Function Prediction

Quan Zou,Arun Kumar Sangaiah,Dariusz Mrozek

New Approaches of Protein Function Prediction from Protein Interaction Networks Jingyu Hou,2017-01-13 New Approaches of Protein Function Prediction from Protein Interaction Networks contains the critical aspects of PPI network based protein function prediction, including semantically assessing the reliability of PPI data, measuring the functional similarity between proteins, dynamically selecting prediction domains, predicting functions, and establishing corresponding prediction frameworks. Functional annotation of proteins is vital to biological and clinical research and other applications due to the important roles proteins play in various biological processes. Although the functions of some proteins have been annotated via biological experiments, there are still many proteins whose functions are yet to be annotated due to the limitations of existing methods and the high cost of experiments. To overcome experimental limitations, this book helps users understand the computational approaches that have been rapidly developed for protein function prediction. Provides innovative approaches and new developments targeting key issues in protein function prediction Presents heuristic ideas for further research in this challenging area

Machine Learning Techniques on Gene Function Prediction Quan Zou, Arun Kumar Sangaiah, Dariusz Mrozek, 2019-12-04

Protein Function Prediction for Omics Era Daisuke Kihara,2011-04-19 Gene function annotation has been a central question in molecular biology. The importance of computational function prediction is increasing because more and more large scale biological data, including genome sequences, protein structures, protein-protein interaction data, microarray expression data, and mass spectrometry data, are awaiting biological interpretation. Traditionally when a genome is sequenced, function annotation of genes is done by homology search methods, such as BLAST or FASTA. However, since these methods are developed before the genomics era, conventional use of them is not necessarily most suitable for analyzing a large scale data. Therefore we observe emerging development of computational gene function prediction methods, which are targeted to analyze large scale data, and also those which use such omics data as additional source of function prediction. In this book, we overview this emerging exciting field. The authors have been selected from 1) those who develop novel purely computational methods 2) those who develop function prediction methods which use omics data 3) those who maintain and update data base of function annotation of particular model organisms (E. coli), which are frequently referred

Protein Function Prediction Daisuke Kihara,2017-05-20 This volume presents established bioinformatics tools and databases for function prediction of proteins. Reflecting the diversity of this active field in bioinformatics, the chapters in this book discuss a variety of tools and resources such as sequence-, structure-, systems-, and interaction-based function prediction methods, tools for functional analysis of metagenomics data, detecting moonlighting-proteins, sub-cellular localization prediction, and pathway and comparative genomics databases. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, step-by-step instructions of how to use software and web resources, use cases, and tips on troubleshooting and avoiding known pitfalls. Thorough and cutting-edge, Protein Function Prediction: Methods and Protocols is a valuable and practical guide for using bioinformatics tools for investigating protein function

Prediction of Protein Structures, Functions, and Interactions Janusz M. Bujnicki,2008-12-23 The growing flood of new experimental data generated by genome sequencing has provided an impetus for the development of automated methods for predicting the functions of proteins that have been deduced by sequence analysis and lack experimental characterization. Prediction of Protein Structures, Functions and Interactions presents a comprehensive overview of methods for prediction of protein structure or function, with the emphasis on their availability and possibilities for their combined use. Methods of modeling of individual proteins, prediction of their interactions, and docking of complexes are put in the context of predicting gene ontology (biological process, molecular function, and cellular component) and discussed in the light of their contribution to the emerging field of systems biology. Topics covered include: first steps of protein sequence analysis and structure prediction automated prediction of protein function from sequence template-based prediction of three-dimensional protein structures: fold-recognition and comparative modelling template-free prediction of three-dimensional protein structures quality assessment of protein models prediction of Protein Structures, Functions and Interactions focuses on the methods that have performed well in CASPs, and which are constantly developed and maintained, and are freely available to academic researchers either as web servers or programs for local installation. It is an essential guide to the newest, best methods for prediction of protein structures and functions, for researchers and advanced students working in structural bioinformatics, protein chemistry, structural biology and drug discovery. **Protein Function Prediction Prediction Prediction Prediction on Protein Structures**.

Bayesian Markov Random Field Analysis for Integrated Network-based Protein Function Prediction Yiannis A. I. Kourmpetis, 2011

Cellular Function Prediction for Hypothetical Proteins Using High-throughput Data ,2003 We have developed an integrated probabilistic prediction method, which combines the information from protein-protein interactions, protein complexes, microarray gene-expression profiles and functional annotations for known proteins. Our approach differs from the other approaches to use high-throughput data in a variety of ways. First, we utilize the GO biological process functional annotation in comparison to the MIPS classification followed by others. Second, we incorporate information from multiple sources of high-throughput data, including genetic interactions, to develop a better model for function prediction. By incorporating information from the multiple sources of high-throughput data, we identify the parameters important for protein function prediction. Third, we estimate the probability for the proteins to have a function of interest by designing a new statistical method for function prediction. Fourth, our approach assigns multiple functions to the hypothetical proteins and allows confidence assessment, based on the supportive evidences from the high-throughput data. Our work demonstrates the power of integrating multiple sources of high-throughput data with biological functional annotations, in the function prediction for unknown proteins. In addition to this, we have also developed a Web server for function prediction in yeast as well as other organisms. We have applied our method to the Saccharomyces cerevisiae proteome and are able to assign function to 1548 out of the 2472 unannotated proteins in yeast with our approach.

Big Data Analytics in Genomics Ka-Chun Wong, 2016-10-24 This contributed volume explores the emerging intersection between big data analytics and genomics. Recent sequencing technologies have enabled high-throughput sequencing data generation for genomics resulting in several international projects which have led to massive genomic data accumulation at an unprecedented pace. To reveal novel genomic insights from this data within a reasonable time frame, traditional data analysis methods may not be sufficient or scalable, forcing the need for big data analytics to be developed for genomics. The computational methods addressed in the book are intended to tackle crucial biological guestions using big data, and are appropriate for either newcomers or veterans in the field. This volume offers thirteen peer-reviewed contributions, written by international leading experts from different regions, representing Argentina, Brazil, China, France, Germany, Hong Kong, India, Japan, Spain, and the USA. In particular, the book surveys three main areas: statistical analytics, computational analytics, and cancer genome analytics. Sample topics covered include: statistical methods for integrative analysis of genomic data, computation methods for protein function prediction, and perspectives on machine learning techniques in big data mining of cancer. Self-contained and suitable for graduate students, this book is also designed for bioinformaticians, computational biologists, and researchers in communities ranging from genomics, big data, molecular genetics, data mining, biostatistics, biomedical science, cancer research, medical research, and biology to machine learning and computer science. Readers will find this volume to be an essential read for appreciating the role of big data in genomics, making this an invaluable resource for stimulating further research on the topic.

R and Data Mining Yanchang Zhao, 2012-12-31 R and Data Mining introduces researchers, post-graduate students, and analysts to data mining using R, a free software environment for statistical computing and graphics. The book provides practical methods for using R in applications from academia to industry to extract knowledge from vast amounts of data. Readers will find this book a valuable guide to the use of R in tasks such as classification and prediction, clustering, outlier detection, association rules, sequence analysis, text mining, social network analysis, sentiment analysis, and more. Data mining techniques are growing in popularity in a broad range of areas, from banking to insurance, retail, telecom, medicine, research, and government. This book focuses on the modeling phase of the data mining process, also addressing data exploration and model evaluation. With three in-depth case studies, a guick reference guide, bibliography, and links to a wealth of online resources, R and Data Mining is a valuable, practical guide to a powerful method of analysis. Presents an introduction into using R for data mining applications, covering most popular data mining techniques Provides code examples and data so that readers can easily learn the techniques Features case studies in real-world applications to help readers apply the techniques in their work

Protein Function Prediction Using Phylogenomics, Domain Architecture Analysis, Data Integration, and Lexical Scoring Asis Hallab, 2015 Homology Molecular Modeling Rafael Trindade Maia, Rômulo Maciel de Moraes Filho, Magnólia De Araújo Campos, 2021-03-10 Homology modeling is an extremely useful and versatile technique that is gaining more and more space and demand in research in computational and theoretical biology. This book, "Homology Molecular Modeling -Perspectives and Applications", brings together unpublished chapters on this technique. In this book, 7 chapters are intimately related to the theme of molecular modeling, carefully selected and edited for academic and scientific readers. It is an indispensable read for anyone interested in the areas of bioinformatics and computational biology. Divided into 4 sections, the reader will have a didactic and comprehensive view of the theme, with updated and relevant concepts on the subject. This book was organized from researchers to researchers with the aim of spreading the fascinating area of molecular modeling by homology.

Introduction to Protein Structure Prediction Huzefa Rangwala, George Karypis, 2011-03-16 A look at the methods and algorithms used to predict proteinstructure A thorough knowledge of the function and structure of proteinsis critical for the advancement of biology and the life sciences aswell as the development of better drugs, higher-vield crops, andeven synthetic bio-fuels. To that end, this reference sheds lighton the methods used for protein structure prediction and reveals the key applications of modeled structures. This indispensable bookcovers the applications of modeled protein structures and unravelsthe relationship between pure sequence information andthree-dimensional structure, which continues to be one of thegreatest challenges in molecular biology. With this resource, readers will find an allencompassingexamination of the problems, methods, tools, servers, databases, and applications of protein structure prediction and they willacquire unique insight into the future applications of the modeledprotein structures. The book begins with a thorough introduction tothe protein structure prediction problem and is divided into fourthemes: a background on structure prediction, the prediction ofstructural elements, tertiary structure prediction, and functionalinsights. Within those four sections, the following topics arecovered: Databases and resources that are commonly used for proteinstructure prediction The structure prediction flagship assessment (CASP) and theprotein structure initiative (PSI) Definitions of recurring substructures and the computational approaches used for solving sequence problems Difficulties with contact map prediction and how sophisticated machine learning methods can solve those problems Structure prediction methods that rely on homology modeling, threading, and fragment assembly Hybrid methods that achieve high-resolution proteinstructures Parts of the protein structure that may be conserved and usedto interact with other biomolecules How the loop prediction problem can be used for refinement of the modeled structures The computational model that detects the differences betweenprotein structure and its modeled mutant Whether working in the field of bioinformatics or molecularbiology research or taking courses in protein modeling, readerswill find the content in this book invaluable.

Prediction of Protein Structure and the Principles of Protein Conformation G.D. Fasman, 2012-12-06 The prediction of the conformation of proteins has developed from an intellectual exercise into a serious practical endeavor that has great promise to yield new stable enzymes, products of pharmacological significance, and catalysts of great potential. With the application of predic tion gaining momentum in various fields, such as enzymology and immunology, it was deemed time that a volume be published to make available a thorough evaluation of present methods, for researchers in this field to expound fully the virtues of various algorithms, to open the field to a wider audience, and to offer the scientific public an opportunity to examine carefully its successes and failures. In this manner the practitioners of the art could better evaluate the tools and the output so that their expectations and applications could be more realistic. The editor has assembled chapters by many of the main contributors to this area and simultaneously placed their programs at three national resources so that they are readily available to those who wish to apply them to their personal interests. These algorithms, written by their originators, when utilized on pes or larger computers, can instantaneously take a primary amino

acid sequence and produce a two-or three-dimensional artistic image that gives satisfaction to one's esthetic sensibilities and food for thought concerning the structure and function of proteins. It is in this spirit that this volume was envisaged.

Interpretable Machine Learning Christoph Molnar,2020 This book is about making machine learning models and their decisions interpretable. After exploring the concepts of interpretability, you will learn about simple, interpretable models such as decision trees, decision rules and linear regression. Later chapters focus on general model-agnostic methods for interpreting black box models like feature importance and accumulated local effects and explaining individual predictions with Shapley values and LIME. All interpretation methods are explained in depth and discussed critically. How do they work under the hood? What are their strengths and weaknesses? How can their outputs be interpreted? This book will enable you to select and correctly apply the interpretation method that is most suitable for your machine learning project.

From Protein Structure to Function with Bioinformatics Daniel J. Rigden,2017-04-06 This book is about protein structural bioinformatics and how it can help understand and predict protein function. It covers structure-based methods that can assign and explain protein function based on overall folds, characteristics of protein surfaces, occurrence of small 3D motifs, protein-protein interactions and on dynamic properties. Such methods help extract maximum value from new experimental structures, but can often be applied to protein models. The book also, therefore, provides comprehensive coverage of methods for predicting or inferring protein structure, covering all structural classes from globular proteins and their membrane-resident counterparts to amyloid structures and intrinsically disordered proteins. The book is split into two broad sections, the first covering methods to generate or infer protein structure, the second dealing with structure-based function annotation. Each chapter is written by world experts in the field. The first section covers methods ranging from traditional homology modelling and fold recognition to fragment-based ab initio methods, and includes a chapter, new for the second edition, on structure prediction using evolutionary covariance. Membrane proteins interaction. The second section includes chapters covering functional diversity within protein folds and means to predict modes of protein and recurring motifs. Further chapters cover the key roles of protein dynamics in protein function and use of automated servers for function inference. The book concludes with two chapters covering case studies of structure prediction, based respectively on crystal structures and protein models, providing numerous examples of real-world usage of the methods mentioned previously. This book is targeted at postgraduate students and academic researchers. It is most obviously of interest to protein bioinformaticians and structural biologists, but should also serve as a guide to biologists more broadly by

Prediction, Learning, and Games Nicolo Cesa-Bianchi, Gabor Lugosi, 2006-03-13 This important text and reference for researchers and students in machine learning, game theory, statistics and information theory offers a comprehensive treatment of the problem of predicting individual sequences. Unlike standard statistical approaches to forecasting, prediction of individual sequences does not impose any probabilistic assumption on the data-generating mechanism. Yet, prediction algorithms can be constructed that work well for all possible sequences, in the sense that their performance is always nearly as good as the best forecasting strategy in a given reference class. The central theme is the model of prediction using expert advice, a general framework within which many related problems can be cast and discussed. Repeated game playing, adaptive data compression, sequential investment in the stock market, sequential pattern analysis, and several other problems are viewed as instances of the experts' framework and analyzed from a common nonstochastic standpoint that often reveals new and intriguing connections.

<u>Gene Prediction: Applying Ontology and Machine Learning (Volume II)</u> Casper Harvey,2023-09-26 Gene prediction refers to the process of identifying the regions of genomic DNA that encodes genes using computational methods. It is an important part of bioinformatics. Gene prediction is the first step for annotating large and contiguous sequences. It aids in identifying the essential elements of the genome including functional genes, intron, splicing sites, exon, and regulatory sites. It is also used in describing the individual genes based on their functions. Protein function prediction is an important part of genome annotation. Lately, high-throughput sequencing technologies have led to development of prediction methods. Gene ontology (60) is one of the databases that are available for identifying the functional properties of proteins. Research in this domain is now focused on efficiently predicting the G0 terms. Researches are ongoing on the use of machine learning algorithms for functional prediction as these algorithms use rule-based approaches to integrate large amounts of heterogeneous data and detect patterns. mSplicer, mGene, and CONTRAST are methods that use machine learning techniques for gene prediction. Gene prediction methods are widely used in fields like structural genomics, functional genomics, and genome studies. This book traces the progress of gene prediction and the application of ontology and machine learning. It is appropriate for students seeking detailed information in this area of study as well as for experts.

Novel Computational Methods for Accurate Quantitative and Qualitative Protein Function Prediction Kai Wang, 2005

Information-Theoretic Evaluation for Computational Biomedical Ontologies Wyatt Travis Clark,2014-01-23 The development of effective methods for the prediction of ontological annotations is an important goal in computational biology, yet evaluating their performance is difficult due to problems caused by the structure of biomedical ontologies and incomplete annotations of genes. This work proposes an information-theoretic framework to evaluate the performance of computational protein function prediction. A Bayesian network is used, structured according to the underlying ontology, to model the prior probability of a protein's function. The concepts of misinformation and remaining uncertainty are then defined, that can be seen as analogs of precision and recall. Finally, semantic distance is proposed as a single statistic for ranking classification models. The approach is evaluated by analyzing three protein function predictors of gene ontology terms. The work addresses several weaknesses of current metrics, and provides valuable insights into the performance of protein function prediction tools.

Decoding Function Prediction: Revealing the Captivating Potential of Verbal Expression

In a time characterized by interconnectedness and an insatiable thirst for knowledge, the captivating potential of verbal expression has emerged as a formidable force. Its power to evoke sentiments, stimulate introspection, and incite profound transformations is genuinely awe-inspiring. Within the pages of "Function **Prediction**," a mesmerizing literary creation penned by a celebrated wordsmith, readers set about an enlightening odyssey, unraveling the intricate significance of language and its enduring impact on our lives. In this appraisal, we shall explore the book is central themes, evaluate its distinctive writing style, and gauge its pervasive influence on the hearts and minds of its readership.

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