

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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Database Modeling for Industrial Data Management: Emerging Technologies and Applications Ma, Zongmin,2005-12-31

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