

ALGORITHMS AND HARDNESS RESULTS IN COMPUTATIONAL HOMOLOGY

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ABSTRACT

In this thesis, we address various issues concerning characterizing topological features in computation.

First, we define metrics on homology classes. This definition uses the discrete metric and the induced geodesic distance. A polynomial algorithm is provided to compute these measure. Besides, this work leads to the definition and algorithm of a canonical basis of the homology group, namely, the optimal homology basis. A straightforward algorithm and an improved algorithm are given.

Second, we discuss the problem of homology localization, namely, localizing a homology class with a cycle which is concise in geometry. This problem is posed as an optimization problem. Different objective function is discussed. For the volume function, we show that the problem is NP-hard to approximate within constant factor. Other objective functions are also discussed, namely, the diameter and the radius.

Third, we study the problem of enriching persistent homology. The objective is to reveal structural relationship between persistent homology classes by computing canonical representative cycles. Various definitions are provided basing on an extension of persistent homology. However, it has been proven that these definitions are not stable with regard to the change of filter function.

Fourth, we apply computation topology method in ribosome drug docking problem. More specifically, we compute the pockets/cavities relating to the drug docking sites. Interesting insights about ribosome are revealed by our work. However, the results are not specific enough for studying drug docking sites.