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Introduction to Bioinformatics in Medicine and Medical Systems

This section covers topics related to inferring gene function from expression data, genome sequence data, integrating expression data with other genome-wide data for functional annotation, functional study of specific molecular and pathway analysis, genome annotation and comparative genomics bioinformatics algorithm and tool development, RNAseq and microarray gene expression data analysis, gene regulatory network construction and Next-Generation Sequencing (NGS) analysis. Furthermore, this section covers topics related to translational bioinformatics, protein sequencing and classification, protein structure prediction, protein function analysis, protein interactions, protein subcellular localization prediction.

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The emerging advances of Bioinformatics have already contributed toward the establishment of better next generation medicine and medical systems by putting emphasis on improvement of prognosis, diagnosis and therapy of diseases including better management of medical systems. The purpose of this chapter is to explore ways by which the use of Bioinformatics and Smart Data Analysis will provide an overview and solutions to challenges in the fields of genomics, medicine and Health Informatics. The focus of this chapter would be on Smart Data Analysis and ways needed to filter out the noise. The chapter addresses challenges researchers and data analysts are facing in terms of the developed computational methods used to extract insights from NGS and high-throughput screening data. In this chapter the concept "Wise Data" is proposed reflecting the distinction between individual health and wellness on the one hand, and social improvement, cohesion and sustainability on the other, leading to more effective medical systems, healthier individuals and more socially cohesive societies.

Chapter 2

Bioinformatics: Applications and Implications 26

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This chapter describes the overview of bioinformatics; bioinformatics, data mining, and data visualization; bioinformatics and secretome analysis; bioinformatics, mass spectrometry, and chemical cross-linking reagents; bioinformatics and Software Product Line (SPL); bioinformatics and protein kinase; bioinformatics and MicroRNAs (miRNAs); and clinical bioinformatics and cancer. Bioinformatics is the application of computer technology to the management and analysis of biological data. Bioinformatics is an interdisciplinary research area that is the interface between biology and computer science. The primary goal of bioinformatics is to reveal the wealth of biological information hidden in the large amounts of data and obtain a clearer insight into the fundamental biology of organisms. Bioinformatics entails the creation and advancement of databases, algorithms, computational and statistical techniques, and theory to solve the formal and practical problems arising from the management and analysis of biological data.

Chapter 3

Protein Structure Prediction 48

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Abhijit Datta, Jhargram Raj College, India

The great disagreement between the number of known protein sequences and the number of experimentally determined protein structures indicate an enormous necessity of rapid and accurate protein structure prediction methods. Computational techniques such as comparative modeling, threading and *ab initio* modelling allow swift protein structure prediction with sufficient accuracy. The three phases of computational protein structure prediction comprise: the pre-modelling analysis phase, model construction and post-modelling refinement. Protein modelling is primarily comparative or *ab initio*. Comparative or template-based methods such as homology and threading-based modelling require structural templates for constructing the structure of a target sequence. The *ab initio* is a template-free modelling approach which proceeds by satisfying various physics-based and knowledge-based parameters. The chapter will elaborate on the three phases of modelling, the programs available for performing each, issues, possible solutions and future research areas.

Chapter 4

Proteomics in Personalized Medicine: An Evolution Not a Revolution 80

Srijan Goswami, Institute of Genetic Engineering, Badu, India

The idea of personalized medicine system is an evolution of holistic approach of treatment and in more evidence based manner. The chapter begins with an introduction of how body system works naturally and impact of modern medicine on overall health, followed by a historical background and brief review of literature providing the description that the concept of personalized medicine is not new but a very old ideology which stayed neglected until the development in the field of medical genetics, followed by the role of omics in modern medicine, the comparison of modern medicine and personalized medicine, medical concepts relevant to proteomics in personalized medicine, impact of proteomics in drug development and clinical safety and finally closing the chapter with future prospects and challenges of proteomics in personalized medicine.

Chapter 5

The Much Needed Security and Data Reforms of Cloud Computing in Medical Data Storage 99

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Cloud computing has shifted our old documents up into the clouds, with the advancement of technology. Fast-growing virtual document storage platforms provide amenities with minimal expense in the corporate society. Despite living in the 20th century, even the first world countries have issues with the maintenance of document storage. Cloud computing resolves this issue for business and clinic owners as it banishes the requirement of planning, provisioning, and allows corporations to advance their filing system according to service demands. Medical practices heavily, rely on document storage as; almost all information contained in medical files is stored in a printed format. Medical practices urgently need to revolutionize their storage standards, to keep up with the growing population. The traditional method of paper storage in medical practice has completely been obsolete and needs to improve in order to assist patients with faster diagnosis in critical situations. Obtaining Knowledge and sharing it is an important part of medical practice, so it needs immediate attention to reach its full service potential. This chapter has analyzed content from literature that highlights issues regarding data storage and recommends solution. This inquiry has found a useful tool that can be beneficial for the development of this problem which is, 'data mining' as it gives the option of predictive, and preventative health care options, when medical data is searched. The functionality and worthiness of each algorithm and methods are also determined in this study. By using cloud and big data services to improve the analysis of medical data in network of regional health information system, has huge advancements that assure convenient management, easy extension, flexible investment, and low requirements for low technical based private medical units.

Section 2

Bioinformatics in the Fields of Genomics and Proteomics as Applied to Medicine, Health Issues, and Medical Systems

This section covers topics related to computational systems biology, machine learning in protein fold recognition, integrative data analysis, structural class prediction of protein, functional study of specific molecular and pathway analysis, data mining in proteomics, homology detection and sequence alignment methods, protein expression analysis, protein sequencing and classification, molecular dynamics simulation, protein docking and drug design, homology detection and sequence alignment methods, multiscale network construction. Environment and health issues as related to integration of big data analytics with bioinformatics, integrated exposure modelling assimilation of exposure measurements and human biomonitoring, data statistics and big data analytics for exposome-wide association studies.

Chapter 6

Informatics and Data Analytics to Support Exposome-Based Discovery: Part 1 - Assessment of External and Internal Exposure 115

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This chapter provides a comprehensive overview of the state of the art and beyond regarding modelling and data analytics towards refined external and internal exposure assessment, for elucidating the human exposome. This includes methods for more accurate measurement of personal exposure (using wearable sensors) and for extrapolation to larger population groups (agent-based modelling). A key component in the modern risk and health impact assessment is the translation of external exposure into internal exposure metrics, accounting for age, gender, genetic and route of exposure dependent differences. The applicability of biokinetics covering a large chemical space is enhanced using quantitative structure activity relationships, especially when the latter are estimated using machine learning tools. Finally, comprehensive biomonitoring data interpretation and assimilation are supported by exposure reconstruction algorithms coupled with biokinetics

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Informatics and Data Analytics to Support Exposome-Based Discovery: Part 2 - Computational Exposure Biology..... 145

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This chapter aims at outlining the current state of science in the field of computational exposure biology and in particular at demonstrating how the bioinformatics techniques and algorithms can be used to support the association between environmental exposures and human health and the deciphering of the molecular and metabolic pathways of induced toxicity related to environmental chemical stressors. Examples of the integrated bioinformatics analyses outlined herein are given concerning exposure to airborne chemical mixtures, to organic compounds frequently found in consumer goods, and to mixtures of organic chemicals and metals through multiple exposure pathways. Advanced bioinformatics are coupled with big data analytics to perform studies of exposome-wide associations with putative adverse health outcomes. In conclusion, the chapter gives the reader an outline of the available computational tools and paves the way towards the development of future comprehensive applications that are expected to support efficiently exposome research in the 21st century.

Chapter 8

Transcriptomics to Metabolomics: A Network Perspective for Big Data..... 188

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A lot of omics data is generated in a recent decade which flooded the internet with transcriptomic, genomics, proteomics and metabolomics data. A number of software, tools, and web-servers have developed to analyze the big data omics. This review integrates the various methods that have been employed over the years to interpret the gene regulatory and metabolic networks. It illustrates random networks, scale-free networks, small world network, bipartite networks and other topological analysis which fits in biological networks. Transcriptome to metabolome network is of interest because of key enzymes identification and regulatory hub genes prediction. It also provides an insight into the understanding of omics technologies, generation of data and impact of in-silico analysis on the scientific community.

Chapter 9

Protein Docking and Drug Design 207

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Protein docking is integral to structure-based drug design and molecular biology. The recent surge of big data in biology, the demand for personalised medicines, evolving pathogens and increasing lifestyle-associated risks, asks for smart, robust, low-cost and high-throughput drug design. Computer-aided drug design techniques allow rapid screening of ultra-large chemical libraries within minutes. This is immensely necessary to the drug discovery pipeline, which is presently burdened with high attrition rates, failures, huge capital and time investment. With increasing drug resistance and difficult druggable targets, there is a growing need for novel drug scaffolds which is partly satisfied by fragment based drug design and *de novo* methods. The chapter discusses various aspects of protein docking and emphasises on its application in drug design.

Section 3

Big Data Analytics for Medical and Health informatics

This section covers topics related to health analytics and informatics, medical and health informatics by using “-omics” data, system biology, disease control, predictive model of disease state, translational medicine, drug design, combinatorial drug discovery, proteomics in personalized medicine, image processing including medical imaging, healthcare and healthcare delivery, healthcare policy research, healthcare outcomes research, monitoring and evaluation, hospital information system, Electronic Medical Record and Electronic Health Record, population health management, decision support systems, telemedicine, Human-Machine Interfaces, ICT, Ageing and Disability, Mobile technologies for Healthcare applications (m-Health), Evaluation and use of Healthcare IT, Health Knowledge Management, Healthcare Management and Information Systems, Software Systems in Medicine, Data Mining and Visualization, Virtual Healthcare Teams, e-Health for Public Health integrating genetics with e-health.

Chapter 10

Effective and Efficient Business Intelligence Dashboard Design: Gestalt Theory in Dutch Long-Term and Chronic Healthcare 243

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This research focuses on the design process of an effective and efficient dashboard which displays management information for an Electronic Health Record (EHR) in Dutch long-term and chronic healthcare. It presents the actual design and realization of a management dashboard for the YBoard 2.0 system, which is a popular solution on the Dutch market. The design decisions in this investigation were based on human perception and computer interaction theory, in particular Gestalt theory. The empirical interviews with medical professionals supplemented valuable additional insights into what the users wanted to see most of all in a dashboard in their daily practices. This study successfully shows how effective and efficient dashboard design can benefit from theoretical insights related to human perception and computer interaction such as Gestalt theory, in combination with integrated end user requirements from daily practices.

Chapter 11

Role of Online Data from Search Engine and Social Media in Healthcare Informatics..... 272

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Search engines and social media are two different online data sources where search engines can provide health related queries logs and Internet users' discuss their diseases, symptoms, causes, preventions and even suggest treatment by sharing their views, experiences and opinions on social media. This chapter hypothesizes that online data from Google and Twitter can provide vital first-hand healthcare information. An approach is provided for collecting twitter data by exploring contextual information gleaned from Google search queries logs. Furthermore, it is investigated that whether it is possible to use tweets to track, monitor and predict diseases, especially Influenza epidemics. Obtained results show that healthcare institutes and professional's uses social media to provide up-to date health related information and interact with public. Moreover, proposed approach is beneficial for extracting useful information regarding disease symptoms, side effects, medications and to track geographical location of epidemics affected area.

Chapter 12

An Optimized Semi-Supervised Learning Approach for High Dimensional Datasets..... 294

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The semi-supervised learning is one of the most interesting fields for research developments in the machine learning domain beyond the scope of supervised learning from data. Medical diagnostic process works mostly in supervised mode, but in reality, we are in the presence of a large amount of unlabeled samples and a small set of labeled examples characterized by thousands of features. This problem is known under the term "the curse of dimensionality". In this study, we propose, as solution, a new approach in semi-supervised learning that we would call Optim Co-forest. The Optim Co-forest algorithm combines the re-sampling data approach with two selection strategies. The first one involves selecting random subset of parameters to construct the ensemble of classifiers following the principle of Co-forest. The second strategy is an extension of the importance measure of Random Forest (RF). Experiments on high dimensional datasets confirm the power of the adopted selection strategies in the scalability of our method.

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Predicting patterns to extract knowledge can be a tough task but it is worth. When you want to accomplish that task you have to take your time analysing all the data you have and you have to adapt it to the algorithms and technologies you are going to use after analysing. So you need to know the type of data that you own. When you have finished making the analysis, you also need to know what you want to find out and, therefore, which methodologies you are going to use to accomplish your objectives. At the end of this chapter you can see a real case making all that process. In particular, a Classification problem is shown as an example when using machine learning methodologies to find out if a hospital patient should be admitted or not in Cardiology department.

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Selection of Pathway Markers for Cancer Using Collaborative Binary Multi-Swarm	
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Pathway information for cancer detection helps to find co-regulated gene groups whose collective expression is strongly associated with cancer development. In this paper, a collaborative multi-swarm binary particle swarm optimization (MS-BPSO) based gene selection technique is proposed that outperforms to identify the pathway marker genes. We have compared our proposed method with various statistical and pathway based gene selection techniques for different popular cancer datasets as well as a detailed comparative study is illustrated using different meta-heuristic algorithms like binary coded particle swarm optimization (BPSO), binary coded differential evolution (BDE), binary coded artificial bee colony (BABC) and genetic algorithm (GA). Experimental results show that the proposed MS-BPSO based method performs significantly better and the improved multi swarm concept generates a good subset of pathway markers which provides more effective insight to the gene-disease association with high accuracy and reliability.

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The diseases and health problems are concerns of managers of the Unified Health System has costs in more sophisticated care sector are high. The World Health Organization focused on prevention of chronic diseases to prevent millions of premature deaths in the coming years, bringing substantial gains

in economic growth by improving the quality of life. Few countries appear to be aimed at prevention, if not note the available knowledge and control of chronic diseases and may represent an unnecessary risk to future generations. Early diagnosis of these diseases is the first step to successful treatment in any age group. The objective is to build a model, from the establishment of a Bayesian network, for the early diagnosis of nursing to identify eating disorders bulimia and anorexia nervosa in adolescents, from the characteristics of the DSM-IV and Nursing Diagnoses The need for greater investment in technology in public health actions aims to increase the knowledge of health professionals, especially nurses, contributing to prevention, decision making and early treatment of problems.

Chapter 16

Image Processing Including Medical Liver Imaging: Medical Image Processing from Big Data

Perspective, Ultrasound Liver Images, Challenges..... 380

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Medical diagnosis has been gaining importance in everyday life. The diseases and their symptoms are highly varying and there is always a need for a continuous update of knowledge needed for the doctors. The diseases fall into different categories and a small variation of symptoms may leave to different categories of diseases. This is further supplemented by the medical analysts for a continuous treatment process. The treatment generally starts with a diagnosis and further goes through a set of procedures including X-ray, CT-scans, ultrasound imaging for qualitative analysis and diagnosis by doctors. A small level of error in disease identification introduces overhead in diagnosis and difficult in treatment. In such cases, an automated system that could retrieve medical images based on user's interest. This chapter deals with various techniques, methodologies that correspond to the classification problem in data analysis process and its methodological impacts to big data.

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