6 GRADIENT BOOSTING, SHAP VALUES

Another important class of algorithms that uses decision trees, besides random forest, is the gradient boosting method.

6.1 Gradient Boosting

We have seen how a single Decision Tree (DT) can be unstable. Small changes to the training set such as changing of a few sample points or instances and its related features/explanatory variables, or choice of different sub-sets of features (or omitting some) can produce different trees with different predictions on a test sample. A RF on the collection or ensemble of independently trained DTs may "average" the variability of each DT and yield a more accurate forecast. RF also randomizes selection of features and resamples for computing different DTs – the bagging approach.

Like the random forest (RF) method, the gradient boosting (GB) method is also an ensemble of decision trees (DTs). However, RF and GB differ in the way they combine the decision trees. Random forest combines all independently generated DTs at the end while the gradient boosting method combines the DTs as each subsequent DT is generated in a dependent way from the previous DTs. Each subsequent DT may have a different set of target values, and the DT is also called a boosting tree. The idea of GB is to start with weak trees and then strengthens them as the algorithm proceeds to "solve" for the net errors left from the past DTs.

There are GB methods (GBM) for continuous or discrete target variable fitting and GB methods for binary and multi-class classifications. We first provide an illustration of the GB methods for continuous or discrete target variable fitting.

A gradient boosting method (or GB Trees) initially constructs a weak predictor and checks for the training error on each sample point. In regression, the initial weak predictor could be just the sample mean $\sum_{j=1}^{N} Y_j/N$ as predictor for every Y_j where Y_j is the target value for the j^{th} training sample point. Call this initial predictor $F_0 \equiv \bar{Y}$. The initial errors of fitting for each sample point in the training set data are $e_{(0)j} = Y_j - \bar{Y}$, for each j in the training sample.

GBT then builds a first DT, DT(1), to fit/predict $e_{(0)j}$ using features of each sample point j. This mapping or DT works by using each feature value X_{jk} (each feature k) to decide which next sub-group the sample point j belongs to, until sample point j is led by its features $\{X_{jk}\}$ and by the DT(1) decision rules to a terminal leaf with a fitted/predicted value. The fitting follows the splitting criterion of minimizing weighted mean squared errors (MSE) in DT. Let the terminal value for a $e_{(0)j}$ be h_{1j}.

The process can be depicted as follows in Figure 6.1.

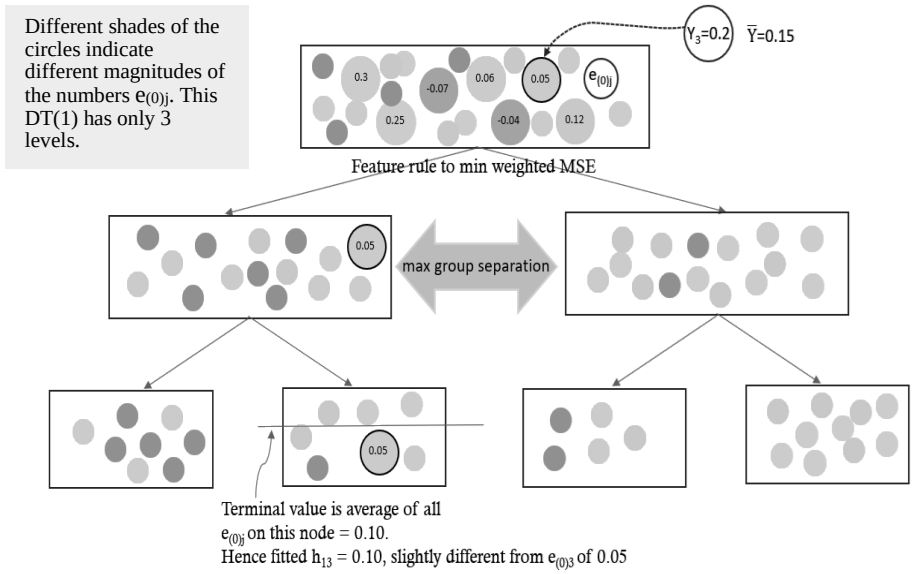


Figure 6.1

In general, we expect to see small differences in targets of $e_{(0)j}$ in DT(1) and the predicted values of h_{1j}. But a good training tree would make this difference close to zero. Even if the DT(1) should in this training data set produce h_{13} exactly equal to $e_{(0)3}$ = 0.05, when the leaf node (final node on tree) is thoroughly resolved to contain only the point or points predicting the same $e_{(0)j}$ values of 0.05, the DT(1) decision rules when applied to a test sample point with approximately similar features may still yield a slightly different predicted h_{1j} as the features are not identical to that in the training sample point. And if the features are identical, but the test sample point has a slightly

different target value than that in the training sample point, then there is still a slight error in prediction.

In GB, to prevent overshooting (rising above the target from below or falling below the target from above), a learning rate (hyperparameter) $\alpha \in (0,1]$, e.g., $\alpha = 0.1$, is imposed on the predicted value h_{1j} within the algorithm. This regularization does not typically occur in a standalone DT. In the case here, the GB algorithm produces the fitted value/predictor of $e_{(0)j}$ as $F_{1j} = \alpha h_{1j}$. The updated value of the prediction of Y_j is $F_0 + F_{1j}$. The fitting/prediction error from DT(1) is then $e_{(1)j} = Y_j - F_0 - F_{1j} = e_{(0)j} - F_{1j}$, for each j in the training sample. Note how the training data set enables use of the label Y_j to determine the next errors $e_{(1)j}$ (for each sample point j in training set) to fit.

Suppose some measure of the total errors $e_{(1)j}$ for all j is not small enough. GBT then builds a second DT in the next stage to train a better DT. And then a third tree to improve on the training, and so on. Thus, unlike the RF method where independent DTs are produced for "averaging", GBT adjusts the algorithm for the next and subsequent DTs (hence dependence of the DTs) to improve on the training based on fitting errors in earlier DTs.

In DT(2), let the terminal (predicted) value for a $e_{(1)j}$ be h_{2j}. The GB algorithm produces the fitted value/predictor of $e_{(1)j}$ as $F_{2j} = \alpha h_{2j}$. The updated value of the prediction of Y_j is $F_0 + F_{1j} + F_{2j}$. The fitting/prediction error from DT(2) is then $e_{(2)j} = Y_j - F_0 - F_{1j} - F_{2j} = e_{(1)j} - F_{2j}$, for each j in the training sample.

Suppose some measure of the total errors $e_{(2)j}$ for all j is still not small enough. The third DT(3) is built to predict $e_{(2)j}$ for all j. The GB algorithm produces the fitted value/predictor of $e_{(2)j}$ as $F_{3j} = \alpha h_{3j}$. The updated value of the prediction of Y_j is $F_0 + F_{1j} + F_{2j} + F_{3j}$. The fitting/prediction error from DT(3) is then $e_{(3)j} = Y_j - F_0 - F_{1j} - F_{2j} - F_{3j} = e_{(2)j} - F_{3j}$, for each j in the training sample. When the maximum number of DTs as in DT(n) is reached or till the measure of errors $e_{(n)j}$, for all j, becomes smaller than a pre-determined size, then the GB tree prediction is $F_0 + F_{1j} + F_{2j} + F_{3j} + \ldots + F_{nj}$ for each Y_j. The boosting regression trees are additive.

Note that in a GB Tree algorithm, the DTs are constructed sequentially in a dependent way whereby previous training errors are considered in building the next tree. Finally, all the trees are added up to form the prediction. The outputs for each of the sequential trees are in a fixed order. This is unlike the RF where each DT can be independently evaluated and hence can be computed

in parallel. GB algorithms typically start with weak trees, i.e., trees that produce large errors. Then, stronger trees are subsequently built to predict those errors and add the predicted errors up to form the final prediction. In this sense, subsequent trees put more "weight" or consideration to sample points in previous trees with larger errors for subsequent error predictions (as larger errors carry more "weight" for fitting in squared error sense for optimal splitting). Computationally, GBT is generally more intensive.

We provide a numerical example of the above procedure as follows. Suppose N = 4 and the set of target values, initial predictor (sample mean), and initial fitting errors are shown.

Y_j	0.5	1.0	1.2	1.3
F_0	1.0	1.0	1.0	1.0
$e_{(0)j}$	-0.5	0.0	0.2	0.3

Next, DT(1) computes h_{1j}, hence F_{1j}. Note $F_{1j} = \alpha h_{1j}$ where $\alpha = 0.1$ here. Next error is $e_{(1)j} = e_{(0)j} - F_{1j}$.

h_{1j}	-0.8	-0.5	0.4	0.9
F_{1j}	-0.08	-0.05	0.04	0.09
$e_{(1)j}$	-0.42	0.05	0.16	0.21

Next, DT(2) computes h_{2j}, hence F_{2j}. Next error is $e_{(2)j} = e_{(1)j} - F_{2j}$.

h_{2j}	-0.5	0.4	0.7	1.5
F_{2j}	-0.05	0.04	0.07	0.15
$e_{(2)j}$	-0.37	0.01	0.09	0.06

We can see that if the algorithm works, $e_{(n)j}$ gets smaller toward zero.

More formally, a Gradient Boosting Model develops stronger trees sequentially by minimizing a loss function at each new tree. The loss function in a GB algorithm is directly connected with setting up the next target variable (the "error") to fit, in the subsequent boosting trees in a GB approach. We just saw how the subsequent target = "error" = original target less updated fitted/predicted value, viz., $e_{(1)j} = Y_j - (F_0 + F_{1j})$, $e_{(2)j} = Y_j - (F_0 + F_{1j} + F_{2j})$, $e_{(3)j} = Y_j - (F_0 + F_{1j} + F_{2j} + F_{3j})$, and so on.

Subsequent trees put more "weight" or consideration to sample points in previous trees with larger errors such as in squared error sense. The loss function as in mean squared error (MSE) puts more importance to fit outliers as these impute larger losses. However, if outliers are erroneous, e.g., due to data entry error, then such fitting would produce poor forecasts as the model overfitted outliers. Using mean absolute error (MAE) as loss function would be more robust to effect of outliers in fitting but may not perform well if the outliers reflect genuine higher risk cases.

We assume outliers are removed or that they posed as genuine possibilities. Suppose the loss function L is MSE or is quadratic in the fitted/predicted "error". $L = \frac{1}{2}\sum_{j=1}^{N}\left(Y_j - \sum_{i=0}^{n} F_{ij}\right)^2$ (for an optimal n number of GB trees) where N is the sample size of the training data set. Typically, n < N. At each boosting stage, e.g., in the algorithm of the mth (m ≤ n) tree, the training loss function would be $\frac{1}{2}\sum_{j=1}^{N}\left(Y_j - F_0 - F_{1j} - \ldots - F_{m-2,j} - F_{m-1,j}\right)^2$. To find the minimum of the loss function, supposing $F_{m-1,j}$ is some function of the features X_{jk}, we could set the following derivatives to zeros, i.e.,

$$\frac{\partial F_{m-1,j}}{\partial X_{jk}}\frac{\partial}{\partial F_{m-1,j}}\ \frac{1}{2}\sum_{j=1}^{N}\left(Y_j - F_0 - F_{1j} - \ldots - F_{m-2,j} - F_{m-1,j}\right)^2$$
$$= -\ \frac{\partial F_{m-1,j}}{\partial X_{jk}}\ \sum_{j=1}^{N}\left(Y_j - F_0 - F_{1j} - \ldots - F_{m-2,j} - F_{m-1,j}\right) = 0.$$

In principle, the minimum loss could be attained when $\sum_{j=1}^{N} F_{m-1,j} = \sum_{j=1}^{N} Y_j - F_0 - F_{1j} - \ \ldots - F_{m-2,j}$. However, as we are dealing with DTs, it is not possible to explicitly derive an analytical function of $F_{m-1,j}$ in terms of X_{jk} for every j such that $\sum_{j=1}^{N} F_{m-1,j} = \sum_{j=1}^{N} Y_j - F_0 - F_{1j} - \ \ldots - F_{m-2,j}$. But we can try to find for each j, $F_{m-1,j}$ that is close to $Y_j - F_0 - F_{1j} - \ \ldots - F_{m-2,j} = e_{(m-2)j}$ using the DT algorithm. And we can try to find for each j, $F_{m,j}$ that is close to $Y_j - F_0 - F_{1j} - \ \ldots - F_{m-2,j} - F_{m-1,j} = e_{(m-1)j}$ and so on.

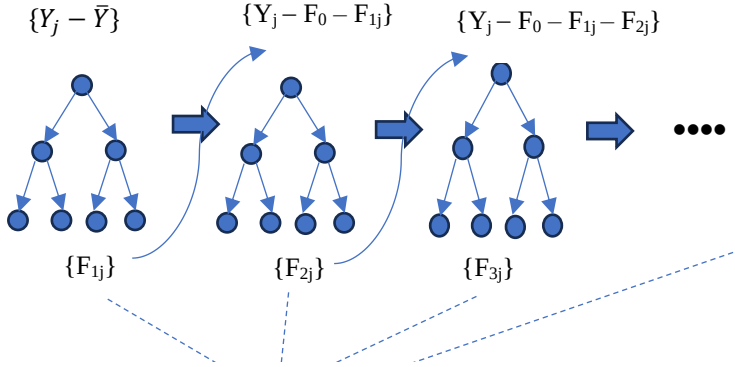
Note that the "error" $e_{(m-1)j}$ as the target value (for every j) of the mth boosting tree, $e_{(m-1)j} = Y_j - F_0 - F_{1j} - \ \ldots - F_{m-1,j}$, is also element in the negative of the gradient term $\frac{\partial L}{\partial F_{m-1,j}}$

$$-\ \sum_{j=1}^{N}\left(Y_j - F_0 - F_{1j} - \ldots - F_{m-2,j} - F_{m-1,j}\right)$$

with respect to the loss function. Hence this approach via reducing "errors" or reducing the gradients toward zeros is thus called gradient boosting method.

Reducing the loss function is directly connected with setting up the next target errors $e_{(m-1)j}$ for fitting.

Visually, GB regression trees for fitting training data can be seen as follows. Note that the features are typically randomly selected for different boosting trees. The quantities on the top line $\{Y_j - \bar{Y}\}$, $\{Y_j - F_0 - F_{1j}\}$, $\{Y_j - F_0 - F_{1j} - F_{2j}\}$, etc., denote the target errors $e_{(0)j}$, $e_{(1)j}$, $e_{(2)j}$ for the trees DT(1), DT(2), DT(3), and so on. The bottom line quantities $\{F_{1j}\}$, $\{F_{2j}\}$, $\{F_{3j}\}$, etc. denote the predicted errors of the DTs.



GB fit for each j in training data is $F_0 + F_{1j} + F_{2j} + F_{3j} + \ldots + F_{nj}$ for n trees

Figure 6.2

For the test sample or prediction of any test sample point given its features, a regression DT(1) is illustrated.

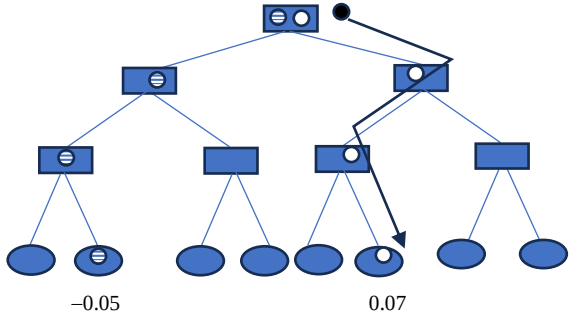
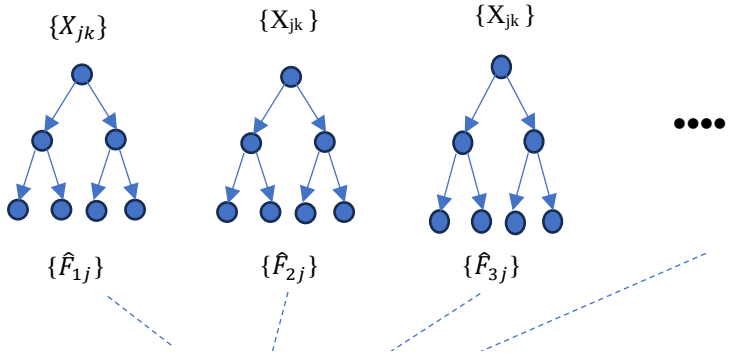


Figure 6.3

The training was done by training data points starting from the root node. The test point (black circle)'s features X_{jk} were used in the DT(1) rules to lead to 0.07.

The trained GB trees DT(1) to DT(n) are used to predict each test sample point j via $\hat{F}_{1j}$ =0.07 from DT(1), $\hat{F}_{2j}$ from DT(2), and so on, without employing the test point's label. Then the GB predictor for the test point j is $\hat{F}_{0j} + \hat{F}_{1j} + \hat{F}_{2j} + \hat{F}_{3j} + \ldots + \hat{F}_{nj}$. Start term $\hat{F}_{0j}$ could be the same as F_{0j} as it does not involve information from the test point label.



GB prediction for each j in test data is $\hat{F}_{0j} + \hat{F}_{1j} + \hat{F}_{2j} + \hat{F}_{3j} + \ldots + \hat{F}_{nj}$ for n trees

Figure 6.4

The loss function is typically synonymous with the splitting criterion in the case of a single DT or RF. However, in a GB algorithm, the loss function, and the splitting criterion for building decision rules in each of the DTs may be different. In the sklearn GradientBoostingRegressor, the loss function could be squared error L as seen earlier. The splitting criterion can be "mean squared error" as seen in minimizing weighted mean squared error in RF, but it can also be Friedman mean squared error which is finding the split (optimal feature and its threshold) yielding maximum information gain

$$\frac{w_L w_R}{w_L + w_R}(\bar{Y}^L - \bar{Y}^R)^2$$

where $\bar{Y}^L$ is mean of L training sample points' labels $e_{(m-1)j}$ (for some j) on left node on the mth tree at any level, $\bar{Y}^R$ is mean of R training sample points'

labels $e_{(m-1)j*}$ (for some other j*) on right node on the m[th] tree at the same level, w_L is weight given by $\sum_{j=1}^{L} \hat{p}_j(1-\hat{p}_j)$, w_R is weight given by $\sum_{j*=1}^{R} \hat{p}_{j*}(1-\hat{p}_{j*})$, and $\hat{p}_j$, $\hat{p}_{j*}$ are probability estimates of label y=1 from a pre-trained training set logistic regression of labels of 1 or 0 on the features (or a simpler implementation such as empirical probabilities). The information gain is larger for the same $(\bar{Y}^L - \bar{Y}^R)^2$ when the uncertainties contained in w_L and w_R are larger, i.e., $\frac{w_L w_R}{w_L + w_R}$ is larger.

We next provide explanation of the GB method for binary classification. Here instead of fitting sequential errors of continuous variable predictions, we fit sequential residuals that are differences between the observed classification value (1 or 0) and the predicted probability of the case in class 1.

As more training proceeds with sequential or boosting DTs, the probability estimates get more accurate, the residuals (or pseudo residuals – since the probability estimates are model driven and not explicitly observed attributes) reduce toward zero, and eventually the probability estimate for each case j is used to decide if a target belongs to one category or the other. If the case or target has probability > ½, then prediction is that it is in class 1. If the case or target has probability ≤ ½, then prediction is that it is in class 0.

We provide a numerical example of a typical GB Classification algorithm as follows. The targets are credit ratings of firms, belonging to either investment grade (BBB and above) or else speculative grade (BB and below). Suppose there are 10 firms, N = 10. Each firm has features that are accounting variables of the firm. Let the 4 available features be X_{1j}, X_{2j}, X_{3j}, and X_{4j}, where j = 1,2,…,10. Let firm j have target rating of Y_j =1 for investment grade, or else Y_j = 0 for speculative grade. The target values of the firms are shown below.

j	1	2	3	4	5	6	7	8	9	10
Y_j	0	1	0	0	0	1	1	1	0	0

The empirical unconditional probability of Y_j = 1 for each j is 0.4 since 4 out of 10 in the sample have values as 1. A gradient boosting method initially constructs a weak initial predictor of the probability of Y_j = 1 for each Y_j, as 0.4. Note that at the end of the GB algorithm, the final prediction of Y_j is 1 if the final predicted probability is greater than ½, and the final prediction of Y_j is 0 if the final predicted probability is less than or equal to ½.

Call the initial predicted probability p_0, of Y_j =1, to be 0.4. The initial pseudo residuals in the probability fitting of the training data is actual $Y_j - p_0$, either 1 – 0.4 = 0.6 or 0 – 0.4 = – 0.4. The first DT(1) is used to fit/predict $Y_j - p_0$. The DT(1) is shown as follows. Three features were randomly selected to form the decision rules. (The feature values are just examples.) The splitting criterion is Friedman mean squared error.

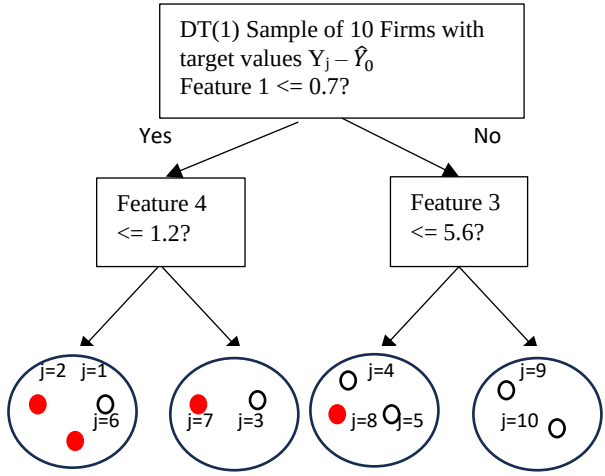


Figure 6.5

In the terminal nodes, the coloured circles represent firms with pseudo residual 0.6 (Y_j =1) while the uncoloured circles represent firms with pseudo residual – 0.4 (Y_j = 0). The splits are performed based on the Friedman MSE criterion or else weighted mean squared errors criterion on the pseudo residuals. Thus, at the terminal nodes based on the randomly selected features, we obtain some separation of those firms with 0.6 versus those with –0.4. The initial log odds corresponding to $p_0 = \sum_{j=1}^{10} Y_j/10$ is $x_0 = \log[\frac{p_0}{(1-p_0)}]$. Note that the training set allows identification of j (labels) amongst the circles.

To continue with the next boosting tree DT(2), however, the pseudo residuals have to be updated. This requires specification of a loss function L. A typical loss function for classification problems is the log loss function. Note that the loss criterion L is different from the splitting criterion in the GB trees.

$$L = -\sum_{j=1}^{N}\left(Y_j \log p + \left(1 - Y_j\right)\log(1-p)\right) > 0 \qquad (6.1)$$

where p ∈ [0,1] is probability of $Y_j = 1$. There is no loss of generality with any constant multiple on L as these loss functions will have the same solution of p for minimum when L is convex ($\partial^2 L/\partial p^2 > 0$). Log-loss measures "distance" of the predicted probability p to the target values Y_j in the binary classification. Eq. (6.1) can also be expressed as monotonic transform

$$\exp(L) = 1/\left(p^{\sum_{j=1}^{N} Y_j}(1-p)^{\sum_{j=1}^{N}(1-Y_j)}\right) > 1 \qquad (6.2)$$

In Eq. (6.2), higher likelihood function of $p^{\sum_{j=1}^{N} Y_j}(1-p)^{\sum_{j=1}^{N}(1-Y_j)}$ implies that L (loss) is smaller. Lower likelihood function of $p^{\sum_{j=1}^{N} Y_j}(1-p)^{\sum_{j=1}^{N}(1-Y_j)}$ implies that L (loss) is higher. Higher likelihood function and hence smaller loss L implies more accurate prediction of p. Inaccurate predictions are penalized with higher loss values.

We want to find a way to minimize the loss function such that the boosting trees could increment the predicted probability. This can be done using log odds in the argument.

If we let x = log (odds), i.e., log p/(1-p), then $p = e^x/(1+e^x)$. Then the log loss function can be written as $L = -\sum_{j=1}^{N}\left(Y_j x - \log(1+e^x)\right)$ in terms of x.

At any node when number of sample points on the node is n ≤ N, i.e., it calculates the loss on that node:

$$L(x) = -\sum_{j=1}^{n}\left(Y_j x - \log(1+e^x)\right) = -\sum_{j=1}^{n} Y_j x + n\log(1+e^x).$$

Using Taylor series expansion around x_0, an initial estimate of the log odds, we have

$$L(x) = L(x_0) + (x-x_0)\left[-\sum_{j=1}^{n} Y_j + \frac{ne^{x_0}}{(1+e^{x_0})}\right] + \frac{1}{2}(x-x_0)^2\left[\frac{ne^{x_0}}{(1+e^{x_0})^2}\right]$$

Higher terms involving higher derivatives of $\frac{ne^x}{(1+e^x)^2}$ and so on are small and are ignored. This approximation of the log loss function in x allows taking the derivative

$$\left.\frac{dL}{dx}\right|_{x_0} = 0 + \left[-\sum_{j=1}^{n} Y_j + \frac{ne^{x_0}}{(1+e^{x_0})}\right] + (x-x_0)\left[\frac{ne^{x_0}}{(1+e^{x_0})^2}\right] = 0$$

that is set to zero on the right to obtain the optimal x. The second order condition satisfies the case for minimum L. Then,

$$(x - x_0) = \frac{\sum_{j=1}^{n} Y_j - \frac{ne^{x_0}}{(1+e^{x_0})}}{\frac{ne^{x_0}}{(1+e^{x_0})^2}}$$

or,

$$x = x_0 + \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)}$$

where $Y_j - p_0$ is the initial pseudo residual. Note that $p_0 = \frac{e^{x_0}}{(1+e^{x_0})}$. The new value of $x = x_1$ is meant to reduce the loss function optimally in DT(1). The new updated x_1 increases from x_0 if at the particular terminal node of DT(1), there are more Y_j's =1 than that at the start. It decreases from x_0 if there are less Y_j's =1 than that at the start. Obviously, for any j, a x_{1j} different from x_0 (higher for some j, lower for others) indicates the DT(1) is working well toward separating the types.

The updating involves terms in the gradient dL/dx. However, the algorithm typically puts in a learning rate, e.g., $\alpha = 0.1$, so

$$x_{1j} = x_0 + \alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)}$$

A subscript j is added to x_1 to indicate that now each new log odd may be different for different case or sample point as each may reside in different lower nodes, i.e., in DT(1), $x_{1j} \neq x_{1j^*}$ for different instances j and j*. Recall each final splitting produces two terminal nodes with differential pseudo residual values in the two nodes. The $\sum_{j=1}^{n} Y_j$ will be different for each node depending on n points in that node and the sum of Y_j's with target value 1. From this new set of x_{1j}'s for every j in training set, the updated probability estimate is

$$p_{1j} = \frac{e^{x_{1j}}}{1+e^{x_{1j}}}$$

and the updated pseudo residuals are $Y_j - p_{1j}$ for every j. These are then used as labels to train DT(2).

Note that by this stage, the different sample points Y_j may have different corresponding pseudo residuals. Refer to the example in Figure 6.5. The new labels to the same training sample points are shown as follows. Note that $x_0 = \log_e(0.4/0.6) = -0.40547$.

On the left-most leaf in DT(1),

$$\alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)} = 0.1 \times \frac{0.6 + 0.6 - 0.4}{3(0.4)(0.6)} = 0.111111.$$

On the second leaf from the left,

$$\alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)} = 0.1 \times \frac{0.6 - 0.4}{2(0.4)(0.6)} = 0.041667.$$

On the third leaf from the left,

$$\alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)} = 0.1 \times \frac{0.6 - 0.4 - 0.4}{3(0.4)(0.6)} = -0.027778.$$

On the right-most leaf,

$$\alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)} = 0.1 \times \frac{-0.4 - 0.4}{2(0.4)(0.6)} = -0.166667.$$

Hence on the left-most leaf in DT(1), $x_{1j} = x_0 + \alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)}$ = −0.40547 + 0.11111 = − 0.29435. This means every node j = 1,2,6 in that leaf has the same x_{1j} value of − 0.29435. On the second leaf from the left, $x_{1j} = x_0 + \alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)}$ = −0.40547 + 0.041667 = − 0.36380. This means every node j = 3,7 in that leaf has the same x_{1j} value of − 0.36380. On the third leaf from the left, $x_{1j} =$ −0.40547 − 0.02778 = − 0.43324. This means every node j = 4,5,8 in that leaf has the same x_{1j} value of – 0.43324. On the right-most leaf, $x_{1j} =$ −0.40547 − 0.16667 = − 0.57213. This means every node j = 9,10 in that leaf has the same x_{1j} value of − 0.57213.

The corresponding p_{1j}' s as in $p_{1j} = \frac{e^{x_{1j}}}{1+e^{x_{1j}}}$ can then be computed. Then the updated pseudo residuals $Y_j - p_{1j}$'s can then be computed for all j. These are shown in the following Table.

Table 6.1

j	Y_j	$\alpha \frac{\sum_{j=1}^{n}(Y_j - p_0)}{np_0(1-p_0)}$	x_{1j}	$p_{1j} = \frac{e^{x_{1j}}}{1+e^{x_{1j}}}$	Updated pseudo residual $Y_j - p_{1j}$	$\Delta p_{1j} = p_{1j} - p_0$
1	0	0.111111	-0.29435	0.426938	-0.42694	0.026938
2	1	0.111111	-0.29435	0.426938	0.573062	0.026938
3	0	0.041667	-0.36380	0.41004	-0.41004	0.01004
4	0	-0.027778	-0.43324	0.393352	-0.39335	-0.00665
5	0	-0.027778	-0.43324	0.393352	-0.39335	-0.00665
6	1	0.111111	-0.29435	0.426938	0.573062	0.026938
7	1	0.041667	-0.36380	0.41004	0.58996	0.01004
8	1	-0.027778	-0.43324	0.393352	0.606648	-0.00665
9	0	-0.166667	-0.57213	0.360745	-0.36075	-0.03925
10	0	-0.166667	-0.57213	0.360745	-0.36075	-0.03925

Next the second boosting tree, DT(2), is built to fit/predict the new pseudo residuals or targets $Y_j - p_{1j}$. Nodes or leaves (not just end leaves) have updated log-odds as follows.

$$x_{2j} = x_{1j} + \alpha \frac{\sum_{j=1}^{n}(Y_j - p_{1j})}{\sum_{j=1}^{n} p_{1j}(1-p_{1j})}$$

for j's within each node. Basically, at each m^{th} boosting tree, x_{mj} is updated. This leads to new fitted p_{mj}, new updated pseudo residual $Y_j - p_{mj}$, next tree fitting and so on.

The algorithm then continues in the same way until there is no significant improvement in the log odds, i.e., x_{nj}. At the end of n trees, i.e., at end of DT(n), the probability estimates p_{nj} for each j are fitted and the GB trees DT(1) up to DT(n) can now be used to predict p_{nk} for each test sample point k.

An alternative way to think about it is as follows. At the end of n trees, i.e., at end of DT(n), the probability estimates p_{nj} for each j are computed as $p_{nj} = \Delta p_{nj} + \Delta p_{n-1,j} + \ldots\ldots + \Delta p_{3j} + \Delta p_{2j} + \Delta p_{1j} + p_0$. If $p_{nj} > ½$, then that j^{th} case is predicted as $Y_j = 1$. Otherwise, it will be predicted as $Y_j = 0$. The number of boosting trees n can be large, e.g., 100, especially if the learning rate α is kept low and if the depths of the trees are kept small. It is common for an effective GB algorithm in a well-defined data set to enable a close to, if not, 100% training fit or accuracy in training.

Visually, GB classification trees for fitting training data can be seen as follows. The quantities on the top line denote the updated pseudo residuals. The quantities on the bottom line denotes the adjustments in predicted probabilities from the previous DT.

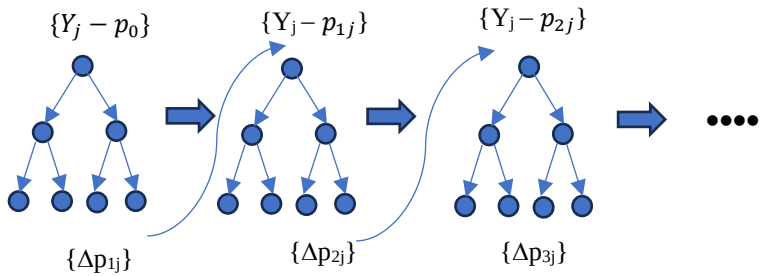


Figure 6.6

Note that the features are typically randomly selected for different boosting trees. GB probability predictor for each j is $p_0 + \Delta p_{1j} + \Delta p_{2j} + \Delta p_{3j} + \ldots\ldots + \Delta p_{nj}$.

For the test sample or prediction of any sample point j given its features, the trained GB classification trees DT(1) to DT(n) are used to predict Δp_{1j} from DT(1), Δp_{2j} from DT(2), and so on. Then the GB probability predictor for each j is $p_0 + \Delta p_{1j} + \Delta p_{2j} + \ldots + \Delta p_{nj}$. If $p_{nj} > ½$, then that j^{th} case is predicted as $Y_j = 1$. Otherwise, it will be predicted as $Y_j = 0$.

There are several points worth noting. Firstly, a different loss function such as the mean squared error may not work as well here as $L(x) = \frac{1}{N}\sum_{j=1}^{N}(Y_j - p)^2 = \frac{1}{N}\sum_{i=j}^{N}\left(Y_j - \frac{e^x}{1+e^x}\right)^2$ is non-convex given Y_j's for some x. Non-convexity does not allow a global minimum to be found and local minimum may not lead to effective predictors. If we try to find the minimum in $\frac{1}{N}\sum_{j=1}^{N}(Y_j - p)^2$ by directly taking p as the control variable, then its

solution is just $\hat{p} = \frac{1}{N}\sum_{j=1}^{N} Y_j$ which is just the proportion of Y_j taking the value 1. $\hat{p}$ is also the initial predictor p_0 in the above example. It is the same for all sample points j, so it is not a strong or effective predictor.

Secondly, if in the terminal node of each tree we had used updated estimate of p directly as the empirical probability on that node, e.g., $p_1 = 2/3$ (based on j=1,2,6 on the left-most leaf) without going through the gradient involving log odds, then the DT becomes an ordinary DT without boosting as the levels on the DT can continue to grow without the need to update the targets.

Thirdly, unlike RF where bagging uses bootstrapping – random sampling with replacements, GB may use random sampling of a smaller set of training sample points without replacements (i.e., no repeated sample points) for the boosting trees. The smaller set enables faster computations. This alternative is sometimes called stochastic gradient boosting.

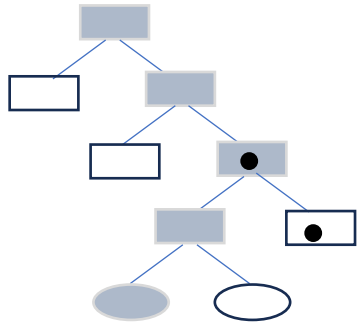
Fourthly, many different varieties of GB based on different loss functions, different split criteria, and different ways of combining the boosting trees, can be built. There are some general comparisons but specifically how one ensemble tree algorithm will perform relative to another depends also on the data.

Fifthly, GB trees may require more tuning of the hyperparameter(s) – setting learning rate, pruning some nodes, setting maximum number of levels per tree, etc.

6.2 Popular Alternatives

An example of a popular alternative to the Gradient Boosting algorithm is the LightGBM (light gradient-boosting machine). LightGBM (from a different original builder and is not part of sklearn) generally has faster speed and places less burden on computer memory. In LightGBM (which can apply to both RF and boosting method), each tree grows not level-wise as in traditional trees, but leaf-wise. Instead of extending the levels down with two nodes at the next level, then 4 nodes, etc., the nodes are only extended down from the previous node with the largest information gain or minimum loss. In principle, if we can grow the trees as long as possible, the lightGBM should produce closely similar prediction result with the regular GB method. However, with regularizations such as limiting the branching and limiting maximum depth of

trees, the lightGBM can perform marginally better. The following diagram shows how one lightGBM tree is constructed in the training data.



Shaded decision nodes and final leaf indicate the path with maximum Gini impurity decrease or maximum decrease in mean square error, depending on whether it is a classification or an estimation tree. The tree does not grow in the non-shaded nodes. Different versions of lightGBM may use different methods of splitting. When a sample point (black) is "stuck" in an upper node – that node's score/values become its predicted value. Score refers to regression estimate using mean of sample labels in node, and other information. Values refer to numbers of the types and can be used to compute the empirical probability in a RF for binary classification.

Figure 6.7

Another popular alternative is the XGBoost (Extreme Gradient Boosting). It is in basic terms similar in approach to the GB method, but it offers some extra bells and whistle. XGBoost incorporates various regularization techniques to prevent overfitting and improve the generalization capability of the models. These regularizations occur where optimization procedures are required in the gradient boosting. Regularization methods such as L1 and L2 regularization (i.e., Lasso and Ridge regularization) penalize complex models, helping to control model complexity and reduce overfitting.

XGBoost employs tree pruning algorithms to control the size of decision trees, reducing overfitting and improving computational efficiency. Tree pruning techniques such as depth-based pruning (to reduce too much depth) and weight-based (to reduce nodes with too little weights) pruning remove unnecessary branches from decision trees. In additional XGBoost employs parallel processing techniques to maximize the computational efficiency.

XGBoost also provides a built-in support for handling missing values in the dataset during training and prediction. It automatically estimates the best imputation strategy for missing values, and fills in the necessary missing data.

When comparing the performances of GBM and XGBoost, the former may be computationally slower as it lacks early stopping such as tree pruning. XGBoost also appears to have a more user-friendly interface and better

customizations although as in most software development, competitors can adapt and catch up fast.

6.3 Worked Example GB – Data

We continue with the credit rating accounting data set corporate_rating2.csv used in chapter 5 for the DT and RF algorithms. The program file is Chapter6-1.ipynb. Recall there are 2029 firms/instances with either ratings BBB up to AAA (Class "1") or ratings BB and below (Class "0").

After standardizing the features using sklearn StandardScalar, the data set "corporate_rating2.csv" is split into 75% training set (X_train, y_train) with 1521 rows and 25% test set (X_test, y_test) with 508 rows in code lines [13]-[14]. The data consist of 25 features.

```
[13]: TT=pd.concat([df_ratios['Class'],df_ratios_new],axis=1)
      TT.shape
      TT.tail()
```

[13]:

	Class	currentRatio	quickRatio	cashRatio	daysOfSalesOutstanding	netProfitMargin	...
2024	1	0.186827	0.135444	1.783407	-0.074822	-0.036575	...
2025	0	-0.012870	-0.041268	-0.066739	-0.068183	-0.073966	...
2026	0	-0.060074	-0.054997	-0.120995	-0.041872	-0.047159	...
2027	0	-0.059442	-0.057857	-0.099558	-0.045460	-0.031518	...
2028	0	-0.055507	-0.049416	-0.129463	-0.040959	-0.084191	...

5 rows × 26 columns

```
[14]: Train, Test = train_test_split(TT,
                                    test_size=0.25,
                                    random_state=0)

      X_train, y_train = Train.iloc[:,1:26], Train.iloc[:,0] ### choose the 25 features
      X_test, y_test = Test.iloc[:,1:26], Test.iloc[:,0]
```

```
[15]: X_train.shape, y_train.shape, X_test.shape, y_test.shape
```

```
[15]: ((1521, 25), (1521,), (508, 25), (508,))
```

Sklearn GradientBoostingClassifier is used with specification of 1000 DTs (n_estimators = 1000). We can set random selection of features, e.g., max_features = 'sqrt' which means that each DT randomly uses $\sqrt{25} = 5$

features of the 25 total in constructing the branching in each of the 1000 DTs. However, because of the learning to solve for the net error in subsequent DTs, there is a learning rate just as in Gradient Descent. Here we fine-tune the learning rate to attain a higher accuracy or lower loss function. See code line [17].

Gradient Boosting

[17]:
```
from sklearn.ensemble import GradientBoostingClassifier
###   Example:
###   class sklearn.ensemble.GradientBoostingClassifier(*, loss='log_loss',
###   learning_rate=0.1, n_estimators=100,subsample=1.0, criterion='friedman_mse',
###   min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0,
###   max_depth=3, min_impurity_decrease=0.0, init=None, random_state=None,
###   max_features=None, verbose=0, max_leaf_nodes=None, warm_start=False,
###   validation_fraction=0.1, n_iter_no_change=None, tol=0.0001, ccp_alpha=0.0)

GB_model = GradientBoostingClassifier(n_estimators=1000, random_state=1, \
           max_features="sqrt", learning_rate=0.01, max_depth=24)
GB_model.fit(X_train, y_train)

y_pred_GB = GB_model.predict(X_test)
Accuracy_GB = metrics.accuracy_score(y_test, y_pred_GB)
print("GB Accuracy:",Accuracy_GB)
```

```
GB Accuracy: 0.8051181102362205
```

The confusion matrix and the classification report for the test are shown in code lines [18] and [19].

[18]:
```
from sklearn.metrics import confusion_matrix
confusion_matrix = confusion_matrix(y_test, y_pred_GB)
print(confusion_matrix)
```

```
[[151  64]
 [ 35 258]]
```

[19]:
```
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred_GB))
```

```
              precision    recall  f1-score   support

           0       0.81      0.70      0.75       215
           1       0.80      0.88      0.84       293

    accuracy                           0.81       508
   macro avg       0.81      0.79      0.80       508
weighted avg       0.81      0.81      0.80       508
```

In this investment grade/speculative grade prediction problem, the accuracy of the GB here is 80.51%. The prediction performance is marginally better than RF with accuracy of 79.53% seen in Chapter 5.

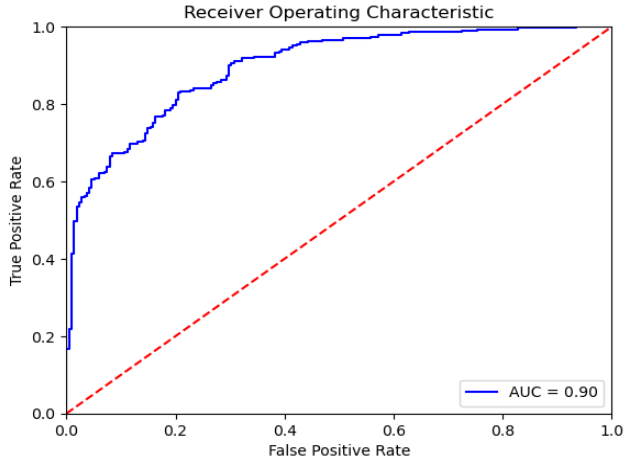
The ROC curve is shown below after computing the various True positive rates and False positive rates based on different threshold probabilities.
Code lines [20] and [21] show the computation of the AUC of the ROC as 89.57%. This is marginally better than the 88.69% in RF.

```
[20]: import sklearn.metrics as metrics
      # calculate the fpr and tpr for all thresholds of the classification
      preds_GB = GB_model.predict_proba(X_test)[:,1]

      fpr, tpr, thresholds = metrics.roc_curve(y_test, preds_GB)
      ### matches y_test of 1's and 0's versus pred prob of 1's for each
      ###  of the 508 test cases
      ### sklearn.metrics.roc_curve(y_true, y_score,...) requires y_true as 0,1
      ###  input and y_score as prob inputs
      ### This metrics.roc_curve returns fpr, tpr, thresholds (Decreasing thresholds
      ###  used to compute fpr and tpr)
      roc_auc_GB = metrics.auc(fpr, tpr)
      ### sklearn.metrics.auc(fpr,tpr) returns AUC using trapezoidal rule
      roc_auc_GB

[20]: 0.89569013413763

[21]: import matplotlib.pyplot as plt
      plt.title('Receiver Operating Characteristic')
      plt.plot(fpr, tpr, 'b', label = 'AUC = %0.2f' % roc_auc_GB)
      plt.legend(loc = 'lower right')
      plt.plot([0, 1], [0, 1],'r--')
      plt.xlim([0, 1])
      plt.ylim([0, 1])
      plt.ylabel('True Positive Rate')
      plt.xlabel('False Positive Rate')
      plt.show()
```



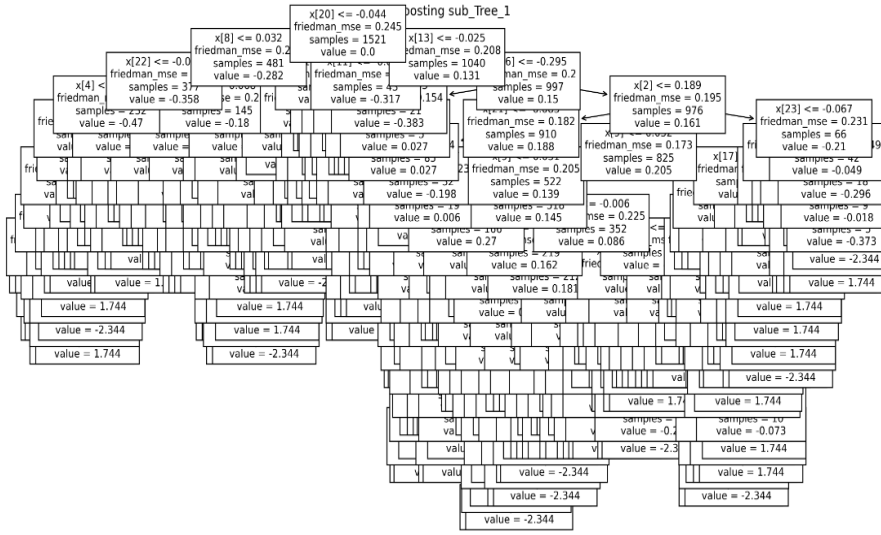
Any one of the 1000 GB trees can be plotted. The first DT(1) is shown as follows.

Visualizing a boosting tree

```
[23]: ### Classifier
GB_model.fit(X_train, y_train)
### Get the tree number 1
sub_tree_1 = GB_model.estimators_[0,0]
### Visualization

from sklearn.tree import plot_tree
fig, axes = plt.subplots(nrows = 1,ncols = 1,figsize = (15,8), dpi=300)

### plot tree
plot_tree(sub_tree_1, fontsize=10)  # set plot size (denoted in inches)
plt.title("Boosting sub_Tree_1")
plt.show()
```



A text representation can be obtained via:

"from sklearn import tree
text_representation = tree.export_text(GB_model.estimators_[n,0])
print(text_representation)"

where "n" indicates the n+1 tree or DT(n+1). The first splitting into binary nodes from the root node uses the 20th feature ("companyEquityMultiplier") <= –0.044 with a minimum Friedman MSE criterion shown in the root node. Higher Equity multiplier means that more of the firm's assets are financed by shareholder equity rather than debt. The right node leads to higher credit rating probability or higher probability of Class "1" in this context. The values

(different apps will use slightly different representations) indicate sum of the pseudo residuals. As the branching produces clearer separation of the classes, the left node and the right node will indicate opposite signed numbers since the side with instances closer to Class "1" will show more positive residuals, being sum of pseudo residuals or (1 – estimated probability) over all instances in that node. The other side with instances further away from Class "1" will show more negative residuals, being sum of pseudo residuals or (0 – estimated probability) over all instances in that node.

In the case of the LightGBM (see code lines [26] – [33]), the prediction accuracy is 83.27%, higher than GB.

Light GBM

[26]:
```
pip install --upgrade pip
```

```
Requirement already satisfied: pip in c:\users\vista\anaconda3\lib\site-packages (24.3.1)
Note: you may need to restart the kernel to use updated packages.
```

[27]:
```
!pip3 install lightgbm
```

```
Requirement already satisfied: lightgbm in c:\users\vista\anaconda3\lib\site-packages (4.5.0)
Requirement already satisfied: numpy>=1.17.0 in c:\users\vista\anaconda3\lib\site-packages (from lightgbm) (1.26.4)
Requirement already satisfied: scipy in c:\users\vista\anaconda3\lib\site-packages (from lightgbm) (1.11.4)
```

[28]:
```
import lightgbm as lgb
from lightgbm.sklearn import LGBMClassifier
```

[29]:
```
# Creating an object for model and fitting it on training data set
LGBMmodel = LGBMClassifier(learning_rate=0.1)
LGBMmodel.fit(X_train, y_train)

# Predicting the Target variable
predLGBM = LGBMmodel.predict(X_test)
print(predLGBM)
accuracy = LGBMmodel.score(X_test, y_test)
print(accuracy)
```

```
0.8326771653543307
```

[30]:
```
from sklearn.metrics import confusion_matrix
confusion_matrix = confusion_matrix(y_test, predLGBM)
print(confusion_matrix)
```

```
[[160  55]
 [ 30 263]]
```

[31]:
```
from sklearn.metrics import classification_report
print(classification_report(y_test, predLGBM))
```

```
              precision    recall  f1-score   support

           0       0.84      0.74      0.79       215
           1       0.83      0.90      0.86       293

    accuracy                           0.83       508
   macro avg       0.83      0.82      0.83       508
weighted avg       0.83      0.83      0.83       508
```

The Light GBM precision and recall on the test data set are also slightly higher than those in GB, showing the advantages of regularization in complex trees.

In the case of the XGBoost (see code lines [35] – [40]), the prediction accuracy is 80.91%, marginally higher than GB.

XGBoost

[35]:
```
pip install xgboost
```

```
Requirement already satisfied: xgboost in c:\users\vista\anaconda3\lib\site-packages (2.1.0)
Requirement already satisfied: numpy in c:\users\vista\anaconda3\lib\site-packages (from xgboost) (1.26.4)
Requirement already satisfied: scipy in c:\users\vista\anaconda3\lib\site-packages (from xgboost) (1.11.4)
Note: you may need to restart the kernel to use updated packages.
```

[36]:
```
# XGBoost
from xgboost import XGBClassifier
XG_model = XGBClassifier(n_estimators=1000, random_state=1, \
           max_features="sqrt", learning_rate=0.02, max_depth=24, \
           objective='binary:logistic')

### Note for multiclass, objective='multi:softprob'
XG_model.fit(X_train,y_train)

### XG_model follows GB model to have n_estimators = 1000 and max_depth = 24
y_pred_XG = XG_model.predict(X_test)
Accuracy_XG = metrics.accuracy_score(y_test, y_pred_XG)
print("XG Accuracy:",Accuracy_XG)
```

```
XG Accuracy: 0.8090551181102362
```

[37]:
```
from sklearn.metrics import confusion_matrix
confusion_matrix = confusion_matrix(y_test, y_pred_XG)
print(confusion_matrix)
```

```
[[152  63]
 [ 34 259]]
```

[38]:
```
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred_XG))
```

```
              precision    recall  f1-score   support

           0       0.82      0.71      0.76       215
           1       0.80      0.88      0.84       293

    accuracy                           0.81       508
   macro avg       0.81      0.80      0.80       508
weighted avg       0.81      0.81      0.81       508
```

The XGBoost precision and recall on the test data set are only marginally higher than those in GB.

For comparison, we use the sklearn LogisticRegression for prediction. The results are shown below. It is seen that the various GB Trees perform significantly better than the logit regression – indicating the efficacy of non-parametric methods when there is a large number of features in a complex manner of data patterns.

Logistic Regression

[42]:
```
# Logistic Regression
from sklearn.linear_model import LogisticRegression
LR = LogisticRegression(random_state=1,
                        multi_class='multinomial',
                        solver='newton-cg')
LR = LR.fit(X_train, y_train)
y_pred_LR = LR.predict(X_test)
Accuracy_LR = metrics.accuracy_score(y_test, y_pred_LR)
print("LR Accuracy:",Accuracy_LR)
```

```
LR Accuracy: 0.6476377952755905
```

[43]:
```
from sklearn.metrics import confusion_matrix
confusion_matrix = confusion_matrix(y_test, y_pred_LR)
print(confusion_matrix)
```

```
[[ 70 145]
 [ 34 259]]
```

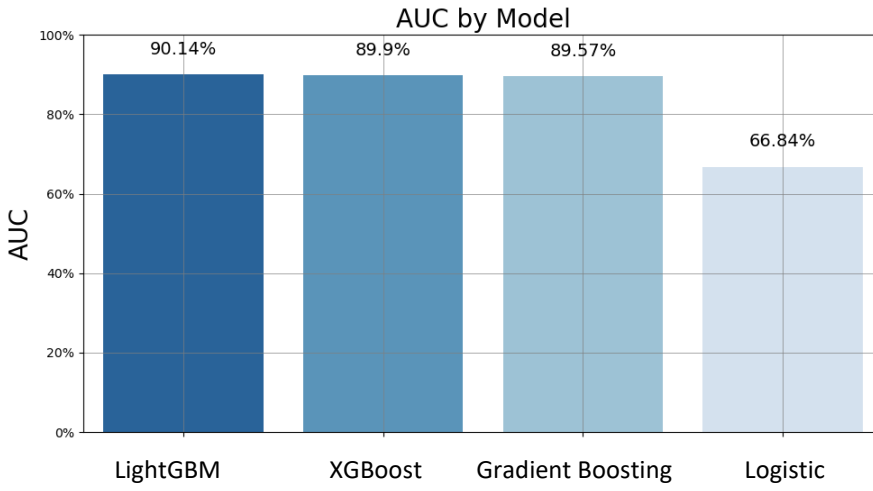
[44]:
```
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred_LR))
```

```
              precision    recall  f1-score   support

           0       0.67      0.33      0.44       215
           1       0.64      0.88      0.74       293

    accuracy                           0.65       508
   macro avg       0.66      0.60      0.59       508
weighted avg       0.65      0.65      0.61       508
```

The comparison of AUC performances of these various methods are shown as follows.



6.4 Shapley and SHAP Values

We have seen how feature importance is a way of measuring how significantly a feature contributes to the prediction accuracy of a DT and RF. The percentage contribution of a feature to the overall Gini importance or overall Gini weighted impurity decrease signifies its importance in a DT and a RF algorithm. In a similar way, the percentage contribution of a feature to the overall weighted MSE or Friedman MSE decrease signifies its importance in a GB Tree and its close relatives.

In XGBoost, Feature Importance is shown in code lines [51] – [52].

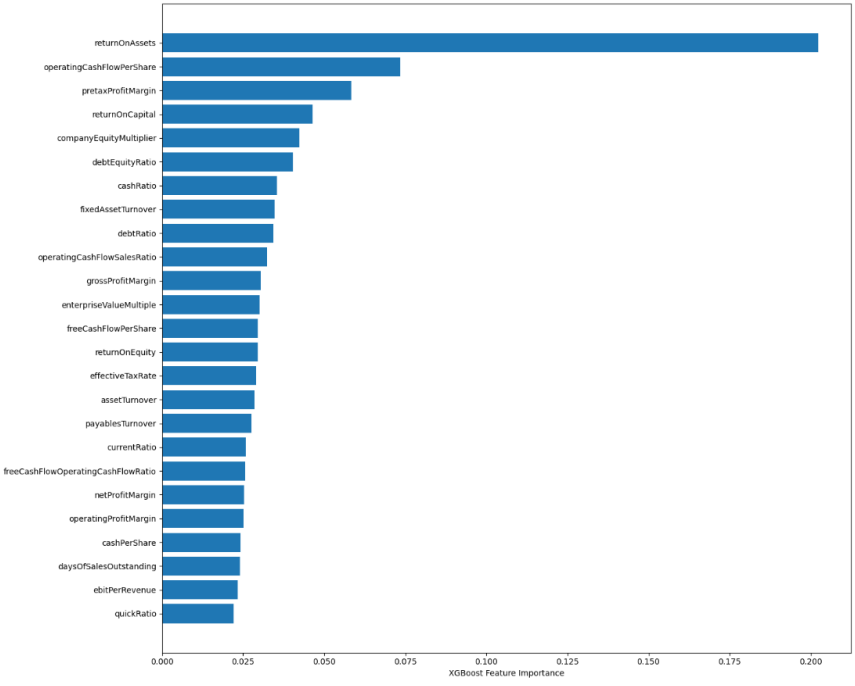
```
[51]: print(XG_model.feature_importances_)
```

```
[0.02575384 0.02205251 0.03534279 0.02407188 0.02522108 0.05827876
 0.03048301 0.02512895 0.20236763 0.04647086 0.02949365 0.02840674
 0.03474097 0.04035477 0.03425717 0.02903091 0.0256409  0.02956792
 0.02413125 0.04235359 0.02329668 0.03009087 0.07348198 0.03233119
 0.0276501 ]
```

```
[52]: ### representation

      fig, ax = plt.subplots(figsize=(15,12))

      sorted_idx = XG_model.feature_importances_.argsort()
      plt.barh(X_train.columns[sorted_idx],XG_model.feature_importances_[sorted_idx])
      plt.xlabel("XGBoost Feature Importance")
      plt.figure(figsize=(20, 15), dpi=80)
      fig.tight_layout()
```



In the XGBoost Tree, the percentage contributions of the 4 main features of "return on assets", "operating cash flow per share", "pretax profit margin", and "return on capital" are 20.24%, 7.35%, 5.83%, and 4.64%. In the case of the RF in Chapter 5, the 4 main features of "operating cash flow per share", "return on assets", "return on capital", and "net profit margin" are 8.06%, 6.06%, 5.75%, and 5.59%. Three of the main features are common to both tree algorithms. However, they are not exactly similar.

Though useful, Feature Importance, however, does not measure explicitly the impact of a feature on the predicted outcome, be it a target value or probability of a classification. This is unlike a linear regression where after fitting, we can state that a feature value times its weight (fitted coefficient) contributes their product value as a percentage of the expected outcome of the target or dependent variable.

We want to consider how much each feature explicitly contributes to the predicted outcome of a ML algorithm. This idea is similar to how much each player in a coalition game contributes to the outcome of a game. This contribution is called the Shapley value. In ML, it is equivalent to the contribution of a feature to the predicted outcome.

We first talk about the coalition (cooperative) game of N players. To understand the meaning of cooperation, let's first think of a non-cooperative game that involves Nash equilibrium. A simple example is the well-known Prisoner's Dilemma problem.

Two robbery suspects, X and Y, were caught and the police believe they are the culprits. However, there is insufficient evidence unless one or both of them testify against the other. Each suspect is interrogated independently, and the outcomes for each of them is given as follows, depending on their responses in the interrogations. If both pleaded innocence, they still have to be in a lock-up for 3 months pending more investigations.

	A: Y does not testify against X	B: Y testifies against X
X does not testify against Y	Lock-up for 3 months	X jailed for 3 years, Y goes free
X testifies against Y	Y jailed for 3 years, X goes free	Both jailed for 2 Years

This is a non-cooperative game with a Nash equilibrium solution. X considers Y's possible responses (assuming Y makes a response and sticks to it) if X does not testify against Y. In this case, X either gets lock-up for 3 months (event A) or jailed for 3 years (event B). Then X considers Y's possible responses if X testifies against Y. In this case, X either goes free (event A) or jailed for 2 years (event B). In both A and B, X is always better off by choosing to testify against Y. By the same argument, Y will also choose to testify against X, so both were jailed for 2 years.

Now think of a cooperative game involving $N > 0$ players trying to work together in a game of making earnings (such as in a sales force) denominated in \$. Assume that outside of the game, any member would make zero earning. But the team will make earnings $\$V[N] > 0$ and any player j in the total coalition of N will receive an allocation $\$\phi_j(V[N]) \geq 0$ with at least one team player having positive allocation. So it makes sense for all N players to join the game together and there is no incentive for any to break away from the total coalition of N. We also assume $V([0]) = 0$ where [0] denotes the null set of no players.

Let each unique player be denoted as player {j} where j is one number of 1, 2, 3,….,N. The problem here is how to determine an efficient and fair allocation $\phi_j(V[N]) \geq 0$ for every player {j}. Clearly, it is not enough to know just V[N]. And distribution such as V[N]/N for each player may not be fair as some players could have contributed more toward earning \$V. In order to be able to find out who contributes more, more observations of between-player interactions are required. In Shapley cooperative game, it is assumed that we can observe the marginal (incremental) contribution by a player {j} when he/she is added to various smaller coalitions. Whether practically this is observable or not is a separate matter.

Smaller coalitions or groupings consist of 0, 1, 2, 3, ….., N-1 players respectively. For example, coalition [S] consists of S players, for $0 \leq S \leq N-1$. We include the null set or coalition [0]. There are ${}^{N-1}P_S = (N-1)!/(N-1-S)!$ number of permutations of selecting S players in an ordered sequence from a pool of N-1 players to form coalition [S].

In the Shapley game, the total coalition earnings \$V[N] is made in the following way. A coalition [1] (one player only – suppose player {7}) is formed and sales is V({7}). Argument {7} denotes the earning is obtained with

player {7}. {7}'s marginal or incremental contribution to earnings is V({7}) – V([0]) = V({7}).

Next suppose a new player {3} is added to form coalition [2] (two players), and the earning is now V({7} ∪ {3}) where ∪ denotes "union" or united effort of {7} and {3}. In this case {3}'s marginal contribution is V({7} ∪ {3}) – V({7}). Suppose {5} is next added to form coalition [3], then {5}'s marginal contribution is V({7} ∪ {3} ∪ {5}) – V({7} ∪ {3}). And so on.

Suppose the addition of new players to a larger coalition till total coalition [N] is in the order: {7}, {3}, {5}, ……., {N}, {4}, {6}. Eventually a total coalition earning consists of the marginal contributions of each added player as the coalitions increase to size N, i.e.,

V[N] = V([0]) + [V({7}) – V([0])] + [V({7} ∪ {3}) – V({7})] + [V({7} ∪ {3} ∪ {5}) – V({7} ∪ {3})] + ……..
+ [V({7} ∪ {3} ∪ {5} ∪ …. ∪ {N} ∪ {4}) – V({7} ∪ {3} ∪ {5} ∪ …. ∪ {N})] + [V({7} ∪ {3} ∪ {5} ∪ …. ∪ {N} ∪ {4} ∪ {6})– V({7} ∪ {3} ∪ {5} ∪ …. ∪ {N} ∪ {4})]

Thus V[N] of the total coalition is V({7} ∪ {3} ∪ {5} ∪ …. ∪ {N} ∪ {4} ∪ {6}).

In Shapley game (not other types of games), a coalition [S] consisting of the same set of players will have the same value despite having different ordered sequences of the players. For example, coalition [2] comprising ({7} ∪ {3}) has value V({7} ∪ {3}) = V({3} ∪ {7}). But coalitions [S] with different sets of players can have different values. For example, V({7} ∪ {3}) ≠ V({{8} ∪ {1}) though ({7} ∪ {3}) and ({{8} ∪ {1}) are both coalition [2].

In the sequence of coalition [1], coalition [2], coalition [3], …… , coalition [N], it is seen that {7}'s marginal contribution is [V({7}) – V([0])] = V({7}) which is observable by the Shapley game. {3}'s marginal contribution is [V({7} ∪ {3}) – V({7})] which is observable by the Shapley game. {5}'s marginal contribution is [V({7} ∪ {3} ∪ {5}) – V({7} ∪ {3})] which is observable by the Shapley game. It is important to note that we observe just one sequence {7}, {3}, {5}, ……, {N}, {4}, {6} of many possible sequences based on different ways of forming the coalition [S], for each S. For example, another sequence {2}, {4}, {N},……,{9}, {3} will produce different marginal contributions. {4}'s marginal contribution is now [V({2} ∪ {4}) – V({2})]. {3}'s marginal contribution is now [V[N] – V({2} ∪ {4} ∪ {N} ∪ …. ∪

{9})]. It is important to note that the sum of all marginal contributions in any sequence is always V[N].

In general, player j or {j} can enter the coalition [S] in N number of ways at S = 0, 1, 2,……, N-1. At each entry, its marginal contribution is V([S] ∪ {j}) – V([S]) for different S=0,1,2, …., N-1. For different S, V([S] ∪ {j}) – V([S]) will likely be different. Even for the same S, V([S] ∪ {j}) – V([S]) will likely be different for different player composition in the coalition [S].

The number of different marginal contributions of player {j} for coalition [S] is $^{N-1}C_S$ = (N-1)!/[(N-1-S)!S!] where $^{N-1}C_S$ is the number of different combinations of making up the coalition [S] from the remaining N-1 members of the team. We can denote the different values for same coalition [S] as S_k. Hence we denote value of coalition [S] (for S < N) as V[k,S] where k denotes a specific one of the $^{N-1}C_S$ combinations.

There are $^{N-1}P_S$ = (N-1)! / (N-1-S)! number of permutations of selecting S players in an ordered sequence from a pool of N-1 players to form coalition [S]. After {j} is added as the S+1th player, there are (N-1-S)! permutations of the players to finish up the sequencing to total coalition [N]. The different permutations or combinations that come after {j} is added do not affect the marginal contribution of {j}. The total number of permutations in N players is seen as N! = N × $^{N-1}P_S$ × (N-1-S)! = N × $^{N-1}C_S$ × S! × (N-1-S)! where multiplication by N indicates the number of the entry position {j} can take.

The Shapley Value of player j or {j} refers to his/her fair contribution ϕ_j(V[N]) to the game payout V([N]) as the average of his/her marginal contributions over all possible sequencings, N!.

$$\phi_j(V[N]) = \frac{1}{N!}\sum_{S=0}^{N-1} S! \times (N-1-S)! \{\sum_{k=1}^{C_S^{N-1}} [V([k,S] \cup \{j\}) - V([k,S])] \}$$

where $0 \le S \le N-1$. (6.1)

The Shapley value is a unique solution concept for allocation of V[N] that holds some nice properties.

(1) The allocation is efficient: $\sum_{j=1}^{N} \phi_j(V[N]) = V[N]$. There is no leakage or wastage in distributing V[N].

(2) Symmetry: If two players i, j, contribute the same in joining every identical coalition [S], i.e., V([k,S] ∪ {i}) = V([k,S] ∪ {j}) , then $\phi_i(V[N]) = \phi_j(V[N])$

(3) Nullity: If any player j contributes nothing, i.e., V([k,S] ∪ {j}) = V([k,S]), then $\phi_j(V[N]) = 0$

(4) Linearity or Additivity:

$\phi_j(a\,V_1[N] + bV_2[N]) = a\,\phi_j(V_1[N]) + \mathrm{b}\,\phi_j(V_2[N])$

provided any player's marginal contribution scales linearly with total coalition payouts.

Hence Shapley allocation is "fair".

We want to use the concept in the Shapley game to measure how each feature (player) of a set of N features X (N players) in an algorithm (game) F contributes to the predicted outcome F(X).

F(.) could be a nonlinear ML algorithm such as RF or NN. Feature space X is made of T number of sample points, $X_{T\,x\,N}$. Each tabular row in X has N feature observations and is associated with a target value. However, the Shapley value or Shap value has to do with computing contributions by features in a prediction and they do not require target or label in the computation F(.). Hence Shapley and Shap values can be computed on both the training as well as the test data sets.

Let one row be (x_1, x_2, x_3, …, x_N). The ML algorithm produces a prediction outcome or output F (x_1, x_2, x_3, …, x_N). We want to find out how much does a feature x_j explain output F (x_1, x_2, x_3, …, x_j, …, x_N).

Let (z_1, z_2, …., z_S) be a particular permutation choosing S ≤ N-1 elements of (x_1, x_2, x_3, …, x_{j-1}, x_{j+1}, …., x_N) from any row of sample size T. Let (z_{S+2}, z_{S+3}, …., z_N) be a particular permutation choosing N-S-1 elements of the remaining features in (x_1, x_2, x_3, …, x_{j-1}, x_{j+1}, …., x_N) from the same row of sample size T. Then F (z_1, z_2, …., z_S, $\mathbf{x_j}$, z_{S+2}, z_{S+3}, …., z_N) – F (z_1, z_2, …., z_S, $\mathbf{r_j}$, z_{S+2}, z_{S+3}, …., z_N) is equivalent to V({z_1}, {z_2}, …., {z_S}, {x_j}) – V({z_1}, {z_2}, …., {z_S}), where r_j is a randomly selected element from feature j in any of the T rows. The full set of N features is included in computing the marginal contribution of feature $\mathbf{x_j}$ as required in the ML algorithm. In practice, for higher accuracy, the random selection of r_j can be repeated and the average is taken for F (z_1, z_2, …., z_S, $\mathbf{x_j}$, z_{S+2}, z_{S+3}, …., z_N) − F (z_1, z_2, …., z_S, $\mathbf{r_j}$, z_{S+2}, z_{S+3}, …., z_N).

To compute Shapley value of feature x_j:

$$\phi_j(V[N]) \equiv \frac{1}{N!}\sum_{S=0}^{N-1} S! \times (N-1-S)! \times$$

$$\{\sum_{k=1}^{C_S^{N-1}}\left[\mathrm{F}(z_1, z_2, \ldots., z_S, x_j, z_{S+2}, \ldots., z_N) - \mathrm{F}(z_1, z_2, \ldots., z_S, r_j, z_{S+2}, \ldots., z_N)\right]\}$$

where $0 \le S \le N-1$. (6.2)

Eq. (6.2) follows Eq. (6.1) where the value addition by feature j is in

$\left[\mathrm{F}(z_1, z_2, \ldots., z_S, x_j, z_{S+2}, \ldots., z_N) - \mathrm{F}(z_1, z_2, \ldots., z_S, r_j, z_{S+2}, \ldots., z_N)\right]$.

The Shapley value of a feature value is the average change in the prediction when the feature value joins an existing coalition of features. However, the above exact method in (6.2) is computationally too tedious for every x_j as it involves too many C_S^{N-1} (for each $S \leq N-1$) number of combinatorial computations of F(.), especially when the number of features N is large. In practice some approximation methods are used.

One approximation method is to use Monte Carlo sampling. We want to find the approximate Shapley value/contribution of the j^{th} feature of $x = (x_1, x_2, x_3, \ldots, x_j, \ldots, x_N)$. This is finding feature x_j's Shapley value $\phi_j(V[N])$.

Let an iteration m involve the following.

(1) Randomly draw a row from feature matrix $X_{T\times N}$. Call this draw $Z = (z_1, z_2, z_3, \ldots, z_N)$.

(2) Perform a random permutation of the order of the features – call this permutation "*", but leaving out the j^{th} feature of x_j. For example, $*(z_1, z_2, z_3, \ldots, z_j, \ldots, z_N)$ becomes $(z_5, z_7, z_1, \ldots, z_j, \ldots, z_6)$. This simulates the different sequencings or permutations in Shapley value calculation while keeping x_j intact.

(3) Form two new instances based on a row of X (going from row 1 to T, or if more data are required, re-sampling some of these rows) and the randomly drawn Z. Permutate these instances based on "*" in step (2). Call these permutated sequences x_{j*}'s and z_{j*}'s.

(4) Adjust one of the two permutated instances by replacing the j+1, j+2, …, N elements of the permutated X sequence with $z_{j+1*}, \ldots., z_{N*}$.
Hence $x_{+j} = (x_{1*}, x_{2*}, x_{3*}, \ldots, x_{j-1*}, x_j, z_{j+1*}, \ldots., z_{N*})$.
Adjust the other permutated instance by replacing the j, j+1, j+2, …, N elements of the permutated X sequence with $z_{j*}, z_{j+1*}, \ldots., z_{N*}$. Here, z_{j*} replaces x_j. Hence $x_{-j} = (x_{1*}, x_{2*}, x_{3*}, \ldots, x_{j-1*}, z_{j*}, z_{j+1*}, \ldots., z_{N*})$.

(5) Compute $\phi_j^m = F(x_{+j}) - F(x_{-j})$. This is marginal contribution of x_j in one constructed iteration.

(6) Repeat iterations for m = 1, …, M for a large M.

Compute approximate Shapley value as average: $\phi_j(x) = \frac{1}{M}\sum_{m=1}^{M} \phi_j^m$. In the above Shapley value computations, we assume that the value is dependent on the order of the features in the first coalition [S]. The formula in (6.2) and the

approximation formula are, however, valid even if a particular ML algorithm does not differentiate amongst the order of entry in the feature input.

Shap Values (Shapley Additive exPlanations)

The concept in Shapley method is to measure how each feature (player) of a set of N features X (N players) in an algorithm (game) F contributes to the predicted outcome F(x) when features in x = (x_1, x_2, x_3, …, x_j, …, x_N) are used. In Eq. (6.2), suppose the features are arranged as (x_3, x_8, x_5, x_{11} ,…, x_N , x_4 , … , x_7 , x_9) which is some permutation of the original x.

This permutation of the N number of represented features will produce contribution of F(x_3, r_8 , r_5 , …, r_N , …, r_9) – F(r_3, r_8 , r_5 , …, r_N , …, r_9) by feature 3, contribution of F(x_3, x_8 , r_5 , …, r_N , …, r_9) – F(x_3, r_8 , r_5 , …, r_N , …, r_9) by feature 8, contribution of F(x_3, x_8 , x_5 , r_{11} , …, r_N , …, r_9) – F(x_3, x_8 , r_5 , r_{11} , …, r_N , …, r_9) by feature 5, ……. , contribution of F(x_3, x_8 , x_5 , …, x_N , r_4 , …, r_9) – F(x_3, x_8 , x_5 , …, r_N , r_4 , …, r_9) by feature N, …….., and contribution of F(x_3, x_8, x_5, x_{11} ,…, x_N , x_4 , … , x_7 , x_9) – F(x_3, x_8, x_5, x_{11} ,…, x_N , x_4 , … , x_7 , r_9) by feature 9 where r_j represents a random draw from feature j. Suppose we write the sum of all the above items in a k^{th} permutation as $Z_{(k)}$. Then $Z_{(k)}$ = F (x_3, x_8, x_5, x_{11} ,…, x_N , x_4 , … , x_7 , x_9) – F(r_3, r_8 , r_5 , r_{11} ,…, r_N , r_4 , … , r_7 , r_9). Now suppose F(x) value is independent of the order of the features in x. Then the average across all the N! permutations of x, i.e., $\frac{1}{N!}\sum_{k=1}^{N!} Z_{(k)}$ = F(x) – $\frac{1}{N!}\sum_{k=1}^{N!} F\left(r_{(k)}\right)$ where $r_{(k)}$ is a k^{th} random vector draw from feature vector of X.

With the independence of F(x) from the order of the features in x, $\frac{1}{N!}\sum_{k=1}^{N!} Z_{(k)}$ can also be expressed $\sum_{j=1}^{N} \phi_j(F[x])$ from Eq. (6.2). Then F(x) – $\frac{1}{N!}\sum_{k=1}^{N!} F\left(r_{(k)}\right) = \sum_{j=1}^{N} \phi_j(F[x])$. Let $\phi_0 = \frac{1}{N!}\sum_{k=1}^{N!} F\left(r_{(k)}\right)$. Thus,

$$F(x) = \phi_0 + \sum_{j=1}^{N} \phi_j(F[x]) \qquad (6.3)$$

for a particular x = (x_1, x_2, x_3, …, x_j, …, x_N) from a row of X. ϕ_0 can be considered as the expectation of the predictions by F(.) over random x. Eq. (6.3) provides the Shap values $\phi_j(F[x])$ of different j features for the ML algorithm prediction F[x]. The Shap values are additive and together help explain the predicted value of F(x). Shap values also obtain similar nice properties as in the Shapley game. This linearized construction still may not help directly in solving for the Shap values ϕ_j. Some ML algorithm such as

Trees, may however, provide for each instance that leads up to the final predicted probability the computation of contributions of features in arriving at that predicted probability.

In general, to solve for Shap values, we can implement some approximation methods. For highly nonlinear ML algorithm where finding $\phi_j(F[x])$ directly is a problem due to the enormous amount of computations, approximations of F (x) by a simpler f (x) (with faster computing) in the neighborhood of each x in X may be done. One popular method is called LIME (Local Interpretable Model-agnostic Explanations) model.

Basically, we search for f (x) that minimizes the loss function L (square error loss) over all sample points i in the neighborhood of each x in X.

$$\min_{f} L(F, f, w) = \Sigma_j^T w_j [\ F(x_j) - \hat{f}(x_j)\ ]^2 + \Omega(f)$$

where w is some weighting and Ω(f) is a penalty function that gets larger if the model f is more complex. For example, if f is linear regression, complexity could be reduced by limiting the number of and size of the coefficients. This leads to regularized linear regression. If f is Decision Tree method, complexity could be reduced by limiting the depth of the tree. Typically, the same type of LIME f (x) is used for the X. In principle, as the LIME method can be applied to whatever F(x), it is called a model-agnostic method.

Suppose the prediction or value function is F (x_1, x_2, x_3, …,x_N) for a given row of features x in X. Suppose we approximate F(x) by a linear ridge regression f(x). For each x, randomly generate M local neighborhood points $x^{(1)}$, $x^{(2)}$,….,$x^{(M)}$ where each vector $x^{(i)}$ is Nx1. Weigh more distant point $x^{(i)}$ from original x by smaller weight, e.g., $w^{(i)} = \exp(-\|x^{(i)} - x\|^2)/D$ where D > 0 is a hyperparameter denoting extent of circle of influence. Larger D means all weights increase. Hence weighted point $x^{(i)}$ becomes $x^{*(i)} = w^{(i)}x^{(i)}$.

Using the ML algorithm F(.), find $F(x^{*(1)}) = Y_1$, $F(x^{*(2)}) = Y_2$, ……, $F(x^{*(M)}) = Y_M$. Then perform linear regression $Y_i = b_0 + b_1 x_1^{*(i)} + b_2 x_2^{*(i)} + ….. + b_N x_N^{*(i)} + e_i$ for i = 1,2,…,M, with coefficient constraints.

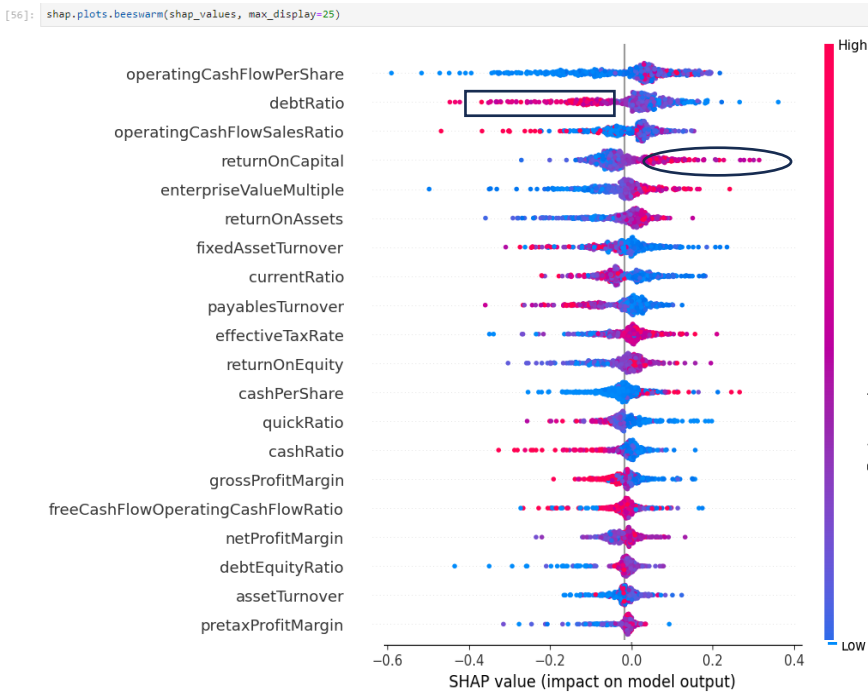
The regression produces estimates $\hat{b}_0$, $\hat{b}_j$'s from $x^{(i)}$'s. Then find f(x) = $\hat{b}_0 + \sum_{j=1}^{N} \hat{b}_j x_j$ with the original x_j's. For this instance or sample point x, we can take expectation over the probability space of X in that neighborhood to obtain

$$E[f(X)] = \hat{b}_0 + \sum_{j=1}^{N} \hat{b}_j E(x_j).$$

Then, f(x) – E[f(X)] = $\sum_{j=1}^{N} \hat{b}_j [x_j - E(x_j)]$ or f(x) = E[f(X)] + $\sum_{j=1}^{N} \hat{b}_j [x_j - E(x_j)]$.

We can treat E[f(X)] = ϕ_0 and $\sum_{j=1}^{N} \hat{b}_j [x_j - E(x_j)] = \sum_{j=1}^{N} \phi_j$ as in Eq. (6.3), thus obtaining $\hat{b}_j [x_j - E(x_j)]$ as the j^{th} feature Shap value for instance x. The sum of the Shap values from all the N features in this instance x gives $\sum_{j=1}^{N} \phi_j$ = f(x) – E[f(X)].

Continuing with Chapter6-1.ipynb, we analyse the XGBoost predictions on the test data set of 508 sample points. The percentage (mean) of the predicted values of "1"s in Class "1" is 0.615. Using the implementation of "import shap" and its shap explainer, we display the beeswarm plot (partial display) of Shap values of each feature in each instance represented by the dots.



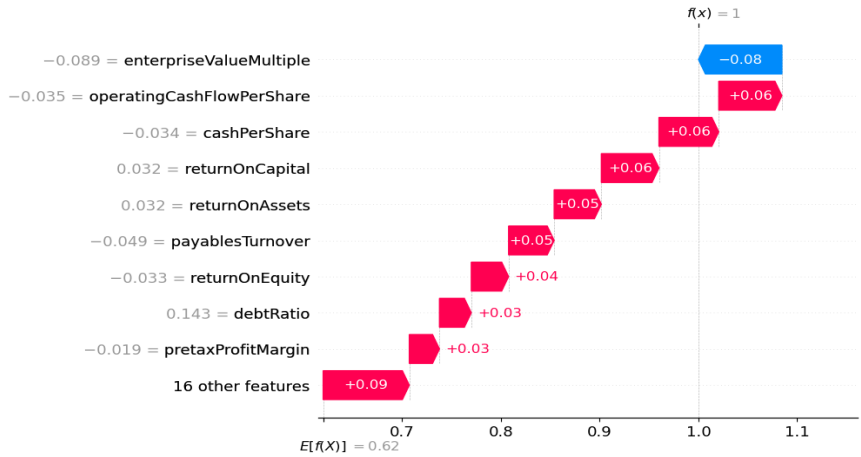
There are 508 points on each feature. For example, in the "return on capital" feature, most of the points in the oval have positive contributions to the predicted probability and they are features with high positive values. This is intuitively correct as high return on capital for a firm implies higher probability

of being in Class “1” or of higher credit rating. In the “debt-ratio” feature, points in the rectangle have high debts and this feature on those points or instances or firms implies lower predicted probability of being in Class “1” and hence higher probability of being in Class “0” or of a lower credit rating.

Code line [57] shows the tabulation of average absolute Shap value per instance across all the features. It is seen that “operating cash flow per share” and “debt ratio” have the largest contributions to predicted probability of being Class “1”. “operating cash flow per share” is also one of the 4 dominant features in features importance. Note that only the partial graph is shown due to space constraint.

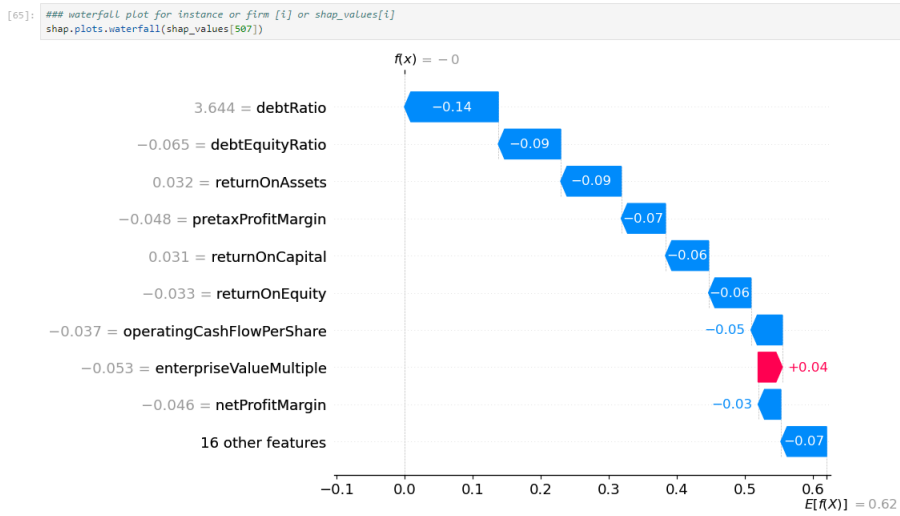
```
[57]: shap.plots.bar(shap_values,max_display=25)
      ### SHAP bar plot will take the mean absolute value of each feature
      ###  over all the instances (rows) of the dataset.
```


```
[59]: ### waterfall plot for instance or firm [i] or shap_values[i]
      shap.plots.waterfall(shap_values[0])
```



We also show in code line [59] the ‘waterfall’ plot of the Shap values of features in contribution to the predicted probability of Class “1” of the first firm or instance in the test data set. In this case, the predicted probability f(x) = 1. The sum of Shap values of all the 25 features is equal to f(x) – E[f(x)] =

1 – 0.62 = 0.38 where 0.62 is the mean of the predicted values of "1"s in Class "1". For this first firm, the main features with highest Shap value contribution to the predicted probability of Class "1" are "operating cash flow per share", "return on capital", "return on assets", etc. The negative contribution of "enterprise value multiple" is due to a lower than average multiple.



We show in code line [65] the 'waterfall' plot of the Shap values of features in contribution to the predicted probability of Class "1" of the last firm or instance in the test data set. In this case, the predicted probability f(x) = 0. The sum of Shap values of all the 25 features is equal to f(x) – E[f(x)] = – 0.62. For this last firm, the main features with largest negative Shap value contribution to the predicted probability of Class "1" are "debt ratio", "debt-equity ratio", "return on assets" (low feature value), etc.

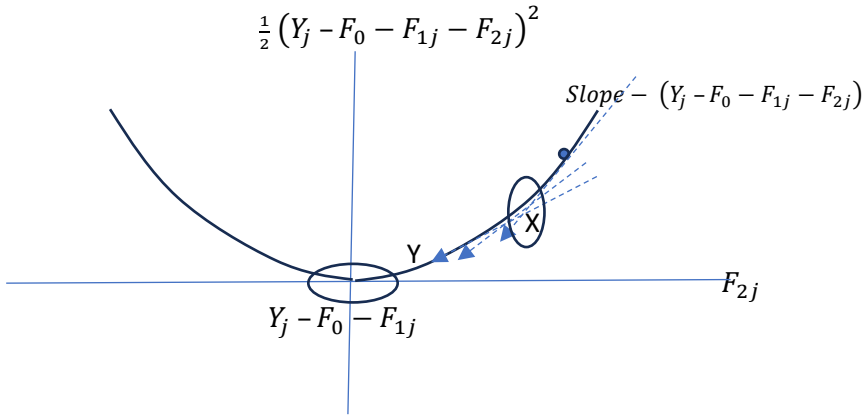
6.5 Concluding Thoughts

In summary, ensemble methods include the bagging approach of RF and the gradient boosting approach of GB, LightGBM, XGBoost, and others. Each DT in a RF of say 500 trees produces a prediction x_i. The prediction of the trees used the same decision rules formulated in the training sample for each of the ensemble of trees. Thus, it is possible that the formulated rules could produce

a biased estimate and hence biased prediction. For regression trees, the RF basically yields an averaged prediction from the 500 trees. The variance of this average is $var\left(\frac{1}{500}\sum_{i=1}^{500} x_i\right) \approx \frac{1}{500} var(x_i)$ which is much smaller than the variability of an individual DT prediction, assuming the predictions from different trees are approximately independent. Hence bagging decreases variance in the prediction but may not decrease the bias if there is any.

For gradient boosting, the idea is to use gradient to boost subsequent trees to reduce the loss function toward zero. Typically, if the loss function gets to near-zero, the prediction would be very accurate. Hence the gradient boosting approach reduces bias in trees toward zero, but the variability may be larger than in RF.

The above idea can be illustrated as follows in the regression tree for continuous or discrete target variable fitting. Suppose the loss function L = $\frac{1}{2}\sum_{j=1}^{N}\left(Y_j - \sum_{i=0}^{n} F_{ij}\right)^2$ for n trees is MSE or is quadratic in the fitted/predicted "error". Suppose n = 2.



In RF, suppose most re-sampled test data trees based on the trained decision rules predict with a bias and end up close to point X (circled region). The averaged prediction of the RF ensemble would also in general be biased but with less variance. The GB trees however would sequentially improve by training on the gradients toward $Y_j - F_0 - F_{1j}$ so that the prediction would have less bias, but perhaps more variance (circled region). Note F_{1j} was also trained using gradient adjustment.

In GB, if the learning rate is too small, the algorithm will require many subsequent trees (iterations) to get close to the minimum. But if the learning rate is too high, the prediction may overshoot the target and end up having the next iteration or tree to revert the other direction. Thus, the learning may take longer.

XGBoost is GB method with added regularizations on the optimization of the loss function. With adequate hyperparameter tuning, it can produce slightly better predictive performance than the GBM. AdaBoost is another boosting method that is popular.

Besides the popular bagging via RF and the boosting gradient models in ensemble prediction, another ensemble approach is stacking. Stacking uses different models, e.g., RF, GB, SVM, NN to perform predictions. The different model predictions (from the different machine learners), called the intermediate predictions, are then possibly averaged to obtain the final ensemble prediction. This final prediction is said to be stacked on top of the intermediate models.

In this chapter, we also see how the Shap values can contribute a better understanding or explanation of the prediction in every instance, in addition to feature importance computations in trees. Specific additions or subtractions to predicted probability by features can help decision-making in improving features to directly affect the probability.

References

Aurelien Geron, (2019), "Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow", 2nd ed., O'Reilly Publisher.

Erik Štrumbelj and Igor Kononenko, (2014), "Explaining prediction models and individual predictions with feature contributions", Knowledge and Information Systems, Vol 41, 647–665.

https://safjan.com/kernelshap-treeshap-two-most-popular-variations-of-the-shap-method/

Jerome H. Friedman, (2002), "Stochastic Gradient Boosting", Computational Statistics & Data Analysis, Vol.38 (4), 367—378.

Lundberg, Scott M., and Su-In Lee, (2017), "A unified approach to interpreting model predictions", Advances in Neural Information Processing Systems.

Marcos Lopez De Prado (2018), “Advances in Financial Machine Learning”, Wiley.