

CAPSTONE PROJECT 2024

Title: IMPORTANCE OF DRUG FEATURES IN

DRUG - DRUG INTERACTION Domain: MACHINE LEARNING

Batch No: 106



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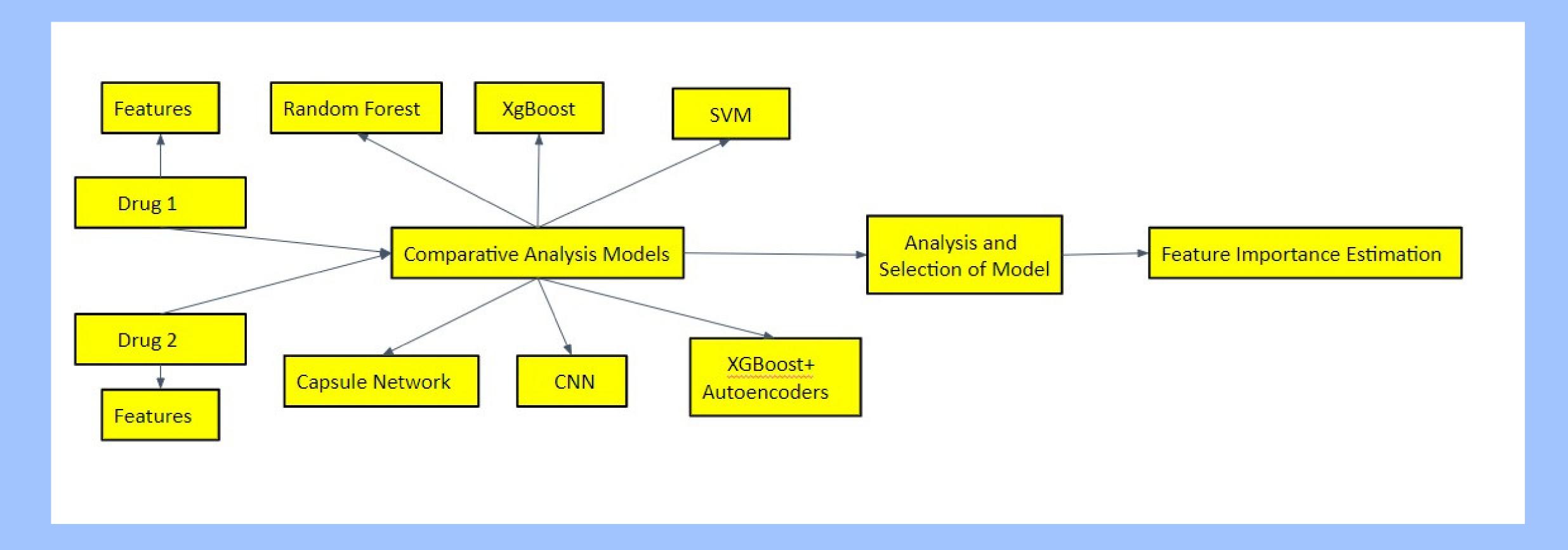


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Abstract:

A comparitive study to estimate the important features of responsible for drug-drug interaction. CNN, XgBoost, Capsule Network and other machine learning models have been trained on a large dataset of known drug-drug interactions. The estimation of feature importance in drug repurposing can accelerate the drug discovery process and can bring new and better therapies to patients faster.

Architectural Flow / Data Flow Diagram:



Results and Discussion:

- Dataset had various parameters like logP, Pka, Pkb, etc.
- Of all the models Random Forest had the highest accuracy of 95.60.
- The important feature was given as a result if any interaction between 2 drugs existed as well as a feature importance bar graph is produced.