Application of Tensor Networks for Rapid Protein-Protein Docking

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Abstract

Protein-protein docking is a complex problem in the study of molecular interactions, with significant implications for drug design and biological research. In this work, we focus on improving protein docking through tensor networks with Tensor Cross Interpolation (TCI) techniques that are highly effective for estimating high-rank tensor functions. Tensor networks within the docking process efficiently handle the high-dimensional score functions characteristic of protein docking, enabling faster convergence to optimal docking poses. This optimization is agnostic to initial conditions, making it well-suited for complex biological systems that involve statistical interaction landscapes with numerous local minima. By incorporating tensor networks, our approach accelerates the docking process and enhances the accuracy of identifying biologically relevant protein-protein interactions. Our method demonstrates significant potential for improving the speed and precision of protein-protein docking, contributing to the advancement of computational biology and drug discovery.