



### **CS316: INTRODUCTION TO AI AND DATA SCIENCE**

# CHAPTER 7 CLASSIFICATION

# LECTURE 1 INTRODUCTION TO CLASSIFICATION

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www.riotu-lab.org

## **Learning Outcomes**

### 1. Explain Classification Concepts:

- Differentiate between binary and multi-class classification.
- Identify and describe accuracy, precision, recall, and F1-score.

### 2. Apply Logistic Regression:

Understand and implement logistic regression, interpreting its parameters.

### 3. Interpret a Classification Report:

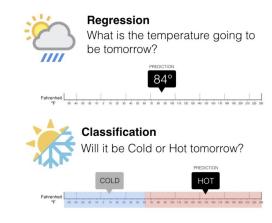
Analyze classification reports to evaluate model accuracy and effectiveness.

### 4. Use ROC for Model Evaluation:

 Construct and interpret ROC curves and calculate the Area Under the Curve (AUC) to assess model performance.

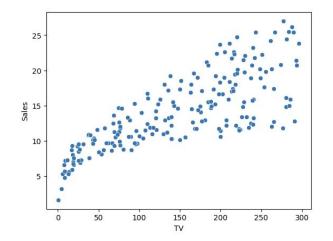
### Introduction to Classification

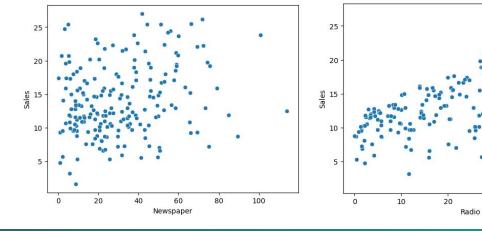
- Definition:
  - Classification: Assign labels from a finite set based on input features.
- Mathematical Framework:
  - ullet Let  $X\subseteq\mathbb{R}^n$  be the feature space and  $Y=\{y_1,y_2,\ldots,y_k\}$  the label set.
  - Seek function  $f:X \to Y$ .
- . Comparison with Regression:
  - Regression:  $\hat{y} = f(x)$ ,  $f: X \to \mathbb{R}$  (Continuous output).
  - Classification:  $\hat{y} = f(x), f: X \to Y$  (Discrete output).



## Regression Use Case

	ID	TV	Radio	Newspaper	Sales
0	1	230.1	37.8	69.2	22.1
1	2	44.5	39.3	45.1	10.4
2	3	17.2	45.9	69.3	9.3
3	4	151.5	41.3	58.5	18.5
4	5	180.8	10.8	58.4	12.9





40

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30

### **Classification - Heart Disease Prediction**

#### · Features Explained:

- . Age: Patient's age in years.
- Sex: Patient's gender (1 = male, 0 = female).
- Cp (Chest Pain Type): Type of chest pain experienced (values from 1 to 4).
- Trestbps (Resting Blood Pressure): Resting blood pressure in mm Hg.
- . Chol (Serum Cholesterol): Serum cholesterol in mg/dl.
- Fbs (Fasting Blood Sugar): Fasting blood sugar > 120 mg/dl (1 = true, 0 = false).
- Restecg (Resting ECG Results): Results of electrocardiogram at rest (0, 1, or 2).
- Thalach (Max Heart Rate Achieved): Maximum heart rate achieved.
- Exang (Exercise Induced Angina): Angina induced by exercise (1 = yes, 0 = no).
- Oldpeak: ST depression induced by exercise relative to rest.
- Slope: Slope of the peak exercise ST segment.
- · Ca: Number of major vessels colored by fluoroscopy.
- Thal: Thalassemia (3 = normal; 6 = fixed defect; 7 = reversible defect).
- . Target Variable (Highlighted):
- Num (Diagnosis of Heart Disease): The degree of heart disease (0 = no presence, 1-4 indicate varying degrees of heart disease).

	age	sex	ср	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	num	Target
0	63	1	1	145	233	1	2	150	0	2.3	3	0.0	6.0	0	NO
1	67	1	4	160	286	0	2	108	1	1.5	2	3.0	3.0	2	YES
2	67	1	4	120	229	0	2	129	1	2.6	2	2.0	7.0	1	YES
3	37	1	3	130	250	0	0	187	0	3.5	3	0.0	3.0	0	NO
4	41	0	2	130	204	0	2	172	0	1.4	1	0.0	3.0	0	NO

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**CLASSIFICATION TECHNIQUES** 

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## **Major Classification Techniques**

### Purpose of Classification:

 To categorize data into predefined labels based on their attributes, aiding in predictive analysis across diverse applications.

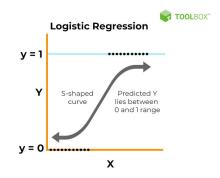
### Major Classification Techniques:

### . Logistic Regression:

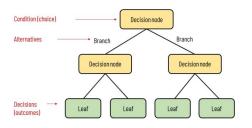
- Suitable for binary classification tasks. Models the probability of the default class via the logistic function.
- Equation:  $logit(p) = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n$

### Decision Trees:

- Splits the data into branches to make decisions. Useful for both categorical and continuous input and output variables.
- · Criteria: Information Gain, Gini Impurity.



### Elements of a decision tree



## **Major Classification Techniques**

### Support Vector Machines (SVM):

- Finds the hyperplane that best divides a dataset into classes with the maximum margin.
- Equation: minimize  $\frac{1}{2} \|\mathbf{w}\|^2$  subject to  $y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1, \forall i$

#### Random Forests:

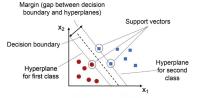
- An ensemble of decision trees designed to improve classification accuracy and control overfitting.
- Mechanism: Each tree votes for a class, and the majority vote decides the final class.

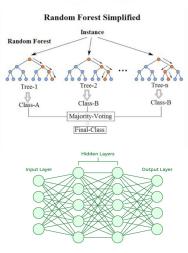
#### Neural Networks:

- . Mimics the workings of the human brain to classify data based on deep learning techniques.
- . Layers: Input, hidden, and output layers with activation functions like Sigmoid, ReLU.

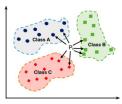
### . k-Nearest Neighbors (k-NN):

- · Classifies new cases based on a similarity measure (e.g., distance functions).
- . Rule: Assign the class most common among the nearest k neighbors.





K Nearest Neighbors



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**OUTPUT ENCODING** 

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### **Encoding the OUTPUT in Classification**

### · Purpose of Encoding:

 Convert categorical variables into a numerical format suitable for algorithmic processing, enabling integration into mathematical models.

### · Label Encoding:

- Definition: Map each unique category to a unique integer.
- Example for 'Target': Map 'NO' → 0 and 'YES' → 1.

• Mathematical Representation: 
$$\mathrm{Target}_{\mathrm{encoded}} = \begin{cases} 0 & \mathrm{if} \ \mathrm{Target} = \mathrm{'NO'} \\ 1 & \mathrm{if} \ \mathrm{Target} = \mathrm{'YES'} \end{cases}$$

Target	num	thal	ca	slope
NO	0	6.0	0.0	3
YES	2	3.0	3.0	2
YES	1	7.0	2.0	2
NO	0	3.0	0.0	3
NO	0	3.0	0.0	1

## **Encoding the Target Variable in Python**

- Purpose of Label Encoding:
  - Convert categorical text data into a model-readable numerical format.
- Using Pandas for Label Encoding:
  - Code Example:

```
import pandas as pd
data = {'Target': ['NO', 'YES', 'NO', 'YES']}
df = pd.DataFrame(data)
df['Target_encoded'] = df['Target'].astype('category').cat.codes
print(df)
```

	Target	Target_encoded
0	N0	0
1	YES	1
2	NO	0
3	YES	1

- Key Points:
  - Label encoding is straightforward but introduces a numerical order that may not exist, influencing some model types.

## **One-Hot Encoding**

### One Hot Encoding:

- **Definition:** Convert each category value into a binary vector representing the presence (1) or absence (0) of the feature.
- Mathematical Representation: Define indicator function  $\mathbf{1}_{\mathrm{category}}(x)$  for each category in the variable.
- Example for 'Target':
  - 'NO' → [1, 0]
  - 'YES' → [0, 1]
- Vector Form:
  - $Target_{NO} = \mathbf{1}_{'NO'}(Target)$
  - $Target_{YES} = \mathbf{1}_{'YES'}(Target)$

slope	ca	thal	num	Target
3	0.0	6.0	0	NO
2	3.0	3.0	2	YES
2	2.0	7.0	1	YES
3	0.0	3.0	0	NO
1	0.0	3.0	0	NO

## One-Hot Encoding - Scikit-learn

### Purpose of One-Hot Encoding:

- Converts each category into a distinct binary column, which is crucial for models that do not assume any ordinal relationship between categories.
- Updated Code for Scikit-learn One-Hot Encoding:
  - · Here's how to handle the one-hot encoding correctly using the latest Scikit-learn methods:

```
python

from sklearn.preprocessing import OneHotEncoder

encoder = OneHotEncoder(sparse_output=False) # Corrected parameter usage
encoded = encoder.fit_transform(df[['Target']]) # Assuming df is predefined
df_encoded = pd.DataFrame(encoded, columns=encoder.get_feature_names_out(['Target']])
df = pd.concat([df, df_encoded], axis=1)
print(df)
```

- . Key Updates and Considerations:
  - The use of `get\_feature\_names\_out()` to retrieve column names from the encoder, replacing
    deprecated `get\_feature\_names()`.
  - Specifying `sparse\_output=False` to handle the deprecation notice about the `sparse` parameter.

## One-Hot Encoding with Scikit-learn

	Target	Target_N0	Target_YES
0	NO	1.0	0.0
1	YES	0.0	1.0
2	NO	1.0	0.0
3	YES	0.0	1.0

## One-Hot Encoding - Pandas

- Alternative Method with Pandas:
  - Often simpler and more direct for handling within a DataFrame context.
- Using Pandas for One-Hot Encoding:
  - Code Example:

```
python

df_one_hot = pd.get_dummies(df['Target'], prefix='Target')

df = pd.concat([df, df_one_hot], axis=1)
print(df)
```

- Considerations:
  - 'get\_dummies' is very efficient and directly integrates with pandas DataFrames, making it ideal for exploratory data analysis and preliminary data processing.

<b>One-Hot Encodi</b>	ng
with Pandas	

	Target	Target_N0	Target_YES	Target_N0	Target_YES
0	NO	1.0	0.0	True	False
1	YES	0.0	1.0	False	True
2	NO	1.0	0.0	True	False
3	YES	0.0	1.0	False	True

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**Logistic Function (Sigmoid)** 

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### **LOGISTIC REGRESSION**

### Definition:

 Logistic Regression is a statistical method for binary classification that models the probability of a binary response based on one or more predictor variables.

### · Mathematical Representation:

• It estimates probabilities using the logistic function, which is an S-shaped curve that maps any real-valued number into the (0, 1) interval, making it suitable for modeling probability.

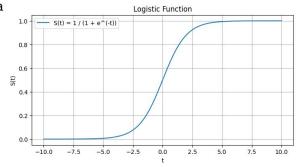
### • Logistic Function:

· The logistic function is defined as:

$$\sigma(z)=rac{1}{1+e^{-z}}$$

 Where z is the linear combination of the input features X and their corresponding coefficients β, expressed as:

$$z = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$



#### Purpose:

- **Predictive Modelling:** Predicts the probability P that an observation falls into the category Y=1 (positive class), as opposed to Y=0 (negative class).
- Decision Boundary: The decision boundary in logistic regression, which is set at  $\sigma(z)=0.5$ , determines the threshold at which the probability output is converted into class labels.
- · Mathematical Goal:
- Maximize Likelihood: The parameters β are typically estimated using maximum likelihood estimation (MLE), which seeks to maximize the likelihood function, ensuring the best model coefficients that predict the observed outcomes.

## Logit in Logistic Regression

### · Logit to Sigmoid Relationship:

• The logistic regression model begins with a linear combination of input features  $x_i$  and their respective coefficients  $\beta_i$ :

$$z = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

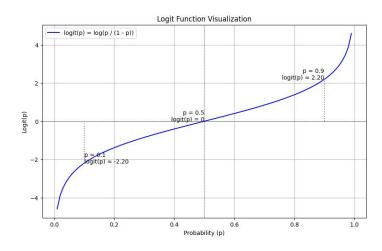
 The linear combination z then becomes the input to the logit function, which computes the logodds of a positive outcome:

$$\operatorname{logit}(P(Y=1|X)) = \log\left(rac{P(Y=1|X)}{1-P(Y=1|X)}
ight) = z$$

• This relationship can be expressed more explicitly:

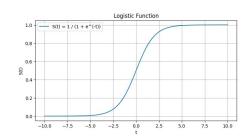
$$\operatorname{logit}(P(Y=1|X)) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

 Thus, the logit function provides a direct link between the linear combination of features and the log-odds of a positive outcome.



- p = 0.1: Here, the probability is low, and the logit value is negative, indicating a decreased likelihood of the positive outcome.
- p = 0.5: This point corresponds to equal odds (logit = 0), meaning the likelihood of positive and negative outcomes is balanced.
- p = 0.9: At this high probability, the logit value is positive and large, signifying a higher likelihood of
  the positive outcome.

## **Logit vs Sigmoid**



### Sigmoid (Logistic) Function:

 The sigmoid function is the inverse of the logit function and converts the linear combination z into a probability between 0 and 1:

$$\sigma(z) = rac{1}{1+e^{-z}}$$

 Substituting the linear combination into the sigmoid function, we can predict the probability of the positive outcome as:

$$P(Y=1|X)=rac{1}{1+e^{-(eta_0+eta_1x_1+eta_2x_2+\cdots+eta_nx_n)}}$$

 This relationship translates the linear combination of features and coefficients into a probability of the positive outcome by applying the nonlinear sigmoid transformation.

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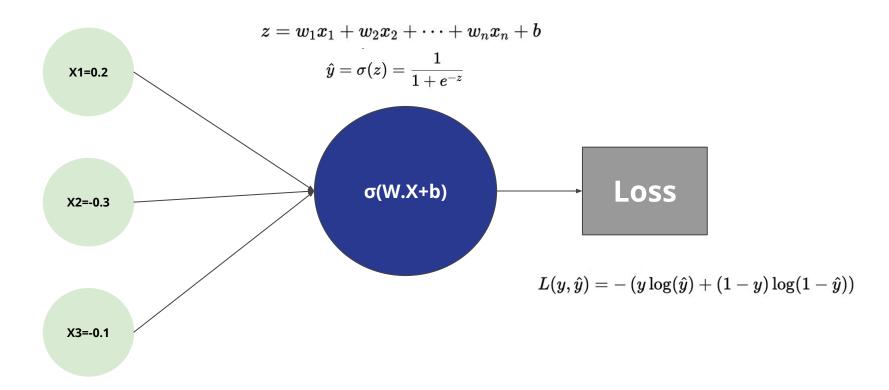
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**LOGISTIC REGRESSION** 

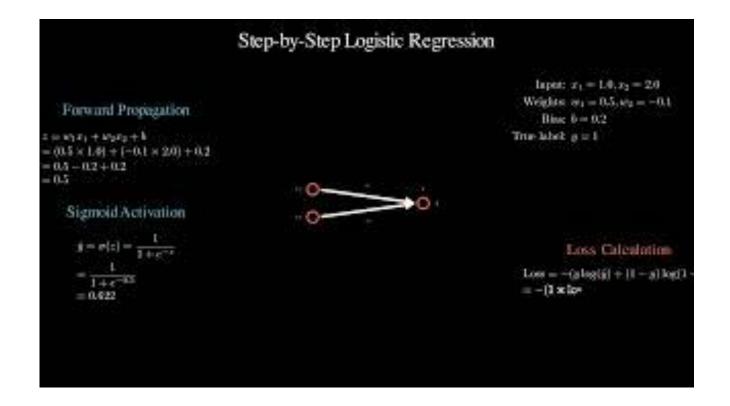
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## Logistic Regression as Perceptron



## Logistic Regression as Perceptron



## Logistic Regression: Bridging Perceptron

### Logistic Regression as a Perceptron

1. Input Features:

$$\mathbf{x} = [x_1, x_2, \dots, x_n]$$

2. Weights and Bias:

$$\mathbf{w} = [w_1, w_2, \dots, w_n], \quad b$$

3. Linear Combination:

$$z = \mathbf{w} \cdot \mathbf{x} + b$$

- Weighted sum of input features plus bias.
- 4. Sigmoid Activation:

$$\sigma(z)=rac{1}{1+e^{-z}}$$

Maps z to a value between 0 and 1 (probability).

## Logistic Regression: Mathematical Formulation

### **Mathematical Representation of Logistic Regression**

1. Linear Combination (Weighted Sum):

$$z=w_1x_1+w_2x_2+\cdots+w_nx_n+b$$

- Computes the linear combination of input features  $\mathbf{x}=[x_1,x_2,\ldots,x_n]$  and weights  $\mathbf{w}=[w_1,w_2,\ldots,w_n]$ , adding the bias b.
- 2. Sigmoid Activation Function:

$$\hat{y}=\sigma(z)=rac{1}{1+e^{-z}}$$

- Transforms the linear combination z into a probability  $\hat{y}$ , mapping the result between 0 and 1.
- 3. Log-Loss Function:

$$L(y, \hat{y}) = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$$

Measures the performance of a classification model whose output is a probability between 0
and 1. The loss increases as the predicted probability diverges from the actual label y.

## **Gradient Descent: Optimizing Weights and Bias**

### **Optimizing Logistic Regression Model**

### **Gradient Descent Method:**

- Purpose: Minimize the loss function L to find the best parameters (w and b).
- Update Rules:

$$w_j := w_j - \eta rac{\partial L}{\partial w_j}, \quad b := b - \eta rac{\partial L}{\partial b}$$

- $\eta$  (eta) is the learning rate, controlling the size of the update step.
- $w_i$  are the weights, b is the bias.

### **Partial Derivatives:**

· Gradient with respect to weights:

$$rac{\partial L}{\partial w_{i}}=(y-\hat{y})x_{j}$$

· Gradient with respect to bias:

$$rac{\partial L}{\partial b} = (y - \hat{y})$$

- $\hat{y}$  is the predicted probability from the sigmoid function.
- y is the actual label.
- $x_j$  is the input feature corresponding to weight  $w_j$ .

## **Sigmoid Function**

#### Definition:

 Logistic Regression is a statistical method for binary classification that models the probability of a binary response based on one or more predictor variables.

#### · Mathematical Representation:

 It estimates probabilities using the logistic function, which is an S-shaped curve that maps any real-valued number into the (0, 1) interval, making it suitable for modeling probability.

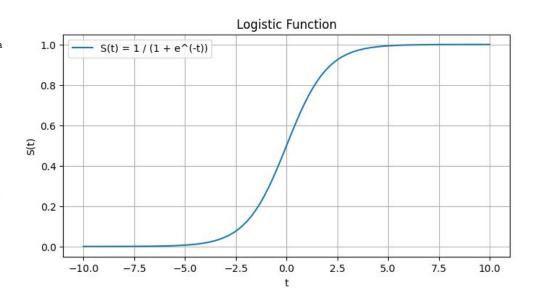
#### · Logistic Function:

• The logistic function is defined as:

$$\sigma(z)=rac{1}{1+e^{-z}}$$

• Where z is the linear combination of the input features X and their corresponding coefficients  $\beta$ , expressed as:

$$z = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n$$



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TRAINING A LOGISTIC REGRESSION CLASSIFICATION MODEL

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## **Preparing the Heart Disease Dataset**

### **Input Features**

### **Output**

	age	sex	ср	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	num	Target
0	63	1	1	145	233	1	2	150	0	2.3	3	0.0	6.0	0	NO
1	67	1	4	160	286	0	2	108	1	1.5	2	3.0	3.0	2	YES
2	67	1	4	120	229	0	2	129	1	2.6	2	2.0	7.0	1	YES
3	37	1	3	130	250	0	0	187	0	3.5	3	0.0	3.0	0	NO
4	41	0	2	130	204	0	2	172	0	1.4	1	0.0	3.0	0	NO

## Separate Features from Target

- Data Loading:
  - Import dataset from a URL into a pandas DataFrame.
- Target Variable Creation:
  - · Generate a new binary 'Target' column:
    - 'YES' for heart disease (num > 0)
    - 'NO' for no heart disease (num = 0)
- · Data Segmentation:
  - . Separate the dataset into features (X) and target (y).
- · Tools and Functions:
  - `pd.read\_csv() `: Reads data from URL.
  - `.apply() `: Applies a lambda function for binary classification.

```
import pandas as pd
    from sklearn.model_selection import train_test_split
    from sklearn.linear_model import LogisticRegression
    from sklearn.metrics import log loss
    from sklearn.preprocessing import OneHotEncoder
 6
    # URL of the dataset
    url = "https://www.riotu-lab.org/cs313/heart_data.csv"
 9
    # Read the dataset from the URL
    df = pd.read_csv(url)
11
12
13
    # Add a new column 'Response' based on the 'num' column
    df['Target'] = df['num'].apply(lambda x: 'YES' if x > 0 else 'NO')
14
15
16
    # Display the first few rows of the dataset
17
    print("Sample dataset:")
18
    #print(df.head())
19
    # Separate features and target variable
    X = df.drop(['num', 'Target'], axis=1)
    v = df['Target']
22
```

### One-Hot Encoding Categorical Features

### Purpose:

Convert categorical variables into a form that can be provided to machine learning algorithms to

improve model performance.

#### Process:

- Identify Categorical Features:
  - · List of categorical variables: 'sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal'.
- · Apply One-Hot Encoding:
  - Use 'OneHotEncoder' to transform these features into binary columns.
  - Handle unknown categories by ignoring them ('handle\_unknown='ignore'').

### · Integration:

- Create a new DataFrame 'X encoded' from the encoded data.
- Name new columns using the original feature names to maintain clarity.
- Merge encoded features back with the non-categorical features.

### Key Functions Used:

- 'OneHotEncoder()': Transforms categorical values into a binary matrix.
- 'fit\_transform()': Fits the encoder to the data and transforms it.
- 'get\_feature\_names\_out() ': Retrieves column names for the new binary matrix.
- `pd.concat()`: Combines the original numeric features with the new encoded data.

```
# Perform one-hot encoding on categorical features
categorical_features = ['sex', 'cp', 'fbs', 'restecg', 'exang', 'slope', 'ca', 'thal']
encoder = OneHotEncoder(handle_unknown='ignore')
X_encoded = pd.DataFrame(encoder.fit_transform(X[categorical_features]).toarray())
X_encoded.columns = encoder.get_feature_names_out(categorical_features)
X_encoded = pd.concat([X_encoded, X.drop(categorical_features, axis=1)], axis=1)

[50] 1    X_encoded.columns = encoder.get_feature_names_out(categorical_features)
2    X_encoded.columns

Index(['sex_0', 'sex_1', 'cp_1', 'cp_2', 'cp_3', 'cp_4', 'fbs_0', 'fbs_1', 'restecg_0', 'restecg_1', 'restecg_2', 'exang_0', 'exang_1', 'slope_1', 'slope_2', 'slope_3', 'ca_0.0', 'ca_1.0', 'ca_2.0', 'ca_3.0', 'ca_nan', 'thal_3.0', 'thal_6.0', 'thal_7.0', 'thal_nan'],
dtype='object')
```

# Training and Testing the Logistic Regression Model

### · Data Splitting:

 Objective: Partition the data into training and testing subsets to evaluate the model's performance on unseen data.

#### · Method:

- Use 'train\_test\_split' from scikit-learn.
- Assign 20% of the data to the test set ('test\_size=0.2').
- Ensure consistency across runs with `random\_state=42`.

### Model Training:

- · Logistic Regression Setup:
  - · Initialize the Logistic Regression model.
- Training Process:
  - Fit the model on the training data using `model.fit(X\_train, y\_train)`.
- . Key Functions Used:
  - `train\_test\_split()`: Splits the dataset into separate training and testing sets.
  - LogisticRegression(): Creates a logistic regression model.
  - 'fit()': Trains the logistic regression model on the training data.

## **Evaluating Model Performance**

- Accuracy as a Performance Metric:
  - Purpose: Evaluate the accuracy of the logistic regression model on the test dataset.
  - Method: `model.score(X\_test, y\_test)` calculates the accuracy, the
    proportion of correct predictions.
- · Code and Output:
  - · Python Execution:

```
python

log_likelihood = model.score(X_test, y_test) # Note: This is actu
print("Final log-likelihood:", log_likelihood)
```

- Interpretation: The reported score, labeled as 'log-likelihood', is actually the
  accuracy of the model, which is approximately 0.869. This means the model
  correctly predicts the outcome for 86.9% of the test cases.
- · Key Python Function:
  - 'model.score()': Computes the accuracy, not the log-likelihood, contrary to what the variable name suggests.

```
# Get the final log-likelihood
log_likelihood = model.score(X_test, y_test)
print("Final log-likelihood:", log_likelihood)
```

Final log-likelihood: 0.8688524590163934

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PREDICTION WITH A LOGISTIC REGRESSION MODEL

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## **Making Predictions with Logistic Regression**

```
# Make predictions on the test set
     y_pred = model.predict(X_test)
     # Display a sample of predictions
     print("Sample predictions:")
     pd.DataFrame({'Actual': y_test, 'Predicted': y_pred}).head(10)
Sample predictions:
     Actual Predicted
 179
         NO
                    NO
 228
        YES
                   YES
 111
        YES
                   YES
 246
        YES
                   YES
 60
        YES
                   YES
  9
        YES
                   YES
 119
        YES
                   YES
        YES
 223
                   YES
```

- Model Prediction:
- · Objective: Use the trained logistic regression model to make predictions on the test dataset.
- · Process:
- Predict using `model.predict(X\_test)`, which classifies each instance in the test set based on the learned parameters.
- . Displaying Predictions:
  - · Sample Output:
  - Combine actual and predicted labels in a DataFrame to compare results visually.
  - · Code Snippet:

```
python

y_pred = model.predict(X_test)
sample_predictions = pd.DataFrame({'Actual': y_test, 'Predicted': y_pred}).head
print("Sample predictions:", sample_predictions)
```

- . Key Functions Used:
  - 'model.predict()': Generates label predictions for the given input data.
  - `pd.DataFrame()`: Constructs a DataFrame from the actual and predicted labels for easy comparison.

YES

NO

NO

YES

268

33

## **Making Predictions with Logistic Regression**

### Beyond Accuracy:

- What limitations does relying solely on accuracy present?
- · How might different thresholds affect model evaluation?

### Understanding Errors:

- What can precision, recall, and F1-score tell us that accuracy cannot?
- How does the confusion matrix provide deeper insights into model performance?

### · Handling Imbalance:

- How should we adjust our evaluation for imbalanced datasets?
- What methods like SMOTE or cost-sensitive learning could be applied?

### · Testing Generalization:

- · How robust is the model against new, unseen data?
- · What validation techniques ensure the model generalizes well?

### · Deep Dive into Model Assessment:

- Why is cross-validation critical for assessing model reliability?
- How does the ROC-AUC curve help in understanding class differentiation?

## END OF LECTURE 1