

Nearest Neighbor Classification in 3D Protein Databases

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Abstract

In molecular databases, structural classification is a basic task that can be successfully approached by nearest neighbor methods. The underlying similarity models consider spatial properties such as shape and extension as well as thematic attributes. We introduce 3D shape histograms as an intuitive and powerful approach to model similarity for solid objects such as molecules. Errors of measurement, sampling, and numerical rounding may result in small displacements of atomic coordinates. These effects may be handled by using quadratic form distance functions. An efficient processing of similarity queries based on quadratic forms is supported by a filter-refinement architecture. Experiments on our 3D protein database demonstrate the high classification accuracy of more than 90% and the good performance of the technique.

Keywords: 3D Protein Databases, Nearest Neighbor Classification, Geometric Similarity Search, Machine Learning

1 Introduction

One important task for modern database applications in the areas molecular biology, astronomy, mechanical engineering, medical imaging, and meteorology is efficient and accurate classification. In protein databases, each year a high number of new 3D structures of molecules is determined either by crystallography or by NMR techniques or by automated structure prediction. A basic question is to which class the new objects belong. The classes represent collections of objects that have characteristic properties in common and thus are similar, whereas different classes contain objects that have more or less strong dissimilarities. After classification, subsequent investigations may be guided by the class information: predictions of primary and secondary effects of drugs, docking prediction in general etc.

Typically, the classes are obtained from class information about objects that are already classified by exploiting domain and expert knowledge. Nearest neighbor classifiers, as a common approach, assign the class label of the most similar object in the previously classified database to the new object. As a basis for nearest neighbor classification, an appropriate similarity model has to be provided. In all of the mentioned applications, the geometric shape of the objects is

an important similarity criterion. Along with the geometry, also thematic attributes such as physical and chemical properties have an influence on the similarity of objects.

As for most real-world applications, the available data about 3D protein structures inherently suffer from errors, including errors of measurement, calibration, sampling errors, numerical rounding errors, displacements of reference frames, and small shifts as well as rotations of the entire object or of local details of the shapes. Although no full invariance against rotations is required if the objects are already provided in a standardized orientation, these errors have to be taken into account. In this paper, we introduce a flexible similarity model that considers these problems of local inaccuracies and may be adapted by the users to their specific requirements or individual preferences.

The remainder of this introduction surveys related work from molecular biology, machine learning, and geometric similarity search. In Section 2, we introduce the components of our similarity model: 3D shape histograms for object representation, and a flexible similarity distance function. Due to the large and increasing size of current databases, the performance of query processing is an important task and, therefore, we present an efficient multistep system architecture in Section 3. The experimental results concerning the effectiveness and efficiency of our technique are presented in Section 4, and Section 5 concludes the paper.

1.1 Classification in Protein Databases

Structural classification schemes for protein databases are already available. In many systems, classifying new objects when inserting them into the database requires supervision by experts that are very experienced and have a deep knowledge of the domain of molecular biology. What is desired, is an efficient classification algorithm that may act as a fast filter for further investigation and that may be restricted e.g. to geometric aspects.

A sophisticated classification is available from the FSSP database (*Families of Structurally Similar Proteins*) generated by the DALI system (Holm and Sander 1994) (Holm and Sander 1998). The similarity of two proteins is based on their secondary structure. The evaluation of a pair of proteins is very expensive, and query processing for a single molecule

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Data Classification Charu C. Aggarwal, 2014-07-25 Comprehensive Coverage of the Entire Area of Classification Research on the problem of classification tends to be fragmented across such areas as pattern recognition database data mining and machine learning Addressing the work of these different communities in a unified way *Data Classification Algorithms and Applications* explores the underlying *Database Modeling for Industrial Data Management: Emerging Technologies and Applications* Ma, Zongmin, 2005-12-31 This book covers industrial databases and applications and offers generic database modeling techniques Provided by publisher *3D Shape Analysis* Hamid Laga, Yulan Guo, Hedi Tabia, Robert B. Fisher, Mohammed Bennamoun, 2019-01-07 An in depth description of the state of the art of 3D shape analysis techniques and their applications This book discusses the different topics that come under the title of 3D shape analysis It covers the theoretical foundations and the major solutions that have been presented in the literature It also establishes links between solutions proposed by different communities that studied 3D shape such as mathematics and statistics medical imaging computer vision and computer graphics The first part of 3D Shape Analysis Fundamentals Theory and Applications provides a review of the background concepts such as methods for the acquisition and representation of 3D geometries and the fundamentals of geometry and topology It specifically covers stereo matching structured light and intrinsic vs extrinsic properties of shape Parts 2 and 3 present a range of mathematical and algorithmic tools which are used for e g global descriptors keypoint detectors local feature descriptors and algorithms that are commonly used for the detection registration recognition classification and retrieval of 3D objects Both also place strong emphasis on recent techniques motivated by the spread of commodity devices for 3D acquisition Part 4 demonstrates the use of these techniques in a selection of 3D shape analysis applications It covers 3D face recognition object recognition in 3D scenes and 3D shape retrieval It also discusses examples of semantic applications and cross domain 3D retrieval i e how to retrieve 3D models using various types of modalities e g sketches and or images The book concludes with a summary of the main ideas and discussions of the future trends 3D Shape Analysis Fundamentals Theory and Applications is an excellent reference for graduate students researchers and professionals in different fields of mathematics computer science and engineering It is also ideal for courses in computer vision and computer graphics as well as for those seeking 3D industrial commercial solutions *Three-Dimensional Model Analysis and Processing* Faxin Yu, Zheming Lu, Hao Luo, Pinghui Wang, 2011-02-03 With the increasing popularization of the Internet together with the rapid development of 3D scanning technologies and modeling tools 3D model databases have become more and more common in fields such as biology chemistry archaeology and geography People can distribute their own 3D works over the Internet search and download 3D model data and also carry out electronic trade over the Internet However some serious issues are related to this as follows 1 How to efficiently transmit and store huge 3D model data with limited bandwidth and storage capacity 2 How to prevent 3D works from being

pirated and tampered with 3 How to search for the desired 3D models in huge multimedia databases This book is devoted to partially solving the above issues Compression is useful because it helps reduce the consumption of expensive resources such as hard disk space and transmission bandwidth On the downside compressed data must be decompressed to be used and this extra processing may be detrimental to some applications 3D polygonal mesh with geometry color normal vector and texture coordinate information as a common surface representation is now heavily used in various multimedia applications such as computer games animations and simulation applications To maintain a convincing level of realism many applications require highly detailed mesh models However such complex models demand broad network bandwidth and much storage capacity to transmit and store To address these problems 3D mesh compression is essential for reducing the size of 3D model representation

Cumulated Index Medicus, 1992 **Image and Video Retrieval** Michael S. Lew, Nicu Sebe, John P. Eakins, 2003-08-02 This book constitutes the refereed proceedings of the International Conference on Image and Video Retrieval CIVR 2002 held in London UK in July 2002 The 30 revised full papers presented together with an introduction by the volume editors were carefully reviewed and selected from 82 submissions The papers are organized in topical sections on image retrieval modeling feature based retrieval semantics and learning video retrieval and evaluation and benchmarking

Proceedings Thomas Lengauer, 1999 **Preclinical Development Handbook** Shayne Cox Gad, 2008-03-21 A clear straightforward resource to guide you through preclinical drug development Following this book's step by step guidance you can successfully initiate and complete critical phases of preclinical drug development The book serves as a basic comprehensive reference to prioritizing and optimizing leads dose formulation ADME pharmacokinetics modeling and regulations This authoritative easy to use resource covers all the issues that need to be considered and provides detailed instructions for current methods and techniques Each chapter is written by one or more leading experts in the field These authors representing the many disciplines involved in preclinical toxicology screening and testing give you the tools needed to apply an effective multidisciplinary approach The editor has carefully reviewed all the chapters to ensure that each one is thorough accurate and clear Among the key topics covered are Modeling and informatics in drug design Bioanalytical chemistry Absorption of drugs after oral administration Transporter interactions in the ADME pathway of drugs Metabolism kinetics Mechanisms and consequences of drug drug interactions Each chapter offers a full exploration of problems that may be encountered and their solutions The authors also set forth the limitations of various methods and techniques used in determining the safety and efficacy of a drug during the preclinical stage This publication should be readily accessible to all pharmaceutical scientists involved in preclinical testing enabling them to perform and document preclinical safety tests to meet all FDA requirements before clinical trials may begin **Chemical Identification and its Quality Assurance** Boris L. Milman, 2013-06-17 This is the first book to show how to apply the principles of quality assurance to the identification of analytes qualitative chemical analysis After presenting the principles of identification and metrological basics the author

focuses on the reliability and the errors of chemical identification This is then applied to practical examples such as EPA methods EU FDA or WADA regulations Two whole chapters are devoted to the analysis of unknowns and identification of samples such as foodstuffs or oil pollutions Essential reading for researchers and professionals dealing with the identification of chemical compounds and the reliability of chemical analysis **Essays in Bioinformatics** David S. Moss, Sibila Jelaska, Sándor Pongor, 2005

Advances in Spatial Databases Ralf H. Güting, Dimitris Papadias, Fred Lochovsky, 2003-05-21 This book constitutes the refereed proceedings of the 6th International Symposium on Spatial Databases SSD 99 held in Hong Kong China in July 1999 The 17 revised full papers presented were carefully selected from 55 submissions Also included are short papers corresponding to three invited talks and industrial applications presentations The papers are organized in chapters on multi resolution and scale indexing moving objects and spatio temporal data spatial mining and classification spatial join uncertainty and geological hypermaps and industrial and visionary application track

ICT Innovations 2009 Danco Davcev, Jorge Marx Gómez, 2010-01-06 This book is the result of the first International Conference ICT Innovations 2009 The ICT Innovations conference is the primary scientific action of the Macedonian Society on Information and Communication Technologies ICT ACT It promotes the publication of scientific results of the international community related to innovative fundamental and applied research in ICT Today ICT has enlarged its horizons and it is practiced under multidisciplinary contexts that introduce new challenges to theoretical and technical approaches The ICT Innovations 2009 conference gathered academics professionals and practitioners reporting their valuable experiences in developing solutions and systems in the industrial and business arena especially innovative commercial implementations novel applications of technology and experience in applying recent research advances to practical situations in any ICT areas The conference focuses on issues concerning a variety of ICT fields like Multimedia Information Systems Artificial Intelligence Pervasive and Ubiquitous Computing Eco and Bio Informatics Internet and Web Applications and Services Wireless and Mobile Communications and Services Computer Networks Security and Cryptography Distributed Systems GRID and Cloud Computing ICT Innovations 2009 Conference was held in Ohrid Macedonia in September 28-30 2009 Local arrangements provided by the members of the Macedonian Society on Information and Communication Technologies ICT ACT mainly consisting of teaching and research staff of Computer Science Department at Faculty of Electrical Engineering and Information Technologies and Institute of Informatics at Faculty of Natural Sciences both at Ss Cyril and Methodius University in Skopje Macedonia **Advances in Geometric Modeling and Processing** Falai Chen, Bert Jüttler, 2008-04-30 Geometric Modeling and Processing GMP is a biennial international conference on geometric modeling simulation and computing which provides researchers and practitioners with a forum for exchanging new ideas discussing new applications and presenting new solutions Previous GMP conferences were held in Pittsburgh 2006 Beijing 2004 Tokyo 2002 and Hong Kong 2000 This the 5th GMP conference was held in Hangzhou one of the most beautiful cities in China GMP 2008 received 113

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Machine Learning Abdelhamid Mellouk, Abdennasser Chebira, 2009-01-01 Machine Learning can be defined in various ways related to a scientific domain concerned with the design and development of theoretical and implementation tools that allow building systems with some Human Like intelligent behavior Machine learning addresses more specifically the ability to improve automatically through experience

Hybrid Artificial Intelligence Systems Emilio Corchado, Xindong Wu, Erkki Oja, Bruno Barua, 2009-06-22 The 4th International Conference on Hybrid Artificial Intelligence Systems HAIS 2009 as the name suggests attracted researchers who are involved in developing and applying symbolic and sub-symbolic techniques aimed at the construction of highly robust and reliable problem solving techniques and bringing the most relevant achievements in this field Hybrid intelligent systems have become increasingly popular given their capabilities to handle a broad spectrum of real world complex problems which come with inherent imprecision uncertainty and vagueness high dimensionality and nonstationarity These systems provide us with the opportunity to exploit existing domain knowledge as well as raw data to come up with promising solutions in an effective manner Being truly multidisciplinary the series of HAIS conferences offers an interesting research forum to present and discuss the latest theoretical advances and real world applications in this exciting research field This volume of Lecture Notes in Artificial Intelligence LNAI includes accepted papers presented at HAIS 2009 held at the University of Salamanca Salamanca Spain June 2009 Since its inception the main aim of the HAIS conferences has been to establish a broad and interdisciplinary forum for hybrid artificial intelligence systems and associated learning paradigms which are playing increasingly important roles in a large number of application areas

Proceedings of the ... ACM CIKM, 2002

Pattern Recognition and Image Analysis Sameer Singh, Maneesha Singh, Chid Apte, Petra Pernert, 2005-08-17 The two volume set LNCS 3686 and LNCS 3687 constitutes the refereed proceedings of the Third International Conference on Advances in Pattern Recognition ICAPR 2005 held in Bath UK in August 2005 The papers submitted to ICAPR 2005 were thoroughly reviewed by up to three referees per paper and less than 40% of the submitted papers were accepted The first volume includes 73 contributions related to Pattern Recognition and Data Mining which included papers from the tracks of pattern recognition methods knowledge and learning and data mining topics addressed are pattern recognition data mining signal processing and OCR document analysis The second volume

contains 87 contributions related to Pattern Recognition and Image Analysis which included papers from the applications track and deals with security and surveillance biometrics image processing and medical imaging It also contains papers from the Workshop on Pattern Recognition for Crime Prevention **Encyclopedia of Data Warehousing and Mining** Wang, John, 2005-06-30 Data Warehousing and Mining DWM is the science of managing and analyzing large datasets and discovering novel patterns and in recent years has emerged as a particularly exciting and industrially relevant area of research Prodigious amounts of data are now being generated in domains as diverse as market research functional genomics and pharmaceuticals intelligently analyzing these data with the aim of answering crucial questions and helping make informed decisions is the challenge that lies ahead The Encyclopedia of Data Warehousing and Mining provides a comprehensive critical and descriptive examination of concepts issues trends and challenges in this rapidly expanding field of data warehousing and mining DWM This encyclopedia consists of more than 350 contributors from 32 countries 1 800 terms and definitions and more than 4 400 references This authoritative publication offers in depth coverage of evolutions theories methodologies functionalities and applications of DWM in such interdisciplinary industries as healthcare informatics artificial intelligence financial modeling and applied statistics making it a single source of knowledge and latest discoveries in the field of DWM **Image and Video Retrieval** Wee-Kheng Leow, Michael S. Lew, Tat-Seng Chua, Wei-Ying Ma, Lekha Chaisorn, Erwin M. Bakker, 2005-07-14 It was our great pleasure to host the 4th International Conference on Image and Video Retrieval CIVR at the National University of Singapore on 20 22 July 2005 CIVR aims to provide an international forum for the discussion of research challenges and exchange of ideas among researchers and practitioners in image video retrieval technologies It addresses innovative research in the broad eld of image and video retrieval A unique feature of this conference is the high level of participation by researchers from both academia and industry Another unique feature of CIVR this year was in its format it o ered both the traditional oral presentation sessions as well as the short presentation cum poster sessions The latter provided an informal alternative forum for animated discussions and exchanges of ideas among the participants We are pleased to note that interest in CIVR has grown over the years The number of submissions has steadily increased from 82 in 2002 to 119 in 2003 and 125 in 2004 This year we received 128 submissions from the international communities with 81 63 3% from Asia and Australia 25 19 5% from Europe and 22 17 2% from North America After a rigorous review process 20 papers were accepted for oral presentations and 42 papers were accepted for poster presentations In addition to the accepted submitted papers the program also included 4 invited papers 1 keynote industrial paper and 4 invited industrial papers Altogether we o ered a diverse and interesting program addressing the current interests and future trends in this area **State-of-the-Art in Content-Based Image and Video Retrieval** Remco C. Veltkamp, Hans Burkhardt, Hans-Peter Kriegel, 2013-04-17 Images and video play a crucial role in visual information systems and multimedia There is an extraordinary number of applications of such systems in entertainment business art engineering and science

Such applications often involved large image and video collections and therefore searching for images and video in large collections is becoming an important operation. Because of the size of such databases efficiency is crucial. We strongly believe that image and video retrieval need an integrated approach from fields such as image processing, shape processing, perception, database indexing, visualization, and querying etc. This book contains a selection of results that was presented at the Dagstuhl Seminar on Content Based Image and Video Retrieval in December 1999. The purpose of this seminar was to bring together people from the various fields in order to promote information exchange and interaction among researchers who are interested in various aspects of accessing the content of image and video data. The book provides an overview of the state of the art in content based image and video retrieval. The topics covered by the chapters are integrated system aspects as well as techniques from image processing, computer vision, multimedia databases, graphics, signal processing, and information theory. The book will be of interest to researchers and professionals in the fields of multimedia, visual information, database systems, computer vision, and information retrieval.

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