World Academy of Science, Engineering and Technology
International Journal of Computer and Information Engineering
Vol:11, No:02, 2017

Artificial Intelligence in Bioscience: The Next Frontier

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Abstract : With recent advances in computational power and access to enough data in biosciences, artificial intelligence methods are increasingly being used in drug discovery research. These methods are essentially a series of advanced statistics based exercises that review the past to indicate the likely future. Our goal is to develop a model that accurately predicts biological activity and toxicity parameters for novel compounds. We have compiled a robust library of over 150,000 chemical compounds with different pharmacological properties from literature and public domain databases. The compounds are stored in simplified molecular-input line-entry system (SMILES), a commonly used text encoding for organic molecules. We utilize an automated process to generate an array of numerical descriptors (features) for each molecule. Redundant and irrelevant descriptors are eliminated iteratively. Our prediction engine is based on a portfolio of machine learning algorithms. We found Random Forest algorithm to be a better choice for this analysis. We captured non-linear relationship in the data and formed a prediction model with reasonable accuracy by averaging across a large number of randomized decision trees. Our next step is to apply deep neural network (DNN) algorithm to predict the biological activity and toxicity properties. We expect the DNN algorithm to give better results and improve the accuracy of the prediction. This presentation will review all these prominent machine learning and deep learning methods, our implementation protocols and discuss these techniques for their usefulness in biomedical and health informatics.

Keywords : deep learning, drug discovery, health informatics, machine learning, toxicity prediction
Conference Title : ICKDML 2017 : International Conference on Knowledge Discovery, Mining and Learning
Conference Location : Mumbai, India
Conference Dates : February 07-08, 2017