Strathmore
UNIVERSITY

Institute of Mathematical Sciences

MASTER OF SCIENCE IN BIOMATHEMATICS

END OF SEMESTER EXAMINATION

BMA 8303: Computational Systems Biology

Date: 18th April, 2024 **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]

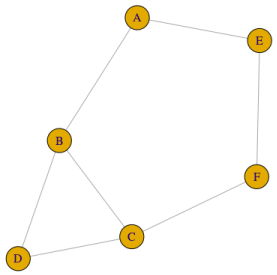


Figure 1: Network **G**

(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 $R = 8.31 JK^{-1}mol^{-1}$. [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.

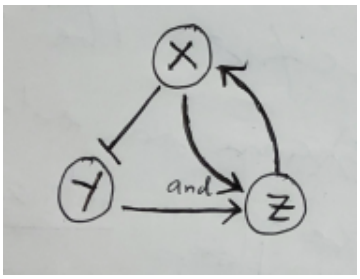


Figure 2

(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]

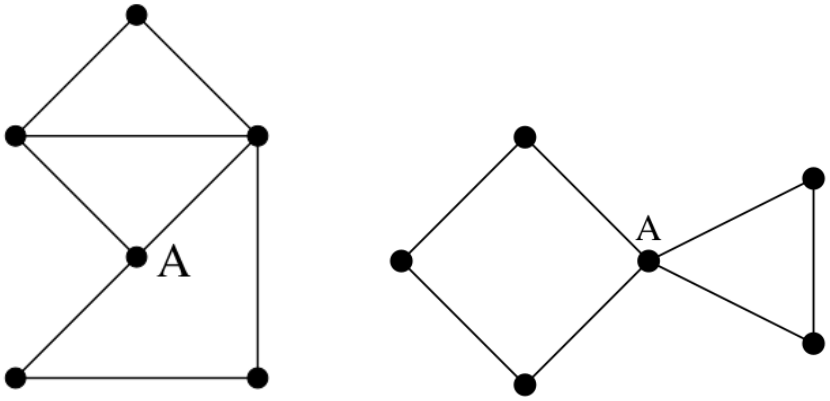
Experiment 1		Experiment 2	
$[A]$(M)	time(s)	$[A]$(M)	time(s)
0.800	0	0.400	0
0.775	40	0.390	64
0.750	83	0.380	132
0.725	129	0.370	203
0.700	179	0.360	278

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 diffential 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.

$$2HgCl_2(aq) + C_2O_4^{2-}(aq) \rightarrow 2Cl^-(aq) + 2CO_2(g) + Hg_2Cl_2(s)$$

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]

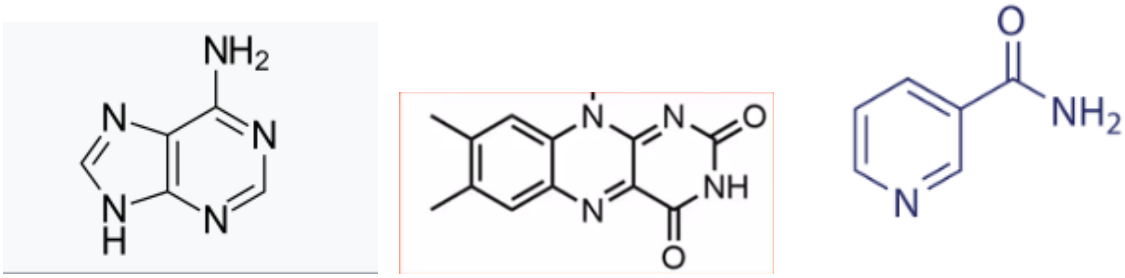
(ii) What is the value of the rate constant k? [2 Marks]

(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] $moldm^{-3}$	[B] $moldm^{-3}$	[C] $moldm^{-3}$	Rate $moldm^{-3}s^{-1}$
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