Introduction:

In machine learning, there are many algorithms to select for a model. What algorithm to choose can be filtered by analysing the problem and the data. After the filtration process, we are often left with multiple algorithms to select for a model. In this case, if feasible, we should train and tune multiple algorithms to find the best algorithm. In this report, we dive into the practice of using and tuning different models. The report will go through each step involved in solving a machine learning problem:

1. We will define a problem.
2. We will tweak our data to fit the problem.
3. We will define and tune the models.
4. We will compare and evaluate the models.

The three models to be used in the report are:

1. XGBoost
2. Logistic Regression
3. Neural network

Problem Formulation:

The problem presented in the report is from the Jane Street Market Prediction competition. The competition involves predicting whether a trade will be profitable or not given the input. The competition's evaluation uses a utility function; however, our evaluation will be which model has more significant profit potential.

Data used to train/validation/test the model contains the date, weight, four resp (return) columns, and 130 feature columns. Each row represents a trade, and different resp values represent the different returns. For simplicity, we will ignore the multiple resp value and weights. We will use one of the resp columns to evaluate if the trade should be taken or not. If the resp is below 0, we will label 0, and 1 if resp above 1. The goal of our model will be to predict if a given trade should be 0 or 1. In other words, this is a binary classification problem.

In the end, we will compare which model can predict profitable trades more while minimizing losing trades. The model that does it the best will classify as a better model.

Preparing the data:

Before initializing the models, we need to clean and prepare our data. We will first clear all the zero weights. Second, we will replace all the missing features with an arbitrary number. We will then extract our features and binary labels.

Since there are ~2 million data entries, we will split it into 55% train – 20% Validation – 25% Test.

Finally, now that our data is ready, we can start designing models.

Approaches:

The three models mentioned in the introduction will train along with a baseline model in this section. We will make all our models use the same loss function and the same evaluation metrics for a more accurate comparison. For the loss function, we will use the binary cross-entropy/Log-Loss function. Log-Loss is taking a negative log of the predicted probability and multiplying it with the actual result. For the evaluation metric, we will use the Area Under Curve. As seen in the figure, AUC is an area under the curve that models False-Positive vs. True-Positive rate. We want the area to be high as possible, as a higher area means better predictions. More information on the loss function and AUC is under the Appendix.

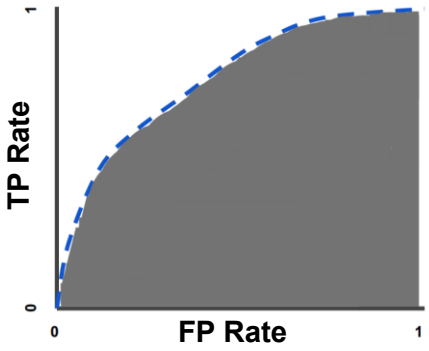


Figure 1: AUC curve

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

Figure 2: Log-Loss function

Baseline:

For the baseline, we will utilize scikit-learn's dummy classifier. For classification, we will be using the most frequent classifier. The most frequent classifier will always predict the most frequent label in the training set.

We do not need to tune/optimize our dummy model as it is an inherently flawed model.

	precision	recall	f1-score	support
0.0	0.00	0.00	0.00	245475
1.0	0.50	1.00	0.67	249847
accuracy			0.50	495322
macro avg	0.25	0.50	0.34	495322
weighted avg	0.25	0.50	0.34	495322

Accuracy: 0.5044132907482405

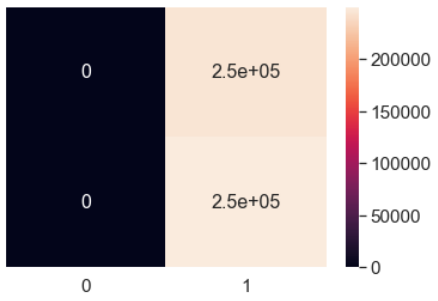


Figure 3: Classification report and confusion matrix

Xtreme Gradient Boosting:

```
print(optimal_param.best_params_)
```

```
{'learning_rate': 0.01, 'max_depth': 15, 'n_estimators': 1200}
```

Figure 4: Optimal parameter generated

The second model we are going to try is one of Kaggle's favourite learning algorithm. XGBoost is known for its speed and its predictive power. XGBoost is a decision tree algorithm combined with other optimizing algorithms such as Parallel Learning to achieve speed and power.

There are numerous parameters to play around with in XGBoost. We will optimize XGBoost by optimizing three hyperparameters. Explanations for the three hyperparameters are below.

- Learning rate: The rate at which the algorithm updates. Range: [0.01, 0.05, 0.005]
- N_esimators: Number of trees. Range: [600, 1000, 1200]
- Max_depth: Maximum depth of the decision tree. Greater depth makes the model more powerful but could overfit. Range: [6, 11, 15]

To prevent overfitting, we can introduce randomness in the data. For randomness, we will put sub_sample to 0.70 and colsample_bytree to 0.50. Sub_sample 0.70 will randomly select 0.70 of data every boosting iteration, and colsample_bytree 0.50 will drop 50% of the columns when training.

To select the best combination of parameters, we will be using the grid search cross-validation from sklearn.

Figure 4 shows the validation AUC while training the model with the parameters from figure 3.

Figures 6 and 7 are our classification report and confusion matrix generated from our inference on the test data. We will explain and compare them under discussion.

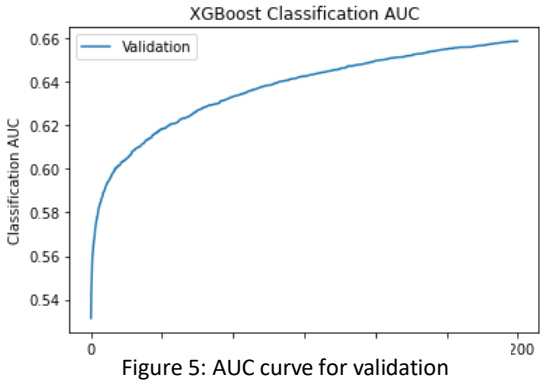


Figure 5: AUC curve for validation

	precision	recall	f1-score	support
0.0	0.61	0.58	0.59	245475
1.0	0.60	0.63	0.62	249847
accuracy			0.60	495322
macro avg	0.60	0.60	0.60	495322
weighted avg	0.60	0.60	0.60	495322

Accuracy: 0.6039445047867852

Figure 6: Classification report of XGBoost

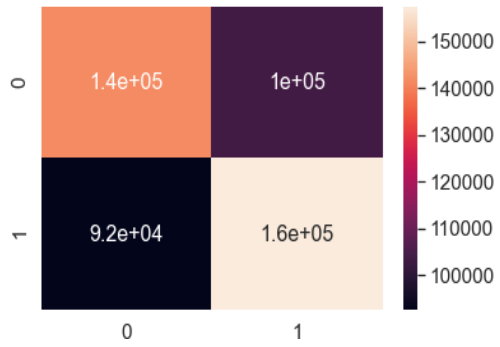


Figure 7: Confusion Matrix

The breakdown from figure 6:

True-Negative: 1.4

False-Positive: 1.0

False-Negative: 0.92

True-Positive: 1.6

Logistic regression:

The third model we will implement is a simple logistic regression model. We will be using Keras from TensorFlow to implement it. For logistic regression, we will be optimizing two hyperparameters. One is the epochs, and another is the learning rate. Running grid search on full data takes a long time; therefore, we will be tuning our parameter with only 100,000 data entries.

```
print(grid.best_params_)
```

```
{'epochs': 700, 'learning_rate': 0.001}
```

Figure 8: Optimal parameter generated

For the optimization algorithm, we will be using Adam's optimizer as it has shown to be one of the better optimizers from time to time.

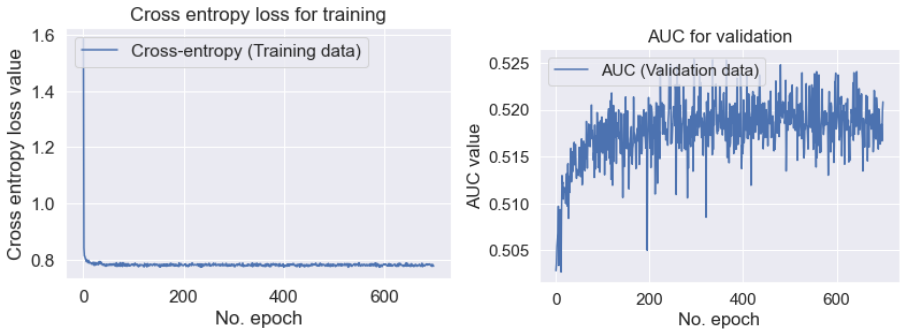


Figure 9: Training loss and AUC validation

	precision	recall	f1-score	support
0.0	0.51	0.40	0.45	245475
1.0	0.52	0.63	0.57	249847
accuracy			0.52	495322
macro avg	0.52	0.51	0.51	495322
weighted avg	0.52	0.52	0.51	495322

Accuracy: 0.5156060098279504

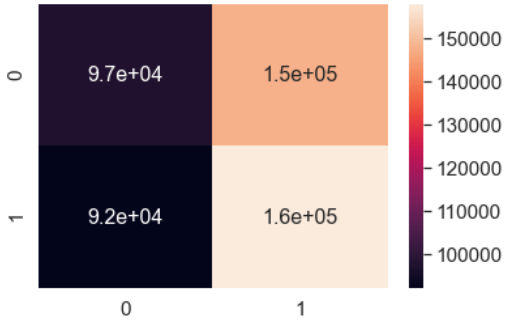


Figure 10: Classification report and confusion matrix

Our accuracy for logistic regression is 52%, and the breakdown for each category is listed below:

True-Negative: 0.97

False-Positive: 1.5

False-Negative: 0.92

True-Positive: 1.6

2-layer neural network:

In this model, we try to solve our problem using a neural network. We will be using two hidden layers to compute an output. For the hidden layers' activation function, we decided to go with Swish. A popular choice for activation function is ReLU, but according to the research conducted by Ramachandran et. Al.[1], swish outperformed ReLU. Therefore, we will be conducting our experiment with Swish.

The formula for swish is $x\sigma(\beta x)$ where beta is a constant or trainable constant. We will use TensorFlow's swish function for the experiment, where the beta is 1.

Like the previous model, we will be using Adam's optimization. We will be tuning the number of units in the hidden layer and the learning rate for hyperparameter tuning.

In a neural network with many data entries, we often run into the problem of overfitting. To prevent overfitting, we will be using a dropout technique. Dropout is dropping a portion of units that feed into the next layer. A paper published in 2014[2] proves dropout a successful strategy in preventing overfitting.

We will be using a fixed dropout rate of 50%. Ideally, this parameter is also tuned, but we will be using a fixed rate due to the excessive tuning time.

To further decrease grid search time, we reduced the number of data entries to 100000. The optimal parameter for hidden units came out to be 64, and the training rate of 0.001. We used it to train on our training set and made inferences on the test data. Below figures display the finding.

[1] Searching for Activation Functions (arxiv.org)

[2] srivastava14a.pdf (jmlr.org)

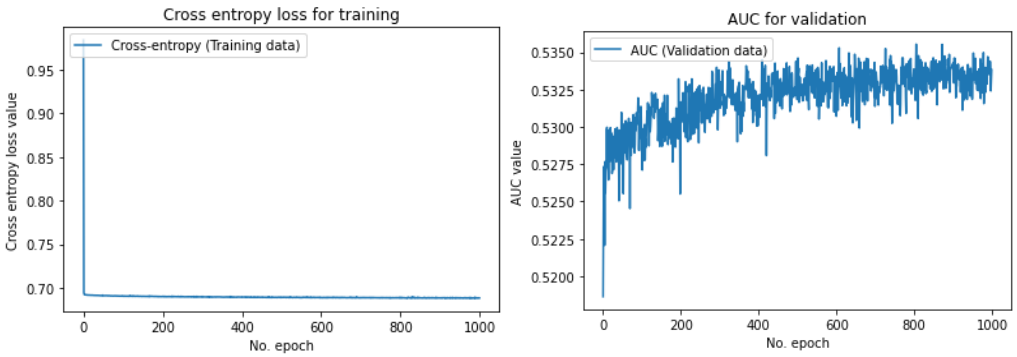
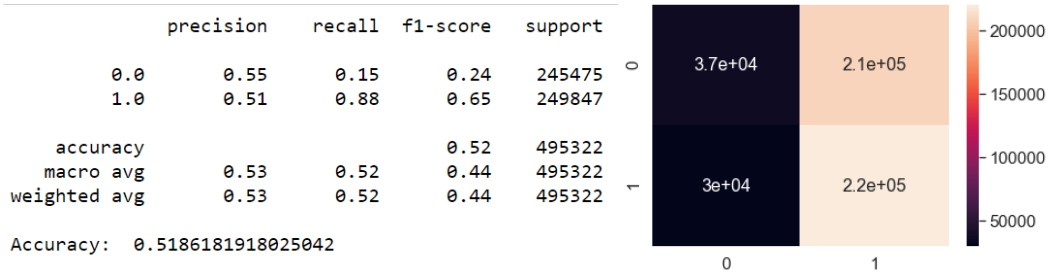


Figure 11: Training loss and AUC validation



	precision	recall	f1-score	support
0.0	0.55	0.15	0.24	245475
1.0	0.51	0.88	0.65	249847
accuracy			0.52	495322
macro avg	0.53	0.52	0.44	495322
weighted avg	0.53	0.52	0.44	495322

Accuracy: 0.5186181918025042

Figure 12: Classification report and confusion matrix

Our accuracy for logistic regression is 52%, and the breakdown for each category is listed below:

True-Negative: 0.37

False-Positive: 2.1

False-Negative: 0.3

True-Positive: 2.2

Discussion:

Comparing to the baseline model, all models did better. Accuracy of the baseline is 0.50, XGBoost is 0.60, logistic regression and neural network is 0.52. We notice that the accuracy of logistic regression and neural network is only slightly better. If all our model gave accuracy close to the baseline, we would need to reconsider the data or the approach. Since our XGBoost did much better than baseline, we can move forward for additional comparison to select the final candidate.

If we compare three models amongst each other, we see that XGBoost has the highest accuracy.

However, accuracy is not enough. We want to minimize the loss when we are risking money. The only time we are risking money is when the model predicts 1. As a result, we should look at the precision of our positive predictions. Precision will tell us how often the trade we execute is profitable.

$$Precision = \frac{TP}{TP + FP}$$

Looking at the classification report for each model, we find XGBoost has a precision of 0.60, logistic regression has a precision of 0.52 and a neural network with a precision of 0.51.

Comparing the accuracy and precision, XGBoost has the edge over the other two models.

The third edge of XGBoost comes from its time to train. Training on XGBoost only took about 10 minutes, where our other two models took more than an hour to train. The time is a considerable advantage for XGBoost over the two.

Conclusion and Future Work:

We successfully trained three models and compared them against the baseline. Our results indicated that the accuracy of logistic regression and neural network is 2% better than the baseline. XGBoost produced an accuracy that is 10% higher than the baseline. Comparing the three with each other, we found XGBoost has the edge over the other two models in terms of accuracy, precision, and training time. XGBoost is the best suitable solution to our problem.

To further improve our results, there are a couple of things we can do. Firstly, we can factor in the weights and various types of return values. Secondly, we can do further exploratory data analysis to get to know our data more closely. We can also perform various algorithms, such as Boruta[3], to help us filter our irrelevant features. All three points can help us obtain a more relevant and accurate dataset. In terms of models, we can perform more in-depth hyperparameter tuning. Instead of tuning hyperparameter on a subset of data, we can perform tuning on the whole dataset. To make tuning faster, we can even consider a random search instead of a grid search.

[3] Is this the Best Feature Selection Algorithm "BorutaShap"? | by Eoghan Keany | Analytics Vidhya | Medium

Appendix:

Cross-Entropy Loss: Understanding binary cross-entropy / log loss: a visual explanation | by Daniel Godoy | Towards Data Science

AUC curve: Classification: ROC Curve and AUC | Machine Learning Crash Course (google.com)