Introduction to Scikit-Learn -by Mithun

1. Introduction

In Python, **scikit-learn (sklearn)** is the most popular library for implementing ML algorithms efficiently. It provides ready-to-use tools for:

- Loading datasets
- Splitting data
- Training ML models
- Evaluating performance
- Visualizing results

This report explains each step of a basic ML project using the **California Housing Dataset**.

2. Dataset and Objective

We use the California Housing Dataset from scikit-learn.

It contains information about California districts such as:

- Median income
- Average number of rooms
- Population
- Proximity to the ocean and the target variable (y) is the median house price.

Objective:

To build an ML model that predicts housing prices based on these features.

3. Step-by-Step ML Workflow

Step 1: Import Required Libraries

We import essential libraries for dataset handling, model building, and visualization:

from sklearn.datasets import fetch_california_housing from sklearn.model_selection import train_test_split, GridSearchCV from sklearn.preprocessing import StandardScaler from sklearn.linear_model import LinearRegression from sklearn.neighbors import KNeighborsRegressor from sklearn.metrics import mean_squared_error, r2_score import matplotlib.pyplot as plt

- datasets: For loading sample data
- model_selection: For splitting and tuning models
- preprocessing: For scaling features
- metrics: For evaluating performance
- matplotlib: For plotting results

Step 2: Load the Dataset

data = fetch_california_housing() X, y = data.data, data.target

- X = Input features (independent variables)
- y = Output or target variable (dependent variable)

This gives us a feature matrix (X) and a label vector (y).

Step 3: Split the Dataset

We divide the dataset into **training** and **testing** parts.

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

- Training set (80%) → used to train the model.
- Testing set (20%) → used to evaluate how well the model generalizes.

Why split?

If we test on the same data we trained on, the model might "memorize" instead of learning — this is called **overfitting**.

Step 4: Data Preprocessing (Scaling)

Different features may have different ranges (e.g., population vs. rooms).

To make sure no feature dominates others, we scale the data:

```
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X test = scaler.transform(X test)
```

Why scale?

Algorithms like **KNN** and **SVM** are distance-based; scaling ensures fairness across all features.

Step 5: Choose and Train a Model

We try two models:

a) Linear Regression

This assumes a straight-line relationship between input and output.

```
Ir_model = LinearRegression()
Ir_model.fit(X_train, y_train)
```

b) K-Nearest Neighbors (KNN)

This model predicts output based on the average of its nearest data points.

```
knn_model = KNeighborsRegressor(n_neighbors=5)
knn_model.fit(X_train, y_train)
```

Why two models?

Different algorithms behave differently on the same dataset.

Trying multiple models helps compare performance.

Step 6: Make Predictions

Once trained, we test the models on unseen data:

```
y_pred_lr = lr_model.predict(X_test)
y_pred_knn = knn_model.predict(X_test)
```

- y_pred_1r → predictions from Linear Regression
- y_pred_knn → predictions from KNN

Step 7: Evaluate Model Performance

We measure how close predictions are to real values.

```
print("Linear Regression:")
print("MSE:", mean_squared_error(y_test, y_pred_lr))
print("R² Score:", r2_score(y_test, y_pred_lr))

print("\nKNN Regressor:")
print("MSE:", mean_squared_error(y_test, y_pred_knn))
print("R² Score:", r2_score(y_test, y_pred_knn))
```

Metrics Explained:

- MSE (Mean Squared Error): Lower = better
- R² Score: Closer to 1 = better model fit

Step 8: Visualize the Results

Plotting helps us visually check how accurate the predictions are.

```
plt.figure(figsize=(6,6))
plt.scatter(y_test, y_pred_lr, color="blue", alpha=0.5, label="Linear Regression")
plt.scatter(y_test, y_pred_knn, color="red", alpha=0.5, label="KNN")
plt.xlabel("Actual Values")
plt.ylabel("Predicted Values")
plt.legend()
plt.title("Actual vs Predicted Housing Prices")
plt.show()
```

Interpretation:

If the points are close to the diagonal line, predictions are accurate.

Step 9: Hyperparameter Tuning using GridSearchCV

Instead of manually guessing the best n_neighbors for KNN, we can use **GridSearchCV** to test multiple values automatically.

```
param_grid = {'n_neighbors': [3, 5, 7, 9]}
grid = GridSearchCV(KNeighborsRegressor(), param_grid, cv=5)
grid.fit(X_train, y_train)
print("Best parameters:", grid.best_params_)
```

How it works:

GridSearchCV trains and tests models for each parameter combination using **cross-validation**, and picks the one with the best accuracy.

4. Summary of the Workflow

Ste p	Task	Description
1	Import Libraries	Load sklearn, numpy, matplotlib, etc.
2	Load Dataset	Fetch California Housing data
3	Split Data	Divide into training/testing
4	Scale Data	Standardize feature values
5	Train Model	Fit Linear Regression or KNN
6	Predict	Generate predictions for test data
7	Evaluate	Check performance using metrics
8	Visualize	Plot actual vs predicted
9	Tune	Optimize hyperparameters with GridSearchCV

5. Key Takeaways

- Scikit-learn offers a modular approach to machine learning.
- Always partition data to mitigate overfitting.
- Feature scaling is essential for distance-based algorithms.
- Employ multiple models to facilitate performance comparison.
- Hyperparameter tuning with GridSearchCV aids in identifying optimal configurations.
- Visualization is instrumental in interpreting model quality.

PREPOCESSING

2. StandardScaler

2.1 Concept

The **StandardScaler** standardizes features by removing the mean and scaling to unit variance. It transforms each feature such that it has a mean of 0 and a standard deviation of 1.

Formula:

```
(X_{scaled} = \frac{X - \mu}{\sigma})
```

Where:

- (\mu) is the mean of the feature
- (\sigma) is the standard deviation

2.2 Limitation: Sensitivity to Outliers

StandardScaler is **not robust** to outliers. A single extreme value can distort the mean and standard deviation, leading to misleading scaling. For example, if one feature value is significantly higher than the others, the scaled data will be compressed around zero, and the model might underperform.

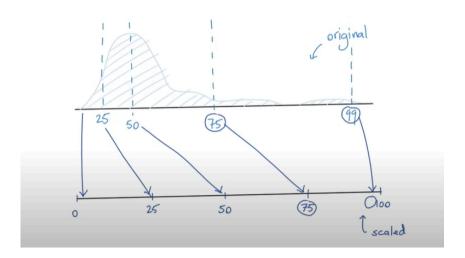
3. Quantiles and QuantileTransformer

3.1 Understanding Quantiles

Quantiles divide the data into equal-sized intervals. For instance:

- The 25th percentile (Q1) marks the point below which 25% of data lies.
- The 50th percentile (Q2 or median) marks the halfway point.

• The 75th percentile (Q3) indicates that 75% of data lies below it.



3.2 QuantileTransformer

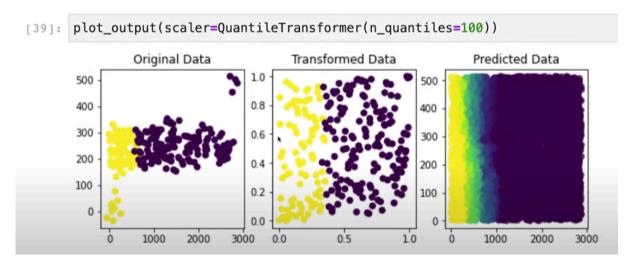
The **QuantileTransformer** maps the original data distribution to a uniform or normal distribution based on quantiles. This technique helps to mitigate the influence of outliers and create a smoother, more balanced scale for features.

3.3 Visual Representation

The provided diagram demonstrates how quantile transformation works. Original data points (e.g., 25, 50, 75, 99) from a skewed distribution are mapped linearly to a new scale (0–100). This makes the transformed data uniformly spaced, removing skewness and reducing the impact of extreme values.

3.4 Use Cases

- When data contains significant outliers.
- When features follow a non-Gaussian distribution.
- For models sensitive to feature scaling, such as SVM or KNN.



4. Polynomial Features

4.1 Concept

Linear models can only capture straight-line relationships. However, many real-world problems involve nonlinear relationships between features and the target variable. **Polynomial features** extend linear models by adding nonlinear combinations of input features.

4.2 Example

If we have a single feature (x), the model can be expanded as: $(y = w_0 + w_1x + w_2x^2 + w_3x^3 + 1)$

In scikit-learn, this is done using:

from sklearn.preprocessing import PolynomialFeatures poly = PolynomialFeatures(degree=2) X_poly = poly.fit_transform(X)

4.3 Benefit

Adding polynomial terms allows models such as **Linear Regression** or **Logistic Regression** to fit curved patterns, improving accuracy on datasets with nonlinear relationships.

5. OneHotEncoder

5.1 Purpose

Most machine learning models require numerical input. The **OneHotEncoder** converts categorical features into numerical form by creating binary columns (0 or 1) for each category.

5.2 Example

Color	Red	Blue	Green
Red	1	0	0
Blue	0	1	0
Gree n	0	0	1

In scikit-learn:

from sklearn.preprocessing import OneHotEncoder encoder = OneHotEncoder(sparse_output=False)

5.3 Advantages

- Prevents numerical ordering in categorical data.
- Helps models understand distinct categories.
- Especially useful for tree-based and regression models.

5.4 Limitations

- May create many columns if a feature has numerous categories (known as the curse of dimensionality).
- Does not handle unknown categories unless explicitly configured.

6. Summary

Technique	Purpose	Best Used When	Limitation
StandardScaler	Standardize features to mean=0, std=1	Data is approximately normal and outliers are minimal	Sensitive to outliers
QuantileTransform er	Map data to uniform/normal distribution	Data is skewed or contains outliers	May distort small datasets
PolynomialFeature s	Add nonlinear feature combinations	When data relationships are nonlinear	May cause overfitting
OneHotEncoder	Encode categorical variables	When data has text categories	Increases feature space size

7. Conclusion

Data preprocessing is the foundation of effective machine learning. Choosing the right preprocessing method depends on the data distribution, feature type, and model sensitivity. Techniques like **QuantileTransformer** make data robust to outliers, while **PolynomialFeatures** expand model capability to capture complex patterns. **OneHotEncoder** ensures categorical variables are properly represented, improving model interpretability and accuracy.

METRICS

```
n_jobs=-1
) given that i prealet traud
) how accurate aux i
: from sklearn.metrics import precision_score, recall_score
recall_score(y, grid.predict(X))
: 0.5918367346938775

did i get all the fraud cases
```

META ESTIMATORS

Meta-Estimators in Scikit-learn

1. Introduction

Meta-estimators are models that build upon other models. Instead of relying on a single algorithm, they combine the predictions of multiple estimators to produce more robust and accurate results. Scikit-learn provides several meta-estimators, such as **VotingClassifier**, **BaggingClassifier**, and **StackingClassifier**. These methods enhance model stability, reduce overfitting, and balance performance across datasets.

2. Voting Classifier

2.1 Concept

The **VotingClassifier** is a simple ensemble technique that aggregates predictions from multiple models (also called base estimators). The final prediction is determined either by majority voting or by averaging probabilities.

- **Hard Voting:** Each model votes for a class label, and the class with the most votes becomes the final prediction.
- Soft Voting: Each model predicts class probabilities, and the final prediction is based on the
 average of these probabilities.

This method assumes that combining several weak or moderately strong models can lead to a more reliable and stable prediction overall.

2.2 Example

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC

log_clf = LogisticRegression()
knn_clf = KNeighborsClassifier()
svc_clf = SVC(probability=True)

voting_clf = VotingClassifier(
    estimators=[('lr', log_clf), ('knn', knn_clf), ('svc', svc_clf)],
    voting='soft'
)
```

from sklearn.ensemble import VotingClassifier

from sklearn.linear_model import LogisticRegression

The VotingClassifier combines the strengths of Logistic Regression, KNN, and SVM to make a collective decision.

2.3 Difference Between Logistic Regression and KNN

Feature	Logistic Regression	K-Nearest Neighbors
Туре	Parametric (learns weights)	Non-parametric (memory-based)
Learning Approach	Learns a decision boundary during training	Makes predictions based on nearest data points
Complexity	Fast to train, slower to converge for nonlinear data	Slow at prediction time due to distance calculations
Interpretability	Provides coefficients and probabilities	Difficult to interpret, depends on data distribution
Usage in VotingClassifier	Learns a global relationship	Adds local neighborhood-based decisions

The difference in nature between these models helps improve ensemble diversity, which is key to a strong voting classifier.

3. Scikit-Lego

3.1 Overview

Scikit-lego is an extension library for scikit-learn that introduces additional transformers, estimators, and tools designed for more flexible workflows. It complements scikit-learn by providing practical utilities that are often needed in real-world machine learning pipelines.

3.2 Features

- Extra meta-estimators and pipeline utilities
- Transformers for data cleaning and feature engineering
- Model inspection tools and wrappers

Example usage:

from sklego.meta import EstimatorTransformer from sklearn.linear_model import LogisticRegression

model = EstimatorTransformer(LogisticRegression())

This library enables scikit-learn users to extend standard functionality without rewriting core components.

4. HumanLearn

4.1 Concept

HumanLearn is a library built to bridge the gap between human reasoning and machine learning models. It allows the creation of interpretable rules based on human-understandable logic rather than complex algorithms.

4.2 Purpose

The main objective of HumanLearn is to make models explainable, auditable, and easier to understand. It focuses on rule-based decision making rather than opaque statistical fitting.

Example:

```
from humanlearn import RuleLearner rules = [
    (lambda x: x['age'] > 50, 1),
    (lambda x: x['income'] < 20000, 0)
]
model = RuleLearner(rules=rules)
```

This provides a structured way to express model logic similar to human decision-making.

5. Conclusion

Meta-estimators in scikit-learn represent a shift from relying on single models to combining multiple approaches for greater reliability. The **VotingClassifier** exemplifies this by merging diverse algorithms like Logistic Regression and KNN, improving performance and generalization. Tools such as **scikit-lego** and **HumanLearn** extend scikit-learn's capabilities, promoting more expressive, interpretable, and adaptable workflows for modern machine learning tasks.