

NETASA: neural network based prediction of solvent accessibility

ABSTRACT

Motivation: Prediction of the tertiary structure of a protein from its amino acid sequence is one of the most important problems in molecular biology. The successful prediction of solvent accessibility will be very helpful to achieve this goal. In the present work, we have implemented a server, NETASA for predicting solvent accessibility of amino acids using our newly optimized neural network algorithm. Several new features in the neural network architecture and training method have been introduced, and the network learns faster to provide accuracy values, which are comparable or better than other methods of ASA prediction.

Results: Prediction in two and three state classification systems with several thresholds are provided. Our prediction method achieved the accuracy level upto 90% for training and 88% for test data sets. Three state prediction results provide a maximum 65% accuracy for training and 63% for the test data. Applicability of neural networks for ASA prediction has been confirmed with a larger data set and wider range of state thresholds. Salient differences between a linear and exponential network for ASA prediction have been analysed.

Keyword: Artificial neural network; Protein tertiary structure; Computer program; Prediction