

With a DVD of color figures, **Clustering in Bioinformatics and Drug Discovery** provides an expert guide on extracting the most pertinent information from pharmaceutical and biomedical data. It offers a concise overview of common and recent clustering methods used in bioinformatics and drug discovery.

Setting the stage for subsequent material, the first three chapters of the book introduce statistical learning theory, exploratory data analysis, clustering algorithms, different types of data, graph theory, and various clustering forms. In the following chapters on partitional, cluster sampling, and hierarchical algorithms, the book provides readers with enough detail to obtain a basic understanding of cluster analysis for bioinformatics and drug discovery. The remaining chapters cover more advanced methods, such as hybrid and parallel algorithms, as well as details related to specific types of data, including asymmetry, ambiguity, validation measures, and visualization.

Features

- Covers the clustering of small and large data sets, parallelization of clustering algorithms, validation and visualization, asymmetric clustering, and clustering ambiguity
- Presents over 20 algorithms in pseudocode
- Provides real-world examples from industrial settings, such as combinatorial library design and compound databases
- Offers primers on matrix algebra, probability theory, and number theory for those new to the mathematics of clustering

This book explores the application of cluster analysis in the areas of bioinformatics and cheminformatics as they relate to drug discovery. Clarifying the use and misuse of clustering methods, it helps readers understand the relative merits of these methods and evaluate results so that useful hypotheses can be developed and tested.

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an informa businesswww.crcpress.com6000 Broken Sound Parkway, NW
Suite 300, Boca Raton, FL 33487
270 Madison Avenue
New York, NY 10016
2 Park Square, Milton Park
Abingdon, Oxon OX14 4RN, UK

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