Approximation of knowledge-based potential function using b-splines in discrimination of native structure

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Abstract: Proteins are functional molecules in the cells. The function of proteins is dictated by its structure. There is a large gap between known sequence and structure of proteins. Therefore, one of the most important problems is the prediction of protein structure. It is generally assumed that proteins take the minimum energy. So, at first, we need to define energy function. Knowledge-based potentials are simplified potentials designed to improve the quality of the protein models. Actually, these potentials are energy functions extracted from the analysis of databases of protein structures. By calculating the total energy of each structure, decoy structures should be ranked according to their closeness to the native structure. In addition, it is assumed that the difference in energy between a decoy structure and the corresponding native structure is linearly related to the distance between the two structures [1]. To determine the distance between two structures, commonly four metrics are defined: Root mean square deviation (RMSD), global distance test where TS stands for total score (GDT-TS), Q is a distance measure that quantifies the changes of a contact map between two models for the same structure, and MT is corresponding variant of FlexE, and FlexE is a new measure of similarity between protein structures that is introduced as an attempt to distinguish those changes that are biologically relevant. Note that GDT-TS is a quantity between 0 and 1, with low values corresponding to low resemblances, and high values (close to or equal to 1) indicating that the two models are highly similar. This similarity measure converts into a distance by considering GDT-TS* = 1- GDT-TS and likely Q* = 1-Q [1]. In this study, we interpolate energy functions using b-splines. The b-spline functions have considerable properties, e.g. the b-spline curve is a piecewise curve with each component a curve of degree p, allows us to design complex shapes with lower degree polynomials.

Keywords: Knowledge-based Potential; B-spline

References

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