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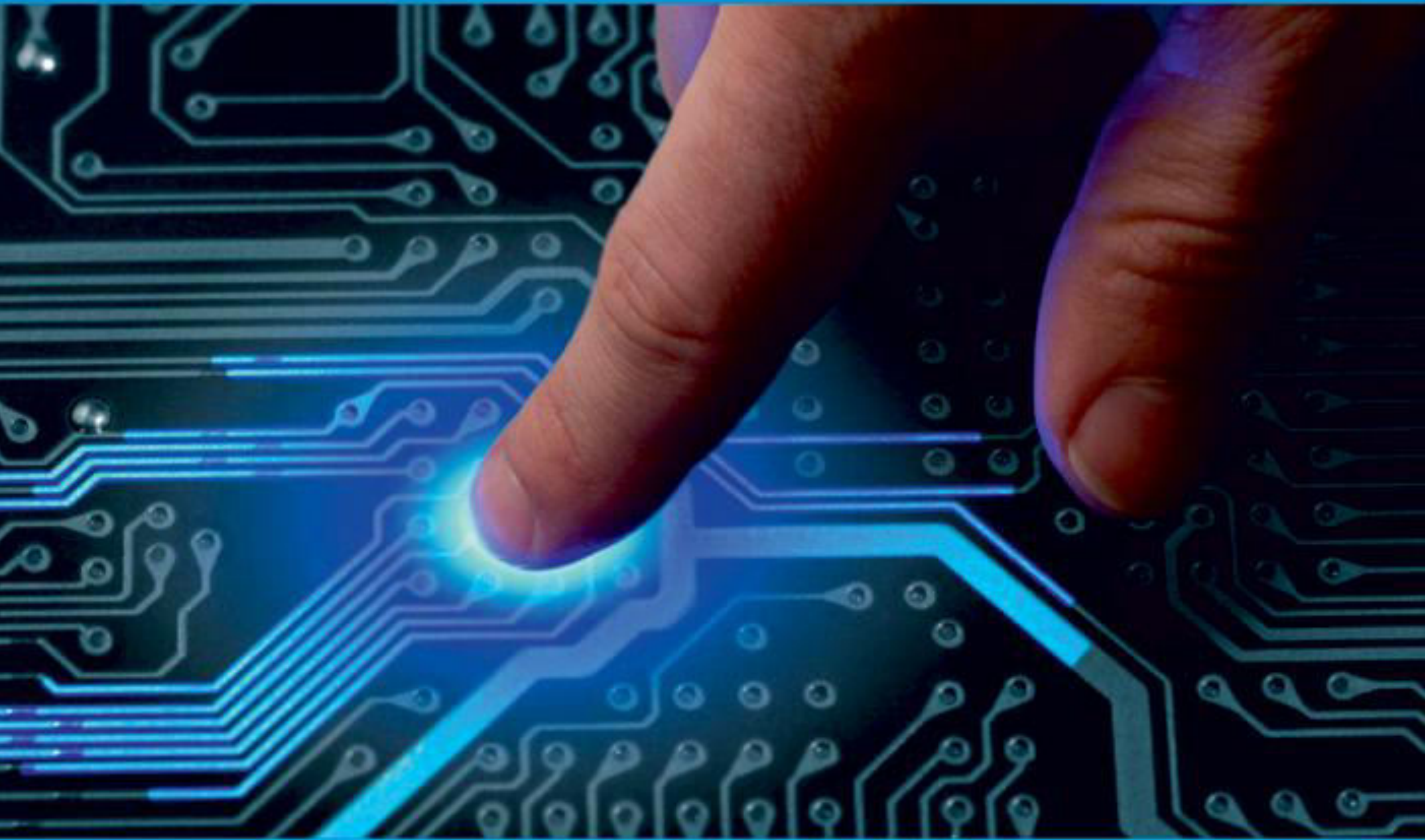

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Mathematical Biology: Modelling Biological Systems

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ABSTRACT: Mathematical biology bridges mathematics and biology to understand and predict the behaviour of biological systems. The field translates biological phenomena into mathematical language, using equations and algorithms to model interactions such as gene regulation and population dynamics. This interdisciplinary approach dates back to early 20th-century pioneers like Vito Volterra and Alfred Lotka, and it now includes diverse techniques from differential equations to machine learning. Deterministic models provide unique outcomes based on fixed rules, while stochastic models incorporate randomness, reflecting biological variability. Parameter estimation ensures model reliability by deriving accurate values from experimental data using techniques like maximum likelihood estimation and Bayesian inference. Analytical techniques such as sensitivity and bifurcation analysis further enhance model robustness and understanding. Applications in synthetic and systems biology demonstrate the field's practical impact, guiding the design of biological circuits and integrating data across biological scales. Mathematical biology exemplifies the power of interdisciplinary collaboration, driving innovations in medicine, environmental science, and biotechnology.

KEYWORDS: Mathematical Modelling, Deterministic Models, Stochastic Processes.

I. INTRODUCTION

Mathematical biology, an interdisciplinary field at the intersection of mathematics and biology, employs mathematical techniques and models to understand and predict the behaviour of biological systems. As biological research has advanced, the complexity of biological systems and the vast amounts of data generated have necessitated the development of sophisticated mathematical models. These models serve as crucial tools for synthesizing data, elucidating underlying mechanisms, and making predictions about biological processes. One of the fundamental aspects of mathematical biology is its ability to translate biological phenomena into mathematical language. This translation involves creating equations and algorithms that represent biological interactions, such as gene regulation, enzyme kinetics, population dynamics, and the spread of infectious diseases. By formulating these interactions mathematically, researchers can simulate and analyze complex biological systems, providing insights that are often unattainable through experimental approaches alone. The use of mathematical models in biology dates back to the early 20th century with seminal work by pioneers such as Vito Volterra and Alfred Lotka, who developed models to describe predator-prey dynamics. Since then, the field has expanded significantly, incorporating diverse mathematical techniques ranging from differential equations and stochastic processes to network theory and machine learning. These models can be broadly classified into deterministic and stochastic frameworks. Deterministic models, based on fixed rules and initial conditions, predict a unique outcome for a given set of parameters. In contrast, stochastic models incorporate randomness, reflecting the inherent variability and unpredictability of biological systems [1,2].

Parameter estimation and optimization are critical components of mathematical modelling in biology. Accurate parameter values are essential for model reliability and predictive power. These parameters, often derived from experimental data, define the rates of biological processes and interactions within the model. Optimization techniques, such as maximum likelihood estimation and Bayesian inference, are employed to refine these parameters, ensuring that the models accurately represent the biological system under study. Mathematical biology also emphasizes the importance of analyzing model behaviour through techniques like sensitivity analysis and bifurcation analysis. Sensitivity analysis assesses how variations in model parameters affect the output, identifying critical parameters that influence system behaviour. Bifurcation analysis explores how changes in parameters can lead to qualitative changes in system dynamics, such as the transition from stable to oscillatory behaviour. These analyses are vital for understanding the robustness and stability of biological systems. Moreover, mathematical modelling plays a pivotal role in synthetic biology and systems biology. In synthetic biology, models guide the design and construction of novel biological circuits, ensuring that engineered systems function as intended. Systems biology uses models to integrate data from multiple biological scales, from molecular to ecological, providing a holistic understanding of biological networks and pathways [2].

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II. SYSTEMATIC REVIEW

Zheng et al., (2010) Mathematical modelling is essential in synthetic biology, bridging conceptual and practical aspects of biological circuits. This review various modelling concepts, assumptions, and methodologies relevant to synthetic biology. They discuss deterministic and stochastic frameworks and emphasize parameter estimation and optimization. Analytical techniques like sensitivity and bifurcation analysis help identify conditions for desired circuit behaviour. The review also covers modelling's role in phenotype analysis and available modelling standards and software. Case studies of a metabolic oscillator, a synthetic counter, and a bottom-up gene regulatory network illustrate the integral role of mathematical modelling in synthetic circuit design.

Naylor et al. (2010) Highlight the challenges in medical practice due to the complexity and variability of human biology. They emphasize the importance of understanding individual human complexity and population variability. Systems biology, aided by analytical platforms and bioinformatics tools, offers a systematic approach to these challenges. The review discusses how systems biology can elucidate key pathways and networks, aiding personalized medicine. By addressing human complexity and variability, systems biology holds potential for improving disease treatment and health outcomes at both individual and population levels, showcasing exciting opportunities in personalized medicine.

Tay et al. (2010) Investigate how mammalian cells respond to varying concentrations of TNF-α using high-throughput microfluidic cell culture, fluorescence microscopy, and mathematical modelling. They find that NF-κB activation is heterogeneous and digital at the single-cell level. Parameters such as NF-κB peak intensity and response time modulate the outcome. A developed stochastic model reproduces the observed dynamics and gene expression profiles. These findings underscore the importance of single-cell resolution measurements in understanding biological systems, providing insights into the cell-to-cell communication and genetic circuitry in dynamic environments like the mammalian immune response.

Jungck, J. R. (2011) Presents a special issue on biomathematics education, showcasing the work of fifteen groups. The highlighted modules integrate current biomathematics research, focusing on classroom adoption and innovative pedagogies. Unlike traditional calculus-based models, these modules emphasize discrete mathematics. Examples range from DNA nanostructures to ecosystem problems, providing contemporary applications for both biology and mathematics classrooms. This issue emphasizes the importance of discrete models and innovative teaching methods, offering easily adaptable resources for educators. It contextualizes quantitative reasoning and modelling within biomathematics education, promoting a modern approach to teaching these interdisciplinary subjects.

Momeni et al., (2011) The diverse symbiotic interactions in nature, from competition to mutualism, and their ecological and evolutionary implications. They review how artificial systems, both abstract and living, can model these interactions to address key questions about symbiosis. With their reduced complexity and increased controllability, artificial systems offer valuable insights into the origins, persistence, and ecological patterns of symbiosis. The review highlights the contributions of artificial systems in understanding natural symbioses, providing a controlled environment to study the underlying principles and dynamics of these interactions, and enhancing our ecological and evolutionary knowledge.

Brigandt, I. (2013) Discusses how systems biology integrates mechanistic and mathematical model explanations. He critiques traditional mechanistic explanations for not incorporating mathematical models and highlights the need for a broader philosophical conception. Systems biology uses mathematical modelling to explain functional-dynamical aspects, feedback loops, and system-wide properties like robustness. Brigandt illustrates this with cases from systems biology, showing that quantitative models are indispensable for explaining qualitative phenomena. This integrative approach underscores the importance of mathematical models in understanding complex biological systems, offering new insights into the interplay between mechanistic research and mathematical modelling.

Rosvall et al., (2014) The limitations of first-order Markov models in network dynamics, advocating for second-order models to capture higher-order dependencies. They demonstrate that ignoring these dynamics can affect community detection, ranking, and information spreading. Their findings, based on various systems, reveal significant differences in outcomes when second-order dynamics are considered. For instance, air traffic patterns and multidisciplinary journals are better understood using second-order models. This review suggests that incorporating higher-order memory in network analysis provides a more accurate understanding of how real systems are organized and function, highlighting the importance of advanced modelling techniques.

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Chiacchio et al., (2014) The use of agent-based modelling and cellular automata in studying the mammalian immune system. These discrete mathematical approaches allow entities (agents) to interact locally based on predefined rules, leading to emergent global behaviours. The review highlights the unpredictability and complexity of immune responses modelled through these techniques. NetLogo, a multi-agent programming language, is discussed for its applications in immunology, aiding hypothesis development and experimental investigations. The review underscores the strengths of agent-based modelling in revealing insights into immunological processes, offering a valuable tool for both research and education in complex biological systems.

Ji et al., (2017) The challenges in understanding cancer progression through biological and clinical perspectives. They emphasize the role of high-throughput technologies and systems biology in developing precise models for complex diseases. Computational and mathematical models help interpret omics data, elucidating molecular mechanisms and aiding in drug discovery. The review covers various modelling approaches, their applications, and limitations, and suggests potential research directions. By bridging the gap between high-throughput technologies and systemic modelling, the review highlights the importance of computational approaches in advancing cancer research and improving treatment strategies.

Yang et al., (2018) The role of reactive oxygen species (ROS) in cancer and chemotherapy. They discuss the challenges in quantitatively detecting ROS levels in clinical settings and the potential of mathematical modelling to predict ROS dynamics during treatment. The review analyzes methods for ROS detection and the application of modelling techniques in understanding tumor biology and treatment responses. It highlights the mixed results of ROS-targeting therapies and provides insights for future development of effective anticancer agents. This review underscores the importance of modelling in advancing our understanding of ROS's role in cancer treatment and improving therapeutic outcomes.

Fages, F. (2020). Systems Biology aims at elucidating the high-level functions of the cell from their biochemical basis at the molecular level. A lot of work has been done for collecting genomic and post-genomic data, making them available in databases and ontologies, building dynamical models of cell metabolism, signalling, division cycle, apoptosis, and publishing them in model repositories. In this chapter we review different applications of AI to biological systems modelling. We focus on cell processes at the unicellular level which constitutes most of the work achieved in the last two decades in the domain of Systems Biology. We show how rule-based languages and logical methods have played an important role in the study of molecular interaction networks and of their emergent properties responsible for cell behaviours.

III. INTERDISCIPLINARY NATURE

Mathematical biology epitomizes the intersection of mathematics and biology, harnessing the power of mathematical techniques to unravel the complexities of biological systems. This interdisciplinary field transcends traditional boundaries by applying mathematical frameworks to model biological phenomena, enabling researchers to simulate and predict intricate biological behaviours. The synergy between these two disciplines allows for a deeper understanding of biological processes that are often too complex to dissect through empirical methods alone. Mathematics provides the tools to abstract, simplify, and quantify biological interactions, making it possible to analyse systems ranging from molecular pathways to ecosystem dynamics. This interdisciplinary approach is not merely a blend of two fields but a transformative integration that enhances both. For instance, mathematical models of gene regulation can reveal insights into genetic control mechanisms, while population dynamics models can predict the impact of environmental changes on species survival. The collaboration between mathematicians and biologists fosters innovative methodologies, such as the development of new statistical techniques for parameter estimation and the creation of sophisticated algorithms for simulating biological processes. Furthermore, the interdisciplinary nature of mathematical biology facilitates the translation of theoretical models into practical applications, such as in drug development, where models predict the behaviour of biological targets under different conditions. This collaborative spirit extends to educational initiatives, where interdisciplinary training programs prepare the next generation of scientists to navigate and contribute to this converging landscape. By bridging the gap between mathematical abstraction and biological complexity, mathematical biology not only advances our theoretical understanding but also drives practical innovations that address real-world challenges in medicine, environmental science, and biotechnology. The field exemplifies how the integration of diverse scientific perspectives can lead to groundbreaking discoveries and solutions, highlighting the essential role of interdisciplinary collaboration in advancing scientific knowledge [3].

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IV. MODELLING FRAMEWORKS

Mathematical biology employs diverse modelling frameworks to capture the intricate behaviours of biological systems, primarily through deterministic and stochastic approaches. Deterministic models use fixed rules and initial conditions to predict unique outcomes, providing clear, reproducible insights into systems like metabolic pathways or gene regulation networks. In contrast, stochastic models incorporate randomness and variability, reflecting the inherent unpredictability of biological processes such as molecular interactions or population dynamics in fluctuating environments. These frameworks allow researchers to simulate biological systems under various conditions, exploring how small changes can lead to different outcomes. By employing both deterministic and stochastic models, mathematical biology offers a comprehensive toolkit to understand and predict the multifaceted nature of life, from cellular mechanisms to ecological interactions [4,5].

V. PARAMETER ESTIMATION

Parameter estimation is a critical aspect of mathematical modelling in biology, ensuring that models accurately reflect the biological systems they aim to simulate. This process involves determining the values of parameters such as reaction rates, growth rates, or interaction strengths that define the behaviour of a model. Accurate parameter estimation is essential for model reliability and predictive power. Techniques such as maximum likelihood estimation, Bayesian inference, and least squares optimization are commonly used to derive these parameters from experimental data. By refining parameter values, these methods enhance the model's ability to mimic real biological processes, allowing for precise simulations and robust predictions. Parameter estimation not only improves model accuracy but also helps in identifying key drivers of biological behaviour, facilitating a deeper understanding of underlying mechanisms and aiding in the development of targeted interventions in fields like drug development, disease modelling, and ecological conservation [6,7].

VI. ANALYTICAL TECHNIQUES

Sensitivity Analysis: Sensitivity analysis is a key analytical technique used in mathematical biology to determine how variations in model parameters affect the output of the model. By systematically altering parameters and observing the resulting changes in the system's behaviour, researchers can identify which parameters are most influential. This helps in understanding the robustness of the model and pinpointing critical factors that drive biological processes. Sensitivity analysis is crucial for refining models, guiding experimental designs, and ensuring that predictions remain reliable under different conditions.

Bifurcation Analysis: Bifurcation analysis examines how changes in model parameters can lead to qualitative shifts in the behaviour of a biological system, such as transitioning from stable to oscillatory dynamics. This technique helps identify thresholds and critical points where small changes in parameters can result in significant changes in system dynamics. By understanding these bifurcation points, researchers can predict and control complex behaviours in biological systems, such as the onset of diseases, population outbreaks, or the stability of ecological systems. Bifurcation analysis is essential for exploring the nonlinear nature of biological systems and their responses to environmental or internal changes.

VII. APPLICATIONS IN BIOLOGY

Mathematical models are integral to various biological disciplines, offering profound insights and practical solutions. In ecology, models predict population dynamics and ecosystem interactions, guiding conservation efforts and understanding species' responses to environmental changes. Epidemiological models forecast the spread of infectious diseases, informing public health strategies and intervention measures. In neuroscience, models simulate neural activity and brain function, advancing our comprehension of cognition, behaviour, and neurological disorders. Evolutionary biology benefits from models that explore genetic and phenotypic changes over time, elucidating mechanisms of natural selection and adaptation. These applications demonstrate the versatility and impact of mathematical modelling in addressing complex biological questions and contributing to advancements in medicine, environmental science, and biotechnology [8,9, 10,11].

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VIII. CONCLUSION

Mathematical biology, an interdisciplinary field, effectively harnesses mathematical techniques to decode complex biological systems. By translating biological interactions into mathematical language, it enables precise simulations and robust predictions. Parameter estimation and analytical techniques ensure model reliability and deepen understanding. Applications span synthetic biology, systems biology, and beyond, highlighting the field's practical significance. The collaborative nature of mathematical biology drives innovations across medicine, environmental science, and biotechnology, demonstrating its crucial role in advancing scientific knowledge and addressing real-world challenges.

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