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An improved deep learning method for predicting DNA-binding proteins based on contextual features in amino acid sequences

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ABSTRACT

With the explosively increased amount of newly discovered proteins, predicting the function of these proteins from amino acid sequencesis becoming one of the main challenges in functional annotation of genomes. Nowadays a number of computational approaches have been developed to predict DNA-binding proteins effectively and accurately from amino acid sequences, such as SVM, DNABP and CNN-RNN. However, these methods do not consider the context in amino acid sequences, which makes it difficult for them to capture sequence features adequately. In this paper, we propose CNN-BiLSTM, a new method for predicting DNA-binding proteins, elaborately reconciling convolution neural network and bi-directional long short-term memory recurrent neural network. CNN-BiLSTM can explore the potential contextual relationships of amino acid sequences to obtain more features than traditional models. The experimental results show that the predication accuracy of the proposed CNN-BiLSTM method on the test set is 96.5%, which is 7.8% higher than that of SVM, 9.6% higher than that of DNABP and 3.7% higher than that of CNN-RNN respectively. Being tested on 20, 000 independent samples provided by UniProt that weren't involved in model training, the accuracy of CNN-BiLSTM is 94.5%, which is 12% higher than that of SVM, 4.9% higher than that of DNABP and 4% higher than that of CNN-RNN respectively. The model training process is visualized and compared with that of CNN-RNN, and it is found that the training process of CNN-BiLSTMsupport better generalization from the training data set, which shows that CNN-BiLSTM has a wider range of adaptations to protein sequences. On the independent samples set, CNN-BiLSTM presents better credibility, for its predicted scores are closer to the labels of the samples than those of CNN-RNN. Therefore, the proposed CNN-BiLSTM is a more powerful method for identifying DNA-binding proteins.

EXTERNAL LINK

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model structure.pdf

GUIDELINES

This is a method of recognizing DNA binding proteins by deep learning.

MATERIALS TEXT

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SAFETY WARNINGS

Pay attention to the proper use of the computer.

BEFORE STARTING

What you need to prepare:
Python 3
TensorFlow
Keras

1 Prepare the dataset:
In the process of extracting protein data from UniProt, we removed those sequences with length less than 50 or greater than 1,280 amino acids, resulting in 17,651 DNA-binding protein sequences are selected as positive samples. At the same time, we got 50,500 non-DNA-binding protein sequences as negative samplesin UniProt that are 50 to 1,280 in length. We took 500 sequences from both positive and negative samples as independent test samples, respectively. For the remaining 17, 151 positive and 50,000 reverse samples, we randomly selected 85% of them as training sets and the remaining 15% as test sets to participate in model training.

2 Build model:
The deep learning model is composed of four parts: coding layer, embedding layer, convolution layer and Bi-LSTM layer. The coding layer represents each amino acid as a particular number. The embedding layer translates amino acid sequences into continuous vectors. The convolution layer consists of two convolutions and two maximal pooling operations. The mission of the Bi-LSTM layer is to grasp the context features of amino acid sequences.We use the Keras platform to build this model.

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3 Model training:
The data is trained in the built model, and this process is carried out on the GPU.At the end of this process, we get a DNA binding protein predictor.

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