



Advances in Protein Prediction: From Sequence to Structure and Function

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Description

Proteins are the workhorses of the cell, performing a wide variety of functions, from catalyzing chemical reactions to transmitting signals within and between cells. Understanding protein structure and function is essential for a range of fields, including drug discovery, biotechnology, and molecular biology. Protein prediction, the process of inferring protein structure and function from sequence data, has undergone tremendous advances in recent years. In this manuscript, we review the state-of-the-art in protein prediction, focusing on the latest techniques for predicting protein structure, function, and interactions. Protein prediction is a crucial area of research in the life sciences. The ability to predict protein structure and function from sequence data can provide insights into protein function, disease mechanisms, and potential drug targets. In recent years, advances in machine learning and bioinformatics have led to significant improvements in protein prediction, enabling researchers to predict protein structure and function with increasing accuracy. One of the major areas of protein prediction is protein structure prediction. The three-dimensional structure of a protein is critical for its function, and predicting protein structure from sequence data has been a long-standing challenge in the field. The latest techniques for protein structure prediction include deep learning methods, such as neural networks and Convolutional Neural Networks (CNNs), as well as

physics-based modeling methods, such as molecular dynamics simulations.

Deep learning methods have shown promise in predicting protein structure, particularly when used in combination with experimental data. For example, AlphaFold, a deep learning-based method developed by Deep Mind, was able to predict protein structure with unprecedented accuracy in the recent CASP13 and CASP14 competitions. AlphaFold uses a combination of neural networks and physical models to predict protein structure, and its success has led to a renewed interest in using deep learning methods for protein structure prediction. In addition to deep learning methods, physics-based modeling methods, such as molecular dynamics simulations, have also been used for protein structure prediction. These methods simulate the physical interactions between atoms in a protein to predict its three-dimensional structure. While these methods can be computationally intensive, they have the potential to accurately predict protein structure without the need for experimental data. In addition to predicting protein structure, predicting protein function is also an important area of research. Protein function is determined by the specific interactions between the protein and other molecules in the cell, and predicting these interactions from sequence data can provide insights into protein function and potential drug targets. Machine learning methods, such as Support Vector Machines (SVMs) and random forests, have been used to predict protein function from sequence data. These methods use known examples of proteins with a particular function to train a model that can predict the function of unknown proteins.

Finally, predicting protein-protein interactions is another critical area of protein prediction. Proteins often function by interacting with other proteins in the cell, and predicting these interactions can provide insights into protein function and potential drug targets. Deep learning methods, such as CNNs and Recurrent Neural Networks (RNNs), have been used to predict protein-protein interactions from sequence data. These methods use known examples of protein-protein interactions to train a model that can predict the likelihood of interaction between two proteins. Protein prediction is a rapidly evolving field, with new techniques and methods being developed all the time. Advances in machine learning and bioinformatics have enabled researchers to predict protein structure, function, and interactions with increasing accuracy. As these techniques continue to improve, we can expect to gain deeper insights into the fundamental workings of cells and develop new drugs and therapies to treat a range of diseases.

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