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APPENDIX

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Appendix I

Publications

- [I] Kasemsant Kuphanumat and Chidchanok Lursinsap, “Prediction of protein secondary structure by combination of support vector machine and Markov models”, *2nd International Conference on Bioinformatics 2003 (InCoB2003)*, September 2003.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Prediction of Protein Secondary Structure by Combination of Support Vector Machine and Markov models

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Support Vector Machine (SVM) currently is a novel approach for protein secondary structure prediction. Based on statistical learning theory and its generalization, SVM was reported to have out-performed results for many applications on Bioinformatics. Even through the method of protein secondary structure prediction based on SVM achieved a good performance, it did not produce the remarkably high results. The primary obstacle that vastly inhibits the power of the predicting model is an inappropriately encoding scheme of protein sequence data. Thus, finding an efficiently representative set of input features for protein sequences is, extremely, an important process to achieve the goal of protein secondary structure prediction. In our research, we introduce a new method based on Markov process to encode the protein sequences. With this simple method, input vectors that contain the essential features of protein sequence can be extracted and efficiently used to train SVM classifiers. Our method achieved the highest results that out-perform other advanced methods at present. The SVM together with Markov transition matrix encoding scheme produces the performance of three-state overall per-residue accuracy measure $Q_3 = 81.39$ and segment overlap accuracy measure $SOV = 78.64\%$ through a seven-folded cross validation on the data set of 513 non-homologous protein chains (CB513). That is the next improving step closing to the theoretical limitation.

Availability: The programs' source code and data sets are available upon request.

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Keywords: Protein secondary structure prediction, Support Vector Machine (SVM), Markov transition matrix, Machine learning, Patterns classification.

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