Gradient Boosting Trees

Maria Rigaki

30-11-2018

Ensemble Methods

- Combine the predictions of several base estimators in order to improve generalization and robustness
- **Bagging** or averaging methods build several estimators independently and average their predictions. Ex: Random Forests
- **Boosting** methods build estimators sequentially. Combining several weak estimators to produce an ensemble. Ex: AdaBoost, Gradient Tree Boosting, etc

Bagging methods reduce the variance (on average).
Boosting methods try to reduce the bias.

Gradient Boosting

High level idea

- Fit an additive model (ensemble) in a forward stage-wise manner.
- In each stage, introduce a weak learner to compensate the shortcomings of existing weak learners.
- "shortcomings" are identified by gradients.
- Gradients tell us how to improve the model.

A simple Boosting algorithm

Dataset: $D = \{(x_1, y_1), (x_2, y_2)...(x_n, y_n)\}$
Task: Fit a model $F(X)$ to minimize square loss $L = (Y - F(X))^2$

1. Initialize $F_0(X) = \frac{1}{N} \sum y_i$
2. **for** $m = 1$ to M:
3. let $r_{m-1} = Y - F_{m-1}(X)$ be the residual vector
4. train a regression tree $h_m(X)$ on r_{m-1}
5. Update $F_m(X) = F_{m-1}(X) + h_m(X)$
6. **end**

Illustration

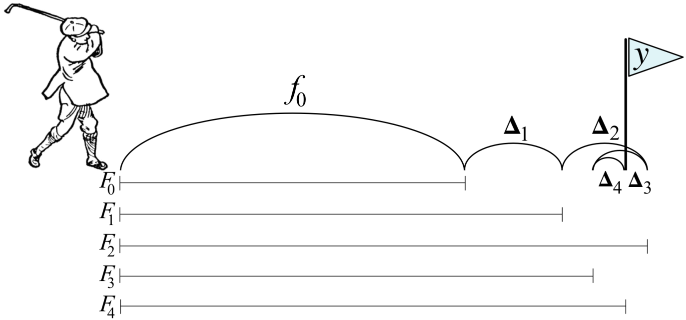
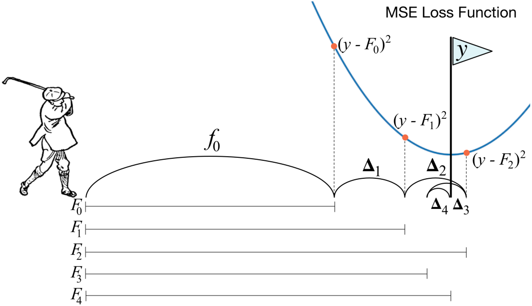


Figure 1: Intuition behind Gradient Boosting (From explained.ai)

Example

Simple Boosting demo

What about the Gradient part?



- It turns out that when using the square loss, the residual is equal to the negative gradient
- In essence, when we update F we use the negative gradient
- Gradient descent on F (not on the model parameters)

Final Formulation

Additive model of the form:

$$F(X) = \sum_m \gamma_m h_m(X)$$

where the new tree h_m tries to minimize the loss L

$$h_m = argmin \sum_i L(y_i, F_{m-1}(x_i) + h_{m-1}(x_i))$$

and the update rule is:

$$F_m(X) = F_{m-1}(X) - \gamma_m \sum_i \nabla_F L(y_i, F_{m-1}(x_i)))$$

Loss Functions (regression)

- Changing from residuals to gradients allows us to change the loss functions
- Square loss is mostly used but it emphasizes the outliers.
- Absolute loss and Huber loss are also used when robustness to outliers is required.
- Other options are Least Absolute Deviation and Quantile.

Challenges

- Models can overfit
- **Regularization** is achieved using shrinkage or subsampling
- **Shrinkage** is reducing the impact of each added learner.
- **Subsampling** is a combination of boosting and bagging.

Shortcomings

- Scalability
- What if the data do not fit in the memory?
- Can it be used in more than one CPUs or machines?

XGBoost (Chen & Guestrin, 2016)

- Scalable gradient boosting trees
- Very popular algorithm in ML competitions
- It can be used for regression, ranking and classification
- Parallel, Distributed computing and Out of core computing
- Cache aware access

Algorithmic improvements

Tree building

How to find the best split points?
How to choose the feature to split?

Approximate algorithm

Most algorithms use an *exact greedy* approach that requires sorting.
XGBoost proposes candidate splitting points according to percentiles of feature distribution.

Sparsity Aware split finding

Parameter Tuning

- General parameters (number of threads)
- Boosting parameters (stepsize, regularization, tree parameters, etc)
- Task parameters (objective, evaluation metric)

LightGBM (Ke et al., 2017)

- Open source algorithm developed by Microsoft
- Gains in popularity and has won ML competitions
- Speed and Memory Usage optimizations
- Sparsity Optimization
- Accuracy optimizations
- Parallel Learning (feature, data and voting parallelization)

Algorithmic improvements

Gradient-based One-Side Sampling

Exclude a significant proportion of data instances with small gradients, and only use the rest to estimate the information gain.

Exclusive Feature Bundling

Bundle mutually exclusive features (i.e., they rarely take nonzero values simultaneously), to reduce the number of features without hurting the accuracy.

System improvements

- Data, Feature and Voting parallelization
- Network communication
- GPU support

Parameter Tuning

- Learning Controls (tree related parameters, bagging regularization)
- IO (verbosity, outputs, binarization)
- Objectives
- Metrics
- Network (num_machines, connectivity, etc)
- GPU

Demo time

Testing XGBoost, LightGBM and Random Forests in a security dataset.

Ember dataset (Anderson & Roth, 2018)

- A collection of pre-processed Windows binary files
- Features extracted from 1.1M binaries from 2017
- 900K training samples (300K malicious, 300K benign, 300K unlabeled)
- 200K test samples (100K malicious, 100K benign)

Features

- File information: size, imported and exported functions
- Raw bytes histograms, Byte entropy histograms
- Header information
- Strings, etc
- 2351 model features

Results I

- Using a subset of the data: 150K training samples and 50K test samples.
- Training set was 1/3 malicious, 2/3 benign.

Algorithm	AUC	FPR	FNR	Training (sec)	Prediction (sec)
XGBoost	0.944	0.037	0.07	136	1.62
LightGBM	**0.966**	0.019	**0.05**	**75**	**0.87**
RF	0.959	**0.010**	0.07	272	1.43

Table 1: Results on smaller dataset

Results II

- Same settings as before, only with the full dataset: 600K training samples, 200K test samples.
- Balanced dataset.

Algorithm	AUC	FPR	FNR	Training (sec)	Prediction (sec)
LightGBM	0.986	0.011	0.01	**283**	**3.43**
RF	**0.989**	0.011	0.01	2258	8.67

Table 2: Results on the full dataset

Conclusions

- LightGBM perfomed surprising well with no tuning
- XGBoost required some setting even with the smaller dataset
- Random Forests performed really well but the training time required was significantly longer.
- The above do NOT mean that XGBoost is a worse library!
- Both Gradient Boosting libraries have a large number of parameters.

Links

https://explained.ai/gradient-boosting/index.html

https://lightgbm.readthedocs.io/en/latest/index.html

https://xgboost.readthedocs.io/en/latest/

http://arogozhnikov.github.io/2016/06/24/gradient_boosting_explained.html

References I

Anderson, H.S. and Roth, P., 2018. EMBER: An Open Dataset for Training Static PE Malware Machine Learning Models. arXiv preprint arXiv:1804.04637.

Chen, T. and Guestrin, C., 2016, August. *Xgboost: A scalable tree boosting system.* In Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining (pp. 785-794). ACM.

Friedman, J.H., 2001. *Greedy function approximation: a gradient boosting machine.* Annals of statistics, pp.1189-1232.

Ke, G., Meng, Q., Finley, T., Wang, T., Chen, W., Ma, W., Ye, Q. and Liu, T.Y., 2017. *Lightgbm: A highly efficient gradient boosting decision tree.* In Advances in Neural Information Processing Systems (pp. 3146-3154).