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Advances in Protein Molecular and Structural Biology Methods

DUNCAN WHITAKER

Fast Computational Methods for Predicting Protein Structure from Primary Amino Acid Sequence

Computational Methods for Protein Structure Prediction and ModelingVolume 1: Basic Characterization

This volume presents a diverse collection of methodologies used to study various problems at the protein sequence and structure level. The chapters in this book look at issues ranging from broad concepts like protein space to specifics like antibody modeling. Topics include point mutations, gene duplication, de novo emergence of new genes, pairwise correlated mutations, ancestral protein reconstruction, homology modelling, protein stability and dynamics, and protein-protein interactions. The book also covers a wide range of computational approaches, including sequence and structure alignments, phylogenies, physics-based and mathematical approaches, machine learning, and more. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions

to their respective topics, lists of the necessary materials and prerequisites, step-by-step, readily reproducible computational protocols (using command line or graphical user interfaces, sometimes including computer code), and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and authoritative, Computational Methods in Protein Evolution is a valuable resource that offers useful workflows and techniques that will help both novice and expert researchers working with proteins computationally. Computational Structural Biology Springer Science & Business Media 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. *Computational Methods in Protein Structure Comparison and Analysis of Protein Interaction Networks* Springer Science & Business Media The second volume in a series which aims to focus on advances in computational biology. This volume discusses such topics as: statistical analysis of protein sequences; progress in large-scale sequence analysis; and the architecture of loops in proteins. Structure and Function Springer Nature This book presents applications of bioinformatics tools that experimental research scientists use in "daily practice." Its interdisciplinary approach combines computational and experimental methods to solve scientific problems. The book begins with reviews of computational methods for protein sequence-structure-function analysis, followed by methods that use experimental data obtained in the laboratory to improve functional predictions. *Development of Computational Methods for the Prediction of Protein Structure, Protein Binding, and Mutational Effects Using Free Energy*

Calculations Springer Science & Business Media Abstract: Protein-protein interactions play a key role in the functioning of cells and pathways, and understanding these interactions on a physical and structural level can help greatly in developing therapeutics for diseases. The large amount of protein structures available presents an immense opportunity to model and predict protein interactions using computational techniques. Here we describe the development of algorithms to predict protein complex structures (referred to as protein docking) and to design proteins to improve their interaction affinities. We also present experimental results validating our protein design approach. The protein docking work we present includes the symmetric multimer docking program M-ZDOCK as well as ZRANK which rescores docking predictions using a weighted potential. Both programs have been successful when applied to docking benchmarks and in the CAPRI experiment. In addition, we have used the M-ZDOCK program to produce a tetrameric model for a disease-associated protein, the

latent nuclear antigen of the Kaposi's sarcoma-associated herpesvirus. We have also developed a protein design algorithm to improve the binding between two proteins, given their complex structure This was applied to a T cell receptor (TCR) to enhance its binding to the Major Histocompatibility Complex and peptide. Several of the point mutations predicted by our algorithm were verified experimentally to bind several times stronger than wild type; we then combined these mutations to produce a TCR with approximately 100-fold affinity improvement. Further testing of combinations of TCR point mutations has led to striking results regarding the kinetics and cooperativity of the mutations. Finally, we have used our protein design algorithm to predict designability of protein complexes from the Protein Data Bank, and identified the complex between CD4 and HIV gp120 as a target for future structure-based design efforts. Preliminary results for this project are given.

Protein Structure Prediction

Elsevier

Protein-protein interactions underlie all biological processes and are a field of study that has wide

implications throughout many other fields including medicine, genetics, biology, and ecology. Proteins are the building blocks and primary actors of life. They work together to accomplish virtually every task within a cell, including, metabolism, signal propagation, immune responses, and cell signaling. This problem is a logical successor to the Human Genome Project: now that we know so much about the DNA of living organisms, how do we advance our knowledge? The Human Genome and other DNA sequencing efforts have provided complete genetic sequences for more than 180 living organisms. However, these efforts fall short of describing or predicting life processes because the sequence of a protein is not enough to elucidate its function. Knowing this, the National Institute of Health started the Protein Structure Initiative, which seeks to increase knowledge of protein structure and has led to an increase in the number of known proteins structures. Unfortunately, even these efforts fall short as there are over 80,000 known protein structures but the function of many is completely unknown. The fledgling field of interface

prediction seeks to use this wealth of structural information to be able to describe protein function and drastically increase our understanding of life processes. Presented herein is a novel methodology for solving the protein-protein interface prediction problem leveraging a variety of Computer Science techniques. Specifically detailed is a process for decomposing this 3-dimensional problem into a feature extraction and classification problem using algorithms from computer vision and machine learning. Applications of Computational Methods for Protein Structure Prediction Humana Press Abstract: Nearly all major processes in living cells are carried out by complex apparatus consisting of protein molecules. This thesis describes computational tools developed to help investigate two fundamental questions about proteins that underlie cell functions: how they interact with each other and form complex structures; and how they are expressed and modified in different cell states. In order to address the first question, several methods are developed to predict protein-

protein complex structures. Protein interactions are energy driven processes. The prediction of protein complex structures is the search for the global minimum on the binding free-energy landscape. An approach is described that uses Van der Wools energy, desolvation energy and shape complementarity as the scoring functions and a five-dimensional fast Fourier transform algorithm to expedite the search. Two methods to screen and optimize the predicted protein complex structures are also introduced. They incorporate additional energy terms and clustering algorithms to provide more precise estimations of the binding free-energy. The same methods can also be used to predict hot spots, the mutations of which significantly alter the binding kinetics. To study the protein expression profiles, a two-step approach for protein identification using peptide mass fingerprinting data is developed. Peptide mass fingerprinting uses peptide masses determined by mass spectrometry to identify the peptides and subsequently, the proteins in the sample Peaks in the mass spectrum are associated

with known peptide sequences in the database based on log-likelihood ratio test. A statistical algorithm is then used to identify proteins by comparing the probability of each protein's presence in the sample, given the peak assignments with the background probability. This method also discovers post-translational modifications in the identified proteins. The protein binding prediction program successfully predicts protein complex structures that closely resemble their native forms, as observed by x-ray crystallography or NMR. The refinements and hot spot predictions also give accurate and consistent results. The database search program that interprets mass spectrometry data is evaluated with artificial and experimental data. The program identifies proteins in the sample with high sensitivity and specificity. The results presented in this thesis demonstrate that computational methods help to better understand the structure and the composition of the protein machineries. All of the methods described herein have been implemented and made available for the research community

over the Internet. *Advances in Computational Biology* Springer Nature The Beauty of Protein Structures and the Mathematics behind Structural Bioinformatics Providing the framework for a one-semester undergraduate course, Structural Bioinformatics : An Algorithmic Approach shows how to apply key algorithms to solve problems related to macromolecular structure. Helps Students Go Further in Their Study of Structural Biology Following some introductory material in the first few chapters, the text solves the longest common subsequence problem using dynamic programming and explains the science models for the Nussinov and MFOLD algorithms. It then reviews sequence alignment, along with the basic mathematical calculations needed for measuring the geometric properties of macromolecules. After looking at how coordinate transformations facilitate the translation and rotation of molecules in a 3D space, the author introduces structural comparison techniques, superposition algorithms, and algorithms that compare relationships within a protein. The final chapter explores how regression

and classification are becoming more useful in protein analysis and drug design. At the Crossroads of Biology, Mathematics, and Computer Science Connecting biology, mathematics, and computer science, this practical text presents various bioinformatics topics and problems within a scientific methodology that emphasizes nature (the source of empirical observations), science (the mathematical modeling of the natural process), and computation (the science of calculating predictions and mathematical objects based on mathematical models). Computational Methods in Molecular Biology Springer This book discusses a broad range of basic and advanced topics in the field of protein structure, function, folding, flexibility, and dynamics. Starting with a basic introduction to protein purification, estimation, storage, and its effect on the protein structure, function, and dynamics, it also discusses various experimental and computational structure determination approaches; the importance of molecular interactions and water in protein stability, folding and dynamics; kinetic and thermodynami

c parameters associated with protein-ligand binding; single molecule techniques and their applications in studying protein folding and aggregation; protein quality control; the role of amino acid sequence in protein aggregation; muscarinic acetylcholine receptors, antimuscarinic drugs, and their clinical significances. Further, the book explains the current understanding on the therapeutic importance of the enzyme dopamine beta hydroxylase; structural dynamics and motions in molecular motors; role of cathepsins in controlling degradation of extracellular matrix during disease states; and the important structure-function relationship of iron-binding proteins, ferritins. Overall, the book is an important guide and a comprehensive resource for understanding protein structure, function, dynamics, and interaction.

Computational Methods for Protein Folding, Volume 120

John Wiley & Sons

The present invention provides a method utilizing primary amino acid sequence of a protein, energy minimization, molecular dynamics and protein vibrational modes to predict three-dimensional structure of a protein. The present invention also

determines possible intermediates in the protein folding pathway. The present invention has important applications to the design of novel drugs as well as protein engineering. The present invention predicts the three-dimensional structure of a protein independent of size of the protein, overcoming a significant limitation in the prior art.

What We Can Learn from Computational Methods

Humana Press

Understanding the synthesis, structures and functions of proteins draws vital attention in computational biology as proteins participate in virtually every cellular function in an organism. In appropriate environment, a protein folds spontaneously into unique three dimensional structure of minimum energy termed as native state. Protein Structure Prediction (PSP) refers to

the computational approach of predicting protein tertiary structure from amino acid sequence. Protein synthesis, on the other hand, is a multi-step process where nuclear DNA is transcribed into protein-coding messenger RNA (mRNA), which is then translated into unique amino acid sequence. MicroRNAs (miRNAs) bind to target mRNAs through complementar

y base-pairing and regulate protein production by translational repression or target degradation. A miRNA can bind to another mRNA from a po¬tentially large mRNA pool and computational prediction of such target mRNA set is referred to as miRNA Target Prediction. -- Incomplete knowledge of folding mechanism, absence of an established perfect energy function, and apparently complex and irregular tertiary structure make the PSP problem ever so difficult, which encourages researchers adopting simplified lattice and energy models to ease the computa¬tion al hardness of the problem so as to explain essential functional properties of proteins. This thesis aims at developing several stochastic optimisation approaches to ab initio PSP in triangular lattice models and comparing their relative efficacy. Triangular lattice models are chosen because of their ability to capture more compact folded structures. In search for a faster and efficient local search method, a new neighbourhoo d relation is developed that is shown complete and efficient in finding minimum energy structures when incorporated

into tabu search and logarithmic simulated annealing algorithm.

Molecular Modeling of Proteins

Elsevier

This book discusses topics related to bioinformatics, statistics, and machine learning, presenting the latest research in various areas of bioinformatics. It also highlights the role of computing and machine learning in knowledge extraction from biological data, and how this knowledge can be applied in fields such as drug design, health supplements, gene therapy, proteomics and agriculture.

From Quantum to Coarse-Grained Methods

Springer

Computational biology is a rapidly expanding field, and the number and variety of computational methods used for DNA and protein sequence analysis is growing every day. These algorithms are extremely valuable to biotechnology companies and to researchers and teachers in universities. This book explains the latest computer technology for analyzing DNA, RNA, and protein sequences. Clear and easy to follow, designed specifically for the non-computer scientist, it will help biologists make better choices on which

algorithm to use. New techniques and demonstrations are elucidated, as are state-of-the-art problems, and more advanced material on the latest algorithms. The primary audience for this volume are molecular biologists working either in biotechnology companies or academic research environments, individual researchers and the institutions they work for, and students. Any biologist who relies on computers should want this book. A secondary audience will be computer scientists developing techniques with applications in biology. An excellent reference for leading techniques, it will also help introduce computer scientists to the biology problems. This is an outstanding work which will be ideal for the increasing number of scientists moving into computational biology.

Computational Optimization Algorithms for Protein Structure Refinement

World Scientific

Proteins lie at the heart of almost all biological processes and have an incredibly wide range of activities. Central to the function of all proteins is their ability to adopt, stably or sometimes transiently, structures that allow for interaction

with other molecules. An understanding of the structure of a protein can therefore lead us to a much improved picture of its molecular function. This realisation has been a prime motivation of recent Structural Genomics projects, involving large-scale experimental determination of protein structures, often those of proteins about which little is known of function. These initiatives have, in turn, stimulated the massive development of novel methods for prediction of protein function from structure. Since model structures may also take advantage of new function prediction algorithms, the first part of the book deals with the various ways in which protein structures may be predicted or inferred, including specific treatment of membrane and intrinsically disordered proteins. A detailed consideration of current structure-based function prediction methodologies forms the second part of this book, which concludes with two chapters, focusing specifically on case studies, designed to illustrate the real-world application of these methods. With bang up-to-date texts from world experts, and abundant links to publicly

available resources, this book will be invaluable to anyone who studies proteins and the endlessly fascinating relationship between their structure and function.

Computational Methods for Protein Structure Prediction and Modeling

Academic Press

The seven-volume set LNCS 12137, 12138, 12139, 12140, 12141, 12142, and 12143 constitutes the proceedings of the 20th International Conference on Computational Science, ICCS 2020, held in Amsterdam, The Netherlands, in June 2020.* The total of 101 papers and 248 workshop papers presented in this book set were carefully reviewed and selected from 719 submissions (230 submissions to the main track and 489 submissions to the workshops). The papers were organized in topical sections named: Part I: ICCS Main Track Part II: ICCS Main Track Part III: Advances in High-Performance Computational Earth Sciences: Applications and Frameworks; Agent-Based Simulations, Adaptive Algorithms and Solvers; Applications of Computational Methods in Artificial Intelligence and Machine Learning; Biomedical and Bioinformatics Challenges for

Computer Science Part IV: Classifier Learning from Difficult Data; Complex Social Systems through the Lens of Computational Science; Computational Health; Computational Methods for Emerging Problems in (Dis-)Information Analysis Part V: Computational Optimization, Modelling and Simulation; Computational Science in IoT and Smart Systems; Computer Graphics, Image Processing and Artificial Intelligence Part VI: Data Driven Computational Sciences; Machine Learning and Data Assimilation for Dynamical Systems; Meshfree Methods in Computational Sciences; Multiscale Modelling and Simulation; Quantum Computing Workshop Part VII: Simulations of Flow and Transport: Modeling, Algorithms and Computation; Smart Systems: Bringing Together Computer Vision, Sensor Networks and Machine Learning; Software Engineering for Computational Science; Solving Problems with Uncertainties; Teaching Computational Science; UNcErtainty QUantIficatiOn for ComputationAl modeLs *The conference was canceled due to the COVID-19 pandemic. **Computational Methods**

for Protein Structure Prediction and Modeling Humana

This volume presents a diverse collection of methodologies used to study various problems at the protein sequence and structure level. The chapters in this book look at issues ranging from broad concepts like protein space to specifics like antibody modeling. Topics include point mutations, gene duplication, de novo emergence of new genes, pairwise correlated mutations, ancestral protein reconstruction, homology modelling, protein stability and dynamics, and protein-protein interactions. The book also covers a wide range of computational approaches, including sequence and structure alignments, phylogenies, physics-based and mathematical approaches, machine learning, and more. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and prerequisites, step-by-step, readily reproducible computational protocols (using command line or graphical user interfaces, sometimes including computer code), and

tips on troubleshooting and avoiding known pitfalls. Cutting-edge and authoritative, Computational Methods in Protein Evolution is a valuable resource that offers useful workflows and techniques that will help both novice and expert researchers working with proteins computationally.

Development of Structure-based Computational Methods for Prediction and Design of Protein-protein Interactions John Wiley & Sons

This book provides a comprehensive overview of modern computer-based techniques for analyzing the structure, properties and dynamics of biomolecules and biomolecular processes. It is organized in four main parts; the first one deals with methodology of molecular simulations; the second one with applications of molecular simulations; the third one introduces bioinformatics methods and the use of experimental information in molecular simulations; the last part reports on selected applications of molecular quantum mechanics. This second edition has been thoroughly revised and updated to include the latest progresses made in the respective field of research.

Computational Methods for Protein

Structure Prediction and Energy Minimization Springer Understanding sequence-structure relationships of proteins is a central theme of computational structural biology. To create accurate mapping between sequences and structures is a big computational challenge, because the inherent dynamics of protein molecules requires any structure to be seen as an ensemble containing a large number of structural states. In this thesis, I focus on developing new structural modeling methods representing two routes towards efficient sequence-structure mapping that are compatible with this ensemble view of structures. First, I will show that the relationships between the sequence and the structural ensemble of a protein can be revealed by breaking down the protein into constituent structural fragments, for which ensemble statistics can be obtained from the protein structure database. Second, sequence-structure relationships can be also extracted by combining explicit atomistic modeling of ensembles and statistical tools reducing the overall computational cost. Implications in structure

prediction, mutational analysis, and design of protein-interaction modulators will be presented and discussed, showing the great promise held by these methods in further improving the state-of-the-art in a broad spectrum of applications in computational structural biology.

Computational Methods for Protein Structure and Micro Ribonucleic Acid Target Prediction

CRC Press

This book covers elements of both the data-driven comparative modeling approach to structure prediction and also recent attempts to simulate folding using explicit or simplified models. Despite the unsolved mystery of how a protein folds, advances are being made in predicting the interactions of proteins with other molecules. Also rapidly advancing are the methods for solving the inverse folding problem, the problem of finding a sequence to fit a structure. This book focuses on the various computational methods for prediction, their successes and their limitations, from the perspective of their most well known practitioners.

Tesi Per Il Conseguimento Del Titolo Di Dottore Di Ricerca

Springer Science & Business Media

This book – in

conjunction with the volumes LNCS 8588 and LNAI 8589 – constitutes the refereed proceedings of the 10th International Conference on Intelligent Computing, ICIC 2014, held in Taiyuan, China, in August 2014. The 58 papers of this volume were carefully reviewed and selected from numerous submissions. The papers are organized in topical sections such as machine learning; neural networks; image processing; computational systems biology and medical informatics; biomedical informatics theory and methods; advances on bio-inspired computing; protein and gene bioinformatics : analysis, algorithms, applications.