Computational Medicine: Tools and Challenges

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Computational methodologies and modeling play a growing role for investigating mechanisms, and for the diagnosis and therapy of human diseases. This progress gave rise to computational medicine, an interdisciplinary field at the interface of computer science and medicine. The main focus of computational medicine lies in the development of data analysis methods and mathematical modeling as well as computational simulation techniques specifically addressing medical problems. In this book, we present a number of computational medicine topics at several scales: from molecules to cells, organs, and organisms. At the molecular level, tools for the analysis of genome variations as well as cloud computing resources for medical genetics are reviewed. Then, an analysis of gene expression data and the application to the characterization of microbial communities are highlighted. At the protein level, two types of analyses for mass spectrometry data are reviewed: labeled quantitative proteomics and lipidomics, followed by protein sequence analysis and a 3D structure and drug design chapter. Finally, three chapters on clinical applications focus on the integration of biomolecular and clinical data for cancer research, biomarker discovery, and network-based methods for computational diagnostics.

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