Gradient Boosting Algorithm - Part 2. Classification

Algorithm explained with an example, math, and code

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib as mpl
import seaborn as sns
import scipy.stats as stats
from sklearn.tree import DecisionTreeRegressor

import plotly.graph_objects as go
import plotly.express as px
from plotly.subplots import make_subplots

sns.set()
```

Algorithm with an Example

Gradient boosting is one of the variants of ensemble methods where you create multiple weak models (they are often decision trees) and combine them to get better performance as a whole. In this section, we are building a gradient boosting classification model using very simple example data to intuitively understand how it works.

The picture below shows the example data. It has the binary class y (0 and 1) and two features (x and x_2).

```
import sklearn.datasets as datasets
from matplotlib.colors import ListedColormap

data = datasets.make_circles(n_samples=100, factor=0.5, noise=0.15, random_state=0)
x, y = data[0], data[1]

# make it imbalance
idx = np.sort(np.append(np.where(y != 0)[0], np.where(y == 0)[0][:-10]))
x, y = x[idx], y[idx]

plt.figure(figsize=(7, 5))
plt.scatter(x[y==0, 0], x[y==0, 1], c='orange', edgecolors='w', s=100, label='class 0')
plt.scatter(x[y==1, 0], x[y==1, 1], c='crimson', edgecolors='w', s=100, label='class 1')
plt.xlabel('x1')
plt.ylabel('x2')
plt.legend(fontsize=14)
plt.show()
```


```
c_scale = [[0, "rgb(247, 168, 84)"], [1, "rgb(209, 0, 0)"]]

def create_scatter(x, y, plot_type):

    return go.Scatter3d(
                x=x[:, 0], y=x[:, 1], z=y,
                mode="markers",
                marker=dict(
                    size=6,
                    color=y,
                    colorscale=c_scale if plot_type == "pred" else "Blugrn",
                    line=dict(width=4, color="White"),
                ),
            )

def format_plot(fig):
  return fig.update_layout(
      scene=dict(
          xaxis_title="x1",
          yaxis_title="x2",
          zaxis_title="y"
      ),
      height=400,
      width=600,
      margin=dict(l=10, r=10, t=40, b=20),
  )

fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))
fig = format_plot(fig)
fig.show()
```

Our goal is to build a gradient boosting model that classifies those two classes. The first step is making a uniform prediction on a probability of class 1 (we will call it p) for all the data points. The most reasonable value for the uniform prediction might be the proportion of class 1 which is just a mean of y.

$$p = P(y = 1) = \bar{y}$$

Here is a 3D representation of the data and the initial prediction. At this moment, the prediction is just a plane which has the uniform value $p = mean(y)$ on the y axis all the time.

```
# creating mesh data to visualize prediction planes
x1_min, x1_max = x[:, 0].min() - 0.5, x[:, 0].max() + 0.5
x2_min, x2_max = x[:, 1].min() - 0.5, x[:, 1].max() + 0.5

h = 0.02  # step size in the mesh
x1_mesh, x2_mesh = np.meshgrid(np.arange(x1_min, x1_max, h), np.arange(x2_min, x2_max, h))


def create_surface(x1, x2, y, plot_type):

    return go.Surface(x=x1, y=x2, z=y,
                      showscale=False,
                      opacity=0.5,
                      colorscale="Peach" if plot_type == "pred" else "Tealgrn",
                      )


p = y.mean()

fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, np.full(x1_mesh.shape, p), "pred"))
fig = format_plot(fig)
fig.show()
```

In our data, the mean of y is 0.56. As it is bigger than 0.5, everything is classified into class 1 with this initial prediction. Some of you might feel that this uniform value prediction does not make sense, but don't worry. We will improve our prediction as we add more weak models to it.

To improve our prediction quality, we might want to focus on the residuals (i.e. prediction error) from our initial prediction as that is what we want to minimize. The residuals are defined as $r_{\mathrm{i}} = y_{\mathrm{i}} - p$ (i represents the index of each data point). In the figure below, the residuals are shown as the brown lines that are the perpendicular lines from each data point to the prediction plane.

```
def create_residual_lines(x, y, pred):

    #create the coordinate list for the lines
    x_list, y_list, z_list = [], [], []
    for i in range(len(x)):
        x_list.extend([x[i, 0], x[i, 0], None])
        y_list.extend([x[i, 1], x[i, 1], None])
        z_list.extend([y[i], pred[i], None])

    return go.Scatter3d(x=x_list,
                        y=y_list,
                        z=z_list,
                        mode='lines',
                        line=dict(
                            color='brown',
                            width=5
                        ))
```

```
fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, np.full(x1_mesh.shape, p), "pred"))
fig.add_trace(create_residual_lines(x, y, np.full(y.shape, p)))
fig = format_plot(fig)
fig.update_layout(showlegend=False)
fig.show()
```

To minimize these residuals, we are building a regression tree model with both x and x_2 as its features and the residuals r as its target. If we can build a tree that finds some patterns between x and r, we can reduce the residuals by utilizing that created tree. To simplify the demonstration, we are building very simple trees each of that only has one split and two terminal nodes which is called "stump". Please note that gradient boosting trees usually have a little deeper trees such as ones with 8 to 32 terminal nodes. Here we are creating the first tree predicting the residuals with two different values $r = \{0.1, -0.6\}$.

```
def train_and_update(x, y, Fm, x1_mesh, x2_mesh, Fm_mesh, learing_rate=0.1, print_tree=True):

    p = np.exp(Fm) / (1 + np.exp(Fm))
    r = y - p
    tree = DecisionTreeRegressor(max_depth=1, random_state=0)
    tree.fit(x, r)
    ids = tree.apply(x)

    if print_tree:
      print_tree_structure(tree)

    x_mesh = np.c_[x1_mesh.ravel(), x2_mesh.ravel()]
    r_pred_mesh = tree.predict(x_mesh).reshape(x1_mesh.shape)

    for j in np.unique(ids):
        fltr = ids == j
        num = r[fltr].sum()
        den = (p[fltr]*(1-p[fltr])).sum()
        gamma = num / den
        Fm[fltr] += learing_rate * gamma

        # update prediction value in the tree
        tree.tree_.value[j, 0, 0] = gamma

    gamma_update_mesh = tree.predict(x_mesh).reshape(x1_mesh.shape)
    Fm_mesh += learing_rate * gamma_update_mesh

    p_mesh = np.exp(Fm_mesh) / (1 + np.exp(Fm_mesh))

    return tree, r, Fm, r_pred_mesh, Fm_mesh
```

```
# this function print out tree structures. adapted from https://scikit-learn.org/stable/auto_examp
def print_tree_structure(clf):

    n_nodes = clf.tree_.node_count
    children_left = clf.tree_.children_left
    children_right = clf.tree_.children_right
    feature = clf.tree_.feature
    threshold = clf.tree_.threshold

    node_depth = np.zeros(shape=n_nodes, dtype=np.int64)
    is_leaves = np.zeros(shape=n_nodes, dtype=bool)
    stack = [(0, 0)]  # start with the root node id (0) and its depth (0)
    while len(stack) > 0:
        # `pop` ensures each node is only visited once
        node_id, depth = stack.pop()
        node_depth[node_id] = depth

        # If the left and right child of a node is not the same we have a split
        # node
        is_split_node = children_left[node_id] != children_right[node_id]
        # If a split node, append left and right children and depth to `stack`
        # so we can loop through them
        if is_split_node:
            stack.append((children_left[node_id], depth + 1))
            stack.append((children_right[node_id], depth + 1))
        else:
            is_leaves[node_id] = True

    print('-'*80)
    print(
        "The binary tree structure has {n} nodes and has "
        "the following tree structure:\n".format(n=n_nodes)
    )
    for i in range(n_nodes):
        if is_leaves[i]:
            print(
                "{space}node={node} is a leaf node.".format(
                    space=node_depth[i] * "\t", node=i
                )
            )
            print(node_depth[i] * '\t', f"prediction: {clf.tree_.value[i, 0, 0]:.1f}")
        else:
            print(
                "{space}node={node} is a split node: "
                "go to node {left} if X[:, {feature}] <= {threshold} "
                "else to node {right}.".format(
                    space=node_depth[i] * "\t",
                    node=i,
                    left=children_left[i],
                    feature=feature[i],
                    threshold=threshold[i],
                    right=children_right[i],
                )
            )
    print('-'*80)
```

```
F0 = np.log(p/(1-p))
F0 = np.full(len(y), F0)
F0_mesh = np.full(x1_mesh.shape, F0[0])
learing_rate = 0.9
tree, r, Fm, r_pred_mesh, Fm_mesh = train_and_update(x, y, F0, x1_mesh, x2_mesh, F0_mesh, learing_

fig = go.Figure()
fig.add_trace(create_scatter(x, r, "res"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, r_pred_mesh, "res"))
fig = format_plot(fig)
fig.update_layout(showlegend=False)
fig.show()
```

```
--------------------------------------------------------------------------------
The binary tree structure has 3 nodes and has the following tree structure:

node=0 is a split node: go to node 1 if X[:, 0] <= 0.6397739946842194 else to node 2.
        node=1 is a leaf node.
         prediction: 0.1
        node=2 is a leaf node.
         prediction: -0.6
--------------------------------------------------------------------------------
```

You might now think we want to add these predicted values to our initial prediction p to reduce its residuals if you already read [the post talking about the regression algorithm](), but things are slightly different with the classification. The values (we call it γ gamma) that we are adding to our initial prediction is computed in the following formula:

$$\frac{\sum_{x_i \in R_j}(y_i - p)}{\sum_{x_i \in R_j} p(1-p)}$$

$\Sigma x_i \in R$□ means we are aggregating the values in the sigma Σ on all the sample x_is that belong to the terminal node R□. j represents the index of each terminal node. You might notice that the numerator of the fraction is the sum of the residuals in the terminal node j. We will go through all the calculations that give us this formula, but let's just use it to calculate γ for now. Below is the computed values of γ□ and γ_2.

$$\gamma_1 = \frac{\sum_{x_i \in R_1}(y_i - 0.56)}{\sum_{x_i \in R_1} 0.56(1-0.56)} = 0.3$$

$$\gamma_2 = \frac{\sum_{x_i \in R_2}(y_i - 0.56)}{\sum_{x_i \in R_2} 0.56(1-0.56)} = -2.2$$

```
print_tree_structure(tree)
```

```
--------------------------------------------------------------------------------
The binary tree structure has 3 nodes and has the following tree structure:

node=0 is a split node: go to node 1 if X[:, 0] <= 0.6397739946842194 else to node 2.
        node=1 is a leaf node.
         prediction: 0.3
        node=2 is a leaf node.
         prediction: -2.2
--------------------------------------------------------------------------------
```

This γ is not simply added to our initial prediction p. Instead, we are converting p into log-odds (we will call this log-odds converted value $F(x)$), then adding γ to it. For those who are not familiar with log-odds, it is defined below. You might have seen it used in [logistic regression]().

$$log(odds) = log(\frac{p}{1-p})$$

One more tweak on the prediction update is that γ is scaled down by **learning rate** ν, which ranges between 0 and 1, and then added to the log-odds-converted prediction$F(x)$. This helps the model not to overfit the training data.

$$F_1(x) = F_0(x) + \nu \bullet \gamma$$

In this example, we use a relatively big learning rate $\nu = 0.9$ to make the optimization process easier to understand, but it is usually supposed to be a much smaller value such as 0.1. By substituting actual values for the variables in the right side of the above equation, we get our updated prediction $F_1(x)$.

$$F□(x) = \begin{cases} log(\frac{0.56}{1-0.56}) + 0.9 \bullet 0.3 = 0.5 & \text{if } x \leq 0.64 \\ log(\frac{0.56}{1-0.56}) - 0.9 \bullet 2.2 = -1.7 & \text{otherwise} \end{cases}$$

If we convert log-odds $F(x)$ back into the predicted probability $p(x)$ (we will cover how we can convert it in the next section), it looks like a stair-like object below.

```
def create_prev_surface(x1, x2, y, plot_type):

    return go.Surface(x=x1, y=x2, z=y,
                      showscale=False,
                      opacity=0.5,
                      colorscale="Purples",
                      surfacecolor=np.ones(x1.shape),
                      )


p_mesh = np.exp(Fm_mesh) / (1 + np.exp(Fm_mesh))

fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))
fig.add_trace(create_prev_surface(x1_mesh, x2_mesh, np.full(x1_mesh.shape, p), "pred"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, p_mesh, "pred"))
fig = format_plot(fig)
fig.update_layout(showlegend=False)
fig.show()
```

The purple-colored plane is the initial prediction p_0 and it is updated to the red and yellow plane p_1. Now, the updated residuals r looks like this:

```
p = np.exp(Fm) / (1 + np.exp(Fm))

fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, p_mesh, "pred"))
fig.add_trace(create_residual_lines(x, y, p))
fig = format_plot(fig)
fig.update_layout(title="Updated Residuals", showlegend=False)
fig.show()
```

Updated Residuals

In the next step, we are creating a regression tree again using the same x_1 and x_2 as the features and the updated residuals r as its target. Here is the created tree:

```
p_mesh_prev = p_mesh
tree, r, Fm, r_pred_mesh, Fm_mesh = train_and_update(x, y, Fm, x1_mesh, x2_mesh, Fm_mesh, learing_

fig = go.Figure()
fig.add_trace(create_scatter(x, r, "res"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, r_pred_mesh, "res"))
fig = format_plot(fig)
fig.update_layout(showlegend=False)
fig.show()
```

```
--------------------------------------------------------------------------------
The binary tree structure has 3 nodes and has the following tree structure:

node=0 is a split node: go to node 1 if X[:, 0] <= -0.6295882761478424 else to node 2.
        node=1 is a leaf node.
         prediction: -0.5
        node=2 is a leaf node.
         prediction: 0.1
--------------------------------------------------------------------------------
```

We apply the same formula to compute γ. The calculated γ along with the updated prediction $F_2(x)$ are as follows.

$$F_2(x) = \begin{cases} F_1(x) - \nu \bullet 2.3 = 0.5 - 0.9 \cdot 2.3 = -1.6 & \text{if } x_1 \leq -0.63 \\ F_1(x) + \nu \bullet 0.4 = 0.5 + 0.9 \cdot 0.4 = 0.9 & \text{else if } -0.63 < x_1 \leq 0.64 \\ F_1(x) + \nu \bullet 0.4 = -1.7 + 0.9 \cdot 0.4 = -1.3 & \text{otherwise} \end{cases}$$

Again, if we convert log-odds $F_2(x)$ back into the predicted probability $p_2(x)$, it looks like something below.

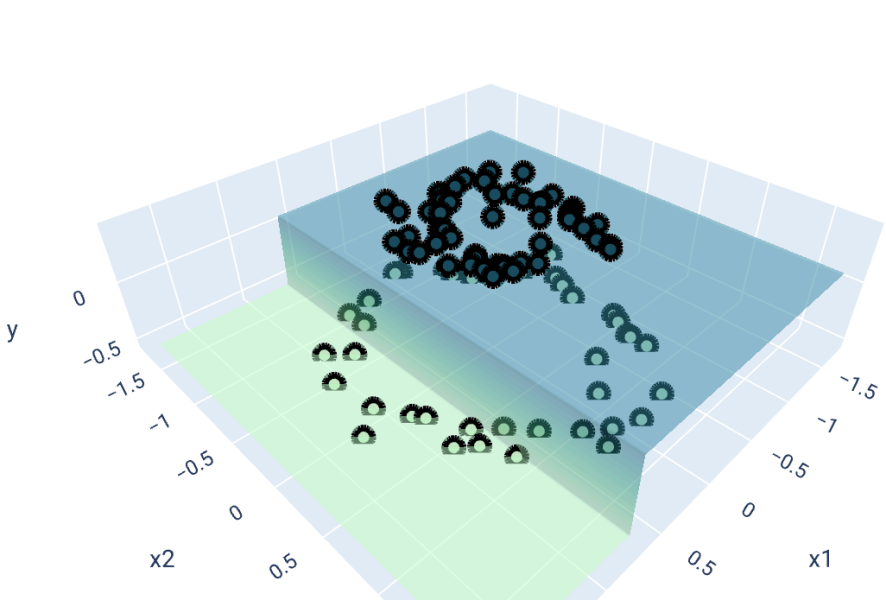
```
p_mesh = np.exp(Fm_mesh) / (1 + np.exp(Fm_mesh))

fig = go.Figure()
fig.add_trace(create_scatter(x, y, "pred"))

fig.add_trace(create_prev_surface(x1_mesh, x2_mesh, p_mesh_prev, "pred"))
fig.add_trace(create_surface(x1_mesh, x2_mesh, p_mesh, "pred"))
p = np.exp(Fm) / (1 + np.exp(Fm))
# fig.add_trace(create_residual_lines(x, y, pred))
fig = format_plot(fig)
fig.update_layout(showlegend=False)
fig.show()
```

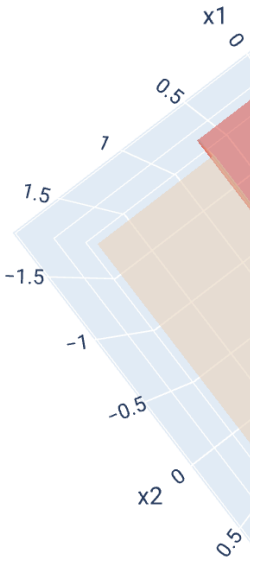
We iterate these steps until the model prediction stops improving. The figures below show the optimization process from 0 to 4 iterations.

```
def create_subplots(iter_num):

    return make_subplots(
        rows=1, cols=2,
        specs=[[{"is_3d": True}, {"is_3d": True}]],
        horizontal_spacing=0,
        subplot_titles=(f"Residuals of iteration {iter_num}", f"Predictions of iteration {iter_num
    )

def format_subplots(fig):
    fig.update_layout(
        scene=dict(
            xaxis_title="x1",
            yaxis_title="x2",
            zaxis_title="y"
        ),
        scene2=dict(
            xaxis_title="x1",
            yaxis_title="x2",
            zaxis_title="y"
        ),
        height=400,
        width=1200,
        margin=dict(l=10, r=10, t=20, b=20),
    )
    fig.update_layout(showlegend=False)
    return fig


p = y.mean()
F0 = np.log(p/(1-p))

learing_rate = 0.9
Fm_mesh = np.full(x1_mesh.shape, F0)
Fm = np.full(len(y), F0)
n_estimators = 4
p = y.mean()

fig = create_subplots(0)
fig.append_trace(create_scatter(x, y, "pred"), row=1, col=2)
fig.append_trace(create_surface(x1_mesh, x2_mesh, np.full(x1_mesh.shape, p), "pred"), row=1, col=2
fig = format_subplots(fig)
fig.show()

for i in range(n_estimators):
    tree, r, Fm, r_pred_mesh, Fm_mesh = train_and_update(x, y, Fm, x1_mesh, x2_mesh, Fm_mesh,
                                                         learing_rate=learing_rate, print_tree=Fal
    p_mesh = np.exp(Fm_mesh) / (1 + np.exp(Fm_mesh))

    fig = create_subplots(i+1)
    fig.append_trace(create_scatter(x, r, "res"), row=1, col=1)
    fig.append_trace(create_surface(x1_mesh, x2_mesh, r_pred_mesh, "res"), row=1, col=1)
    fig.append_trace(create_scatter(x, y, "pred"), row=1, col=2)
    fig.append_trace(create_surface(x1_mesh, x2_mesh, p_mesh, "pred"), row=1, col=2)

    fig = format_subplots(fig)
    fig.show()
```

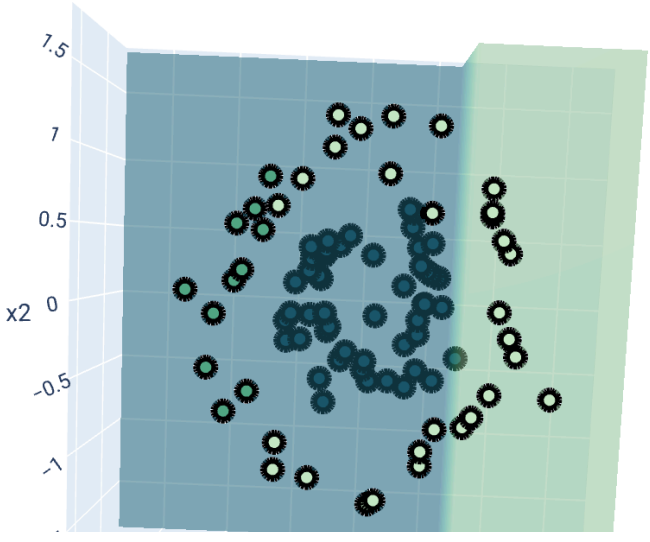
Residuals of iteration 0

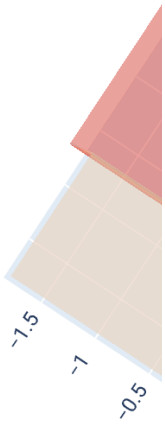
Residuals of iteration 1



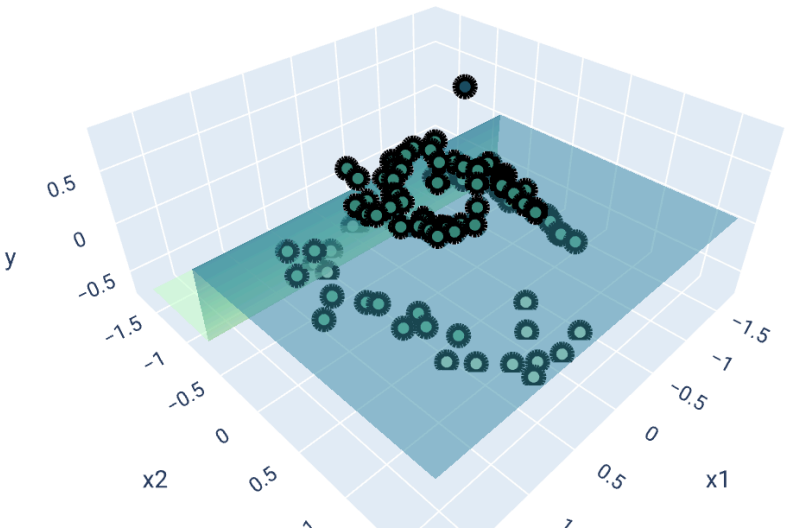


Residuals of iteration 2

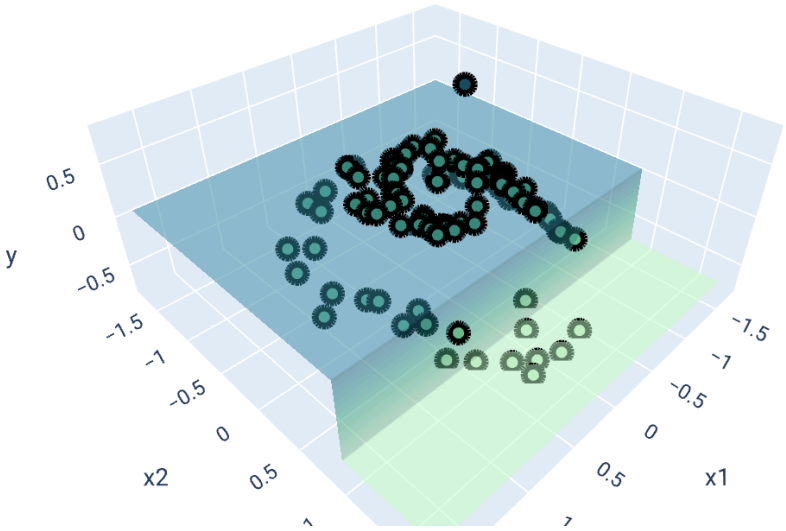




Residuals of iteration 3



Residuals of iteration 4



You can see the combined prediction $p(x)$ (red and yellow plane) is getting closer to our target y as we add more trees into the combined model. This is how gradient boosting works to predict complex targets by combining multiple weak models.

Code