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Bioinformatics up to Date

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Inside…..

About us

The Bioinformatics Infrastructure Facility (BIF) at Biotechnology division, CSIR NEIST, Jorhat runs under the Biotechnology Information System Network (BTISnet) programme of DBT, Ministry of Science & Technology, and Government of India. The Centre was established on 2nd February, 2008 to promote innovation in Biological research and education through Bioinformatics accomplishment. The main goal is to facilitate and expose students and researchers from different academic institutions of North East India in Bioinformatics. The center conduct training and workshops for enlightening the use of bioinformatics applications in biological research and development. The Centre has access to global information through 24 hour high speed internet facility, and also e-journal facilities with DeLCON, Science Direct etc. To date the Centre has profoundly extended support in R & D work with a great intensity to different biological discipline including medicinal chemistry, computer aided drug design, genomics and proteomic data analysis etc.

CRDS: A docking web tool for drug-target identification.

Identification of potential drug targets is a significant process for explaining the mechanism of drug interaction against multiple targets to finding a new therapeutic agents for existing drugs. One of the key method of drug-target identification is to use the molecular docking. Molecular docking is one of the important approach in structure based drug design. However, its utilization has been delayed by the lack of user friendly publicly available servers. Therefore, it is essential for researchers to develop a advance computational tool or package for drug-target identification by molecular docking.

Figure: Home page of CRDS web tool

In this study, a fully computerized web tool named CRDS (Consensus Reverse Docking System) developed for prediction of potential binding site of a particular drug. They developed a approach of consent scoring for improvement of hit rates of drug-target interaction. These web tool CRDS carried out reverse docking against 5,254 candidate protein by using three different scoring functions (GoldScore, Vina, and LeDock from GOLD version 5.7.1, AutoDock Vina version 1.1.2, and LeDock version 1.0, respectively). And they combined those binding scores into a single binding score named CDS (Consensus Docking Score). Then the web server provides the list of top fifty predicted binding sites, docking conformations, ten most significant pathways, and the distribution of consensus docking scores. Homepage of CRDS was shown in the figure.

Source: Source: Aeri Lee, J Oxford Bioinformatics,2019

AI model for prediction of the progression of diabetic kidney disease using machine learning approach

Diabetes mellitus (DM) is a leading chronic metabolic disorder in world wide. Among various diabetic related disease, diabetic kidney disease (DKD), such as diabetic nephropathy, is the most common cause of (HD) and is associated with cardiovascular diseases. Hemodialysis or dialysis, is a process of purifying the blood of a person whose kidneys are not working normally.

Microalbuminuria is known to be a good predictor of further progression of diabetic nephropathy and subsequent cardiovascular diseases5 and early intervention for DKD, such as anti-hypertensive medicine, could induce remission of DKD with microalbuminuria. However, a more precise predictive model is needed for the very early intervention in DKD to prevent its further progression in diabetes patients without apparent symptoms or signs.

Artificial intelligence (AI) is increasingly becoming an advance approach in our daily life and in health science. AI has two main branches, virtual and physical. The physical branch includes robotics, which can support surgery and rehabilitation. The other one virtual branch includes informatics, which is expected to help physicians in their clinical diagnosis and disease treatment. Currently, the recent advancement of machine-learning(ML), with big data analysis, is contributing greatly in the field of pharmacokinetics, genetics and oncology. However, there is a predictive models for prognosis or progression of complications in various daily life diseases, such as T2DM.

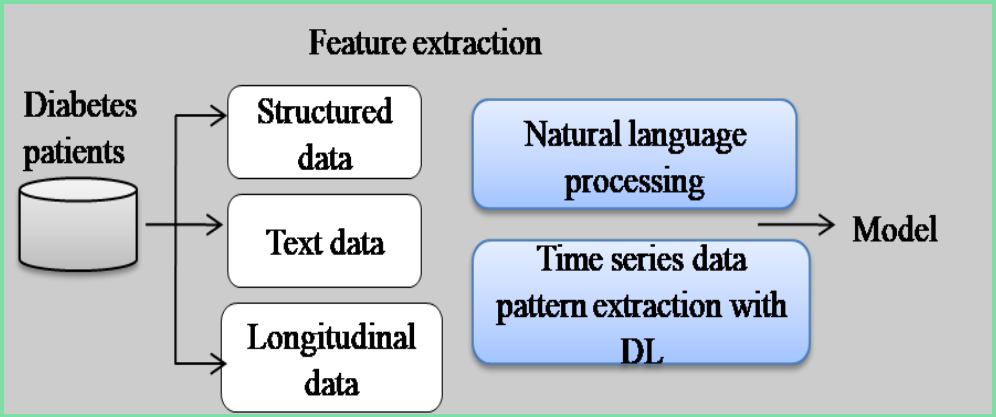


Figure: Overall workflow of AI model for DKD

AI is expected to support in the field of medicine. Some of the researchers constructed a new predictive model for diabetic kidney diseases (DKD). They used AI, processing natural language and longitudinal data with big data machine learning approaches to developed their model on the basis of electronic medical records (EMR) of 64,059 diabetes patients. AI extracted raw features of DKD aggravation, using a convolutional autoencoder. AI constructed the predictive model with 3,073 features, including time series data using logistic regression analysis. AI can predict DKD aggravation with 71% accuracy. In addition, the group with DKD aggravation had a significantly higher incidence of hemodialysis than the non-aggravation group. This newly constructed predictive model could detect progression of DKD and it may contribute to more effective and accurate intervention to reduce hemodialysis.

Source: Masaki Makino *et al.,* Sci Reports 2019

Bioinformatics Animation

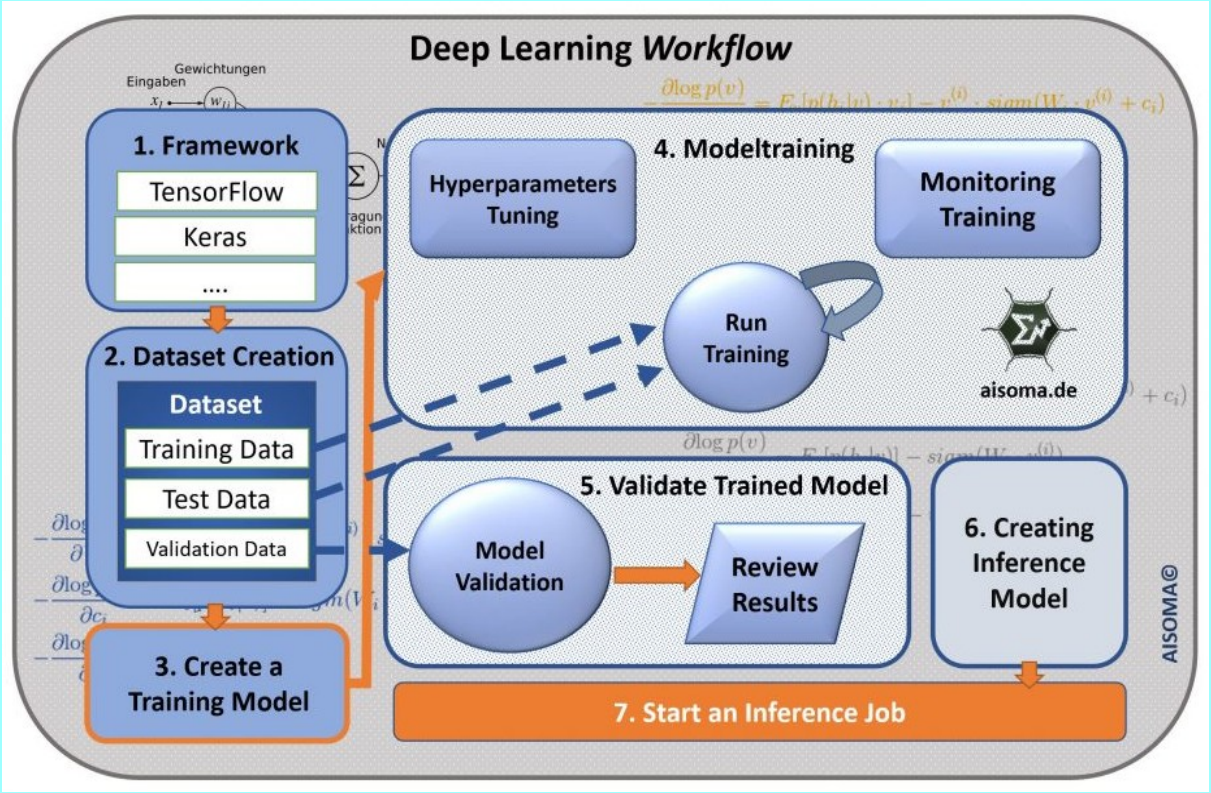
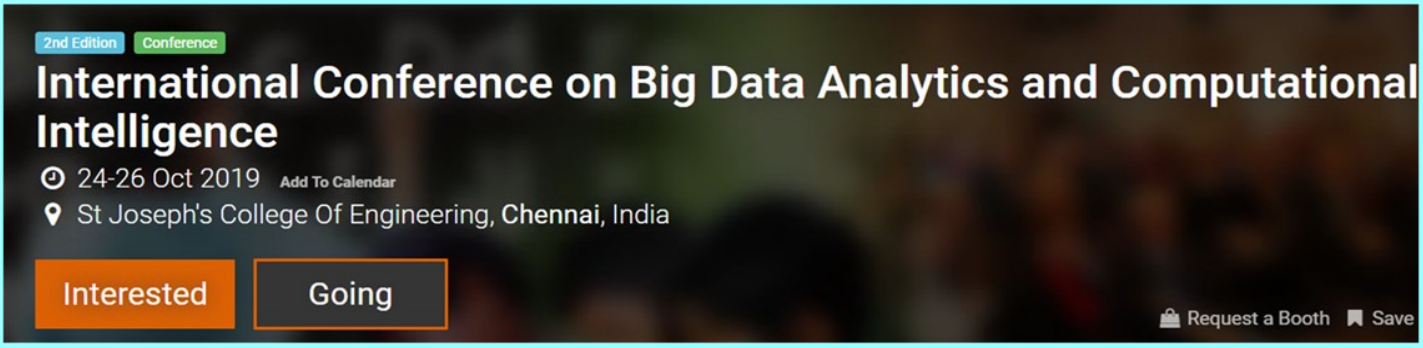


Figure: Deep learning workflow
*Source:*https://www.aisoma.de/10-useful-ai-ml-slides/

Upcoming Events



https://10times.com/dmip-shanghai
https://10times.com/icbdaci

Molecule of the month

Cyclin and Cyclin-dependent Kinase

Cyclin-dependent kinases (CDKs) are the families of protein kinases and this protein first discovered for their role in regulating the cell cycle. Cyclins and cyclin-dependent kinases control when cells divide, making them important targets for cancer therapy. A cyclins and CDK together control when cells divide and when they don't. Uncontrolled growth is one of the key point of cancer so control is essential in our life.

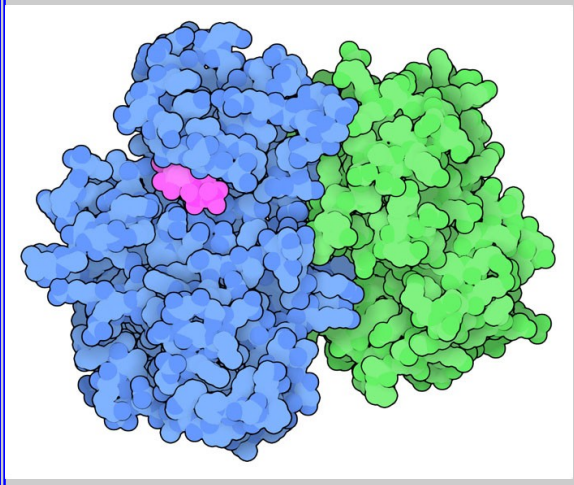


Figure 1:Cyclin A (green) and cyclin-dependent kinase 2 (blue) with ATP (magenta).

Cycles and Checkpoints

In cell cycle regulation process, transitions occurs between the phases are controlled by different cyclins and CDKs, which can also protect checkpoints that allow from one phase into the next.

CDK in Anticancer Drugs

In some of the study reported that CDK enzymes are targets for cancer chemotherapy, by blocking them. They can block the abnormal growth of tumor cells and much effort has been focused on CDK4 and CDK6, which protect a key restriction point before the cell starts DNA replication. In the Figure 2, they mention about the chemical structures of 3 US FDA-approved drugs (PDB entries 2euf, 5l2t and 5l2s) and all were revealed through structure-based drug design. They all have different chemical structures, but they interacted with a similar way at the active site region of the enzyme.

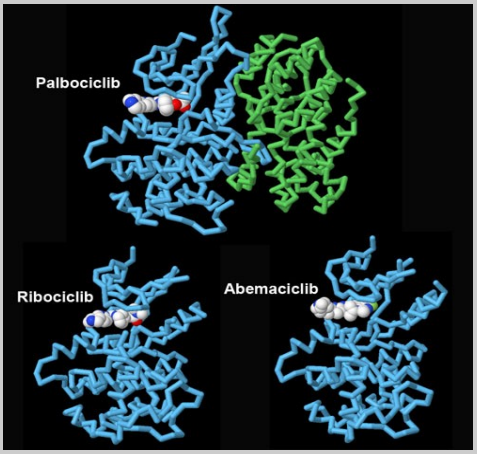


Figure 2:Drug bind with target at active site region of target

Source: http://pdb101.rcsb.org/motm/236

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