

How Math and AI are Revolutionizing Biosciences

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Abstract

Mathematics underpins fundamental theories in physics such as quantum mechanics, general relativity, and quantum field theory. Nonetheless, its success in modern biology, namely cellular biology, molecular biology, biochemistry, genomics, and genetics, has been quite limited. Artificial intelligence (AI) has fundamentally changed the landscape of science, technology, industry, and social media in the past few years and holds a great future for discovering the rules of life. However, AI-based biological discovery encounters challenges arising from the structural complexity of macromolecules, the high dimensionality of biological variability, the multiscale entanglement of molecules, cells, tissues, organs, and organisms, the nonlinearity of genotype, phenotype, and environment coupling, and the excessiveness of genomic, transcriptomic, proteomic, and metabolomic data. We tackle these challenges mathematically. Our work focuses on reducing the complexity, dimensionality, entanglement, and nonlinearity of biological data in AI. We have introduced evolutionary de Rham-Hodge, persistent cohomology, persistent Laplacian, and persistent sheaf theories to model complex, heterogeneous, multiscale biological systems and thus significantly enhance AI's ability to handle biological datasets. Using our mathematical AI approaches, my team has been the top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design and discovery for years. Using over two million genomes isolates from patients, we discovered the mechanisms of SARS-CoV-2 evolution and transmission and accurately forecast emerging SARS-CoV-2 variants.