Exercise Sheet 7

Due: June 10, 2021 12:00

Submit your solutions to andreas.denger@bioinformatik.uni-saarland.de with two attachments: (1) A ZIP file containing all your source code files, potential result files, figures and whatever else is needed to generate your solution, (2) a PDF file containing your answers. Subject of the email should be in the following format: BI3 A7 LastName1 LastName2.

Co-expression Correlation and Master Regulatory Genes

Exercise 7.1: Co-expression based on Correlation and Mutual Information (60 points)

Mutual information (I) and Pearson correlation coefficient (Corr) between two random variables are defined as:

$$I(X,Y) = \sum_{x \in X} \sum_{y \in Y} p(x,y) \times log\left(\frac{p(x,y)}{p(x) \times p(y)}\right)$$
$$Corr(X,Y) = \frac{\sum_{i=1}^{n} (x_i - \mu_X) \times (y_i - \mu_Y)}{\sqrt{\sum_{i=1}^{n} (x_i - \mu_X)^2} \times \sqrt{\sum_{i=1}^{n} (y_i - \mu_Y)^2}}$$

, where p(x, y) is the joint probability distribution of expression levels x and y, p(x) is the marginal probability of expression value x, and μ_X is the (arithmetic) mean expression for gene X.

(a) Calculate the Pearson correlation coefficient and mutual information for the data given below. Here, the data is comprised of two genes whose expression were measured over 6 time series. An expressed gene is denoted by value 1. Solve this task by hand.

Gene	t1	t2	t3	t4	t5	t6
gene1	0	0	1	1	1	0
gene2	0	1	0	0	1	1

- (b) Explain the main difference between mutual information and Pearson correlation.
- (c) What is the advantage of using rank-based correlation coefficients?
- (d) Write a program that reads the time-series gene expression data given in the supplement and calculates the Pearson correlation coefficients for all pairs of genes.
- (e) Plot the distribution of correlation coefficients between pairs of genes, for example by using the displot function from the Python package *seaborn*. Ignore pairs that contain the same gene twice.

Interpret the shape of the plot and include it in your submission.

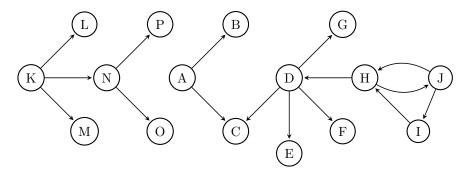
- (f) Take a look at the correlation scores between the gene ITGB2 and the other genes. Write a function that finds the gene with the:
 - Highest correlation to ITGB2
 - Lowest correlation to ITGB2

• Correlation to ITGB2 that is closest to zero

Next, for each of these three genes, create a scatter plot with a linear regression model fit between its expression values and those of *ITGB2*, for example with the regplot function from the Python package *seaborn*.

Include the three plots in your submission and describe what you see.

Exercise 7.2: Identification of master-regulatory genes (40 points)



- (a) Which dominating sets exist in the network shown above?
- (b) What is the minimum dominating set (MDS) of this network?
- (c) List the following sets of nodes and their sizes:
 - Largest connected component in the directed graph
 - Largest strongly connected component in the directed graph
 - Largest connected component in the underlying undirected graph

Find the minimum connected dominating set (MCDS) for each of the three sets.

(d) Compare the MDS and MCDS in terms of size.