

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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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

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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

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3D Object Processing Jean-Luc Dugelay, Atilla Baskurt, Mohamed Daoudi, 2008-06-03 The arrival and continuing evolution of high quality 3D objects has been made possible by recent progress in 3D scanner acquisition and 3D graphics rendering With this increasing quality comes a corresponding increase in the size and complexity of the data files and the necessity for advances in compression techniques Effective indexing to facilitate the retrieval of the 3D data is then required to efficiently store search and recapture the objects that have been compressed The application of 3D images in fields such as communications medicine and the military also calls for copyright protection or watermarking to secure the data for transmission Written by expert contributors this timely text brings together the three important and complementary topics of compression retrieval and watermarking techniques for 3D objects 3D object processing applications are developing rapidly and this book tackles the challenges and opportunities presented focusing on the secure transmission sharing and searching of 3D objects on networks and includes an introduction to the commonly used 3D representation schemes the characteristics advantages and limitations of polygonal meshes surface based models and volumetric models 3D compression techniques the 3D coding and decoding schemes for reducing the size of 3D data to reduce transmission time and minimize

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pullman family lives here in a town house it s in present day upper manhattan in new york city beecher prep auggie s middle school is within walking distance from home