

Protein Scoring Functions: Empiricism, Optimization and Optimism

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Abstract

Protein force fields and scoring functions do not have to be dreary tables of numbers which scare students. Instead, they can be entertaining creations coming from an optimization calculation, if one has the right quantity to optimize. We will discuss building a score function for the limited case of protein threading and how this can be done without serious physics or hiding behind a Boltzmann relation. Furthermore, how one can use optimization methods to improve protein sequence to structure alignments as might be used for protein threading or protein modeling in general.