An Interactive Adverse Drug Effect Network

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Problem

In the USA, 64.8% of adults are taking prescription medications.

When taken concurrently with other medications, such as Over-The-Counter (OTC) medications, this can cause Adverse Drug Reactions (ADRs).

Project Goals: 1) Create a network visualization tool that maps relationships between medications based on ADRs 2) Predict OTC medications that may cause ADRs using machine learning.
Problem: No tool allows users to input just a single drug and receive results
Why care? Adverse drug reactions occur frequently and can lead to various harmful reactions

Data

- **DDInter Database**: Provides node (drug) and edge (drug pair) data, including interaction severity (Minor, Moderate, Major).
- **FDA Adverse Event Reporting System (FAERS)**: Real-world adverse event data to calculate adverse event frequency and severity scores for drug pairs.
- **DrugBank**: Chemical structure (via SMILES) and protein target data for feature extraction. Training and testing data for ML model (drug pairs).

Approach

- Interactive network visualization tool with:
  - 1) **Search** function to allow users to select a drug and view its top 10 most common DDIs.
  - 2) **Predict** function: predict potential DDIs for drugs without prior interaction data using a machine learning model (ML).
- Feature Engineering + ML prediction.
  - Tanimoto coefficient to measure chemical similarity between two drugs.

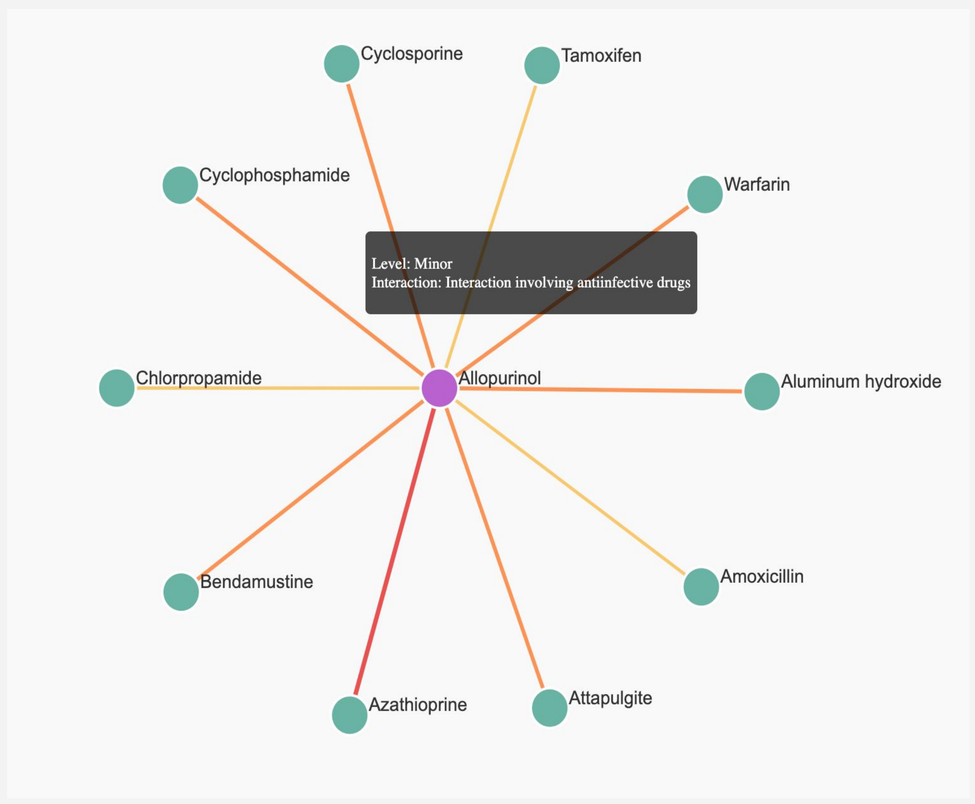
$$TC(A,B) = \frac{|A \cap B|}{|A \cup B|}$$

  - Calculation of adverse event severity scores.
  - Counting number of adverse events per drug pair.
  - Similarity between protein targets of drug pair.

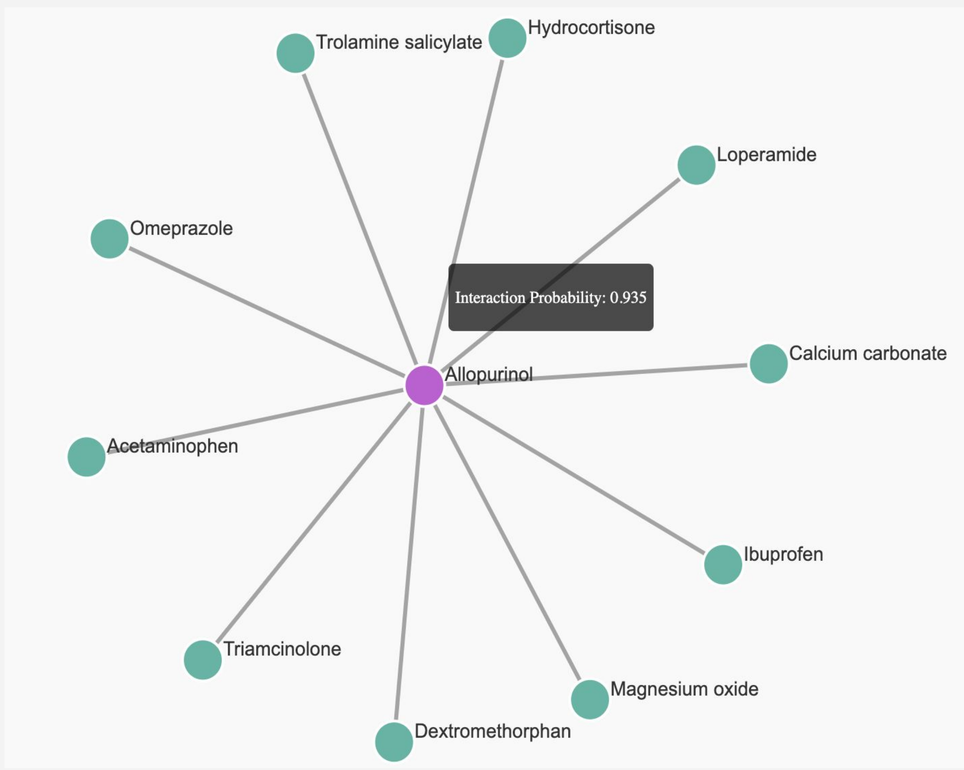
$$Jaccard\_similarity(A,B) = \frac{|A \cap B|}{|A \cup B|}$$

- ML prediction using random forest classifier algorithm.

Search Function

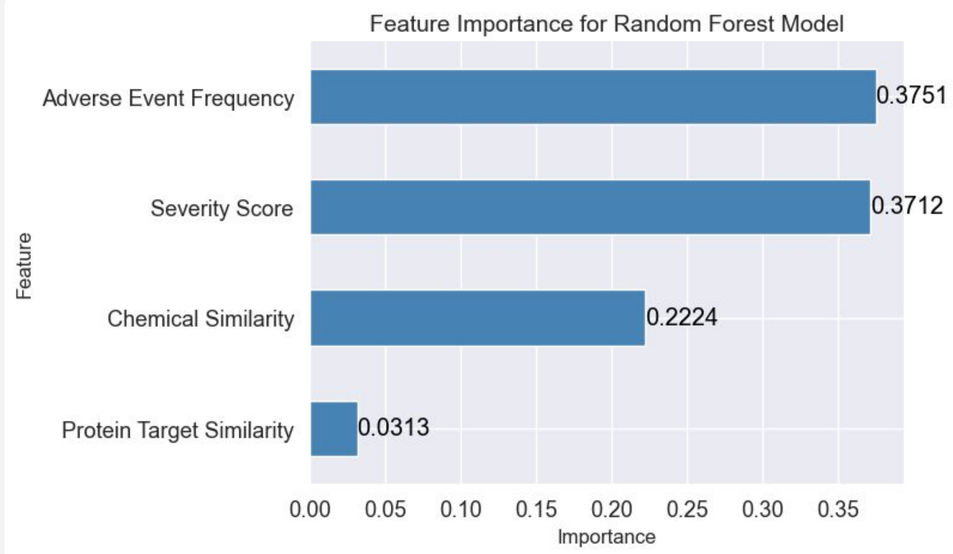


Predict Function

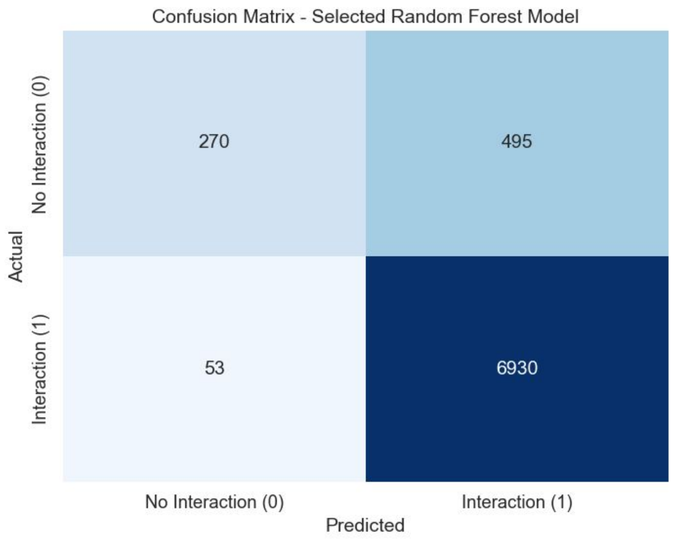


Evaluation

- Network was evaluated through user feedback
- Changes made to improve readability (eg. separate predicted drugs, reduce mouseover features)
- ML model was evaluated using various metrics (recall, minimizing false negatives, etc)



Feature importance plot from the selected random forest model. The longer bars indicate greater importance in predicting DDIs.



This confusion matrix shows the performance of the random forest model in predicting adverse drug interactions and minimizing the number of false negatives, 53.