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# LightGBM Model

LightGBM (Light Gradient Boosting Machine) is a distributed high-performance framework that uses decision trees for ranking, classification, and regression tasks (Saha, 2023). In contrast to the level-wise(horizontal) growth in XGBoost, LightGBM carries out leaf-wise (vertical) growth that results in more loss reduction, and higher accuracy while being faster (Saha, 2023). However, this approach may lead to the overfitting of the training data (Saha, 2023).

For the experiment and the improvement attempts, the training data set will be used. The data set will be split for cross-validation with k = 10. The experiments with LightGBM are organized as below:

* Exploring preprocessing techniques:
  + An initial run was done with all the features available in the training data set, using Scikit-learn’s TimeSeriesSplit for Cross-Validation, without scaling the data using the StandardScaler(), and using all default hyperparameter values of LGBMRegressor.
  + Test the effect of applying StandardScaler() with the rest of the processing and setting equal to the initial run.
  + Test the effect of using normal k-fold cross-validation (non-time series data) with the rest of the processing and setting equal to the initial run.
  + Test the effect of applying PCA (principal component analysis) on the training data set
* Exploring Feature Engineering
  + The first test will check if removing seemingly unrelated features will affect or improve the training performance.
  + The second test will check if extra engineered features help.
    - First extra sets– incorporate the movement of the reference price, this includes the first derivative, which is the price of the current minus the price of the previous 10 seconds, and the second derivative, which is the change of the first derivative in the last 10 seconds.
    - Second extra sets – add the first and second derivatives for all 8 prices.
    - Third extra sets – Add the imbalance factors
  + The third test set tries to predict the two dependent variables which define the final target separately and combine the result.
* Exploring hyperparameter tunings of the LightGBM model
  + The hyperparameters considered include n\_estimators, learning\_rate, num\_leavers, max\_depth, min\_data\_in\_leaf, max\_bin, min\_gain\_to\_split and subsample.

# Exploring preprocessing techniques

## Initial Trial

Figure 1 shows the training and validation scores for the initial run using all features available in the training data set and Scikit-learn’s TimeSeriesSplit of 10 for cross-validation. The main observations are as follows:

Observation 1: The average validation scores are about 5% higher than the average training scores, this indicates potential overfitting of the model to the training data.

Observation 2: The validation score seems to be improving when more data is used for training. This indicates that the series might be stationary without a trend or seasonal component. Note when using the Scikit-learn’s TimeSeriesSplit function, the testing data of the first fold is added to the training data of the second fold (see Figure 2 for illustration), thus the training data set will continue to expand.

Since the number of days in the training data set is 480, one concern is the original split (TimeSeriesSplit of 10 will split the training data set into 11 parts) may contain fractional data of the day which affect the performance of the model. A quick test was performed using the TimeSeriesSplit setting of 9 (which split the data into 10 parts) with the result shown in table 1. As the resulting models didn’t perform significantly better than the previous models, it is concluded that the number of splits has no significant effect on the performance.

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Figure : Training scores and Validation scores for the initial run

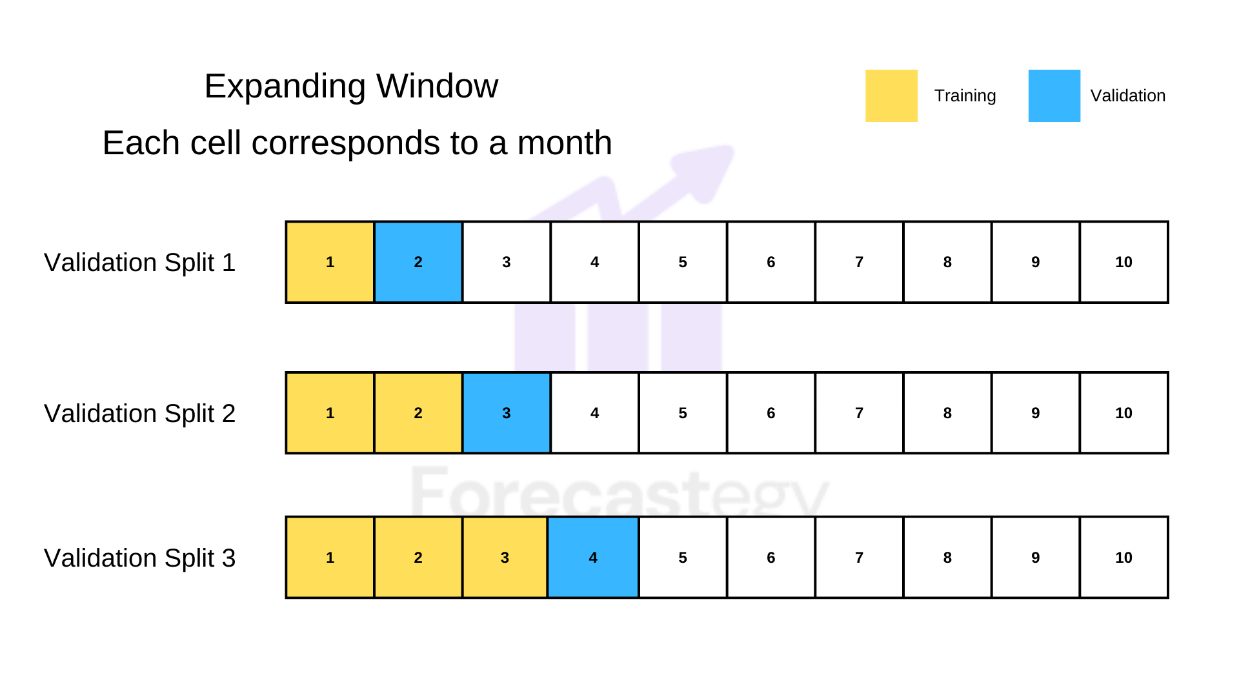


Figure : Expanding Window Time Series Split Validation (Source: (Filho, 2023))

## Initial Trial with Standard Scaler Applied

This test applied StandardScaler() to the following numerical categories: imbalance\_size, reference\_price, matched\_size, far\_price, near\_price, bid\_price, bid\_size, ask\_price and ask\_size. The results are shown in Table 1. It doesn’t seem to have significant improvement compared to training data without StandardScaler() applied.

## Initial Trial with k-fold cross-validation

This test uses the k-fold instead of TimeSeriesSplit for cross-validation. The results are shown in Figure 3. On average the model performs better compared to the model trained using the TimeSeriesSplit. Besides, there are two observations:

Observation 1: The is one part of the data (the first part) where the model predicts well.

Observation 2: The model performs better in the validation set when it is underfitting the training data. This happens when the validation score is lower than the training score achieved.

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Figure : Training scores and Validation scores for the initial run with k-fold cross validation

## Initial Trial with PCA

In this trial, Principle Component Analysis (PCA) was performed on the training data set hoping to improve the decision boundaries for the LightGBM model. However as PCA does not handle NaN values, there are two choices. The first choice is to drop all rows whenever one of the columns contains NaN values. However, there are too many NaN values in the far\_price and near\_price (about 2.8 million each), and dropping them will reduce the training data size to about 0.4 of the original. Although this approach yields good results (see Table 1), the good results applied only to the smaller dataset with NaN values available. Furthermore, the model won't be able to deal with new testing data that contains the NaN values. Hence this approach was not selected.

The second choice is to replace all the NaN values in the far\_price and near\_price columns with 0 while dropping other rows with NaN values. This approach preserves more than 99% of the training data. As shown in Table 1, this approach yields a minimal improvement compared to training with data without the PCA transformation.

## Summary of Preprocessing Techniques

Table 1 shows the summary of the comparison of the performance of the models using different preprocessing techniques. Based on the results, it can be concluded that,

* The training data exhibits stationary property with variations independent of time, hence processing the data in time series is not necessary.
* The best-performing model is likely to be the model that underfits the training data.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Test Title | Training Score | | Validation Score | |
| Average | Best Validate | Average | Best |
| Initial Run | 6.14128 | 6.34218 | 6.47656 | 5.88523 |
| With TimeSeriesSplit of 9 | 6.15360 | 6.34312 | 6.47738 | 5.90742 |
| With StandardScaler | 6.14125 | 6.34143 | 6.48478 | 5.88302 |
| With kfold | 6.29844 | 6.42056 | 6.32005 | 5.23449 |
| With PCA | 6.29813 | 6.42039 | 6.31976 | 5.23347 |
| With PCA(drop na) | 5.59804 | 5.69312 | 5.63493 | 4.77072 |

Table : Summary comparison of the performance of the models for different preprocessing techniques

# Exploring Feature Engineering

Figure 4 shows the feature importance (Gain) for all the features used to train the best model. It seems that the feature ask\_size and bid\_size play a significant role compared to the other features. Figure 5 shows the feature importance (Split) for all the features used to train the best model. The distribution of the feature importance is more even compared to the feature importance (Gain).

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Figure : Feature Importance (Gain) for the base model

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Figure : Feature Importance (Split) for the base model

## Removing Less Important Features

Based on the feature importance (Gain & Split) for the best base model shown before, an experiment was carried out by removing the four least important features (near\_price, stock\_id, far\_price, imbalance\_buy\_sell\_flag). The results are shown in table 2. Compared with the initial run, there is a slight drop in the average training score and validation score performance. As the extra features don’t affect the training speed and contribute slightly to the performance of the models, it is decided to keep these four features for future training.

## Adding First and Second Derivatives

The idea is to try to capture the movement trend (first and second derivative) for the eight potential trending features (matched\_size, bid\_price, ask\_price, wap, ask\_size, bid\_size, reference\_price, and imbalance\_size). Taking the reference price as an example, the hope is that if the model knows the relative movement of the reference price (change in price in last 10 seconds) and the relative change in movement (change of change in price in last 10 seconds) it can learn better the direction where the target is heading.

Figures 6 & 7 show the performance and feature importance (gain & split) for the model trained with the first and second derivatives of the reference price. As shown in the figure the first and second derivatives have a minor impact on the gain and split of the model. As shown in Table 2, there is minimal improvement in the training results compared to the initial base model.

Figures 8 & 9 show the performance and feature importance (gain & split) for the model trained with the first and second derivatives of the eight potential trending features. the first and second derivatives have a minor impact on the gain and split of the model, with the second derivatives generally having less impact compared to the first derivatives. As shown in Table 2, there is a minimal improvement in the training results compared to the initial base model, and negligible improvement compared with the model trained using additional first and second derivatives of the reference price.

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Figure : Feature Importance (Gain) for model trained with first and second derivatives of reference price

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Figure : Feature Importance (Gain) for model trained with first and second derivatives of reference price

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Figure : Feature Importance (Gain) for model trained with first and second derivatives of 8 features

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Figure : Feature Importance (Split) for a model trained with first and second derivatives of 8 features.

## Adding Imbalance Features

The imbalance features were proposed by one of the Kaggle competition participants (zhezhou, 2023). The results are shown in Table 2, Figures 10 & 11. As compared to the base model in Table 2, there is a minor improvement in the training results with the imbalanced features added in.

Based on Figures 10 & 11, one might wonder if only two imbalance features (imb\_s1 and imb\_s2) will be enough to improve the result. The test was carried out with only these two additional imbalance features. As shown in Table 2, there is a minor degradation of the overall training performance when only using two imbalanced features. Hence the suggestion is to keep all imbalanced features. The resulting test score using test data provided by the competition is 5.39 as shown in figure 13.

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Figure : Feature Importance (Gain) for model trained with imbalance features

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Figure : Feature Importance (Split) for model trained with imbalance features

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Figure : Test scores for the model trained with imbalance features

## Separate Model for the dependent variable

The prediction target is defined using the following formula (Forbes et al., 2023):

From the formula, only is known by the model, the model needs to predict both and . Thus the idea is to check if we create a model to predict these two term separately, will it perform better compared to the model predicting their result (the Target) directly?

Tests were conducted using two models with and without the imbalance factors with results shown in Table 2. It can be concluded that the two model approaches didn’t yield any improvement, probably due to the errors being compounded between the two models.

Pearson correlation and Spearman Correlation analysis were carried out between the columns and the target wap and target change in index separately. The results are shown in Figures 13 & 15. Based on the results, for target wap, only the columns wap, ask\_price, bid\_price, and reference\_price have moderate (absolute value of 0.3 – 0.5) relationship with the future wap, and this coincides well with the feature importance (gain & split) shown in figure 14 for the model to predict future wap.

For target change in the index, besides the target\_wap & target, none of the columns have a moderate or stronger relationship. The top five columns with weak relationships are wap, reference\_price, bid\_price, ask\_price, and near\_price. This coincides well with the feature importance (gain & split) shown in Figure 16 for the model to predict future wap.

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Figure : Correlation between the columns and the target\_wap, sorted by absolute value

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Figure : Feature Importance (Gain & Split) for the model to predict future wap

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Figure : Correlation between the columns and the target\_index, sorted by absolute value

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Figure : Feature Importance (Gain & Split) for the model to predict change in index

## Summary of feature engineering

Based on the experiment done against a set of features, it can be concluded that the best feature set will include the derivatives on the reference price and all the imbalance features. A final test was run using the best feature set. As shown in Table 2, this indeed generates the best average training scores, best average validation scores, and best validation scores from the cross-validation.

However, as it will be difficult to obtain the first and second derivatives with the test data provided, it is decided to use the imbalance factors only as extra features. The resulting test score is 5.39. The 2 models approach to predict the dependent variables separately was not selected as the validation scores and test scores are no better than the single model approach.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Test Title | Training Score | | Validation Score | | Test Score  (Submission) |
| Average | Best Validate | Average | Best |
| Initial Run with kfold | 6.29844 | 6.42056 | 6.32005 | 5.23449 | N/A |
| 4 features removed | 6.30591 | 6.42768 | 6.32560 | 5.23688 | N/A |
| With derivatives on Reference price | 6.29823 | 6.41934 | 6.31806 | 5.23228 | N/A |
| With derivatives on all trend features | 6.29823 | 6.41934 | 6.31804 | 5.23228 | N/A |
| With all imbalance features | 6.26616 | 6.38593 | 6.28535 | 5.1937 | 5.39 |
| With only two imbalance features | 6.29743 | 6.41905 | 6.31597 | 5.22403 | N/A |
| With derivatives on reference price & all imbalance features | 6.26397 | 6.38409 | 6.28376 | 5.19254 | N/A |
| 2 model | 6.42320 | 6.54786 | 6.47963 | 5.28060 | 5.4613 |
| 2 model with imbalance features | 6.39075 | 6.51506 | 6.43437 | 5.26175 | 5.4391 |

Table : Summary comparison of the performance of the models for different feature sets

# Exploring Hyperparameter Tuning

An experiment with Hyperparameter tuning was carried out using the Optuna library with reference to one of the online guides (T., 2023).

Selected Hyperparameter for tuning are as follows:

* n\_estimators (default=100) – set to 10,000, controls the number of decision trees, a higher number may result in overfitting and longer training time. Often tuned together with the learning rate.
* learning\_rate (default=0.1) - range between 0.01 – 0.3, controls the learning speed. A smaller number leads to a slower learning rate, and the need to use early stopping rounds to terminate the training early to avoid excessive long training duration.
* num\_leaves (default=31) range between 20 – 3000, controls the number of decision leaves in a single tree. Range limit also depends on the max\_depth and should be 2^(max\_depth) according to LGBM documentation.
* max\_depth(default=-1) – range between 3 – 12, control the level of the tree. Lower numbers may lead to underfitting, higher numbers may lead to overfitting.
* min\_data\_in\_leaf(default=20) – range between 200 – 10000, specifies the minimum number of observations that fit the decision criteria in a leaf. Lower numbers may lead to overfitting.
* max\_bin(default=255) – range between 63 – 256. Smaller values increase the training speed while larger values increase the accuracy (Bahmani, 2023). For GPU training max\_bin limit is 256.
* min\_gain\_to\_split(default=0) – range between 0 – 15. Similar to XGBoosts’s gamma. Can be used as extra regularization in large parameter grids.

Figure 17 shows the best hyperparameter setting obtained from the first run. Figure 18 & Figure 19 shows the Optimization history and hyperparameter importance. As can be seen from Table 3, the model trained with tuned parameters performs slightly better with better average & best training and validation scores, as well as test score upon submission.

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Figure 17: Best hyperparameters setting for first tuning (note optimization goal is minimum validation score achieved)

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Figure 18: Optimization History Plot for first tuning

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Figure 19: Hyperparameter Importance ranking for first tuning.

The second run included all parameter choices from the first run with the following additions/modifications:

* subsample (or bagging\_fraction, default=1) – specify the percentage of rows used per tree building iteration. Improved generalization but also speed of training (Bahmani, 2023).
* Change the n\_estimators to 1000
* Modify the range for num\_leaves to be within 2^(max\_depth-1) – 2^(max\_depth)
* Modify the range for max\_bin to between 32 and 256.

The best hyperparameter settings obtained are shown in Figure 20. As shown in Table 3, the average training scores and validation scores improved compared to the baseline, but the submission test score is slightly worse.

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Figure 20: Best hyperparameters setting for second tuning (note optimization goal is minimum average validation score achieved)

The third run included all parameter choices from the second run with only one modification:

* Change the n\_estimators setting from the default value (1000) to a suggestion range between 50 to 500 with a step of 50. As higher n\_estimators increased the training time required significantly with a potential risk of overfitting, this attempt is to find the n\_estimator that allows the model to train fast and generalize better.

The best hyperparameter settings obtained are shown in Figure 21. As shown in Table 3, the average training scores and validation scores improved compared to the baseline, and the submission test score is the best achieved thus far.

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Figure : Best hyperparameters setting for third tuning (note optimization goal is minimum average validation score achieved)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Test Title | Training Score | | Validation Score | | Test Score  (Submission) |
| Average | Best Validate | Average | Best |
| Baseline (with imbalance factors) | 6.26616 | 6.38593 | 6.28535 | 5.1937 | 5.39 |
| First Tuning | 6.19929 | 6.31821 | 6.27048 | 5.1798 | 5.3823 |
| Second Tuning | 6.22611 | 6.34055 | 6.27049 | 5.1807 | 5.3906 |
| Third Tuning | 6.23874 | 6.35838 | 6.27021 | 5.1807 | 5.3785 |

Table 3: Summary comparison of the performance of the models for different hyperparameter tuning trial

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