Energy-based Neural Networks as a Tool for Harmony-based Virtual Screening

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Abstract

© 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. In Energy-Based Neural Networks (EBNNs), relationships between variables are captured by means of a scalar function conventionally called "energy". In this article, we introduce a procedure of "harmony search", which looks for compounds providing the lowest energies for the EBNNs trained on active compounds. It can be considered as a special kind of similarity search that takes into account regularities in the structures of active compounds. In this paper, we show that harmony search can be used for performing virtual screening. The performance of the harmony search based on two types of EBNNs, the Hopfield Networks (HNs) and the Restricted Boltzmann Machines (RBMs), was compared with the performance of the similarity search based on Tanimoto coefficient with "data fusion". The AUC measure for ROC curves and 1 %-enrichment rates for 20 targets were used in the benchmarking. Five different scores were computed: the energy for HNs, the free energy and the reconstruction error for RBMs, the mean and the maximum values of Tanimoto coefficients. The performance of the harmony search was shown to be comparable or even superior (significantly for several targets) to the performance of the similarity search. Important advantages of using the harmony search for virtual screening are very high computational efficiency of prediction, the ability to reveal and take into account regularities in active structures, flexibility and interpretability of models, etc.

Keywords

harmony search, Hopfield nets, neural networks, Restricted Boltzmann Machines, virtual screening

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