# Explorations Of Mathematical Models In Biology With Matlab

Explorations Of Mathematical Models In Biology With Matlab Explorations of Mathematical Models in Biology with MATLAB Mathematical Biology MATLAB Modeling Biological Systems Simulation Differential Equations Population Dynamics Epidemiology Systems Biology Bioinformatics Imagine a bustling city teeming with life where every individual interacts competes and cooperates all within a complex web of relationships This city however isnt made of brick and mortar its a living organism a biological system Understanding its dynamics predicting its future and intervening when necessary requires a powerful tool mathematical modeling And in the realm of computational biology MATLAB stands as a potent engine driving these explorations forward This article delves into the fascinating world of mathematical modeling in biology showcasing how MATLAB empowers scientists to unravel the intricate complexities of life Well journey from simple population growth models to sophisticated simulations of gene regulatory networks all while illuminating the practical applications of this powerful combination The Power of Abstraction From Reality to Equations Before diving into MATLAB its crucial to understand the essence of mathematical modeling Its an act of creative abstraction translating the messy nuanced reality of biological systems into a simplified yet insightful mathematical representation Think of it as building a miniature replica of a city focusing on key aspects like traffic flow population density and resource allocation to understand the overall behavior of the system Consider the classic example of the LotkaVolterra equations which model the predatorprey interaction between rabbits and foxes These equations although relatively simple capture the cyclical nature of population dynamics revealing how changes in one population directly influence the other Implementing these equations in MATLAB allows us to simulate these cycles visualize the results and explore the impact of different parameters like birth rates death

rates and predation efficiency MATLAB The Architect of Biological Simulations MATLAB with its intuitive syntax and extensive toolboxes provides the perfect environment 2 for building analyzing and visualizing these models Its powerful numerical computing capabilities enable the efficient solving of differential equations a cornerstone of many biological models For instance simulating the spread of an infectious disease requires solving complex differential equations that describe the rate of infection recovery and death MATLABs builtin functions and specialized toolboxes streamline this process allowing researchers to focus on the biological implications rather than the intricacies of numerical computation Beyond PredatorPrey Exploring Diverse Applications The applications of mathematical modeling in biology extend far beyond simplistic predator prey interactions Here are a few compelling examples Epidemiology Modeling the spread of infectious diseases predicting outbreaks and evaluating the efficacy of vaccination strategies MATLAB allows for simulating various scenarios such as the impact of social distancing or the effectiveness of different treatments Population Dynamics Studying the growth and decline of populations considering factors such as resource availability competition and environmental changes MATLABs ability to handle large datasets makes it ideal for analyzing realworld population data and validating models Systems Biology Investigating complex interactions within biological networks such as gene regulatory networks or metabolic pathways MATLABs graphical capabilities facilitate the visualization of these networks helping researchers understand the flow of information and the impact of perturbations Bioinformatics Analyzing biological data such as gene expression profiles or protein sequences to identify patterns and predict functions MATLABs statistical and machine learning toolboxes are invaluable for extracting meaningful insights from this vast amount of data A Personal Anecdote Unveiling the Secrets of Cancer Growth During my doctoral studies I used MATLAB to model the growth and spread of cancerous tumors We developed a model that incorporated factors like cell proliferation apoptosis programmed cell death and angiogenesis formation of new blood vessels By tweaking parameters within the model we were able to simulate the effects of different cancer therapies gaining valuable insights into their mechanisms of action and potential limitations The visual representation of tumor growth generated by MATLAB was particularly illuminating allowing us

to identify key stages in tumor development and pinpoint potential 3 therapeutic targets This experience underscored the immense potential of MATLAB in translating biological observations into actionable predictions Actionable Takeaways Learn MATLAB Investing time in learning MATLAB opens doors to a vast world of biological modeling and simulation Numerous online resources and tutorials are available to get you started Start Simple Begin with simpler models and gradually increase complexity as you gain experience Mastering the fundamentals is crucial before tackling intricate systems Collaborate Connect with researchers in your field and exchange knowledge and expertise Collaborative efforts often lead to more comprehensive and impactful models Validate Your Models Compare your model predictions with realworld data to ensure accuracy and reliability This iterative process of model refinement is essential for producing meaningful results Frequently Asked Questions FAQs 1 What background is required to use MATLAB for biological modeling A basic understanding of mathematics particularly calculus and differential equations is helpful Prior programming experience is beneficial but not strictly necessary 2 What are the limitations of mathematical models in biology Models are inherently simplifications of reality They may not capture all the complexities of biological systems and their predictions should be interpreted with caution 3 Are there any free alternatives to MATLAB Yes there are opensource alternatives like R and Python each with its own strengths and weaknesses The choice depends on the specific needs of the project and the users familiarity with different programming languages 4 How can I visualize the results of my MATLAB simulations MATLAB offers a wide range of plotting and visualization tools allowing you to create graphs charts and even animations to represent your model outputs 5 Where can I find more information on mathematical modeling in biology Numerous textbooks research articles and online resources cover this topic extensively Searching for specific keywords related to your area of interest will yield relevant results The journey into the world of mathematical modeling in biology is both challenging and rewarding With MATLAB as your trusty companion youll be empowered to decipher the 4 intricate code of life making significant contributions to scientific discovery and potentially revolutionizing healthcare environmental management and beyond So embark on this exciting adventure and witness firsthand the power of mathematical modeling in

unraveling the secrets of the living world

Dynamic Models in BiologyStochastic Models in BiologyMathematical Models in BiologyModels in BiologyMathematical Models in BiologyA Primer in Mathematical Models in BiologyModeling BiologyMathematical Models in BiologyMathematical Models in BiologyTheoretical Models in BiologyMathematical Models for Society and BiologyNeutral Models in BiologyMathematical Models in Biology and MedicineLinear Models in BiologyDynamical Models in BiologySingle-Cell-Based Models in Biology and MedicineModeling Biological Systems:Mathematical Modeling in Systems BiologyModel-Based Hypothesis Testing in BiomedicineLectures on Nonlinear-differential-equation Models in Biology Stephen P. Ellner Narendra S. Goel Valeria Zazzu David Brown Elizabeth Spencer Allman Lee A. Segel Manfred Dietrich Laubichler Elisabeth S. Allman Elizabeth S. Allman Glenn W. Rowe Edward Beltrami Matthew H. Nitecki IFIP-TC4 Working Conference on Mathematical Models in Biology and Medicine$ (1972 : Varna, Bulgarie) Michael R. Cullen Mikl? s Farkas Alexander Anderson James W. Haefner Brian P. Ingalls Rikard Johansson James Dickson Murray

Dynamic Models in Biology Stochastic Models in Biology Mathematical Models in Biology Models in Biology Mathematical Models in Biology A Primer in Mathematical Models in Biology Modeling Biology Mathematical Models in Biology Mathematical Models in Biology Theoretical Models in Biology Mathematical Models for Society and Biology Neutral Models in Biology Mathematical Models in Biology and Medicine Linear Models in Biology Dynamical Models in Biology Single-Cell-Based Models in Biology and Medicine Modeling Biological Systems: Mathematical Modeling in Systems Biology Model-Based Hypothesis Testing in Biomedicine Lectures on Nonlinear-differential-equation Models in Biology *Stephen P. Ellner Narendra S. Goel Valeria Zazzu David Brown Elizabeth Spencer Allman Lee A. Segel Manfred Dietrich Laubichler Elisabeth S. Allman Elizabeth S. Allman Glenn W. Rowe Edward Beltrami Matthew H. Nitecki IFIP-TC4 Working Conference on Mathematical Models in Biology and Medicine$ (1972 : Varna, Bulgarie) Michael R. Cullen Mikl? s Farkas Alexander Anderson James W. Haefner Brian P. Ingalls Rikard Johansson James Dickson Murray*

FROM CONTROLLING DISEASE OUTBREAKS TO PREDICTING HEART ATTACKS DYNAMIC MODELS ARE INCREASINGLY CRUCIAL FOR UNDERSTANDING BIOLOGICAL PROCESSES MANY UNIVERSITIES ARE STARTING UNDERGRADUATE PROGRAMS IN COMPUTATIONAL BIOLOGY TO INTRODUCE STUDENTS TO THIS RAPIDLY GROWING FIELD IN DYNAMIC MODELS IN BIOLOGY THE FIRST TEXT ON DYNAMIC MODELS SPECIFICALLY WRITTEN FOR UNDERGRADUATE STUDENTS IN THE BIOLOGICAL SCIENCES ECOLOGIST STEPHEN ELLNER AND MATHEMATICIAN JOHN GUCKENHEIMER TEACH STUDENTS HOW TO UNDERSTAND BUILD AND USE DYNAMIC MODELS IN BIOLOGY DEVELOPED FROM A COURSE TAUGHT BY ELLNER AND GUCKENHEIMER AT CORNELL UNIVERSITY THE BOOK IS ORGANIZED AROUND BIOLOGICAL APPLICATIONS WITH MATHEMATICS AND COMPUTING DEVELOPED THROUGH CASE STUDIES AT THE MOLECULAR CELLULAR AND POPULATION LEVELS THE AUTHORS COVER BOTH SIMPLE ANALYTIC MODELS THE SORT USUALLY FOUND IN MATHEMATICAL BIOLOGY TEXTS AND THE COMPLEX COMPUTATIONAL MODELS NOW USED BY BOTH BIOLOGISTS AND MATHEMATICIANS LINKED TO A SITE WITH COMPUTER LAB MATERIALS AND EXERCISES DYNAMIC MODELS IN BIOLOGY IS A MAJOR NEW INTRODUCTION TO DYNAMIC MODELS FOR STUDENTS IN THE BIOLOGICAL SCIENCES MATHEMATICS AND ENGINEERING

STOCHASTIC MODELS IN BIOLOGY DESCRIBES THE USEFULNESS OF THE THEORY OF STOCHASTIC PROCESS IN STUDYING BIOLOGICAL PHENOMENA THE BOOK DESCRIBES ANALYSIS OF BIOLOGICAL SYSTEMS AND EXPERIMENTS THOUGH PROBABILISTIC MODELS RATHER THAN DETERMINISTIC METHODS THE TEXT REVIEWS THE MATHEMATICAL ANALYSES FOR MODELING DIFFERENT BIOLOGICAL SYSTEMS SUCH AS THE RANDOM PROCESSES CONTINUOUS IN TIME AND DISCRETE IN STATE SPACE THE BOOK ALSO DISCUSSES POPULATION GROWTH AND EXTINCTION THROUGH MALTHUS LAW AND THE WORK OF MACARTHUR AND WILSON THE TEXT THEN EXPLAINS THE DYNAMICS OF A POPULATION OF INTERACTING SPECIES THE BOOK ALSO ADDRESSES POPULATION GENETICS UNDER SYSTEMATIC EVOLUTIONARY PRESSURES KNOWN AS DETERMINISTIC EQUATIONS AND GENETIC CHANGES IN A FINITE POPULATION KNOWN AS STOCHASTIC EQUATIONS THE TEXT THEN TURNS TO STOCHASTIC MODELING OF BIOLOGICAL SYSTEMS AT THE MOLECULAR LEVEL PARTICULARLY THE KINETICS OF BIOCHEMICAL REACTIONS THE BOOK ALSO PRESENTS VARIOUS USEFUL EQUATIONS SUCH AS THE DIFFERENTIAL EQUATION FOR GENERATING FUNCTIONS FOR BIRTH AND DEATH PROCESSES THE TEXT CAN PROVE VALUABLE FOR BIOCHEMISTS CELLULAR BIOLOGISTS AND RESEARCHERS IN THE MEDICAL AND CHEMICAL FIELD WHO ARE TASKED TO PERFORM DATA ANALYSIS

THIS BOOK PRESENTS AN EXCITING COLLECTION OF CONTRIBUTIONS BASED ON THE WORKSHOP BRINGING MATHS TO LIFE HELD OCTOBER 27 29 2014 IN NAPLES ITALY THE STATE OF THE ART RESEARCH IN BIOLOGY AND THE STATISTICAL AND ANALYTICAL CHALLENGES FACING HUGE MASSES OF DATA COLLECTION ARE TREATED IN THIS WORK SPECIFIC TOPICS EXPLORED IN DEPTH SURROUND THE SESSIONS AND SPECIAL INVITED SESSIONS OF THE WORKSHOP AND INCLUDE GENETIC VARIABILITY VIA DIFFERENTIAL EXPRESSION MOLECULAR DYNAMICS AND MODELING COMPLEX BIOLOGICAL SYSTEMS VIEWED FROM QUANTITATIVE MODELS AND MICROSCOPY IMAGES PROCESSING TO NAME SEVERAL IN DEPTH DISCUSSIONS OF THE MATHEMATICAL ANALYSIS REQUIRED TO EXTRACT INSIGHTS FROM COMPLEX BODIES OF BIOLOGICAL DATASETS TO AID DEVELOPMENT IN THE FIELD NOVEL ALGORITHMS METHODS AND SOFTWARE TOOLS FOR GENETIC VARIABILITY MOLECULAR DYNAMICS AND COMPLEX BIOLOGICAL SYSTEMS ARE PRESENTED IN THIS BOOK RESEARCHERS AND GRADUATE STUDENTS IN BIOLOGY LIFE SCIENCE AND MATHEMATICS STATISTICS WILL FIND THE CONTENT USEFUL AS IT ADDRESSES EXISTING CHALLENGES IN IDENTIFYING THE GAPS BETWEEN MATHEMATICAL MODELING AND BIOLOGICAL RESEARCH THE SHARED SOLUTIONS WILL AID AND PROMOTE FURTHER COLLABORATION BETWEEN LIFE SCIENCES AND MATHEMATICS

THIS TEXT PROVIDES AN INTRODUCTION TO THE USE OF MATHEMATICAL MODELS IN BIOLOGY THE STATISTICAL TECHNIQUES FOR FITTING AND TESTING THEM AND ASSOCIATED COMPUTING METHODS THE PROPERTIES OF MODELS AND METHODS OF FITTING AND TESTING ARE DEMONSTRATED BY COMPUTER SIMULATION ILLUSTRATIONS

A TEXTBOOK ON MATHEMATICAL MODELLING TECHNIQUES WITH POWERFUL APPLICATIONS TO BIOLOGY COMBINING THEORETICAL EXPOSITION WITH EXERCISES AND EXAMPLES

EXPERTS EXAMINE NEW MODELING STRATEGIES FOR THE INTERPRETATION OF BIOLOGICAL DATA AND THEIR INTEGRATION INTO THE CONCEPTUAL FRAMEWORK OF THEORETICAL BIOLOGY DETAILING APPROACHES THAT FOCUS ON MORPHOLOGY DEVELOPMENT BEHAVIOR OR EVOLUTION ABSTRACT AND CONCEPTUAL MODELS HAVE BECOME AN INDISPENSABLE TOOL FOR ANALYZING THE FLOOD OF HIGHLY DETAILED EMPIRICAL DATA GENERATED IN RECENT YEARS BY ADVANCED TECHNIQUES IN THE BIOSCIENCES SCIENTISTS ARE DEVELOPING NEW MODELING STRATEGIES FOR ANALYZING DATA INTEGRATING RESULTS INTO THE CONCEPTUAL FRAMEWORK OF THEORETICAL BIOLOGY AND FORMULATING NEW HYPOTHESES IN MODELING BIOLOGY LEADING SCHOLARS INVESTIGATE NEW MODELING STRATEGIES IN THE DOMAINS OF MORPHOLOGY DEVELOPMENT BEHAVIOR AND EVOLUTION THE EMPHASIS

ON MODELS IN THE BIOLOGICAL SCIENCES HAS BEEN ACCOMPANIED BY A NEW FOCUS ON CONCEPTUAL ISSUES AND A MORE COMPLEX UNDERSTANDING OF EPISTEMOLOGICAL CONCEPTS CONTRIBUTORS TO MODELING BIOLOGY DISCUSS MODELS AND MODELING STRATEGIES FROM THE PERSPECTIVES OF PHILOSOPHY HISTORY AND APPLIED MATHEMATICS INDIVIDUAL CHAPTERS DISCUSS SPECIFIC APPROACHES TO MODELING IN SUCH DOMAINS AS BIOLOGICAL FORM DEVELOPMENT AND BEHAVIOR FINALLY THE BOOK ADDRESSES THE MODELING OF THESE PROPERTIES IN THE CONTEXT OF EVOLUTION WITH A PARTICULAR EMPHASIS ON THE EMERGING FIELD OF EVOLUTIONARY DEVELOPMENTAL BIOLOGY OR EVO DEVO CONTRIBUTORS GIORGIO A ASCOLI CHANDRAJIT BAJAJ JAMES P COLLINS LUCIANO DA FONTOURA COSTA KERSTIN DAUTENHAHN NIGEL R FRANKS SCOTT GILBERT MARTA IBA? ES MIGUEZ JUAN CARLOS IZPIS? A BELMONTE ALEXANDER S KLYUBIN THOMAS J KOEHNLE MANFRED D LAUBICHLER SABINA LEONELLI JAMES A R MARSHALL GEORGE R MCGHEE JR GERD B M? LLER CHRYSTOPHER L NEHANIV KARL J NIKLAS LARS OLSSON EIRIKUR PALSSON DANIEL POLANI DIEGO RASSKIN GUTMAN HANS J? RG RHEINBERGER ALEXEI V SAMSONOVICH JEFFREY C SCHANK HARRY B M UYLINGS JAAP VAN PELT IAIN WERRY

THIS INTRODUCTORY TEXTBOOK ON MATHEMATICAL BIOLOGY FOCUSES ON DISCRETE MODELS ACROSS A VARIETY OF BIOLOGICAL SUBDISCIPLINES BIOLOGICAL TOPICS TREATED INCLUDE LINEAR AND NON LINEAR MODELS OF POPULATIONS MARKOV MODELS OF MOLECULAR EVOLUTION PHYLOGENETIC TREE CONSTRUCTION GENETICS AND INFECTIOUS DISEASE MODELS THE COVERAGE OF MODELS OF MOLECULAR EVOLUTION AND PHYLOGENETIC TREE CONSTRUCTION FROM DNA SEQUENCE DATA IS UNIQUE AMONG BOOKS AT THIS LEVEL COMPUTER INVESTIGATIONS WITH MATLAB ARE INCORPORATED THROUGHOUT IN BOTH EXERCISES AND MORE EXTENSIVE PROJECTS TO GIVE READERS HANDS ON EXPERIENCE WITH THE MATHEMATICAL MODELS DEVELOPED MATLAB PROGRAMS ACCOMPANY THE TEXT MATHEMATICAL TOOLS SUCH AS MATRIX ALGEBRA EIGENVECTOR ANALYSIS AND BASIC PROBABILITY ARE MOTIVATED BY BIOLOGICAL MODELS AND GIVEN SELF CONTAINED DEVELOPMENTS SO THAT MATHEMATICAL PREREQUISITES ARE MINIMAL

THIS BOOK SURVEYS THEORETICAL MODELS IN THREE BROAD AREAS OF BIOLOGY THE ORIGIN OF LIFE THE IMMUNE SYSTEM AND MEMORY IN THE BRAIN INTRODUCING MATHEMATICAL AND MAINLY COMPUTATIONAL MODELS THAT HAVE BEEN USED TO CONSTRUCT SIMULATIONS MOST CURRENT BOOKS ON THEORETICAL BIOLOGY FALL INTO ONE OF TWO CATEGORIES A BOOKS THAT SPECIALIZE IN ONE AREA OF BIOLOGY AND TREAT THEORETICAL MODELS IN CONSIDERABLE DEPTH AND B BOOKS THAT CONCENTRATE ON PURELY MATHEMATICAL MODELS WITH

COMPUTERS USED ONLY TO FIND NUMERICAL SOLUTIONS TO DIFFERENTIAL EQUATIONS FOR EXAMPLE ALTHOUGH SOME MATHMATICAL MODELS ARE CONSIDERED IN THIS BOOK THE MAIN EMPHASIS IS ON STOCHASTIC COMPUTER MODLES OF BIOLOGICAL SYSTEMS SUCH TECHNIQUES HAVE A MUCH GREATER POTENTIAL FOR PRODUCTING DETAILED REALISTIC MODELS OF INDIVIDUAL SYSTEMS AND ARE LIKELY TO BE THE PREFERRED MODELLING METHODS OF THE FUTURE BY CONSIDERING THREE DIFFERENT AREAS IN BIOLOGY THE BOOK SHOWS HOW SEVERAL OF THESE MODELLING TECHNIQUES HAVE BEEN SUCCESSFULLY APPLIED IN DIVERSE AREAS PUT SIMPLY THIS BOOK IS IMPORTANT BECUASE IT SHOWS HOW THE POWER OF MODERN COMPUTERS IS ALLOWING RESEARCHERS IN THEORETICAL BIOLOGY TO BREAK FREE OF THE CONSTRAINTS ON MODELLING THAT WERE IMPOSED BY THE TRADITIONAL DIFFERENTIAL EQUATION APPROACH ANYONE WHO IS INTERESTED IN THE THEORETICAL MODELS OF COMPLICATED LIVING SYSTEMS SHOULD HAVE THIS IN HIS OR HER LIBRARY G B ERMENTROUT BULLETIN OF MATHEMATICAL BIOLOGY

MATHEMATICAL MODELING FOR SOCIETY AND BIOLOGY ENGAGINGLY RELATES MATHEMATICS TO COMPELLING REAL LIFE PROBLEMS IN BIOLOGY AND CONTEMPORARY SOCIETY IT SHOWS HOW MATHEMATICAL TOOLS CAN BE USED TO GAIN INSIGHT INTO THESE MODERN COMMON PROBLEMS TO PROVIDE EFFECTIVE REAL SOLUTIONS BELTRAMI S CREATIVE NON THREATENING APPROACH DRAWS ON A WEALTH OF INTERESTING EXAMPLES PERTAINING TO CURRENT SOCIAL AND BIOLOGICAL ISSUES CENTRAL IDEAS APPEAR AGAIN IN DIFFERENT CONTEXTS THROUGHOUT THE BOOK SHOWING THE GENERAL UNITY OF THE MODELING PROCESS THE MODELS ARE STRIKINGLY NOVEL AND BASED ON ISSUES OF REAL CONCERN MOST HAVE NEVER APPEARED IN BOOK FORM THROUGH THE RELEVANCE OF THESE MODELS MATHEMATICS BECOMES NOT JUST FIGURES AND NUMBERS BUT A MEANS TO A MORE REFINED UNDERSTANDING OF THE WORLD

NEUTRAL MODELS ARE CONSTRUCTED TO HELP SCIENTISTS UNDERSTAND COMPLEX PATTERNS OF FORM STRUCTURE OR BEHAVIOR THAT MAY NOT BE OBSERVED DIRECTLY IN THIS UNIQUE VOLUME EIGHT DISTINGUISHED SCIENTISTS PRESENT A COMPREHENSIVE STUDY OF THE USE OF NEUTRAL MODELS IN TESTING BIOLOGICAL THEORIES THEY DESCRIBE THE PRINCIPLES OF MODEL TESTING AND EXPLORE HOW THEY ARE APPLIED TO RESEARCH IN MOLECULAR BIOLOGY GENETICS ECOLOGY EVOLUTION AND PALEONTOLOGY IN ADDITION TO THE EDITORS THE CONTRIBUTORS INCLUDE STEPHEN STIGLER DAVID RAUP PAUL HARVEY L B SLOBODKIN STUART KAUFFMAN WILLIAM WIMSATT AND JAMES CROW

DYNAMIC MODELS IN BIOLOGY OFFERS AN INTRODUCTION TO MODERN MATHEMATICAL BIOLOGY THIS BOOK PROVIDES A SHORT INTRODUCTION TO MODERN MATHEMATICAL METHODS IN MODELING DYNAMICAL PHENOMENA AND TREATS THE BROAD TOPICS OF POPULATION DYNAMICS EPIDEMIOLOGY EVOLUTION IMMUNOLOGY MORPHOGENESIS AND PATTERN FORMATION PRIMARILY EMPLOYING DIFFERENTIAL EQUATIONS THE AUTHOR PRESENTS ACCESSIBLE DESCRIPTIONS OF DIFFICULT MATHEMATICAL MODELS RECENT MATHEMATICAL RESULTS ARE INCLUDED BUT THE AUTHOR S PRESENTATION GIVES INTUITIVE MEANING TO ALL THE MAIN FORMULAE BESIDES MATHEMATICIANS WHO WANT TO GET ACQUAINTED WITH THIS RELATIVELY NEW FIELD OF APPLICATIONS THIS BOOK IS USEFUL FOR PHYSICIANS BIOLOGISTS AGRICULTURAL ENGINEERS AND ENVIRONMENTALISTS KEY TOPICS INCLUDE CHAOTIC DYNAMICS OF POPULATIONS THE SPREAD OF SEXUALLY TRANSMITTED DISEASES PROBLEMS OF THE ORIGIN OF LIFE MODELS OF IMMUNOLOGY FORMATION OF ANIMAL HIDE PATTERNS THE INTUITIVE MEANING OF MATHEMATICAL FORMULAE EXPLAINED WITH MANY FIGURES APPLYING NEW MATHEMATICAL RESULTS IN MODELING BIOLOGICAL PHENOMENA MIKLOS FARKAS IS A PROFESSOR AT BUDAPEST UNIVERSITY OF TECHNOLOGY WHERE HE HAS RESEARCHED AND INSTRUCTED MATHEMATICS FOR OVER THIRTY YEARS HE HAS TAUGHT AT UNIVERSITIES IN THE FORMER SOVIET UNION CANADA AUSTRALIA VENEZUELA NIGERIA INDIA AND COLUMBIA PROF FARKAS RECEIVED THE 1999 BOLYAI AWARD OF THE HUNGARIAN ACADEMY OF SCIENCE AND THE 2001 ALBERT SZENTGYORGYI AWARD OF THE HUNGARIAN MINISTRY OF EDUCATION A DOWN TO EARTH INTRODUCTION TO THE GROWING FIELD OF MODERN MATHEMATICAL BIOLOGY ALSO INCLUDES APPENDICES WHICH PROVIDE BACKGROUND MATERIAL THAT GOES BEYOND ADVANCED CALCULUS AND LINEAR ALGEBRA

MANY DIFFERENT SINGLE CELL BASED MODELS HAVE BEEN DEVELOPED AND APPLIED TO BIOLOGICAL AND MEDICAL PROBLEMS COMPUTATIONAL APPROACHES USED ARE MONTE CARLO SIMULATIONS ENERGY MINIMISATION TECHNIQUES VOLUME CONSERVATION LAWS SOLUTIONS OF THE EQUATIONS OF MOTION FOR EACH INDIVIDUAL CELL OR FOR EACH POINT ON THE CELL MEMBRANE THEY DIFFER IN THE LEVEL OF DETAIL THAT DEFINES THE CELL STRUCTURE AND SUBSEQUENTLY IN THE NUMBER OF INDIVIDUAL CELLS THAT THE MODEL CAN INCORPORATE THIS VOLUME PRESENTS A COLLECTION OF MATHEMATICAL AND COMPUTATIONAL SINGLE CELL BASED MODELS AND THEIR APPLICATION THE MAIN SECTIONS COVER FOUR GENERAL MODEL GROUPINGS HYBRID CELLULAR AUTOMATA CELLULAR POTTS LATTICE FREE CELLS AND VISCOELASTIC CELLS EACH SECTION IS INTRODUCED BY A DISCUSSION OF THE APPLICABILITY OF THE PARTICULAR MODELLING APPROACH AND ITS ADVANTAGES AND

disadvantages which will make the book suitable for students starting research in mathematical biology as well as scientists modelling multicellular processes

i principles 1 1 models of systems 3 1 1 systems models and modeling 3 1 2 uses of scientific models 4 1 3 example island biogeography 6 1 4 classifications of models 10 1 5 constraints on model structure 12 1 6 some terminology 12 1 7 misuses of models the dark side 13 1 8 exercises 15 2 the modeling process 17 2 1 models are problems 17 2 2 two alternative approaches 18 2 3 an example population doubling time 24 2 4 model objectives 28 2 5 exercises 30 3 qualitative model formulation 32 3 1 how to eat an elephant 32 3 2 forrester diagrams 33 3 3 examples 36 3 4 errors in forrester diagrams 44 3 5 advantages and disadvantages of forrester diagrams 44 3 6 principles of qualitative formulation 45 3 7 model simplification 47 3 8 other modeling problems 49 viii contents 3 9 exercises 53 4 quantitative model formulation i 4 1 from qualitative to quantitative finite difference equations and differential equations 4 2 4 3 biological feedback in quantitative models 4 4 example model 4 5 exercises 5 quantitative model formulation i1 81 5 1 physical processes 81 5 2 using the toolbox of biological processes 89 5 3 useful functions 96 5 4 examples 102 5 5 exercises 104 6 numerical techniques 107 6 1 mistakes computers make 107 6 2 numerical integration 110 6 3 numerical instability and stiff equations 115

an introduction to the mathematical concepts and techniques needed for the construction and analysis of models in molecular systems biology systems techniques are integral to current research in molecular cell biology and system level investigations are often accompanied by mathematical models these models serve as working hypotheses they help us to understand and predict the behavior of complex systems this book offers an introduction to mathematical concepts and techniques needed for the construction and interpretation of models in molecular systems biology it is accessible to upper level undergraduate or graduate students in life science or engineering who have some familiarity with calculus and will be a useful reference for researchers at all levels the first four chapters cover the basics of mathematical modeling in molecular systems biology the last four chapters address specific biological domains treating

modeling of metabolic networks of signal transduction pathways of gene regulatory networks and of electrophysiology and neuronal action potentials chapters 3 8 end with optional sections that address more specialized modeling topics exercises solvable with pen and paper calculations appear throughout the text to encourage interaction with the mathematical techniques more involved end of chapter problem sets require computational software appendixes provide a review of basic concepts of molecular biology additional mathematical background material and tutorials for two computational software packages xppaut and matlab that can be used for model simulation and analysis

the utilization of mathematical tools within biology and medicine has traditionally been less widespread compared to other hard sciences such as physics and chemistry however an increased need for tools such as data processing bioinformatics statistics and mathematical modeling have emerged due to advancements during the last decades these advancements are partly due to the development of high throughput experimental procedures and techniques which produce ever increasing amounts of data for all aspects of biology and medicine these data reveal a high level of inter connectivity between components which operate on many levels of control and with multiple feedbacks both between and within each level of control however the availability of these large scale data is not synonymous to a detailed mechanistic understanding of the underlying system rather a mechanistic understanding is gained first when we construct a hypothesis and test its predictions experimentally identifying interesting predictions that are quantitative in nature generally requires mathematical modeling this in turn requires that the studied system can be formulated into a mathematical model such as a series of ordinary differential equations where different hypotheses can be expressed as precise mathematical expressions that influence the output of the model within specific sub domains of biology the utilization of mathematical models have had a long tradition such as the modeling done on electrophysiology by hodgkin and huxley in the 1950s however it is only in recent years with the arrival of the field known as systems biology that mathematical modeling has become more commonplace the somewhat slow adaptation of mathematical modeling in biology is partly due

to historical differences in training and terminology as well as in a lack of awareness of showcases illustrating how modeling can make a difference or even be required for a correct analysis of the experimental data in this work I provide such showcases by demonstrating the universality and applicability of mathematical modeling and hypothesis testing in three disparate biological systems in paper II we demonstrate how mathematical modeling is necessary for the correct interpretation and analysis of dominant negative inhibition data in insulin signaling in primary human adipocytes in paper III we use modeling to determine transport rates across the nuclear membrane in yeast cells and we show how this technique is superior to traditional curve fitting methods we also demonstrate the issue of population heterogeneity and the need to account for individual differences between cells and the population at large in paper IV we use mathematical modeling to reject three hypotheses concerning the phenomenon of facilitation in pyramidal nerve cells in rats and mice we also show how one surviving hypothesis can explain all data and adequately describe independent validation data finally in paper I we develop a method for model selection and discrimination using parametric bootstrapping and the combination of several different empirical distributions of traditional statistical tests we show how the empirical log likelihood ratio test is the best combination of two tests and how this can be used not only for model selection but also for model discrimination in conclusion mathematical modeling is a valuable tool for analyzing data and testing biological hypotheses regardless of the underlying biological system further development of modeling methods and applications are therefore important since these will in all likelihood play a crucial role in all future aspects of biology and medicine especially in dealing with the burden of increasing amounts of data that is made available with new experimental techniques anv□ ndandet av matematiska verktyg har inom biologi och medicin traditionellt sett varit mindre utbredd j□ mf□ rt med andra □ mnen inom naturvetenskapen s□ som fysik och kemi ett □ kat behov av verktyg som databehandling bioinformatik statistik och matematisk modellering har tr□ tt fram tack vare framsteg under de senaste decennierna dessa framsteg □ r delvis ett resultat av utvecklingen av storskaliga datainsamlingstekniker inom alla omr□ den av biologi och medicin s□ har dessa data avsl□ jat en h□ g niv□ av interkonnektivitet mellan komponenter verksamma p□ m□ nga kontrollniv□ er och med

flera ? terkopplingar b? de mellan och inom varje niv? av kontroll tillg? ng till storskaliga data ? r emellertid inte synonymt med en detaljerad mekanistisk f? rst? else f? r det underliggande systemet snarare uppn? s en mekanisk f? rst? else f? rst n? r vi bygger en hypotes vars prediktioner vi kan testa experimentellt att identifiera intressanta prediktioner som ? r av kvantitativ natur kr? ver generellt sett matematisk modellering detta kr? ver i sin tur att det studerade systemet kan formuleras till en matematisk modell s? som en serie ordin? ra differentialekvationer d? r olika hypoteser kan uttryckas som precisa matematiska uttryck som p? verkar modellens output inom vissa delomr? den av biologin har utnyttjandet av matematiska modeller haft en l? ng tradition s? som den modellering gjord inom elektrofysiologi av Hodgkin och Huxley p? 1950 talet det ? r emellertid just p? senare ? r med ankomsten av f? ltet systembiologi som matematisk modellering har blivit ett vanligt inslag den n? got l? ngsamma adapteringen av matematisk modellering inom biologi ? r bl a grundad i historiska skillnader i tr? ning och terminologi samt brist p? medvetenhet om exempel som illustrerar hur modellering kan g? ra skillnad och faktiskt ofta ? r ett krav f? r en korrekt analys av experimentella data i detta arbete tillhandah? ller jag s? dana exempel och demonstrerar den matematiska modelleringens och hypotestestningens allm? ngiltighet och till? mpbarhet i tre olika biologiska system i arbete II visar vi hur matematisk modellering ? r n? dv? ndig f? r en korrekt tolkning och analys av dominant negativ inhiberingsdata vid insulinsignalering i prim? ra humana adipocyter i arbete III anv? nder vi modellering f? r att best? mma transporthastigheter ? ver cellk? rnmembranet i j? stceller och vi visar hur denna teknik ? r ? verl? gsen traditionella kurvpassningsmetoder vi demonstrerar ocks? fr? gan om populationsheterogenitet och behovet av att ta h? nsyn till individuella skillnader mellan celler och befolkningen som helhet i arbete IV anv? nder vi matematisk modellering f? r att f? rkasta tre hypoteser om hur fenomenet facilitering uppst? r i pyramidala nervceller hos r? ttor och m? ss vi visar ocks? hur en ? verlevande hypotes kan beskriva all data inklusive oberoende valideringsdata slutligen utvecklar vi i arbete I en metod f? r modellselektion och modelldiskriminering med hj? lp av parametrisk bootstrapping samt kombinationen av olika empiriska f? rdelningar av traditionella statistiska tester vi visar hur det empiriska log likelihood ratio testet ? r den b? sta kombinationen av tv? tester och hur testet ? r applicerbart inte bara f? r modellselektion utan

ocks f r modelldiskriminering sammanfattningsvis r matematisk modellering ett v rdefullt verktyg f r att analysera data och testa biologiska hypoteser oavsett underliggande biologiskt system vidare utveckling av modelleringsmetoder och till mpningar r d rf r viktigt eftersom dessa sannolikt kommer att spela en avg rande roll i framtiden f r biologi och medicin s rskilt n r det g ller att hantera belastningen fr n kande datam ngder som blir tillg nglig med nya experimentella tekniker

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