

MOLECULAR COMMUNICATION IN BIOLOGICAL CELLS: FOUNDATIONAL  
STUDY AND DEVELOPMENT OF COMPUTATIONAL TECHNIQUES

by

Zahmeeth Sayed Sakkaff

A DISSERTATION

Presented to the Faculty of

The Graduate College at the University of Nebraska

In Partial Fulfilment of Requirements

For the Degree of Doctor of Philosophy

Major: Engineering

(Computer Engineering-Computer Science)

Under the Supervision of Professor Massimiliano Pierobon

Lincoln, Nebraska

July, 2019

MOLECULAR COMMUNICATION IN BIOLOGICAL CELLS: FOUNDATIONAL  
STUDY AND DEVELOPMENT OF COMPUTATIONAL TECHNIQUES

Zahmeeth Sayed Sakka, Ph.D.

University of Nebraska, 2019

Adviser: Massimiliano Pierobon

Your abstract

## ACKNOWLEDGMENTS

Your ack

## Table of Contents

<b>List of Figures</b>	<b>v</b>
<b>List of Tables</b>	<b>vi</b>
<b>1 Introduction</b>	<b>1</b>
<b>2 Background</b>	<b>2</b>
2.1 Motivation . . . . .	2
2.2 Biological Pathways . . . . .	2
2.2.1 Gene Regulation . . . . .	3
<b>3 Conclusion and Future Directions</b>	<b>4</b>
<b>Bibliography</b>	<b>5</b>

## List of Figures

2.1	Graphical representation of the interconnection of signal transduction, gene regulation and metabolic pathways. . . . .	2
-----	--	---

## List of Tables

2.1	Mutual information values for different sugars. . . . .	3
-----	---	---

## Chapter 1

### Introduction

Your intro

Reference [1].

Refere section or subsetion ??.

Equations (2.1).

## Chapter 2

## Background

### 2.1 Motivation

Your background

### 2.2 Biological Pathways

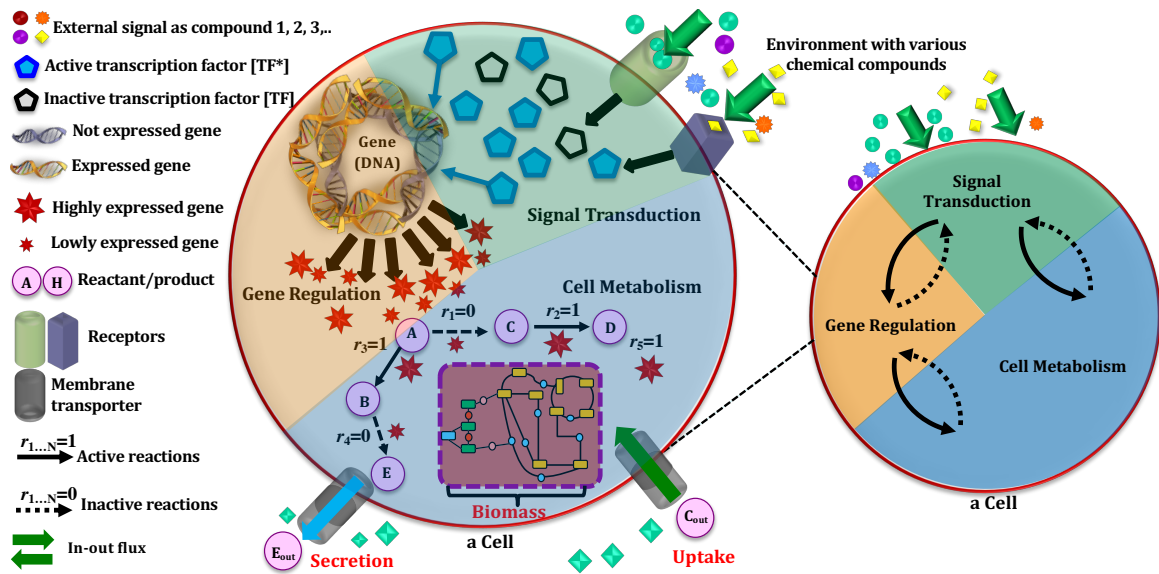


Figure 2.1: Graphical representation of the interconnection of signal transduction, gene regulation and metabolic pathways.



---

**Algorithm 1:** Probability Histograms for Equation (??)

---

**Data:**  $R$  simulation runs for each of  $I$  input concentrations containing values for all  $N$  simulation steps

**Result:** For each protein  $j$ ,  $p_{Y_j}$  and  $p_{X|\{y_{j,t_n}\}_{n=0}^N}$

- 1 **for** *each simulation time step*  $t_n$  **do**
- 2     Create  $\{Z_{i,r}\}_{t_n}$  by extracting protein  $j$  concentration for each simulation run  $r$  and input concentration  $i$
- 3     Map each value of  $\{Z_{i,r}\}_{t_n}$  in  $N_{j,t_n}$  equally-spaced bins (with index  $b_{t_n}$ ) between min and max values, expressed as  $(\{Z_{i,r}\}_{t_n}, b_{t_n})$
- 4 **end**
- 5 Obtain matrix  $M$  of size  $C$  by  $N$  by combining all the mapped bin indices  $b_{t_n}$  for each simulation run  $(i, r)$  and each time step  $t_n$
- 6 Compute the multidimensional histogram considering each row of  $M$  as a datapoint:  
 $p_{Y_j}(\{y_{j,t_n}\}_{n=0}^N)$
- 7 **for** *each bin in the multidimensional histogram* **do**
- 8     Take all the input values corresponding to the values  $\{y_{j,t_n}\}_{n=0}^N$  that define the current multidimensional bin
- 9     Compute the histogram  $p_{X|\{y_{j,t_n}\}_{n=0}^N}$  by mapping the input values found at Step 8 into  $S_{\{y_{j,t_n}\}_{n=0}^N}$  equally space bins between min and max values
- 10    If no input value from Step 8, set  $p_{X|\{y_{j,t_n}\}_{n=0}^N} = 0$
- 11 **end**

---

### 2.2.1 Gene Regulation

$$N_{j,t_n} = 1 + \log_2(C) + \log_2 \left( 1 + \frac{g_{Y_j}(t_n)}{\sigma_{g_{Y_j}(t_n)}} \right). \quad (2.1)$$

Table 2.1: Mutual information values for different sugars.

Sugar Type	$\tilde{H}(X)$	$\tilde{H}(X bm(t_c))$	$\tilde{H}(X) - \tilde{H}(X bm(t_c))$
Glucose	6.6295	5.2694	1.3601
Lactose	6.6295	5.2851	1.3444
Glucose6P	6.6295	5.8971	0.7324

## Chapter 3

### Conclusion and Future Directions

Your conclusion

- AAA
- BBB

## Bibliography

- [1] S Mahner, C Baasch, J Schwarz, S Hein, L Wlber, F Jnicke, and K Milde-Langosch. C-fos expression is a molecular predictor of progression and survival in epithelial ovarian carcinoma. *Br. J. Cancer*, 99(8):1269–1275, October 2008.