Capturing Surface Complementarity in Proteins using Unsupervised Learning and Robust Curvature Measure

Abhijit Gupta[1] and Arnab Mukherjee[1]

[1]Indian Institute of Science Education Research Pune Centre of Excellence in Epigenetics

November 10, 2021

Abstract

The structure of a protein plays a pivotal role in determining its function. Often, the protein surface's shape and curvature dictate its nature of interaction with other proteins and biomolecules. However, marked by corrugations and roughness, a protein's surface representation poses significant challenges for its curvature-based characterization. In the present study, we employ unsupervised machine learning to segment the protein surface into patches. To measure the surface curvature of a patch, we present an algebraic sphere fitting method that is fast, accurate, and robust. Moreover, we use local curvatures to show the existence of "shape complementarity" in protein-protein, antigen-antibody, and protein-ligand interfaces. We believe that the current approach could help understand the relationship between protein structure and its biological function and can be used to find binding partners of a given protein.

Hosted file

SurfaceCurvature_MS_Proteins.docx available at https://authorea.com/users/445509/articles/545010-capturing-surface-complementarity-in-proteins-using-unsupervised-learning-and-robust-curvature-measure