



CZ4041: Machine Learning



Project: NYC taxi trip duration prediction (Kaggle)





Presented by Group 21

Meet the Team

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Build a model that predicts the ride durations of Taxi Trips in New York City

NYC Taxi Trip Duration Dataset

id
vendor_id - taxi company
pickup_datetime, dropoff_datetime
passenger_count
pickup long/lat, dropoff long/lat
store_and_fwd_flag - trip record
submitted manually?
trip_duration - duration of the trip
in seconds

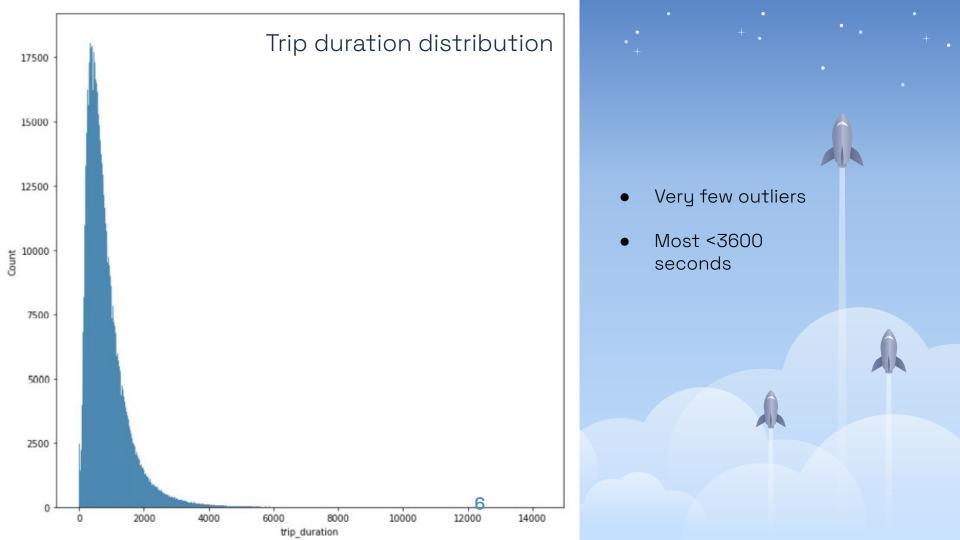
NYC Taxi with OSRM

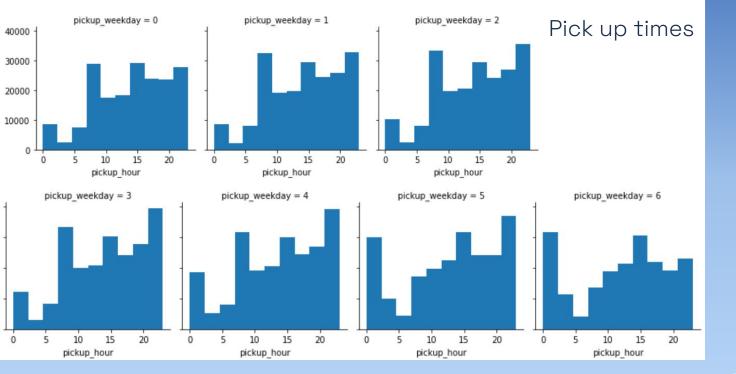
starting_street end_street total_distance total_travel_time number_of_steps - step consists of some driving and a turn or going on to a highway street_for_each_step - a list of streets where each step occurs distance_per_step travel_time_per_step step_maneuvers - e.g. taking turn step_direction **step_location_list** - the coordinates for each action





1. Exploratory Data Analysis





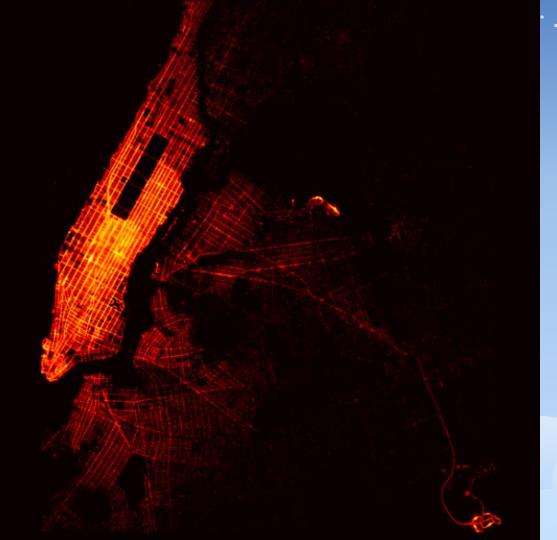


- Peak after midnight during weekends
- Very consistent!







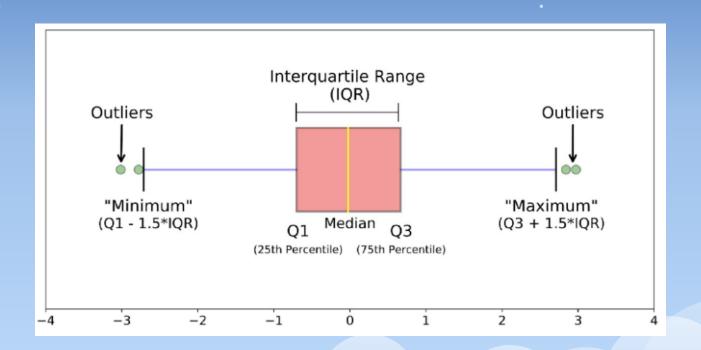


Trip start/endpoint heatmap

- Streets clearly visible
- Mostly around center of Manhattan
- None in Central Park















Feature Engineering & Selection

Date time features extracted from raw timestamp

PCA on longitude/latitude

Manhattan-Haversine distance of trip

OSRM - calculate theoretical fastest (shortest) path









2. Extreme Gradient Boosting (XGBoost)



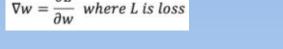


Gradient Boosting

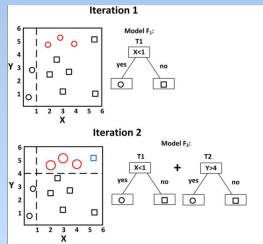
Gradient Descent

$$\nabla w = w - \eta \nabla w$$

$$\nabla w = \frac{\partial L}{\partial w} \text{ where } L \text{ is loss}$$



Ensemble of weak learners -> strong learner



One new decision tree at a time

Address shortcomings of other weak learners







Techniques

Backwards **tree pruning** for each weak learner **Cross-validation** to tune hyperparameters

Parallelisation and cached gradient vectors





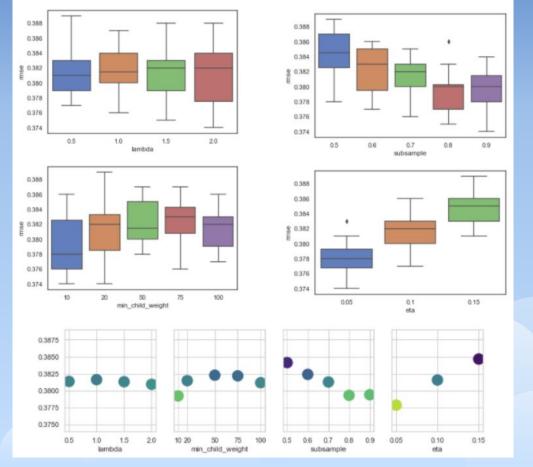
Objective Function

RMSE loss + regularization





Hyperparam Optimisation







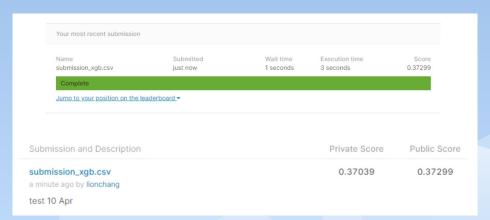


Final results XGB

Training RMSE: 0.13582

Validation (k-fold): 0.36754

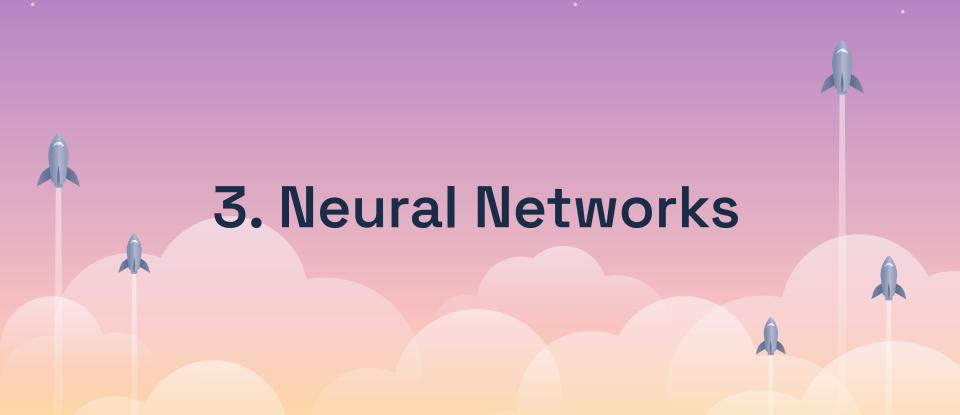
Test (Kaggle): 0.37299











Neural Network Overview & Architecture

- Neural networks are a subset of machine learning and form the basis of deep learning algorithms.
- A feed forward network architecture was created using TensorFlow (Keras) for this project.
- All hidden layers in the network are Dense (Fully Connected).
- Batch normalization (BN) layers are introduced to improve the training stability, allowing for quicker convergence.
- Training data is split into batches, and for each batch of inputs to each BN layer, inputs are normalized with respect to their batch in both batch size and input size dimensions.



Hyperparameters Tuned

- Number of Dense (FC) Layers Network Depth
 - Between 4 and 64 layers
- Number of Neurons per Dense Layer Network Breadth:
 - Between 16 and 512 neurons per layer
- Optimizers for Gradient Descent
 - Stochastic Gradient Descent (SGD), Momentum, RMSProp, and Adam.
- Learning Rate (α)
 - Tested α values from the range: 10^-2 < α < 10^-4
- Regularization
 - None vs. L2 Kernel/Bias vs. Dropout Regularization







Neural Network Experiments

- Random Search used for Hyperparameter tuning.
- Model was overfitting quickly so training was usually stopped at 100 epochs.
- Experimented with different batch sizes initially [16, 32, 64, 128, 256], but final batch size was 128.
 - Trade-off between no. of gradient descent updates per epoch & training time per epoch (larger batches => less time).
 - Dataset is large (>1.4 million training examples).
- Used a Train-Validation split of 80:20.







Important Results

Hyperparameters	Train RMSE	Validation RMSE	Leaderboard Score (Public)
16 layers, 256 neurons per layer, SGD, no regularization, learning rate = 1e-2	0.43314	0.43201	0.47360
16 layers, 256 neurons per layer, Adam, no regularization, learning rate = 1e-3	0.42165	0.42784	0.46209
16 layers, 256 neurons per layer, Adam, L2 reg. factor = 1e-5, learning rate = 1e-3	0.41398	0.41239	0.43442
16 layers, 256 neurons per layer, Adam, Dropout w/drop-rate = 0.2, learning rate = 1e-3	0.41887	0.43542	0.45930
32 layers, 256 neurons per layer, Adam, L2 reg. factor = 1e-5, learning rate = 1e-3	0.40480	0.39246	0.41522
40 layers, 400 neurons per layer, Adam, L2 reg. factor = 5e-5, learning rate = 1e-3	0.39921	0.38803	0.39963

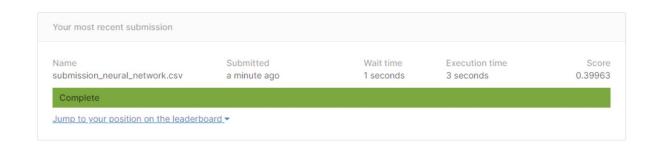
Table of Results for Neural Networks with Various Combinations of Hyperparameters

- Table shows main results.
- Best (final) model highlighted in green.
- Best optimizer: Adam (vs. SGD, RMSProp, etc.).
- Error decreased with increasing network depth and breadth.
- Learning rate adjusted based on Adam (α = 1e-3).
- L2 regularization helped improve ability of NN to generalize to new data.





Results of Final Neural Network Model



Submission and Description	Private Score	Public Score
submission_neural_network.csv a minute ago by Abhinandan Padhi	0.39758	0.39963

add submission details



Analysis of Experimental Results

- Clearly, XGBoost performed better than Neural Networks for predicting NYC Trip Duration. Why?
- Possible reasons:
 - XGBoost has the big advantage of Ensemble learning, NN does not.
 Ensemble Learners are especially popular for NYC dataset.
 - Further hyperparameter tuning could have improved NN performance, but is difficult due to computational and time constraints.
- While XGBoost allows for Top 6% Kaggle LB rank, higher performance might have been possible with Weather data or more external data.
- Some taxis/drivers may be faster or "more aggressive" than others, so predicting trip duration would be complicated further.







Summary of The Project

- We have explored various types of Exploratory Data Analysis
 (EDA) techniques to better understand trends/patterns in the NYC
 data.
- Applied outlier detection using IQR and Z-score approach.
- Performed feature engineering and selection on our dataset.
- For prediction, we experimented with two types of models:
 XGBoost and Neural Networks.
- Experiments and analysis shows that XGBoost outperformed the Neural Network models.
- Thus, XGBoost is a great solution to the NYC Taxi Trip Duration prediction problem.





Challenges Faced

- 1. Data was noisy and contained both outright errors and non-standard behaviour.
- 2. Trip duration was affected by various factors, e.g. time of the day, speed, and trip distance.
- 3. NYC data had relatively few features per training example, so external data was required.
- 4. Training Machine/Deep Learning models was computationally expensive and time-consuming.
- 5. Division of work was difficult due to dependencies between different aspects of our project.







Our Solutions to the Challenges

- 1. Discovered ways to filter bad data to improve prediction accuracy.
- 2. Explored factors and created new features to account for these factors.
- 3. Used NYC-OSRM dataset from Kaggle, though processing and merging with the original data was challenging.
- 4. Had to use cloud services for computation, e.g. Google Colaboratory and Kaggle GPUs.
- 5. We attempted to collaborate on the code by sharing code on a group GitHub repository and using Google Colaboratory.







Possible Future Improvements

- 1. Different methods for outlier removal and data cleaning.
- 2. Engineer more (and better) features and select features more carefully.
- 3. Experiment with other complex models to see if performance is better.







