Computational methods for analyzing bistability in biochemical reaction networks

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***Abstract*—Bistability plays a key role in important biological processes, such as cell division, differentiation, and apoptosis. Examples show that there is a very delicate relationship between the structure of a reaction network and its capacity for bistable behavior. We describe mathematical methods that discriminate between networks that have the capacity for bistability and those that do not, as well as algorithms derived from these methods. We have implemented some of these algorithms in the software package BioNetX. We present results obtained by using this package to analyze random samples from a comprehensive database of reaction networks.**

I. Introduction

A chemical reaction network is usually given by a finite list of reactions that involve a finite set of chemical species. As an example, consider the reaction network with two species A_1 and A_2 schematically given in the diagram (1).

$$2A_1 \rightleftarrows A_1 + A_2 \rightleftarrows 2A_2 \tag{1}$$

To keep track of the temporal variation of the state of this chemical system, we define the functions $c_{A_1}(t)$ and $c_{A_2}(t)$ to be the molar concentrations of the species A_1, A_2 at time t. The chemical reactions in the network are responsible for changes in the concentrations; for instance, whenever the reaction $A_1 + A_2 \to 2A_1$ occurs, there is a net gain of a molecule of A_1, whereas one molecule of A_2 is lost. Similarly, the reaction $2A_2 \to 2A_1$ results in the the creation of two molecules of A_1 and the loss of two molecules of A_2.

We will assume that the rate of change of the concentration of each species is governed by *mass-action kinetics* [12], i.e., that each reaction takes place at a rate that is proportional to the product of the concentrations of the species being consumed in that reaction. For example, under the mass-action kinetics assumption, the contribution of the reaction $A_1 + A_2 \to 2A_2$ to the rate of change of c_{A_2} has the form $k_{A_1+A_2\to 2A_2} c_{A_1} c_{A_2}$, where $k_{A_1+A_2\to 2A_2}$ is a positive number called *reaction rate constant*. Collecting these contributions from all the reactions, we obtain the following system of differential equations:

$$\begin{aligned} \dot{c}_{A_1} = & -k_{2A_1\to A_1+A_2} c_{A_1}^2 + k_{A_1+A_2\to 2A_1} c_{A_1} c_{A_2} + \\ & + k_{2A_2\to A_1+A_2} c_{A_2}^2 - 2k_{2A_1\to 2A_2} c_{A_1}^2 + 2k_{2A_2\to 2A_1} c_{A_2}^2 \\ \dot{c}_{A_2} = & \ k_{2A_1\to A_1+A_2} c_{A_1}^2 - k_{A_1+A_2\to 2A_1} c_{A_1} c_{A_2} - \\ & - k_{2A_2\to A_1+A_2} c_{A_2}^2 + 2k_{2A_1\to 2A_2} c_{A_1}^2 - 2k_{2A_2\to 2A_1} c_{A_2}^2 \end{aligned} \tag{2}$$

We now introduce the standard terminology of Chemical Reaction Network Theory (see [12], [5] for more details). We denote by $\mathbb{R}$ the set of real numbers, by $\mathbb{R}_+$ the set of strictly positive real numbers, and by $\mathbb{R}_+$ the set of nonnegative real numbers. For an arbitrary finite set I we denote by $\mathbb{R}^I$, $\mathbb{R}^I_+$ and $\mathbb{R}^I_+$ the sets of formal sums $\alpha = \sum_{i\in I} \alpha_i i$ with $\alpha_i \in \mathbb{R}$, $\alpha_i \in \mathbb{R}_+$ and $\alpha_i \in \mathbb{R}_+$ respectively. The *support* of an element $\alpha \in \mathbb{R}^I$ is $supp(\alpha) = \{i \in I : \alpha_i \neq 0\}$.

A *chemical reaction network* is a triple $(\mathcal{S}, \mathcal{C}, \mathcal{R})$, where $\mathcal{S}$ is the set of chemical *species*, $\mathcal{C} \subseteq \mathbb{R}^{\mathcal{S}}_+$ is the set of *complexes* (i.e., the objects on the left or right side of reaction arrows), and $\mathcal{R}$ is a relation on $\mathcal{C}$, denoted $y \to y'$ and represents the set of *reactions* in the network. Moreover, the set $\mathcal{R}$ must satisfy the following three conditions: (i) it cannot contain elements of the form $y \to y$; (ii) for any $y \in \mathcal{C}$ there exists some $y' \in \mathcal{C}$ such that either $y \to y'$ or $y' \to y$; (iii) the union of the supports of all $y \in \mathcal{C}$ is $\mathcal{S}$.

For the network (1), the set of species is $\mathcal{S} = \{A_1, A_2\}$, the set of complexes is $\mathcal{C} = \{2A_1, A_1 + A_2, 2A_2\}$ and the set of reactions is $\mathcal{R} = \{2A_1 \rightleftarrows A_1 + A_2, 2A_2 \rightleftarrows 2A_1, 2A_2 \to A_1 + A_2\}$, and consists of 5 reactions, represented as two reversible reactions and one irreversible reaction.

Note that we regard the complexes as non-negative linear combinations of the species; on the other hand, it will be useful to also think of the complexes as (column) vectors of dimension equal to the number of elements of $\mathcal{S}$, via an identification given by a fixed ordering of the species. For example, the complexes above are

$$2A_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}, A_1 + A_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \text{ and } 2A_2 = \begin{bmatrix} 0 \\ 2 \end{bmatrix}.$$

This slight abuse of notation provides a convenient way of representing the *reaction vectors* $y' - y$ for all $y \to y' \in \mathcal{R}$.

We may now define mass-action systems and the set of differential equations that governs mass-action kinetics. First we introduce a useful notation. Given two vectors $u = \sum_{s\in\mathcal{S}} u_s s$ and $v = \sum_{s\in\mathcal{S}} v_s s$ in $\mathbb{R}^{\mathcal{S}}_+$, we denote $u^v = \prod_{s\in\mathcal{S}} (u_s)^{v_s}$, with the convention $0^0 = 1$.

A *mass-action system* is a quadruple $(\mathcal{S}, \mathcal{C}, \mathcal{R}, k)$, where $(\mathcal{S}, \mathcal{C}, \mathcal{R})$ is a chemical reaction network and $k \in \mathbb{R}^{\mathcal{R}}_+$, where $k_{y\to y'}$ is the *reaction rate constant* of the reaction $y \to y' \in \mathcal{R}$. The *system of differential equations* for the mass-action

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Algorithms And Computational Methods For Biochemical And Evolutionary Networks

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Evolutionary Computation and the journal of Genetic Programming and Evolvable Machines Nasimul Noman is a lecturer in the School of Electrical Engineering and Computer Science at the University of Newcastle NSW Australia From 2002 to 2012 he was a faculty member at the University of Dhaka Bangladesh Noman is an Editor of the BioMed Research International journal His research interests include computational biology synthetic biology and bioinformatics **Combinatorial Pattern Matching** Moshe Lewenstein,Gabriel Valiente,2006-07-01 This book constitutes the refereed proceedings of the 17th Annual Symposium on Combinatorial Pattern Matching CPM 2006 held in Barcelona Spain July 2006 The book presents 33 revised full papers together with 3 invited talks organized in topical sections on data structures indexing data structures probabilistic and algebraic techniques applications in molecular biology string matching data compression and dynamic programming **Computational Methods in Systems Biology** Pierpaolo Degano,Roberto Gorrieri,2009-08-27 This volume contains the proceedings of the 7th Conference on Computational Methods in Systems Biology CMSB 2009 held in Bologna from August 31 to September 1 2009 The rst CMSB was held in Trento in 2003 bringing together life scientists computer scientists engineers and physicists The goal was to promote the c vergence of di erent disciplines aiming at a new understanding and description of biological systems rmly ground in formal models supported by compu tionallanguagesandtools ando eringnew methodsofanalysis The conference then moved to Paris in 2004 Edinburgh in 2005 Trento in 2006 Edinburgh in 2007 and Rostock Warnemunde in 2008 This year the conference attracted about 45 submissions form 18 countries mainly from Europe and North America but also from Asia and Australia We wish to thank all authors for their interest in CMSB 2009 After careful disc sions the Programme Committee eventually selected 18 papers for presentation at the conference Each of them was accurately refereed by at least three viewers who delivered detailed and insightful comments and suggestions The Conference Chairmen warmly thank all the members of the Programme C mittee and all their sub referees for the excellent support they gave as well as for the friendly and constructive discussions We also would like to thank the authorsfor havingrevisedtheir papers to addressthe comments andsuggestions by the referees

Computational Methods in Systems Biology Luca Bortolussi,Guido Sanguinetti,2019-09-16 This book constitutes the refereed proceedings of the 17th International Conference on Computational Methods in Systems Biology CMSB 2019 held in Trieste Italy in September 2019 The 14 full papers 7 tool papers and 11 posters were carefully reviewed and selected from 53 submissions Topics of interest include formalisms for modeling biological processes models and their biological applications frameworks for model verification validation analysis and simulation of biological systems high performance computational systems biology and parallel implementations model inference from experimental data model integration from biological databases multi scale modeling and analysis methods computational approaches for synthetic biology and case studies in systems and synthetic biology Computational Intelligence in Sustainable Computing and Optimization Balamurugan Balusamy,Vinayakumar Ravi,Rajesh Kumar Dhanaraj,Sudha Senthilkumar,Brindha K,2024-10-08 Computational Intelligence

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Computational Techniques for Biological Sequence Analysis Saiyed Umer,Ranjeet Kumar Rout,Monika Khandelwal,Smitarani Pati,2025-06-17 This book provides an overview of basic and advanced computational techniques for analyzing and understanding protein RNA and DNA sequences It covers effective computing techniques for DNA and protein classifications evolutionary and sequence information analysis evolutionary algorithms and ensemble algorithms Furthermore the book reviews the role of machine learning techniques artificial intelligence ensemble learning and sequence based features in predicting post translational modifications in proteins DNA methylation and mRNA methylation along with their functional implications The book also discusses the prediction of protein protein and protein DNA interactions protein structure and function using computational methods It also presents techniques for quantitative analysis of protein DNA interactions and protein methylation and their involvement in gene regulation Additionally the use of nature inspired algorithms to gain insights into gene regulatory mechanisms and metabolic pathways in human diseases is explored This book acts as a useful reference for bioinformaticians and computational biologists working in the fields of molecular biology genomics and bioinformatics Key Features Reviews machine learning techniques for DNA sequence classification and protein structure prediction Discusses genetic algorithms for analyzing multiple sequence alignments and predicting protein protein interaction sites Explores computational methods for quantitative analysis of protein DNA interactions Examine the role of nature inspired algorithms in understanding the gene regulation and metabolic pathways Covers evolutionary algorithms and

sequence based features in predicting post translational modifications *Simulation Algorithms for Computational Systems Biology* Luca Marchetti,Corrado Priami,Vo Hong Thanh,2017-09-27 This book explains the state of the art algorithms used to simulate biological dynamics Each technique is theoretically introduced and applied to a set of modeling cases Starting from basic simulation algorithms the book also introduces more advanced techniques that support delays diffusion in space or that are based on hybrid simulation strategies This is a valuable self contained resource for graduate students and practitioners in computer science biology and bioinformatics An appendix covers the mathematical background and the authors include further reading sections in each chapter *Handbook of Computational Intelligence in Manufacturing and Production Management* Laha, Dipak,Mandal, Purnendu,2007-11-30 During the last two decades computer and information technologies have forced great changes in the ways businesses manage operations in meeting the desired quality of products and services customer demands competition and other challenges The Handbook of Computational Intelligence in Manufacturing and Production Management focuses on new developments in computational intelligence in areas such as forecasting scheduling production planning inventory control and aggregate planning among others This comprehensive collection of research provides cutting edge knowledge on information technology developments for both researchers and professionals in fields such as operations and production management Web engineering artificial intelligence and information resources management Handbook of Research on Computational Methodologies in Gene Regulatory Networks Das, Sanjoy,Caragea, Doina,Welch, Stephen,Hsu, William H.,2009-10-31 This book focuses on methods widely used in modeling gene networks including structure discovery learning and optimization Provided by publisher Networks in Systems Biology Fabricio Alves Barbosa da Silva,Nicolas Carels,Marcelo Trindade dos Santos,Francisco José Pereira Lopes,2020-10-03 This book presents a range of current research topics in biological network modeling as well as its application in studies on human hosts pathogens and diseases Systems biology is a rapidly expanding field that involves the study of biological systems through the mathematical modeling and analysis of large volumes of biological data Gathering contributions from renowned experts in the field some of the topics discussed in depth here include networks in systems biology the computational modeling of multidrug resistant bacteria and systems biology of cancer Given its scope the book is intended for researchers advanced students and practitioners of systems biology The chapters are research oriented and present some of the latest findings on their respective topics *Handbook of Bioinspired Algorithms and Applications* Stephan Olariu,Albert Y. Zomaya,2005-09-29 The mystique of biologically inspired or bioinspired paradigms is their ability to describe and solve complex relationships from intrinsically very simple initial conditions and with little or no knowledge of the search space Edited by two prominent well respected researchers the Handbook of Bioinspired Algorithms and Applications reveals the **Bio-Inspired Algorithms and Devices for Treatment of Cognitive Diseases Using Future Technologies** Gupta, Shweta,2022-02-11 As there are no proper medical tests available to predict certain diseases such as

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