Bioinformatics III

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Winter Semester 2020

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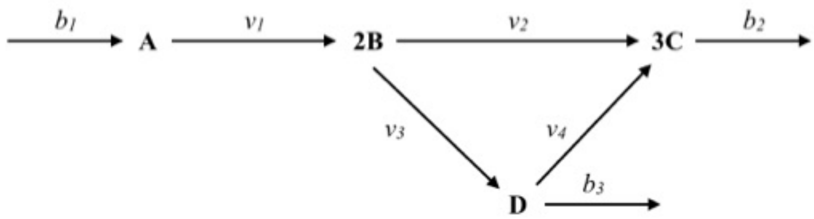
Tutor

Exercise Sheet 9
Graph and Pathways of Metabolic Networks
Due: June 29, 2021 12:00

Submit your solutions to pratiti.bhadra@bioinformatik.uni-saarland.de (a PDF file containing your answers). Subject of the email should be in the following format: *BI3 A9 LastName1 LastName2.*

Please feel free to contact me for any clarifications either via email or you can reach me in building E2.1, Room 3.01 (preferably between 3 pm and 4 pm).

Q1 Stoichiometric Matrix and Extreme Pathways (*50 points*)



Metabolites are A,B,C and D. There are four internal flux reactions v_1-v_4 and three unconstrained external fluxes b_1, b_2 and b_3.

(a) Determine the stoichiometric Matrix (*10 points*)

(b) Calculate the extreme pathways of the above network. Show step wise calculation. Give the extreme pathways as a sum of the individual reactions, and sketch them with a layout similar to the given network. (*25 points*)

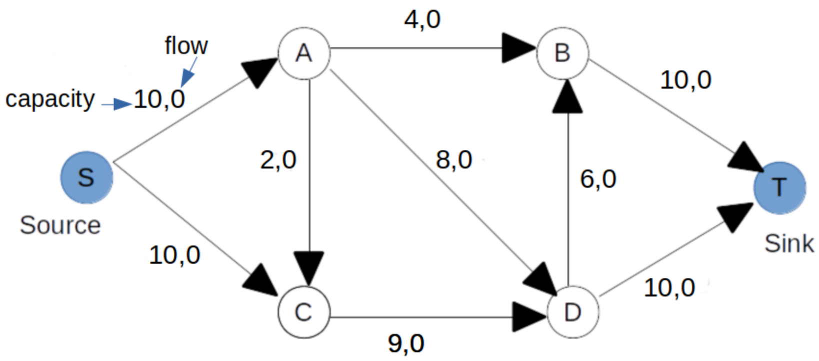
(c) Determine the pathway length matrix. Which information does it provide? (*5 points*)

(d) Determine the reaction participation matrix. Which reaction(s) contribute(s) to the most pathways. (*5 points*)

(e) Now assume that reaction b_2 is essential for the organism, i.e. it dies if there is no output via b_2 . Determine from the extreme pathways which (combinations of) internal reactions are essential, i.e. if they are blocked, then the output via b_2 is blocked, too. (*5 points*)

Q2 Max-flow-min-cut (*40 points*)

(a) Find the minimum capacity over all S-T cuts of the given graph. (*hint: Ford Fulkerson algorithm*) (*20 points*)



(b) The counts of supply and demand of four different kinds of food are given in the following table (*20 points*)

Food type	Vegan	Vegetarian Type A	Vegetarian Type B	Non-Vegetarian
Supply	50	36	11	8
Demand	45	42	8	3

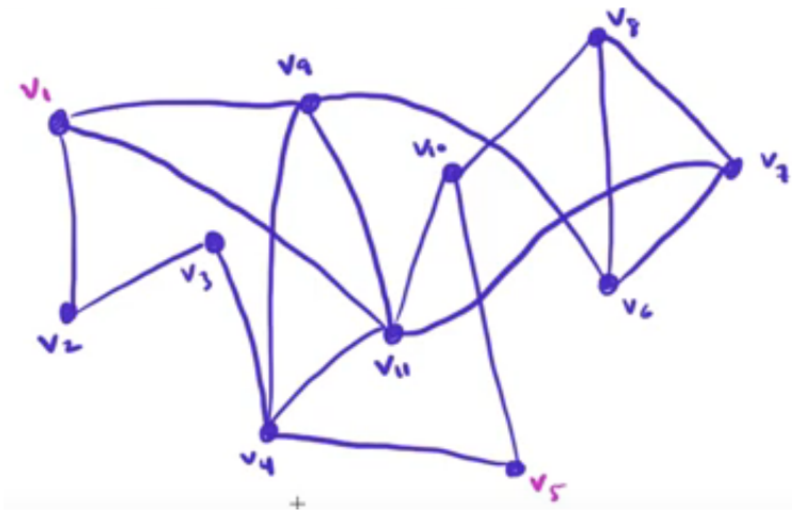
'Vegetarian Type A' can only have 'Vegetarian Type A' or 'Vegan' food; 'Vegetarian Type B' can eat only 'Vegetarian Type B' or 'Vegan'; 'Vegan' can have only 'Vegan' food; and 'Non-vegetarian' can eat any of the four types.

Model the problem as a flow network problem. Draw the corresponding network. (*hint: In the network, there will be one source node, one sink node, 4 nodes for the supply of each food type and 4 nodes for the demand of each food type.*)

Is it possible to meet the full demand? Explain why or why not, using an argument based on a min cut. If it is not possible to meet the full demand, the output of your algorithm still is meaningful. What does it tell you?

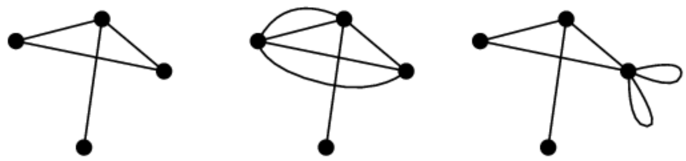
(c) Graph connectivity (*10 points*)

(a) How many internally disjoint V_1-V_5 paths are in the following graph G? How can you explain this? (*3 points*)
internally disjoint path (edge-independent path): Paths are internally disjoint if they have no common internal vertex.



(b) Let G be a 3-regular graph. The vertex-connectivity of G is equal to 3, $k_v(G) = 3$. Find out the edge-connectivity of the graph G, $k_e(G) = ?$. (*3 points*)
A graph is **r-regular** if every vertex has degree **r**.

(c) "There exists a connected n-vertex simple graph with n+1 edges". If the above statement is true give an example or if it is false explain why (*4* points).
simple graph: An unweighted, undirected graph containing no graph loops or multiple edges. A simple graph may be either connected or disconnected.



simple graph *nonsimple graph with multiple edges* *nonsimple graph with loops*