

DINABANDHU BEHERA

Data Scientist

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EXPERIENCE

Data Scientist

AIRA MATRIX

Oct 2020 – present

Thane, India

Drug Induces Liver Injury Prediction | POC

- Data has been scrapped from Pubchem website which contains SMILES and their corresponding dili level.
- The task is to predict dili level (0-6) of the drug like molecules.
- Mainly we are applying Graph Neural Network architecture to predict the classes. (Still working on it)

Liver Toxicity Prediction pre-clinical | POC

- The animal study data has been collected from TG-GATES database and NTP website. In total 400 labeled molecules were there in dataset.
- It was a multi-label classification problem, where we have to classify each molecules to 10 different liver lesions. classes.
- We have used XGB, RF, Catboost, ANN, Graph Neural Network for modeling and used Optuna for hyperparameter optimization. Also implemented a web demo using Streamlit for client presentation.

Skin Toxicity Prediction | POC

- The data has been collected from open source websites for this binary classification problem.
- We have used multi-modal approach using features from tabular data, image data and graph data to predict the skin toxicity.
- Also implemented a Flask based web application for the demo of the project.

Machine Learning Engineering

Virtusa, xLabs

Aug 2018 – Aug 2020

Bengaluru, India

Retail recommendation system based on click-stream data | POC

- The goal was to develop and deploy recommendation system for retail website using Google Cloud Platform (GCP) services and user click-stream data.
- We have used open source divolte collector, flask, app engine, cloud bigquery, google cloud dataprep services from GCP to implement the solution.

Determining frequent opiate prescriber | Client IBM Watson

- Our objective was to reduce fatalities due to drug overdose.
- We classified the prescription data based on how frequent an opiate-drug had been prescribed in an year.
- We applied tree-based algorithms such as Random Forest and XGboost for classification and developed a flask API for the same.

Precision Medicine for Cancer | Client IBM Watson

- Developed a binary classifier to classify blood cell cancer types (ALL/ AML), such that appropriate treatment could be provided to the patients.
- The problem belongs to HDLSS problem class, with dimension (rows:38 + 34, cols:7129) ($p \gg N$). We used techniques and algorithms such as PCA, Lasso, HSIC Lasso, SVM and XGboost and flask API for interaction.

EDUCATION

IIT Bombay - M.Tech

Aug 2016 – Aug 2018

Biomedical (Imaging)

IIT Guwahati - B.Tech

July 2012 – May 2016

Electrical and Electronics

SKILLS

Technologies - AI/ML Cloud Health care

Languages - Python Matlab C++ (basic)

Web - Web-Scrapping Streamlit Flask Git

Non-Tech - Team-work Leadership Research

ACHIEVEMENTS / PUBLICATIONS

- Certified as an Associate Google Cloud Engineer.
- Contributed to open-source soft-wares on github e.g. <https://github.com/ecrl/padelpy>
- " Multi-modal approach for prediction of skin toxicity in small molecules " at EUROTOX 2021, year 2021, Poster presentation
- " Multi-label classification model for the prediction of Mechanism-of-Action of small molecules " at Pharmacology 2021, British Pharmaceutical Society, year 2021, Oral presentation

OTHERS

Mechanism of Action prediction | Kaggle Competition

- Secured a rank of 707 out of 4373 total participants with a single model prediction.
- It is a multi-class classification problem. We used Pytorch to implement a 3 layered neural network along with clever preprocessing to predict the outputs.

Bristol-Myers Squibb – Molecular Translation | Kaggle Competition

- Problem here is to predict InChI string representation from scanned molecular structure.
- We are approaching this problem as an image captioning problem. And we are still working on this competition.

Vehicle Routing Optimization Problem (IoT) | Nestle

- Used google OR-Tool to find out the optimal vehicle route.
- Developed a web interface to intake warehouse position details and display the optimal route on website.

Real Time vehicle location tracking (IoT) | Nestle

- In this project, I have used NodeRED for real time vehicle location tracking simulation.
- I used open-source "CloudMQTT website" as the pub/sub broker and displayed real-time location, vehicle speed on NodeRED dashboard.