



Strathmore
UNIVERSITY

Institute of Mathematical Sciences
MASTER OF SCIENCE IN BIOMATHEMATICS
END OF SEMESTER EXAMINATION
BMA 8303: Computational Systems Biology

Date: 11 January, 2023

Time: 2.5 Hours

Instructions

1. This examination consists of **FIVE** questions.
2. Answer **Question ONE (COMPULSORY)** and any other **TWO** questions.

QUESTION ONE (20 MARKS)

- (a) Discuss briefly the following biological networks. [4 Marks]
- (i) Protein-protein interaction networks
 - (ii) Cell signalling networks

- (b) Following are two statements pertaining to the reaction $2A + B \rightarrow 2C$, for which the rate law is

$$rate = k[A][B].$$

Identify which statement is true and which is false, and explain your reasoning. [2 Marks]

- (i) The value of k is independent of the initial concentrations $[A]_0$ and $[B]_0$.
 - (ii) The unit of the rate constant for this reaction can be expressed either as s^{-1} or min^{-1} .
- (c) (i) Use Euler's method to obtain a numerical solution of the differential equation $\frac{dy}{dx} + y = 2x$, given the initial conditions that at $x = 0, y = 1$, for the range $x = 0(0.2)1.0$. Draw the graph of the solution in this range. [5 Marks]
- (ii) Determine the percentage error at $x = 0.4$. [3 Marks]
- (d) (i) Determine the **eccentricity**, **diameter** and **radius** of the Biological Network **G** shown in Figure 1 below. [3 Marks]

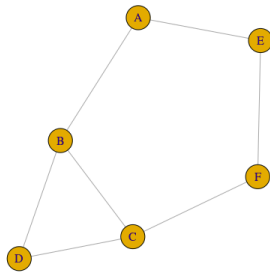


Figure 1: Network G

- (ii) Find the betweenness centrality for vertex **b** in Network G [3 Marks]

QUESTION TWO (20 MARKS)

- (a) Calculate the activation energy, ϵ_a (in $Jmol^{-1}$), of a reaction at 330K and a rate constant $1.30 \times 10^{-6}s^{-1}$. Assume $A = 5.44 \times 10^{13}$ and $R = 8.31JK^{-1}mol^{-1}$. [3 Marks]
- (b) Consider the following gene regulatory network. X enhances Y, X and Y enhances Z (that is, both X and Y need to be present to enhance Z) and X inhibits Y.

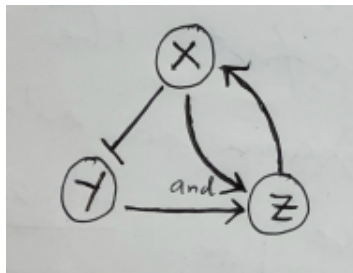


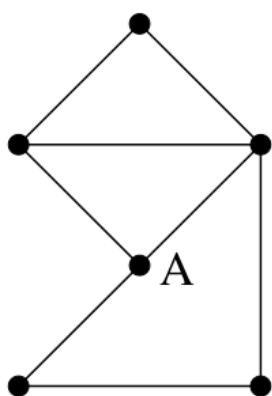
Figure 2

- (i) Write down the Boolean network for the above gene regulatory network. [3 Marks]
- (ii) Given that $(X, Y, Z)_0 = (0, 1, 1)$, determine $(X, Y, Z)_1$, $(X, Y, Z)_2$ and $(X, Y, Z)_3$ [4 Marks]
- (c) The following data were obtained in two separate experiments in the reaction: $A \rightarrow$ products. Determine the rate law for this reaction, including the value of the rate constant k . [10 Marks]

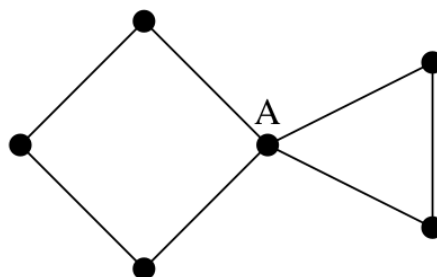
Experiment 1		Experiment 2	
[A](M)	time(s)	[A](M)	time(s)
0.800	0	0.400	0
0.775	40	0.390	64
0.750	83	0.380	132
0.725	129	0.370	203
0.700	179	0.360	278

QUESTION THREE (20 MARKS)

- (a) (i) Obtain a numerical solution of the differential equation: $\frac{dy}{dx} = 3(1+x) - y$ in the range 1.0(0.2)1.4, using the fourth order Runge-Kutta (RK4) method, given the initial conditions that $x = 1.0$ when $y = 4.0$. [11 Marks]
- (ii) Using analytical method, determine the exact solution to the given differential equation and hence the percentage error at $x = 1.4$ by RK4 method. [3 Marks]
- (b) Determine the degree centrality, closeness centrality and betweenness centrality for the vertex A in the following networks: [6 Marks]



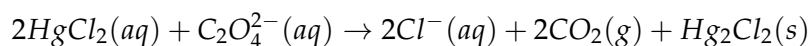
(a) Network



(b) Network

QUESTION FOUR (20 MARKS)

- (a) State two quantities that must be measured to establish the rate of a chemical reaction and cite two factors that affect the rate of a chemical reaction. [4 Marks]
- (b) In the reaction $H_2O_2(aq) \rightarrow H_2O(l) + \frac{1}{2}O_2$, the initial concentration of H_2O_2 is $0.2546M$, and the initial rate of reaction is $9.32 \times 10^{-4} Ms^{-1}$. What will be $[H_2O_2]$ at $t = 35s$? [4 Marks]
- (c) The rate of the following reaction in aqueous solution is monitored by measuring the number of moles of Hg_2Cl_2 that precipitate per liter per minute. The data obtained are listed in the following table.

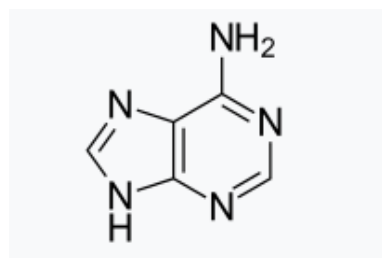


Experiment	$[HgCl_2](M)$	$[C_2O_4^{2-}](M)$	Initial rate ($molL^{-1}min^{-1}$)
1	0.105	0.15	1.8×10^{-5}
2	0.105	0.15	1.8×10^{-5}
3	0.052	0.30	7.1×10^{-5}
4	0.052	0.15	8.9×10^{-6}

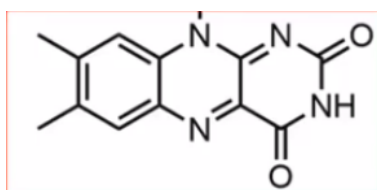
- (i) Determine the order of reaction with respect to $HgCl_2$, with respect to $C_2O_4^{2-}$ and overall. [6 Marks]
- (ii) What is the value of the rate constant k ? [2 Marks]
- (iii) What would be the initial rate of reaction if $[HgCl_2] = 0.094M$ and $[C_2O_4^{2-}] = 0.19M$? [2 Marks]
- (iv) Are all four experiments necessary to answer parts (a) – (c)? Explain. [2 Marks]

QUESTION FIVE (20 MARKS)

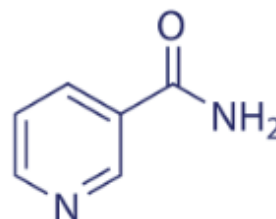
- (a) In the final stage of Catabolism, Acetyl CoA get oxidised in the citric acid cycle to liberate CO_2 and there is formation Nicotinamide-Adenine-Dinucleotide-Hydrogen and Flavin-Adenine-Dinucleotide-Di-Hydrogen. Name the biological molecules whose structures are given below. [3 Marks]



(a)



(b)



(c)

Figure 4: Pictures of animals

- (b) Derive the rate law based on the following experimental data. [7 Marks]

Experiment	[A] $mol\,dm^{-3}$	[B] $mol\,dm^{-3}$	[C] $mol\,dm^{-3}$	Rate $mol\,dm^{-3}\,s^{-1}$
1	0.1	0.5	0.25	0.1
2	0.2	0.5	0.25	0.2
3	0.1	1.0	0.25	0.4
4	0.1	0.5	0.5	0.1

- (c) A ball at $1200\,K$ is allowed to cool down in air at an ambient temperature of $300\,K$. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.3067 \times 10^{-12}(\theta^4 - 81 \times 10^8), \quad \theta(0) = 1200K$$

where θ is in K and t in seconds. Find the temperature at $t = 480$ seconds using Runge-Kutta 4th order method. Assume a step size of $h = 240$ seconds. [10 Marks]

END OF PAPER