[Jupyter Notebook] Exact Greedy Algorithm for Split Finding

April 28, 2024

[1]:

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import copy
import numpy as np
import matplotlib.pyplot as plt


class XGBTree:
    def __init__(self, max_depth, reg_lambda, gamma, tree_type="regressor"):
        self.max_depth = max_depth
        self.reg_lambda = reg_lambda
        self.gamma = gamma
        self.tree_type = tree_type
        self.root_node = None
        self.backup_root_node = None
        self.features = None
        self.target_residual = None
        self.previous_predictions = None

    def calculate_node_split(self, indices):
        lambda_reg, num_features = self.reg_lambda, self.features.shape[1] #␣
↪Dòng số 1 trong thuật toán
        sum_gradient, sum_hessian = (
            self.target_residual[indices].sum(), # Biểu thức số (13) và (22),␣
↪dòng số 4 trong thuật toán
            (self.previous_predictions[indices] * (1 - self.
↪previous_predictions[indices])).sum() # Biểu thức số (26), dòng số 5 trong␣
↪thuật toán
            if self.tree_type == "binary_classifier"
            else indices.shape[0], # Biểu thức số (15), dòng số 5 trong thuật␣
↪toán
        )
        # Dòng số 14 trong thuật toán
        best_score, maximum_gain, best_feature_index, best_split_point =␣
↪(sum_gradient**2) / (sum_hessian + lambda_reg), -np.inf, None, None

        # Dòng số 6 trong thuật toán
        for feature_index in range(num_features):
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            gradient_left, hessian_left = 0.0, 0.0 # Dòng số 7 và 8 trong thuật toán
            feature_values, unique_values = self.features[indices, feature_index], np.unique(self.features[indices, feature_index])
            split_candidates = [(unique_values[i - 1] + unique_values[i]) / 2 for i in range(1, len(unique_values))]

            # Dòng số 9 trong thuật toán
            for split in split_candidates:
                left_indices, right_indices = indices[feature_values <= split], indices[feature_values > split]
                gradient_left, hessian_left = (
                    self.target_residual[left_indices].sum(), # Biểu thức số (13) và (22), dòng số 10 trong thuật toán
                    (self.previous_predictions[left_indices] * (1 - self.previous_predictions[left_indices])).sum() # Biểu thức số (26), dòng số 11 trong thuật toán
                    if self.tree_type == "binary_classifier"
                    else left_indices.shape[0], # Biểu thức số (15), dòng số 11 trong thuật toán
                )

                # Dòng số 12 và 13 trong thuật toán
                gradient_right, hessian_right = sum_gradient - gradient_left, sum_hessian - hessian_left

                # Dòng số 14 trong thuật toán
                gain = (gradient_left**2) / (hessian_left + lambda_reg) + (gradient_right**2) / (hessian_right + lambda_reg) - best_score

                # Dòng số 15 trong thuật toán
                if gain > maximum_gain:
                    maximum_gain, best_feature_index, best_split_point, _ = gain, feature_index, split, split

        return (
            {
                "feature_index": best_feature_index,
                "split_point": best_split_point,
                "left_indices": indices[self.features[indices, best_feature_index] <= best_split_point],
                "right_indices": indices[self.features[indices, best_feature_index] > best_split_point],
            }
            if maximum_gain >= self.gamma
            else None
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        )

    def split_node(self, node, depth):
        if depth < self.max_depth and isinstance(node, dict):
            for side in ["left_indices", "right_indices"]:
                child_node = self.calculate_node_split(node[side])
                if child_node:
                    node[side] = child_node
                    self.split_node(node[side], depth + 1)

    def calculate_output_value(self, indices):
        lambda_reg, sum_hessian = (
            self.target_residual[indices],
            (self.previous_predictions[indices] * (1 - self.previous_predictions[indices])).sum()
            if self.tree_type == "binary_classifier"
            else indices.shape[0],
        )
        return self.target_residual[indices].sum() / (sum_hessian + self.reg_lambda)

    def calculate_leaf_values(self, node):
        if isinstance(node, dict):
            for side in ["left_indices", "right_indices"]:
                if isinstance(node[side], dict):
                    self.calculate_leaf_values(node[side])
                else:
                    node[side] = self.calculate_output_value(node[side])

    def fit(self, features, target, initial_predictions):
        self.features, self.target_residual, self.previous_predictions = features, target, initial_predictions
        root = self.calculate_node_split(np.arange(features.shape[0]))
        if root:
            self.split_node(root, depth=1)
            self.root_node = root
            self.backup_root_node = copy.deepcopy(root)
            self.calculate_leaf_values(self.backup_root_node)
        return self.backup_root_node

    def predict_single_instance(self, node, feature_instance):
        while isinstance(node, dict):
            node = node["left_indices"] if feature_instance[node["feature_index"]] <= node["split_point"] else node["right_indices"]
        return node
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    def predict(self, features_test):
        return (
            np.array([self.predict_single_instance(self.backup_root_node,␣
↪feature_instance) for feature_instance in features_test])
            if isinstance(self.backup_root_node, dict)
            else self.previous_predictions * np.ones(features_test.shape[0])
        )


class XGBModel:
    def __init__(
        self,
        n_estimators=10,
        max_depth=3,
        eta=0.3,
        gamma=0.0,
        reg_lambda=0.0,
        initial_score=0.5,
        tree_type="regressor",
    ):
        self.n_estimators = n_estimators
        self.max_depth = max_depth
        self.eta = eta
        self.gamma = gamma
        self.reg_lambda = reg_lambda
        self.initial_score = initial_score
        self.tree_type = tree_type
        self.trees = []

    @staticmethod
    def sigmoid(x):
        return 1 / (1 + np.exp(-x))

    def fit(self, features, target):
        if self.tree_type == "binary_classifier":
            cumulative_predictions = np.log(self.initial_score / (1 - self.
↪initial_score))
            cumulative_predictions = np.repeat(cumulative_predictions, features.
↪shape[0])
            loss_function = lambda target, predicted: (
                -(target * np.log(predicted + 1e-8)) + (1 - target) * np.log(1␣
↪- predicted + 1e-8)
            ).sum()
        else:
            cumulative_predictions = self.initial_score
            loss_function = lambda target, cumulative_predictions: ((target -␣
↪cumulative_predictions) ** 2).sum()
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        predictions = self.sigmoid(cumulative_predictions) if self.tree_type == "binary_classifier" else cumulative_predictions
        self.loss_history = []

        for m in range(self.n_estimators):
            residual = target - predictions
            tree = XGBTree(
                max_depth=self.max_depth,
                reg_lambda=self.reg_lambda,
                gamma=self.gamma,
                tree_type=self.tree_type,
            )
            tree.fit(
                features,
                residual,
                predictions if self.tree_type == "binary_classifier" else residual.mean(),
            )
            update = tree.predict(features)
            cumulative_predictions += self.eta * update
            predictions = self.sigmoid(cumulative_predictions) if self.tree_type == "binary_classifier" else cumulative_predictions

            self.trees.append(tree)
            self.loss_history.append(loss_function(target, predictions))

    def predict(self, features_test, probability=False):
        cumulative_predictions = np.zeros(shape=(features_test.shape[0],)) + self.initial_score

        for tree in self.trees:
            cumulative_predictions += self.eta * tree.predict(features_test)

        if self.tree_type == "binary_classifier":
            probabilities = self.sigmoid(cumulative_predictions)
            return probabilities if probability else (probabilities > 0.5).astype("uint8")

        return cumulative_predictions
```

[2]:
```python
X = np.random.rand(300).reshape(-1, 1)
y = 2.0 * np.sin(4.0 * np.pi * X).flatten() + np.random.normal(0.0, 0.5, 300) + 3.0

model = XGBModel(
    n_estimators=20,
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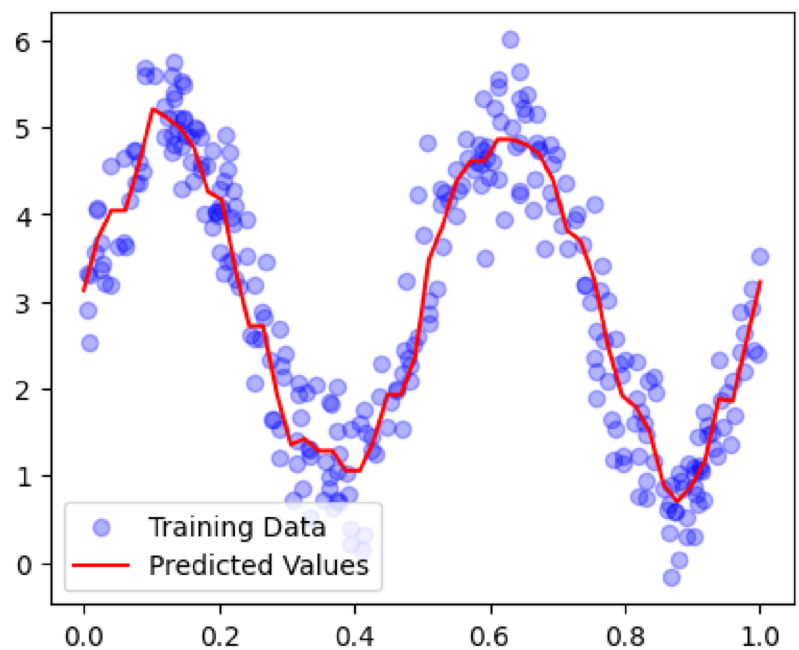
    max_depth=3,
    eta=0.3,
    gamma=0.01,
    reg_lambda=1,
    initial_score=y.mean(),
    tree_type='regressor'
)

model.fit(X, y)

X_test = np.linspace(0, 1, 50).reshape(-1, 1)
y_pred = model.predict(X_test)

plt.figure(figsize=(5, 4))
plt.scatter(X, y, c='b', alpha=0.3, label='Training Data')
plt.plot(X_test, y_pred, c='r', label='Predicted Values')
plt.legend()
plt.show()
```



[3]:
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X = np.random.randn(300, 2)
y = np.logical_xor(X[:, 0] > 0, X[:, 1] > 0)

model = XGBModel(
    n_estimators=20,
    max_depth=3,
```

```
    eta=0.3,
    gamma=0.01,
    reg_lambda=1,
    initial_score=y.mean(),
    tree_type='binary_classifier'
)

model.fit(X, y)

X_test = np.random.uniform(-3, 3, (500, 2))
y_pred = model.predict(X_test)

plt.figure(figsize=(5,5))
color = ['r' if a == 1 else 'b' for a in y_pred]
plt.scatter(X_test[:, 0], X_test[:, 1], s=100, c=color, alpha=0.3)
plt.xlim(-4, 4)
plt.ylim(-4, 4)
plt.show()
```