Introduction To Computational Proteomics Protein

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Introduction to Computational Proteomics Springer
The definitive introduction to data analysis in quantitativeproteomics This book provides all the necessary knowledge about massspectrometry based proteomics methods and computational andstatistical approaches to pursue the planning, design and analysisof quantitative proteomics experiments. The author’scarefully constructed approach allows readers to easily make thetransition into the field of quantitative proteomics. Throughdetailed descriptions of wet-lab methods, computational approachesand statistical tools, this book covers the full scope of aquantitative experiment, allowing readers to acquire new knowledgeas well as acting as a useful reference work for more advancedreaders. Computational and Statistical Methods for ProteinQuantification by Mass Spectrometry: Introduces the use of mass spectrometry in proteinquantification and how the bioinformatics challenges in this fieldcan be solved using statistical methods and various softwareprograms. Is illustrated by a large number of figures and examples aswell as numerous exercises. Provides both clear and rigorous descriptions of methods andapproaches. Is thoroughly indexed and cross-referenced, combining thestrengths of a text book with the utility of a reference work. Features detailed discussions of both wet-lab approaches andstatistical and computational methods. With clear and thorough descriptions of the various methods andapproaches, this book is accessible to biologists, informaticians,and statisticians alike and is aimed at readers across the academicspectrum, from advanced undergraduate students to post doctoratesentering the field.
Bioinformatics and Functional Genomics Springer Science & Business Media
Wiley is proud to announce the publication of the first ever broad-based textbook introduction to Bioinformatics and Functional Genomics by a trained biologist, experienced researcher, and award-winning instructor. In this new text, author Jonathan Pevsner, winner of the 2001 Johns Hopkins University "Teacher of the Year" award, explains problem-solving using bioinformatic approaches using real examples such as breast cancer, HIV-1, and retinal-binding protein throughout. His book includes 375 figures and over 170 tables. Each chapter includes: Problems, discussion of Pitfalls, Boxes explaining key techniques and math/stats principles, Summary, Recommended Reading list, and URLs for freely available software. The text is suitable for professionals and students at every level, including those with little to no background in computer science.
Protein-Protein Interactions Academic Press
Where did SARS come from? Have we inherited genes from Neanderthals? How do plants use their internal clock? The genomic revolution in biology enables us to answer such questions. But the revolution would have been impossible without the support of powerful computational and statistical methods that enable us to exploit genomic data. Many universities are introducing courses to train the next generation of bioinformaticians: biologists fluent in mathematics and computer science, and data analysts familiar with biology. This readable and entertaining book, based on successful taught courses, provides a roadmap to navigate entry to this field. It guides the reader through key achievements of bioinformatics, using a hands-on approach. Statistical sequence analysis, sequence alignment, hidden Markov models, gene and motif finding and more, are introduced in a rigorous yet accessible way. A companion website provides the reader with Matlab-related software tools for reproducing the steps demonstrated in the book.
Computational Methods for Mass Spectrometry Proteomics Springer Science & Business Media
Proteomics is the science of understanding the dynamic protein content of an organism's cells (its proteome), which is one of the largest current challenges in biology. Computational proteomics is an active research area that involves in-silico methods for the analysis of high-throughput protein identification data. Current methods are based on a technology called tandem mass spectrometry (MS/MS) and suffer from low coverage and accuracy, reliably identifying only 20-40% of the proteome. This dissertation addresses recall, precision, speed and scalability of computational proteomics experiments. This research goes beyond the traditional paradigm of analyzing MS/MS experiments in isolation, instead learning priors of protein presence from the joint analysis of various systems biology data sources. This integrative "systems" approach to protein identification is very effective, as demonstrated by two new methods. The first, MSNet, introduces a social model for protein identification and leverages functional dependencies from genome-scale, probabilistic, gene functional networks. The second, MSPresso, learns a gene expression prior from a joint analysis of mRNA and proteomics experiments on similar samples. These two sources of prior information result in more accurate estimates of protein presence, and increase protein recall by as much as 30% in complex samples, while also increasing precision. A comprehensive suite of benchmarking datasets is introduced for evaluation in yeast. Methods to assess statistical significance in the absence of ground truth are also introduced and employed whenever applicable. This dissertation also describes a database indexing solution to improve speed and scalability of protein identification experiments. The method, MSFound, customizes a metric-space database index and its associated approximate k-nearest-neighbor search algorithm with a semi-metric distance designed to match noisy spectra. MSFound achieves an order of magnitude speedup over traditional spectra database searches while maintaining scalability.
Computational Methods for Protein Structure Prediction and Modeling John Wiley & Sons
The field of proteomics has developed rapidly over the past decade nurturing the need for a detailed introduction to the various informatics topics that underpin the main liquid

chromatography tandem mass spectrometry (LC-MS/MS) protocols used for protein identification and quantitation. Proteins are a key component of any biological system, and monitoring proteins using LC-MS/MS proteomics is becoming commonplace in a wide range of biological research areas. However, many researchers treat proteomics software tools as a black box, drawing conclusions from the output of such tools without considering the nuances and limitations of the algorithms on which such software is based. This book seeks to address this situation by bringing together world experts to provide clear explanations of the key algorithms, workflows and analysis frameworks, so that users of proteomics data can be confident that they are using appropriate tools in suitable ways.

Statistical Analysis of Proteomics, Metabolomics, and Lipidomics Data Using Mass Spectrometry CRC Press

Volume Two of this two-volume sequence presents a comprehensive overview of protein structure prediction methods and includes protein threading, De novo methods, applications to membrane proteins and protein complexes, structure-based drug design, as well as structure prediction as a systems problem. A series of appendices review the biological and chemical basics related to protein structure, computer science for structural informatics, and prerequisite mathematics and statistics.

Computational Medicine CRC Press

This book presents a focus on proteins and their structures. The text describes various scalable solutions for protein structure similarity searching, carried out at main representation levels and for prediction of 3D structures of proteins. Emphasis is placed on techniques that can be used to accelerate similarity searches and protein structure modeling processes. The content of the book is divided into four parts. The first part provides background information on proteins and their representation levels, including a formal model of a 3D protein structure used in computational processes, and a brief overview of the technologies used in the solutions presented in the book. The second part of the book discusses Cloud services that are utilized in the development of scalable and reliable cloud applications for 3D protein structure similarity searching and protein structure prediction. The third part of the book shows the utilization of scalable Big Data computational frameworks, like Hadoop and Spark, in massive 3D protein structure alignments and identification of intrinsically disordered regions in protein structures. The fourth part of the book focuses on finding 3D protein structure similarities, accelerated with the use of GPUs and the use of multithreading and relational databases for efficient approximate searching on protein secondary structures. The book introduces advanced techniques and computational architectures that benefit from recent achievements in the field of computing and parallelism. Recent developments in computer science have allowed algorithms previously considered too time-consuming to now be efficiently used for applications in bioinformatics and the life sciences. Given its depth of coverage, the book will be of interest to researchers and software developers working in the fields of structural bioinformatics and biomedical databases.

Computational Biology Springer Science & Business Media

This book reflects more than three decades of research on Cellular Automata (CA), and nearly a decade of work on the application of CA to model biological strings, which forms the foundation of 'A New Kind of Computational Biology' pioneered by the start-up, CARLBio. After a brief introduction on Cellular Automata (CA) theory and functional biology, it reports on the modeling of basic biological strings with CA, starting with the basic nucleotides leading to codon and anti-codon CA models. It derives a more involved CA model of DNA, RNA, the entire translation process for amino acid formation and the evolution of protein to its unique structure and function. In subsequent chapters the interaction of Proteins with other bio-molecules is also modeled. The only prior knowledge assumed necessary is an undergraduate knowledge of computer programming and biology. The book adopts a hands-on, "do-it-yourself" approach to enable readers to apply the method provided to derive the CA rules and comprehend how these are related to the physical 'rules' observed in biology. In a single framework, the authors have presented two branches of science - Computation and Biology. Instead of rigorous molecular dynamics modeling, which the authors describe as a Bottoms-Up model, or relying on the Top-Down new age Artificial Intelligence (AI) and Machine Language (ML) that depends on extensive availability of quality data, this book takes the best from both the Top-Down and Bottoms-up approaches and establishes how the behavior of complex molecules is represented in CA. The CA rules are derived from the basic knowledge of molecular interaction and construction observed in biological world but mapped to a few subset of known results to derive and predict results. This book is useful for students, researchers and industry practitioners who want to explore modeling and simulation of the physical world complex systems from a different perspective. It raises the inevitable the question - 'Are life and the universe nothing but a collection of continuous systems processing information'.

A New Kind of Computational Biology John Wiley & Sons

One of the most pressing tasks in biotechnology today is to unlock the function of each of the thousands of new genes identified every day. Scientists do this by analyzing and interpreting proteins, which are considered the task force of a gene. This single source reference covers all aspects of proteins, explaining fundamentals, synthesizing the latest literature, and demonstrating the most important bioinformatics tools available today for protein analysis, interpretation and prediction. Students and researchers of biotechnology, bioinformatics, proteomics, protein engineering, biophysics, computational biology, molecular modeling, and drug design will find this a ready reference for staying current and productive in this fast evolving interdisciplinary field. Explains all aspects of proteins including sequence and structure analysis, prediction of protein structures, protein folding, protein stability, and protein interactions Presents a cohesive and accessible overview of the field, using illustrations to explain key concepts and detailed exercises for students.

Computational Biology Springer Science & Business Media

Gabriel Waksman Institute of Structural Molecular Biology, Birkbeck and University College London, Malet Street, London WC1E 7HX, United Kingdom Address for correspondence: Professor Gabriel Waksman Institute of Structural Molecular Biology Birkbeck and University College London Malet Street London WC1E 7H United Kingdom Email: g. waksman@bbk. ac. uk and g. waksman@ucl. ac. uk Phone: (+44) (0) 207 631 6833 Fax: (+44) (0) 207 631 6833 URL: http://people. cryst. bbk. ac. uk/?ubcg54a Gabriel Waksman is Professor of Structural Molecular Biology at the Institute of Structural Molecular Biology at UCL/Birkbeck, of which he is also the director. Before joining the faculty of UCL and Birkbeck, he was the Roy and Diana Vagelos Professor of Biochemistry and Molecular Biophysics at the Washington University School of Medicine in St Louis (USA). The rapidly evolving ?eld of protein science has now come to realize the ubiquity and importance of protein–protein interactions. It had been known for some time that proteins may interact with each other to form functional complexes, but it was thought to be the property of only a handful of key proteins. However, with the advent of hi- throughput proteomics to monitor protein–protein interactions at an organism level, we can now safely state that protein–protein interactions are the norm and

not the exception.

Proteome Bioinformatics CRC Press

This book provides a comprehensive overview of the fundamental aspects of protein-protein interactions (PPI), including a detailed account of the energetics and thermodynamics involved in these interactions. It also discusses a number of computational and experimental approaches for the prediction of PPI interactions and reviews their principles, advantages, drawbacks, and the recent developments. Further, it offers structural and mechanistic insights into the formation of protein-protein complexes and maps different PPIs into networks to delineate various pathways that operate at the cellular level. Lastly, it describes computational protein-protein docking techniques and discusses their implications for further experimental research. Given its scope, this book is a valuable resource for students, researchers, scientists, entrepreneurs, and medical/healthcare professionals.

Computational Biology and Genome Informatics Royal Society of Chemistry

Computational biology is an interdisciplinary field that applies mathematical, statistical, and computer science methods to answer biological questions, and its importance has only increased with the introduction of high-throughput techniques such as automatic DNA sequencing, comprehensive expression analysis with microarrays, and proteome analysis with modern mass spectrometry. In Computational Biology, expert practitioners present a broad survey of computational biology methods by focusing on their applications, including primary sequence analysis, protein structure elucidation, transcriptomics and proteomics data analysis, and exploration of protein interaction networks. As a volume in the highly successful Methods in Molecular BiologyTM series, this work provides the kind of detailed description and implementation advice that is crucial for getting optimal results. Authoritative and easy to use, Computational Biology is an ideal guide for all scientists interested in quantitative biology.

Scalable Big Data Analytics for Protein Bioinformatics CRC Press

Probabilistic models are becoming increasingly important in analysing the huge amount of data being produced by large-scale DNA-sequencing efforts such as the Human Genome Project. For example, hidden Markov models are used for analysing biological sequences, linguistic-grammar-based probabilistic models for identifying RNA secondary structure, and probabilistic evolutionary models for inferring phylogenies of sequences from different organisms. This book gives a unified, up-to-date and self-contained account, with a Bayesian slant, of such methods, and more generally to probabilistic methods of sequence analysis. Written by an interdisciplinary team of authors, it aims to be accessible to molecular biologists, computer scientists, and mathematicians with no formal knowledge of the other fields, and at the same time present the state-of-the-art in this new and highly important field.

Computational and Statistical Methods for Protein Quantification by Mass Spectrometry Cambridge University Press

In this, the post-genomic age, our knowledge of biological systems continues to expand and progress. As the research becomes more focused, so too does the data. Genomic research progresses to proteomics and brings us to a deeper understanding of the behavior and function of protein clusters. And now proteomics gives way to neuroproteomics as we begin to unravel the complex mysteries of neurological diseases that less than a generation ago seemed opaque to our inquiries, if not altogether intractable. Edited by Dr. Oscar Alzate, Neuroproteomics is the newest volume in the CRC Press Frontiers of Neuroscience Series. With an extensive background in mathematics and physics, Dr. Alzate exemplifies the newest generation of biological systems researchers. He organizes research and data contributed from all across the world to present an overview of neuroproteomics that is practical and progressive. Bolstered by each new discovery, researchers employing multiple methods of inquiry gain a deeper understanding of the key biological problems related to brain function, brain structure, and the complexity of the nervous system. This in turn is leading to new understanding about diseases of neurological deficit such as Parkinson's and Alzheimer's. Approaches discussed in the book include mass spectrometry, electrophoresis, chromatography, surface plasmon resonance, protein arrays, immunoblotting, computational proteomics, and molecular imaging. Writing about their own work, leading researchers detail the principles, approaches, and difficulties of the various techniques, demonstrating the questions that neuroproteomics can answer and those it raises. New challenges wait, not the least of which is the identification of potential methods to regulate the structures and functions of key protein interaction networks. Ultimately, those building on the foundation presented here will advance

Applied Bioinformatics Springer

Starting by describing the structure of proteins and explaining how these structures can be studied, this book goes on to illustrate the wide range of protein functions by showing how the shape of a protein is intimately linked to its function.

Introduction to Protein Science World Scientific

This book contains articles written by experts on a wide range of topics that are associated with the analysis and management of biological information at the molecular level. It contains chapters on RNA and protein structure analysis, DNA computing, sequence mapping, genome comparison, gene expression data mining, metabolic network modeling, and phyloinformatics. The important work of some representative researchers in bioinformatics is brought together for the first time in one volume. The topic is treated in depth and is related to, where applicable, other emerging technologies such as data mining and visualization. The goal of the book is to introduce readers to the principle techniques of bioinformatics in the hope that they will build on them to make new discoveries of their own. Contents: Exploring RNA Intermediate Conformations with the Massively Parallel Genetic Algorithm; Introduction to Self-Assembling DNA Nanostructures for Computation and Nanofabrication; Mapping Sequence to Rice FPC; Graph Theoretic Sequence Clustering Algorithms and their Applications to Genome Comparison; The Protein Information Resource for Functional Genomics and Proteomics; High-Grade Ore for Data Mining in 3D Structures; Protein Classification: A Geometric Hashing Approach; Interrelated Clustering: An Approach for Gene Expression Data Analysis; Creating Metabolic Network Models Using Text Mining and Expert Knowledge; Phyloinformatics and Tree Networks. Readership: Molecular biologists who rely on computers and mathematical scientists with interests in biology.

Proteomics and Protein-Protein Interactions Springer

Volume One of this two-volume sequence focuses on the basic characterization of known protein structures, and structure prediction from protein sequence information. Eleven chapters survey of the field, covering key topics in modeling, force fields, classification, computational methods, and structure prediction. Each chapter is a self contained review covering definition of the problem and historical perspective; mathematical formulation; computational methods and algorithms; performance results; existing software; strengths, pitfalls, challenges, and future research.

Introduction to Proteins Humana

This book constitutes the thoroughly refereed post-proceedings of

two joint RECOMB 2006 satellite events: the Second Annual Workshop on Systems Biology, RSB 2006, and the First Biennial Workshop on Computational Proteomics, RCP 2006, held in San Diego, CA, USA in December 2006. The papers cover various aspects of systems biology and explore the use of computational mass spectrometry in various proteomic applications.

Ten Most Wanted Solutions in Protein Bioinformatics Springer Science & Business Media

Protein Interaction Networks, Volume 131 in the Advances in Protein Chemistry and Structural Biology series, highlights new advances in the field, with this new volume presenting interesting chapters written by an international board of authors. Provides the authority and expertise of leading contributors from an international board of authors Presents the latest release in the Advances in Protein Chemistry and Structural Biology series Includes the latest information on protein design and structure

Computational Methods for Protein Structure Prediction and Modeling Springer Science & Business Media

Bioinformatics is an evolving field that is gaining popularity due to genomics, proteomics and other high-throughput biological methods. The function of bioinformatic scientists includes biological data storage, retrieval and in silico analysis of the results from large-scale experiments. This requires a grasp of knowledge mining algorithms, a thorough understanding of biological knowledge base, and the logical relationship of entities that describe a process or the system. Bioinformatics researchers are required to be trained in multidisciplinary fields of biology, mathematics and computer science. Currently the requirements are satisfied by ad hoc researchers who have specific skills in biology or mathematics/computer science. But the learning curve is steep and the time required to communicate using domain specific terms is becoming a major bottle neck in scientific productivity. This workbook provides hands-on experience which has been lacking for qualified bioinformatics researchers.