

SECOND EDITION

COMPUTATIONAL SYSTEMS BIOLOGY

FROM MOLECULAR MECHANISMS TO DISEASE

Edited by
Roland Eils
and **Andres Kriete**



Computational Systems Biology Second Edition From Molecular Mechanisms To Disease

**Julien Delile, René Doursat, Nadine
Peyriéras**



Computational Systems Biology Second Edition From Molecular Mechanisms To Disease:

Computational Systems Biology Andres Kriete,Roland Eils,2013-11-26 This comprehensively revised second edition of Computational Systems Biology discusses the experimental and theoretical foundations of the function of biological systems at the molecular cellular or organismal level over temporal and spatial scales as systems biology advances to provide clinical solutions to complex medical problems In particular the work focuses on the engineering of biological systems and network modeling Logical information flow aids understanding of basic building blocks of life through disease phenotypes Evolved principles gives insight into underlying organizational principles of biological organizations and systems processes governing functions such as adaptation or response patterns Coverage of technical tools and systems helps researchers to understand and resolve specific systems biology problems using advanced computation Multi scale modeling on disparate scales aids researchers understanding of dependencies and constraints of spatio temporal relationships fundamental to biological organization and function **Computational Systems Biology** Helder I Nakaya,2013-11-26 **Computational Systems**

Biology Stefan M. Kallenberger,Stefan Legewie,Roland Eils,2013-11-26 Apoptosis is a form of cellular suicide central to various aspects in biology including tissue homeostasis and embryonic development It is typically dysregulated in cancer Understanding the apoptotic signal transduction network is thus a central goal of cancer research Quantitative modeling approaches provided valuable insights into determinants of cell fate decisions and promise to become a valuable tool to optimize therapeutic strategies In this chapter we summarize modeling approaches used in systems biology of apoptosis In addition we give an overview of apoptosis related research questions that can be addressed by modeling Moreover we review top down and bottom up modeling approaches applied to apoptosis and particularly focus on ordinary differential equation ODE modeling We describe bistability temporal switching crosstalk between death and survival and discuss approaches to model cell to cell variability Computational Systems Biology Juergen Eilsa,Elena Herzoga,Baerbel Felder,Christian

Lawrenza,Roland Eils,2013-11-26 Systems biology combines experimental and computational research to facilitate understanding of complex biological processes In this chapter we describe data repositories data standards modeling and visualization tools as prerequisites for systems biology research in order to help us to better study and understand biological processes In addition we propose improvements of these tools providing an example application JUMMP developed in our laboratory We suggest that flexibility interoperability and modularity of novel applications contribute to better acceptance and further development of these tools We also emphasize that having flexible and extendable standards describing complex and incomplete biological data allow new discoveries to be incorporated in a seamless way into systems biology tools Overall we discuss here advances challenges and perspectives of data and other platforms in systems biology which we believe will continue to make an impact on biomedical research **Computational Systems Biology** Joseph Xu Zhou,Xiaojie

Qiu,Aymeric Fouquier d'Herouel,Sui Huang,2013-11-26 In this chapter we introduced the basic concepts of cell attractors

and showed that Waddington's metaphoric epigenetic landscape has a formal basis in the attractor landscape. This conceptual framework helps to understand core properties of cell differentiation and ultimately multicellularity. Specifically, we developed the concept of relative stability of network states on the epigenetic landscape, thus providing the elevation in the landscape picture a formal quantifiable basis. We proposed methods to quantify the relative stability of attractor states in discrete gene networks models. We show in two examples that even with incomplete information about network structures, the use of Boolean networks can capture the essential outlines of cell fate dynamics and more importantly permit the estimation of relative stability and the attractor transition barriers. These measures hold great promise for the rational design of the perturbation protocols for cell reprogramming in regenerative medicine. As the knowledge of the structure of GRNs for the development of various tissues will undoubtedly increase in the next decade, the utilization of such network information for therapeutic reprogramming may benefit from the concepts developed here.

Computational Systems Biology Robert B. Russell, Gordana Apic, Olga Kalinina, Leonardo Trabuco, Matthew J. Betts, Qianhao Lu, 2013-11-26. The best understanding of complex biological systems ultimately comes from details of the underlying atomic structures within it. In the absence of known structures of all protein complexes and interactions in a system, structural bioinformatics or modeling fill an important niche in providing predicted mechanistic information which can guide experiments, aid the interpretation of high throughput datasets and help provide key details to model biological systems. This introductory review discusses the current state of this field and suggests how current datasets in systems studies can profit from a better integration of predicted or known structural information.

Computational Systems Biology Hans V. Westerhoff, Fei He, Ettore Murabito, Frédéric Crémazy, Matteo Barberis, 2013-11-26. Systems Biology brings the potential to discover fundamental principles of Life that cannot be discovered by considering individual molecules. This chapter discusses a number of early, more recent and upcoming discoveries of such network principles. These range from the balancing of fluxes through metabolic networks, the potential of those networks for truly individualized medicine, the time dependent control of fluxes and concentrations in metabolism and signal transduction, the ways in which organisms appear to regulate metabolic processes, various limitations therein, tradeoffs in robustness and fragility, and a relation between robustness and time dependences in the cell cycle. The robustness considerations will lead to the issue whether and how evolution has been able to put in place design principles of control engineering such as infinite robustness and perfect adaptation in the hierarchical biochemical networks of cell biology.

Computational Systems Biology Julien Delile, René Doursat, Nadine Peyri  ras, 2013-11-26. We propose a theoretical yet realistic agent based model and simulation platform of animal embryogenesis called MecaGen, centered on the physico-chemical coupling of cell mechanics with gene expression and molecular signaling. This project aims to investigate the multiscale dynamics of the early stages of biological morphogenesis. Here, embryonic development is viewed as an emergent self-organized phenomenon based on a myriad of cells and their genetically regulated and regulating

biomechanical behavior Cells mechanical properties such as division rate adhesion strength or intrinsic motility are closely correlated with their spatial location and temporal state of genetic and molecular dynamics such as internal protein and external ligand concentrations and affect each other concurrently In a second part we illustrate our model on artificial data gene regulation motifs and cell sorting then demonstrate a customization and application to a real biological case study in the zebrafish early development We use as an example the episode of intercalation patterns appearing during the first phase of epiboly and the movements of the deep cells between the yolk and the enveloping layer A domain of the model s multidimensional parameter space is explored systematically while experimental data obtained from microscopy imaging of live embryos is used to measure the fitness of the virtual embryo and validate our hypotheses **Computational Systems**

Biology Hong-Wu Ma, An-Ping Zeng, 2013-11-26 Understanding the complex interactions among cellular components genes proteins and metabolites at a network level is a key issue in systems biology In this chapter we give an overview of metabolic network reconstruction from genome information and its structural analysis First two approaches for genome scale metabolic network reconstruction high throughput reconstruction and high quality reconstruction are discussed Then the various means for mathematical representation of metabolic networks are explained with particular emphasis on the problem arising from currency metabolites Several topological features of metabolic network such as the power law connection degree distribution and the bow tie global connectivity structure are explained in detail In the last section we discuss the different types of methods for network decomposition which can be used to identify somehow structurally and functionally independent modules in a complex network This allows us to understand the functional organization of metabolic network from a modular perspective Computational Systems Biology John Cole, Michael J. Hallock, Piyush Labhsetwar, Joseph R. Peterson, John E. Stone, Zaida Luthey-Schulten, 2013-11-26 All chemical reactions are inherently random discrete events while large numbers of reacting species in well stirred vessels may appear to be governed by deterministic expressions the biochemistry at the heart of the living cell which may involve only a single copy of a gene or only a handful of proteins can exhibit significant fluctuations from mean behavior Here we describe the Lattice Microbes software for the stochastic simulation of biochemical reaction networks within realistic models of cells and explore its application to two model systems The first is the lac genetic switch which illustrates how stochastic gene expression can drive identical cells in macroscopically identical environments toward very different cell fates and the second is the MinDE system whose oscillatory behavior along the length of the E coli cell illustrates the necessity of detailed spatial resolution in accurately modeling cellular biochemistry We conclude by describing the use of a hybrid methodology that couples the Lattice Microbes reaction diffusion modeling capability with a genome scale flux balance model of metabolism in order to describe the collective metabolism of a dense colony of cells Computational Systems Biology Jean-Luc Bouchot, William L. Trimble, Gregory Ditzler, Yemin Lan, Steve Essinger, Gail Rosen, 2013-11-26 Recent advances in next generation sequencing have enabled high

throughput determination of biological sequences in microbial communities also known as microbiomes. The large volume of data now presents the challenge of how to extract knowledge, recognize patterns, find similarities and find relationships from complex mixtures of nucleic acid sequences currently being examined. In this chapter we review basic concepts as well as state of the art techniques to analyze hundreds of samples which each contain millions of DNA and RNA sequences. We describe the general character of sequence data and describe some of the processing steps that prepare raw sequence data for inference. We then describe the process of extracting features from the data, assigning taxonomic and gene labels to the sequences. Then we review methods for cross sample comparisons: 1) using similarity measures and ordination techniques to visualize and measure differences between samples and 2) feature selection and classification to select the most relevant features for discriminating between samples. Finally, in conclusion, we outline some open research problems and challenges left for future research.

Computational Systems Biology Stanley Gu, Herbert Sauro, 2013-11-26. With the sequencing of the human genome, it has become apparent that systems biology, the understanding of cellular networks through dynamical analysis, is becoming an important part of research for mainstream biologists. One of the indicative trends to emerge in recent years is the development of model interchange standards that permit biologists to easily exchange dynamical models between different software tools. This chapter describes the current and rising standards in systems biology that facilitate knowledge management and physiological model exchange. In addition, software platforms that implement these standards and enable the reuse of software code are discussed. Finally, the range of possible computational applications is described, highlighting the most commonly used and emerging tools in the field.

Computational Systems Biology Jean-Christophe Leloup, Didier Gonze, Albert Goldbeter, 2013-11-26. Circadian rhythms originate from intertwined feedback processes in genetic regulatory networks. Computational models of increasing complexity have been proposed for the molecular mechanism of these rhythms which occur spontaneously with a period on the order of 24h. We show that deterministic models for circadian rhythms in *Drosophila* account for a variety of dynamical properties such as phase shifting or long term suppression by light pulses and entrainment by light dark cycles. Stochastic versions of these models allow us to examine how molecular noise affects the emergence and robustness of circadian oscillations. Finally, we present a deterministic model for the mammalian circadian clock and use it to address the dynamical bases of physiological disorders of the sleep wake cycle in humans.

Computational Systems Biology Christina Kiel, Luis Serrano, 2013-11-26. This chapter brings mammalian signal transduction to the center of quantitative and integrative sciences. Historically imbedded within human physiology, thanks to proteomics, interactomics and molecular biology approaches, signaling is now far beyond the black box principle. However, despite the large amount of data available, we still have only limited insight into general design principles and we lack knowledge on how cell type specific signaling is achieved. Here we summarize recent efforts in elucidating cell type specific signaling and, in particular, the role of protein abundances, signaling complexes and modules. We further discuss the potential

of using synthetic biology approaches to decipher signaling networks All of this is discussed in light of complementary quantitative mathematical modeling approaches Signaling more than any other discipline needs computational biology to capture the dynamic systems behavior and to reach its final goal to be truly predictive for both the physiological and disease perturbed cellular conditions

Computational Systems Biology Seiya Imoto,Hiroshi Matsuno,Satoru Miyano,2013-11-26 This chapter describes the computational methods for estimating modeling and simulating biological systems It also presents two approaches to understand biological systems and describes a method and a software tool developed by our research group Bayesian network is a mathematical model for representing causal relationships among random variables by using conditional probabilities The conditional probabilities describe the parent child relationships and can be viewed as an extension of the deterministic models like Boolean networks This model is suited for modeling qualitative relations between genes and allows mathematical and algorithmic analyses We also devised a method to infer a gene network in terms of a linear system of differential equations from time course gene expression data A software tool is developed based on Petri net to modeling and simulation of gene networks With this software tool various models have been constructed and its utility has been demonstrated in practice

Computational Systems Biology Roland Eils,Andres Kriete,2013-11-26

Network Bioscience, 2nd Edition Marco Pellegrini,Marco Antoniotti,Bud Mishra,2020-03-27 Network science has accelerated a deep and successful trend in research that influences a range of disciplines like mathematics graph theory physics statistics data science and computer science just to name a few and adapts the relevant techniques and insights to address relevant but disparate social biological technological questions We are now in an era of big biological data supported by cost effective high throughput genomic transcriptomic proteomic metabolomic data collection techniques that allow one to take snapshots of the cells molecular profiles in a systematic fashion Moreover recently also phenotypic data data on diseases symptoms patients etc are being collected at nation wide level thus giving us another source of highly related causal big data This wealth of data is usually modeled as networks aka binary relations graphs or webs of interactions including protein protein metabolic signaling and transcription regulatory interactions The network model is a key view point leading to the uncovering of mesoscale phenomena thus providing an essential bridge between the observable phenotypes and omics underlying mechanisms Moreover network analysis is a powerful hypothesis generation tool guiding the scientific cycle of data gathering data interpretation hypothesis generation and hypothesis testing A major challenge in contemporary research is the synthesis of deep insights coming from network science with the wealth of data often noisy contradictory incomplete and difficult to replicate so to answer meaningful biological questions in a quantifiable way using static and dynamic properties of biological networks

Artificial Neural Network for Drug Design, Delivery and Disposition Munish Puri,Yashwant Pathak,Vijay Kumar Sutariya,Srinivas Tipparaju,Wilfrido Moreno,2015-10-15 Artificial Neural Network for Drug Design Delivery and Disposition provides an in depth look at the use of artificial neural networks ANN in

pharmaceutical research With its ability to learn and self correct in a highly complex environment this predictive tool has tremendous potential to help researchers more effectively design develop and deliver successful drugs This book illustrates how to use ANN methodologies and models with the intent to treat diseases like breast cancer cardiac disease and more It contains the latest cutting edge research an analysis of the benefits of ANN and relevant industry examples As such this book is an essential resource for academic and industry researchers across the pharmaceutical and biomedical sciences Written by leading academic and industry scientists who have contributed significantly to the field and are at the forefront of artificial neural network ANN research Focuses on ANN in drug design discovery and delivery as well as adopted methodologies and their applications to the treatment of various diseases and disorders Chapters cover important topics across the pharmaceutical process such as ANN in structure based drug design and the application of ANN in modern drug discovery Presents the future potential of ANN based strategies in biomedical image analysis and much more

Examining the Causal Relationship Between Genes, Epigenetics, and Human Health Wambuguh, Oscar J.,2019-03-22 For as much as we know about DNA and gene expression many more mysteries remain to be solved Epigenetics and epigenomics seek to study heritable modifications in gene expression that do not involve underlying DNA sequences to further human health changes Examining the Causal Relationship Between Genes Epigenetics and Human Health provides innovative research methods and applications of chemical activation or deactivation of genes without altering the original DNA sequence While highlighting topics including gene expression personalized medicine and public policy this book is ideal for researchers geneticists biologists medical professionals students and academics seeking current research on the expanding fields of genomics epigenomics proteomics pharmacogenomics and genome wide association studies

Bioinformatics of Genome Regulation, Volume I, 2nd Edition Yuriy L. Orlov,Ancha Baranova,Tatiana V. Tatarinova, Publisher's note In this 2nd edition the following article has been updated Orlov YL Tatarinova TV Oparina NY Galieva ER and Baranova AV 2021 Editorial Bioinformatics of Genome Regulation Volume I Front Genet 12 803273 doi 10.3389/fgene.2021.803273

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