Predicting side effects of unknown drugs using the Simplified Molecular Input Line Entry System (SMILES)

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Background

What does our application do?

- Displays the structural representation and the SMILE of a compound given the compound ID number assigned to it
- Predicts the presence of side effects of a particular drug
- Reports data regarding the accuracy of the model's prediction

Practical Applications

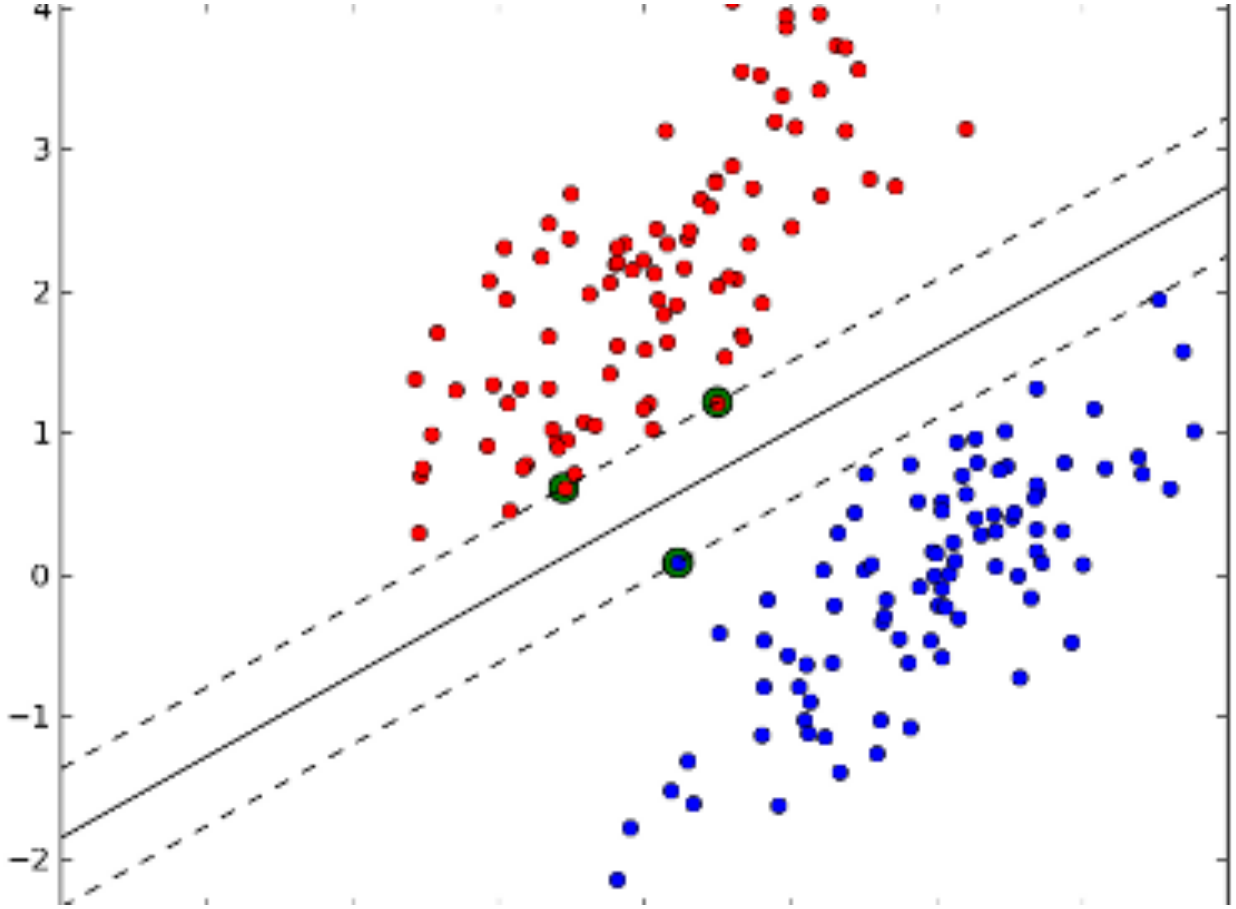
Why use this application?

- Often times side effect testing for drugs is an expensive and lengthy procedure
- Saves time by cutting down on side effect clinical testing expenses
- Warns the producers of a possible side effect to look for
- Confirms discovered side effects of FDA approved drugs

Methods

- Used a Support Vector Machine (SVM) classification model to predict side effects
- Separates data points into two groups based on a "best fit line" or ***decision boundary***
- The value of the unknown data point can be predicted based on it's location relative to the decision boundary

SVM Example



Code

- All code was written in Python
- Imported Python libraries
  - RDKit, Scikit, Tkinter
  - Purpose of importing libraries
- SVM
  - Divide the dataset into training and testing models
  - Train the model
  - Predict and find four metrics
  - Import

Live Demonstration

Further Improvements

- Incorporated more machine learning techniques
  - Linear, K-Nearest Neighbors, Decision Trees, Ridge, Lasso, etc.
- Expand the dataset
  - Use data, such as the compound structural representation, besides SMILES for side effect predictions
- Minor GUI Adjustments
  - Make the program more user-friendly and organized

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