

Study of the effectiveness of SVMs methods for the prediction of protein ω angles

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In protein structure prediction, the relationship between sequence and structure is essential to understand, but lacks clear rules. The prediction of protein backbone dihedral angles ϕ and ψ from their sequences has been widely studied in the literature, but the prediction of ω angles has been much less explored because it presents more difficulties, in particular since these angles vary in narrower intervals than the other dihedral angles of the backbone. Nevertheless, the analysis of protein structure computation from local geometry information has shown that variations in stereochemistry are essential to consider (da Rocha et al., 2024), and in particular, variations in ω torsion angles. Therefore, we are exploring the use of kernel classification methods to predict ω angle values from the protein’s primary sequence (Guermeur, 2012). Our prediction results show that SVMs (Support Vector Machine) methods are effective for datasets composed of proteins displaying sequence alignment, however, our results are more modest for datasets composed of proteins of low sequence identity belonging to the same CATH family. We also observed that when we take sequence of peptides restricted to smaller values of B factors, most of our predictions it improves.

References:

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