XGBoost_Report

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1 XGBoost

1.0.1 Group Name: BYD2060

1.0.2 Link to the github repo: https://github.com/Yangxinyee/XGboost_for_BYD

2 Overview of XGBoost

XGBoost, or Extreme Gradient Boosting, is an efficient, scalable machine learning algorithm used primarily for supervised learning tasks like classification and regression. It builds upon gradient boosting principles to create an ensemble of weak learners that sequentially correct the errors of previous models to improve accuracy.

2.1 How XGBoost Works

1. **Initialization**:
   - Starts with an initial prediction (average value for regression or a default probability for classification).
2. **Iterative Model Training**:
   - In each step, a new weak learner (we are using decision tree) is trained to minimize residual errors from previous models.
   - The weak learner is trained on a modified dataset where the target is now the residual error from the last iteration.
3. **Gradient Boosting with Regularization**:
   - XGBoost includes regularization terms in the objective function to control overfitting:

$$\text{Objective} = \sum_{i=1}^{N} L(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k)$$

   where $L(y_i, \hat{y}_i)$ is the loss function, $\Omega(f_k)$ is the regularization term for tree f_k, N is the numble of samples, and K is the number of trees (Chen & Guestrin, 2016).
4. **Shrinking (Learning Rate)**:
   - Applies a learning rate to scale each weak learner's contribution, ensuring gradual model improvement to prevent overfitting.
5. **Tree Pruning**:

- Uses constraints like "max depth" to limit tree depth, preventing overfitting.

6. **Weighted Data and Column Sampling**:
   - Row and column sampling prevent overfitting, making the model more robust to noisy data.
7. **Final Prediction**:
   - Predictions are generated by aggregating the outputs of all weak learners, often by summing their outputs.

2.2 Advantages of XGBoost

1. **Highly Efficient and Scalable**:
   - Optimized for speed, utilizing CPU/GPU resources for large datasets.
2. **Regularization**:
   - L1 and L2 regularization helps reduce overfitting, improving generalization (Friedman, 2001).
3. **Custom Loss Functions**:
   - Allows custom loss functions, adapting well to various tasks and metrics.
4. **Handles Missing Values**:
   - Automatically learns the best direction for missing values during training.
5. **Parallel and Distributed Computing**:
   - Supports parallel tree boosting, and distributed training, making it suitable for very large datasets.
6. **Feature Importance and Interpretability**:
   - Provides feature importance scores for insight into feature contributions.

2.3 Disadvantages of XGBoost

1. **Complexity in Tuning**:
   - Many hyperparameters require tuning; poor parameter settings may lead to suboptimal performance.
2. **Sensitive to Noise**:
   - Can overfit noisy data or when trees are too deep, despite regularization.
3. **High Memory Consumption**:
   - Memory-intensive on large datasets with high-dimensional data.
4. **Not Ideal for Small Datasets**:
   - On small datasets, simpler models may perform better with fewer resources.
5. **Black-box Nature**:
   - Though feature importance scores provide some interpretability, XGBoost can still be difficult to fully interpret.

2.4 Representation of XGBoost

In XGBoost with Decision Tree as the weak learner, predictions are made by combining the outputs of a sequence of decision trees. Here's how XGBoost generates a single prediction from feature values:

1. **Initialization**:

- The model starts with an initial prediction for all samples, often set to zero or the average target value if it's a regression task. Let's denote this initial prediction as $F^{(0)}(x)$.

2. **Training Decision Trees**:
   - In each boosting round t, a new Decision Tree $f_t(x)$ is trained to predict the residuals (the difference between the true values y_i and the current predictions $F^{(t-1)}(x_i)$.
   - At each split, the Decision Tree splits the data based on a single feature and threshold, recursively creating a set of rules. The final prediction for each sample is determined by the leaf node it falls into after traversing the tree.

3. **Tree Prediction**:
   - For a feature x and a threshold θ, a single split in the Decision Tree assigns predictions to samples based on the threshold:

$$f_t(x) = \begin{cases} y_{\text{left}} & \text{if } x_i < \theta \\ y_{\text{right}} & \text{otherwise} \end{cases}$$

   - Here, y_{left} and y_{right} represent the predicted values for the samples on each side of the split. These predictions are often chosen to minimize the overall error in the objective function (Hastie, Tibshirani & Friedman, 2009).

4. **Updating the Overall Prediction**:
   - The model's prediction is updated by adding a scaled version of the Decision Tree's prediction. The learning rate η controls how much each tree contributes to the final model:

$$F^{(t)}(x) = F^{(t-1)}(x) + \eta f_t(x)$$

   - This update means each Decision Tree contributes only a small correction to the existing prediction, allowing the model to make gradual adjustments rather than large changes.

5. **Final Prediction**:
   - After T boosting rounds, the final prediction for a data point x is the sum of all weak learners' contributions:

$$F(x) = \sum_{t=1}^{T} \eta f_t(x)$$

   - Each Decision Tree captures patterns by recursively splitting data based on features and thresholds. By combining multiple trees, XGBoost can approximate complex relationships in the data (Chen & Guestrin, 2016).

2.5 Loss of XGBoost

The loss is used to measure the error between predicted and actual values. XGBoost supports various loss functions tailored to different types of tasks, including regression and classification tasks.

Loss Function:

For the regression task, we can use Mean Squared Error(MSE) or Mean Absolute Error (MAE) (Hastie, Tibshirani & Friedman, 2009)

Mean Squared Error(MSE):

$$L(F^{(\mathbf{t})}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - F^{(\mathbf{t})}(\mathbf{x}_i))^2$$

Mean Absolute Error (MAE):

$$L(F^{(\mathbf{t})}) = \frac{1}{N}\sum_{i=1}^{N}|y_i - F^{(\mathbf{t})}(\mathbf{x}_i)|$$

For the binary classification task, we can use Binary Cross Entropy Loss Binary Cross Entropy Loss:

$$L_S(F^{(\mathbf{t})}) = -\frac{1}{N}\sum_{i=1}^{N}\left[y \cdot \log(\hat{y}) + (1-y) \cdot \log(1 - F^{(\mathbf{t})}(\mathbf{x}_i))\right]$$

For the multiclass classification task, we can use Cross Entropy Loss Cross Entropy Loss (Bishop, 2006):

$$L_S(F^{(\mathbf{t})}) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{K}\mathbb{1}[y_i = j]\log F^{(\mathbf{t})}(\mathbf{x}_i)_j$$

where:

- y_i is the i-th actual value
- N is the number of samples
- K is the number of classes
- j is the j-th class
- $F^{(\mathbf{t})}$ is the model at the t-th iteration.

2.6 XGBoost with Decision Tree as Weak Learner: Optimizer Update

In this configuration, XGBoost uses a decision tree as the weak learner. The optimizer is updated to account for the decision tree mechanism, which recursively splits the data based on features and thresholds. Each leaf node assigns a constant value to the samples it contains. The prediction update process incorporates a learning rate η to scale the contribution of each tree, ensuring gradual and controlled adjustments to the model (Quinlan, 1996).

2.6.1 Objective Function

The objective function consists of the loss and regularization terms:

$$\text{Objective} = \sum_{i=1}^{N} L(y_i, \hat{y}_i) + \sum_{k=1}^{K}\Omega(f_k)$$

where $L(y_i, \hat{y}_i)$ is the loss function, typically squared error or logistic loss, measuring the difference between the true values y_i and predictions $\hat{y}_i$. $\Omega(f_k)$ is the regularization term to control model complexity.

At each iteration t, the model updates the prediction with the new decision tree's prediction, scaled by the learning rate η:

$$F^{(t)}(x) = F^{(t-1)}(x) + \eta f_t(x)$$

where $f_t(x)$ represents the decision tree's prediction.

2.6.2 Weak Learner

For a feature x and a threshold θ, a single split in the Decision Tree assigns predictions to samples based on the threshold:

$$f_t(x) = \begin{cases} y_{\text{left}} & \text{if } x_i < \theta \\ y_{\text{right}} & \text{otherwise} \end{cases}$$

Here, y_{left} and y_{right} represent the predicted values for the samples on each side of the split. These predictions are often chosen to minimize the overall error in the objective function.

2.6.3 Approximation with Taylor Expansion

To facilitate optimization, we apply a second-order Taylor expansion around the current prediction $F^{(t-1)}$ to approximate the loss function $L(F^{(t)})$:

$$L(F^{(t)}) \approx \sum_{i=1}^{N} \left[L(y_i, F^{(t-1)}(x_i)) + g_i f_t(x_i) + \frac{1}{2} h_i f_t(x_i)^2 \right] + \Omega(f_t)$$

where: - $g_i = \frac{\partial L(y_i, F^{(t-1)}(x_i))}{\partial F^{(t-1)}(x_i)}$ is the first derivative of the loss with respect to the previous prediction (the gradient). - $h_i = \frac{\partial^2 L(y_i, F^{(t-1)}(x_i))}{\partial F^{(t-1)}(x_i)^2}$ is the second derivative (the Hessian).

2.6.4 Regularization and Optimal Leaf Weights

The regularization term for a decision tree $\Omega(f_t)$ is given by:

$$\Omega(f_t) = \gamma N + \frac{1}{2} \lambda \sum_{j=1}^{N} w_j^2$$

where: - N is the number of leaf nodes, - w_j is the weight assigned to each leaf, - γ controls the complexity penalty, and λ controls the weight shrinkage.

The optimal weight for each leaf j is obtained by minimizing the regularized objective:

$$w_j^* = -\frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} h_i + \lambda}$$

where I_j is the set of sample indices for leaf j.

2.6.5 Gain Calculation and Tree Update

The gain for adding a new tree, which represents the improvement in the objective function, is:

$$\text{Gain} = \frac{1}{2}\sum_{j=1}^{N} \frac{\left(\sum_{i\in I_j} g_i\right)^2}{\sum_{i\in I_j} h_i + \lambda} - \gamma N$$

This gain metric helps determine the best split points and decide whether further splitting is beneficial.

2.6.6 Prediction Update

Finally, the model's prediction is updated at each iteration with the contribution from the newly added decision tree:

$$F^{(t)}(x) = F^{(t-1)}(x) + \eta f_t(x)$$

where η is the learning rate.

2.7 XGBoost Pseudo-code

Input:
- Training set $S = \{(x_1, y_1), \ldots, (x_m, y_m)\}$
- Weak learner $f_t(x)$ (Decision Tree)
- Number of boosting rounds T
- Learning rate η
- Regularization parameters λ, γ

Initialize:
$F^{(0)}(x) = 0$

for $t = 1, \ldots, T$:
1. **Compute gradients and Hessians**:
$g_i = \frac{\partial L(y_i, F^{(t-1)}(x_i))}{\partial F^{(t-1)}(x_i)}$
$h_i = \frac{\partial^2 L(y_i, F^{(t-1)}(x_i))}{\partial F^{(t-1)}(x_i)^2}$

2. **Find the best split**:
   - For each feature and threshold θ:
     - Split data into left and right groups based on θ
     - Compute split gain using gradients and Hessians
   - Select feature and threshold θ with the highest gain
3. **Train decision tree** $f_t(x)$:
   - Fit $f_t(x)$ using the selected splits

- Assign values y_{left} and y_{right} to leaf nodes

- Compute optimal weights w_j for each leaf node

4. **Update model**:
   $F^{(t)}(x) = F^{(t-1)}(x) + \eta f_t(x)$

Output:
Final model prediction: $F(x) = F^{(T)}(x)$

3 XGBoost Model

Class DecisionTree

[23]:
```python
import numpy as np
import random

class DecisionTree:
    """
    A class representing a decision tree model used in gradient boosting.
    Attributes:
        max_depth (int): Maximum depth of the tree.
        min_samplessplit (int): Minimum number of samples required to split a␣
↪node.
        tree (dict or float): The root of the tree, represented as a dictionary␣
↪or a leaf value.
    """
    def __init__(self, max_depth=3, min_samplessplit=2):
        """
        Initializes the DecisionTree with maximum depth and minimum samples␣
↪required to split.
        @params:
            max_depth (int): The maximum depth of the tree. Default is 3.
            min_samplessplit (int): Minimum samples required to split a node.␣
↪Default is 2.
        """
        self.max_depth = max_depth
        self.min_samplessplit = min_samplessplit
        self.tree = None

    def train(self, X, y, grad, hess):
        """
        Trains the decision tree using the given data, gradients, and hessians.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪training data.
            y (numpy.ndarray): A 1D array of shape (n_samples,) with target␣
↪values.
```

```
            grad (numpy.ndarray): A 1D array of gradients for each sample.
            hess (numpy.ndarray): A 1D array of hessians for each sample.
        """
        self.tree = self.build_tree(X, y, grad, hess)

    def split(self, X, y, grad, hess):
        """
        Finds the best split for the data to maximize the gain.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪training data.
            y (numpy.ndarray): A 1D array of shape (n_samples,) with target␣
↪values.
            grad (numpy.ndarray): A 1D array of gradients for each sample.
            hess (numpy.ndarray): A 1D array of hessians for each sample.
        @return:
            tuple: The best feature index and threshold for the split.
        """
        best_gain = -np.inf
        best_split = None
        # Iterate over all features to find the best split point
        for feature_index in range(X.shape[1]):
            # Sort feature values and compute threshold for splits
            sorted_index = np.argsort(X[:, feature_index])
            X_sorted, grad_sorted, hess_sorted = X[sorted_index,␣
↪feature_index], grad[sorted_index], hess[sorted_index]
            # Initialize left and right sum of gradients and Hessians
            G_L, H_L = 0, 0
            G_R, H_R = np.sum(grad_sorted), np.sum(hess_sorted)

            # Iterate over feature values to find the best split point
            for i in range(1, len(X_sorted)):
                G_L += grad_sorted[i - 1]
                H_L += hess_sorted[i - 1]
                G_R -= grad_sorted[i - 1]
                H_R -= hess_sorted[i - 1]

                # Check if the split meets the minimum sample requirement
                if i < self.min_samplessplit or len(X_sorted) - i < self.
↪min_samplessplit:
                    continue

                # Calculate gain for this split using a separate function
                gain = self.gain(G_L, H_L, G_R, H_R)

                # Update the best gain and split if the current gain is higher
                if gain > best_gain:
```

```
                    best_gain = gain
                    best_split = (feature_index, (X_sorted[i - 1] +␣
↪X_sorted[i]) / 2)

        return best_split

    def gain(self, G_L, H_L, G_R, H_R):
        """
        Calculates the gain of a split using left and right gradient and␣
↪Hessian sums.
        @params:
            G_L (float): Sum of gradients for the left split.
            H_L (float): Sum of Hessians for the left split.
            G_R (float): Sum of gradients for the right split.
            H_R (float): Sum of Hessians for the right split.
        @return:
            float: The calculated gain for the split.
        """
        # Gain formula using left and right gradient and Hessian sums
        gain = 0.5 * ((G_L ** 2) / (H_L + 1e-10) + (G_R ** 2) / (H_R + 1e-10) -␣
↪((G_L + G_R) ** 2) / (H_L + H_R + 1e-10))
        return gain

    def build_tree(self, X, y, grad, hess, depth=0):
        """
        Recursively builds the decision tree based on the provided data.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪training data.
            y (numpy.ndarray): A 1D array of target values.
            grad (numpy.ndarray): A 1D array of gradients for each sample.
            hess (numpy.ndarray): A 1D array of hessians for each sample.
            depth (int): The current depth of the tree.
        @return:
            dict or float: A dictionary representing the subtree or a leaf␣
↪value.
        """
        if depth == self.max_depth or len(y) < self.min_samplessplit:
            # Return leaf value if maximum depth is reached or samples are␣
↪insufficient
            leaf_value = -np.sum(grad) / (np.sum(hess) + 1e-10)
            return leaf_value

        best_split = self.split(X, y, grad, hess)
        if not best_split:
            # Return leaf value if no valid split is found
```

```
            return -np.sum(grad) / (np.sum(hess) + 1e-10)

        feature_index, threshold = best_split
        left_mask = X[:, feature_index] < threshold
        right_mask = ~left_mask

        # Recursively build left and right subtrees
        left_subtree = self.build_tree(X[left_mask], y[left_mask],␣
↪grad[left_mask], hess[left_mask], depth + 1)
        right_subtree = self.build_tree(X[right_mask], y[right_mask],␣
↪grad[right_mask], hess[right_mask], depth + 1)
        return {"feature_index": feature_index, "threshold": threshold, "left":␣
↪left_subtree, "right": right_subtree}

    def predict_single(self, x, tree):
        """
        Predicts the value for a single sample using the decision tree.
        @params:
            x (numpy.ndarray): A 1D array of feature values for a single sample.
            tree (dict or float): The decision tree or leaf value to predict␣
↪with.
        @return:
            float: The predicted value for the sample.
        """
        if not isinstance(tree, dict):
            # Return the leaf value if the node is a leaf
            return tree

        feature_index = tree["feature_index"]
        threshold = tree["threshold"]
        # Traverse left or right subtree based on the feature value
        if x[feature_index] < threshold:
            return self.predict_single(x, tree["left"])
        else:
            return self.predict_single(x, tree["right"])

    def predict(self, X):
        """
        Predicts the values for multiple samples using the decision tree.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪input data.
        @return:
            numpy.ndarray: A 1D array of predicted values for each sample.
        """
        return np.array([self.predict_single(x, self.tree) for x in X])
```

```
    def print_tree(self, tree=None, node_id=0, depth=0):
        """
        Prints the structure of the decision tree with node IDs.
        """
        if tree is None:
            tree = self.tree

        # initialize queue and node number
        queue = [(tree, 0)]
        node_map = {}
        node_counter = 0

        # number the nodes in breadth-first order
        while queue:
            node, parent_id = queue.pop(0)
            node_id = node_counter
            node_map[id(node)] = node_id
            node_counter += 1
            if isinstance(node, dict):
                queue.append((node["left"], node_id))
                queue.append((node["right"], node_id))

        # print node in depth-first order
        def depth_first_traversal(node, depth):
            node_id = node_map[id(node)]
            if isinstance(node, dict):
                # print current split node
                feature_index = node["feature_index"]
                threshold = node["threshold"]
                left_id = node_map[id(node["left"])]
                right_id = node_map[id(node["right"])]
                print(
                    "\t" * depth
                    + f"{node_id}:[f{feature_index}<{threshold:.6f}] yes={left_id},no={right_id},missing={right_id}"
                )
                # print left and right sub-tree recursively
                depth_first_traversal(node["left"], depth + 1)
                depth_first_traversal(node["right"], depth + 1)
            else:
                # leaf node
                print("\t" * depth + f"{node_id}:leaf={node:.6f}")

        depth_first_traversal(tree, depth=0)
```

Class XGBoost

[2]:
```
class XGBoost:
    """
    XGBoost for binary classification.
    Attributes:
        num_trees (int): Number of boosting rounds (trees).
        max_depth (int): Maximum depth of each decision tree.
        min_samplessplit (int): Minimum number of samples required to split an␣
↪internal node.
        learning_rate (float): Step size shrinkage used in update to prevent␣
↪overfitting.
        trees (list): List of trained decision tree models.
    """
    def __init__(self, num_trees=10, max_depth=3, min_samplessplit=2,␣
↪learning_rate=0.3):
        """
        Initializes the XGBoost model with the specified parameters.
        @params:
            num_trees (int): Number of trees to fit. Default is 10.
            max_depth (int): Maximum depth of each tree. Default is 3.
            min_samplessplit (int): Minimum samples required to split a node.␣
↪Default is 2.
            learning_rate (float): Learning rate for the model. Default is 0.3.
        """
        self.num_trees = num_trees
        self.max_depth = max_depth
        self.min_samplessplit = min_samplessplit
        self.learning_rate = learning_rate
        self.trees = []

    def train(self, X, y, detailed=False):
        """
        Trains the XGBoost model using the training data.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪the training data.
            y (numpy.ndarray): A 1D array of shape (n_samples,) with the target␣
↪labels.
            detailed (boolean): Whether to print the current tree when␣
↪interating. Default is true.
        """
        # Initialize predictions with zeros
        y_pred = np.zeros_like(y, dtype=float)

        # Train each tree iteratively
        for i in range(self.num_trees):
            # Compute gradients and hessians
```

```python
            grad, hess = self.gradient(y, y_pred)

            # Initialize and train a new decision tree
            tree = DecisionTree(max_depth=self.max_depth, min_samplessplit=self.
↪min_samplessplit)
            tree.train(X, y, grad, hess)

            # Make predictions using the trained tree
            predictions = tree.predict(X)

            # Update predictions with the learning rate
            y_pred += self.learning_rate * predictions
            self.trees.append(tree)

            if detailed:
                # Print the structure of the current tree
                print(f"Tree {i + 1}:")
                tree.print_tree()
                # Calculate and print the cross-entropy loss using sigmoid
                loss = self.cross_entropy_loss(y, 1 / (1 + np.exp(-y_pred)))
                print(f"Loss after Tree {i + 1}: {loss}")
                print("\n")

    def gradient(self, y, y_pred):
        """
        Computes the gradients and hessians for the loss function.
        @params:
            y (numpy.ndarray): A 1D array of target labels.
            y_pred (numpy.ndarray): A 1D array of current predictions.
        @return:
            tuple: A tuple containing:
                - grad (numpy.ndarray): A 1D array of gradients for each sample.
                - hess (numpy.ndarray): A 1D array of hessians for each sample.
        """
        # Compute the first derivative (gradient)
        grad = y_pred - y

        # For the squared error loss, the second derivative (hessian) is␣
↪constant and equal to 1
        hess = np.ones_like(y)
        return grad, hess

    def cross_entropy_loss(self, y, y_pred):
        """
        Computes the cross-entropy loss between true and predicted labels.
        @params:
            y (numpy.ndarray): A 1D array of target labels.
```

```
            y_pred (numpy.ndarray): A 1D array of predicted probabilities.
        @return:
            float: The mean cross-entropy loss.
        """
        # Clip predicted probabilities to avoid log(0)
        y_pred = np.clip(y_pred, 1e-15, 1 - 1e-15)
        loss = -np.mean(y * np.log(y_pred) + (1 - y) * np.log(1 - y_pred))
        return loss

    def predict(self, X):
        """
        Outputs predicted labels for the input data using the trained trees.
        @params:
            X (numpy.ndarray): A 2D array of shape (n_samples, n_features) with␣
↪the input data.
        @return:
            numpy.ndarray: A 1D array of predicted values for each sample.
        """
        # Initialize predictions with zeros
        y_pred = np.zeros(X.shape[0])

        # Aggregate predictions from each tree
        for tree in self.trees:
            y_pred += self.learning_rate * tree.predict(X)
        return y_pred
```

4 Check Model

Unit tests and edge cases

[3]:
```
import pytest

# Sets random seed for reproducibility
np.random.seed(0)

# Synthetic dataset 1: Linearly separable data
X_linear = np.array([
    [float(i), float(2 * i + 1)] for i in range(10)
])
y_linear = np.array([0 if x[0] < 5 else 1 for x in X_linear])
y_pred_linear = np.zeros_like(y_linear, dtype=float)

# Synthetic dataset 2: Non-linearly separable data
X_nonlinear = np.random.rand(20, 2) * 10  # Random points in a 10x10 grid
y_nonlinear = np.array([1 if x[0]**2 + x[1]**2 < 50 else 0 for x in␣
↪X_nonlinear])
y_pred_nonlinear = np.zeros_like(y_nonlinear, dtype=float)
```

```python
test_gain_cases = [
    # Format: (G_L, H_L, G_R, H_R, expected_gain)
    (10.0, 5.0, 20.0, 10.0, -2.000000165480742e-10),
    (5.0, 2.0, 15.0, 8.0, 0.3124999997117186),
    (0.0, 1.0, 0.0, 1.0, 0.0),
    (10.0, 0.1, 10.0, 0.1, -4.999999418942025e-07)
]

# Additional edge cases
# Minimal dataset
X_minimal = np.array([[1.0, 2.0]])
y_minimal = np.array([1])

# Zero gradient and Hessian
X_zero_grad = np.array([[1.0, 1.0], [2.0, 2.0]])
y_zero_grad = np.array([0, 1])

# Identical features
X_identical = np.array([[1.0, 1.0], [1.0, 1.0], [1.0, 1.0]])
y_identical = np.array([0, 0, 1])

# Creates a simple parameter dictionary
params = {
    'num_trees': 4,
    'max_depth': 3,
    'min_samplessplit': 2,
    'learning_rate': 0.3
}


# Test model with a minimal dataset (1 sample).
def test_minimal_dataset():
    """
    Validates the DecisionTree model's behavior with the smallest possible␣
 ↪dataset (one sample).
    Purpose: Ensure the model can train and predict with minimal input data.
    """
    tree = DecisionTree(max_depth=1, min_samplessplit=1)
    tree.train(X_minimal, y_minimal, grad=np.zeros_like(y_minimal)-y_minimal,␣
 ↪hess=np.ones_like(y_minimal))
    predictions = tree.predict(X_minimal)
    assert predictions.shape == y_minimal.shape
    assert predictions[0] == pytest.approx(1, .001)
    print(f"Minimal dataset test passed with predictions {predictions[0]:.2f} ")
```

```python
# Test model with zero gradient and Hessian values.
def test_zero_gradient_hessian():
    """
    Checks the DecisionTree's response to a dataset with zero gradients and␣
 ↪Hessians.
    Purpose: Verify that the model handles edge cases where no learning signal␣
 ↪exists.
    """
    tree = DecisionTree(max_depth=2, min_samplessplit=1)
    grad = np.zeros_like(y_zero_grad)
    hess = np.zeros_like(y_zero_grad)
    tree.train(X_zero_grad, y_zero_grad, grad=grad, hess=hess)
    predictions = tree.predict(X_zero_grad)
    print(f"Predictions with zero gradient/hessian: {predictions}")
    assert predictions.shape == y_zero_grad.shape
    print("Zero gradient and Hessian test passed.")


# Test model on dataset with identical feature values.
def test_identical_features():
    """
    Tests the DecisionTree on a dataset where all feature values are identical.
    Purpose: Evaluate the model's ability to handle cases where no meaningful␣
 ↪split is possible.
    """
    tree = DecisionTree(max_depth=2, min_samplessplit=1)
    tree.train(X_identical, y_identical, grad=np.
 ↪zeros_like(y_identical)-y_identical, hess=np.ones_like(y_identical))
    predictions = tree.predict(X_identical)
    print(f"Predictions with identical features: {predictions}")
    assert np.all(predictions == predictions[0]), "Model failed on identical␣
 ↪features dataset."
    print("Identical features test passed.")


# Test gain calculation for various cases.
def test_gain():
    """
    Evaluates the correctness of the gain function used in the tree-splitting␣
 ↪logic.
    Purpose: Ensure gain calculations match expected values for test cases.
    """
    tree = DecisionTree(max_depth=2, min_samplessplit=1)
    # Test each case
    for i, (G_L, H_L, G_R, H_R, expected_gain) in enumerate(test_gain_cases):
        gain = tree.gain(G_L, H_L, G_R, H_R)
```

```python
        assert abs(gain - expected_gain) < 1e-5, f"Test case {i+1} failed:␣
↪expected {expected_gain}, got {gain}"
    print("Gain computation test passed.")


# Test the best split function in the DecisionTree class.
def test_split():
    """
    Assesses the DecisionTree's ability to identify the optimal split point for␣
↪a dataset.
    Purpose: Verify that the split logic works correctly for both linear and␣
↪non-linear datasets.
    """
    tree = DecisionTree(max_depth=2, min_samplessplit=1)
    split_feature1, split_value1 = tree.split(X_linear, y_linear,␣
↪grad=y_pred_linear-y_linear, hess=np.ones_like(y_linear))
    split_feature2, split_value2 = tree.split(X_nonlinear, y_nonlinear, grad=np.
↪ones_like(y_nonlinear), hess=np.ones_like(y_nonlinear))
    assert split_feature1 == 0
    assert split_feature2 == 0
    assert split_value1 == pytest.approx(4.5, .001)
    assert split_value2 == pytest.approx(0.195, .001)
    print("Split test passed.")


# Test DecisionTree on linearly separable data.
def test_decision_tree_with_linear_data():
    """
    Validates the DecisionTree's performance on a linearly separable dataset.
    Purpose: Ensure the model achieves 100% accuracy on simple linearly␣
↪separable data.
    """
    tree = DecisionTree(max_depth=3, min_samplessplit=2)
    tree.train(X_linear, y_linear, grad=y_pred_linear-y_linear, hess=np.
↪ones_like(y_linear))
    predictions = tree.predict(X_linear)
    assert predictions.shape == y_linear.shape
    accuracy = np.mean((predictions > 0.5) == y_linear)
    assert accuracy == 1.0, f"Expected accuracy 1.0, got {accuracy}"
    print(f"DecisionTree accuracy on linear dataset: {accuracy:.2f}")


# Test DecisionTree on non-linearly separable data.
def test_decision_tree_with_nonlinear_data():
    """
    Tests the DecisionTree's performance on a non-linearly separable dataset.
```

```
    Purpose: Check how well the model handles more complex decision boundaries.
    """
    tree = DecisionTree(max_depth=3, min_samplessplit=2)
    tree.train(X_nonlinear, y_nonlinear, grad=y_pred_nonlinear-y_nonlinear,␣
 ↪hess=np.ones_like(y_nonlinear))
    predictions = tree.predict(X_nonlinear)
    assert predictions.shape == y_nonlinear.shape
    accuracy = np.mean((predictions > 0.5) == y_nonlinear)
    print(f"DecisionTree accuracy on non-linear dataset: {accuracy:.2f}")


# Test gradient and hessian computation in the XGBoost model.
def test_compute_gradients():
    """
    Validates gradient and Hessian computation in the XGBoost model for␣
 ↪synthetic datasets.
    Purpose: Ensure that gradient calculations are consistent with expectations.
    """
    model = XGBoost(**params)
    gradients1, _ = model.gradient(y_linear, y_pred_linear)
    gradients2, _ = model.gradient(y_nonlinear, y_pred_nonlinear)
    assert gradients1 == pytest.approx(np.array([0., 0., 0., 0., 0., -1., -1.,␣
 ↪-1., -1., -1.]), .001)
    assert gradients2 == pytest.approx(np.array([0., 0., 0., 0., 0., 0., 0., -1.
 ↪, 0., 0., 0., 0., -1., 0., -1., 0., 0., -1., 0., 0.]), .001)
    print("Gradients computation test passed.")


# Test cross-entropy loss calculation in the XGBoost model.
def test_cross_entropy_loss():
    """
    Verifies the accuracy of cross-entropy loss calculation in XGBoost.
    Purpose: Ensure loss is computed correctly for different datasets.
    """
    model = XGBoost(**params)
    loss1 = model.cross_entropy_loss(y_linear, y_pred_linear)
    loss2 = model.cross_entropy_loss(y_nonlinear, y_pred_nonlinear)
    print(loss1)
    print(loss2)
    assert loss1 == pytest.approx(17.269, .001)
    assert loss2 == pytest.approx(6.907, .001)
    print("Cross entropy loss test passed.")


# Test XGBoost on linearly separable data.
def test_xgboost_with_linear_data():
    """
```

```python
    Tests the XGBoost model's ability to learn from a linearly separable␣
↪dataset.
    Purpose: Validate that XGBoost achieves 100% accuracy on simple datasets.
    """
    model = XGBoost(**params)
    model.train(X_linear, y_linear, detailed=False)
    predictions = model.predict(X_linear)
    assert predictions.shape == y_linear.shape
    accuracy = np.mean((predictions > 0.5) == y_linear)
    assert accuracy == 1.0, f"Expected accuracy 1.0, got {accuracy}"
    print(f"XGBoost accuracy on linear dataset: {accuracy:.2f}")


# Test XGBoost on non-linearly separable data.
def test_xgboost_with_nonlinear_data():
    """
    Evaluates the performance of the XGBoost model on non-linearly separable␣
↪data.
    Purpose: Measure the model's capability to adapt to complex decision␣
↪boundaries.
    """
    model = XGBoost(**params)
    model.train(X_nonlinear, y_nonlinear, detailed=False)
    predictions = model.predict(X_nonlinear)
    assert predictions.shape == y_nonlinear.shape
    accuracy = np.mean((predictions > 0.5) == y_nonlinear)
    print(f"XGBoost accuracy on non-linear dataset: {accuracy:.2f}")


# Run tests with synthetic datasets
test_minimal_dataset()
test_zero_gradient_hessian()
test_identical_features()
test_gain()
test_split()
test_decision_tree_with_linear_data()
test_decision_tree_with_nonlinear_data()
test_compute_gradients()
test_cross_entropy_loss()
test_xgboost_with_linear_data()
test_xgboost_with_nonlinear_data()

print("All tests passed!")
```

```
Minimal dataset test passed with predictions 1.00
Predictions with zero gradient/hessian: [0. 0.]
Zero gradient and Hessian test passed.
```

```
Predictions with identical features: [0.33333333 0.33333333 0.33333333]
Identical features test passed.
Gain computation test passed.
Split test passed.
DecisionTree accuracy on linear dataset: 1.00
DecisionTree accuracy on non-linear dataset: 0.90
Gradients computation test passed.
17.269388197455342
6.907755278982137
Cross entropy loss test passed.
XGBoost accuracy on linear dataset: 1.00
XGBoost accuracy on non-linear dataset: 0.95
All tests passed!
```

4.1 Comparisons of Previous Works Using XGBoost

4.1.1 Introduction of Python XBGoost Module:

The XGBoost Python module is the implementation of the XGBoost algorithm in Python. This module supports loading datasets and training models using the sklearn estimator interface from the sklearn module. With this interface, users can set the loss function based on the task and choose the type of tree used in XGBoost. This allows XGBoost to make predictions on different datasets. The previous works we selected all used this module for training and prediction on different datasets (Pedregosa et al., 2011).

4.1.2 Breast Cancer Diagnosis

This work uses XGBoost to diagnose whether a breast mass is benign or malignant. The dataset used is the Breast Cancer Wisconsin (Diagnostic) Data Set (Wolberg et al., 1993). The features of this dataset are derived from a digitized image of a fine needle aspirate (FNA) of a breast mass. Below is a list of features:

Feature	**Description**
ID number	Identifier for each case
Diagnosis	M = malignant, B = benign
radius	Mean of distances from center to points on the perimeter
texture	Standard deviation of gray-scale values
perimeter	Perimeter of the contour
area	Area within the contour
smoothness	Local variation in radius lengths
compactness	Perimeter^2 / Area - 1.0
concavity	Severity of concave portions of the contour
concave points	Number of concave portions of the contour
symmetry	Symmetry of the contour
fractal dimension	“Coastline approximation” - 1

To facilitate result comparison, we made the following improvements:

- Remove the ID number column as the irrelevant column.
- Encode the values in the Diagnosis column, where M = malignant and B = benign, into Malignant = 1 and Benign = 0.
- Set the number of decision trees used by XGBoost to 5, the maximum depth of the trees to 5, and the learning rate to 0.3.

We split the dataset into 20% training and 80% testing sets, using 5-fold cross-validation to evaluate the accuracy of our model and the previous work's model.

Implementing with OUR XGBoost

[4]:
```
from sklearn.model_selection import train_test_split

# Load the dataset from a CSV file using numpy's genfromtxt
data = np.genfromtxt('../data/breast+cancer+wisconsin+diagnostic/wdbc.data',␣
↪delimiter=',', dtype=str)

# Extract features and convert them to float
X = data[:, 2:].astype(float)  # Features start from the 3rd column (index 2)
# Convert the labels to binary (Malignant -> 1, Benign -> 0)
y = np.where(data[:, 1] == 'M', 1, 0)

# Normalize the features using mean and standard deviation
X = (X - X.mean(axis=0)) / X.std(axis=0)

# Split the dataset into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)

# Use the XGBoost model we implemented earlier
model = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)

# Trains the XGBoost model on the training data.
model.train(X_train, y_train, detailed='true')

# Generates predictions on the test data.
predictions = model.predict(X_test)

# Convert predictions to binary labels (0 or 1) using a threshold of 0.5
predictions = np.where(predictions >= 0.5, 1, 0)

# Calculate the accuracy of the model
accuracy = np.mean(predictions == y_test)
print("Model Accuracy:", accuracy)
```

```
Tree 1:
0:[f7<0.060896] yes=1,no=2,missing=2
        1:[f20<0.116134] yes=3,no=4,missing=4
                3:[f10<0.795390] yes=7,no=8,missing=8
```

```
                        7:[f24<1.870977] yes=15,no=16,missing=16
                                15:[f14<-1.244043] yes=27,no=28,missing=28
                                        27:leaf=0.142857
                                        28:leaf=0.003984
                                16:leaf=0.500000
                        8:leaf=0.666667
                4:[f1<-0.721309] yes=9,no=10,missing=10
                        9:[f0<0.274843] yes=17,no=18,missing=18
                                17:leaf=-0.000000
                                18:[f0<0.594359] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=-0.000000
                        10:[f17<-0.270993] yes=19,no=20,missing=20
                                19:[f0<-0.146918] yes=31,no=32,missing=32
                                        31:leaf=1.000000
                                        32:leaf=1.000000
                                20:leaf=-0.000000
        2:[f27<0.486395] yes=5,no=6,missing=6
                5:[f22<0.237953] yes=11,no=12,missing=12
                        11:[f1<0.410809] yes=21,no=22,missing=22
                                21:[f0<-1.137276] yes=33,no=34,missing=34
                                        33:leaf=-0.000000
                                        34:leaf=-0.000000
                                22:[f0<0.087394] yes=35,no=36,missing=36
                                        35:leaf=1.000000
                                        36:leaf=1.000000
                        12:[f0<0.632701] yes=23,no=24,missing=24
                                23:leaf=1.000000
                                24:[f0<0.876953] yes=37,no=38,missing=38
                                        37:leaf=1.000000
                                        38:leaf=1.000000
                6:[f16<3.440249] yes=13,no=14,missing=14
                        13:[f0<-0.714947] yes=25,no=26,missing=26
                                25:leaf=1.000000
                                26:[f0<-0.562999] yes=39,no=40,missing=40
                                        39:leaf=1.000000
                                        40:leaf=1.000000
                        14:leaf=-0.000000
Loss after Tree 1: 0.6435127119020765


Tree 2:
0:[f27<0.422443] yes=1,no=2,missing=2
        1:[f23<0.135125] yes=3,no=4,missing=4
                3:[f1<0.736599] yes=7,no=8,missing=8
                        7:[f10<0.687294] yes=15,no=16,missing=16
                                15:[f19<-0.938027] yes=25,no=26,missing=26
                                        25:leaf=0.105287
```

```
                                26:leaf=-0.002150
                        16:leaf=0.200000
                8:[f20<0.084036] yes=17,no=18,missing=18
                        17:[f1<0.773832] yes=27,no=28,missing=28
                                27:leaf=0.849402
                                28:leaf=0.047147
                        18:[f0<0.068933] yes=29,no=30,missing=30
                                29:leaf=0.700000
                                30:leaf=0.700000
        4:[f26<-0.390943] yes=9,no=10,missing=10
                9:[f0<0.842871] yes=19,no=20,missing=20
                        19:leaf=-0.000000
                        20:leaf=0.350000
                10:[f15<0.166655] yes=21,no=22,missing=22
                        21:[f0<0.304664] yes=31,no=32,missing=32
                                31:leaf=0.700000
                                32:leaf=0.700000
                        22:[f0<1.028901] yes=33,no=34,missing=34
                                33:leaf=0.700000
                                34:leaf=0.700000
2:[f2<-0.830149] yes=5,no=6,missing=6
        5:[f5<0.876677] yes=11,no=12,missing=12
                11:leaf=-0.001195
                12:leaf=-0.000000
        6:[f11<-1.376912] yes=13,no=14,missing=14
                13:leaf=-0.000598
                14:[f6<-0.030751] yes=23,no=24,missing=24
                        23:[f27<0.553392] yes=35,no=36,missing=36
                                35:leaf=-0.000598
                                36:leaf=0.700000
                        24:[f16<2.994288] yes=37,no=38,missing=38
                                37:leaf=0.701095
                                38:leaf=0.350000
```

```
Loss after Tree 2: 0.613821695762677


Tree 3:
0:[f7<0.060896] yes=1,no=2,missing=2
        1:[f20<0.116134] yes=3,no=4,missing=4
                3:[f10<0.795390] yes=7,no=8,missing=8
                        7:[f21<2.181745] yes=15,no=16,missing=16
                                15:[f14<-1.244043] yes=27,no=28,missing=28
                                        27:leaf=0.096041
                                        28:leaf=-0.000624
                                16:leaf=0.202998
                        8:leaf=0.421952
                4:[f1<-0.721309] yes=9,no=10,missing=10
                        9:[f0<0.594359] yes=17,no=18,missing=18
```

```
                        17:[f0<0.274843] yes=29,no=30,missing=30
                                29:leaf=0.000645
                                30:leaf=0.000645
                        18:leaf=-0.052177
                10:[f17<-0.270993] yes=19,no=20,missing=20
                        19:[f11<0.157207] yes=31,no=32,missing=32
                                31:leaf=0.490000
                                32:leaf=0.542500
                        20:leaf=-0.000000
        2:[f22<0.214124] yes=5,no=6,missing=6
                5:[f21<-0.003619] yes=11,no=12,missing=12
                        11:[f27<0.776462] yes=21,no=22,missing=22
                                21:[f24<-1.361262] yes=33,no=34,missing=34
                                        33:leaf=-0.082500
                                        34:leaf=0.000542
                                22:leaf=0.489672
                        12:[f12<-0.647777] yes=23,no=24,missing=24
                                23:leaf=0.245090
                                24:[f5<-0.046260] yes=35,no=36,missing=36
                                        35:leaf=0.587928
                                        36:leaf=0.487330
                6:[f14<3.783160] yes=13,no=14,missing=14
                        13:[f27<0.419398] yes=25,no=26,missing=26
                                25:[f0<0.760507] yes=37,no=38,missing=38
                                        37:leaf=0.490000
                                        38:leaf=0.490000
                                26:[f6<-0.056552] yes=39,no=40,missing=40
                                        39:leaf=0.490000
                                        40:leaf=0.489672
                        14:leaf=0.542500
Loss after Tree 3: 0.5949167203973654


Tree 4:
0:[f27<0.422443] yes=1,no=2,missing=2
        1:[f23<0.135125] yes=3,no=4,missing=4
                3:[f1<0.531817] yes=7,no=8,missing=8
                        7:[f13<0.246703] yes=15,no=16,missing=16
                                15:[f13<0.183999] yes=25,no=26,missing=26
                                        25:leaf=-0.003007
                                        26:leaf=0.306948
                                16:leaf=-0.210918
                        8:[f18<-0.778813] yes=17,no=18,missing=18
                                17:[f17<-0.797364] yes=27,no=28,missing=28
                                        27:leaf=0.163924
                                        28:leaf=0.778007
                                18:[f7<0.002343] yes=29,no=30,missing=30
                                        29:leaf=0.018677
```

```
                                30:leaf=0.374026
                4:[f26<-0.390943] yes=9,no=10,missing=10
                        9:[f1<-0.096491] yes=19,no=20,missing=20
                                19:leaf=-0.044673
                                20:leaf=0.216125
                        10:[f8<-0.960631] yes=21,no=22,missing=22
                                21:leaf=0.335125
                                22:[f14<-0.682021] yes=31,no=32,missing=32
                                        31:leaf=0.343000
                                        32:leaf=0.343000
        2:[f16<3.440249] yes=5,no=6,missing=6
                5:[f11<-1.376912] yes=11,no=12,missing=12
                        11:leaf=-0.000406
                        12:[f20<-0.292854] yes=23,no=24,missing=24
                                23:[f4<0.792763] yes=33,no=34,missing=34
                                        33:leaf=-0.036998
                                        34:leaf=0.343473
                                24:[f26<-0.211516] yes=35,no=36,missing=36
                                        35:leaf=0.170971
                                        36:leaf=0.345744
                6:[f8<1.233586] yes=13,no=14,missing=14
                        13:leaf=-0.040450
                        14:leaf=-0.000163
Loss after Tree 4: 0.5822573940429663


Tree 5:
0:[f27<0.422443] yes=1,no=2,missing=2
        1:[f20<0.110957] yes=3,no=4,missing=4
                3:[f10<0.795390] yes=7,no=8,missing=8
                        7:[f26<-0.306986] yes=15,no=16,missing=16
                                15:[f14<-1.246544] yes=25,no=26,missing=26
                                        25:leaf=-0.070122
                                        26:leaf=-0.004830
                                16:[f15<-0.731490] yes=27,no=28,missing=28
                                        27:leaf=0.700955
                                        28:leaf=0.005834
                        8:[f5<-0.791527] yes=17,no=18,missing=18
                                17:leaf=0.473599
                                18:leaf=-0.147642
                4:[f1<-0.678258] yes=9,no=10,missing=10
                        9:[f1<-1.328674] yes=19,no=20,missing=20
                                19:leaf=-0.037296
                                20:[f0<0.575898] yes=29,no=30,missing=30
                                        29:leaf=0.001361
                                        30:leaf=0.009292
                        10:[f11<0.780434] yes=21,no=22,missing=22
                                21:[f14<0.001007] yes=31,no=32,missing=32
```

```
                                        31:leaf=0.260225
                                        32:leaf=0.151639
                                22:leaf=0.080938
        2:[f16<3.440249] yes=5,no=6,missing=6
                5:[f11<-1.376912] yes=11,no=12,missing=12
                        11:leaf=-0.000284
                        12:[f20<-0.292854] yes=23,no=24,missing=24
                                23:[f4<0.792763] yes=33,no=34,missing=34
                                        33:leaf=-0.025899
                                        34:leaf=0.240431
                                24:[f6<-0.277770] yes=35,no=36,missing=36
                                        35:leaf=0.093578
                                        36:leaf=0.242399
                6:[f0<-1.129465] yes=13,no=14,missing=14
                        13:leaf=0.005686
                        14:leaf=-0.034114
Loss after Tree 5: 0.573200214537392


Model Accuracy: 0.956140350877193
```

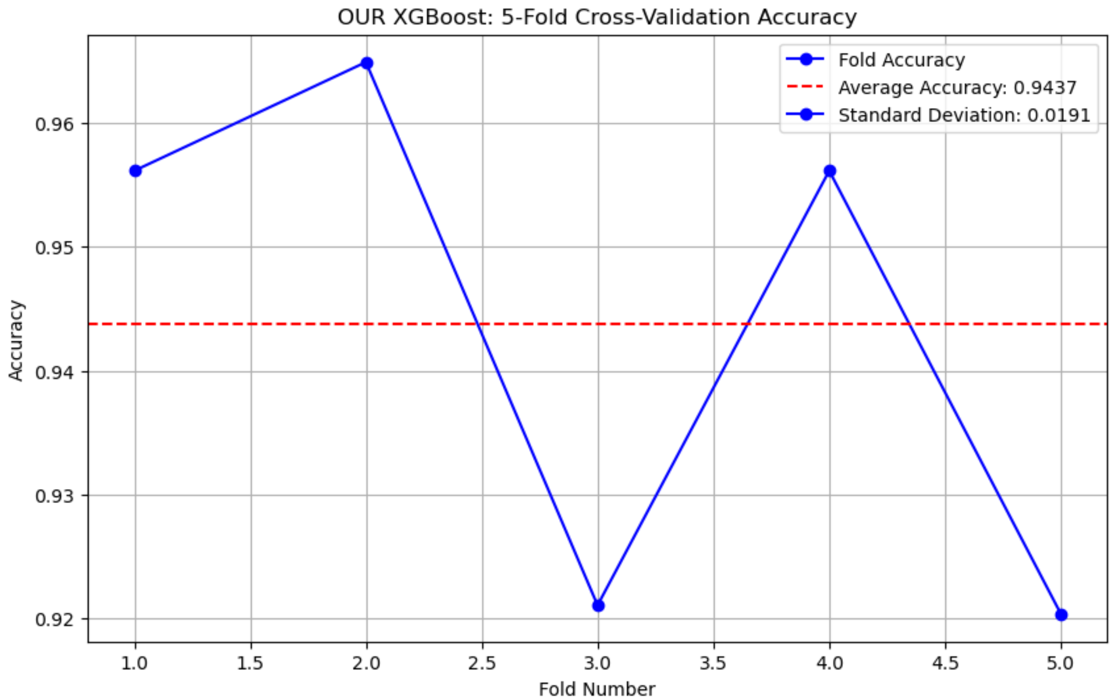
K-Fold Cross Validation

[5]:
```python
from sklearn.model_selection import KFold

# Define 5-Fold Cross Validation
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Initialize a list to store accuracy for each fold
accuracy_scores = []

# Perform 5-Fold Cross-Validation
for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
    # Split data into train and test sets for this fold
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    # Initialize and train the XGBoost model on the training data
    model = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)
    model.train(X_train, y_train, detailed=False)

    # Generate predictions on the test data
    y_prob = model.predict(X_test)

    # Convert predictions to binary labels (0 or 1) using a threshold of 0.5
    predictions = np.where(y_prob >= 0.5, 1, 0)

    # Calculate accuracy for this fold
```

```
    accuracy = np.mean(predictions == y_test)
    accuracy_scores.append(accuracy)
    print(f'Fold {fold} Accuracy: {accuracy:.4f}')

# Calculate the average accuracy across all folds
mean_accuracy = np.mean(accuracy_scores)
std_deviation = np.std(accuracy_scores)

# Print the results
print(f'Average Accuracy: {mean_accuracy:.4f}')
print(f'Standard Deviation: {std_deviation:.4f}')
```

```
Fold 1 Accuracy: 0.9561
Fold 2 Accuracy: 0.9649
Fold 3 Accuracy: 0.9211
Fold 4 Accuracy: 0.9561
Fold 5 Accuracy: 0.9204
Average Accuracy: 0.9437
Standard Deviation: 0.0191
```

[6]:
```
import matplotlib.pyplot as plt

# Plot the accuracy scores for each fold
plt.figure(figsize=(10, 6))
plt.plot(range(1, 6), accuracy_scores, marker='o', linestyle='-', color='b',␣
 ↪label='Fold Accuracy')
plt.axhline(mean_accuracy, color='r', linestyle='--', label=f'Average Accuracy:␣
 ↪{mean_accuracy:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Fold Accuracy',
    f'Average Accuracy: {mean_accuracy:.4f}',
    f'Standard Deviation: {std_deviation:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
 ↪loc='upper right')
plt.xlabel('Fold Number')
plt.ylabel('Accuracy')
plt.title('OUR XGBoost: 5-Fold Cross-Validation Accuracy')
plt.grid(True)
plt.show()
```



Implementing with imported XGBoost

[7]:
```
import numpy as np
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

# Load data from a CSV file
data = np.genfromtxt('../data/breast+cancer+wisconsin+diagnostic/wdbc.data',␣
 ↪delimiter=',', dtype=str)

# Extract features and convert them to float for numerical operations
X = data[:, 2:].astype(float)  # Features start from the 3rd column (index 2)

# Convert labels from 'M' (Malignant) and 'B' (Benign) to binary (1 and 0)
y = np.where(data[:, 1] == 'M', 1, 0)

# Normalize the features by subtracting the mean and dividing by the standard␣
 ↪deviation
X = (X - X.mean(axis=0)) / X.std(axis=0)

# Split the dataset into training and testing sets (80% training, 20% testing)
```

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

# Create an XGBoost model with log loss as the evaluation metric
model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.3,␣
↪tree_method='exact', eval_metric='logloss')

# Fits the XGBoost model to the training data.
model.fit(X_train, y_train)

# Retrieve and print model parameters for reference
params = model.get_params()
print(params)
n_estimators = params['n_estimators']
max_depth = params['max_depth']
learning_rate = params['learning_rate']

print("Number of estimators:", n_estimators)
print("Max depth:", max_depth)
print("Learning rate:", learning_rate)

# Retrieve the trained booster (underlying model) from XGBoost
booster = model.get_booster()

# Iterate over each tree in the model and print its structure
for i, tree in enumerate(booster.get_dump()):
    print(f"Tree {i + 1} structure:\n{tree}\n")

# Make predictions on the test data
y_pred_s = model.predict(X_test)

# Compute and print the accuracy score
accuracy_s = accuracy_score(y_test, y_pred_s)
print("Model Accuracy:", accuracy_s)
```

```
{'objective': 'binary:logistic', 'base_score': None, 'booster': None,
'callbacks': None, 'colsample_bylevel': None, 'colsample_bynode': None,
'colsample_bytree': None, 'device': None, 'early_stopping_rounds': None,
'enable_categorical': False, 'eval_metric': 'logloss', 'feature_types': None,
'gamma': None, 'grow_policy': None, 'importance_type': None,
'interaction_constraints': None, 'learning_rate': 0.3, 'max_bin': None,
'max_cat_threshold': None, 'max_cat_to_onehot': None, 'max_delta_step': None,
'max_depth': 5, 'max_leaves': None, 'min_child_weight': None, 'missing': nan,
'monotone_constraints': None, 'multi_strategy': None, 'n_estimators': 5,
'n_jobs': None, 'num_parallel_tree': None, 'random_state': None, 'reg_alpha':
None, 'reg_lambda': None, 'sampling_method': None, 'scale_pos_weight': None,
'subsample': None, 'tree_method': 'exact', 'validate_parameters': None,
```

```
'verbosity': None}
Number of estimators: 5
Max depth: 5
Learning rate: 0.3
Tree 1 structure:
0:[f7<0.0608958304] yes=1,no=2,missing=1
	1:[f20<0.116133995] yes=3,no=4,missing=3
		3:[f10<0.45829007] yes=7,no=8,missing=7
			7:[f21<2.00098825] yes=15,no=16,missing=15
				15:leaf=-0.461461931
				16:leaf=-0.120359808
			8:leaf=0.0178343765
		4:[f1<-0.721309006] yes=9,no=10,missing=9
			9:leaf=-0.280055076
			10:[f0<0.374247849] yes=17,no=18,missing=17
				17:leaf=0.522711515
				18:leaf=0.156028554
	2:[f22<-0.119477332] yes=5,no=6,missing=5
		5:[f21<0.0403489135] yes=11,no=12,missing=11
			11:leaf=-0.353559196
			12:leaf=0.384283721
		6:[f21<-0.878090024] yes=13,no=14,missing=13
			13:[f7<1.08556175] yes=19,no=20,missing=19
				19:leaf=-0.280055076
				20:leaf=0.468376309
			14:leaf=0.769567907


Tree 2 structure:
0:[f7<0.0608958304] yes=1,no=2,missing=1
	1:[f20<0.116133995] yes=3,no=4,missing=3
		3:[f12<0.619996548] yes=7,no=8,missing=7
			7:[f5<0.580086112] yes=15,no=16,missing=15
				15:[f14<-1.24404335] yes=19,no=20,missing=19
					19:leaf=-0.114919953
					20:leaf=-0.399985224
				16:leaf=-0.0655016676
			8:leaf=0.0298318025
		4:[f1<-0.141869307] yes=9,no=10,missing=9
			9:leaf=-0.192298621
			10:leaf=0.390452296
	2:[f27<0.486395031] yes=5,no=6,missing=5
		5:[f22<0.237952724] yes=11,no=12,missing=11
			11:[f1<0.279329836] yes=17,no=18,missing=17
				17:leaf=-0.343801051
				18:leaf=0.224137589
			12:leaf=0.405573368
		6:[f16<2.31672382] yes=13,no=14,missing=13
```

```
                        13:leaf=0.52348572
                        14:leaf=0.0616371781


Tree 3 structure:
0:[f7<0.0608958304] yes=1,no=2,missing=1
        1:[f20<0.116133995] yes=3,no=4,missing=3
                3:[f13<0.0607889853] yes=7,no=8,missing=7
                        7:[f21<1.23643661] yes=13,no=14,missing=13
                                13:[f19<-0.938026965] yes=19,no=20,missing=19
                                        19:leaf=-0.10479755
                                        20:leaf=-0.368357956
                                14:[f1<1.92689347] yes=21,no=22,missing=21
                                        21:leaf=0.0976544172
                                        22:leaf=-0.247339159
                        8:leaf=0.0508711077
                4:[f1<-0.721309006] yes=9,no=10,missing=9
                        9:leaf=-0.22352621
                        10:[f17<-0.401247859] yes=15,no=16,missing=15
                                15:leaf=0.36783421
                                16:leaf=0.0450727977
        2:[f22<0.214124054] yes=5,no=6,missing=5
                5:[f21<-0.00361891091] yes=11,no=12,missing=11
                        11:[f4<1.41546059] yes=17,no=18,missing=17
                                17:leaf=-0.316982895
                                18:leaf=-0.0404704325
                        12:leaf=0.359822601
                6:leaf=0.428095102


Tree 4 structure:
0:[f22<-0.170113266] yes=1,no=2,missing=1
        1:[f7<0.191929251] yes=3,no=4,missing=3
                3:[f13<0.00545468368] yes=7,no=8,missing=7
                        7:leaf=-0.338304639
                        8:leaf=0.0522898771
                4:leaf=0.0492498875
        2:[f26<-0.311543882] yes=5,no=6,missing=5
                5:[f1<0.0140441973] yes=9,no=10,missing=9
                        9:leaf=-0.266404003
                        10:leaf=0.0214250796
                6:[f21<-0.939156532] yes=11,no=12,missing=11
                        11:[f7<0.895976007] yes=13,no=14,missing=13
                                13:leaf=-0.242309749
                                14:leaf=0.232369795
                        12:[f24<-1.28082311] yes=15,no=16,missing=15
                                15:leaf=-0.0093738595
                                16:leaf=0.377245426
```

```
Tree 5 structure:
0:[f27<0.42244333] yes=1,no=2,missing=1
        1:[f20<0.11095693] yes=3,no=4,missing=3
                3:[f13<0.183998555] yes=7,no=8,missing=7
                        7:[f21<0.727549732] yes=13,no=14,missing=13
                                13:leaf=-0.328899622
                                14:[f20<-0.380864084] yes=17,no=18,missing=17
                                        17:leaf=-0.26351434
                                        18:leaf=0.113017946
                        8:leaf=0.0656299293
                4:[f1<-0.6782583] yes=9,no=10,missing=9
                        9:leaf=-0.198012784
                        10:[f11<0.21798721] yes=15,no=16,missing=15
                                15:leaf=0.321310699
                                16:leaf=0.0138620846
        2:[f20<-0.183100253] yes=5,no=6,missing=5
                5:[f4<0.828345776] yes=11,no=12,missing=11
                        11:leaf=-0.237057492
                        12:leaf=0.230106771
                6:leaf=0.344857752


Model Accuracy: 0.9736842105263158
```

K-Fold Cross Validation

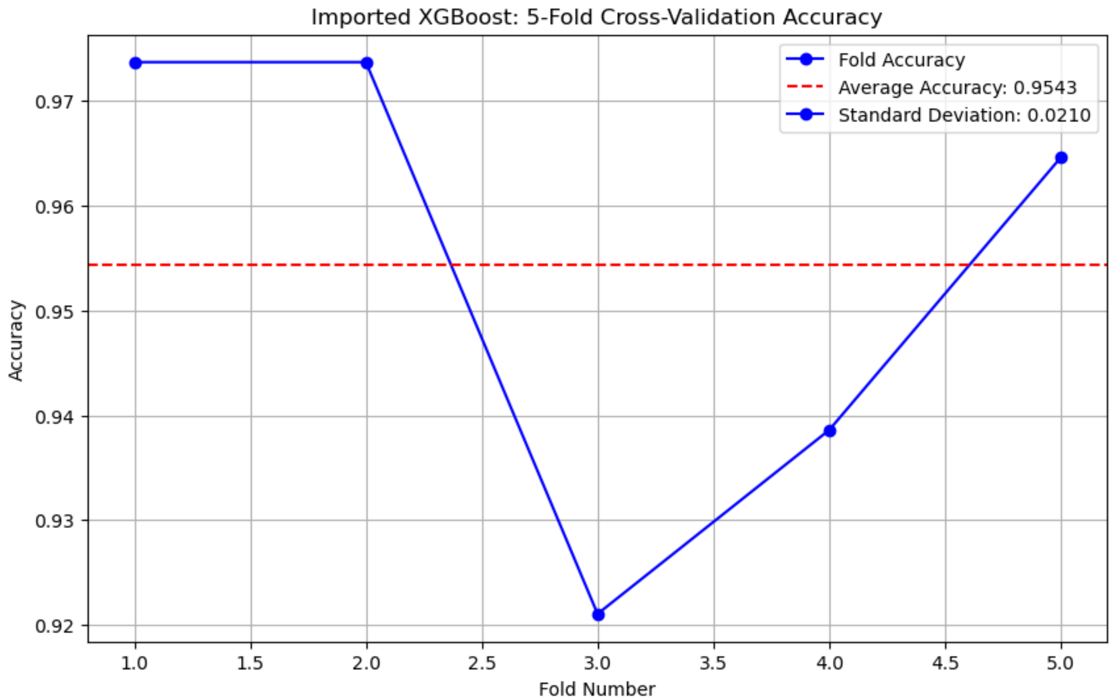
[8]:

```python
from sklearn.model_selection import KFold

# Define 5-Fold Cross Validation
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Initialize a list to store accuracy for each fold
accuracy_scores = []

# Perform 5-Fold Cross-Validation
for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
    # Split data into train and test sets for this fold
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    # Create an XGBoost model with log loss as the evaluation metric
    model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.3,␣
 ↪tree_method='exact', eval_metric='logloss')

    # Fits the XGBoost model to the training data.
    model.fit(X_train, y_train)
```

```
    # Generate predictions
    predictions = model.predict(X_test)

    # Calculate accuracy for this fold
    accuracy = accuracy_score(y_test, predictions)
    accuracy_scores.append(accuracy)
    print(f'Fold {fold} Accuracy: {accuracy:.4f}')

# Calculate the average accuracy across all folds
mean_accuracy_s = np.mean(accuracy_scores)
std_deviation_s = np.std(accuracy_scores)

# Print the results
print(f'Average Accuracy: {mean_accuracy_s:.4f}')
print(f'Standard Deviation: {std_deviation_s:.4f}')
```

```
Fold 1 Accuracy: 0.9737
Fold 2 Accuracy: 0.9737
Fold 3 Accuracy: 0.9211
Fold 4 Accuracy: 0.9386
Fold 5 Accuracy: 0.9646
Average Accuracy: 0.9543
Standard Deviation: 0.0210
```

[9]:
```
# Plot the accuracy scores for each fold
plt.figure(figsize=(10, 6))
plt.plot(range(1, 6), accuracy_scores, marker='o', linestyle='-', color='b',␣
 ↪label='Fold Accuracy')
plt.axhline(mean_accuracy_s, color='r', linestyle='--', label=f'Average␣
 ↪Accuracy: {mean_accuracy_s:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Fold Accuracy',
    f'Average Accuracy: {mean_accuracy_s:.4f}',
    f'Standard Deviation: {std_deviation_s:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
 ↪loc='upper right')
plt.xlabel('Fold Number')
plt.ylabel('Accuracy')
plt.title('Imported XGBoost: 5-Fold Cross-Validation Accuracy')
plt.grid(True)
plt.show()
```



Results 1 From the comparison of the two figures, it can be seen that under the 5-fold experiment, Our average accuracy is 1.06% lower, while our standard deviation is 0.19% lower than those in previous work. This shows that we successfully reproduced the previous work.

4.1.3 Customer Churn Prediction

This work uses XGBoost to predict customer retention based on information such as credit score, age, and income. The dataset used is Churn_Predictions_Personal (Ezzeldean, 2024). This dataset includes the following features:

Feature	Description
RowNumber	The row number in the dataset (used as an index).
CustomerId	A unique identifier for each customer.
Surname	The last name of the customer.
CreditScore	The credit score of the customer.
Geography	The location or country of the customer.
Gender	The gender of the customer (e.g., Male, Female).
Age	The age of the customer.
Tenure	The number of years the customer has been with the provider.
Balance	The account balance of the customer.
NumOfProducts	The number of products the customer has with the provider.
HasCrCard	Whether the customer has a credit card (1 = Yes, 0 = No).
IsActiveMember	Whether the customer is an active member (1 = Yes, 0 = No).
EstimatedSalary	The estimated salary of the customer.

Feature	Description
Exited	Whether the customer exited the bank (1 = Yes, 0 = No).

To facilitate result comparison, we made the following improvements:

- Remove the RowNumber, CustomerId, and Surname columns as the irrelevant columns.
- Encode the Gender and Geography features with the LabelEncoder
- Set the number of decision trees used by XGBoost to 5, the maximum depth of the trees to 5, and the learning rate to 0.3.

We split the dataset into 20% training and 80% testing sets, using 5-fold cross-validation to evaluate the accuracy of our model and the previous work's model.

Implementing with OUR XGBoost

[147]:
```python
from sklearn.preprocessing import LabelEncoder
# Load the Customer dataset
data = pd.read_csv('../data/Customer/Churn_Predictions.csv')
data = data.drop(['RowNumber','CustomerId','Surname'],axis=1)

# Create a sample dataframe with categorical data
Genderr = pd.DataFrame({'Gender': ['Male', 'Female']})
Geographyy = pd.DataFrame({'Geography': ['France', 'Germany','Spain']})

# Create a LabelEncoder object
le = LabelEncoder()

# Fit and transform the categorical data
data['Gender'] = le.fit_transform(data['Gender'])
data['Geography'] = le.fit_transform(data['Geography'])

# Data pre-processing
X = data.drop('Exited', axis=1)
y = data['Exited']
X = X.values if isinstance(X, pd.DataFrame) else X
y = y.values if isinstance(y, pd.Series) else y

# Split the dataset into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
 ↪random_state=42)

# Use the XGBoost model we implemented earlier and train it
model = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)
model.train(X_train, y_train, detailed='true')

# Generates predictions on the test data.
predictions = model.predict(X_test)
```

```python
# Convert predictions to binary labels (0 or 1) using a threshold of 0.5
predictions = np.where(predictions >= 0.5, 1, 0)

# Calculate the accuracy of the model
accuracy = np.mean(predictions == y_test)
print("Model Accuracy:", accuracy)
```

```
Tree 1:
0:[f3<43.000000] yes=1,no=2,missing=2
	1:[f6<2.000000] yes=3,no=4,missing=4
		3:[f3<38.000000] yes=7,no=8,missing=8
			7:[f1<0.000000] yes=13,no=14,missing=14
				13:leaf=-0.000000
				14:[f1<0.000000] yes=23,no=24,missing=24
					23:leaf=-0.000000
					24:leaf=0.132921
			8:[f8<1.000000] yes=15,no=16,missing=16
				15:[f1<0.000000] yes=25,no=26,missing=26
					25:leaf=-0.000000
					26:leaf=0.332530
				16:[f0<592.000000] yes=27,no=28,missing=28
					27:leaf=0.284091
					28:leaf=0.138889
		4:[f6<2.500000] yes=9,no=10,missing=10
			9:[f5<0.000000] yes=17,no=18,missing=18
				17:leaf=-0.000000
				18:[f5<0.000000] yes=29,no=30,missing=30
					29:leaf=-0.000000
					30:leaf=0.044476
			10:[f5<57003.365000] yes=19,no=20,missing=20
				19:[f9<131358.235000] yes=31,no=32,missing=32
					31:leaf=0.393939
					32:leaf=0.857143
				20:[f9<188544.700000] yes=33,no=34,missing=34
					33:leaf=0.959459
					34:leaf=0.250000
	2:[f8<0.000000] yes=5,no=6,missing=6
		5:leaf=-0.000000
		6:[f8<0.000000] yes=11,no=12,missing=12
			11:leaf=-0.000000
			12:[f8<0.000000] yes=21,no=22,missing=22
				21:leaf=-0.000000
				22:[f8<0.000000] yes=35,no=36,missing=36
					35:leaf=-0.000000
					36:leaf=0.415584
Loss after Tree 1: 0.702994294363243
```

```
Tree 2:
0:[f6<3.000000] yes=1,no=2,missing=2
	1:[f3<46.000000] yes=3,no=4,missing=4
		3:[f6<2.000000] yes=7,no=8,missing=8
			7:[f3<39.000000] yes=15,no=16,missing=16
				15:[f1<0.000000] yes=31,no=32,missing=32
					31:leaf=-0.000000
					32:leaf=0.093264
				16:[f8<0.000000] yes=33,no=34,missing=34
					33:leaf=-0.000000
					34:leaf=0.227173
			8:[f5<0.000000] yes=17,no=18,missing=18
				17:leaf=-0.000000
				18:[f5<0.000000] yes=35,no=36,missing=36
					35:leaf=-0.000000
					36:leaf=0.028385
		4:[f8<0.500000] yes=9,no=10,missing=10
			9:[f6<2.000000] yes=19,no=20,missing=20
				19:[f3<49.000000] yes=37,no=38,missing=38
					37:leaf=0.541991
					38:leaf=0.716089
				20:[f3<50.000000] yes=39,no=40,missing=40
					39:leaf=0.079626
					40:leaf=0.475325
			10:[f3<58.000000] yes=21,no=22,missing=22
				21:[f6<1.500000] yes=41,no=42,missing=42
					41:leaf=0.338108
					42:leaf=0.042707
				22:[f3<65.000000] yes=43,no=44,missing=44
					43:leaf=0.065068
					44:leaf=-0.059019
	2:[f3<42.500000] yes=5,no=6,missing=6
		5:[f5<57003.365000] yes=11,no=12,missing=12
			11:[f6<3.000000] yes=23,no=24,missing=24
				23:leaf=-0.000000
				24:[f6<3.000000] yes=45,no=46,missing=46
					45:leaf=-0.000000
					46:leaf=0.372340
			12:[f4<1.000000] yes=25,no=26,missing=26
				25:leaf=-0.000000
				26:[f4<1.000000] yes=47,no=48,missing=48
					47:leaf=-0.000000
					48:leaf=0.646154
		6:[f3<66.000000] yes=13,no=14,missing=14
			13:[f0<568.500000] yes=27,no=28,missing=28
				27:[f5<0.000000] yes=49,no=50,missing=50
					49:leaf=-0.000000
					50:leaf=0.841991
```

```
                                28:[f0<589.000000] yes=51,no=52,missing=52
                                        51:leaf=0.875325
                                        52:leaf=0.875325
                        14:[f6<3.000000] yes=29,no=30,missing=30
                                29:leaf=-0.000000
                                30:[f6<3.000000] yes=53,no=54,missing=54
                                        53:leaf=-0.000000
                                        54:leaf=0.275325
Loss after Tree 2: 0.7042491308758148


Tree 3:
0:[f6<2.000000] yes=1,no=2,missing=2
        1:[f3<42.000000] yes=3,no=4,missing=4
                3:[f1<0.000000] yes=7,no=8,missing=8
                        7:leaf=-0.000000
                        8:[f1<0.000000] yes=15,no=16,missing=16
                                15:leaf=-0.000000
                                16:[f1<0.000000] yes=27,no=28,missing=28
                                        27:leaf=-0.000000
                                        28:leaf=0.075593
                4:[f8<0.000000] yes=9,no=10,missing=10
                        9:leaf=-0.000000
                        10:[f8<0.000000] yes=17,no=18,missing=18
                                17:leaf=-0.000000
                                18:[f8<0.000000] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=0.270872
        2:[f6<2.500000] yes=5,no=6,missing=6
                5:[f5<1884.345000] yes=11,no=12,missing=12
                        11:[f3<43.000000] yes=19,no=20,missing=20
                                19:[f4<10.000000] yes=31,no=32,missing=32
                                        31:leaf=-0.003316
                                        32:leaf=0.016116
                                20:[f2<0.000000] yes=33,no=34,missing=34
                                        33:leaf=-0.000000
                                        34:leaf=-0.069079
                        12:[f3<47.000000] yes=21,no=22,missing=22
                                21:[f5<34556.880000] yes=35,no=36,missing=36
                                        35:leaf=0.978142
                                        36:leaf=0.054606
                                22:[f8<0.000000] yes=37,no=38,missing=38
                                        37:leaf=-0.000000
                                        38:leaf=0.207795
                6:[f3<36.000000] yes=13,no=14,missing=14
                        13:[f5<0.000000] yes=23,no=24,missing=24
                                23:leaf=-0.000000
                                24:[f5<0.000000] yes=39,no=40,missing=40
```

```
                                        39:leaf=-0.000000
                                        40:leaf=0.304076
                        14:[f3<42.000000] yes=25,no=26,missing=26
                                25:[f3<36.000000] yes=41,no=42,missing=42
                                        41:leaf=-0.000000
                                        42:leaf=0.447046
                                26:[f3<42.000000] yes=43,no=44,missing=44
                                        43:leaf=-0.000000
                                        44:leaf=0.573612
Loss after Tree 3: 0.7074395955866944


Tree 4:
0:[f3<45.000000] yes=1,no=2,missing=2
        1:[f6<2.000000] yes=3,no=4,missing=4
                3:[f1<0.000000] yes=7,no=8,missing=8
                        7:leaf=-0.000000
                        8:[f1<0.000000] yes=15,no=16,missing=16
                                15:leaf=-0.000000
                                16:[f1<0.000000] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=0.058931
                4:[f6<3.000000] yes=9,no=10,missing=10
                        9:[f4<0.000000] yes=17,no=18,missing=18
                                17:leaf=-0.000000
                                18:[f4<0.000000] yes=31,no=32,missing=32
                                        31:leaf=-0.000000
                                        32:leaf=0.013776
                        10:[f8<1.000000] yes=19,no=20,missing=20
                                19:[f0<638.000000] yes=33,no=34,missing=34
                                        33:leaf=0.420236
                                        34:leaf=0.255566
                                20:[f6<3.000000] yes=35,no=36,missing=36
                                        35:leaf=-0.000000
                                        36:leaf=0.232531
        2:[f8<1.000000] yes=5,no=6,missing=6
                5:[f3<51.000000] yes=11,no=12,missing=12
                        11:[f6<1.000000] yes=21,no=22,missing=22
                                21:leaf=-0.000000
                                22:[f6<1.000000] yes=37,no=38,missing=38
                                        37:leaf=-0.000000
                                        38:leaf=0.220730
                        12:[f3<73.500000] yes=23,no=24,missing=24
                                23:[f3<51.000000] yes=39,no=40,missing=40
                                        39:leaf=-0.000000
                                        40:leaf=0.451049
                                24:[f8<0.000000] yes=41,no=42,missing=42
                                        41:leaf=-0.000000
```

```
                                42:leaf=-0.151078
                6:[f3<58.000000] yes=13,no=14,missing=14
                        13:[f6<2.000000] yes=25,no=26,missing=26
                                25:[f1<2.000000] yes=43,no=44,missing=44
                                        43:leaf=0.201154
                                        44:leaf=0.004311
                                26:[f6<3.000000] yes=45,no=46,missing=46
                                        45:leaf=0.004643
                                        46:leaf=0.417717
                        14:[f6<3.000000] yes=27,no=28,missing=28
                                27:[f3<71.000000] yes=47,no=48,missing=48
                                        47:leaf=-0.025618
                                        48:leaf=-0.114775
                                28:[f1<0.000000] yes=49,no=50,missing=50
                                        49:leaf=-0.000000
                                        50:leaf=0.213644
Loss after Tree 4: 0.70854362835862


Tree 5:
0:[f8<1.000000] yes=1,no=2,missing=2
        1:[f3<50.000000] yes=3,no=4,missing=4
                3:[f1<0.000000] yes=7,no=8,missing=8
                        7:leaf=-0.000000
                        8:[f1<0.000000] yes=15,no=16,missing=16
                                15:leaf=-0.000000
                                16:[f1<0.000000] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=0.067778
                4:[f3<52.000000] yes=9,no=10,missing=10
                        9:[f9<53957.075000] yes=17,no=18,missing=18
                                17:[f5<103236.255000] yes=31,no=32,missing=32
                                        31:leaf=-0.308940
                                        32:leaf=0.047648
                                18:[f0<450.000000] yes=33,no=34,missing=34
                                        33:leaf=-0.475954
                                        34:leaf=0.266784
                        10:[f8<0.000000] yes=19,no=20,missing=20
                                19:leaf=-0.000000
                                20:[f8<0.000000] yes=35,no=36,missing=36
                                        35:leaf=-0.000000
                                        36:leaf=0.332766
        2:[f6<3.000000] yes=5,no=6,missing=6
                5:[f0<408.500000] yes=11,no=12,missing=12
                        11:[f5<121526.960000] yes=21,no=22,missing=22
                                21:[f0<366.000000] yes=37,no=38,missing=38
                                        37:leaf=0.719274
                                        38:leaf=0.891787
```

```
                        22:leaf=0.324482
                12:[f2<1.000000] yes=23,no=24,missing=24
                        23:[f1<0.000000] yes=39,no=40,missing=40
                                39:leaf=-0.000000
                                40:leaf=0.032354
                        24:[f5<199014.130000] yes=41,no=42,missing=42
                                41:leaf=-0.021032
                                42:leaf=0.609832
        6:[f3<35.000000] yes=13,no=14,missing=14
                13:[f2<1.000000] yes=25,no=26,missing=26
                        25:[f9<183416.770000] yes=43,no=44,missing=44
                                43:leaf=0.323493
                                44:leaf=-0.429829
                        26:[f0<568.500000] yes=45,no=46,missing=46
                                45:leaf=0.413753
                                46:leaf=-0.289327
                14:[f3<35.000000] yes=27,no=28,missing=28
                        27:leaf=-0.000000
                        28:[f3<35.000000] yes=47,no=48,missing=48
                                47:leaf=-0.000000
                                48:leaf=0.239537
Loss after Tree 5: 0.7101325140744678


Model Accuracy: 0.853
```

K-Fold Cross Validation

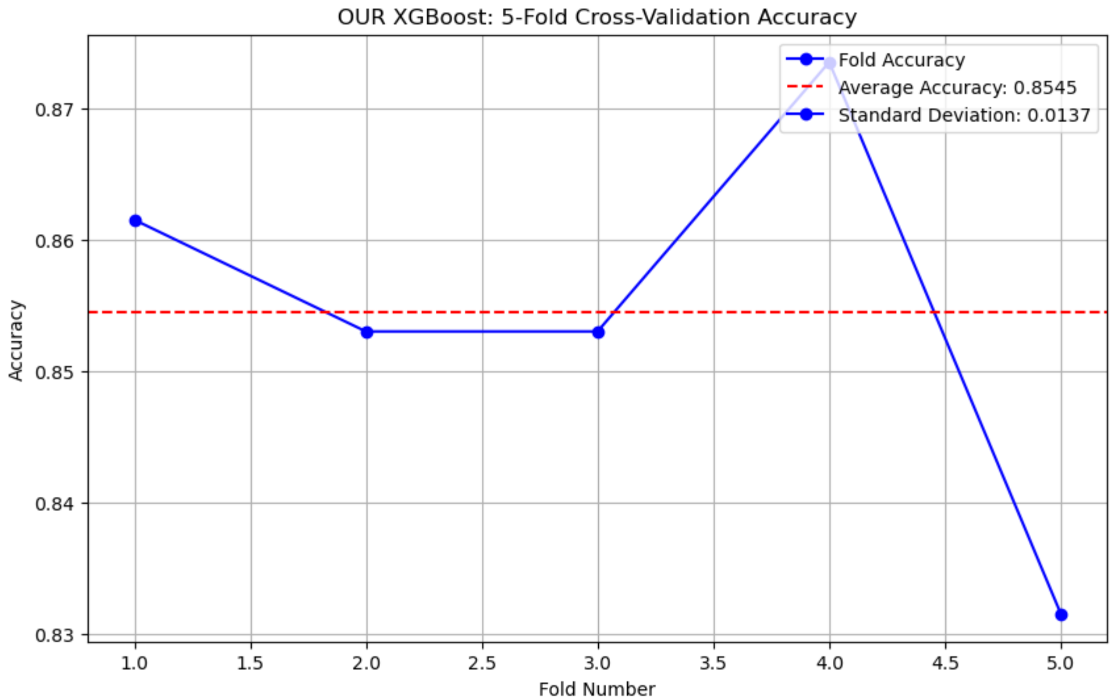
[ ]:
```python
from sklearn.model_selection import KFold

# Define 5-Fold Cross Validation
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Initialize a list to store accuracy for each fold
accuracy_scores = []
# Perform 5-Fold Cross-Validation
for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
    # Split data into train and test sets for this fold
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
    # Initialize and train the XGBoost model on the training data
    model = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)
    model.train(X_train, y_train, detailed=False)

    # Generate predictions on the test data
    y_prob = model.predict(X_test)

    # Convert predictions to binary labels (0 or 1) using a threshold of 0.5
```

```
    predictions = np.where(y_prob >= 0.5, 1, 0)

    # Calculate accuracy for this fold
    accuracy = np.mean(predictions == y_test)
    accuracy_scores.append(accuracy)
    print(f'Fold {fold} Accuracy: {accuracy:.4f}')

# Calculate the average accuracy across all folds
mean_accuracy = np.mean(accuracy_scores)
std_deviation = np.std(accuracy_scores)

# Print the results
print(f'Average Accuracy: {mean_accuracy:.4f}')
print(f'Standard Deviation: {std_deviation:.4f}')
```

```
Fold 1 Accuracy: 0.8615
Fold 2 Accuracy: 0.8530
Fold 3 Accuracy: 0.8530
Fold 4 Accuracy: 0.8735
Fold 5 Accuracy: 0.8315
Average Accuracy: 0.8545
Standard Deviation: 0.0137
```

[155]:

```
# Plot the accuracy scores for each fold
plt.figure(figsize=(10, 6))
plt.plot(range(1, 6), accuracy_scores, marker='o', linestyle='-', color='b',␣
 ↪label='Fold Accuracy')
plt.axhline(mean_accuracy, color='r', linestyle='--', label=f'Average Accuracy:␣
 ↪{mean_accuracy:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Fold Accuracy',
    f'Average Accuracy: {mean_accuracy:.4f}',
    f'Standard Deviation: {std_deviation:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
 ↪loc='upper right')
plt.xlabel('Fold Number')
plt.ylabel('Accuracy')
plt.title('OUR XGBoost: 5-Fold Cross-Validation Accuracy')
plt.grid(True)
plt.show()
```



Implementing with imported XGBoost

[156]:
```python
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)
model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.3,␣
↪tree_method='exact', eval_metric='logloss')
model.fit(X_train, y_train)
# Retrieve and print model parameters for reference
params = model.get_params()
print(params)
n_estimators = params['n_estimators']
max_depth = params['max_depth']
learning_rate = params['learning_rate']

print("Number of estimators:", n_estimators)
print("Max depth:", max_depth)
print("Learning rate:", learning_rate)

# Retrieve the trained booster (underlying model) from XGBoost
booster = model.get_booster()

# Iterate over each tree in the model and print its structure
for i, tree in enumerate(booster.get_dump()):
    print(f"Tree {i + 1} structure:\n{tree}\n")
```

```python
# Make predictions on the test data
y_pred_s = model.predict(X_test)

# Compute and print the accuracy score
accuracy_s = accuracy_score(y_test, y_pred_s)
print("Model Accuracy:", accuracy_s)
```

```
{'objective': 'binary:logistic', 'base_score': None, 'booster': None,
'callbacks': None, 'colsample_bylevel': None, 'colsample_bynode': None,
'colsample_bytree': None, 'device': None, 'early_stopping_rounds': None,
'enable_categorical': False, 'eval_metric': 'logloss', 'feature_types': None,
'gamma': None, 'grow_policy': None, 'importance_type': None,
'interaction_constraints': None, 'learning_rate': 0.3, 'max_bin': None,
'max_cat_threshold': None, 'max_cat_to_onehot': None, 'max_delta_step': None,
'max_depth': 5, 'max_leaves': None, 'min_child_weight': None, 'missing': nan,
'monotone_constraints': None, 'multi_strategy': None, 'n_estimators': 5,
'n_jobs': None, 'num_parallel_tree': None, 'random_state': None, 'reg_alpha':
None, 'reg_lambda': None, 'sampling_method': None, 'scale_pos_weight': None,
'subsample': None, 'tree_method': 'exact', 'validate_parameters': None,
'verbosity': None}
Number of estimators: 5
Max depth: 5
Learning rate: 0.3
Tree 1 structure:
0:[f3<44.5] yes=1,no=2,missing=1
        1:[f6<2.5] yes=3,no=4,missing=3
                3:[f6<1.5] yes=7,no=8,missing=7
                        7:[f3<38.5] yes=15,no=16,missing=15
                                15:[f1<0.5] yes=31,no=32,missing=31
                                        31:leaf=-0.230547518
                                        32:leaf=-0.0919528306
                                16:[f8<0.5] yes=33,no=34,missing=33
                                        33:leaf=0.241346836
                                        34:leaf=-0.0322341733
                        8:[f5<1884.34497] yes=17,no=18,missing=17
                                17:[f3<42.5] yes=35,no=36,missing=35
                                        35:leaf=-0.358693063
                                        36:leaf=-0.249457821
                                18:[f3<36.5] yes=37,no=38,missing=37
                                        37:leaf=-0.29474625
                                        38:leaf=-0.182480931
                4:[f5<57003.3672] yes=9,no=10,missing=9
                        9:[f3<37.5] yes=19,no=20,missing=19
                                19:[f9<123449.453] yes=39,no=40,missing=39
                                        39:leaf=-0.0320933424
                                        40:leaf=0.604930401
                                20:leaf=0.800906122
```

```
                        10:[f9<186808.109] yes=21,no=22,missing=21
                                21:leaf=1.13479555
                                22:leaf=0.228974879
        2:[f8<0.5] yes=5,no=6,missing=5
                5:[f3<51.5] yes=11,no=12,missing=11
                        11:[f6<1.5] yes=23,no=24,missing=23
                                23:[f9<138612.75] yes=41,no=42,missing=41
                                        41:leaf=0.579765379
                                        42:leaf=0.890252292
                                24:[f6<2.5] yes=43,no=44,missing=43
                                        43:leaf=-0.00507485913
                                        44:leaf=1.08584046
                        12:[f3<72.5] yes=25,no=26,missing=25
                                25:[f9<2436.76489] yes=45,no=46,missing=45
                                        45:leaf=0.228974879
                                        46:leaf=1.0812273
                                26:leaf=0.0847412795
                6:[f6<2.5] yes=13,no=14,missing=13
                        13:[f6<1.5] yes=27,no=28,missing=27
                                27:[f3<57.5] yes=47,no=48,missing=47
                                        47:leaf=0.352320939
                                        48:leaf=-0.101905048
                                28:[f5<79687.5391] yes=49,no=50,missing=49
                                        49:leaf=-0.307367653
                                        50:leaf=0.0116048651
                        14:[f3<60.5] yes=29,no=30,missing=29
                                29:leaf=1.101349
                                30:leaf=0.228974879


Tree 2 structure:
0:[f3<41.5] yes=1,no=2,missing=1
        1:[f6<2.5] yes=3,no=4,missing=3
                3:[f6<1.5] yes=7,no=8,missing=7
                        7:[f8<0.5] yes=15,no=16,missing=15
                                15:[f1<0.5] yes=31,no=32,missing=31
                                        31:leaf=-0.123139046
                                        32:leaf=0.0517069176
                                16:[f3<32.5] yes=33,no=34,missing=33
                                        33:leaf=-0.243828058
                                        34:leaf=-0.110126264
                        8:[f5<1884.34497] yes=17,no=18,missing=17
                                17:[f2<0.5] yes=35,no=36,missing=35
                                        35:leaf=-0.298691213
                                        36:leaf=-0.343250066
                                18:[f8<0.5] yes=37,no=38,missing=37
                                        37:leaf=-0.164395511
                                        38:leaf=-0.277632624
```

```
                4:[f5<23194.0801] yes=9,no=10,missing=9
                        9:[f9<131358.234] yes=19,no=20,missing=19
                                19:[f3<32.5] yes=39,no=40,missing=39
                                        39:leaf=-0.140488297
                                        40:leaf=0.24397181
                                20:leaf=0.455020964
                        10:[f4<1.5] yes=21,no=22,missing=21
                                21:leaf=0.112659268
                                22:leaf=0.548208952
        2:[f8<0.5] yes=5,no=6,missing=5
                5:[f3<47.5] yes=11,no=12,missing=11
                        11:[f6<1.5] yes=23,no=24,missing=23
                                23:[f1<0.5] yes=41,no=42,missing=41
                                        41:leaf=0.129033059
                                        42:leaf=0.357695699
                                24:[f6<2.5] yes=43,no=44,missing=43
                                        43:leaf=-0.128731012
                                        44:leaf=0.557621419
                        12:[f3<50.5] yes=25,no=26,missing=25
                                25:[f6<1.5] yes=45,no=46,missing=45
                                        45:leaf=0.409767628
                                        46:leaf=0.143114015
                                26:[f3<69.5] yes=47,no=48,missing=47
                                        47:leaf=0.499052256
                                        48:leaf=0.135661215
                6:[f6<2.5] yes=13,no=14,missing=13
                        13:[f6<1.5] yes=27,no=28,missing=27
                                27:[f3<65.5] yes=49,no=50,missing=49
                                        49:leaf=0.142425805
                                        50:leaf=-0.219705313
                                28:[f5<43031.9688] yes=51,no=52,missing=51
                                        51:leaf=-0.291753232
                                        52:leaf=-0.0132753709
                        14:[f3<62.5] yes=29,no=30,missing=29
                                29:[f3<42.5] yes=53,no=54,missing=53
                                        53:leaf=0.159109443
                                        54:leaf=0.567204833
                                30:leaf=0.0904192328


Tree 3 structure:
0:[f3<39.5] yes=1,no=2,missing=1
        1:[f6<2.5] yes=3,no=4,missing=3
                3:[f6<1.5] yes=7,no=8,missing=7
                        7:[f5<57593.7734] yes=15,no=16,missing=15
                                15:[f3<30.5] yes=29,no=30,missing=29
                                        29:leaf=-0.11751961
                                        30:leaf=0.112188675
```

```
                        16:[f1<0.5] yes=31,no=32,missing=31
                                31:leaf=-0.212003157
                                32:leaf=-0.0582340844
                8:[f5<95672.2188] yes=17,no=18,missing=17
                        17:[f4<0.5] yes=33,no=34,missing=33
                                33:leaf=-0.161258608
                                34:leaf=-0.300384313
                        18:[f5<188051.125] yes=35,no=36,missing=35
                                35:leaf=-0.187877953
                                36:leaf=0.208440915
        4:[f0<690.5] yes=9,no=10,missing=9
                9:[f5<157702.703] yes=19,no=20,missing=19
                        19:leaf=0.426330298
                        20:leaf=0.138677329
                10:[f5<23194.0801] yes=21,no=22,missing=21
                        21:[f4<1.5] yes=37,no=38,missing=37
                                37:leaf=0.266680717
                                38:leaf=-0.266097724
                        22:[f9<129588.812] yes=39,no=40,missing=39
                                39:leaf=0.376982927
                                40:leaf=0.0572154783
    2:[f6<2.5] yes=5,no=6,missing=5
        5:[f6<1.5] yes=11,no=12,missing=11
                11:[f8<0.5] yes=23,no=24,missing=23
                        23:[f3<45.5] yes=41,no=42,missing=41
                                41:leaf=0.11760886
                                42:leaf=0.318599164
                        24:[f1<1.5] yes=43,no=44,missing=43
                                43:leaf=0.120175429
                                44:leaf=-0.116074398
                12:[f5<1884.34497] yes=25,no=26,missing=25
                        25:[f0<627.5] yes=45,no=46,missing=45
                                45:leaf=-0.156297997
                                46:leaf=-0.282667547
                        26:[f2<0.5] yes=47,no=48,missing=47
                                47:leaf=0.147731021
                                48:leaf=-0.0845054984
        6:[f3<66] yes=13,no=14,missing=13
                13:[f3<42.5] yes=27,no=28,missing=27
                        27:[f5<104733.641] yes=49,no=50,missing=49
                                49:leaf=0.123565555
                                50:leaf=0.397861928
                        28:leaf=0.482624292
                14:leaf=0.0303768311


Tree 4 structure:
0:[f3<42.5] yes=1,no=2,missing=1
```

```
        1:[f6<2.5] yes=3,no=4,missing=3
                3:[f6<1.5] yes=7,no=8,missing=7
                        7:[f2<0.5] yes=15,no=16,missing=15
                                15:[f5<179116.719] yes=27,no=28,missing=27
                                        27:leaf=0.00220615743
                                        28:leaf=0.456649184
                                16:[f3<35.5] yes=29,no=30,missing=29
                                        29:leaf=-0.164669454
                                        30:leaf=-0.0337890387
                        8:[f5<108284.734] yes=17,no=18,missing=17
                                17:[f3<35.5] yes=31,no=32,missing=31
                                        31:leaf=-0.284751028
                                        32:leaf=-0.212522194
                                18:[f5<108993.398] yes=33,no=34,missing=33
                                        33:leaf=0.349195987
                                        34:leaf=-0.134200111
                4:[f5<57003.3672] yes=9,no=10,missing=9
                        9:[f9<131358.234] yes=19,no=20,missing=19
                                19:[f9<83460.3672] yes=35,no=36,missing=35
                                        35:leaf=0.128232881
                                        36:leaf=-0.0872453451
                                20:leaf=0.283689499
                        10:[f9<187897.812] yes=21,no=22,missing=21
                                21:leaf=0.362116754
                                22:leaf=-0.0115433987
        2:[f6<2.5] yes=5,no=6,missing=5
                5:[f6<1.5] yes=11,no=12,missing=11
                        11:[f3<71.5] yes=23,no=24,missing=23
                                23:[f5<40737.3359] yes=37,no=38,missing=37
                                        37:leaf=0.27687487
                                        38:leaf=0.101990096
                                24:[f9<171044.047] yes=39,no=40,missing=39
                                        39:leaf=-0.303259224
                                        40:leaf=-0.0630478337
                        12:[f5<42398.0352] yes=25,no=26,missing=25
                                25:[f0<539.5] yes=41,no=42,missing=41
                                        41:leaf=0.024136778
                                        42:leaf=-0.223969236
                                26:[f4<1.5] yes=43,no=44,missing=43
                                        43:leaf=0.27258423
                                        44:leaf=0.0187295284
                6:[f3<66] yes=13,no=14,missing=13
                        13:leaf=0.403459936
                        14:leaf=0.0255268496


Tree 5 structure:
0:[f3<36.5] yes=1,no=2,missing=1
```

```
1:[f6<1.5] yes=3,no=4,missing=3
	3:[f5<57593.7734] yes=7,no=8,missing=7
		7:[f0<574] yes=15,no=16,missing=15
			15:[f0<544.5] yes=29,no=30,missing=29
				29:leaf=0.0627980605
				30:leaf=-0.303245187
			16:[f0<616.5] yes=31,no=32,missing=31
				31:leaf=0.389550507
				32:leaf=0.0381290615
		8:[f1<0.5] yes=17,no=18,missing=17
			17:[f5<175825.344] yes=33,no=34,missing=33
				33:leaf=-0.219364226
				34:leaf=0.383046895
			18:[f1<1.5] yes=35,no=36,missing=35
				35:leaf=0.0504731052
				36:leaf=-0.171664238
	4:[f6<2.5] yes=9,no=10,missing=9
		9:[f5<108284.734] yes=19,no=20,missing=19
			19:[f0<477.5] yes=37,no=38,missing=37
				37:leaf=-0.029379582
				38:leaf=-0.266987354
			20:[f5<109039.023] yes=39,no=40,missing=39
				39:leaf=0.312336385
				40:leaf=-0.157680169
		10:[f5<23194.0801] yes=21,no=22,missing=21
			21:[f7<0.5] yes=41,no=42,missing=41
				41:leaf=0.228500918
				42:leaf=-0.149840653
			22:[f9<159646.219] yes=43,no=44,missing=43
				43:leaf=0.295526922
				44:leaf=-0.02069664
2:[f6<2.5] yes=5,no=6,missing=5
	5:[f8<0.5] yes=11,no=12,missing=11
		11:[f3<49.5] yes=23,no=24,missing=23
			23:[f6<1.5] yes=45,no=46,missing=45
				45:leaf=0.0724150464
				46:leaf=-0.0492360219
			24:[f3<53.5] yes=47,no=48,missing=47
				47:leaf=0.177568972
				48:leaf=0.301647991
		12:[f2<0.5] yes=25,no=26,missing=25
			25:[f3<62.5] yes=49,no=50,missing=49
				49:leaf=0.0454354435
				50:leaf=-0.185750291
			26:[f6<1.5] yes=51,no=52,missing=51
				51:leaf=-0.0545372032
				52:leaf=-0.205473319
	6:[f3<66] yes=13,no=14,missing=13
```

```
13:[f0<461.5] yes=27,no=28,missing=27
        27:leaf=0.0919968858
        28:leaf=0.334728658
14:leaf=0.0214559808
```

```
Model Accuracy: 0.8605
```

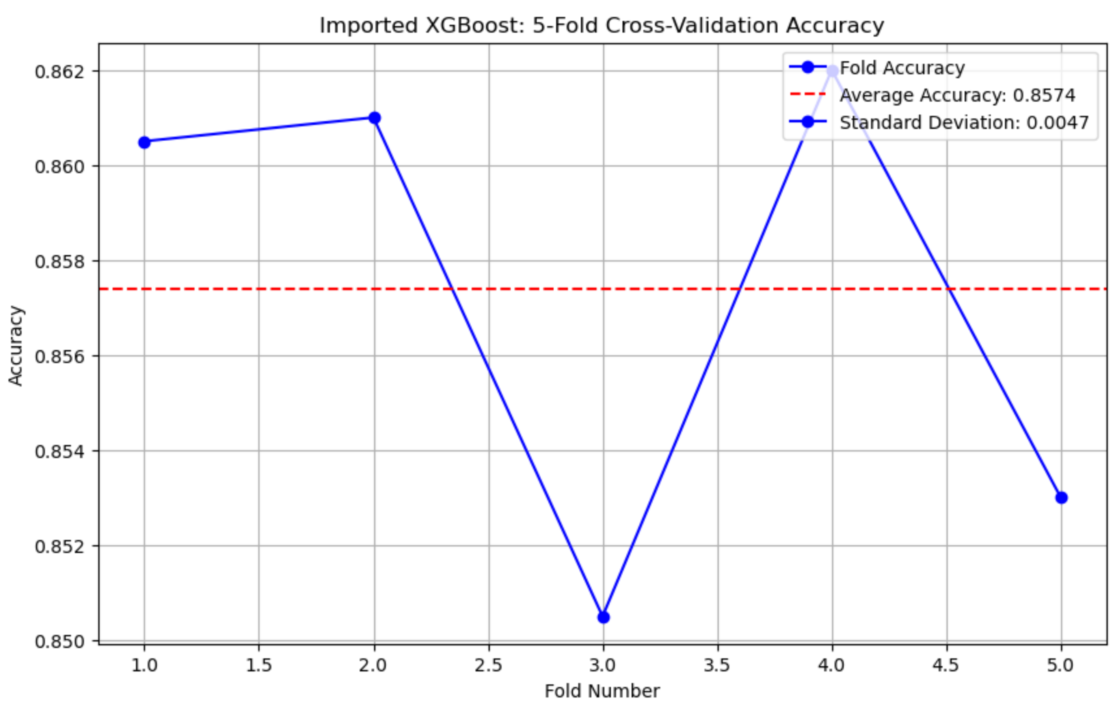
K-Fold Cross Validation

[157]:
```python
from sklearn.model_selection import KFold

# Define 5-Fold Cross Validation
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Initialize a list to store accuracy for each fold
accuracy_scores = []

# Perform 5-Fold Cross-Validation
for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
    # Split data into train and test sets for this fold
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    # Create an XGBoost model with log loss as the evaluation metric
    model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.3,␣
 ↪tree_method='exact', eval_metric='logloss')

    # Fits the XGBoost model to the training data.
    model.fit(X_train, y_train)

    # Generate predictions
    predictions = model.predict(X_test)

    # Calculate accuracy for this fold
    accuracy = accuracy_score(y_test, predictions)
    accuracy_scores.append(accuracy)
    print(f'Fold {fold} Accuracy: {accuracy:.4f}')

# Calculate the average accuracy across all folds
mean_accuracy_s = np.mean(accuracy_scores)
std_deviation_s = np.std(accuracy_scores)

# Print the results
print(f'Average Accuracy: {mean_accuracy_s:.4f}')
print(f'Standard Deviation: {std_deviation_s:.4f}')
```

```
Fold 1 Accuracy: 0.8605
Fold 2 Accuracy: 0.8610
```

```
Fold 3 Accuracy: 0.8505
Fold 4 Accuracy: 0.8620
Fold 5 Accuracy: 0.8530
Average Accuracy: 0.8574
Standard Deviation: 0.0047
```

[152]:
```python
# Plot the accuracy scores for each fold
plt.figure(figsize=(10, 6))
plt.plot(range(1, 6), accuracy_scores, marker='o', linestyle='-', color='b',␣
 ↪label='Fold Accuracy')
plt.axhline(mean_accuracy_s, color='r', linestyle='--', label=f'Average␣
 ↪Accuracy: {mean_accuracy_s:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Fold Accuracy',
    f'Average Accuracy: {mean_accuracy_s:.4f}',
    f'Standard Deviation: {std_deviation_s:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
 ↪loc='upper right')
plt.xlabel('Fold Number')
plt.ylabel('Accuracy')
plt.title('Imported XGBoost: 5-Fold Cross-Validation Accuracy')
plt.grid(True)
plt.show()
```



Results 2 From the comparison of the two figures, it can be seen that under the 5-fold experiment, our average accuracy is 0.29% lower. This shows that we successfully reproduced the previous work.

4.1.4 Titanic Survival Prediction

This work uses XGBoost to predict which passengers would survive the Titanic shipwreck. The dataset used is Titanic - Machine Learning from Disaster (Kaggle, 2024). Below are the features included in the dataset:

Feature	Description
PassengerId	Unique identifier for each Passenger.
Survival	Survival status (0 = No, 1 = Yes).
Pclass	Ticket class (1 = 1st, 2 = 2nd, 3 = 3rd).
Sex	Sex of the passenger.
Age	Age of the passenger in years.
Sibsp	Number of siblings/spouses aboard the Titanic.
Parch	Number of parents/children aboard the Titanic.
Ticket	Ticket number.
Fare	Passenger fare.
Cabin	Cabin number.
Embarked	Port of Embarkation (C = Cherbourg, Q = Queenstown, S = Southampton).

To facilitate result comparison, we made the following improvements:

- Remove the Name, PassengerId, Ticket columns as the irrelevant columns.
- Count the null values in the Cabin and Age columns and set the number of null values into a new feature: 0 means no null values, 1 means one null value, and 2 means all values are nulls.
- Extract the first letter of the Cabin code and map it to a number.
- Fill the missing cells in Fare with the average ticket price of third-class passengers.
- Fill the missing cells in Embarked with the Embarkation Southampton.
- Convert the 'Sex', 'Nulls', 'Cabin_mapped', 'Embarked' columns into one-hot encodings.
- Set the number of decision trees used by XGBoost to 5, the maximum depth of the trees to 5, and the learning rate to 0.3.

We split the dataset into 20% training and 80% testing sets, using 5-fold cross-validation to evaluate the accuracy of our model and the previous work's model.

Implementing with OUR XGBoost

[111]:
```python
import warnings
warnings.filterwarnings('ignore')
train = pd.read_csv('../data/Titanic/train.csv')
test = pd.read_csv('../data/Titanic/test.csv')

# Concatenate training set and test set
X_full = pd.concat([train.drop('Survived', axis = 1), test], axis = 0)
```

```python
# Clean X_full
X_full.drop('PassengerId', axis = 1, inplace=True)
X_full['Nulls'] = X_full.Cabin.isnull().astype('int') + X_full.Age.isnull().
 ↪astype('int')

# Divide the cabin category by simply extracting the first letter
X_full['Cabin_mapped'] = X_full['Cabin'].astype(str).str[0]
cabin_dict = {k:i for i, k in enumerate(X_full.Cabin_mapped.unique())}

# Transform 'Age' and 'Cabin'
X_full.loc[:, 'Cabin_mapped'] = X_full.loc[:, 'Cabin_mapped'].map(cabin_dict)
X_full.drop(['Age', 'Cabin'], inplace = True, axis = 1)

# Assume people with missing fare paid the average price
fare_mean = X_full[X_full.Pclass == 3].Fare.mean()
X_full['Fare'].fillna(fare_mean, inplace = True)
X_full['Embarked'].fillna('S', inplace = True)

# Fit and transform the categorical data
X_full.drop(['Name', 'Ticket'], axis = 1, inplace = True)
X_dummies = pd.get_dummies(X_full, columns = ['Sex', 'Nulls', 'Cabin_mapped',␣
 ↪'Embarked'], drop_first=True)

# Split and construct desired dataset
X = X_dummies[:len(train)]; new_X = X_dummies[len(train):]
y = train.Survived
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
 ↪random_state=42)
model = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)

# Trains the XGBoost model on the training data.
X_train = X_train.values if isinstance(X_train, pd.DataFrame) else X_train
X_test = X_test.values if isinstance(X_test, pd.DataFrame) else X_test
y_train = y_train.values if isinstance(y_train, pd.Series) else y_train
y_test = y_test.values if isinstance(y_test, pd.Series) else y_test
model.train(X_train, y_train, detailed='true')

# Generates predictions on the test data.
predictions = model.predict(X_test)

# Convert predictions to binary labels (0 or 1) using a threshold of 0.5
predictions = np.where(predictions >= 0.5, 1, 0)

# Calculate the accuracy of the model
accuracy = np.mean(predictions == y_test)
print("Model Accuracy:", accuracy)
```

```
Tree 1:
0:[f4<0.500000] yes=1,no=2,missing=2
        1:[f0<3.000000] yes=3,no=4,missing=4
                3:[f7<1.000000] yes=7,no=8,missing=8
                        7:[f5<1.000000] yes=13,no=14,missing=14
                                13:[f0<1.000000] yes=23,no=24,missing=24
                                        23:leaf=-0.000000
                                        24:leaf=1.000000
                                14:[f16<1.000000] yes=25,no=26,missing=26
                                        25:leaf=1.000000
                                        26:leaf=0.959184
                        8:[f2<2.000000] yes=15,no=16,missing=16
                                15:[f3<39.108350] yes=27,no=28,missing=28
                                        27:leaf=0.500000
                                        28:leaf=1.000000
                                16:[f0<1.000000] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=0.600000
                4:[f3<23.350000] yes=9,no=10,missing=10
                        9:[f2<0.000000] yes=17,no=18,missing=18
                                17:leaf=-0.000000
                                18:[f2<0.000000] yes=31,no=32,missing=32
                                        31:leaf=-0.000000
                                        32:leaf=0.585106
                        10:[f0<3.000000] yes=19,no=20,missing=20
                                19:leaf=-0.000000
                                20:[f0<3.000000] yes=33,no=34,missing=34
                                        33:leaf=-0.000000
                                        34:leaf=0.047619
        2:[f0<1.000000] yes=5,no=6,missing=6
                5:leaf=-0.000000
                6:[f0<1.000000] yes=11,no=12,missing=12
                        11:leaf=-0.000000
                        12:[f0<1.000000] yes=21,no=22,missing=22
                                21:leaf=-0.000000
                                22:[f0<1.000000] yes=35,no=36,missing=36
                                        35:leaf=-0.000000
                                        36:leaf=0.186296
Loss after Tree 1: 0.6807310897522159


Tree 2:
0:[f4<0.500000] yes=1,no=2,missing=2
        1:[f0<3.000000] yes=3,no=4,missing=4
                3:[f7<1.000000] yes=7,no=8,missing=8
                        7:[f5<1.000000] yes=13,no=14,missing=14
                                13:[f0<1.000000] yes=21,no=22,missing=22
                                        21:leaf=-0.000000
```

```
                                22:leaf=0.700000
                        14:[f16<1.000000] yes=23,no=24,missing=24
                                23:leaf=0.700000
                                24:leaf=0.671429
                8:[f2<2.000000] yes=15,no=16,missing=16
                        15:[f3<39.108350] yes=25,no=26,missing=26
                                25:leaf=0.350000
                                26:leaf=0.700000
                        16:[f0<1.000000] yes=27,no=28,missing=28
                                27:leaf=-0.000000
                                28:leaf=0.420000
        4:[f15<0.000000] yes=9,no=10,missing=10
                9:leaf=-0.000000
                10:[f15<0.000000] yes=17,no=18,missing=18
                        17:leaf=-0.000000
                        18:[f15<0.000000] yes=29,no=30,missing=30
                                29:leaf=-0.000000
                                30:leaf=0.340870
    2:[f0<1.000000] yes=5,no=6,missing=6
        5:leaf=-0.000000
        6:[f0<1.000000] yes=11,no=12,missing=12
                11:leaf=-0.000000
                12:[f0<1.000000] yes=19,no=20,missing=20
                        19:leaf=-0.000000
                        20:[f0<1.000000] yes=31,no=32,missing=32
                                31:leaf=-0.000000
                                32:leaf=0.130407
Loss after Tree 2: 0.6764992074666439


Tree 3:
0:[f4<0.500000] yes=1,no=2,missing=2
    1:[f0<3.000000] yes=3,no=4,missing=4
        3:[f7<1.000000] yes=7,no=8,missing=8
                7:[f5<1.000000] yes=13,no=14,missing=14
                        13:[f0<1.000000] yes=21,no=22,missing=22
                                21:leaf=-0.000000
                                22:leaf=0.490000
                        14:[f16<1.000000] yes=23,no=24,missing=24
                                23:leaf=0.490000
                                24:leaf=0.470000
                8:[f2<2.000000] yes=15,no=16,missing=16
                        15:[f3<39.108350] yes=25,no=26,missing=26
                                25:leaf=0.245000
                                26:leaf=0.490000
                        16:[f0<1.000000] yes=27,no=28,missing=28
                                27:leaf=-0.000000
                                28:leaf=0.294000
```

```
                4:[f15<0.000000] yes=9,no=10,missing=10
                        9:leaf=-0.000000
                        10:[f15<0.000000] yes=17,no=18,missing=18
                                17:leaf=-0.000000
                                18:[f15<0.000000] yes=29,no=30,missing=30
                                        29:leaf=-0.000000
                                        30:leaf=0.238609
        2:[f0<1.000000] yes=5,no=6,missing=6
                5:leaf=-0.000000
                6:[f0<1.000000] yes=11,no=12,missing=12
                        11:leaf=-0.000000
                        12:[f0<1.000000] yes=19,no=20,missing=20
                                19:leaf=-0.000000
                                20:[f0<1.000000] yes=31,no=32,missing=32
                                        31:leaf=-0.000000
                                        32:leaf=0.091285
Loss after Tree 3: 0.6749888609436842


Tree 4:
0:[f4<0.000000] yes=1,no=2,missing=2
        1:leaf=-0.000000
        2:[f4<0.000000] yes=3,no=4,missing=4
                3:leaf=-0.000000
                4:[f4<0.000000] yes=5,no=6,missing=6
                        5:leaf=-0.000000
                        6:[f4<0.000000] yes=7,no=8,missing=8
                                7:leaf=-0.000000
                                8:[f4<0.000000] yes=9,no=10,missing=10
                                        9:leaf=-0.000000
                                        10:leaf=0.129107
Loss after Tree 4: 0.6823111042588685


Tree 5:
0:[f4<0.000000] yes=1,no=2,missing=2
        1:leaf=-0.000000
        2:[f4<0.000000] yes=3,no=4,missing=4
                3:leaf=-0.000000
                4:[f4<0.000000] yes=5,no=6,missing=6
                        5:leaf=-0.000000
                        6:[f4<0.000000] yes=7,no=8,missing=8
                                7:leaf=-0.000000
                                8:[f4<0.000000] yes=9,no=10,missing=10
                                        9:leaf=-0.000000
                                        10:leaf=0.090375
Loss after Tree 5: 0.6876535336283215
```

Model Accuracy: 0.7653631284916201

K-Fold Cross Validation

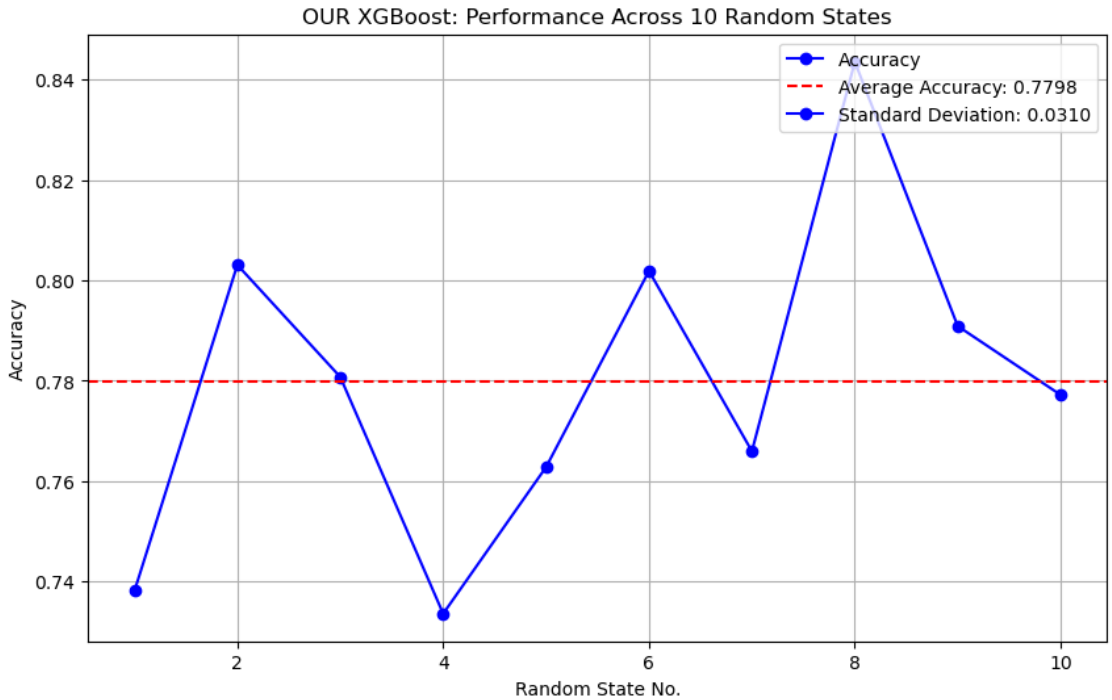
[ ]:
```python
from sklearn.model_selection import KFold

mean_accuracies = []
# Generate 10 random states between 1 and 50
random_states = [x for x in random.sample(range(1, 101), 10)]

# Loop through each random state
for random_state in random_states:

    # Define 5-Fold Cross Validation with the current random state
    kf = KFold(n_splits=5, shuffle=True, random_state=random_state)

    # Initialize a list to store accuracy for each fold
    accuracy_scores = []

    # Perform 5-Fold Cross-Validation
    for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
        # Convert to NumPy arrays if X or y are Pandas objects
        X = X.values if isinstance(X, pd.DataFrame) else X
        y = y.values if isinstance(y, pd.Series) else y

        # Split the data into training and testing sets
        X_train, X_test = X[train_index], X[test_index]
        y_train, y_test = y[train_index], y[test_index]

        # Create and train an XGBoost model with log loss as the evaluation␣
↪metric
        model_x = XGBoost(num_trees=5, max_depth=5, learning_rate=0.3)
        model_x.train(X_train, y_train)

        # Generate predictions
        y_prob = model_x.predict(X_test)
        predictions = np.where(y_prob >= 0.5, 1, 0)

        # Calculate accuracy for this fold
        accuracy = np.mean(predictions == y_test)
        accuracy_scores.append(accuracy)

    # Calculate the mean accuracy for this random state
    mean_accuracy = np.mean(accuracy_scores)
    mean_accuracies.append(mean_accuracy)
    print(f' Accuracy for Random State {random_state}: {mean_accuracy:.8f}')
```

```
# Calculate overall statistics for the generated accuracies
overall_mean_accuracy = np.mean(mean_accuracies)
overall_std_deviation = np.std(mean_accuracies)

# Print the overall results
print(f'  Mean Accuracy Across 10 Random States: {overall_mean_accuracy:.8f}')
print(f'  Standard Deviation Across 10 Random States: {overall_std_deviation:.
↪8f}')
```

```
Accuracy for Random State 1: 0.73809868
Accuracy for Random State 37: 0.80309146
Accuracy for Random State 20: 0.78075764
Accuracy for Random State 22: 0.73357919
Accuracy for Random State 47: 0.76279895
Accuracy for Random State 65: 0.80187371
Accuracy for Random State 25: 0.76595631
Accuracy for Random State 31: 0.84355345
Accuracy for Random State 8: 0.79089511
Accuracy for Random State 30: 0.77717971
 Mean Accuracy Across 10 Random States: 0.77977842
 Standard Deviation Across 10 Random States: 0.03095347
```

[143]:

```
plt.figure(figsize=(10, 6))
plt.plot(range(1, 11), mean_accuracies, marker='o', linestyle='-', color='b',␣
↪label='Fold Accuracy')
plt.axhline(overall_mean_accuracy, color='r', linestyle='--', label=f'Average␣
↪Accuracy: {overall_mean_accuracy:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Accuracy',
    f'Average Accuracy: {overall_mean_accuracy:.4f}',
    f'Standard Deviation: {overall_std_deviation:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
↪loc='upper right')
plt.xlabel('Random State No.')
plt.ylabel('Accuracy')
plt.title('OUR XGBoost: Performance Across 10 Random States')
plt.grid(True)
plt.show()
```



Implementing with imported XGBoost

[144]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42)
model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.3,␣
↪tree_method='exact', eval_metric='logloss')
model.fit(X_train, y_train)
params = model.get_params()
print(params)
n_estimators = params['n_estimators']
max_depth = params['max_depth']
learning_rate = params['learning_rate']

print("Number of estimators:", n_estimators)
print("Max depth:", max_depth)
print("Learning rate:", learning_rate)

# Retrieve the trained booster (underlying model) from XGBoost
booster = model.get_booster()

# Iterate over each tree in the model and print its structure
for i, tree in enumerate(booster.get_dump()):
    print(f"Tree {i + 1} structure:\n{tree}\n")
```

```python
# Make predictions on the test data
y_pred_s = model.predict(X_test)

# Compute and print the accuracy score
accuracy_s = accuracy_score(y_test, y_pred_s)
print("Model Accuracy:", accuracy_s)
```

```
{'objective': 'binary:logistic', 'base_score': None, 'booster': None,
'callbacks': None, 'colsample_bylevel': None, 'colsample_bynode': None,
'colsample_bytree': None, 'device': None, 'early_stopping_rounds': None,
'enable_categorical': False, 'eval_metric': 'logloss', 'feature_types': None,
'gamma': None, 'grow_policy': None, 'importance_type': None,
'interaction_constraints': None, 'learning_rate': 0.3, 'max_bin': None,
'max_cat_threshold': None, 'max_cat_to_onehot': None, 'max_delta_step': None,
'max_depth': 5, 'max_leaves': None, 'min_child_weight': None, 'missing': nan,
'monotone_constraints': None, 'multi_strategy': None, 'n_estimators': 5,
'n_jobs': None, 'num_parallel_tree': None, 'random_state': None, 'reg_alpha':
None, 'reg_lambda': None, 'sampling_method': None, 'scale_pos_weight': None,
'subsample': None, 'tree_method': 'exact', 'validate_parameters': None,
'verbosity': None}
Number of estimators: 5
Max depth: 5
Learning rate: 0.3
Tree 1 structure:
0:[f4<0.5] yes=1,no=2,missing=1
        1:[f0<2.5] yes=3,no=4,missing=3
                3:leaf=0.719301105
                4:[f3<23.3500004] yes=7,no=8,missing=7
                        7:[f16<0.5] yes=13,no=14,missing=13
                                13:[f3<15.3729] yes=21,no=22,missing=21
                                        21:leaf=0.268888533
                                        22:leaf=0.555703223
                                14:[f3<10.8249998] yes=23,no=24,missing=23
                                        23:leaf=0.0170285795
                                        24:leaf=0.275128305
                        8:leaf=-0.351209491
        2:[f0<1.5] yes=5,no=6,missing=5
                5:[f3<26.1437492] yes=9,no=10,missing=9
                        9:leaf=-0.300538749
                        10:[f6<0.5] yes=15,no=16,missing=15
                                15:[f3<32] yes=25,no=26,missing=25
                                        25:leaf=0.132736221
                                        26:leaf=-0.0319211148
                                16:leaf=-0.282738179
                6:[f2<0.5] yes=11,no=12,missing=11
                        11:[f3<43.2833023] yes=17,no=18,missing=17
                                17:leaf=-0.332552314
                                18:leaf=0.0567918941
```

```
                        12:[f3<19.4812508] yes=19,no=20,missing=19
                                19:[f3<15.6208496] yes=27,no=28,missing=27
                                        27:leaf=0.0189113505
                                        28:leaf=0.339164436
                                20:[f0<2.5] yes=29,no=30,missing=29
                                        29:leaf=-0.021240741
                                        30:leaf=-0.344573855


Tree 2 structure:
0:[f4<0.5] yes=1,no=2,missing=1
        1:[f0<2.5] yes=3,no=4,missing=3
                3:leaf=0.477941602
                4:[f3<23.3500004] yes=7,no=8,missing=7
                        7:[f3<7.7437501] yes=13,no=14,missing=13
                                13:[f15<0.5] yes=19,no=20,missing=19
                                        19:leaf=0.480101854
                                        20:leaf=0.104824543
                                14:[f3<15.3729] yes=21,no=22,missing=21
                                        21:leaf=0.039290525
                                        22:leaf=0.298447579
                        8:leaf=-0.294154018
        2:[f3<52.2770996] yes=5,no=6,missing=5
                5:[f8<0.5] yes=9,no=10,missing=9
                        9:[f2<0.5] yes=15,no=16,missing=15
                                15:[f7<0.5] yes=23,no=24,missing=23
                                        23:leaf=-0.265922755
                                        24:leaf=0.0462718122
                                16:[f3<19.4812508] yes=25,no=26,missing=25
                                        25:leaf=0.115782313
                                        26:leaf=-0.189706042
                        10:leaf=0.24892424
                6:[f3<59.0875015] yes=11,no=12,missing=11
                        11:leaf=0.267633855
                        12:[f3<75.1146011] yes=17,no=18,missing=17
                                17:leaf=-0.332445592
                                18:[f12<0.5] yes=27,no=28,missing=27
                                        27:leaf=-0.0390266962
                                        28:leaf=0.273367137


Tree 3 structure:
0:[f4<0.5] yes=1,no=2,missing=1
        1:[f0<2.5] yes=3,no=4,missing=3
                3:leaf=0.383151293
                4:[f3<23.3500004] yes=7,no=8,missing=7
                        7:[f3<8.03960037] yes=13,no=14,missing=13
                                13:[f16<0.5] yes=21,no=22,missing=21
```

```
                                        21:leaf=0.287950784
                                        22:leaf=0.141392544
                                14:[f3<10.8249998] yes=23,no=24,missing=23
                                        23:leaf=-0.176651925
                                        24:leaf=0.167895868
                        8:leaf=-0.252652317
        2:[f3<29.4125004] yes=5,no=6,missing=5
                5:[f8<0.5] yes=9,no=10,missing=9
                        9:[f2<0.5] yes=15,no=16,missing=15
                                15:[f16<0.5] yes=25,no=26,missing=25
                                        25:leaf=-0.160563156
                                        26:leaf=-0.237061515
                                16:[f0<2.5] yes=27,no=28,missing=27
                                        27:leaf=0.158795476
                                        28:leaf=-0.124135755
                        10:leaf=0.250830263
                6:[f3<30.75] yes=11,no=12,missing=11
                        11:[f5<0.5] yes=17,no=18,missing=17
                                17:leaf=0.0455127843
                                18:leaf=0.311205924
                        12:[f3<52.2770996] yes=19,no=20,missing=19
                                19:[f3<39.2999992] yes=29,no=30,missing=29
                                        29:leaf=0.0222998857
                                        30:leaf=-0.340716779
                                20:[f3<59.0875015] yes=31,no=32,missing=31
                                        31:leaf=0.199791178
                                        32:leaf=-0.0512342192


Tree 4 structure:
0:[f4<0.5] yes=1,no=2,missing=1
        1:[f0<2.5] yes=3,no=4,missing=3
                3:[f7<0.5] yes=7,no=8,missing=7
                        7:leaf=0.353156358
                        8:[f2<0.5] yes=15,no=16,missing=15
                                15:[f3<68.9416504] yes=25,no=26,missing=25
                                        25:leaf=0.0723548234
                                        26:leaf=0.270794451
                                16:leaf=0.00226664566
                4:[f3<23.3500004] yes=9,no=10,missing=9
                        9:[f3<7.7437501] yes=17,no=18,missing=17
                                17:[f15<0.5] yes=27,no=28,missing=27
                                        27:leaf=0.34121263
                                        28:leaf=0.039002087
                                18:[f15<0.5] yes=29,no=30,missing=29
                                        29:leaf=0.0141656809
                                        30:leaf=0.218801439
                        10:[f1<3.5] yes=19,no=20,missing=19
```

```
                        19:leaf=-0.252637148
                        20:leaf=-0.0780817792
        2:[f3<29.8500004] yes=5,no=6,missing=5
                5:[f8<0.5] yes=11,no=12,missing=11
                        11:[f1<0.5] yes=21,no=22,missing=21
                                21:[f16<0.5] yes=31,no=32,missing=31
                                        31:leaf=-0.120267779
                                        32:leaf=-0.201506555
                                22:[f3<26.125] yes=33,no=34,missing=33
                                        33:leaf=-0.0136133907
                                        34:leaf=-0.27034995
                        12:leaf=0.198777378
                6:[f3<30.75] yes=13,no=14,missing=13
                        13:leaf=0.229996756
                        14:[f16<0.5] yes=23,no=24,missing=23
                                23:[f5<0.5] yes=35,no=36,missing=35
                                        35:leaf=0.149415001
                                        36:leaf=-0.119995676
                                24:[f3<80.7541504] yes=37,no=38,missing=37
                                        37:leaf=-0.164857775
                                        38:leaf=0.173302799


Tree 5 structure:
0:[f4<0.5] yes=1,no=2,missing=1
        1:[f0<2.5] yes=3,no=4,missing=3
                3:[f7<0.5] yes=7,no=8,missing=7
                        7:leaf=0.314898968
                        8:[f2<0.5] yes=15,no=16,missing=15
                                15:[f3<68.9416504] yes=27,no=28,missing=27
                                        27:leaf=0.0622311793
                                        28:leaf=0.242087945
                                16:leaf=0.00185911614
                4:[f3<23.3500004] yes=9,no=10,missing=9
                        9:[f3<7.7437501] yes=17,no=18,missing=17
                                17:[f15<0.5] yes=29,no=30,missing=29
                                        29:leaf=0.29161948
                                        30:leaf=0.0325987339
                                18:[f3<15.3729] yes=31,no=32,missing=31
                                        31:leaf=-0.0122824134
                                        32:leaf=0.173359826
                        10:[f1<3.5] yes=19,no=20,missing=19
                                19:leaf=-0.228363484
                                20:leaf=-0.0670191646
        2:[f6<0.5] yes=5,no=6,missing=5
                5:[f5<0.5] yes=11,no=12,missing=11
                        11:[f7<0.5] yes=21,no=22,missing=21
                                21:[f1<0.5] yes=33,no=34,missing=33
```

```
                                33:leaf=0.0322490819
                                34:leaf=0.270216137
                        22:[f2<1.5] yes=35,no=36,missing=35
                                35:leaf=-0.141160995
                                36:leaf=0.00775017822
                12:[f7<0.5] yes=23,no=24,missing=23
                        23:[f3<11.3708496] yes=37,no=38,missing=37
                                37:leaf=-0.0722106099
                                38:leaf=-0.14528352
                        24:leaf=0.132358804
        6:[f3<8.08125019] yes=13,no=14,missing=13
                13:leaf=-0.241400629
                14:[f3<14.7749996] yes=25,no=26,missing=25
                        25:leaf=0.249405801
                        26:[f15<0.5] yes=39,no=40,missing=39
                                39:leaf=-0.252804637
                                40:leaf=-0.0422912613
```

```
Model Accuracy: 0.8156424581005587
```

K-Fold Cross Validation

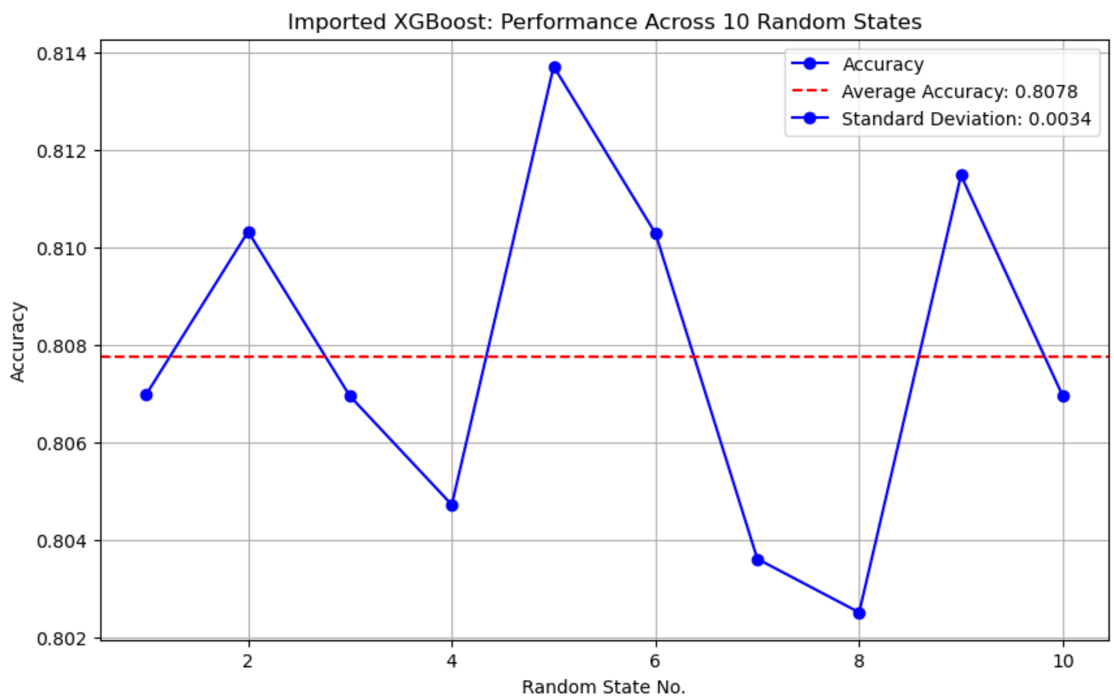
[145]:
```
from sklearn.model_selection import KFold

mean_accuracies = []

# Loop through each random state
for random_state in random_states:

    # Define 5-Fold Cross Validation with the current random state
    kf = KFold(n_splits=5, shuffle=True, random_state=random_state)

    # Initialize a list to store accuracy for each fold
    accuracy_scores = []

    # Perform 5-Fold Cross-Validation
    for fold, (train_index, test_index) in enumerate(kf.split(X), 1):
        # Split data into train and test sets for this fold
        X_train, X_test = X[train_index], X[test_index]
        y_train, y_test = y[train_index], y[test_index]

        # Create an XGBoost model with log loss as the evaluation metric
        model = xgb.XGBClassifier(n_estimators=5, max_depth=5, learning_rate=0.
↪3, tree_method='exact', eval_metric='logloss')

        # Fits the XGBoost model to the training data.
        model.fit(X_train, y_train)
```

```
        # Generate predictions
        predictions = model.predict(X_test)

        # Calculate accuracy for this fold
        accuracy = accuracy_score(y_test, predictions)
        accuracy_scores.append(accuracy)

    # Calculate the mean accuracy for this random state
    mean_accuracy = np.mean(accuracy_scores)
    mean_accuracies.append(mean_accuracy)

# Print the mean accuracies for all random states
for random_state, mean_accuracy in zip(random_states, mean_accuracies):
    print(f' Accuracy for Random State {random_state}: {mean_accuracy:.4f}')

# Calculate overall statistics for the generated accuracies
overall_mean_accuracy = np.mean(mean_accuracies)
overall_std_deviation = np.std(mean_accuracies)

# Print the overall results
print(f'  Mean Accuracy Across 10 Random States: {overall_mean_accuracy:.8f}')
print(f'  Standard Deviation Across 10 Random States: {overall_std_deviation:.
 ↪8f}')
```

```
 Accuracy for Random State 1: 0.8070
 Accuracy for Random State 37: 0.8103
 Accuracy for Random State 20: 0.8070
 Accuracy for Random State 22: 0.8047
 Accuracy for Random State 47: 0.8137
 Accuracy for Random State 65: 0.8103
 Accuracy for Random State 25: 0.8036
 Accuracy for Random State 31: 0.8025
 Accuracy for Random State 8: 0.8115
 Accuracy for Random State 30: 0.8070
  Mean Accuracy Across 10 Random States: 0.80775971
  Standard Deviation Across 10 Random States: 0.00343833
```

[146]:
```
# Plot the accuracy scores for each fold
plt.figure(figsize=(10, 6))
plt.plot(range(1, 11), mean_accuracies, marker='o', linestyle='-', color='b',␣
 ↪label='Accuracy')
plt.axhline(overall_mean_accuracy, color='r', linestyle='--', label=f'Average␣
 ↪Accuracy: {overall_mean_accuracy:.4f}')
handles, labels = plt.gca().get_legend_handles_labels()
custom_labels = [
    'Accuracy',
```

```
    f'Average Accuracy: {overall_mean_accuracy:.4f}',
    f'Standard Deviation: {overall_std_deviation:.4f}'
]
plt.legend(handles=[handles[0], handles[1], handles[0]], labels=custom_labels,␣
 ↪loc='upper right')
plt.xlabel('Random State No.')
plt.ylabel('Accuracy')
plt.title('Imported XGBoost: Performance Across 10 Random States')
plt.grid(True)
plt.show()
```



Results 3 On this dataset, considering the particularity of its data distribution, we conducted more solid experiments. We randomly selected 10 random states, performed 5-fold cross validation on each random state, and used its mean accuracy as the accuracy on that random state. Finally, we calculated the average accuracy and standard deviation on these ten random states.

From a quantitative perspective, the performance of our method shows a mean accuracy of 0.7798 with a standard deviation of 0.031. In contrast, the imported XGBoost model achieves a higher mean accuracy of 0.8078 with a significantly lower standard deviation of 0.0034, indicating more stable and consistent performance. The accuracy of our method fluctuates considerably between approximately 0.73 and 0.84, while the imported model consistently maintains results above 0.79 and peaks at 0.813. This indicates that although our model can achieve performance close to the imported XGBoost, the gap between the two becomes larger compared to the results on the previous two datasets, thus showing inferior robustness.

The Titanic dataset presents specific characteristics that make it a potential candidate for binary classification, yet it also exposes the strengths and weaknesses of different models. The dataset combines categorical features, such as Sex, Pclass, and Embarked, with numerical features, including Age, Fare, SibSp, and Parch. Notably, the Sex and Pclass features are highly discriminative for survival prediction. Women had a significantly higher survival rate than men, and passengers in the first class were far more likely to survive compared to those in the second and third classes. However, the dataset is relatively small, containing only 891 training samples, which increases the risk of overfitting. Furthermore, missing values, especially in Age and Cabin, require careful handling to maintain model performance.

Given these characteristics, the imported XGBoost model outperforms our method due to several key advantages that align well with the dataset's structure. One critical factor is regularization. XGBoost applies both L1 and L2 regularization to prevent the model from overfitting to the limited and potentially noisy training data. This is particularly important in a small dataset like Titanic, where overfitting is a significant challenge. In contrast, our method does not yet incorporate regularization terms into the gain calculation, which makes the resulting trees more prone to overfitting the specific training samples.

The way splits are determined during tree building is another contributing factor to the performance difference. The imported XGBoost uses highly optimized algorithms, including approximate split finding and histogram-based methods, which allow it to efficiently identify the most impactful thresh olds for numerical features like Age and Fare. In contrast, our method relies on sorting and iterating over all possible split points, a process that is not only computationally intensive but also less precise, particularly when working with small datasets.

Furthermore, the Titanic dataset highlights the importance of incorporating randomization into the model training process. XGBoost includes mechanisms such as column subsampling and row subsampling, which reduce the dependency of the model on specific features or data points. This is particularly valuable in the Titanic dataset, where features like Sex might dominate predictions without such safeguards, reducing model generalization. Our method currently lacks these randomization strategies.

In conclusion, the Titanic dataset's small size, feature structure, and binary classification nature emphasize the need for models that can handle overfitting, optimize probabilistic outputs, and incorporate efficient tree-building strategies. Our method, while capturing the core principles of gradient boosting, currently lacks these advanced techniques, which highlights directions for future improvement.

5 Citation and Reference

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