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Editorial: Mathematical modeling of gene networks

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Editorial on the Research Topic
Mathematical modeling of gene networks

All processes occurring in living organisms and responsible for performing vitally necessary functions are carried out by coordinated expression of various groups of genes. A gene regulatory network (GRN) is understood as a set of coordinately expressed genes, their protein products, and the relationships between them. Inferring gene regulatory networks is a fundamental problem in biology that aims to reveal the complex relationships between genes and their regulators. Mathematical methods can be used effectively to solve this and related issues. The existing mathematical approaches are diverse. Among them are thermodynamical models, models using Boolean algebra, graph theory, and models based on the use of dynamical systems. A variety of modeling approaches can be a stimulating prospect for new researchers in this area. The main aim of this Research Topic was to bring together the articles devoted to the contemporary understanding of the application of mathematical methods to the analysis of GRN. Within this topic, six articles have been published that complemented our knowledge of gene networks and their investigations by mathematical methods. Let us look at the articles that were collected in the volume during editorial work.

Understanding control mechanisms in biological systems plays a crucial role in important applications. Cifuentes-Fontanals et al. point out that available approaches to control strategy identification usually focus either on attractor or phenotype control and are unable to deal with more complex control problems, for instance, phenotype avoidance. They present a novel approach to control strategy identification in Boolean networks based on model checking. The method is guaranteed to identify all minimal control strategies and provides maximal flexibility in the definition of the control target. The authors investigate the applicability of the approach by considering a range of control problems for different biological systems, comparing the results, where possible, to those obtained by alternative control methods.

Freitas and Bischof provide the review that examines GRN modeling approaches in aging, encompassing differential equations, Boolean/fuzzy logic decision trees, Bayesian networks, mutual information, and regression clustering. These approaches provide nuanced insights into the intricate gene-protein interactions in aging, unveiling potential therapeutic targets and ARD biomarkers. This review aspires to stimulate further research in aging, fostering the innovation of computational approaches for promoting healthspan and longevity.

Duncan et al. address a problem of correspondence between the dynamics of a parameterized system and the structure of interactions within that system. The structure of interactions is captured by a signed network. A network dynamics is parameterized by collections of multi-level monotone Boolean functions (MBFs), which are organized in a parameter graph PG. Each collection generates dynamics which are captured in a structure of recurrent sets called a Morse graph. The operations on signed graphs are studied. The authors show that duality, a standard operation on MBFs, and switching are dynamically related. They remark that combinatorial description of network dynamics is closely related to switching ODE network models, therefore their results suggest similar results for parameterized sets of smooth ODE network models of the network dynamics.

Nieto-Marín et al. describe the genetic code in terms of numbers that help to find several dual symmetries. Their formulation can even be rewritten regarding the up-down and right-left dual concepts. The authors argue that their work may bring many topological tools to studying the DNA molecule, including the Grassmann-Plucker coordinates, which are important in mathematical and physical contexts.

Nanda and Kirschner acknowledge that mathematical and computational models of biological systems are increasingly complex, typically comprised of hybrid multi-scale methods such as ordinary differential equations, partial differential equations, agent-based and rule-based models, etc. These mechanistic models typically comprise large numbers of parameters and therefore large degrees of freedom. Thus, fitting these models to multiple experimental datasets over time and space presents significant challenges. The authors undertake the task of reviewing, testing, and advancing calibration practices across models and dataset types to compare methodologies for model calibration. The work compares the performance of their model agnostic Calibration Protocol (CaliPro) with approximate Bayesian computing (ABC) to highlight strengths, weaknesses, synergies, and differences among these methods. The authors explore several model implementations and suggest a decision tree for selecting calibration approaches to match dataset types and modeling constraints.

Author contributions

JD: Project administration, Supervision, Writing – original draft, Writing – review & editing. FS: Project administration, Supervision, Writing – original draft, Writing – review & editing, Conceptualization. IS: Writing – original draft, Writing – review & editing.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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