

Ceng 499 Final Part 2.2

Machine Learning works on Covid-19 disease can help speeding up drug discovery process and provide some future insights like antivirals, infection levels and screening patients. This report summarizes works done from different sources.

1. Predicting protein structure and their relation with chemicals to help finding cure with current and new antiviral drugs.
 - a. Deep Learning Based Drug Screening for Novel Coronavirus 2019-nCov (Zhang, et al.): This study focus on predicting current antivirals that can help patients using deep learning. They have used modified DenseNet to predict protein-ligand interactions. Then they use a model of RNA sequence of coronavirus along with chemical compounds to make drugs' functionality test. They have indicated that further work is required. [1]
 - b. Deepmind: from data GISAid and AlphaFold library, aim is predicting protein structure of Covid-19 virus. AlphaFold is virtual library based on chemistry deep learning. Researchers gain knowledge about molecular structure of the virus which might pave the way for faster vaccine or antiviral detection. [2]
 - c. Predicting commercially available antiviral drugs that may act on it. New coronavirus(2019-nCov), Wuhan, China through drug-target interaction deep learning model: Authors look for currently available drugs and trying to train model with different approach. They use network "Molecule Transformer-Drug Target" or MT-DTI. Surprisingly, the more they suspect the familiarity with BERT, architecture is same at its heart. The network trained with SMILES dataset, it can form effective representation of molecules as in textual data. The authors then fine-tuned this pre-trained model to predict 'binding affinity values between commercially available antiviral drugs and target proteins. They have found that '2019-nCoV 3C-like proteinase was predicted to bind to atazanavir.' [3]

2. Forecast infection rates and spread / patient prognosis to allow hospitals / health officials to better plan their resourcing and response.
 - a. Prediction of criticality in patients with severe Covid-19 infection using three clinical features: a machine learning-based prognostic model with clinical data n Wuhan: In this paper, the researchers explained the use of XG-Boost model to make predictions about whether an infected Covid-19 patient can survive based on his/her age and other risky factors. It is good to making advises to people that need to be most isolated in the disease. [4]
 - b. Data-Based Analysis, Modelling and Forecasting of the Covid-19 outbreak: The researches based on the mean field of the Susceptible-Infected-Recovered-Dead (SIRD) model. Based on the dataset(saved data), R0 estimated value calculated from 11 Jan to 18 Jan, using official confirmed cases. Therefore, based on simulation trials of SIRD, the approximate mean value of R0 was found 2.4. [5]
 - c. Using Kalman Filters to predict spread of Coronavirus: Researchers tried to predict the spread of coronavirus for each regions. To produce best short term and long term prediction, fitting time series analysis and statistical algorithms used. [6]
3. Helping diagnosis if technologies such as X-ray or CT reveals Covid-19.
 - a. Deep Learning System for Screening Coronavirus Disease 2019: In this article total number of patients in the dataset is significantly greater. Data obtained from 3 hospitals around 500 patients in China. Surprisingly, the models' precision/recall scores are considerably lower than Chen et. al. Although they have more patients, they scan far few. [7]
 - b. Deep learning-based model for detecting 2019 novel coronavirus pneumonia on high-resolution computed tomography: a prospective study (Chen et. al.): Researchers used UNet++ to identify and extract features from CT scan. From 106 patients they have made 40000 scans and found model with well precision and recall. Clearly, model has 100% per-patient sensitivity, specificity of 93.55%, 95.24% precision etc. in the dataset. [8]

As a result, in order to make models more accurate, the researches need to share the data by keeping data privacy. There are lots of available unused data in the hospitals that need to be used in order to make great research with machine learning.

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