A Machine Learning approach to Biophysics of proteins

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Abstract

Introduction: Computational prediction of protein structure is one of the most promising tools for de novo protein design. Despite significant improvements in this area, most of the tools do not share the same success. The main challenge in the computational design of proteins is the Inverse Protein Folding problem which connects the hierarchy of structures in one protein. Hence, there is an as-yet unmet need for the development of tools and methodology of protein design.

Methods: In Machine Learning approaches, protein descriptors are either obtained experimentally or computationally. Then suitable models are selected based on the nature of the problem (i.e. classification, clustering, and regression). Finally, the results will be investigated using Biophysical golden standard methods.

Results and discussion: The success of a computational tool is typically based upon: (1) Biophysical model for describing proteins and (2) prediction algorithm which works on top of the Biophysical model. Machine Learning fits the scope of the second phase and helps in the determination of Biophysical parameters, sequence, and structure. Accuracy of Machine Learning approaches heavily depends on Biophysical models and there is an urgent need for Biophysical protein descriptor indices.

Conclusion: Despite the challenges facing in the utilization of Machine Learning approaches in Biophysics, it successfully created reliable solutions for designing customized proteins. In this seminar it would be discussed that how designing better Biophysical descriptors of proteins, results in accuracy and efficiency improvements in Machine Learning approaches.

Keywords: Computational protein design, Biophysical protein models, Machine Learning

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