

Tutorial Complex Systems

Freie Universität Berlin, Summer 2020

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Assignment 1

Due date: 24.04.2020 10:00 AM before the lecture

You should upload a single PDF report (with all the important steps of your calculations), code files (with comments and clear function naming) and any additional files requested in the assignment on Whiteboard (KVV). Optimally you should generate your PDF report in Latex, we will also accept *legible* photos/scans grouped into a single PDF file. Form groups of 2 students to solve the problems but remember: everyone has to be able to explain the solutions.

Problem 1 (*30 Points; Gene Networks*). Consider the following RPKM values from 5 RNA-seq experiments for the following genes:

Gene	Exp1	Exp2	Exp3	Exp4	Exp5
A	7	9.2	14.6	20	35.1
B	19	14.2	6.6	14.6	18
C	8.6	7.0	6.5	7.3	8.7
D	6.8	7.9	5.5	2.3	2.9
E	0.9	1.8	3.9	4.8	6.2

Using the package NetworkX for Python 3, draw the gene network with the following criteria for edges:

(A) Draw an edge between genes X and Y if the Euclidean distance:

$$d_E(X, Y) := \sqrt{\sum_{i=1}^n (x_i - y_i)^2} < 11.$$

n is the number of samples (i.e. experiments) and $X, Y \in \{A, B, C, D, E\}$.

(B) Draw an edge between genes X and Y if the correlation coefficient $|r(X, Y)| > 0.75$. Color the edges with positive correlation red and the edges with negative correlation blue.

(C) Draw an edge between genes X and Y if the L_1 -norm:

$$\|X, Y\|_{L_1} := \frac{1}{n} \sum_{i=1}^n |x_i - y_i| < 7$$

(D) Draw an edge between genes X and Y if the mutual information:

$$I(X, Y) := \sum_{x \in X} \sum_{y \in Y} p(x, y) \log\left(\frac{p(x, y)}{p(x)p(y)}\right) > 0.65.$$

To calculate the mutual information, bin the RPKM values for each gene into 3 intervals.

Problem 2 (40 Points; Probabilistic Distribution, Independence, Information Theory). Consider two random variables X and Y from which we drew the following samples:

$$x = (0.3, 0.98, 0.54, 0.49, 0.39, 0.14, 0.03, 0.81, 0.65, 0.18)$$

$$y = (0.74, 0.09, 0.48, 0.15, 0.71, 0.8, 0.53, 0.95, 0.63, 0.88)$$

Therefore the first observation is ($x = 0.3$, $y = 0.74$) and so on (10 observations in total). First, bin the data by dividing the interval of $[0, 1]$ into 4 equally wide sub-intervals. Provide the following calculations *by hand*.

(A) Calculate the joint probability distribution $p_{X,Y}(x, y)$ of the binned data and write it in the following table:

$Y X$	x_1	x_2	x_3	x_4
y_1				
y_2				
y_3				
y_4				

(B) Calculate the marginal distributions $p_X(x)$ and $p_Y(y)$

(C) Calculate the product of the two marginal distributions $p_X(x) \times p_Y(y)^T$ (matrix multiplication!) and compare it with the joint distribution $p_{X,Y}(x, y)$. Are the variables X and Y stochastically independent? Justify your answer.

(D) Calculate the conditional distributions $p_{X|Y}(x|y = y_3)$ and $p_{Y|X}(y|x = x_4)$

(E) Calculate the joint entropy $H(X, Y)$ and the marginal entropies $H(X)$ and $H(Y)$

(F) Calculate the conditional entropies $H(X|Y)$ and $H(Y|X)$ using the chain rule.

(G) Calculate the mutual information $I(X, Y)$ using both, the definition and the relation to entropy. Are both results equal? Why?

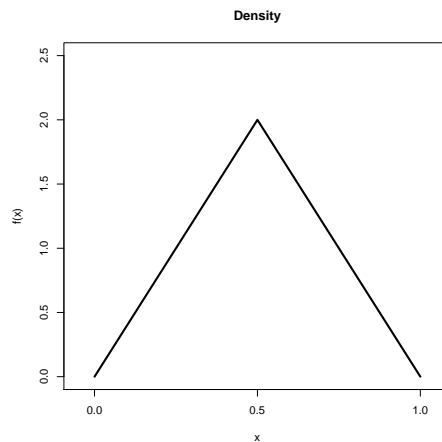
Problem 3 (20 Points; Network topology). Install Cytoscape 3.8 and get familiar with its interface. For subsequent tasks use the package NetworkX for Python 3.

(A) Generate a random network $G(n = 150, p = 0.08)$ according to Erdős-Rényi model where n is the number of nodes and p is the probability of including an edge in the graph (remember to set a random seed, mention it in your report). Analyze your network:

calculate the number and size of connected components, plot histograms for the degree values, closeness and betweenness centralities. Normalize the degree histogram and on top of it plot the theoretically appropriate Poisson probability mass function (you may use `scipy.stats.poisson`). Compare the two. Export the network as GraphML file and the node attributes (centralities, degree) as a csv file. Check what happens when you change the value of p (you do not need to hand in the results for other values of p).

- (B) Import the network and its attributes from the previous task into Cytoscape. Visualize it so that: the size of the node reflects the closeness centrality value (the larger the closeness, the larger the node), betweenness centrality is represented by colour of the node (viridis colour palette - yellow for small values, dark blue for large values) and the degree value is set as the label of the node. Set layout to degree sorted circular and save the resulting visualization as an image. On top of that save an image of a zoom-in on the node with the largest degree. Include it in your report.
- (C) In a separate session in Cytoscape, download the Escherichia coli interactome (File -> Import -> Network from Public Databases) from IMEx. Delete all the nodes for which the Taxonomy ID is not equal to 83333 (which represents the E. coli K-12 strain). Keep only the largest remaining connected component of the network (delete the rest). Run tool Analyze Network (assume the network is not directed). What is the number of nodes and edges that are left after all the previous filtering steps? Export the image of node degree distribution and include it in your report. Is it the same as for the Erdős-Rényi model? Upload your Cytoscape session (*.cys) file to Whiteboard (KVV).

Problem 4 (10 Points; Expected value). Consider the following density function $f_X(x)$ of random variable X :



Calculate the expected value EX and the variance of X .