All You Need to Know about Gradient Boosting Algorithm – Part 1. Regression

Algorithm explained with an example, math, and code

Photo by Luca Bravo on Unsplash

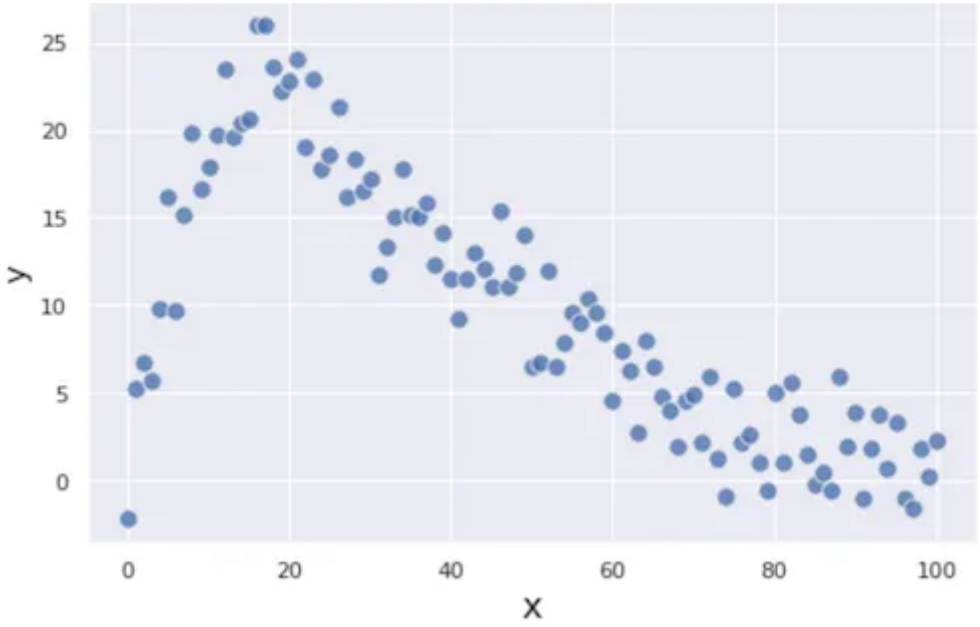
Gradient boosting is one of the most popular machine learning algorithms for tabular datasets. It is powerful enough to find any nonlinear relationship between your model target and features and has great usability that can deal with missing values, outliers, and high cardinality categorical values on your features without any special treatment. While you can build barebone gradient boosting trees using some popular libraries such as XGBoost or LightGBM without knowing any details of the algorithm, you still want to know how it works when you start tuning hyper-parameters, customizing the loss functions, etc., to get better quality on your model.

This article aims to provide you with all the details about the algorithm, specifically its regression algorithm, including its math and Python code from scratch. If you are more interested in the classification algorithm, please look at Part 2.

Algorithm with an Example

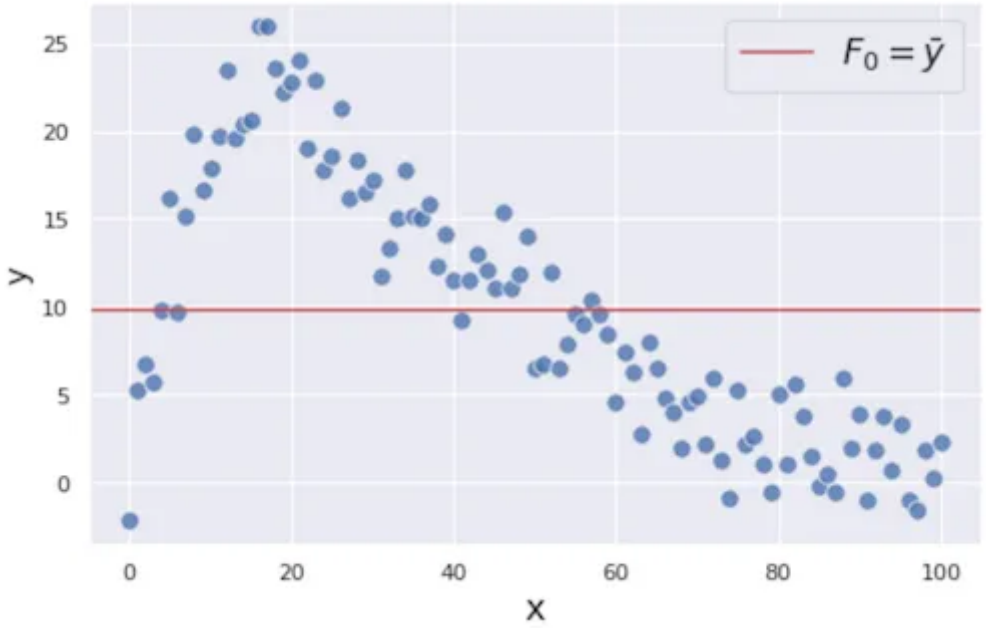
Gradient boosting is one of the variants of ensemble methods where you create multiple weak models and combine them to get better performance as a whole.

In this section, we are building gradient boosting regression trees step by step using the below sample which has a nonlinear relationship between x and y to intuitively understand how it works (all the pictures below are created by the author).



Sample for a regression problem

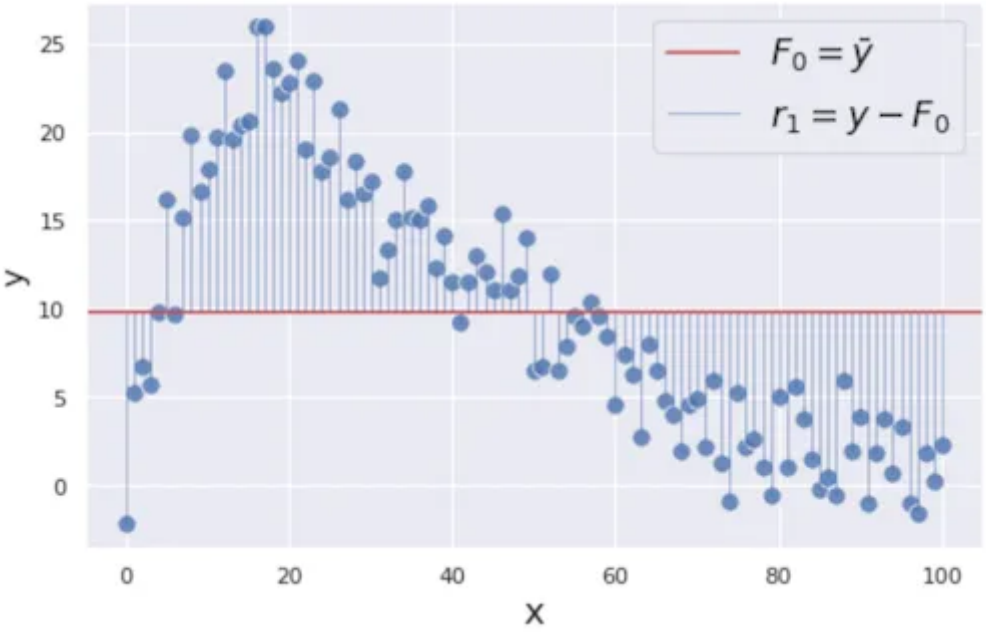
The first step is making a very naive prediction on the target y. We make the initial prediction F_0 as an overall average of y:



Initial prediction: F0 = mean(y)

You might feel using the mean for the prediction is silly, but don't worry. We will improve our prediction as we add more weak models to it.

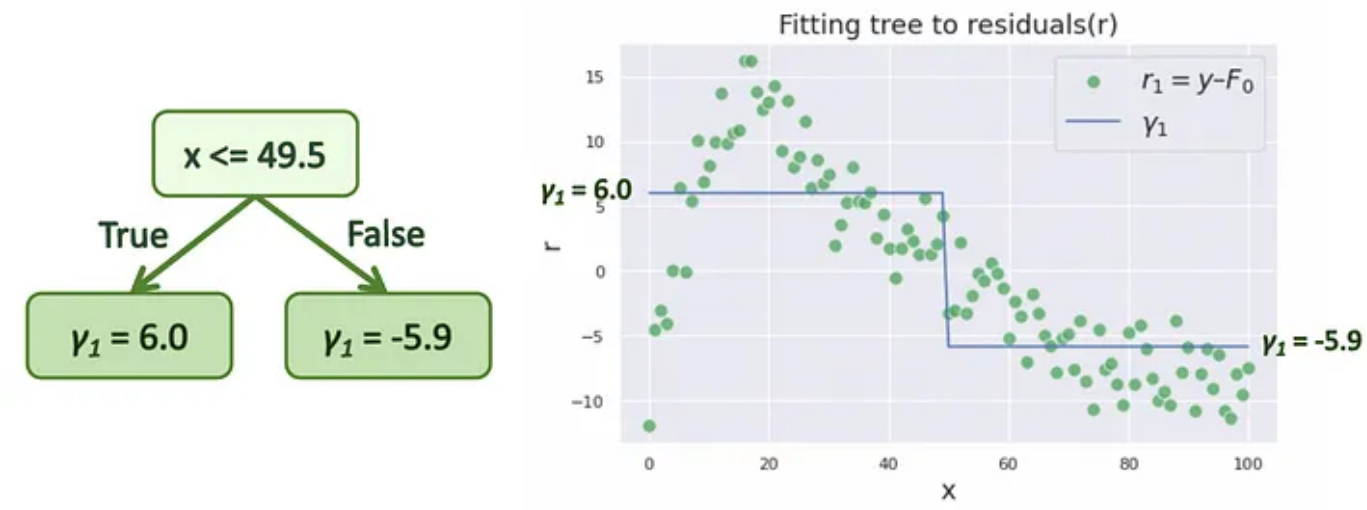
To improve our prediction, we will focus on the residuals (i.e. prediction errors) from the first step because that is what we want to minimize to get a better prediction. The residuals r_1 are shown as the vertical blue lines in the figure below.



To minimize these residuals, we are building a regression tree model with x as its feature and the residuals $r_1 = y - mean(y)$ as its target. The reasoning behind that is if we can find some patterns between x and r_1 by building the additional weak model, we can reduce the residuals by utilizing it.

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 $\gamma_1 = \{6.0, -5.9\}$ (we are using γ (gamma) to denotes the prediction).



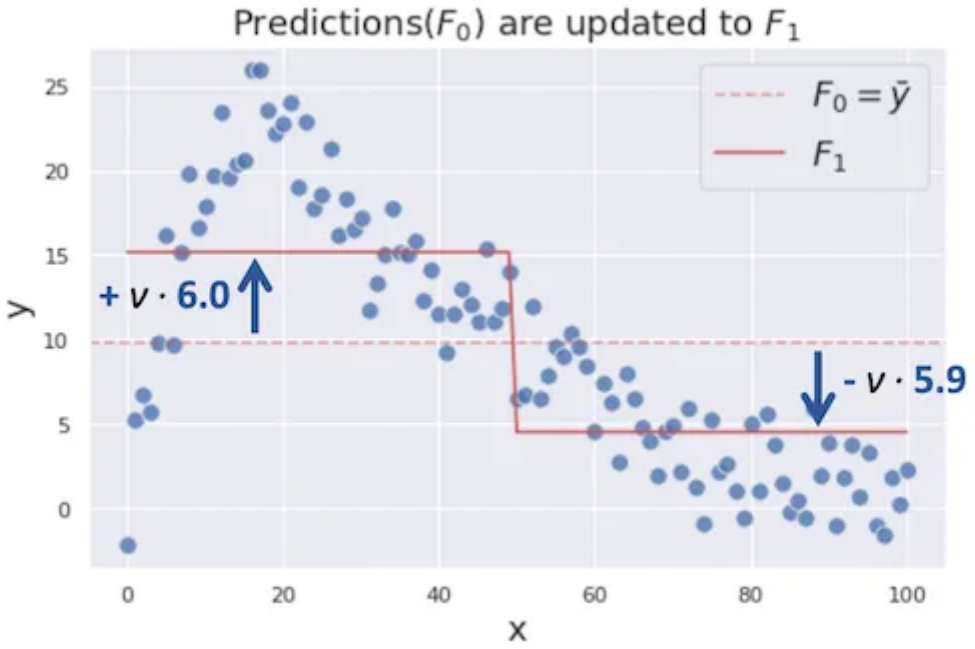
This prediction γ_1 is added to our initial prediction F_0 to reduce the residuals. In fact, gradient boosting algorithm does not simply add γ to F as it makes the model overfit to the training data. Instead, γ is scaled down by **learning rate** ν which ranges between 0 and 1, and then added to F.

$$F_1 = F_0 + \nu \cdot \gamma_1$$

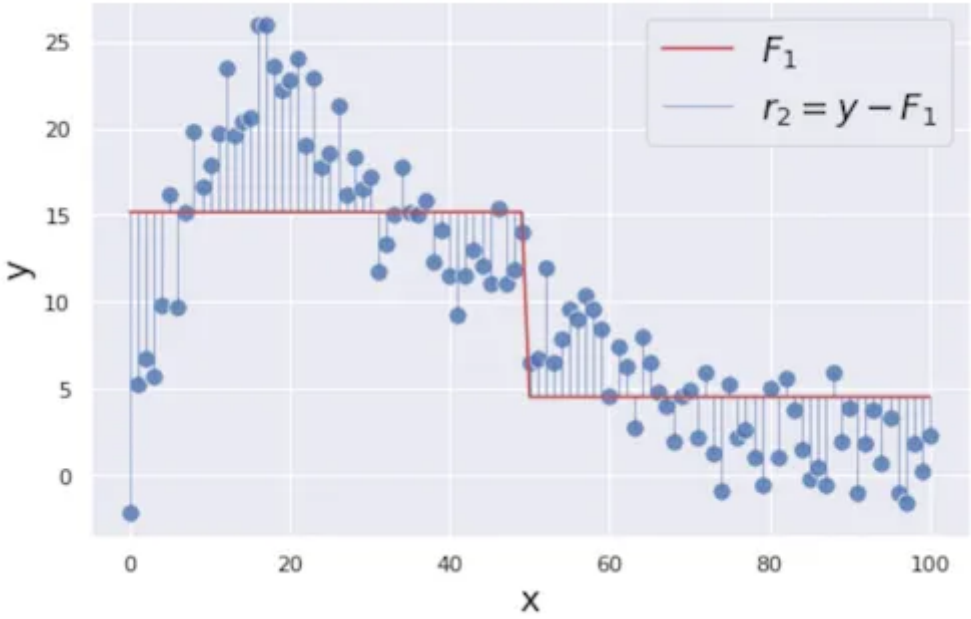
In this example, we use a relatively big learning rate $\nu = 0.9$ to make the optimization process easier to understand, but it is usually supposed to be a much smaller value such as 0.1.

After the update, our combined prediction F_1 becomes:

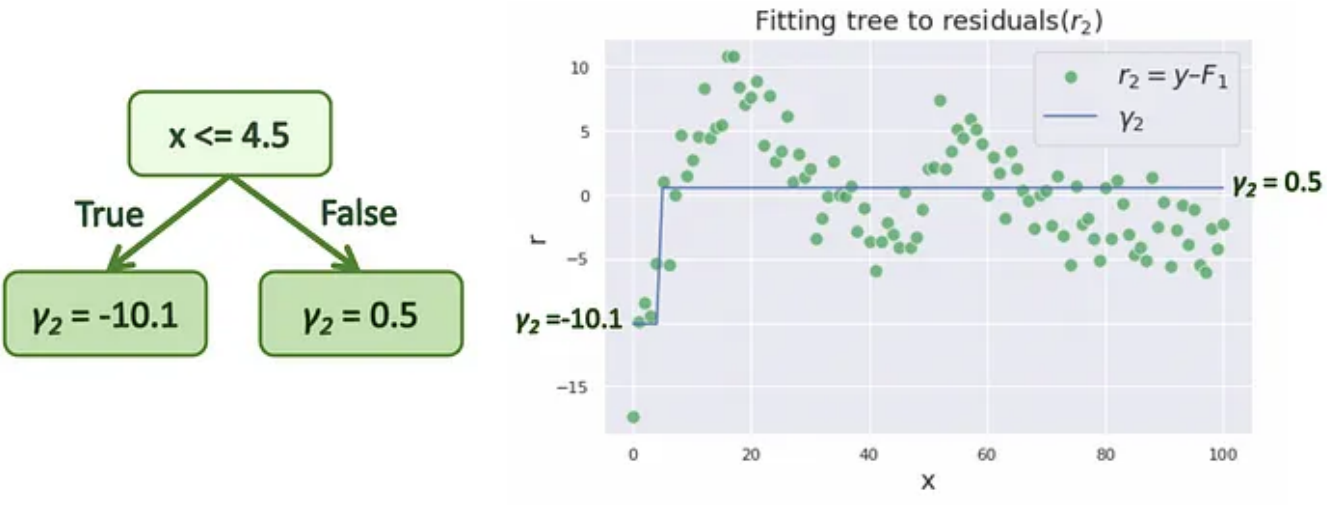
$$F_1 = \begin{cases} F_0 + \nu \cdot 6.0 & if\ x \leq 49.5 \\ F_0 - \nu \cdot 5.9 & otherwise \end{cases}$$



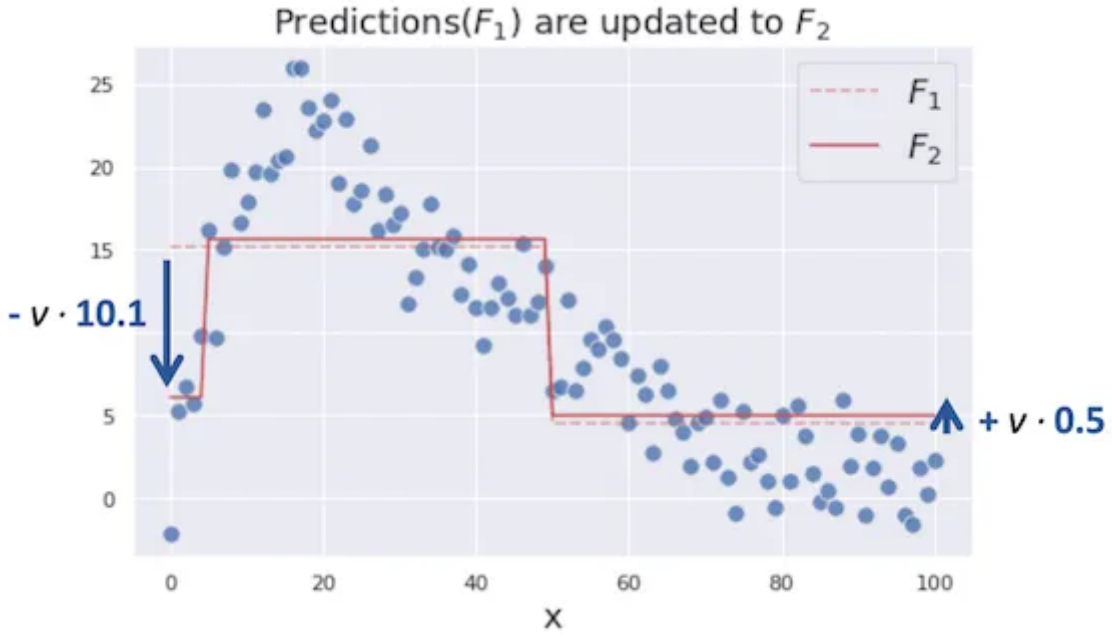
Now, the updated residuals r_2 looks like this:



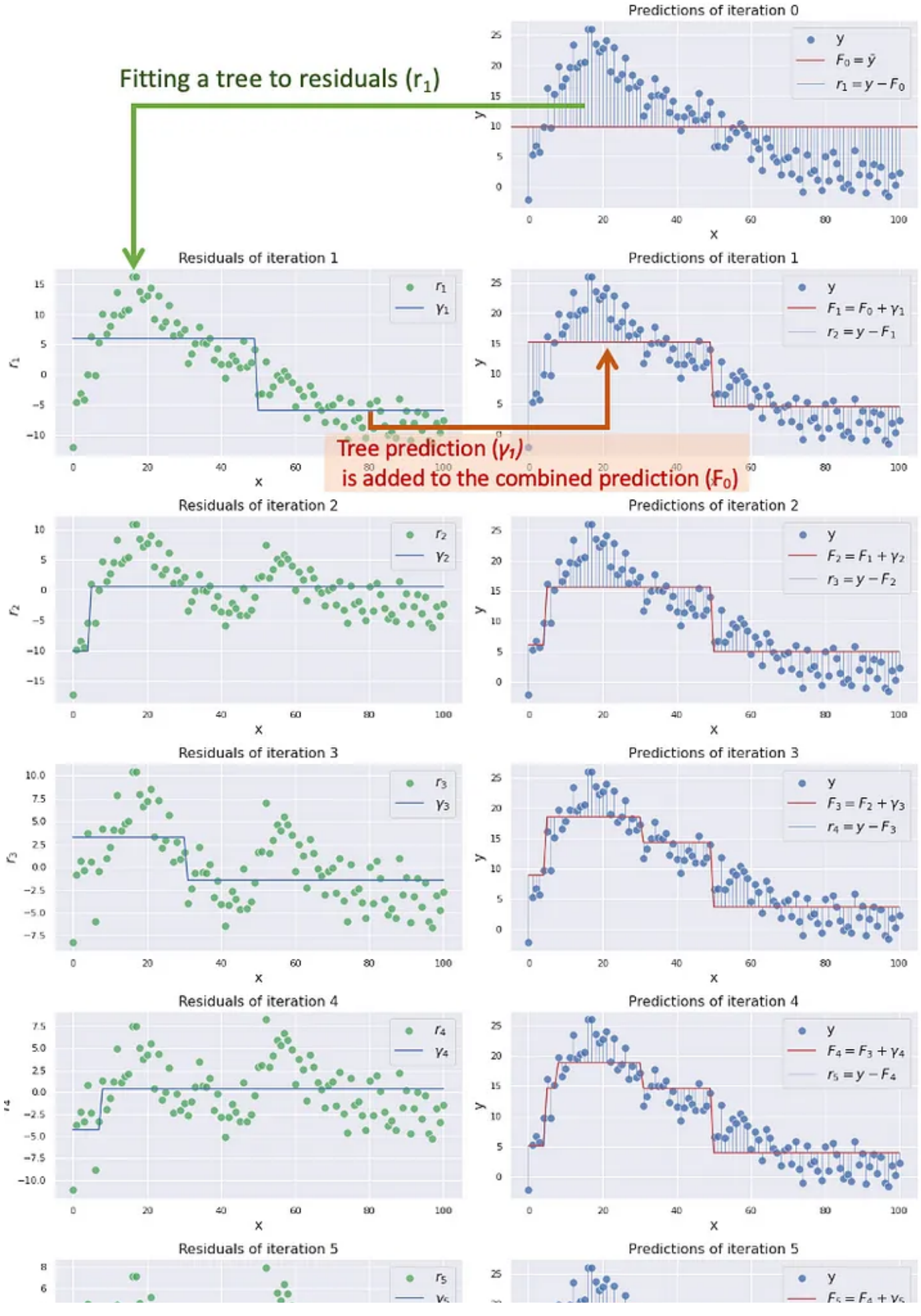
In the next step, we are creating a regression tree again using the same x as the feature and the updated residuals r_2 as its target. Here is the created tree:

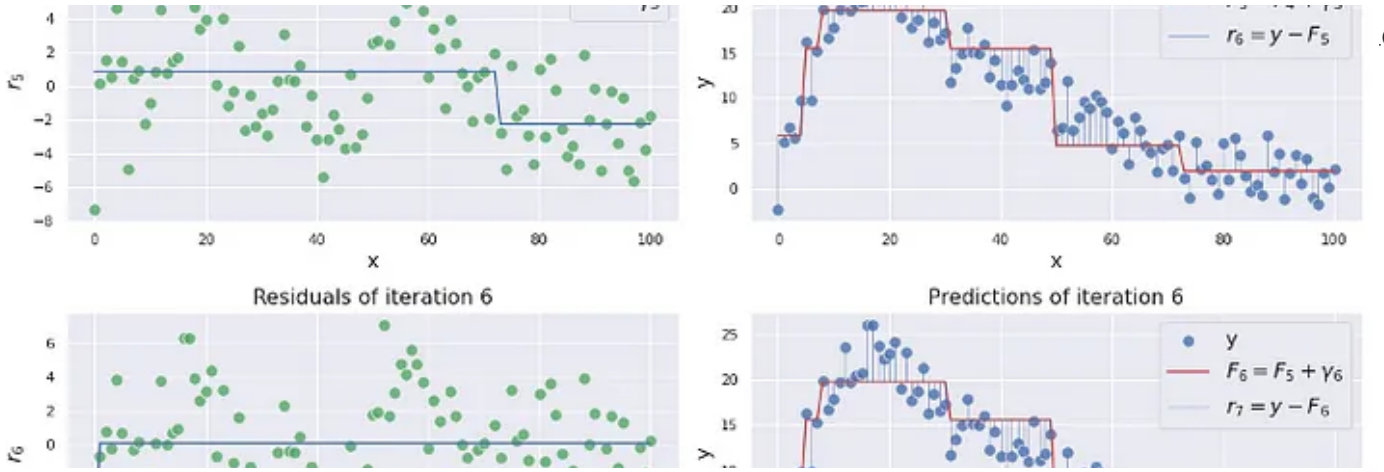


Then, we are updating our previous combined prediction F_1 with the new tree prediction γ_2.



We iterate these steps until the model prediction stops improving. The figures below show the optimization process from 0 to 6 iterations.


Predictions of iteration 0
y
$F_0 = \bar{y}$
$r_1 = y - F_0$
Fitting a tree to residuals (r_1)
Residuals of iteration 1
r_1
γ_1
Predictions of iteration 1
$F_1 = F_0 + \gamma_1$
$r_2 = y - F_1$
Tree prediction (γ_1)
is added to the combined prediction (F_0)
Residuals of iteration 2
r_2
γ_2
Predictions of iteration 2
$F_2 = F_1 + \gamma_2$
$r_3 = y - F_2$
Residuals of iteration 3
r_3
γ_3
Predictions of iteration 3
$F_3 = F_2 + \gamma_3$
$r_4 = y - F_3$
Residuals of iteration 4
r_4
γ_4
Predictions of iteration 4
$F_4 = F_3 + \gamma_4$
$r_5 = y - F_4$
Residuals of iteration 5
r_5
Predictions of iteration 5
x



d

Gradient Boosting Algorithm

1. Initialize model with a constant value:

$$F_0(x) = \underset{\gamma}{argmin} \sum_{i=1}^{n} L(y_i, \gamma)$$

2. for $m = 1$ *to* M:

2-1. Compute residuals $r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)}$ *for* $i = 1,\ldots,n$

2-2. Train regression tree with features x against r and create terminal node reasions R_{jm} for $j = 1,\ldots,J_m$

2-3. Compute $\gamma_{jm} = \underset{\gamma}{argmin} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma)$ *for* $j = 1,\ldots,J_m$

2-4. Update the model:

$$F_m(x) = F_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} 1(x \in R_{jm})$$

Source: adapted from Wikipedia and Friedman's paper

Let's demystify this line by line.

Step 1

1. Initialize model with a constant value:

$$F_0(x) = \underset{\gamma}{argmin} \sum_{i=1}^{n} L(y_i, \gamma)$$

The first step is creating an initial constant value prediction `F₀`. `L` is the loss function and it is squared loss in our regression case.

$$L = (y_i - \gamma)^2$$

`argmin` means we are searching for the value `γ` that minimizes `ΣL(yᵢ,γ)`. Let's compute the value `γ` by using our actual loss function. To find `γ` that minimizes `ΣL`, we are taking a derivative of `ΣL` with respect to `γ`.

$$\begin{aligned} \frac{\partial}{\partial \gamma} \sum_{i=1}^{n} L &= \frac{\partial}{\partial \gamma} \sum_{i=1}^{n} (y_i - \gamma)^2 \\ &= -2 \sum_{i=1}^{n} (y_i - \gamma) \\ &= -2 \sum_{i=1}^{n} y_i + 2n\gamma \end{aligned}$$

And we are finding `γ` that makes `∂ΣL/∂γ` equal to 0.

$$-2\sum_{i=1}^{n} y_i + 2n\gamma = 0$$

$$n\gamma = \sum_{i=1}^{n} y_i$$

$$\gamma = \frac{1}{n}\sum_{i=1}^{n} y_i = \bar{y}$$

It turned out that the value γ that minimizes ΣL is the mean of y. This is why we used y mean for our initial prediction F_0 in the last section.

$$F_0(x) = \overset{*}{\gamma} = \bar{y}$$

Step2

> 2. for $m = 1$ *to* M:

The whole step2 processes from 2–1 to 2–4 are iterated M times. M denotes the number of trees we are creating and the small m represents the index of each tree.

Step 2–1

> 2-1. Compute residuals $r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)}$ *for* $i = 1,\ldots,n$

We are calculating residuals r_{im} by taking a derivative of the loss function with respect to the previous prediction F_{m-1} and multiplying it by −1. As you can see in the subscript index, r_{im} is computed for each single sample i. Some of you might be wondering why we are calling this r_{im} residuals. This value is actually **negative gradient** that gives us guidance on the directions (+/−) and the magnitude in which the loss function can be

minimized. You will see why we are calling it residuals shortly. By the way, this technique where you use a gradient to minimize the loss on your model is very similar to gradient descent technique which is typically used to optimize neural networks. (In fact, they are slightly different from each other. If you are interested, please look at this article detailing that topic.)

Let's compute the residuals here. F_{m-1} in the equation means the prediction from the previous step. In this first iteration, it is F_0. We are solving the equation for residuals r_{im}.

$$
\begin{aligned}
r_{im} &= -\left[\frac{\partial L(y_i,\ F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \\
&= -\frac{\partial (y_i - F_{m-1})^2}{\partial F_{m-1}} \\
&= 2(y_i - F_{m-1})
\end{aligned}
$$

We can take 2 out of it as it is just a constant. That leaves us $r_{im} = y_i - F_{m-1}$. You might now see why we call it residuals. This also gives us interesting insight that the negative gradient that provides us the direction and the magnitude to which the loss is minimized is actually just residuals.

Step 2–2

> 2-2. Train regression tree with features x against r and create terminal node reasions R_{jm} for $j = 1,\ldots, J_m$

j represents a terminal node (i.e. leave) in the tree, m denotes the tree index, and capital J means the total number of leaves.

Step 2–3

2-3. Compute $\gamma_{jm} = \underset{\gamma}{argmin} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma) \quad for\ j = 1,\ldots, J_m$

We are searching for γ_{jm} that minimizes the loss function on each terminal node j. $\Sigma x_i \in R_{jm}\ L$ means we are aggregating the loss on all the sample x_i s that belong to the terminal node R_{jm}. Let's plugin the loss function into the equation.

$$\gamma_{jm} = \underset{\gamma}{argmin} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma)$$

$$= \underset{\gamma}{argmin} \sum_{x_i \in R_{jm}} (y_i - F_{m-1}(x_i) - \gamma)^2$$

Then, we are finding γ_{jm} that makes the derivative of Σ(*) equals zero.

$$\frac{\partial}{\partial \gamma} \sum_{x_i \in R_{jm}} (y_i - F_{m-1}(x_i) - \gamma)^2 = 0$$

$$-2 \sum_{x_i \in R_{jm}} (y_i - F_{m-1}(x_i) - \gamma) = 0$$

$$n_j \gamma = \sum_{x_i \in R_{jm}} (y_i - F_{m-1}(x_i))$$

$$\gamma = \frac{1}{n_j} \sum_{x_i \in R_{jm}} r_{im}$$

Please note that n_j means the number of samples in the terminal node j. This means the optimal γ_{jm} that minimizes the loss function is the average of the residuals r_{im} in the terminal node R_{jm}. In other words, γ_{jm} is the regular prediction values of regression trees that are the average of the target values (in our case, residuals) in each terminal node.

Step 2–4

2-4. Update the model:

$$F_m(x) = F_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} 1(x \in R_{jm})$$

In the final step, we are updating the prediction of the combined model F_m. $\gamma_{jm}1(x \in R_{jm})$ means that we pick the value γ_{jm} if a given x falls in a terminal node R_{jm}. As all the terminal nodes are exclusive, any given single x falls into only a single terminal node and corresponding γ_{jm} is added to the previous prediction F_{m-1} and it makes updated prediction F_m.

As mentioned in the previous section, ν is learning rate ranging between 0 and 1 which controls the degree of contribution of the additional tree prediction γ to the combined prediction F_m. A smaller learning rate reduces the effect of the additional tree prediction, but it basically also reduces the chance of the model overfitting to the training data.

Now we have gone through the whole steps. To get the best model performance, we want to iterate step 2 M times, which means adding M trees to the combined model. In reality, you might often want to add more than 100 trees to get the best model performance.

Some of you might feel that all those maths are unnecessarily complex as the previous section showed the basic idea in a much simpler way without all those complications. The reason behind it is that gradient boosting is designed to be able to deal with any loss functions as long as it is differentiable and the maths we reviewed is a generalized form of gradient boosting algorithm with that flexibility. That makes the formula a little complex, but it is the beauty of the algorithm as it has huge flexibility and convenience to work on a variety of types of problems. For example, if your problem requires absolute loss instead of squared loss, you can just replace the loss function and the whole algorithm works as it is as defined above. In fact, popular gradient boosting implementations such as XGBoost or LightGBM have a wide variety of loss functions, so you can choose whatever loss functions that suit your problem (see the various loss functions available in XGBoost or LightGBM).

Code

In this section, we are translating the maths we just reviewed into a viable python code to help us understand the algorithm further. The code is mostly derived from Matt Bowers' implementation, so all credit goes to his work. We are using `DecisionTreeRegressor` from scikit-learn to build trees which helps us just focus on the gradient boosting algorithm itself instead of the tree algorithm. We are imitating scikit-learn style implementation where you train the model with `fit` method and make predictions with `predict` method.

Please note that all the trained trees are stored in `self.trees` list object and it is retrieved when we make predictions with `predict` method.

Next, we are checking if our `CustomGradientBoostingRegressor` performs as the same as `GradientBoostingRegressor` from scikit-learn by looking at their RMSE on our data.

```
# Output
Custom GBM RMSE:       3.961707263264281
Scikit-learn GBM RMSE: 3.961707263264281
```

As you can see in the output above, both models have exactly the same RMSE.

Conclusion

The algorithm we have reviewed in this post is just one of the options of gradient boosting algorithm that is specific to regression problems with squared loss.