

WiM DRP Fall 2023

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# An Introduction to Explainable AI

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# Motivation

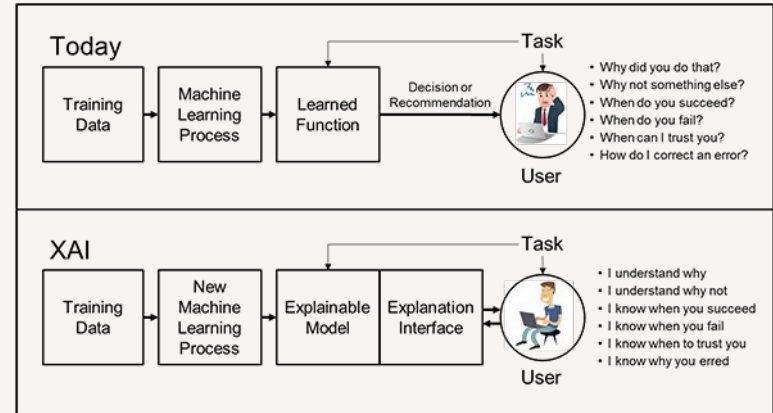
# Motivation

## What is Explainable AI?

- Explainable Artificial Intelligence (AI) is the ability for artificial intelligence systems to provide understandable explanations for their decisions, recommendations, or predictions

## Why do we need Explainable AI?

- AI is becoming a crucial part of our lives
- Models are mostly “black-box” (ie. user does not know how the model actually works)
- Uses of Explainable AI:
  - Accountability & Responsibility
  - Transparency builds trust among users
  - Legal & Ethical Compliance
  - Bias Detection & Mitigation
  - Facilitating user understanding
  - Advancing research & collaboration between humans and AI



# Dataset: Early Classification of Diabetes

According to the World Health Organization (WHO), diabetes is one of the *fastest growing chronic diseases*. Early detection is essential in helping diagnose and treat diabetic patients.

## About the Dataset

- 520 observations (ie. patients) with 16 characteristics/symptoms (ex. Age, gender, etc.)
- Data was collected through questionnaires and diagnosis results from the patients in the Sylhet Diabetes Hospital in Bangladesh

## Objective

- With the use of ML models, **predict the diagnosis of diabetes** using patient's profile + characteristics
- Identify the characteristics/symptoms that have the highest contribution to the diagnosis of diabetes through multiple machine learning models



# Machine Learning Models

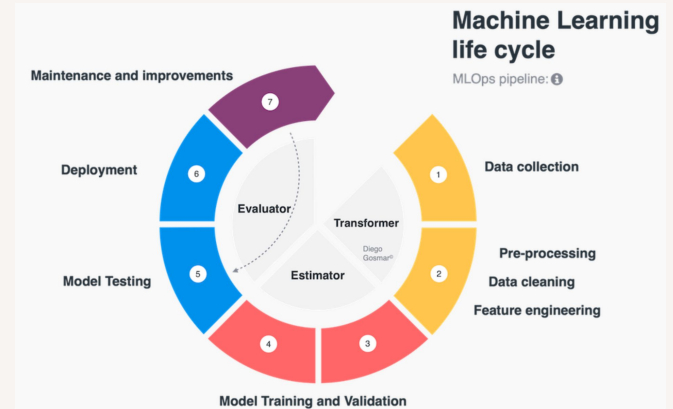
# What are Machine Learning Models?

- **What is the purpose of ML models?**
  - To enable data-based learning, reasoning, and decision making via statistical models and computational algorithms
  - Some other key purposes include: Classification, Regression, Clustering, etc.
- **How do ML models work?**
  - Use mathematical models to generalize from input features and corresponding output labels in training data, allowing them to make predictions on new data
  - The algorithms **iteratively adjust their internal parameters** during training to minimize the difference between predicted and actual outcomes, enabling them to generalize and perform well on diverse datasets



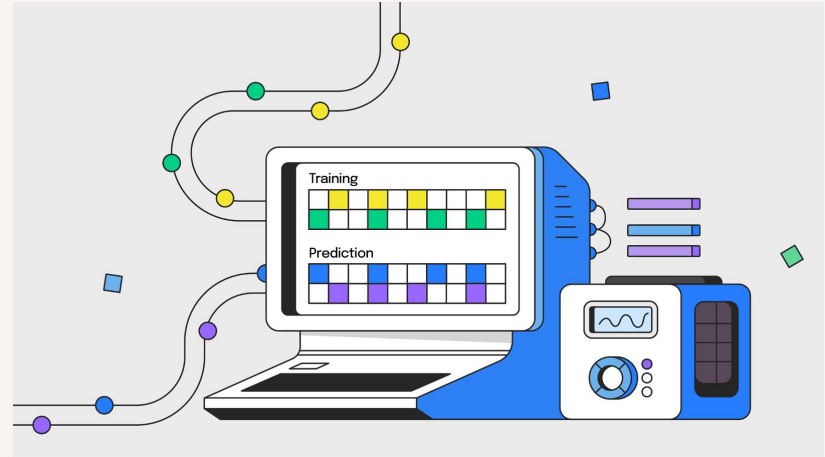
# What are Machine Learning Models? (cont'd)

- **Examples of ML Models:**
  - Linear Regression, Logistic Regression, Decision Trees, Random Forest, K-Nearest Neighbours, Naive Bayes, Neural Networks and many more!
- **How to evaluate ML Models**
  - The choice of evaluation metrics depends on the type of problem (ex. Classification, Regression, Clustering) and the specific goal of the model
  - Regression Models: Mean Absolute Error (MAE), Mean Squared Error (MSE), R-Squared, etc.
  - Classification Models: Precision, Accuracy, Confusion Matrix, F1 Score, etc.
  - Compare the model's performance on the training & test sets.
  - We will be focusing on using the **Mean Squared Error (MSE)**



# What are Machine Learning Models? (cont'd)

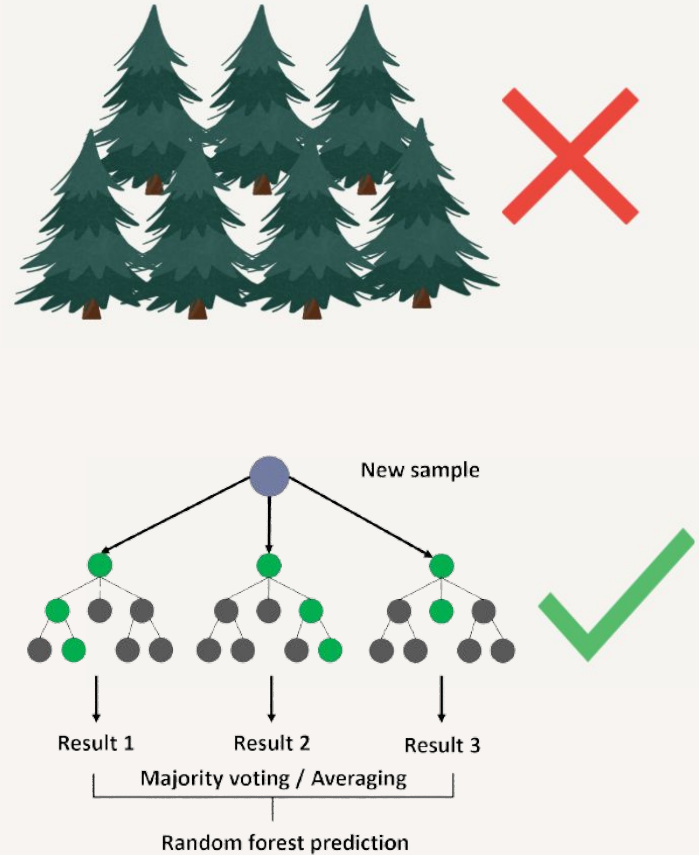
- **How to evaluate ML Models**
  - First, we split the dataset into the training and test data
  - **Training Set:** The data that is used to train the ML model.
    - This data contains true labels.
  - **Test Set:** The data that is used to evaluate the performance of the ML models (ie. using MSE).
    - The true labels are removed and utilize the ML models to make predictions based on the features in the test data.
    - We then compare the predictions with the true labels to evaluate the ML models





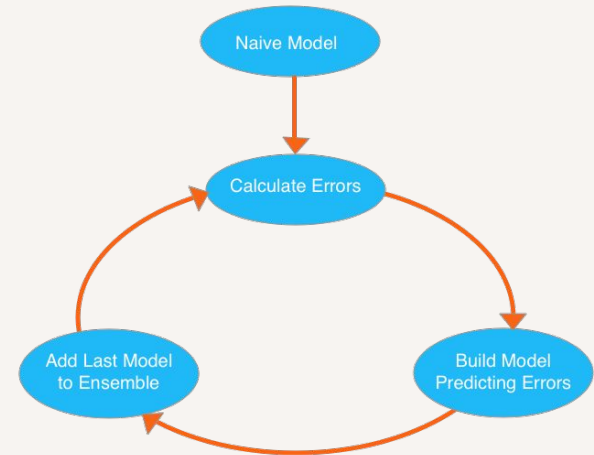
# Random Forest

- **Random forest** is a ML algorithm that uses the results of multiple “decision trees ” to create a single result.
  - What is a “**decision tree**”?
    - A decision tree is a flowchart-like model that represents a decision-making process, where each node denotes result of a decision.
  - Why is it **random**?
    - The data (including the observations and features) used to train the model for each decision tree is randomly selected
- Each decision tree in the forest makes a prediction
- The individual predictions of the ensemble of trees are combined to create a single result
  - This process is also called “**ensemble learning**”



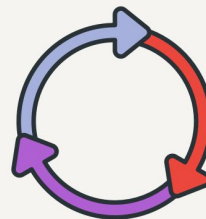
# XGBoost

- **What is an “Ensemble Learning Algorithm”?**
  - A technique of combining the predictions of multiple machine learning models to improve overall performance & robustness
  - Used to reduce overfitting, enhance generalization, and increase predictive accuracy
  - Ex. Random Forest, XGBoost
- **XGBoost (eXtreme Gradient Boosting)** is an ML algorithm that is an implementation of *gradient boosted decision trees*, designed for speed and performance.
  - Works by combining the predictions of multiple weak models (usually decision trees) additively
  - New trees are built based on the performance of old trees
- There is no straightforward way to interpret the XGBoost or Random Forest model because they are “Black-Box Models”



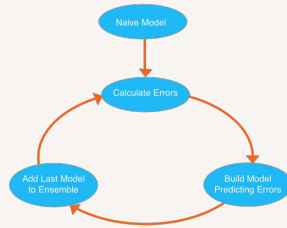
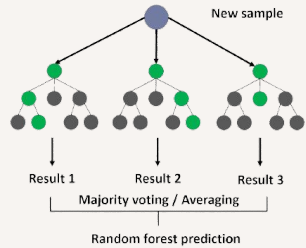
# Permutation Importance

# Permutation Importance



- **What is *Permutation Importance*?**
- Permutation feature importance measures the increase in the prediction error of the model after permuting the feature values.
  - This process breaks the relationship between the feature and the true outcome.
    - i.e. permutation feature importance takes into account both the main feature effect and the interaction effects on model performance
- **How does it work?**
  - To calculate the importance score for each feature:
    - In the test dataset, we permute the observations (rows) within the feature while keeping the other features the same
    - Use the machine learning model to make predictions based on the new test dataset
    - Then we evaluate the prediction error and compare it with the prediction error made using the original dataset
  -

# Permutation Importance



## Input

Machine Learning  
Model

## Process

Permute Each  
Feature

## Output

Feature Importance  
Scores

# Advantages & Disadvantages

- **Advantages**

- **Easy Interpretation**

- Feature importance is the increase in model error when the feature's information is destroyed

- **Comparable**

- Feature importance measurements can be compared across different problems

- **Does Not Require Model Retraining**

- Permuting a feature can save a lot of time: these importance methods go through the process of deleting a feature, retraining the model and then comparing the model error



- **Disadvantages**

- **Requires Access to the True Outcome**

- Permutation importance cannot be calculated without the true results of a dataset

- **Results May Vary**

- The permutation feature importance is determined by shuffling the feature, which adds randomness to the measurement



# Data Analysis

# Overview

- Used R to perform our analyses
- 80% of the data is randomly selected as the training set, and the remaining 20% is the test set
- Used Random Forest, and XGBoost to predict the diagnosis of diabetes based on the characteristics and symptoms of the patient
- Mean Squared Error (MSE): Measures how well a predicted value matches some truth value

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

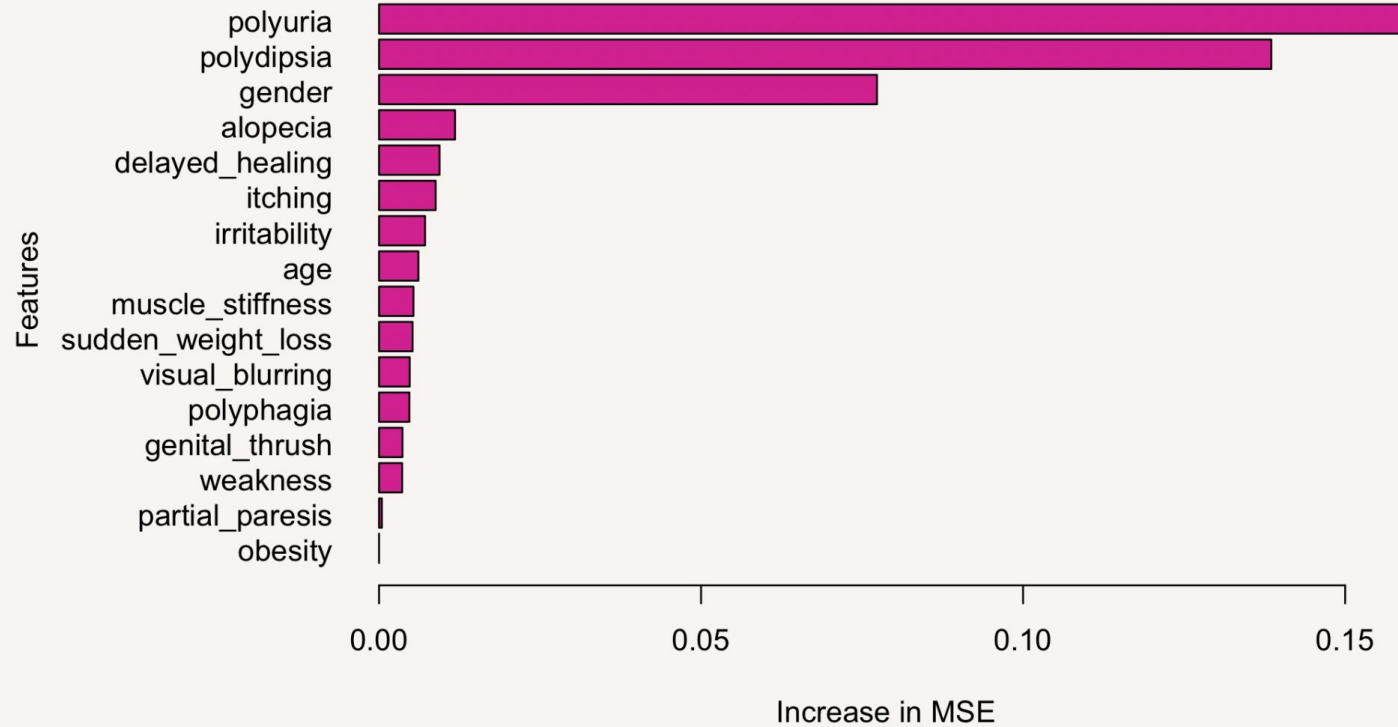
The equation is annotated with blue boxes and labels: 'Mean' above the fraction, 'Error' above the difference term, and 'Squared' above the exponent.

Model	Training Errors	Test Errors
Random Forest	0	0.01923077
XGBoost	5.206861e-06	0.03179245



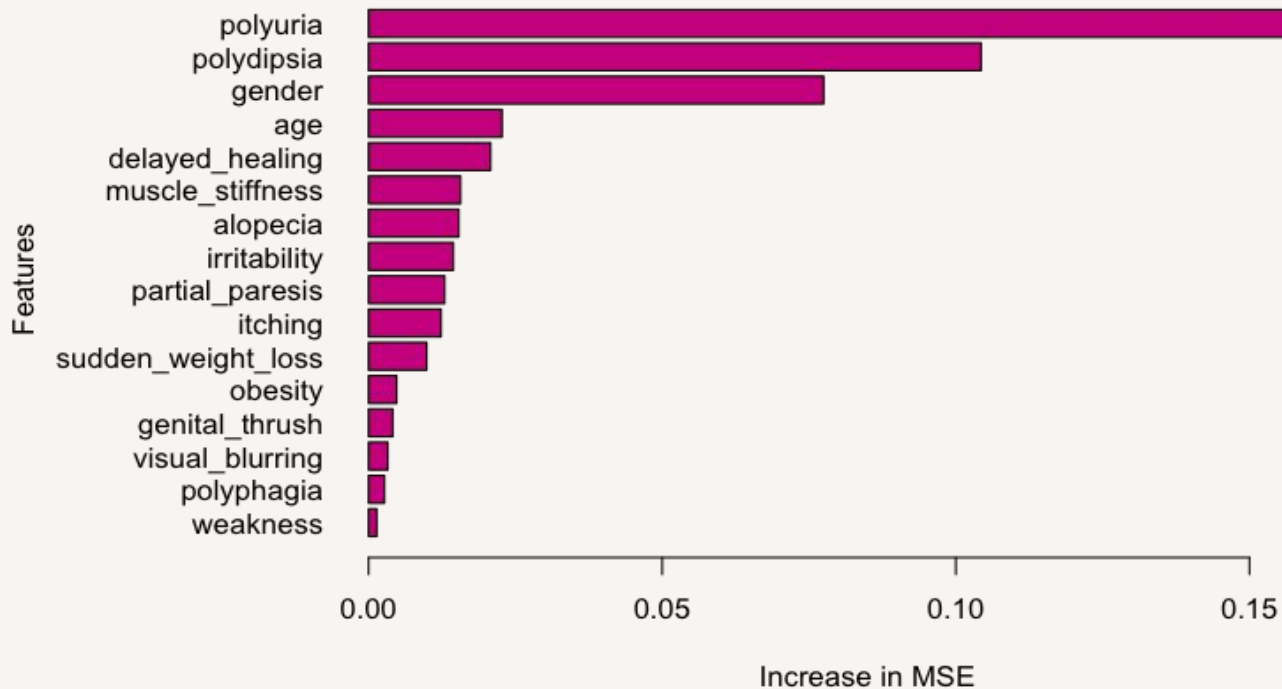
# Random Forest

Feature Importance according to  
Random Forest Model



# XGBoost

Feature Importance according to XGBoost Model



# Importance Analysis

From both the Random Forest and XGBoost models we saw that polyuria, polydipsia and gender were the most important features in diabetes diagnosis:

- **Polyuria:**
  - Whether a patient experienced excessive urination or not
    - Patients with polyuria are more likely to have diabetes than those who do not
- **Polydipsia:**
  - Whether the patient experienced excessive thirst/excessive drinking or not
    - Patients with polydipsia are more likely to have diabetes than those who do not
- **Gender**
  - Females are more likely to have diabetes than males



**Thank You!**