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Computational Intelligence in Bioinformatics

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Since the term 'bioinformatics' was coined in 1970 [1], the field of bioinformatics has become relatively mature allowing high-throughput whole genome sequencing and making computer-aided drug design an essential part of drug discovery. With the needs of addressing ever more complex problems in a faster and more accurate manner, the bioinformatics community has exploited many different paradigms. Among them, 'Computational Intelligence' has proved particularly effective since nature-inspired computational approaches are able to extract patterns from large volumes of data, infer rules from sets of examples and adapt according to changing data and/or contexts [2]. Many of those methods have been applied to bioinformatics; they include: Artificial Immune Systems [3], Bayesian Networks [4], Evolutionary Algorithms [5], Fuzzy Logic [6], Hidden Markov Models [7], Neural Networks [8], Rough Sets [9], Support Vector Machines (SVM) [10] and Swarm Intelligence [11]. In this special issue, we present six papers that illustrate the latest applications of Computational Intelligence in Bioinformatics.

Since more and more protein structure prediction tools are now available, it is crucial to be able to assess the quality of the generated models. Using features extracted from sequence alignment between a target and its template(s), Deng et al. [12] developed a SVM-based method to predict the quality score of a model. High correlation between predicted and actual values showed the effectiveness of their method.

Unlike the previous case, the choice of features may not be intuitive. As a consequence, selection methods are required before classification to prevent redundancy and the "curse of dimensionality". To design a system to identify and classify nuclear receptors into sub-families, Wang and Xiao [13], first, applied the sequential forward selection heuristic method to select the most appropriate sequence based features and, second, fed them to an SVM classifier. Rigorous evaluation revealed average prediction accuracies well-over 90%, which makes their predictor extremely valuable for the discovery of new drug-targets.

When analysing data such as gene expression data where the number of features can be two orders of magnitude higher than the number of samples, advanced feature reduction is essential to produce robust classifiers. Xu et al. [14] presented a new procedure based on the discriminative or predictive ability of variables via bootstrapped ROCAUCs (Area Under Receiver Operating Characteristic Curves). Simulations demonstrated the usefulness of the proposed methodology to build predictive models from bioinformatics data.

Since generally combining predictions of a set of classifiers produces more accurate predictions than the individual classifiers, Nguyen et al. [15] adopted an assemble approach in order to reconstruct metabolic networks. Taking advantage of the duality between metabolic gap filling and protein function prediction, they designed an indirect approach based on retrofitting outputs from several function predictors. Conducted experiments established the validity of their original approach, which would benefit further from integration of additional classifiers.

Also building on the fact that convergent predictions from different sources provide a way to increase result reliability, Holien et al. [16] used two docking algorithms to gain insights into interactions between inhibitors of a picornavirus RNA polymerase and their target. Discovery of structure-activity relationships should contribute to the design of more potent drugs for the treatment of infections.

Exploiting tools relying on dynamic programming and suffix arrays, Anupama et al. [17] performed an evolutionary analysis of Clustered Regularly Interspaced Short Palindrome Repeats (CRISPRs) in archaea genomes. In addition to identification of novel CRISPRs, authors presented evidence supporting that CRISPRs are the product of horizontal gene transfer.

As demonstrated by these articles, usage of Computational Intelligence has been spreading in bioinformatics. The excellent match between this paradigm and, the nature and complexity of bioinformatics problems makes it suitable for a wide range of applications from sequence annotation, microarray interpretation to protein structure analysis. There is no doubt that in the coming years the impact of Computational Intelligence will grow further, leading to even better understanding of biological data.

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