Logistic Regression

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PW SKILLS

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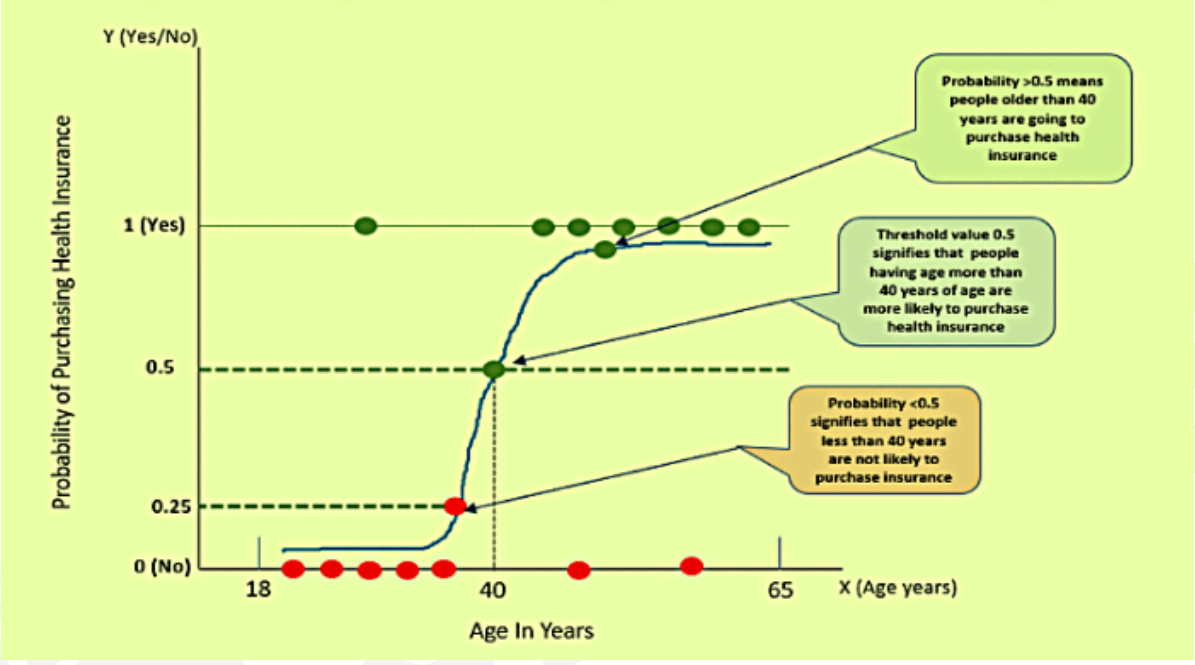
1. What is Logistic Regression

1.1 Definition and Concept

Logistic Regression is a statistical method used for binary classification problems, where the outcome can take one of two possible values (e.g., yes/no, 0/1, malignant/benign). Unlike linear regression, which predicts continuous outcomes, logistic regression predicts the probability of a particular class or event, and the output is a value between 0 and 1.



Logistic Function (Sigmoid Function): The core of logistic regression is the logistic function, which maps any real-valued number into the range [0, 1]. The logistic function is defined as:

$$\text{logistic}(\eta) = \frac{1}{1 + e^{-\eta}}$$

Here, η is the linear combination of the input features and their corresponding weights. This function ensures that the output is always between 0 and 1, making it interpretable as a probability.

1.2 Logistic Regression vs Linear Regression

While both logistic regression and linear regression are used to model relationships between a dependent variable and one or more independent variables, they serve different purposes and have distinct characteristics:

1. Output:

- **Linear Regression:** Predicts a continuous outcome.
- **Logistic Regression:** Predicts a probability that can be mapped to binary outcomes

2. Equation Form:

- **Linear Regression:** y^=β0+β1.x1+...+βp.xp
- **Logistic Regression:** P(y=1)=1/(1+e^-(β0+β1.x1+...+βp.xp))

3. Interpretation:

- **Linear Regression:** Coefficients represent the change in the outcome for a one-unit change in the predictor.
- **Logistic Regression:** Coefficients represent the change in the log-odds of the outcome for a one-unit change in the predictor.

4.Application: Linear regression is used for predicting continuous outcomes (e.g., house prices), while logistic regression is ideal for binary classification problems (e.g., disease diagnosis).

1.3 Applications of Logistic Regression

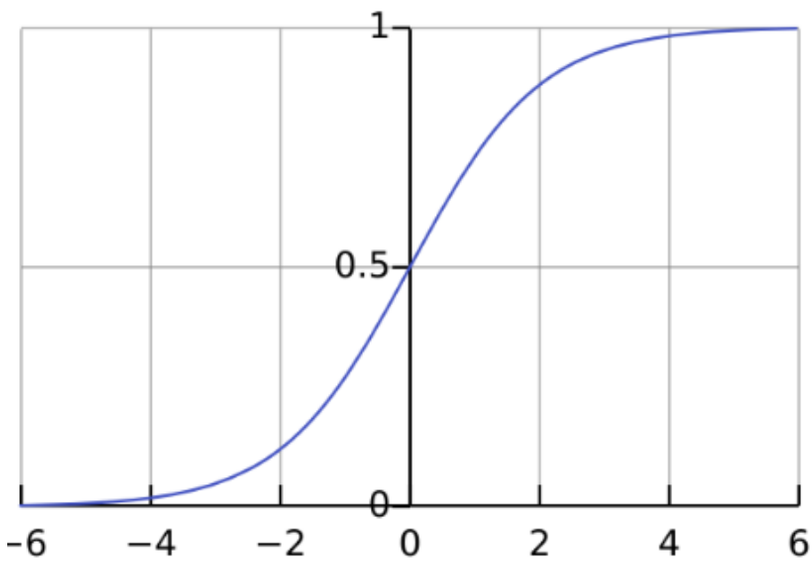
Logistic Regression is widely used in various fields due to its simplicity and interpretability:

- **Medical Diagnosis:** Predicting the probability of a patient having a certain disease based on symptoms or test results.
- **Credit Scoring:** Assessing the likelihood that a borrower will default on a loan.
- **Marketing:** Predicting whether a customer will respond to a marketing campaign (e.g., clicking on an ad, purchasing a product).
- **Risk Management:** Estimating the probability of a certain risk event occurring, such as fraud detection.

2. Mathematics of Logistic Regression

2.1 Sigmoid Function

The Sigmoid function, also known as the logistic function, is the mathematical foundation of logistic regression. It is used to map the output of a linear equation to a probability between 0 and 1.



- **Mathematical Definition:**

$$\text{logistic}(\eta) = \frac{1}{1+e^{-\eta}}$$

where η=β0+β1.x1+...+βp.xp is the linear combination of the model's parameters and input features.
Properties:

- **Range:** The output is bounded between 0 and 1.
- **Interpretation:** The output of the Sigmoid function can be interpreted as the probability that the input belongs to a particular class (e.g., P(y=1)).

Graphical Representation:
The Sigmoid function produces an S-shaped curve. When η=0, the function outputs 0.5, indicating maximum uncertainty. As η increases, the function asymptotically approaches 1, and as η decreases, it approaches 0.

2.2 Cost Function

In logistic regression, the cost function is used to measure the error between the predicted probabilities and the actual class labels. The objective is to find the model parameters that minimize this error.

- Log-Loss (Binary Cross-Entropy Loss): For binary classification, the cost function is the log-loss, defined as:

$$LogLoss = \frac{-1}{N}\sum_{i=1}^{N}\sum_{j=1}^{M} x_{ij} * \ log(p_{ij})$$

where y(i) is the actual label, y^(i) is the predicted probability, and m is the number of training examples.

2.3 Maximum Likelihood Estimation

Maximum Likelihood Estimation (MLE) is the method used to estimate the parameters (β) of the logistic regression model.

- **Likelihood Function:** The likelihood function represents the probability of observing the given data under the current model parameters:

$$L(\beta) = \prod_{i=1}^{m} \hat{y}^{(i)y^{(i)}} \left(1-\hat{y}^{(i)}\right)^{(1-y^{(i)})}$$

where y^(i) is the probability predicted by the model for the i-th example.

- **Log-Likelihood:** Since the likelihood function involves a product, it's often easier to work with the log-likelihood:

$$\log L(\beta) = \sum_{i=1}^{m} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1-y^{(i)}) \log(1-\hat{y}^{(i)})\right]$$

The goal is to find the parameters β that maximize the log-likelihood function.

2.4 Gradient Descent in Logistic Regression

Gradient Descent is an iterative optimization algorithm used to minimize the cost function and find the best parameters for the logistic regression model.

- **Gradient of the Cost Function:** The gradient of the cost function with respect to the parameters β is given by:

$$\frac{\partial J(\beta)}{\partial \beta_j} = \frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^{(i)} - y^{(i)} \right) x_j^{(i)}$$

where xj(i) is the j-th feature of the i-th training example.

- **Gradient Descent Update Rule:** The parameters are updated iteratively using the following rule:

$$\beta_j := \beta_j - \alpha \frac{\partial J(\beta)}{\partial \beta_j}$$

where α is the learning rate, a hyperparameter that controls the step size of the update.

- **Convergence:** The algorithm stops when the parameters converge, i.e., when the change in the cost function is below a certain threshold or after a fixed number of iterations.

3. Hyperparameter Tuning

3.1 Definition of Hyperparameters

Hyperparameters are parameters of the learning algorithm itself, rather than the model. Unlike model parameters, which are learned from the training data (such as the coefficients in logistic regression), hyperparameters must be set before the learning process begins.

- **Examples:**
  - Learning rate (α)
  - Regularization strength (e.g., C in logistic regression)
  - Number of iterations for convergence
- **Distinction from Model Parameters:** Model parameters, like the weights in logistic regression, are optimized by the learning algorithm. Hyperparameters, on the other hand, guide the optimization process but are not derived from the data.

3.2 Importance of Hyperparameter Tuning

Hyperparameter tuning is crucial for improving the performance and generalizability of a machine learning model.

- **Model Performance:** Properly tuned hyperparameters can significantly enhance model accuracy, while poor choices can lead to underfitting or overfitting.
- **Control of Bias-Variance Tradeoff:** Hyperparameters such as the regularization parameter control the balance between bias and variance. Tuning them helps in finding the optimal trade-off, leading to better generalization on unseen data.

Examples:

- A small learning rate might lead to very slow convergence, while a large one might cause the model to overshoot the optimal solution.
- Proper regularization prevents the model from overfitting, especially in cases with high-dimensional data.

3.3 Common Hyperparameters in Logistic Regression

In logistic regression, several key hyperparameters can be tuned to optimize the model's performance.

- **Regularization Parameter (C):**
  - **Description:** Controls the trade-off between fitting the training data well and keeping the model simple (low variance). It's the inverse of the regularization strength (λ).
  - **Effect:**
    - A large C value means less regularization, allowing the model to fit the training data more closely.
    - A small C value applies stronger regularization, which can help prevent overfitting.
  - **Tuning Strategy:** Typically, a range of C values is tested (e.g., using grid search or cross-validation) to find the best value.
- **Penalty Type (L1 or L2):**
- **L1 Regularization (Lasso):** Encourages sparsity in the model by shrinking some coefficients to zero, which can be useful for feature selection.
- **L2 Regularization (Ridge):** Penalizes the sum of the squared coefficients, leading to more evenly distributed non-zero coefficients.
- **Tuning Strategy:** Depending on the problem, one might choose L1 for a simpler model or L2 for a more stable model.

- **Solver:**
  - **Description:** The algorithm used to optimize the logistic regression objective function.
  - **Options:** Common solvers include 'liblinear', 'sag', 'saga', and 'lbfgs'.
  - **Tuning Strategy:** Different solvers might perform better depending on the dataset size, sparsity, and the regularization used.

- **Maximum Number of Iterations (max_iter):**
  - **Description:** The maximum number of iterations taken for the solvers to converge.
  - **Effect:** If the solver fails to converge, increasing this value might help, though it could also increase computational cost.
  - **Tuning Strategy:** Set this value high enough to ensure convergence but not so high that it leads to unnecessary computation time.

4. Grid Search CV

4.1 Concept of Grid Search

Grid Search is a hyperparameter tuning technique that exhaustively searches through a predefined set of hyperparameters for the best possible combination to optimize a machine learning model's performance.

- **How It Works:**
  - **Hyperparameter Grid:** You define a grid of hyperparameters, with each possible value you want to test.
  - **Exhaustive Search:** The Grid Search algorithm tests every possible combination of hyperparameters from this grid.
  - **Cross-Validation:** For each combination, the model is evaluated using cross-validation, ensuring that the selected hyperparameters generalize well to unseen data.
- **Example:** In a logistic regression model, you might use Grid Search to find the best values for hyperparameters like the regularization strength (C) and the solver type.

4.2 Implementation of Grid Search CV

- GridSearchCV in scikit-learn automates the process of performing a grid search with cross-validation. It simplifies finding the optimal hyperparameters for a model.

- **Key Steps:**

1. **Estimator:** Select the machine learning model (estimator) you want to tune.
2. **Param Grid:** Define a dictionary where the keys are the hyperparameter names and the values are lists of the values you want to test.
3. **Scoring:** Specify a metric to evaluate the model performance (e.g., accuracy, precision).
4. **Cross-Validation (CV):** Define the number of folds for cross-validation to ensure the model's robustness.

```python
# Library Importing
import pandas as pd
from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split

# Importing the dataset
df=pd.read_csv('heart.csv')

#separate into X,Y
X = df.drop('target', axis = 1)
y = df['target']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_state = 42)

# Define the model
model = RandomForestClassifier()

# Define the parameter grid
param_grid = {
    'n_estimators': [100, 200, 300],
    'max_depth': [5, 10, 15]
}

# Initialize GridSearchCV
grid_search = GridSearchCV(estimator=model, param_grid=param_grid, cv=5, scoring='accuracy')

# Fit the model
grid_search.fit(X_train, y_train)

# Best parameters and score
print(grid_search.best_params_)
print(grid_search.best_score_)
```

The Output:
{'max_depth': 15, 'n_estimators': 300}
0.8300110741971206

Result: The best combination of hyperparameters will be displayed, along with the cross-validated score for that combination.

4.3 Advantages and Limitations

Advantages:
- **Exhaustive Search:** Tests all possible combinations of hyperparameters, ensuring the best combination is found.
- **Cross-Validation:** Reduces the risk of overfitting by validating the model on multiple subsets of the data.

Limitations:
- **Computationally Expensive:** The exhaustive nature of Grid Search can be very resource-intensive, especially with large datasets or a large number of hyperparameters.
- **Time-Consuming:** As the number of hyperparameters and possible values increases, the time required to perform Grid Search increases exponentially.

Considerations:
- **When to Use:** Grid Search is best used when computational resources are sufficient and the hyperparameter space is not too large.
- **Alternatives:** For very large hyperparameter spaces, Random Search or Bayesian Optimization may be more efficient.

5. Randomized Search CV

5.1 Concept of Randomized Search

Randomized Search Cross-Validation (RandomizedSearchCV) is a hyperparameter tuning technique used to find the optimal combination of hyperparameters for a machine learning model. Unlike GridSearchCV, which exhaustively evaluates all possible combinations within a predefined grid, RandomizedSearchCV randomly samples from a distribution of hyperparameter values. This approach allows for exploring a broader range of hyperparameters in less time, making it especially useful when the hyperparameter space is large and computational resources are limited.

Key Points:

- **Random Sampling:** RandomizedSearchCV selects random combinations of hyperparameters from a specified distribution.
- **Efficiency:** It can be more computationally efficient than GridSearchCV, particularly when dealing with high-dimensional hyperparameter spaces.
- **Flexibility:** It provides the flexibility to define different distributions for different hyperparameters, enabling more targeted exploration.

5.2 Implementation of Randomized Search CV

RandomizedSearchCV can be implemented using the RandomizedSearchCV class from the scikit-learn library. This class requires several inputs, including the machine learning model (estimator), the distribution of hyperparameters to sample from, the number of iterations (n_iter), and the cross-validation strategy (cv).

```python
#Importing Library
from sklearn.model_selection import RandomizedSearchCV
from sklearn.ensemble import RandomForestClassifier
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split

# Load dataset
X, y = load_iris(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

# Define model
rfc = RandomForestClassifier()

# Define hyperparameter distribution
param_dist = {
    'n_estimators': range(10, 200),
    'max_depth': range(1, 20),
    'min_samples_split': range(2, 11)
}

# Initialize and fit RandomizedSearchCV
random_search = RandomizedSearchCV(estimator=rfc, param_distributions=param_dist, n_iter=100, cv=5,
random_state=42)
random_search.fit(X_train, y_train)

# Output best parameters
print("Best Parameters:", random_search.best_params_)
print("Best Score:", random_search.best_score_)

# The Output:
Best Parameters: {'n_estimators': 122, 'min_samples_split': 9, 'max_depth': 13}
Best Score: 0.9523809523809523
```

This code demonstrates how to use RandomizedSearchCV to tune a Random Forest Classifier's hyperparameters.

5.3 Comparison with Grid Search CV

RandomizedSearchCV and GridSearchCV are both effective methods for hyperparameter tuning, but they have key differences:

- **Search Strategy:**
  - **GridSearchCV:** Evaluates all possible combinations of hyperparameters within a predefined grid. This method is exhaustive but can be computationally expensive, especially for large grids.
  - **RandomizedSearchCV:** Samples a fixed number of hyperparameter combinations randomly. This method is less exhaustive but can explore more of the hyperparameter space in less time.
- **Computational Efficiency:**
  - **GridSearchCV:** More suitable for small, well-defined hyperparameter spaces where an exhaustive search is feasible.
  - **RandomizedSearchCV:** More efficient for large hyperparameter spaces or when computational resources are limited.

- **Flexibility**:
  - **GridSearchCV:** Limited to predefined hyperparameter grids, which might miss good combinations if not well-chosen.
  - **RandomizedSearchCV:** Can use distributions for hyperparameters, offering more flexibility and potentially uncovering better-performing models.
- **Performance:**
  - The choice between the two often depends on the problem at hand. GridSearchCV might be more reliable for small grids, while RandomizedSearchCV offers a better trade-off between exploration and computational cost when dealing with a large number of hyperparameters.

In conclusion, both RandomizedSearchCV and GridSearchCV have their strengths and can be chosen based on the specific needs of the model tuning task.

6. Data Leakage

6.1 Definition of Data Leakage

Data leakage occurs when information from outside the training dataset is inadvertently used to create the model, leading to overly optimistic performance estimates during training and validation. Essentially, data leakage provides the model with information it wouldn't have in a real-world scenario, resulting in a model that performs well during testing but fails in production.

Data leakage typically happens when the training data contains information about the target that wouldn't be available at the time predictions are made. This contamination can skew the model's predictions, leading to high accuracy on the training set but poor generalization on new data.

6.2 Types of Data Leakage

There are two main types of data leakage: target leakage and train-test contamination.
Target Leakage:

- **Definition:** Target leakage occurs when predictors in the model include information that will not be available at the time of prediction. This can happen when the model has access to features that are generated or influenced after the target outcome has been established.
- **Example:** Consider a dataset used to predict who will get pneumonia. If the model has access to a feature like took_antibiotic_medicine, which is only true if a person has already contracted pneumonia, then this is a case of target leakage. The model would erroneously learn that those who haven't taken antibiotics won't get pneumonia, leading to misleadingly high accuracy in the training and validation phases.
- **Consequence:** The model will perform well during training and validation but fail when deployed in real-world scenarios where the "leaked" information isn't available at prediction time.

Train-Test Contamination:

- **Definition:** Train-test contamination occurs when the distinction between training data and validation (or test) data is blurred, leading to the model indirectly learning from validation data.
- **Example:** Suppose you perform data preprocessing (like imputing missing values) before splitting your data into training and validation sets. If the imputation is influenced by the entire dataset (including validation data), the model might perform well during validation because it has indirectly learned patterns from the validation set itself. This is particularly dangerous when performing complex feature engineering before data splitting.
- **Consequence:** The model will show high accuracy during validation but will not generalize well to new, unseen data because the validation process has been compromised.

6.3 Preventing Data Leakage

To prevent data leakage, the following best practices should be observed:

1. **Chronological Awareness:** Ensure that any feature created after the target variable is realized should not be included in the model. This prevents target leakage by maintaining a clear temporal distinction between features and the target.
2. **Proper Data Splitting:** Always split your data into training and validation sets before performing any preprocessing or feature engineering. This prevents train-test contamination by ensuring that the model does not inadvertently learn from validation data.
3. **Use of Pipelines:** When using scikit-learn, leverage pipelines to ensure that all preprocessing steps are contained within the training process. This ensures that each fold of cross-validation only sees the training data for preprocessing and fitting, avoiding any contamination from validation data.

By adhering to these practices, you can build models that are more robust and generalize better to new data, minimizing the risk of data leakage and ensuring more accurate predictions in real-world applications.

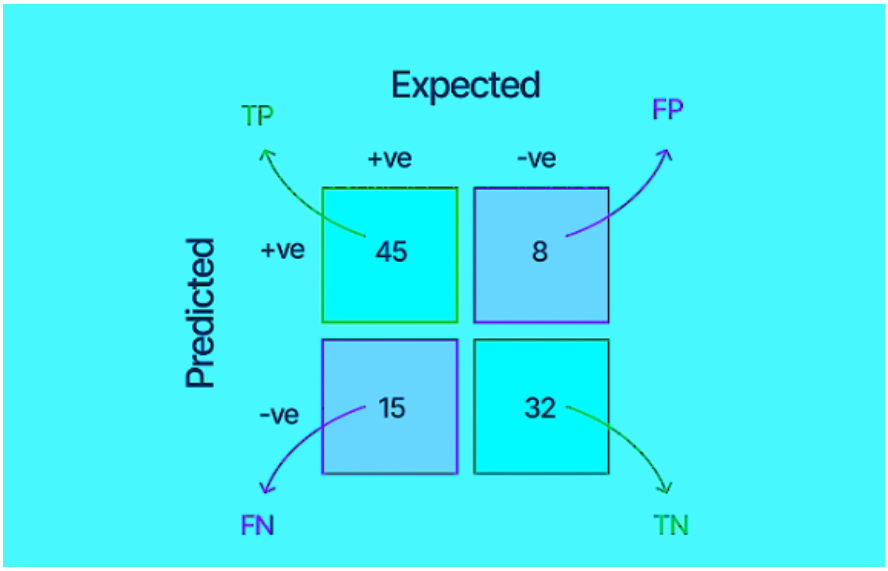
7. Confusion Matrix

7.1 Structure of Confusion Matrix

A confusion matrix is a fundamental tool for evaluating the performance of a classification model. It is a matrix layout that allows visualization of the performance of an algorithm, particularly in the context of supervised learning. The matrix is organized with rows representing the actual class labels and columns representing the predicted class labels by the model.

In a binary classification, the confusion matrix typically consists of four key components:

- **True Positives (TP):** Cases where the actual class is positive, and the model correctly predicts positive.
- **True Negatives (TN):** Cases where the actual class is negative, and the model correctly predicts negative.
- **False Positives (FP):** Cases where the actual class is negative, but the model incorrectly predicts positive.
- **False Negatives (FN):** Cases where the actual class is positive, but the model incorrectly predicts negative.



7.2 Interpreting Confusion Matrix

Interpreting the confusion matrix involves understanding these key terms:

- **Accuracy:** The proportion of correct predictions (TP + TN) among the total number of cases. It gives a general sense of the model's performance.
- **Precision:** The proportion of true positive predictions among all positive predictions (TP / (TP + FP)). Precision measures how many of the positive predictions were actually correct.
- **Recall (Sensitivity):** The proportion of true positive cases that were correctly identified by the model (TP / (TP + FN)). Recall measures the model's ability to capture all positive cases.
- **Specificity:** The proportion of true negative cases correctly identified (TN / (TN + FP)). It's particularly important when distinguishing between classes is critical, like in medical diagnoses.
- **F1 Score:** The harmonic mean of precision and recall, offering a balance between the two metrics (2 * (Precision * Recall) / (Precision + Recall)).

In multi-class classification problems, the confusion matrix expands to accommodate multiple classes, with each row representing the actual class and each column representing the predicted class. Each cell in the matrix shows the count of instances where the actual class was one category and the prediction was another.

7.3 Deriving Metrics from Confusion Matrix

Using the values from the confusion matrix, several key metrics can be derived to assess the model's performance:

- **Global Metrics:**
  - **Accuracy:** (TP + TN) / Total cases
  - **Misclassification Rate (Error Rate):** (FP + FN) / Total cases
- **Class-Specific Metrics:**
  - **Precision:** TP / (TP + FP)
  - **Recall (Sensitivity):** TP / (TP + FN)
  - **Specificity:** TN / (TN + FP)
  - **F1 Score:** 2 * (Precision * Recall) / (Precision + Recall)

In multi-class scenarios, metrics like Micro-Averaged F1 Score and Macro-Averaged F1 Score are used to provide a single metric that summarizes performance across all classes.

8. Precision, Recall, F1 Score

8.1 Precision: Definition and Calculation

Precision is the ratio of correctly predicted positive observations to the total predicted positives. It indicates the accuracy of the positive predictions made by the model. Precision is critical when the cost of false positives is high, such as in spam detection.

- **Formula: Precision = TP / (TP + FP)**

8.2 Recall: Definition and Calculation

Recall, also known as sensitivity, measures the proportion of actual positives that are correctly identified. It is crucial when it is important to capture all positive instances, such as in disease screening.

- **Formula: Recall = TP / (TP + FN)**

8.3 F1 Score: Definition and Calculation

The F1 Score is the harmonic mean of precision and recall, providing a single metric that balances both concerns. It is particularly useful when the class distribution is imbalanced.

- **Formula: F1 Score = 2 * (Precision * Recall) / (Precision + Recall)**

8.4 Trade-off between Precision and Recall

There is often a trade-off between precision and recall. Increasing precision may lower recall and vice versa. This trade-off is usually managed by adjusting the decision threshold in a model. The optimal balance between precision and recall depends on the specific application and the relative costs of false positives and false negatives.

Receiver Operating Characteristic (ROC) curves and Precision-Recall (PR) curves are tools used to visualize and understand these trade-offs better, helping to choose an appropriate threshold for model deployment.

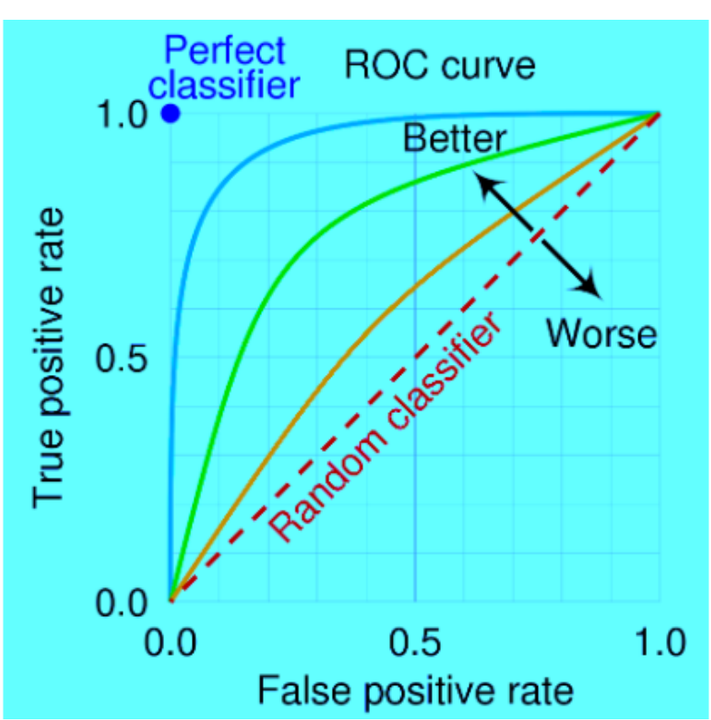
9. ROC (Receiver Operating Characteristic)

9.1 Concept of ROC Curve

The Receiver Operating Characteristic (ROC) curve is a tool used to evaluate the performance of a binary classification model across all possible classification thresholds. It originated from WWII radar detection, where it was used to visualize the performance of radar systems.

To construct an ROC curve, the True Positive Rate (TPR) and False Positive Rate (FPR) are calculated at various threshold values. TPR, also known as sensitivity or recall, is the ratio of correctly predicted positive observations to all actual positives. FPR is the ratio of incorrectly predicted positive observations to all actual negatives. The ROC curve is plotted with TPR on the y-axis and FPR on the x-axis.

A perfect model would achieve a TPR of 1.0 and an FPR of 0.0 at some threshold, represented by a point at (0, 1) on the ROC graph. The curve would then extend from (0, 1) to (1, 1) if all other thresholds are ignored.



9.2 Interpreting ROC Curve

The ROC curve allows us to visually assess the trade-off between the True Positive Rate and False Positive Rate for different thresholds. A model that performs well will have a curve that bows towards the top-left corner of the plot. The closer the curve follows the top-left border, the better the model's performance.

In the context of comparing different models, the area under the ROC curve (AUC) is used. A model with an AUC closer to 1.0 indicates a better performance, as it suggests that the model is good at distinguishing between positive and negative examples. Conversely, an AUC closer to 0.5 indicates a model with performance similar to random guessing.

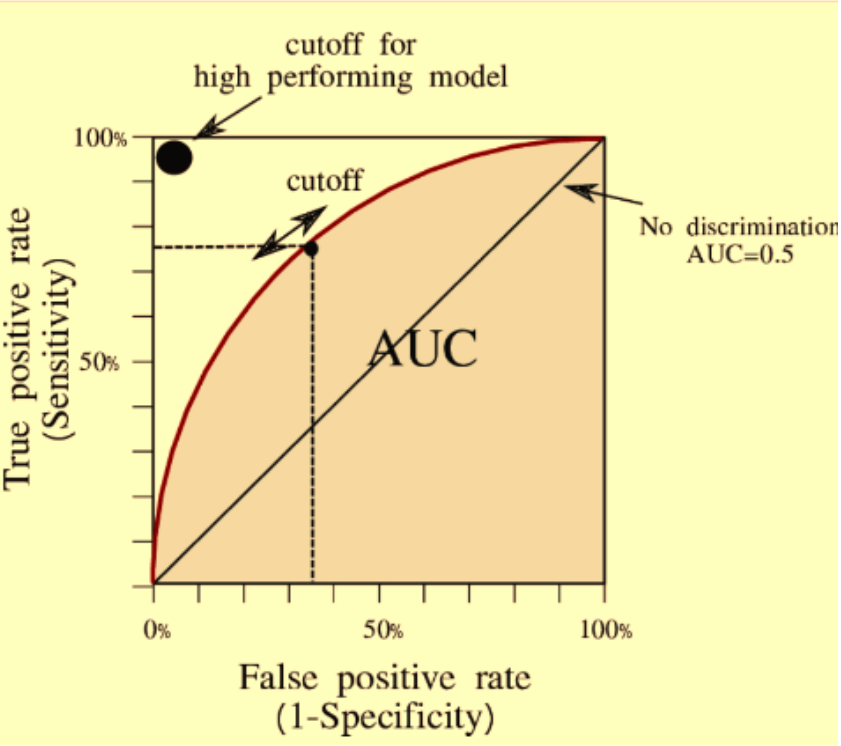
9.3 Limitations of ROC Curve

While the ROC curve is useful, it does have limitations, especially in the case of imbalanced datasets. In scenarios where the positive class is rare compared to the negative class, the ROC curve might present an overly optimistic view of model performance. In such cases, the Precision-Recall Curve (PRC) and its associated AUC can provide a better assessment.

10. AUC (Area Under the Curve)

10.1 Definition of AUC

The Area Under the Curve (AUC) is a single scalar value that quantifies the overall performance of a classification model by summarizing the ROC curve. The AUC represents the probability that a randomly chosen positive instance will be ranked higher than a randomly chosen negative instance by the model.
An AUC of 1.0 indicates a perfect model that correctly ranks all positive instances higher than all negative instances. An AUC of 0.5 indicates that the model performs no better than random guessing.



10.2 Interpreting AUC Values

Interpreting AUC values helps in understanding the effectiveness of the model:

- **AUC = 1.0:** Perfect model, correctly classifies all positive and negative instances.
- **0.5 < AUC < 1.0:** Model performs better than random guessing, with higher values indicating better performance.
- **AUC = 0.5:** Model performs no better than random guessing.
- **AUC < 0.5:** The model performs worse than random guessing. This can occur if the model's predictions are systematically incorrect.

For example, an AUC of 0.65 suggests that there is a 65% probability that the model will correctly rank a randomly chosen positive instance higher than a randomly chosen negative instance. Conversely, an AUC of 0.31 indicates worse-than-chance performance, meaning the model is performing poorly.

10.3 AUC vs Other Metrics

While AUC is a valuable metric, it is not always sufficient for model evaluation:

- **Precision-Recall Curve (PRC):** For imbalanced datasets, PRC and the area under the PRC curve may provide more meaningful insights into model performance, as they focus on the performance of the positive class.
- **F1 Score, Accuracy, Precision, Recall:** These metrics can complement AUC by providing a more detailed view of model performance, particularly in the context of specific application requirements.

AUC is particularly useful for comparing models when the dataset is balanced, but it's important to consider other metrics for a comprehensive evaluation, especially in cases of class imbalance.