

Variational Gradient Boost — Novel Gradient Boosting Method

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Abstract

Purpose — Gradient Boosting is a compelling ensemble method, such as XGBoost. It uses Decision Trees as estimators to create a feed forward loop in order to minimize the residuals errors. Which is prone to overfitting due to irrelevant features, outliers and external noise. Thereby, it is proposed that a variational feed forward loop of a combination of many different estimators should be implemented.

Method — Variation Gradient Boosting (VGBoost), makes an initial prediction as the mean of the dependent feature. Then it calculates the residuals and uses these residuals as the dependent feature for the next layer. In each subsequent layer besides just relying on Decision Trees, it simultaneously trains many linear and non-linear models and chooses the model with least validation mean squared error (mse). This feed forward loop is repeated until the mse value converges to zero or it has exhausted the iterations.

Results — On Scikit-Learn's California housing price dataset, XGBoost and VGBoost had a training and validation mse of 0.692 and 0.236, and 0.681 and 0.482. On Scikit-Learn's Friedman1 dataset, XGBoost and VGBoost had a training and validation mse of 1.047 and 0.058, and 0.477 and 0.201. Further on Scikit-Learn's make_classification dataset, XGBoost and VGBoost had a training and validation F1 score of 89.28. And 100, and 90.65 and 96.53.

Conclusion — The above benchmarking proves that testing various different machine learning models and making a feed forward loop would combat overfitting and thereby also improve the overall metrics ¹.

1 Introduction

Gradient Boosting is an ensemble learning algorithm which creates a sequential feed forward ensemble based on the previous residual errors. In conventional

¹ Mean Squared Error for regression and F1 Score for classification

gradient boosting algorithms [6], first an initial prediction which is the arithmetic mean of the dependent features is made. Then the residuals errors values are calculated which are the difference between the true dependent values and the predicted dependent values which is scaled by a learning rate in order to improve the generalization accuracy [9]. For each subsequent layer a decision tree is used to calculate the current dependent features, this is iterated n number of times where n is a hyper-parameter. Although Decision Trees which are used as the base estimator in gradient boosting are highly prone to over-fitting and having a high variance [3]. As a result, gradient boosted like its base estimators, decision trees, have low bias and high variance [4].

2 Reviewing Current Literature

2.1 Reducing variance and over-fitting in Decision Trees

- (a) Adding noise filters such as ENN, RENN, and ALLKNN for instance reduction [2].
- (b) Further, by pre-pruning and post-pruning the branches of the decision trees [1].
- (c) Making minimum Surfeit and Inaccuracy algorithm based on Kolmogorov complexity and breadth search traversal [5].

2.2 Reducing variance and over-fitting in Gradient Boosting Algorithms

- (a) Tuning hyper parameters such as the learning rate, limiting max depth of base trees and by early-stopping.
- (b) Removing confusing samples and outliers empirically shows that it would reduce the generalization error [8].

Further as a general principle variance can be reduced by early-stopping, network-reduction, data-expansion and regularization [10].

3 Variational Gradient Boosting Algorithm

3.1 Overview

Depending on the dataset, algorithms like Linear Regression, Ridge Regressor, LARS Lasso, RANSAC Regressor et cetera, and non linear algorithms such as SVM, K-nearest Neighbor, Bayesian Ridge et cetera, may have better accuracy than a decision tree.

VGBoost makes the initial prediction as the arithmetic mean of the dependent features, and calculates the difference between the true values and predicted

values as the residual errors. For each subsequent layer it uses multi-threading to simultaneously train various models and chooses the one with the least Mean Squared Error, as defined in Model Selection 3. It simultaneously keeps track of the models which will be later used for making predictions. Then it scales the current predictions by a learning rate α , and calculates the new residuals. This process is repeated till it has exhausted n estimators, or the residual error is zero, or due to early stopping. Classification — It can be directly used for binary classification problem, for rest add Scikit-Learn's [7] OneVsRestClassifier on VGBoost Classifier. The complete implementation of VGBoost is in (github.com/Agnij-Moitra/variational-gradient-boosting).

```

Input: X_train: iterable
Input: y_train: iterable
1      ▷ expects binary feature for classification
Output: None, creates ensemble
2 global init_preds = mean(X_train)
3 residuals[0] = y_train - init_preds
4 global ensemble = list()      ▷ sequential list of models in each layer
5 for  $i \in n_{estimators}$  do
6      $y[i] = residuals[i - 1]$ 
7     do in parallel
8          $train\_test\_split(X\_train, y[i])$ 
9          $train\ all\ models$ 
10         $model = get\ model\ with\ least\ Mean\ Squared\ Error$ 
11     $residuals[i] = y[i] - model.predict(X_{train}) * \alpha$ 
12    global ensemble.append(model)
13    if warm_start then
14         $X_{train}[i] = y[i - 1]$ 
15    if early_stopping or  $residuals[i] == 0$  then
16        break
17
```

Algorithm 1: VGBoost Fit Method

Input: X_{test} : iterable
Output: y_{preds} : numpy array

```

1  $preds[0] = \text{global init\_preds}$ 
2 for  $i$  in range(len(global ensemble)) do
3   |  $\underline{preds}[i] = ensemble[i].predict(X_{test})$ 
4 if classification then
5   |  $row\_preds = row\_wise\_sum(preds)$   $\triangleright$  add prediction of each layer
6   |  $final\_preds = quantize(row\_preds)$   $\triangleright$  quantize value to 0 or 1
7   | return  $final\_preds$ 
8 else
9   |  $final\_preds = row\_wise\_sum(preds)$   $\triangleright$  add prediction of each layer
10  | return  $final\_preds$ 
11
```

Algorithm 2: VGBost Predict Method

3.2 Model Selection

Based on the parameters provided, for each subsequent layer, VGBost uses multi-threading to train the following model and chooses the one with least validation mean squared error ², to change the time complexity of the algorithms used:

²It uses `train_test_split(*, train_size = 0.7)` in for this evaluation.

Input: light = True
Input: complexity = False
Input: custom_models = None
Output: None, sets model list

```

1 if light then
2   models                                     ▷ Least Complexity (Default)
3   ↪ LGBMRegressor, ExtraTreesRegressor, BaggingRegressor,
   RANSACRegressor, LassoLarsIC, BayesianRidge
4 if complexity then
5   models                                     ▷ Maximum Complexity
6   ↪ DecisionTreeRegressor, LinearRegression, BayesianRidge,
   KNeighborsRegressor, HistGradientBoostingRegressor, ElasticNet,
   LassoLars, Lasso, GradientBoostingRegressor,
   ExtraTreesRegressor, BaggingRegressor, NuSVR, XGBRegressor,
   SGDRegressor, KernelRidge, MLPRegressor, LGBMRegressor,
   Ridge, ARDRegression, RANSACRegressor, HuberRegressor,
   TheilSenRegressor, LassoLarsIC
7 else
8   if custom_models then
9     models                                     ▷ Set Custom Models
10    ↪ custom_models
11  else
12    models
13    ↪ DecisionTreeRegressor, LinearRegression,
   BayesianRidge, KNeighborsRegressor, LGBMRegressor,
   ElasticNet, LassoLars, Lasso, SGDRegressor,
   BaggingRegressor, ExtraTreesRegressor, Ridge,
   ARDRegression, RANSACRegressor, LassoLarsIC
  
```

Algorithm 3: Model Selection

4 Results and Interpretation

4.1 Testing

VGBoost was then tested on the following datasets³:

1. `make_regression(n_samples = 20000, flip_y = 0.1)` [7]
2. `X, y = make_friedman1(n_samples = 20000, noise = 0.2)` [7]
3. `X, y = make_friedman2(n_samples = 20000, noise = 0.2)` [7]
4. `X, y = make_friedma3(n_samples = 20000, noise = 0.2)` [7]
5. `X, y = make_classification(n_samples = 20000, noise = 0.2)` [7]

³The noise factors were added in order to simulate real world data

6. $X, y = \text{fetch_california_housing}(\text{as_frame} = \text{True})["\text{data}"]$ [7]

The results of the above datasets are as follow ⁴:

Model	Validation MSE	Training MSE	Time
VGBRegressor (light=True)	0.0397	.0403	12min 43s
VGBRegressor (light=False)	0.0394	0.0405	12min 17s
VGBRegressor (complexity=True)	0.0396	0.0403	1h 4min 17s
XGBRegressor	1347.7776	269.4160	11.8 s
GradientBoostingRegressor	1352.8389	974.4383	1min 40s
ExtraTreesRegressor	3116.4577	6.4210×10^{-26}	1min
RandomForestRegressor	3987.9605	576.5084	2min 51s
BaggingRegressor	4973.3768	1006.1820	17.1 s
AdaBoostRegressor	5888.4974	5522.6421	32.3 s
DecisionTreeRegressor	11298.4037	0.00	2.39 s

Table 1: make_regression Results

Model	Validation MSE	Training MSE	Time
VGBRegressor (light=True)	0.0419	0.0341	33.4 s
VGBRegressor (light=False)	0.0422	0.0343	33.5 s
VGBRegressor (complexity=True)	0.0420	0.0365	8min 35s
XGBRegressor	0.0439	0.0249	734 ms
GradientBoostingRegressor	0.0421	0.0384	2.14 s
RandomForestRegressor	0.0443	0.0060	6.75 s
ExtraTreesRegressor	3987.9605	3.2095×10^{-30}	3.45 s
BaggingRegressor	0.0476	0.0082	727 ms
AdaBoostRegressor	0.0472	0.0447	1.02 s
DecisionTreeRegressor	0.0866	0.00	94 ms

Table 2: make_friedman3 Results

⁴Results can be found in (<https://bit.ly/3FuZPIf>) and (<https://bit.ly/3DmuCoa>)

Model	Validation MSE	Training MSE	Time
VGBRegressor (light=True)	9.0275	2.3473	51 s
VGBRegressor (light=False)	9.6481	2.4882	55.4 s
VGBRegressor (complexity=True)	10.2357	2.5552	10min 31s
XGBRegressor	62.0922	28.2265	732 ms
GradientBoostingRegressor	198.4483	176.8633	2.05 s
RandomForestRegressor	19.9297	2.9441	5 s
ExtraTreesRegressor	7.4181	7.1130×10^{-25}	3.31 s
BaggingRegressor	31.8670	7.9816	535 ms
AdaBoostRegressor	3994.4126	4012.8412	1.09 s
DecisionTreeRegressor	104.0727	0.00	81 ms

Table 3: make_friedman2 Results

Model	Validation MSE	Training MSE	Time
VGBRegressor (light=True)	0.2359	0.1636	56.6 s
VGBRegressor (light=False)	0.2325	0.1642	1min 3s
VGBRegressor (complexity=True)	0.0755	0.0696	12min 38s
XGBRegressor	0.3678	0.1132	1.25 s
GradientBoostingRegressor	0.6261	0.5429	4.87 s
RandomForestRegressor	0.9364	0.1385	11.3 s
ExtraTreesRegressor	0.6838	4.4569×10^{-28}	5.06 s
BaggingRegressor	1.1862	0.2404	1.17 s
AdaBoostRegressor	4.7566	4.6560	2.08 s
DecisionTreeRegressor	2.7734	0.00	81 ms

Table 4: make_friedman1 Results

Model	Validation f1_score	Training f1_score	Time
VGBClassifier (light=True)	0.8471	0.8882	1min 42s
VGBClassifier (light=False)	0.8466	0.9625	2min 23s
VGBClassifier (complexity=True)	0.8499	0.8564	38min 22s
XGBClassifier	0.3678	0.1132	1.25 s
GaussianNB	0.7887	0.7834	75 ms
GradientBoostingClassifier	0.8503	0.8575	11.4 s
RandomForestClassifier	0.8482	1.0	7.66 s
ExtraTreesClassifier	0.8495	1.0	2.49 s
BaggingClassifier	0.8290	0.9883	3.74 s
AdaBoostClassifier	0.8456	0.8479	3.23 s
DecisionTreeClassifier	0.7756	1.0	547 ms

Table 5: make_classification Results

Model	Validation MSE	Training MSE	Time
VGBRegressor (light=False)	0.6816	0.5686	0.8162
VGBRegressor (complexity=True)	0.6972	0.5757	0.8120
XGBRegressor	0.6922	0.5748	0.8133

Table 6: California Housing Results

4.2 Rationale

Thereby, it can be claimed that, using a Variational Gradient Boosting can yield better metrics ⁵ than GradientBoost and XGBoost. This is because VGBoost simultaneously trains many models ³ which individually have a better metrics ⁶ than regular Decision Trees.

Hyper-parameters — based on the above results it can be claimed that having a greater complexity does not necessarily provide better metrics ⁷. Although, setting `complexity = True` did give better results in `friedman1` ⁴, as which yields a more complex dataset than the rest. Further by `light = True` and `light = False` also had similar results, thereby one may also consider the training time of the algorithms.

Drawbacks and further prospects — Compared to GradientBoost and XGBoost, VGBoost has a greater time and memory complexity, as observed in `testing4.1`. Thereby, hardware level optimization and low-level programming language implementation, for example in PyPy or Cython. Maybe used in order to optimize VGBoost.

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⁵Refer footnote 1

⁶Refer footnote 1

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