Binary Classification of Imbalanced data from Bosch Production Line

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1 Background

1.1 Gradient boosting tree

Gradient boosting tree is achieving wide attention in Kaggle competitions. The basic idea of gradient boosting tree is to fit a base tree learner to pseudo-residuals.

$$r_{im} = -[\frac{\delta F(y_i, F(x_i))}{\delta F(x_i)}]_{F(x)=F_{m-1}(x))}, i = 1, ...n$$

Then computer r_m by solving the following one-dimensional optimization problem:

$$\sum_{i=1}^{n} L(y_i, F_{m-1}(x) + rh_m(x_i))$$

And there are many versions of gradient boosting tree. In this paper, we will list five different versions of gradient boosting tree.

Scikit Learn gradient boosting tree: implemented in python and integrated in scikit learn package, relatively slow

SAS Viya: implemented in C and MPI, developed by SAS, supports python and lua API. It only support equal binning now.

xgboost(`https://github.com/dmlc/xgboost`): C language, open sourced and supply good support with python wrapper and R wrapper.

FastBDT(`https://github.com/thomaskeck/FastBDT`): C language, open sourced and currently only suitable for classification problem.

LightGBM(`https://github.com/Microsoft/LightGBM`): C language, developed by Microsoft and open sourced recently, it is said to be much faster than xgboost and can achieve the same accuracy

We mainly focus on xgboost and SAS Viya in our paper

2 Method

2.1 Data Set

The data from an ongoing Kaggle competition: Bosch Production Line Performance (`https://www.kaggle.com/c/bosch-production-line-performance/data`). The data represents measurements of parts as they move through Bosch's production lines and it is a binary classification problem. The raw data has three types of feature: numerical, categorical, and date.

2.2 Machine learning workflow

This project has two challenges: 1) The size of raw data is large(15.4GB) and cannot directly fit into a single machine. We will do data exploration and feature reduction to fit important features into a single memory with 16GB memory. 2) The raw data is highly imbalanced (6879:1176868). We will utilize different methods such as upsampling, downsampling and SMOTE to do the sampling.

Following the above two procedures, we will then train the machine learning models with gradient boosting tree, and then compare its performance with other speeding up gradient boosting tree models, including Xgboost and SAS Viya.

2.3 The magic feature

Some kagglers report that there is magic feature in the competition which will improve the performance in public board from 0.3 to 0.4. The magic feature comes from id and there is a debate if it is a leak. The leak is something that was introduced during data manipulation, either by data owners or by Kaggle. In essence, the leak is an unintentional tipping of the final outcome by those who know the outcome. We've had plenty of leaks that satisfy this definition. In this competition, the id column has leak information and we will use the information.

2.4 Optimizing probabilities for best MCC

The criteria for the competition is Matthews correlation coefficient, the equation to calculate it is as following. We will yield the threshold that yields the best MCC score.

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP+FP)(TP+FN)(TN+FP)(TN+FN)}}$$

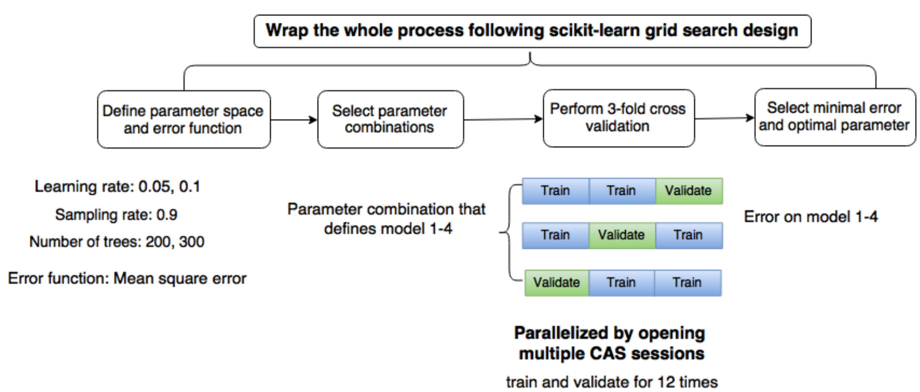
The steps are as following: ordering distinct probabilities, computing TP/TN when assuming the threshold for each distinct probability, computing the MCC , returning the probability row with the maximum MCC.

2.5 Grid Search

For gradient boosting tree, we need to do hyperparameter optimization for tree number, learning rate and other parameters. we tuning or a learning algorithm, usually with the goal of optimizing a measure of the algorithm's performance on an independent data set. In this case it is mcc. The traditional way of performing hyperparameter optimization has been grid search, or a parameter sweep, which is simply an exhaustive searching through a manually specified subset of the hyperparameter space of a learning algorithm

2.6 SAS Viya python wrapper

SAS Viya is the next-generation high-performance and visualization architecture from the leader in analytics. It supplies python interface for gradient boosting tree, but it doesn't support grid search and cross validation APIs. To solve this problem, we wrote python modules for SAS Viya following scikit-learn architecture.

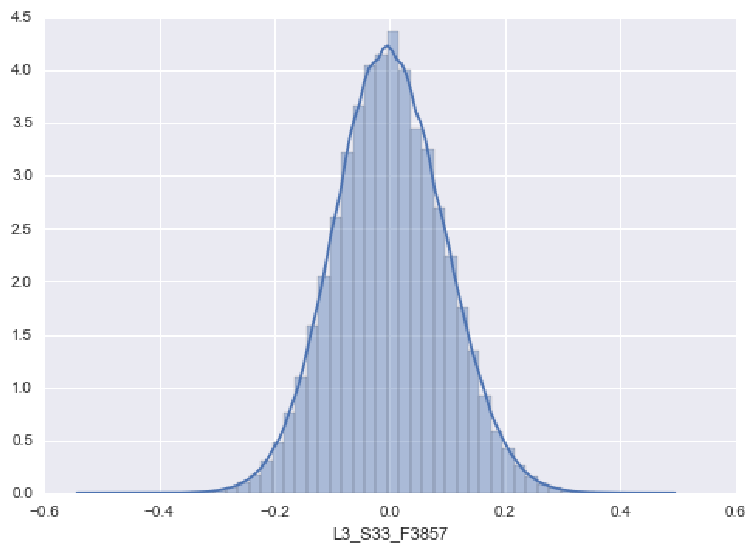


3 Experiment

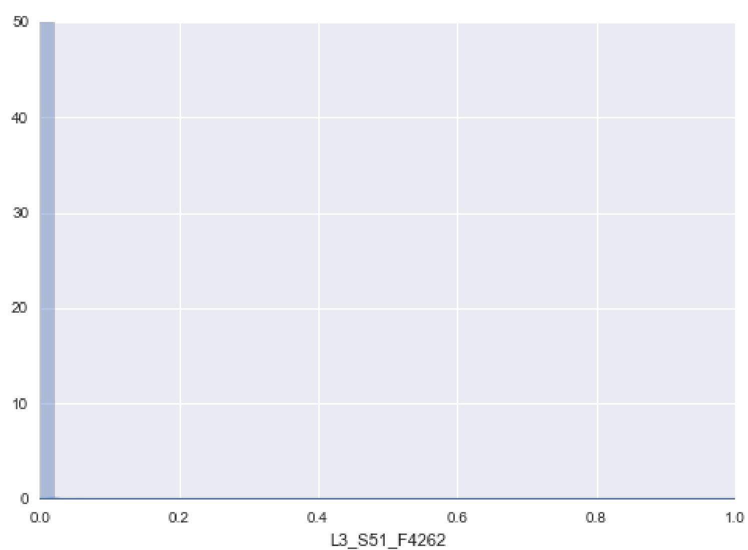
In our experiment, the highest score we got in public board now is 0.19 for SAS Viya

3.1 equal binning vs. quantile binning

Single machine version of xgboost uses exact greedy algorithm that searches overall possible candidates, this can be desirable for deeper trees, and is usually what the user want. But this will slow the training speed when the number of observations is very large. So the gradient boosting implementation In the competition, we do data exploration in different numeric features. We find that some features are normally distributed and others are quite skewed, the distribution of some features are shown below. That's the reason xgboost outperforms SAS Viya, SAS Viya only supports equal binning.

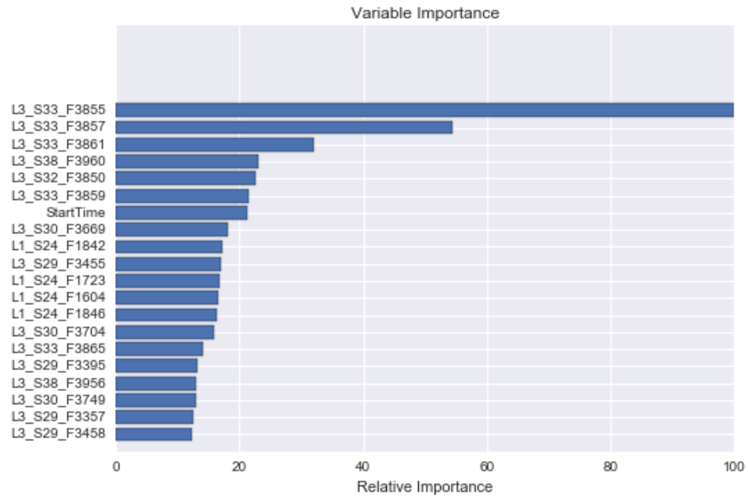


Skewed numeric feature



3.2 Feature Importance

We can get feature importance from numeric data.



4 Reference

[1] Tianqi Chen, & Carlos Guestrin. (2016) XGBoost: A Scalable Tree Boosting System. *KDD*.

[2] Keck T. (2016) A speed-optimized and cache-friendly implementation of stochastic gradient-boosted decision trees for multivariate classification *arXiv preprint arXiv*: 1609.06119.

[3] Chawla, Nitesh V., et al.(2002) SMOTE: synthetic minority over-sampling technique. *Journal of artificial intelligence research*, , pp. 321–357.

5 Teammate and Work Division

Xi & Yeojin: Data exploration and feature reduction, sampling

Weijie & Liang: Tree building, hyperparameter optimization