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Abstract

AI in Computational Drug Discovery

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Abstract:

Conventional drug discovery methods rely primarily in-vitro experiments conducted with a target molecule and a very large set of small molecules to choose a right ligand. With the exploration space for the right ligand being very large, this approach is highly time consuming and requires high capital for facilitation. Virtual screening, a computational technique used for evaluating a large group of molecules to identify lead molecules, can be used for this purpose to speed up the drug discovery process. Ligand based drug design works by building a conceptual model of the target protein. Ligand based virtual screening uses this model to evaluate and separate active molecules for a target protein. A classes of algorithm in machine leaning called Classification algorithm can be used to build the above model. In this abstract, 3 different machine learning approaches to solve virtual screening is described. The first method utilises an efficient virtual screening technique using Random Forest (RF) classifier. Second technique applies SVM classifier for virtual screening. The third method demonstrates the applicability of Self Organizing Map (SOM) as a classifier for screening ligand molecules, which is first of its kind in this area as per the literature. The talk end with comparing the plus and minus of the three techniques. The GPU parallelisation of these methods will be also explained in details.

Biography:

Jayaraj received his Ph.D in Computer Science from National Institute of Technology Calicut, India. His thesis was "GPU based Virtual Screening Techniques for Faster Drug Discovery". Now he is an assistant professor at the

CSE department, NIT Calicut, India. His research interests include Medical-informatics, Computational Drug Design and GPU Computing. He has published many journals as well as conference proceedings. He has attended an International spring school on High Performance Computing (HighPer 2018) at San Sebastian, Spain in April 2018. Following are some of his recent publications

Publication of speakers:

1. P. B. Jayaraj et al. Ligand based Virtual Screening using SVM on GPU, Computational Biology and Chemistry, 2019
2. P. B. Jayaraj et al., GPURFSCREEN: A GPU based virtual screening tool using Random Forest Classifier, Journal of Cheminformatics, 2016
3. Jayaraj, P. B et al., "A GPU based maximum common subgraph algorithm for drug discovery applications." in IPDPS Workshops, 580-588. Chicago, USA, 2016.
4. K. Steiner, M. Binder, M. Schemper, K. Wolff, and H. Pehamberger, "Statistical evaluation of epiluminescence dermoscopy criteria for melanocytic pigmented lesions," Journal of the American Academy of Dermatology, vol. 29, no. 4, pp. 581–588, 1993.

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