Applied-AI-in-Chemical-and-Process-Engineering / 2_MLpipeline_w3.ipynb

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Applied AI in Chemical and Process Engineering

Bulding ML pipeline for Reactor data

Week 3-4

This notebook will build a pipeline to prepare data and develop an ML algorithm

Content

Part 1: Data Preprocessing & Exploration

Step	Description	Key Actions & Tools
Data Preparation	Gather, load, and inspect raw data	- Load dataset (e.g., CSV, DB) - Check data types, shape, initial samples (`df.head()` , `df.info()`)
Data Cleaning	Fix issues in data quality	- Handle missing values (impute or drop) - Remove duplicates - Detect and treat outliers (IQR, Z-score)
Exploratory Data Analysis (EDA)	Understand data distributions and relationships	- Visualizations: histograms, scatter plots, pair plots - Correlation matrix (heatmaps) - Summary statistics

Part 2: Modeling & Interpretation

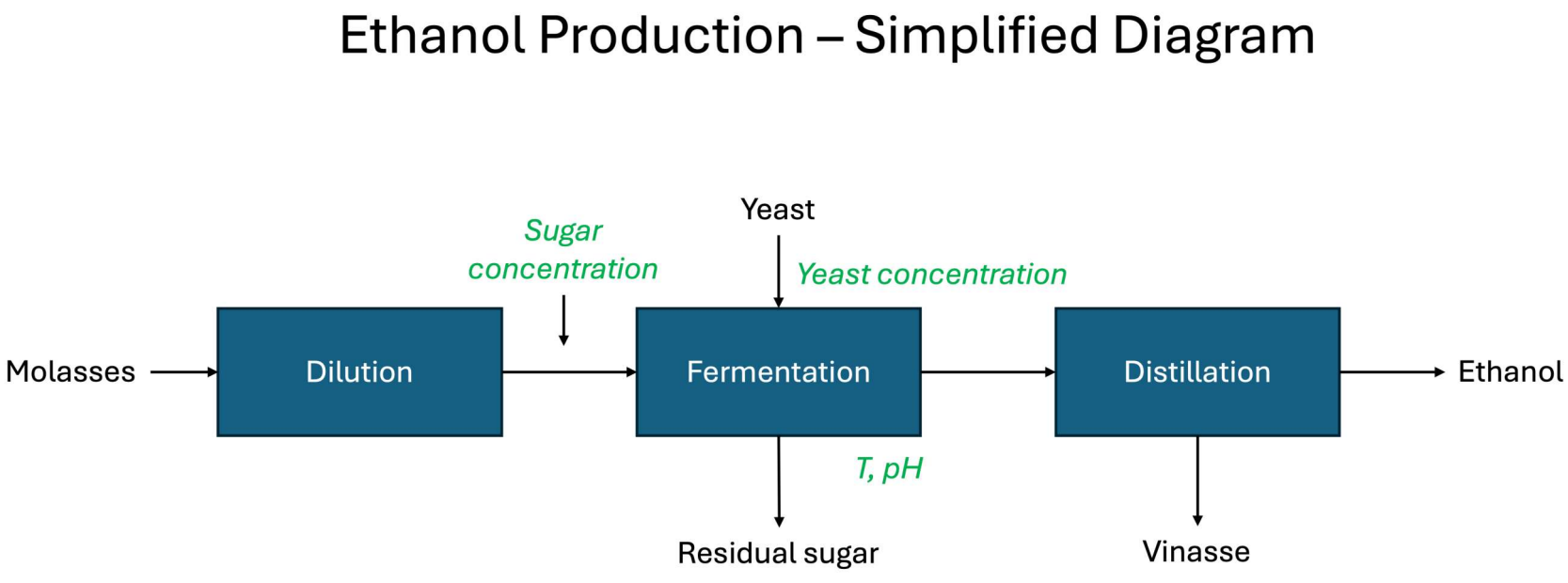
Step	Description	Key Actions & Tools
Normalization	Scale features to same range (e.g., for distance-based models)	- Apply Min-Max Scaling or Standardization - Justify choice based on model needs (e.g., SVM, KNN, Neural Networks)
Model Training, Validation & Testing	Build and evaluate model performance	- Split data: `train_test_split` - Train models (e.g., Linear Regression, Random Forest, XGBoost) - Use cross-validation - Evaluate using metrics (RMSE, MAE, R^2, etc.)
Model Explanation with XAI	Interpret model predictions and feature importance	- Use SHAP, LIME, or feature importance plots - Explain predictions to stakeholders - Ensure transparency and trust

Part 3: Optimization

Apply wide search strategy and Bayseian optimization to find the most optimum operating parameters

Note: Since our example does not have categorical data, we do not encode variables - which is essential if the data is categorical

Ethanol Production - Sugar Industry



Our goal is to model residual sugar. The model can be later used to optimize the fermentation process

Data

- Temperature °C: Fermentation tank
- pH: Fermentation tank
- Yeast Concentration g/L: Fermentation tank
- Sugar Concentration w/v: Dilution tank (input for fermenation)
- Residual Sugar g/L: Post-fermentation

Note: The data is simualted data

Data Preperation

Prompt: Load data from below github https://raw.githubusercontent.com/dissabnd/Applied-AI-in-Chemical-and-Process-Engineering/refs/heads/main/data/Ethanol_Molasses_Dataset.csv

In [ ]:

Prompt:

Print first 15 rows of the table and the dimensions of the table

Data Cleaning

Step	Purpose	Common Methods	Notes
Missing Data	Handle incomplete or null values	- Remove rows/columns - Impute with mean/median/mode - KNN/imputation models	Can bias models; choice depends on amount and reason for missingness
Duplicates	Remove redundant data entries	- Identify and drop duplicate rows - Use `pandas.drop_duplicates()`	Prevents overfitting and skewed results
Outliers	Detect and manage extreme values	- Z-score, IQR method - Visualization (box plots, scatter plots) - Winsorizing	Can distort models; keep if meaningful (e.g., fraud detection)

Check for missing data

Prompt: Check if the table has missing values

Fill the missing data wiht median using imputer

Prompt: Fill the missing data with median value

Check for duplicates

Prompt:

Check if it has duplicates

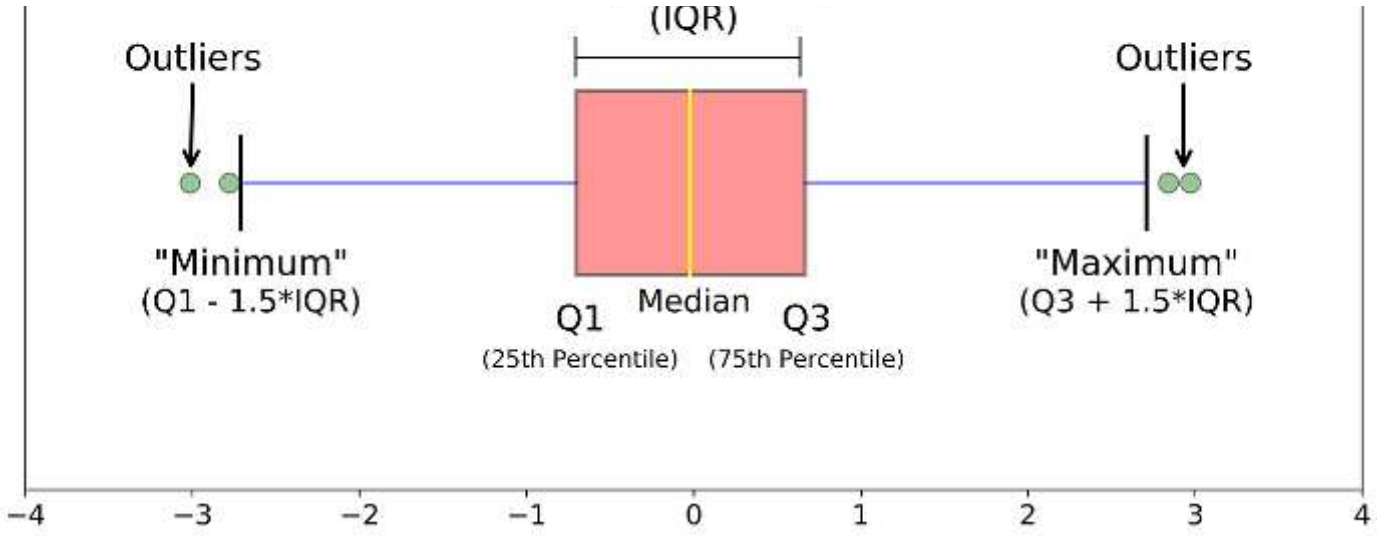
Exploratory Dara Analysis (EDA)

Summary Stats

Prompt:

Data Visualization

Data Visualization with Box Plot



Prompt:

Create box plots for all variables in multiple plots in single figure. show outliers

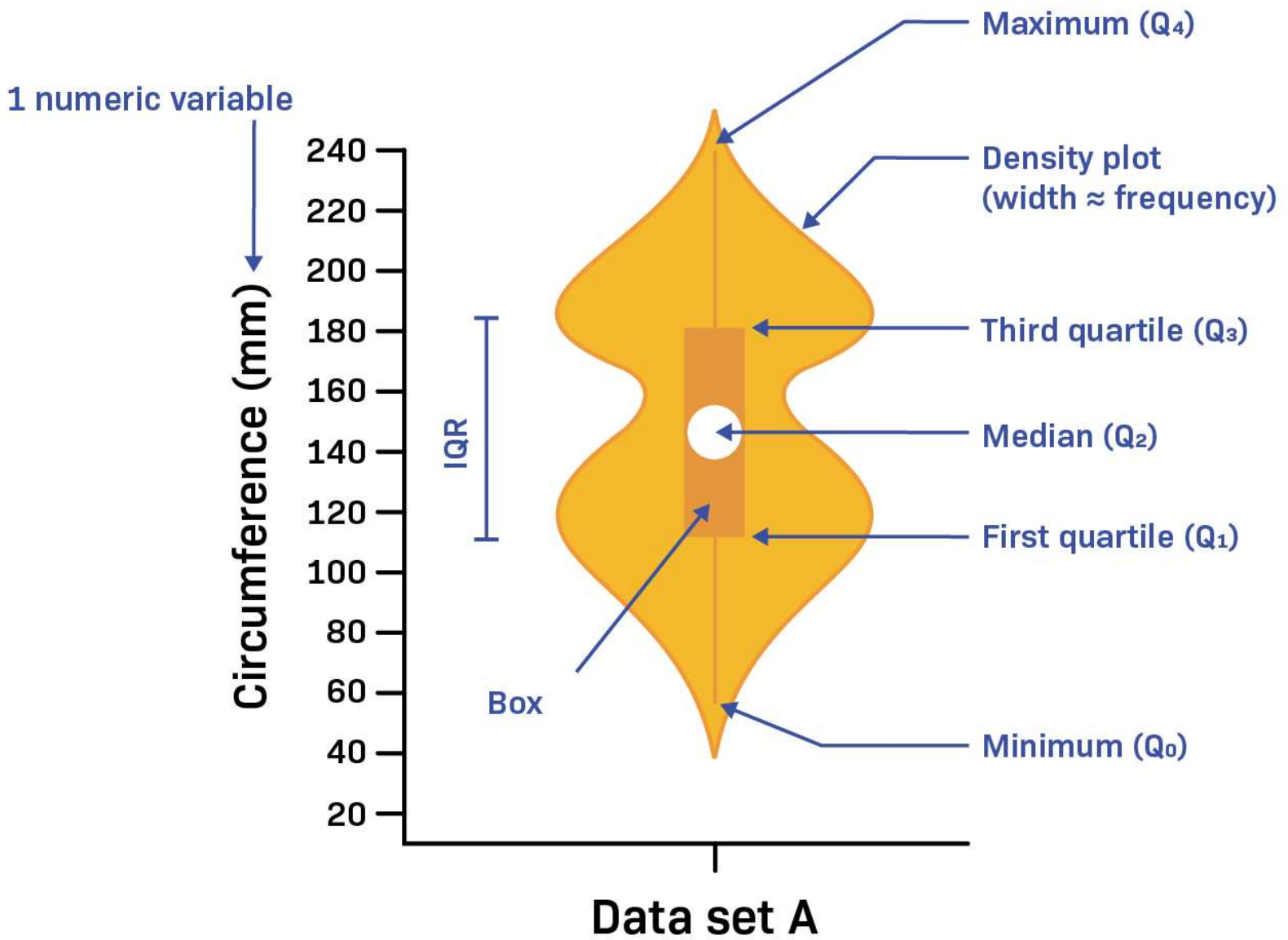
In [7]:
```
df_filled
```

Out[7]:

	Temperature	pH	Yeast_Concentration	Sugar_Concentration	Residual_Sugar
0	28.7	5.0	1.2	12.30	5.3
1	34.5	5.4	2.3	10.00	5.4
2	32.3	5.1	4.1	17.30	3.2
3	31.0	4.3	3.8	19.70	2.7
4	26.6	4.0	4.2	12.20	5.5
...	...	...	...	...	...
967	28.0	5.2	1.9	18.80	7.3
968	30.7	4.7	2.2	15.60	4.7
969	29.8	4.1	2.2	12.30	3.8
970	82.0	0.1	3.0	14.95	4.0
971	74.0	9.0	2.5	14.95	6.0

972 rows × 5 columns

Data Visualization with Violine plot



Prompt:

Create violine plots for all variables in multiple plots in single figure.

Data Visualization with Histogram plot

Prompt:

Create histogram plots for all variables in multiple plots in single figure.

Outliers

Strategy: We will use statistical methods to remove outliers (IQR)

Prompt:

Remove all outliers of df using IQR method and create a table called dfclean

Histogram plot with cleaned data

Prompt:

Create histogram plots for all variables in multiple plots in single figure using dfclean

Corelinearity

Prompt:

Print correlations matrix and do a plot a heatmap of correlation of dfclean

Data Prep for Model

Define Features and Target

Prompt:

'Residual_Sugar' is Y variables and Temperature','pH','Yeast_Concentration','Sugar_Concentration' are features. Plot scatter plot between features and Y

Feature Engineering with Data Scaling

Prompt:

Normalize X data using StandarScaler and plot histogram

Model Selection

Scenario	Recommended Model(s)	Notes
Linear + Few variables	Linear/Logistic Regression	High accuracy if relationship is linear; highly interpretable
Linear + Many variables	Ridge/Lasso	Handles many predictors; requires tuning
Non-linear + Small data	Random Forest	Robust, good accuracy, moderate interpretability
Non-linear + Large data	**Gradient Boosting**	High accuracy, slower, less interpretable
Very large data + High compute	Neural Networks (deep learning)	Best for complex, big data; low interpretability
Need interpretability	Linear, Random Forest, Gradient Boosting (with SHAP/LIME)	Linear most interpretable; others with tools
Time constraints	Linear > Random Forest > Gradient Boosting > Neural Networks	Linear fastest, Neural Networks slowest

XGBoost Model

Note:

Since this is tree model which does not require feature scaling in general, we **will not** use scaled data for model fitting

XGBoost

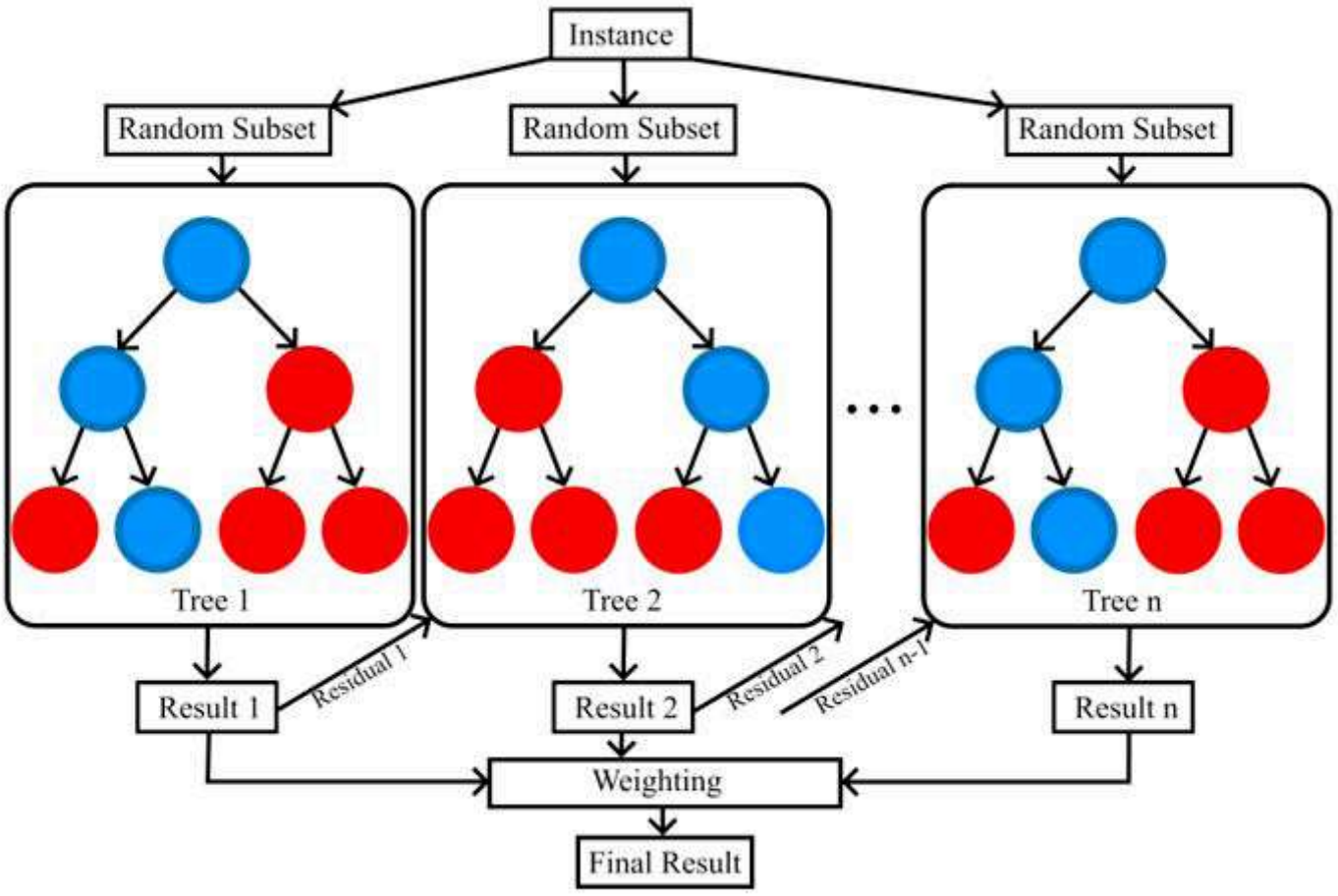
🔘 XGBoost is a machine learning algorithm that builds multiple decision trees one after another, where each new tree tries to fix the errors made by the previous trees.

🔘 It uses a method called gradient boosting, which helps improve prediction accuracy by combining many weak models into a stronger one.

🔘The algorithm includes features to prevent overfitting, such as regularization and controlling how the trees grow.

🔘 XGBoost can handle large datasets efficiently by using parallel processing to speed up training.

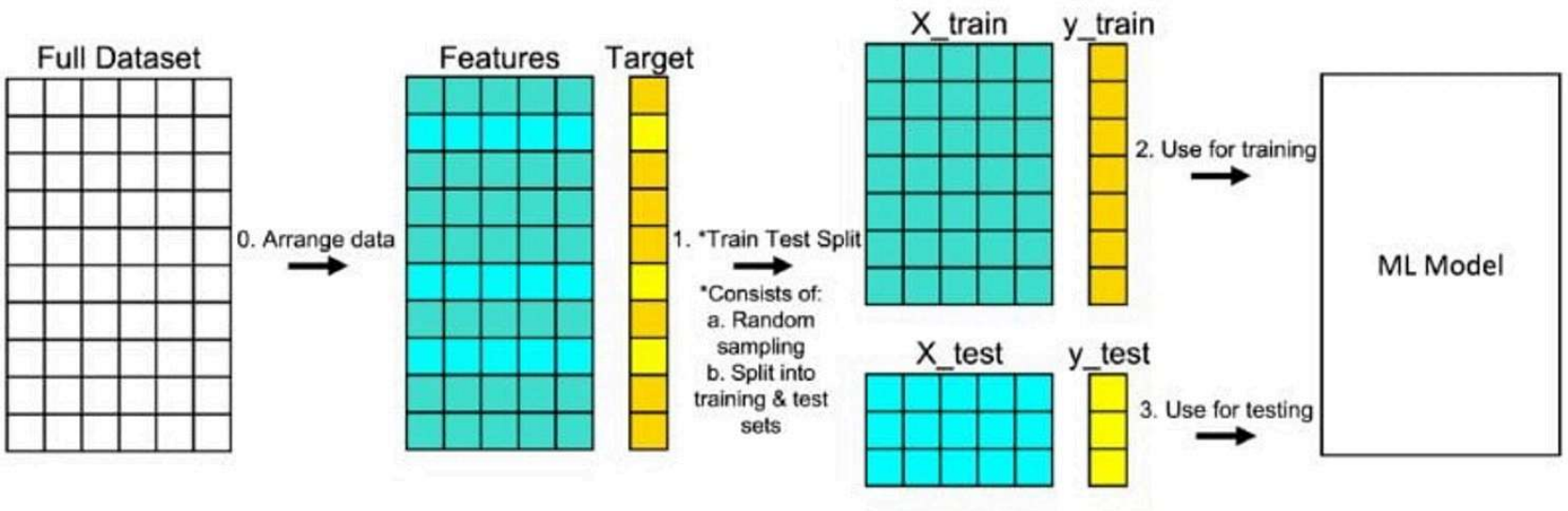
🔘 It is widely used because it is fast, accurate, and works well for tasks like classification and regression, making it popular among beginners and experts alike.



References:

XGboost paper

Data Split



In [ ]:

Prompt

Split the data into training and testing sets.

Hyperparameter Optimization

Parameter	Purpose	Simple Explanation	Default
`n_estimators`	Number of decision trees	More trees = more learning, but too many can overdo it. Like having more experts vote on the answer. ✅ **Typical tuned range:** 100–300	`100`
`max_depth`	How deep each tree can go	Controls complexity. Deeper = more detailed rules, but may memorize data. Like allowing more "if-then" steps. ✅ **Typical tuned range:** 3–10	`6`
`learning_rate`	How fast the model learns	Smaller = slow, steady improvement. Larger = fast but may overshoot. Like step size toward the goal. ✅ **Typical tuned range:** 0.01 – 0.3	`0.3`
`subsample`	% of data used for each tree	Uses only part of the data per tree to avoid overfitting. Like asking different small groups to learn. ✅ **Typical tuned range:** 0.6 – 1.0	`1.0`
`colsample_bytree`	% of features used per tree	Each tree uses only some columns (e.g., size, age, location). Prevents over-reliance on one feature. ✅ **Typical tuned range:** 0.6 – 1.0	`1.0`
`min_child_weight`	Minimum data in a prediction box	Stops trees from splitting too small. "Don't make a rule unless at least a few examples agree." ✅ **Typical tuned range:** 1 – 7	`1`
`gamma`	Minimum improvement to split	Only split if it clearly helps. Like saying: "Only add a rule if it makes things meaningfully better." ✅ **Typical tuned range:** 0 – 0.5	`0`
`reg_alpha`	Simplifies model (L1 penalty)	Shrinks weak signals to zero. Helps when many inputs are noisy or irrelevant. ✅ **Typical tuned range:** 0 – 1	`0`
`reg_lambda`	Smooths predictions (L2 penalty)	Keeps predictions stable by avoiding extreme values. Works like a safety brake. ✅ **Typical tuned range:** 1 – 2	`1`

Grid Search

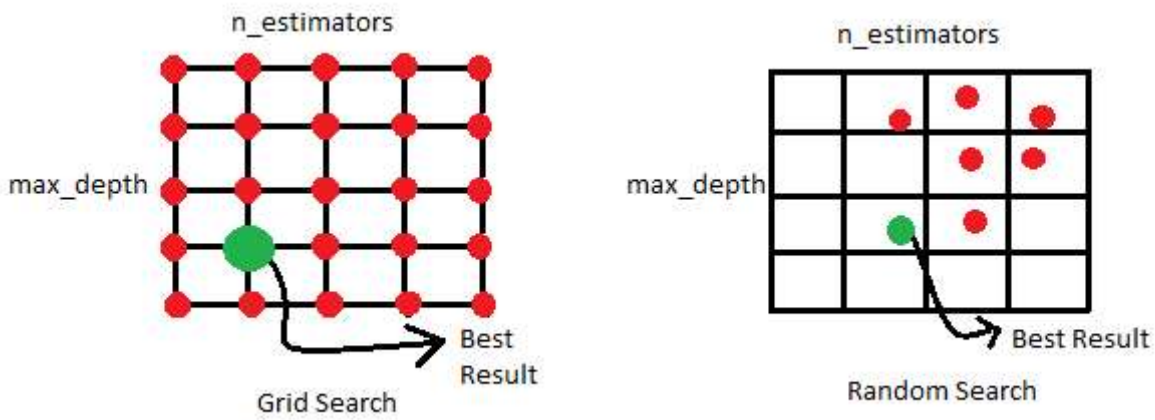
🔘 Grid Search is like trying all possible combinations of settings to find the best one — just like testing different oven temperatures and baking times to make the perfect cake.

🔘 It automatically tests every combination of hyperparameters (like learning_rate=0.1, max_depth=6) you specify, trains the model each time, and picks the one with the best performance.

🔘 It uses cross-validation (e.g., 5-fold) to ensure the result is reliable and not just lucky on one data split.

🔘 Think of it as "brute-force tuning" — thorough, systematic, and great for finding optimal settings, but can be slow with too many parameters.

Example: If you test 5 values for max_depth, and 5 values for n_estimators, Grid Search will try all 5x5=25 combinations and tell you which works best.



K-fold Cross validation

In K-fold cross-validation, the data is split into K equal parts (folds). The model is trained K times, each time leaving out one fold for testing and using the other K-1 folds for training. The final performance metric is averaged over all K runs. This approach uses the entire dataset for both training and testing, providing a more reliable estimate of model performance.

Prompt:

Finetune below hyperparamters of xgboost with 5 fold cross validation. Print R2/RMSE of testing and training

```
param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [3, 6, 9],
    'learning_rate': [0.01, 0.1, 0.3],
    'subsample': [0.6, 0.8, 1.0]
}
```

Training

In [15]:

```
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.metrics import r2_score, mean_squared_error
import xgboost as xgb


# Define features and target
X = dfclean[['Temperature', 'pH', 'Yeast_Concentration', 'Sugar_Concentration']]
y = dfclean['Residual_Sugar']

# Split data into 70/30
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

# Define parameter grid
param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [3, 6, 9],
    'learning_rate': [0.01, 0.1, 0.3],
    'subsample': [0.6, 0.8, 1.0]
}

# Create XGBoost regressor
xgb_model = xgb.XGBRegressor(random_state=42)

# Perform grid search with 5-fold cross-validation
grid_search = GridSearchCV(
    estimator=xgb_model,
    param_grid=param_grid,
    cv=5,
    scoring='r2',
    n_jobs=-1,
    verbose=1
)

# Fit the grid search
grid_search.fit(X_train, y_train)

# Get best model
best_model = grid_search.best_estimator_

# Make predictions
y_train_pred = best_model.predict(X_train)
y_test_pred = best_model.predict(X_test)

# Calculate metrics
train_r2 = r2_score(y_train, y_train_pred)
test_r2 = r2_score(y_test, y_test_pred)
train_rmse = np.sqrt(mean_squared_error(y_train, y_train_pred))
test_rmse = np.sqrt(mean_squared_error(y_test, y_test_pred))

# Print results
print("Best Parameters:", grid_search.best_params_)
print("\nTraining Metrics:")
print(f"R²: {train_r2:.4f}")
print(f"RMSE: {train_rmse:.4f}")
print("\nTesting Metrics:")
print(f"R²: {test_r2:.4f}")
print(f"RMSE: {test_rmse:.4f}")
```

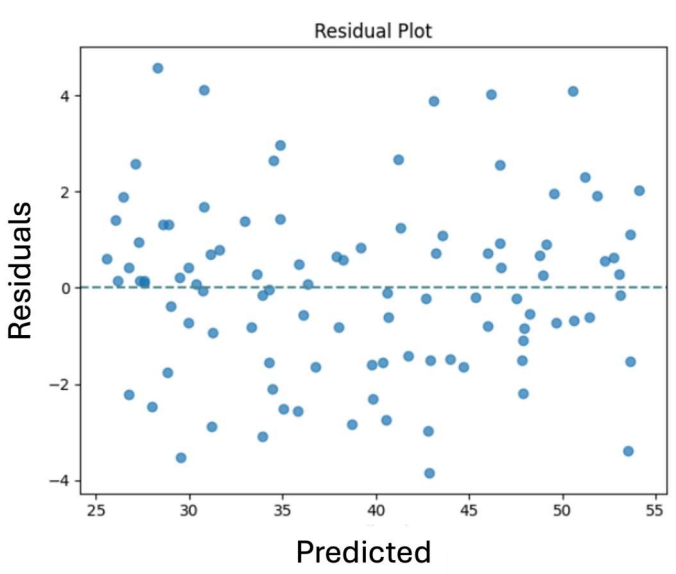
```
Fitting 5 folds for each of 81 candidates, totalling 405 fits
Best Parameters: {'learning_rate': 0.1, 'max_depth': 3, 'n_estimators': 100, 'subsample': 0.6}

Training Metrics:
R²: 0.8699
RMSE: 0.5291

Testing Metrics:
R²: 0.8111
RMSE: 0.6399
```

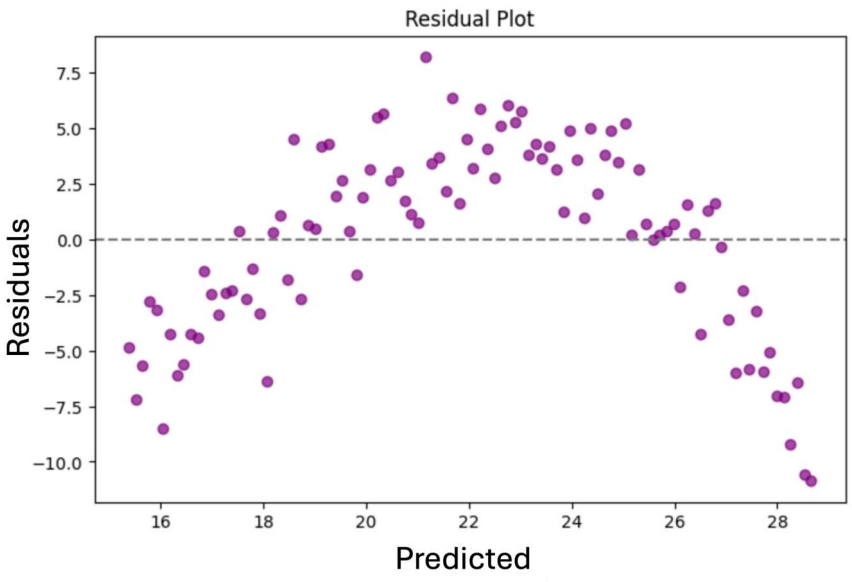
Model Evaluation

Prompt: Evaluate the model as below.

1. Plot actual vs predicted values for both train and test

2. Print R2/RMSE on the graph



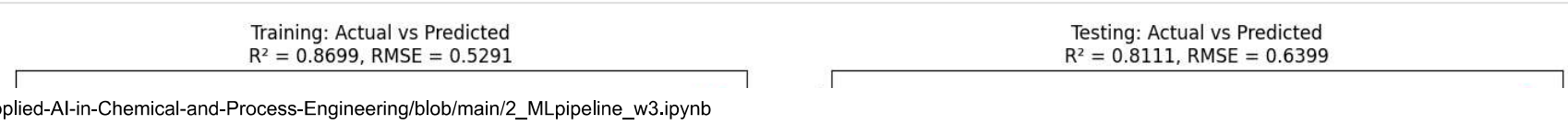


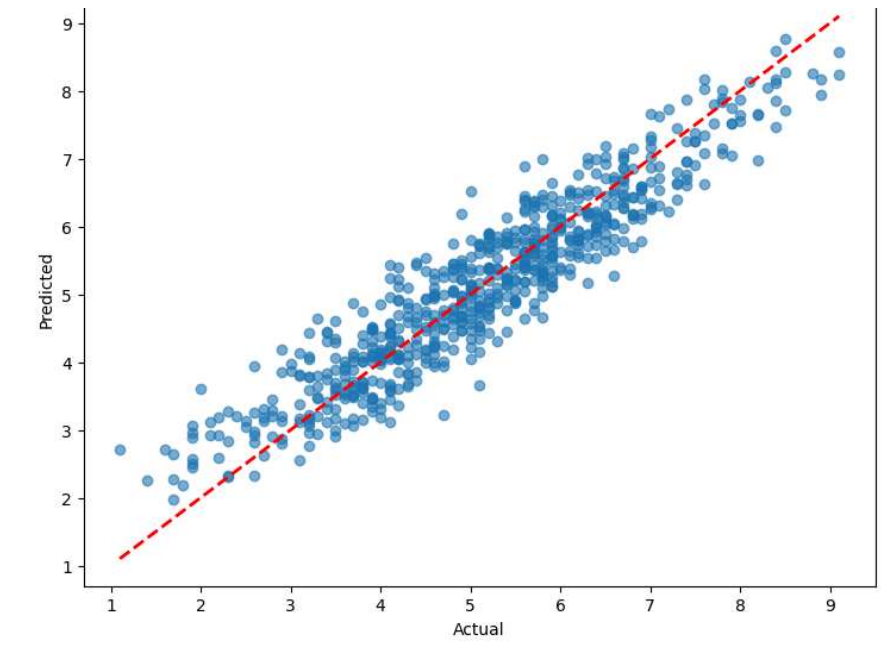
No pattern in residual plot

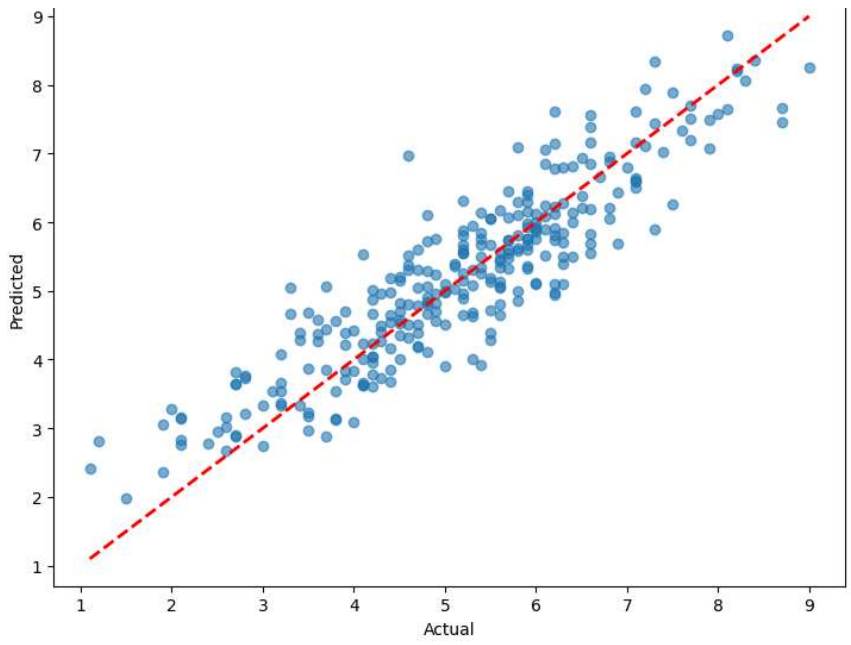
Residual plot has a pattern

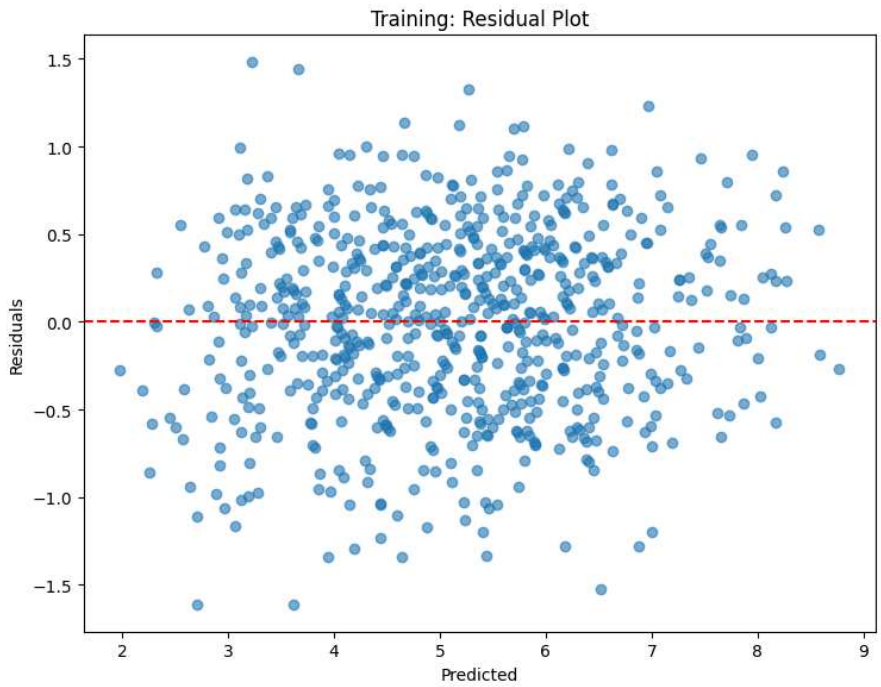
In [16]:

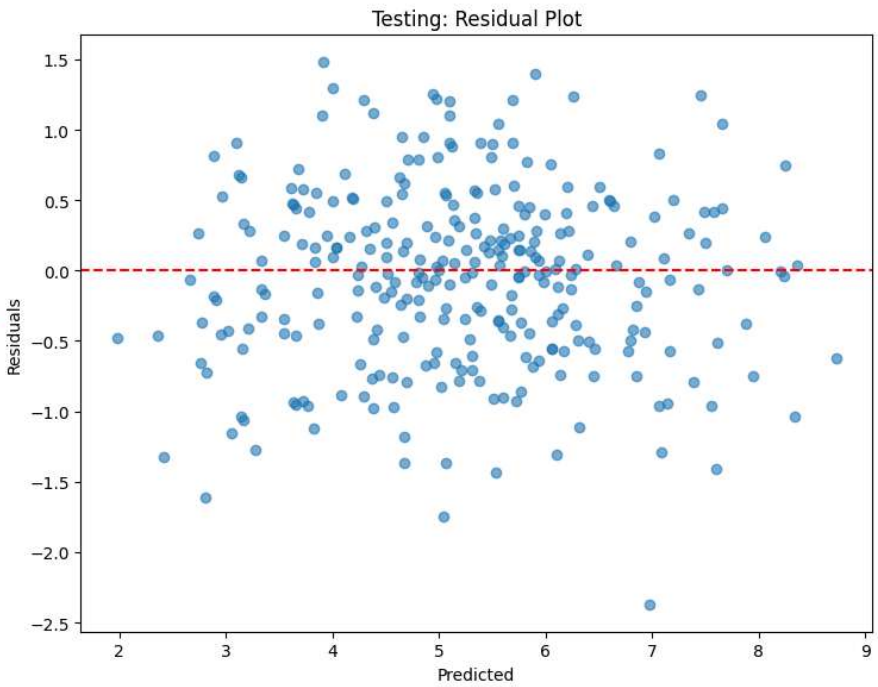
```
# Get best model
best_model = grid_search.best_estimator_

# Make predictions
y_train_pred = best_model.predict(X_train)
y_test_pred = best_model.predict(X_test)

# Calculate metrics
train_r2 = r2_score(y_train, y_train_pred)
test_r2 = r2_score(y_test, y_test_pred)
train_rmse = np.sqrt(mean_squared_error(y_train, y_train_pred))
test_rmse = np.sqrt(mean_squared_error(y_test, y_test_pred))

# Create evaluation plots
fig, axes = plt.subplots(2, 2, figsize=(15, 12))

# Plot 1: Actual vs Predicted for Training
axes[0, 0].scatter(y_train, y_train_pred, alpha=0.6)
axes[0, 0].plot([y_train.min(), y_train.max()], [y_train.min(), y_train.max()], 'r--', lw=2)
axes[0, 0].set_xlabel('Actual')
axes[0, 0].set_ylabel('Predicted')
axes[0, 0].set_title(f'Training: Actual vs Predicted\nR² = {train_r2:.4f}, RMSE = {train_rmse:.4f}')

# Plot 2: Actual vs Predicted for Testing
axes[0, 1].scatter(y_test, y_test_pred, alpha=0.6)
axes[0, 1].plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--', lw=2)
axes[0, 1].set_xlabel('Actual')
axes[0, 1].set_ylabel('Predicted')
axes[0, 1].set_title(f'Testing: Actual vs Predicted\nR² = {test_r2:.4f}, RMSE = {test_rmse:.4f}')

# Plot 3: Residuals for Training
train_residuals = y_train - y_train_pred
axes[1, 0].scatter(y_train_pred, train_residuals, alpha=0.6)
axes[1, 0].axhline(y=0, color='r', linestyle='--')
axes[1, 0].set_xlabel('Predicted')
axes[1, 0].set_ylabel('Residuals')
axes[1, 0].set_title('Training: Residual Plot')

# Plot 4: Residuals for Testing
test_residuals = y_test - y_test_pred
axes[1, 1].scatter(y_test_pred, test_residuals, alpha=0.6)
axes[1, 1].axhline(y=0, color='r', linestyle='--')
axes[1, 1].set_xlabel('Predicted')
axes[1, 1].set_ylabel('Residuals')
axes[1, 1].set_title('Testing: Residual Plot')

plt.tight_layout()
plt.show()

# Print metrics
print("Best Parameters:", grid_search.best_params_)
print("\nTraining Metrics:")
print(f"R²: {train_r2:.4f}")
print(f"RMSE: {train_rmse:.4f}")
print("\nTesting Metrics:")
print(f"R²: {test_r2:.4f}")
print(f"RMSE: {test_rmse:.4f}")
```












```
Best Parameters: {'learning_rate': 0.1, 'max_depth': 3, 'n_estimators': 100, 'subsample': 0.6}

Training Metrics:
R²: 0.8699
RMSE: 0.5291

Testing Metrics:
R²: 0.8111
RMSE: 0.6399
```

Save final model

Prompt:

Save the model in pickle format

Model Explanation with XAI