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Graphs and Graph Theory in Computational Biology

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Message from the Guest Editor

The field of computational biology boasts a rich historical connection with graph theory, where graphs serve as a sophisticated and versatile data structure for modeling a wide range of complex problems. For example, de Bruijn graphs find utility in solving sequence assembly problems, while protein–protein interaction networks, expressed as undirected or directed graphs, illuminate the physical bindings between proteins and their associated regulatory mechanisms. Furthermore, the features of real-world data, such as small-world and scale-free network structures, presented by power-law degree distributions and hub nodes, are identified in biological networks. Recent advancements, like graph neural networks, have revolutionized the analysis of non-Euclidean distance data, providing a mathematical framework for machine learning applications within biological datasets. In light of these developments, this Special Issue embarks on a compelling exploration of how graphs and graph theory are employed in computational biology.

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Message from the Editor-in-Chief

Algorithms are the very core of Computer Science. The whole area has been considered from quite different perspectives, having led to the development of many sub-communities: Complexity theory (limitations), approximation or parameterized algorithms (types of problems), geometric algorithms (subject area), metaheuristics, algorithm engineering, medical imaging (applications), indicates the range of perspectives. Our journal welcomes submissions written from any of these perspectives, so that it may become a forum for exchange of ideas between the corresponding scientific subcommunities.

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