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DEPARTMENT OF COMPUTER SCIENCE ENGINEERING (DATA SCIENCE)

ENHANCING DRUG SIDE EFFECT PREDICTION WITH EXPLAINABLE AI FOR MEDICAL HEALTH APPLICATIONS

PROJECT GUIDE
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ABSTRACT

Drugs are medications that change how the body functions. Some make us feel good when ill, while others treat ongoing health issues. They are in the form of pills, syrups, creams, or injections. Examples: paracetamol, antibiotics, vitamins, allergy medications, blood pressure medication, diabetes medications, and cough syrups. Side effects of drugs are able to result in serious health hazards for patients. Before using a drug, it is important to be aware of the negative effects. This research uses explainable AI (XAI) to improve drug side effect prediction. Machine learning models scan drug and patient information to identify patterns. The doctors are able to understand and trust AI advice because of these explanations. Important elements that could cause negative effects are identified by the system. Improved predictions help provide a more unique, secure drug plan.

INTRODUCTION

- Predicting harmful medicine reactions is important for ensuring patient safety in healthcare environments.
- Artificial intelligence (AI) models help in the analysis of large medical databases to improve the accuracy of side effect predictions.
- This is addressed by explainable AI (XAI), which makes model predictions clear.
- Doctors can use XAI to understand why a medication may have particular negative effects.
- The result facilitates better clinical decision-making and increases confidence in AI solutions.
- These kinds of findings can guide more personalised methods and safer recommendations for drugs.

Motivation

- Many people suffer from unexpected side effects after taking medicines, which can be dangerous or even life-threatening.
- Traditional methods like clinical trials are slow, expensive, and sometimes miss rare side effects.
- There is a large amount of drug-related data available, which can be used to build smart systems that can predict side effects in advance.
- Existing machine learning models are not always accurate and cannot handle multiple side effects at once.

Problem Defination

- Traditional methods for detecting side effects rely heavily on clinical trials and post-marketing surveillance, which are time-consuming, expensive, and often fail to identify rare or long-term side effects.

- Existing machine learning models (e.g., Logistic Regression, SVM, Naïve Bayes) lack the ability to capture complex, nonlinear relationships in high-dimensional medical data, limiting their prediction accuracy.

- The proposed solution aims to build a Multi-Layer Perceptron (MLP) based model, enhanced with Explainable AI (XAI) techniques such as SHAP and LIME, to predict and interpret drug side effects effectively.

Literature Survey

Author	year	Title	work done
Alizadehsani	2020	Explainable Artificial Intelligence for Drug Discovery and Development Comprehensive Survey	The authors explored various XAI techniques like SHAP, LIME, and feature importance methods to offer transparency and explainability. The work also evaluated how the models improve the understanding of drug toxicity and facilitate better clinical decision-making.
R. K. Sheu	2022	A Survey on Medical Explainable AI (XAI): Recent Progress, Explainability Approach, Human Interaction, and Scoring System,	discusses XAI methods and their integration into clinical settings for predicting drug side effects. The authors highlighted the potential of XAI to improve trust in automated predictions and its role inenhancing medical decisions.
T. H. Vo et al	2022	On the Road to Explainable AI in Drug–Drug Interaction Prediction: A Systematic Review.	The authors assessed how XAI approaches like attention mechanisms, LIME, and SHAP have help uncover the decision logic behind complex models. These XAI tools were shown to enhance model interpretability, enabling clinicians to better understand and trust the AI's predictions.
E. Bresso et al.	2020	Investigating ADR Mechanisms with Knowledge Graph Mining and Explainable AI	The authors introduced graph-based AI models to analyze complex relationships between drugs, their mechanisms of action, and potential side effects. They employed graph-based AI models in conjunction with decision trees and rule-based classification methods to ensure that the predictions remained interpretable to clinicians and researchers.

Research Gaps

- Lack of Interpretability: Current models often do not explain how they arrive at predictions, making it hard for clinicians to trust their outputs.

- Insufficient Data Integration: Many models use isolated datasets and fail to combine various sources of information, leading to incomplete insights.

- Challenges in Polypharmacy: Existing models struggle to accurately predict side effects when patients are taking multiple medications simultaneously.

- Limited Real-World Validation: Most models are validated in controlled environments,which may not reflect actual clinical settings, reducing their practical applicability

Proposed system

The research uses explainable AI (XAI) techniques to improve drugs' side effect prediction. Deep learning algorithms are used in research to analyse medication characteristics and patient data. In order for healthcare providers to understand prediction, XAI helps to highlight them. it helps in healthcare, this research promotes greater trust and decision-making.

EXISTING METHODOLOGY : ML ALGORITHMS

1. Logistic Regression Classifier (LRC)

Logistic Regression is a simple yet effective linear model used for binary and multi-label classification tasks. In the context of drug side effect prediction, it models the probability of occurrence of each side effect based on drug features.

- Pros: Fast, interpretable, good for linearly separable data.
- Cons: Struggles with complex, nonlinear patterns.

2. Support Vector Machine (SVM)

SVM is a powerful classifier that finds the optimal hyperplane that separates classes in the feature space. It is effective in high-dimensional spaces and often used for biomedical applications.

- Pros: Handles high-dimensional data well; effective with clear margins.
- Cons: Computationally expensive on large datasets; harder to interpret.

3. Ridge Classifier

Ridge Classifier applies L2 regularization to reduce overfitting, making it robust in the presence of multicollinearity.

- Pros: Reduces overfitting; works well with numerical features.
- Cons: Assumes linearity and may miss complex relationships.

4. Naïve Bayes Classifier

Naïve Bayes is a probabilistic model based on Bayes' theorem with the assumption of feature independence. It is commonly used in text classification and works well with sparse data.

- Pros: Fast, simple, effective with small datasets.
- Cons: Assumes independence between features, which is rarely true in medical data.

5. SGPC (Stochastic Gradient Polynomial Classifier)

SGPC applies stochastic gradient descent with polynomial feature transformation, allowing it to capture some non-linear relationships.

- Pros: Scalable, supports online learning, can handle non-linear patterns.
- Cons: Requires careful tuning of learning rate and regularization; may converge slowly.

OUTPUT OF ML-ALGORITHMS

Logistic Regression Precision : 80.83569296330386
Logistic Regression Recall : 78.4181125165494
Logistic Regression F1-Score : 79.39188781765762
Logistic Regression Accuracy : 74.8

Linear SVC Precision : 72.64485853960768
Linear SVC Recall : 72.90079083915771
Linear SVC F1-Score : 72.54916148108774
Linear SVC Accuracy : 68.7

Ridge Classifier Precision : 67.48374451754387
Ridge Classifier Recall : 37.64780787544186
Ridge Classifier F1-Score : 42.74898916086426
Ridge Classifier Accuracy : 55.00000000000001

Multinomial Naive Bayes Precision : 44.17863598001383
Multinomial Naive Bayes Recall : 49.903205696285845
Multinomial Naive Bayes F1-Score : 45.81278529607516
Multinomial Naive Bayes Accuracy : 49.4

SGDClassifier Precision : 44.17863598001383
SGDClassifier Recall : 49.903205696285845
SGDClassifier F1-Score : 45.81278529607516
SGDClassifier Accuracy : 49.4

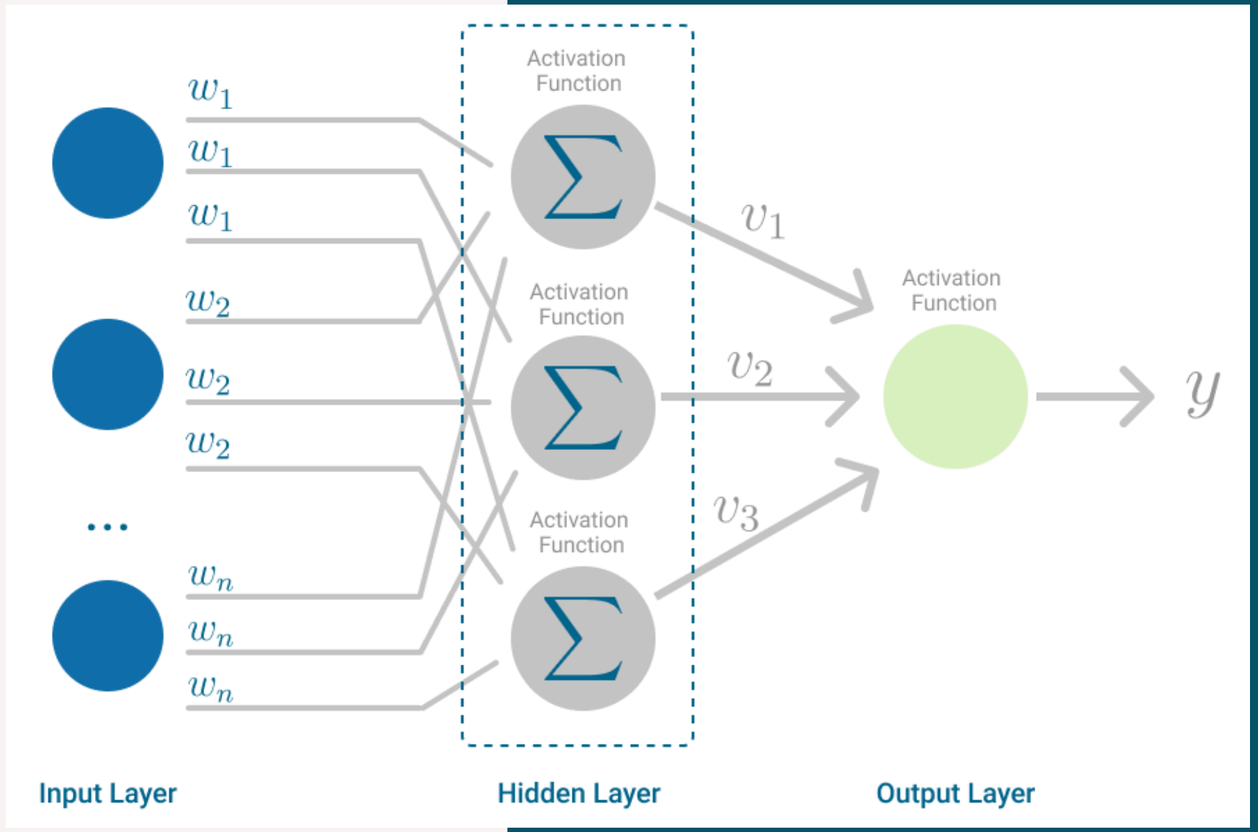
PROPOSED METHODOLOGY :

MLP

MLPs is a type of neural network, meaning data flows in one direction from the input layer to the output layer.

MLPs consist of:

- Input Layer: Receives the input data.
- Hidden Layers: Perform complex computations on the data using weights and biases.
- Output Layer: Produces the final prediction or classification.



- **Fully Connected Neurons:**
  Each neuron in a layer is connected to all neurons in the subsequent layer.

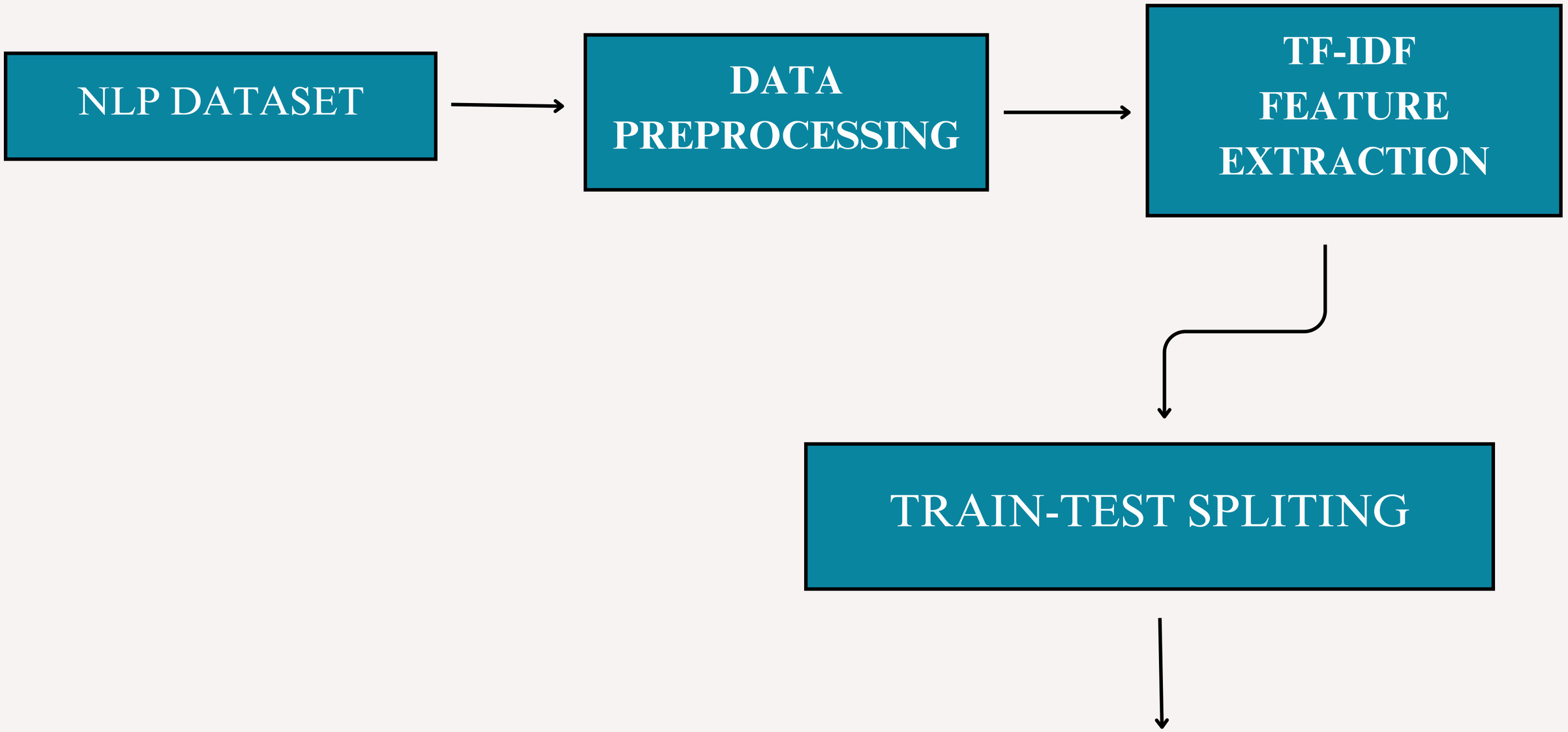
- **Non-linear Activation Functions:**
  Neurons use activation functions (like ReLU, sigmoid, or tanh) to introduce non-linearity, allowing the network to learn complex patterns.

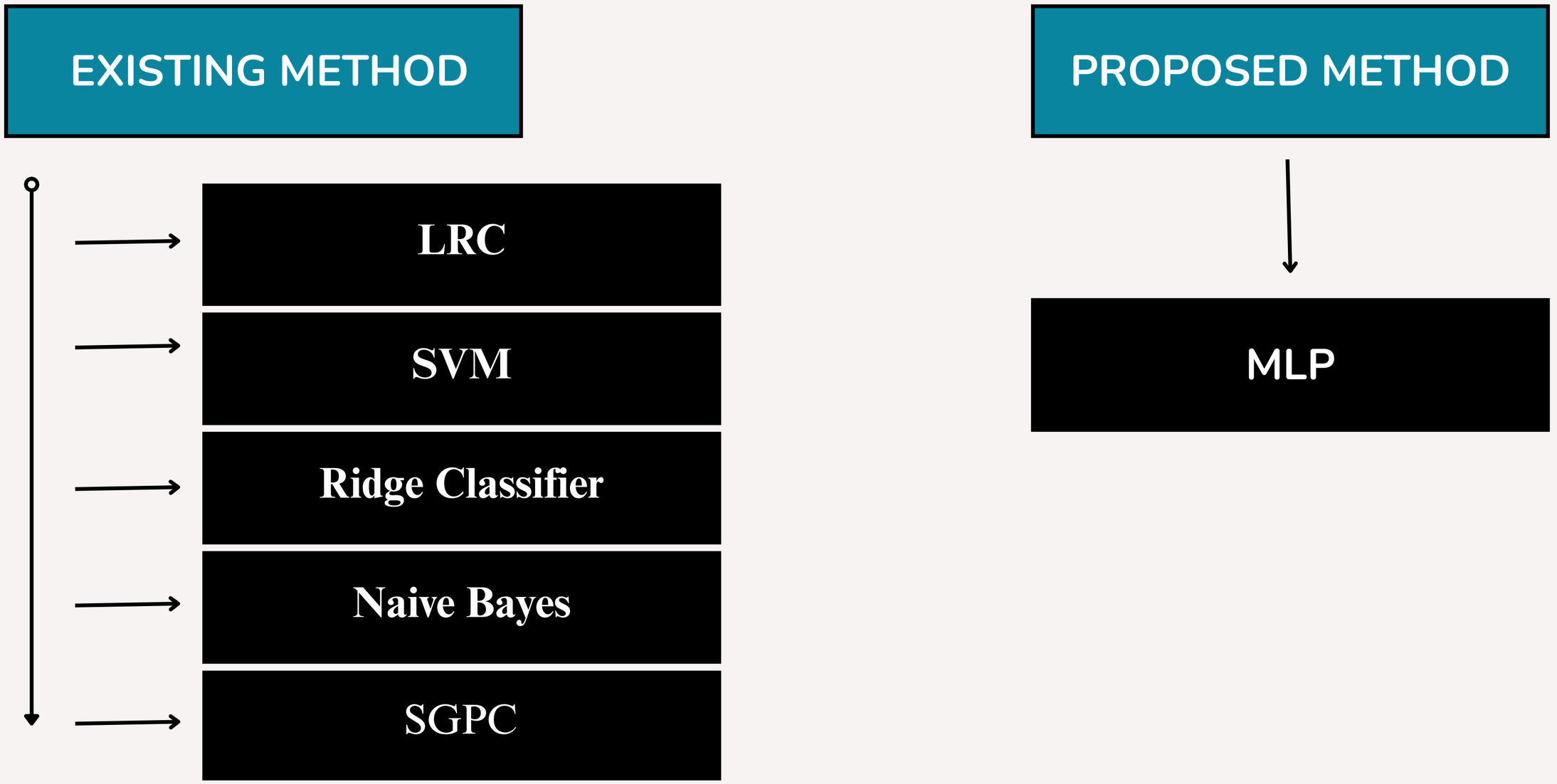
- **Backpropagation:**
  MLPs are trained using backpropagation, an algorithm that adjusts the weights and biases of the network by propagating the error from the output layer back to the input layer

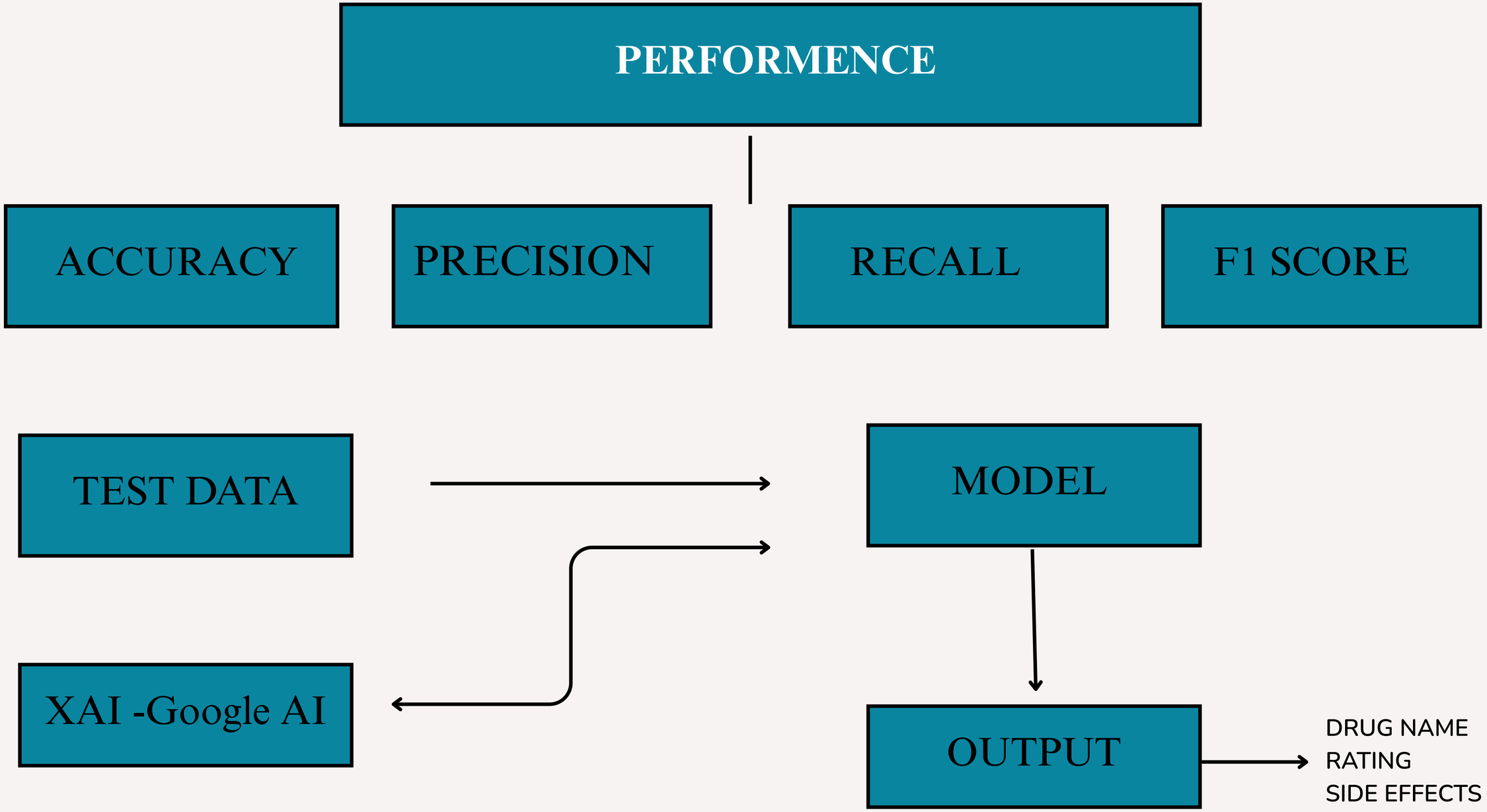
OUTPUT OF MLP:

Multilayer Perceptron Classifier Precision : 99.96784565916398
Multilayer Perceptron Classifier Recall : 99.93506493506494
Multilayer Perceptron Classifier F1-Score : 99.95132365051639
Multilayer Perceptron Classifier Accuracy : 99.9

MODEL


NLP DATASET
DATA PREPROCESSING
TF-IDF FEATURE EXTRACTION
TRAIN-TEST SPLITING


EXISTING METHOD
LRC
SVM
Ridge Classifier
Naive Bayes
SGPC
PROPOSED METHOD
MLP


PERFORMENCE
ACCURACY
PRECISION
RECALL
F1 SCORE
TEST DATA
MODEL
XAI -Google AI
OUTPUT
DRUG NAME
RATING
SIDE EFFECTS

Advantages

- Improved Safety: Reduces the risk of harmful side effects from medications.
  Enhanced Trust: Builds confidence among healthcare professionals and patients through clear explanations of predictions.

- Personalized Medicine: Supports tailored treatment plans based on individual patient characteristics.

- Better Decision-Making: Helps healthcare providers make informed choices about medication management.

- Data Integration: Combines various data sources for a more comprehensive understanding of drug interactions.

Applications

- Clinical Decision Support: Helps doctors identify potential side effects before prescribing medications.
- Drug Safety Monitoring: Improves systems that track and report drug side effects, allowing for faster responses to safety concerns.
- Personalized Treatment: Assists in creating tailored treatment plans based on how Individual patients might react to medications.
- Drug Development: Aids pharmaceutical companies in assessing potential side effects early in the drug development process.
- Patient Education: Provides information to patients about possible side effects, helping them make informed choices about their medications.

Software Details

Programming Language :

-Python 3.x

Development Environment:

- Jupyter Notebook / Google Colab / VS Code

Libraries & Frameworks :

- TensorFlow / Keras (for building and training the MLP model)
- Scikit-learn (for preprocessing, classical models, metrics)
- Pandas, NumPy (for data handling and manipulation)
- Matplotlib / Seaborn (for data visualization)

Future Scope

- The model can be added to hospital software to help doctors predict side effects while prescribing drugs.
- It can be trained with more data like patient age, gender, or other health conditions for better and more accurate results.
- In the future, we can use genetic and biological data to make predictions more personalized.
- More advanced models like Graph Neural Networks can be used to improve performance.
- We can build a mobile or web app so that users and doctors can easily use the system.
- The explainability can be made even better by using new XAI tools specially designed for medical use.

Conclusion

This project presents an intelligent and interpretable system for predicting drug side effects using a Multi-Layer Perceptron (MLP) enhanced with Explainable AI (XAI) techniques such as SHAP and LIME. The system addresses the limitations of traditional machine learning models by offering higher prediction accuracy and supporting multi-label classification, which is crucial as drugs often have multiple side effects.

The integration of XAI provides clear insights into the model's decision-making process, enabling trust, transparency, and accountability — especially important in the medical and healthcare domains. This combination of deep learning with interpretability makes the system not only powerful but also reliable for practical use in clinical environments.

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thankyou....