NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

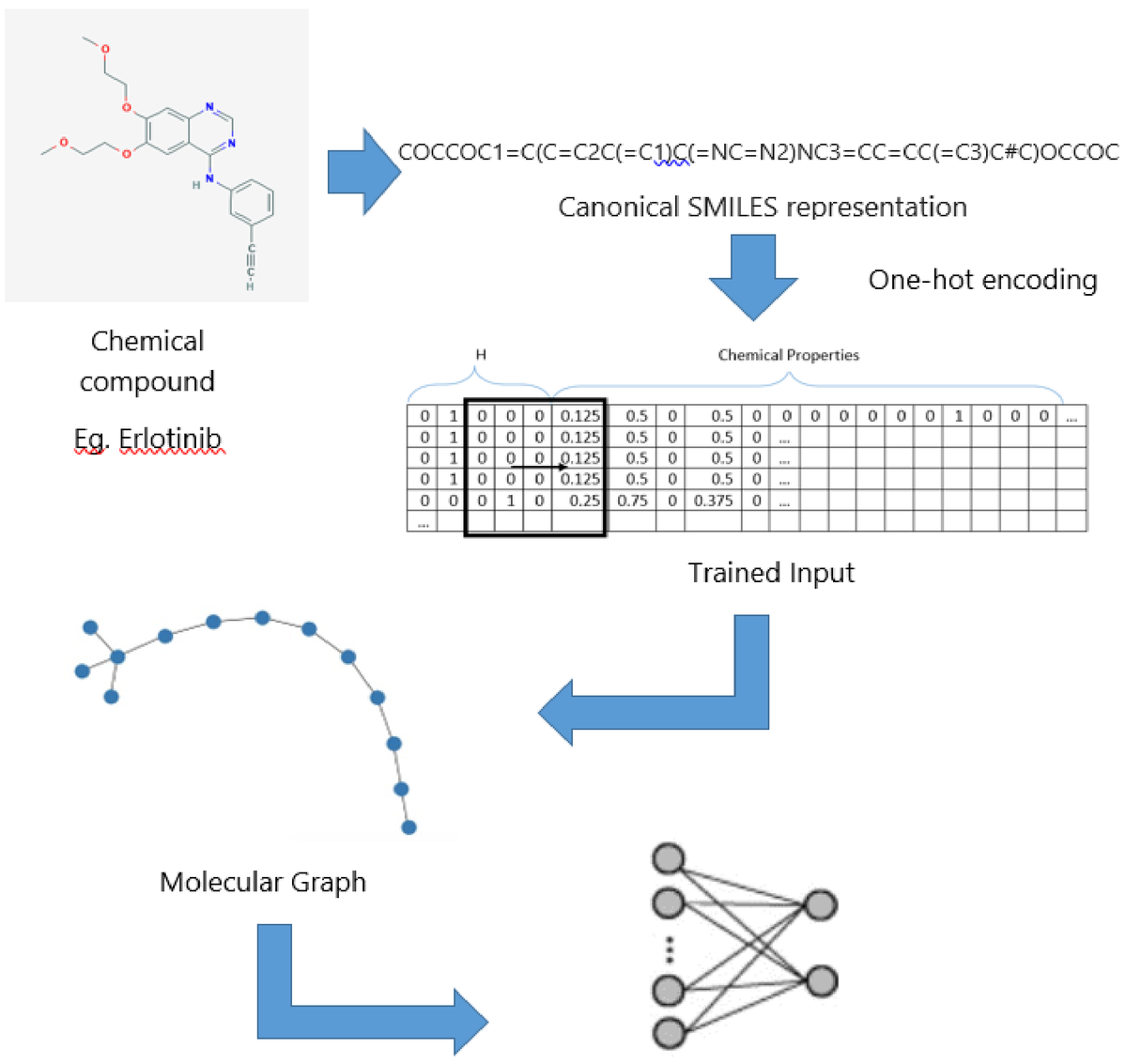
School of Computer Science and Engineering
College of Engineering

Drug Response Prediction from Chemical Features using Deep Neural Networks

Student: Krithika D/O Ramamoorthy Supervisor: Prof Jagath C Rajapakse

Project Objectives:

Develop models with deep neural networks(DNN), convolutional neural networks(CNN) and graph convolutional networks(GCN) to predict drug responses using chemical features accurately.



- Each drug chemical compound is converted to a binary data structure.
- This is done by using RDkit to derive chemical properties from the SMILES notation, one-hot- encode and further convert into a graph structure.
- The train data is fed into DNN, 1D-CNN, 2D-CNN and GCN with different configurations. GCN performed best with around 0.001 loss.

Neural Networks	Best Validation Loss
Deep Neural Network	6.6397
1D Convolutional Neural Network	5.2503
2D Convolutional Neural Network	4.9654
Multi-target 2D CNN	0.4379
Graph Convolutional Network	0.001211