# Gradient Boosting With Piece-Wise Linear Regression Trees (Appendix)

## 1 More on Histograms for GBDT With PL Tree

Histogram is used in several GBDT implementations [Tyree *et al.*, 2011; Chen and Guestrin, 2016; Ke *et al.*, 2017] to reduce the number of potential split points. For each feature, a histogram of all its values in all data points is constructed. The boundaries of bins in the histogram are chosen to distribute the training data evenly over all bins. Each bin accumulates the statistics needed to calculate the loss reduction. When finding the optimal split point, we only consider the bin boundaries, instead of all unique feature values. After the histogram is constructed, we only need to record the bin number of each feature for each data point. Fewer than 256 bins in a histogram is enough to achieve good accuracy [Zhang *et al.*, 2017], thus a bin number can be stored in a single byte. We can discard the original feature values and only store the bin numbers during the boosting process. Thus using histograms produces small memory footprint.

It seems nature to directly use the histogram technique in our algorithm. For LightGBM and XGBoost, each bin in a histogram only needs to record the sum of gradients and hessians of data in that bin. For our algorithm, the statistics in the histogram is more complex. The statistics are used to compute the least squares. Each bin $B$ needs to record both $\sum_{i\in B} h_i \mathbf{x}_i \mathbf{x}_i^T$ and $\sum_{i\in B} g_i \mathbf{x}_i$, where $\mathbf{x}_i$ is the column vector of selected regressors of data $i$. However, the feature values $\mathbf{x}_i$ are needed when fitting linear models in leaves. We still need to access the feature values constantly, which incurs long memory footprint. To overcome this problem, for each feature $j$ and each bin $i$ of $j$, we record the average feature values in bin $j$, denoted as $\overline{x}_{i,j}$. When fitting linear models, we use $\overline{x}_{i,j}$ to replace the original feature value $\mathbf{x}_{k,i}$. Here $\mathbf{x}_{k,i}$ is the value of feature $i$ of data point $\mathbf{x}_k$, and $\mathbf{x}_{k,i}$ falls in bin $j$. In this way, we can still discard the original feature values after preprocessing. Thus we adapt the histogram technique to PL Trees and preserve the small memory footprint.

The histogram technique used in several existing methods (such as XGBoost and LightGBM) only record 2 elements in each bin (sum of gradients and hessians). Our histograms require more than 2 elements (including qudratic terms of feature values). So the detailed implementation is in fact quite different from existing ones. To better utilized the SIMD units when constructing histograms, we use intel intrinsics (which directly indicate the assemble instructions to use) to carefully arrange the calculation.

## 2 Experiment Platform for Training Time Recording

The experiment environment for training time comparison are listed in Table 1.

Table 1: Experiment Platform

| OS | CPU | Memory |
|---|---|---|
| CentOS Linux 7 | 2 × Xeon E5-2690 v3 | DDR4 2400Mhz, 128GB |

## 3 Datasets

The datasets we used in this paper are all from UCI datasets. The number of instances and features can be found in the following table. We will provide details about how we split the datasets into train and testing sets on our github page. [1] For datasets with features of large values, including Year, SUPERCONDUCTOR, Energy and CASP, we first find the minimum and maximum values of each feature in the training set, and rescale the features into range [0, 1] before feeding it into GBDT-PL. This is for numerical stability when computing matrix inversions.

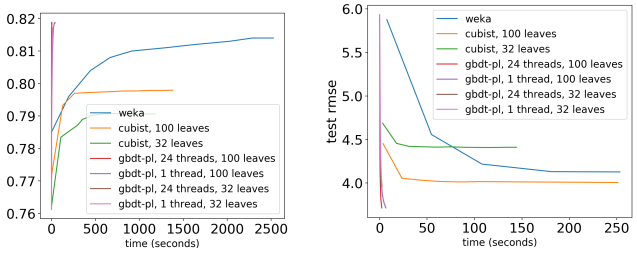
Table 2: Datasets Description

| name | # training | # testing | # features | task |
|---|---|---|---|---|
| HIGGS | 10000000 | 500000 | 28 | classification |
| HEPMASS | 7000000 | 3500000 | 28 | classification |
| CASP | 30000 | 15731 | 9 | regression |
| Epsilon | 400000 | 100000 | 2000 | classification |
| SUSY | 4000000 | 1000000 | 18 | classification |
| SGEMM | 193280 | 48320 | 14 | regression |
| SUPERCONDUCTOR | 17008 | 4255 | 81 | regression |
| CT | 42941 | 10559 | 384 | regression |
| Energy | 15788 | 3947 | 27 | regression |
| Year | 412206 | 103139 | 90 | regression |

[1] https://github.com/GBDT-PL/GBDT-PL.git

## 4 Comparison With Existing Boosted PL Trees

We compare our results with boosted PL Trees in Weka [Hall *et al.*, 2009] and Cubist [Kuhn *et al.*, 2018] packages. The base learner of Weka and Cubist is M5/M5P, a PL Tree proposed by [Quinlan and others, 1992; Wang and Witten, 1996]. The main differences between M5/M5P and our algorithm are: **1**. M5/M5P does not use half-additive fitting, histogram and our system optimization techniques. **2**. M5/M5P grows the tree in a way similar to piecewise constant regression trees (e.g. CART), then fits the linear models at the nodes. Each split in our algorithm considers how much the resultant linear models in the child nodes will reduce the boosting objective. In other words, the split finding in GBDT-PL is greedy and more expensive. Figure 1 shows the results on a small subset of HIGGS dataset with only 100k samples and CASP. All algorithms train 100 trees. GBDT-PL has a significant advantage in efficiency. For example, GBDT-PL finished training 100 32-leaf trees for CASP within 2 seconds, while Cubist takes about 150 seconds.




(a) HIGGS-100k AUC (b) CASP RMSE

Figure 1: Comparison With Weka and Cubist

## 5 Parameter Settings

The parameters we tried are listed in following tables. For big datastes (HIGGS, Epsilon, SUSY and HEPMASS), we only test the learning rate 0.1. We evaluate all different combinations of these values. On small datasets, 96 combinations of parameters are tested for GBDT-PL, and 144 combinations of parameters are tested for XGBoost, LightGBM and CatBoost. The total number of trees (iterations) are chosen according to the learning rate. For XGBoost, LightGBM and GBDT-PL, 500 trees for *learning_rate* 0.1, 1000 trees for *learning_rate* 0.05 and 5000 trees for *learning_rate* 0.01. For CatBoost in *SymmetricTree* mode, instead of controlling maximum leaf number, we tried maximum tree depth of 4, 6, 8, 10 and use 4 times number of trees in other 3 packages. Since CatBoost in *SymmetricTree* mode uses simpler tree structure, it convergences slower. Thus for CatBoost in *SymmetricTree* mode, we use 2000 trees for *learning_rate* 0.1, 4000 trees for *learning_rate* 0.05 and 20000 trees for *learning_rate* 0.01. Subsampling of training data and features are **disabled** in all experiments. For the accuracy and convergence rate experiments, we use the *Ordered* mode of CatBoost for better accuracy. And for the training time experiments, we use *Plain* mode since it is much faster.

For XGBoost, LightGBM and CatBoost, we directly pick up the best result on test set in the best iteration of the best hyperparameter setting. For GBDT-PL, we sample 20% from training data for validation, and pick the iteration and hyperparameter setting performs best in the validation set, then report the corresponding accuracy on test data.

The versions of python packages we used are LightGBM 2.1.0, XGBoost 0.81 and CatBoost 0.14.2.

Table 3: Parameter Settings for LightGBM

| | |
|---|---|
| num_leaves | 16, 64, 256, 1024 |
| max_bin | 63, 255, 1024 |
| min_sum_hessian_in_leaf | 1.0, 100.0 |
| learning_rate | 0.01, 0.05, 0.1 |
| reg_lambda | 0.01, 10.0 |
| min_data_in_leaf | 0, 20 |

Table 4: Parameter Settings for XGBoost

| | |
|---|---|
| max_leaves | 16, 64, 256, 1024 |
| max_bin | 63, 255, 1024 |
| min_child_weight | 1.0, 100.0 |
| eta | 0.01, 0.05, 0.1 |
| lambda | 0.01, 10.0 |
| grow_policy | loss_guided |
| tree_method | hist |

Table 5: Parameter Settings for CatBoost (*SymmetricTree* mode)

| | |
|---|---|
| depth | 4, 6, 8, 10 |
| border_count | 63, 128, 255 |
| min_data_in_leaf | 1, 100 |
| learning_rate | 0.01, 0.05, 0.1 |
| l2_leaf_reg | 0.01, 10.0 |
| grow_policy | SymmetricTree |
| leaf_estimation_method | Newton |
| random_strength | 0.0 |
| bootstrap_type | No |

Table 6: Parameter Settings for CatBoost (*Lossguide* mode)

| | |
|---|---|
| max_leaves | 16, 64, 256, 1024 |
| border_count | 63, 128, 255 |
| min_data_in_leaf | 1, 100 |
| learning_rate | 0.01, 0.05, 0.1 |
| l2_leaf_reg | 0.01, 10.0 |
| grow_policy | Lossguide |
| leaf_estimation_method | Newton |
| random_strength | 0.0 |
| bootstrap_type | No |

Table 7: Parameter Settings for GBDT-PL

| | |
|---|---|
| max_leaf | 16, 64, 256, 1024 |
| max_bin | 63, 255 |
| min_sum_hessian_in_leaf | 1.0, 100.0 |
| learning_rate | 0.01, 0.05, 0.1 |
| l2_reg | 0.01, 10.0 |
| grow_by | leaf |
| leaf_type | half_additive |
| max_vars | 5 |

## References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