DeepSF: Deep Convolutional Neural Network for Mapping Protein Sequences to Folds

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ABSTRACT

Predicting the fold of a protein from its sequence is a challenging and important problem in bioinformatics. In this work, we developed the first deep learning method that can directly classify any protein sequence of arbitrary length into 1,195 known protein folds in the Structural Classification of Proteins (SCOP) database [1]. The method uses one-dimensional convolutional neural networks (1D-CNN) to automatically extract features from raw protein sequence information and compose them to high-level features to predict protein folds, achieving a classification accuracy of 73% on an independent test dataset. This novel machine learning approach is different from traditional alignment methods that rely on the known folds of homologous proteins to recognize the fold of a target protein. It is also more accurate than HHSearch - a top protein profile-profile alignment method in recognizing folds of proteins that have little sequence similarity with proteins with known folds. Moreover, the deep learning method overcomes the shortcoming of the previous machine learning methods that can only classify proteins into dozens of pre-selected folds due to methodological limitations. The hidden features extracted by the deep learning method provide a new semantic representation of proteins that can be used in other protein analysis tasks such as protein clustering and comparison.

CCS CONCEPTS

• **Bioinformatics** → **Protein folding** •

KEYWORDS

Protein fold classification, deep learning, convolutional neural network

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