Supervised Learning Foundations

Data split
Model evaluation
Performance vs Interpretability
Accuracy vs Generalization
Regularization (L1, L2)
Feature Engineering
Hyperparameters

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Training-Test Split

Definition

A train-test split is a method to divide data into two subsets:

- Training set: to train the machine learning model (larger size).
- Test set: to evaluate the performance on unseen data.

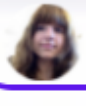
Common methods

1. **Simple split:** dividing the entire dataset.
   Common ratio is 80% training : 20% test
   If dataset size allows: 70% training : 20% validation : 10% test
   Common advanced models ratio is 90% training :10% test or 85 : 15

2. **Cross-validation:** multiple train-test splits to assess the model's performance. Most popular is k-Fold Cross-Validation.

3. **Stratified split (imbalanced datasets):** each class in the dataset is represented proportionally in both train and test sets.

4. **Time Series split (time-dependent data):** common approach is using the most recent observations for test set.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Training-Test Split

Important

- Training set: must be always larger than test set.
- Test set: remains untouched during training (unbiased evaluation)

Scikit-Learn library makes splitting data easy using train_test_split

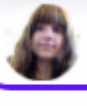
Replace test_size=0.2 indicated 80 : 20 split (replace if needed)

Use stratify=y to ensure proportional representation in sets

```
from sklearn.model_selection import train_test_split

# Assume X (features) and y (target) are already defined
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42, stratify=y
)

print("Training set size:", len(X_train))
print("Test set size:", len(X_test))
```



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Evaluation: Classification Model

Confusion matrix

	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
Actual Negative	False Positive (FP)	True Negative (TN)

Core evalutation metrics

Accuracy : overall correctness. (TP + TN) / (Total Predictions)

Precision: % of correctly predicted positives among all positives. TP / (TP + FP)

Recall: % of correctly predicted positives among all corrects. TP / (TP + FN)

F1 score: model's performance. 2 * (Precision * Recall) / (Precision + Recall)

Secondary evalutation metrics

AUC-ROC curve: discrimination between positives and negatives.
0.5 - random guess, 1.0 - perfect discrimination.

Log Loss: correctness of prediction. 0 - perfect, ∞ - highly inaccurate.

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Evaluation: Classification Model

Precision or Recall?

Precision if the cost of False Positive is high.

Examples: insurance company pay false claim, bank gives a loan to a customer with bad records, cybersecurity (false alarms disrupt operations).

Recall if capturing Positives is more important than avoiding False Positives.

Examples: fraudulent transactions detection, retail recommender system.

Scikit-Learn

```
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score, confusion_matrix, classification_report

# Predictions and true labels
y_true = [1, 0, 1, 1, 0, 1, 0, 0, 1]
y_pred = [1, 0, 1, 0, 0, 1, 1, 0, 1]

# Compute metrics
print("Accuracy:", accuracy_score(y_true, y_pred))
print("Precision:", precision_score(y_true, y_pred))
print("Recall:", recall_score(y_true, y_pred))
print("F1 Score:", f1_score(y_true, y_pred))

# Confusion matrix
matrix = confusion_matrix(y_true, y_pred)
print("Confusion Matrix:\n", matrix)

# Classification Report
print("Full Report:\n", classification_report(y_true, y_pred))
```

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Evaluation: Regression Model

Evalutation metrics

y = target variable value n = number of observations

yi = actual value yi^ = predicted value $\bar{y_i}$ = mean of actual value

MAE (Mean Absolute Error): average absolute difference between the predicted and actual values. Most interpretable. $MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$

MSE (Mean Squared Error): average of the squared difference between the actual and predicted values. Penalizes for large errors. $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

RMSE (Root Mean Squared Error): like MSE, but expressed in the same units as the target variable. $RMSE = \sqrt{MSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$

MAPE (Mean Absolute Percentage Error): average of the absolute percentage differences between the actual and predicted values. $MAPE = \frac{100}{n}\sum_{i=1}^{n}|\frac{y_i - \hat{y}_i}{y_i}|$

R^2 (R-square): percentage of variance explained. $R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \overline{y})^2}$

Adjusted R^2 : if higher than R^2, then the model is too complex (extra predictors do not add value. $Adjusted\ R^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - p - 1}$

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Evaluation: Regression Model

Which metric is the best?

MAE or MAPE: interpretable, larger errors are acceptable as long as they cancel each other. Example: real estate (house prices).

MSE or R^2: relationship is deterministic, precision is critical, larger errors significantly impact conclusions. Example: R&D, engineering.

RMSE: larger errors must be penalized because they lead to system collapse. Example: supply chain, electricity demand forecasting.

MAPE: comparing models with different absolute values of target variable. Example: sales forecast for different countries.

Scikit-Learn

```python
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
import numpy as np

# True values (y) and predicted values (y_pred)
y_true = [100, 200, 300, 400, 500]
y_pred = [110, 190, 310, 420, 490]

# Calculate metrics
mae = mean_absolute_error(y_true, y_pred)
mse = mean_squared_error(y_true, y_pred)
rmse = np.sqrt(mse)
r2 = r2_score(y_true, y_pred)
```

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Performance vs Interpretability

Definitions

Performance: how well a model makes accurate predictions on unseen data. Key focus: **evaluation metrics**, generalization (evaluation on test set).

Interpretability: how easily humans can understand and explain how a model makes predictions. Key focus: **which factors** impact predictions and **how**.

High Interpretability (Simple Models) <-> High Performance (Complex Models)

Models by complexity

Core models

Regression: linear, non-linear, time series

Classification: logistic regression, Naive Bayes, k-NNs

Decision Trees

(tree depth: trade-off between performance and interpretability)

Support Vector Machines

Ensemble: Bagging

Ensemble: Boosting

Neural Networks


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Performance or Interpretability?

Rule of thumb

Performance = Execution. **Interpretability** = Design or Regulations.

Examples

Fast Moving Consumer Goods
Interpretability - Marketing designs go-to-market campaign and needs to know how levels of media budget and its split impact profit.
Performance - Supply Chain Manager splits the forecast into weeks or days to secure stocks but avoid excessive inventory.

Fashion
Interpretability - Merchandiser aims to plan seasonal collections and needs to know which product attributes (e.g., colors, fabrics, styles) drive sales.
Performance - Recommender system for better conversions.

Banking
Interpretability - Credit risk officer wants to determine why a customer is likely to default on a loan (e.g., income instability, spending patterns).
Performance - Fraud detection model flags suspicious transactions in real time during online banking.

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Accuracy and Generalization

Definitions

Bias → Accuracy: how closely a model captures the patterns of the data.

- High Bias: The model oversimplifies, missing important patterns (**underfitting**).
- Low Bias: The model learns the patterns effectively but can become prone to minor changes in data (**overfitting**).

Variance → Generalization: how sensitive a model is to fluctuations in the data.

- High Variance: The model fits the training data very closely but fails to generalize to new data (**overfitting**).
- Low Variance: The model is more stable across datasets but might miss nuanced details (**underfitting**).

Detection

	High bias (underfit)	**High variance (overfit)**
Training error	High	Low
Test error	High	High
Learning curve	Training and Test errors are both high and close	Large gap between Training and Test errors


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Fit detection: classification

F1-score comparison between Training and Test

- Underfitting: both training and test scores are low and unsatisfactory
- Overfitting: training score is high, but test score is much lower
- Balanced Model: training and test scores are similar and satisfactory

Scikit-Learn

```python
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import f1_score

# Load data (replace 'classification_data.csv' with your file)
data = pd.read_csv('classification_data.csv')
X = data.drop(columns=['target'])  # Replace 'target' with your target column name
y = data['target']

# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# Fit logistic regression
model = LogisticRegression()
model.fit(X_train, y_train)

# Calculate F1-Scores
train_f1 = f1_score(y_train, model.predict(X_train))
test_f1 = f1_score(y_test, model.predict(X_test))

print(f"Training F1-Score: {train_f1:.2f}")
print(f"Test F1-Score: {test_f1:.2f}")
```

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Fit detection: regression

RMSE (or another error metric) comparison between Training and Test

- Underfitting: both training and test scores are low and unsatisfactory
- Overfitting: training score is high, but test score is much lower
- Balanced Model: training and test scores are similar and satisfactory

Scikit-Learn

```python
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error
import numpy as np

# Load data (replace 'regression_data.csv' with your file)
data = pd.read_csv('regression_data.csv')
X = data[['feature']]  # Replace with the name of your feature column
y = data['target']     # Replace with the name of your target column

# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# Fit linear regression
model = LinearRegression()
model.fit(X_train, y_train)

# Calculate RMSE
train_rmse = np.sqrt(mean_squared_error(y_train, model.predict(X_train)))
test_rmse = np.sqrt(mean_squared_error(y_test, model.predict(X_test)))

print(f"Training RMSE: {train_rmse:.2f}")
print(f"Test RMSE: {test_rmse:.2f}")
```

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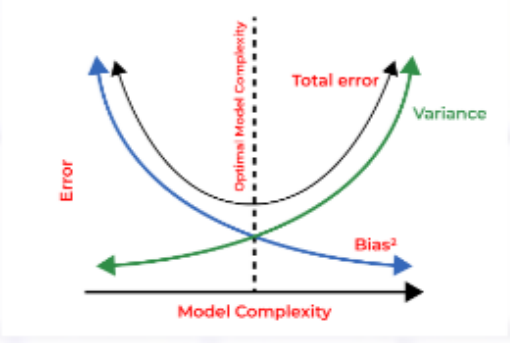
Balancing Bias and Variance

1. Selecting right model complexity!!!



2. Cross-validation

Split the data multiple times to ensure the model generalizes well.

3. Regularization: L1 (Lasso), L2 (Ridge)

Penalizes overly complex models to reduce variance.

4. Other methods

- Decision Tree: pruning, max depth, min samples leaf
- Random Forest: max features, tree constraints
- Boosting: learning rate shrinkage, subsampling
- Neural Networks: dropout, batch normalization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Regularization

Definition

Regularization is a technique used to reduce overfitting by **discouraging complexity** in the model during training. It works after the initial evaluation, not preprocessing.

Types

1. L1 Regularization (Lasso)

Adds a penalty proportional to the absolute values of the model coefficients ($\sum|\text{weights}|$).Drives some weights to exactly 0, leading to sparse models (automatic feature selection).

2. L2 Regularization (Ridge)

Adds a penalty proportional to the squared values of the model coefficients ($\sum\text{weights}^2$). Shrinks coefficients smoothly, preventing extreme weight values and reducing sensitivity.


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Regularization

Application

Scenario
A marketing team is conducting extended A/B testing on ad campaigns. They want to optimize for click-through rate (CTR) and engagement. They experiment with 100+ factors, including variations in layout, headlines, color schemes, audiences, etc. However, some features introduce noise and overload the model.

Problem = Generalization
Unstable or inconsistents results, when applied to new campaigns. Recommendations like *"This shade of blue in Region X leads to CTR spikes during weekdays"*.

After regularization
The team focuses on impactful patterns, like:

- Certain headlines (urgency-related) universally boost CTR.
- Specific color schemes appeal broadly.
- "Buy Now" consistently overperforms “Learn More”.

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Feature Engineering

Definitions

Feature: A measurable property or characteristic of your data that helps the model predict the target outcome.
Example (sales prediction): price, advertising spend, seasonality.

Feature Engineering: the process of creating, transforming, and selecting features to improve model performance. Usually done at data preprocessing, sometimes after initial model evaluation.

Stages

1. **Creation:** deriving features from raw data.
2. **Transformation:** modifying features to make them more interpretable or linear for the model.
3. **Extraction:** seriving high-level features from complex data.
4. **Scaling:** standardizing or normalizing numerical features.

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Feature Engineering

Stage	Libraries and Functions	Example output
Creation	pandas, featuretools	daily sales aggregated to monthly
Transformation	numpy, scipy.stats, sklearn.preprocessing	sales growth %, log transformed sales
Extraction	sklearn.feature_extraction, tensorflow, opencv	lag features, rolling averages
Selection	sklearn.feature_selection, Lasso, RFE	log_1 and rolling_avg_3 are most useful for future predictions
Scaling	sklearn.preprocessing (MinMaxScaler, StandardScaler)	z-score normalization (all values have similar ranges)

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Hyperparameters tuning

Definitions

Hyperparameters: parameters set before training; control learning process.

Hyperparameters tuning: a process to optimize hyperparameters.

Rule of thumb

Simple model (few parameters, less sensitive)
<->
Complex model (may parameters, sensitive)

Key hyperparameters

Linear and Logistic Regressions: regularization strength

Decision Tree: complexity (max_depth, min_samples_split, min_samples_leaf)

SVM: regularization strength, kernel (type, coefficient - gamma)

Random Forest: complexity (n_estimators, max_depth)

Boosting: iterations (n_estimators), shrinking contribution (learning_rate)

Neural Networks: Learning Rate (lr), batch size, layers and neurons, dropout rate, activation functions (relu, sigmoid, tanh), optimizer (adam, sgd, rmsprop)

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