Wine Quality

AWS Sagemaker - XG Boost

Problem Being Solved
&
Dataset

Guidelines

Problem being solved: Can machine learning be used to determine if a wine is good given its physico-chemical properties? If we get a dataset with the amount of chlorides, acidity of a wine, its residual sugars, citric acid, sulfur dioxide and other properties, will an AI find out if a particular wine is of grade 5, 6 or 8 for example? Let's find out.

Dataset and features : The project is based on a dataset donated to the UCI machine learning repository in 2009, https://archive.ics.uci.edu/ml/datasets/wine+quality and it was collected by: Paulo Cortez, University of Minho, Guimarães, Portugal, http://www3.dsi.uminho.pt/pcortez A. Cerdeira, F. Almeida, T. Matos and J. Reis, Viticulture Commission of the Vinho Verde Region(CVRVV), Porto, Portugal @2009

Relationship between the data and problem being solved: The dataset collected seems perfect for the problem. It provides all the physicochemical characteristics of white wines and about 4898 wines analysed. This dataset also looks great for the fact that all the data is completed and there are no empty/blank data in the .csv file.

Guidelines

How an update to the dataset will impact the solution: This dataset is a precious material for sommeliers all over the world. They can get information about a wine's acidity and grade instantly. The idea is that any person can insert all the characteristics of a new wine in the dataset and get an estimated grade about its quality. To update it; the user would need to insert: both fixed & volatile acidity, residual sugars, citric acid, chlorides, free & total sulfur dioxide, pH, sulphates, alcohol, and density to get an estimated quality grade between 1-9. The dataset doesn't regard region of wine production or year; only its chemical information.

The pros and the cons of the available data: The pros is that the data was publicly available. In the field of data science; I'm happy to refer the authors Paulo Cortez, University of Minho, Guimarães, Portugal, http://www3.dsi.uminho.pt/pcortez A. Cerdeira, F. Almeida, T. Matos and J. Reis as an appreciation gesture to their work. The dataset is supervised learning and all the features and labels were completed, with no missing information for the 4898 wines (labels) and its 12 features.

The additional resources that will help to improve the solution and possible means to collect it: Since this dataset is already 11 years old; it would be interesting to get additional recent data to compare and improve the dataset with more reliable data. The only way to collect this would be based on generosity of portuguese white wine producers.

The Dataset

```
!wget -N https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.csv
```

```
--2020-12-03 14:10:49--  https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.csv
Resolving archive.ics.uci.edu (archive.ics.uci.edu)... 128.195.10.252
Connecting to archive.ics.uci.edu (archive.ics.uci.edu)|128.195.10.252|:443... connected.
HTTP request sent, awaiting response... 304 Not Modified
File 'winequality-white.csv' not modified on server. Omitting download.
```

```
!head winequality-white.csv
```

```
"fixed acidity";"volatile acidity";"citric acid";"residual sugar";"chlorides";"free sulfur dioxide";"total sulfur dioxide";"density";"p
H";"sulphates";"alcohol";"quality"
7;0.27;0.36;20.7;0.045;45;170;1.001;3;0.45;8.8;6
6.3;0.3;0.34;1.6;0.049;14;132;0.994;3.3;0.49;9.5;6
8.1;0.28;0.4;6.9;0.05;30;97;0.9951;3.26;0.44;10.1;6
7.2;0.23;0.32;8.5;0.058;47;186;0.9956;3.19;0.4;9.9;6
7.2;0.23;0.32;8.5;0.058;47;186;0.9956;3.19;0.4;9.9;6
8.1;0.28;0.4;6.9;0.05;30;97;0.9951;3.26;0.44;10.1;6
6.2;0.32;0.16;7;0.045;30;136;0.9949;3.18;0.47;9.6;6
7;0.27;0.36;20.7;0.045;45;170;1.001;3;0.45;8.8;6
6.3;0.3;0.34;1.6;0.049;14;132;0.994;3.3;0.49;9.5;6
```

```
import numpy as np  # For matrix operations and numerical processing
import pandas as pd # For munging tabular data
```

```
# https://pandas.pydata.org/pandas-docs/stable/generated/pandas.read_csv.html
data = pd.read_csv('winequality-white.csv', sep=';')
pd.set_option('display.max_columns', 500)     # Make sure we can see all of the columns
pd.set_option('display.max_rows', 50)         # Keep the output on one page
data[:5]
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	6
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	6
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	6
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6

```
data.shape # (number of lines, number of columns)
```

```
(4898, 12)
```

Julien Simon - XGBoost Tutorial

https://medium.com/@julsimon/aws-ai-machine-learning-podcast-episode-11-xgboost-special-492f64356a29
https://www.youtube.com/watch?v=w0F4z0dMdzI&t=206s

His problem: Classification / Direct Marketing Dataset //using just 1 label (y_yes):

XGBoost Classifier: { objective: binary_logistic ; eval_metrics: auc ; max_depth: max_depth}

"**Bibliography**" : https://gitlab.com/juliensimon/ent321/-/blob/master/ENT321%20-%20short%20version.ipynb

4 days stuck in one line of code due to an SDK version update and the clue went straight to my Junkmail folder::

Lauren Yu Inbox - julia...itsencrypted.com December 1, 2020 at 7:54 PM

Re: [aws/sagemaker-python-sdk] SDK 2.0: image_uris.retrieve() fails for XGBoost 1.0-1 (#1748) Details

To: aws/sagemaker-python-sdk, Cc: itsencrypted, Mention,

Reply-To: aws/sagemaker-python-sdk

This message is from a mailing list. Unsubscr

@itsencrypted you need to swap the order of your first two arguments for `retrieve()`:

```
container = sagemaker.image_uris.retrieve('xgboost', region, 'latest')
```

docs: https://sagemaker.readthedocs.io/en/stable/api/utility/image_uris.html#sagemaker.image_uris.retrieve

if you need more assistance, please open a new issue (since this one is closed).

—

You are receiving this because you were mentioned.
Reply to this email directly, view it on GitHub, or unsubscribe.

```
from sagemaker.amazon.amazon_estimator import get_image_uri

container = get_image_uri(boto3.Session().region_name, 'xgboost')
role      = sagemaker.get_execution_role()   # Role when working on a notebook instance
sess      = sagemaker.Session()

xgb = sagemaker.estimator.Estimator(container,
                                    role,
                                    train_instance_count=1,
                                    train_instance_type='ml.m4.2xlarge',
                                    input_mode="File",
                                    output_path='s3://{}/{}/output'.format(bucket, prefix),
                                    sagemaker_session=sess)
```

Jupyter Notebook - Data Manipulation

29	7.2	0.32	0.36	2.00	0.033	37.0	114.0	0.9906	3.10	0.71	12.3	7

In [11]:
```
data.shape # (number of lines, number of columns)
```

Out[11]:
```
(4898, 12)
```

In [27]:
```
one_class = data[data['quality']<=7]
one_class_count = one_class.shape[0]
print("Normal quality wines: %d" % one_class_count)

zero_class = data[data['quality']>=8]
zero_class_count = zero_class.shape[0]
print("Excellent Quality wines: %d" % zero_class_count)

zero_to_one_ratio = zero_class_count/one_class_count
print("Ratio: %.2f" % zero_to_one_ratio)
```

```
Normal quality wines: 4718
Excellent Quality wines: 180
Ratio: 0.04
```

In [30]:
```
[np.min(data['residual sugar']), np.max(data['residual sugar'])]
```

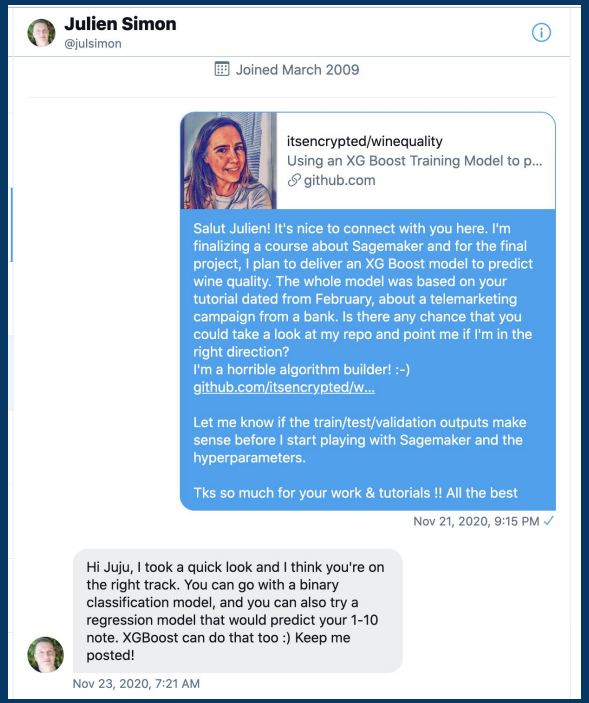
Out[30]:
```
[0.6, 65.8]
```

In [31]:
```
#wines with very high residual sugar are low quality. wines with a balanced residual sugar are better quality
```

In [32]:
```
# Indicator variable to capture when residual sugar takes a value higher than 2.5
# https://docs.scipy.org/doc/numpy-1.15.1/reference/generated/numpy.where.html
data['very sweet'] = np.where(data['residual sugar'] >= 2.5, 1, 0)
data = data.drop(['residual sugar'], axis=1)
```

In [33]:
```
data['fixed acidity'].value_counts()
```

Initial idea: do a classification model and separate the wine between “good quality” = 1 and “not good quality” = 0



Feature Engineering

Feature Engineering

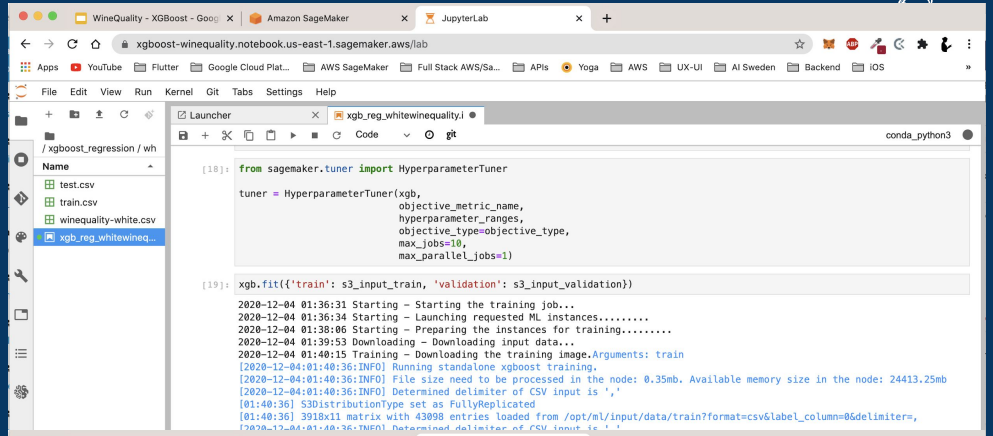
The features and basic characteristics

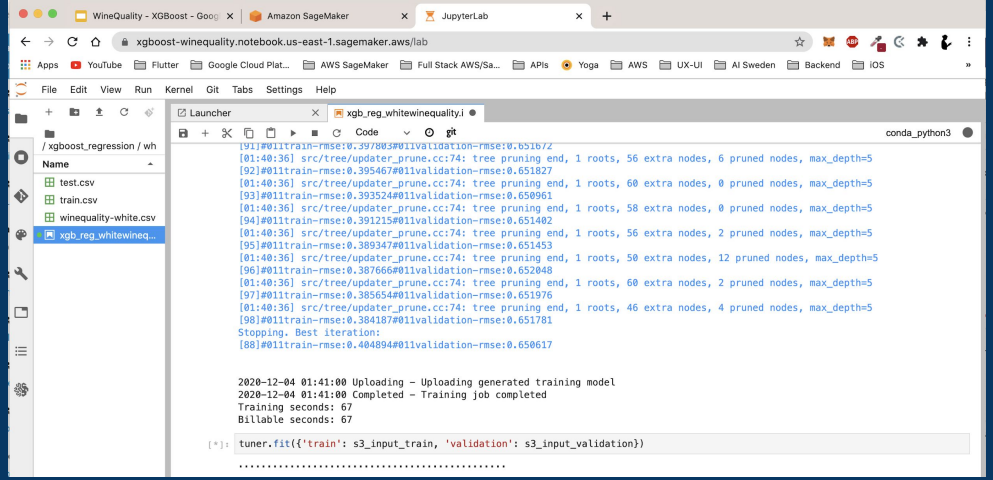
The process of creating features from raw data

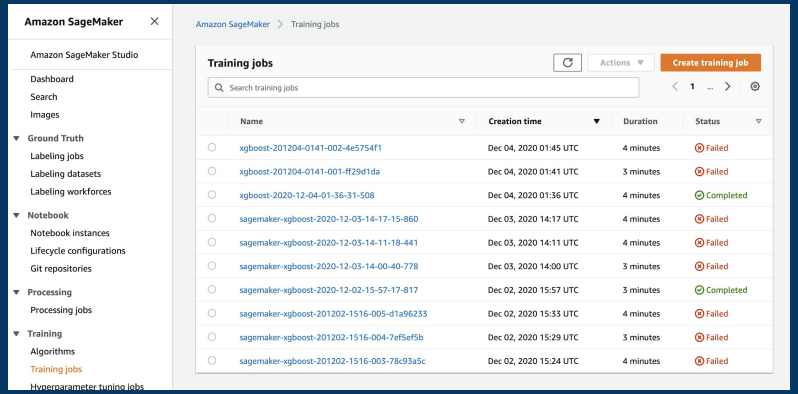
The statistics of the features after feature engineering & comment on possible variations

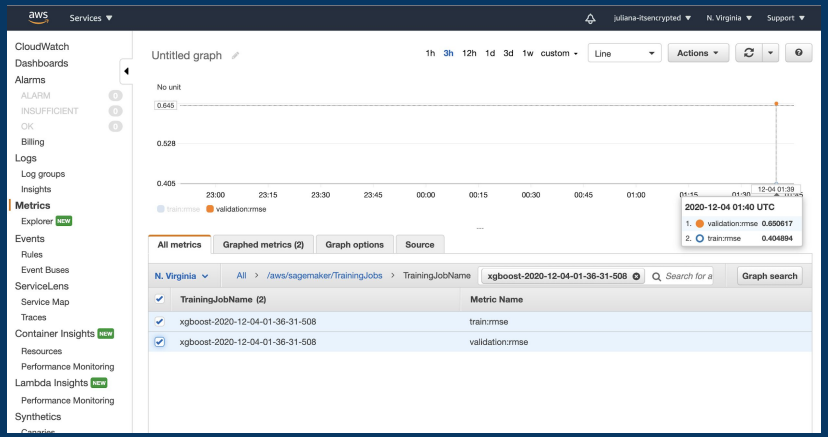
Create multiple datasets with different feature engineering techniques and describe the results

Training Model









About the Algorithm chosen

XGBoost Algorithm

PDF | Kindle | RSS

The XGBoost (eXtreme Gradient Boosting) is a popular and efficient open-source implementation of the gradient boosted trees algorithm. Gradient boosting is a supervised learning algorithm that attempts to accurately predict a target variable by combining an ensemble of estimates from a set of simpler and weaker models. The XGBoost algorithm performs well in machine learning competitions because of its robust handling of a variety of data types, relationships, distributions, and the variety of hyperparameters that you can fine-tune. You can use XGBoost for regression, classification (binary and multiclass), and ranking problems.

You can use the new release of the XGBoost algorithm either as a Amazon SageMaker built-in algorithm or as a framework to run training scripts in your local environments. This implementation has a smaller memory footprint, better logging, improved hyperparameter validation, and an expanded set of metrics than the original versions. It provides an XGBoost `estimator` that executes a training script in a managed XGBoost environment. The current release of SageMaker XGBoost is based on the original XGBoost versions 0.90, 1.0, and 1.2.

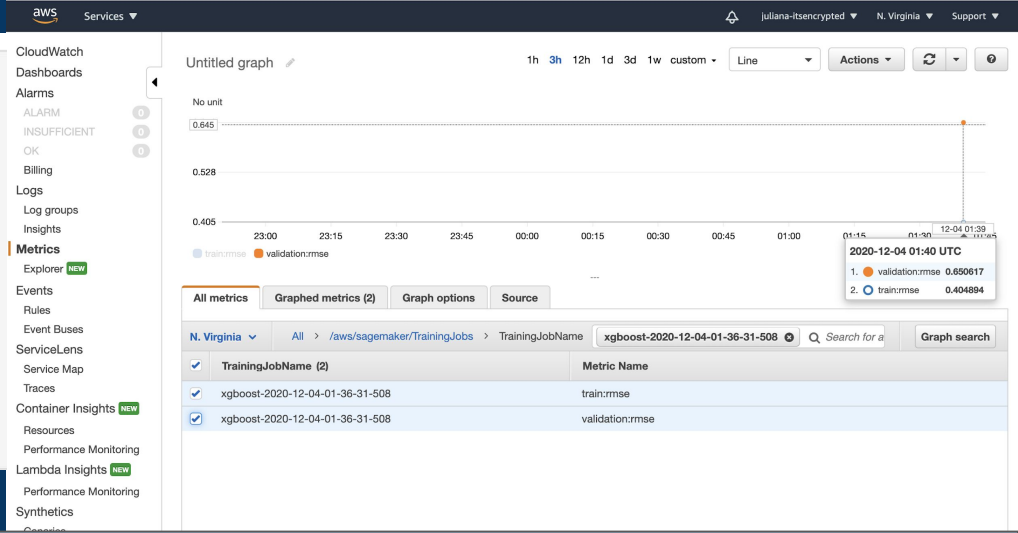
Algorithm Tuning

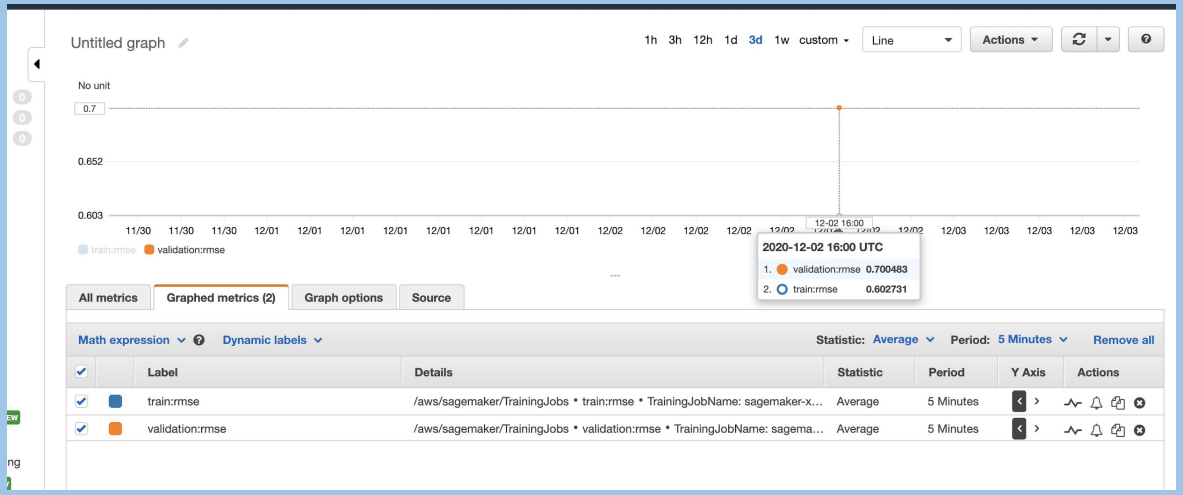
Choose and algorithm and run it with default values - see slides 12, 14, 15 and 16 for screenshots of the hyperparameters chosen with XG Boost Algorithm

Hyperparameter tune different algorithms in a systematic way and choose the best one : this job is an automated feature provided by AWS. The Python SDK (from v. 0.90-2 until its newest stable version 2.0) allowing Data Scientist Developers to run many training jobs in parallel. With only a few lines of code; the SDK finds the best combination of hyperparameters to maximize the training job results. The **tuner.fit()** function takes a few minutes (20' sometimes) to run many jobs and bring the best training job back to become the model to go to deployment/production. (see slides

Hyperparameter tune different algorithms in combination with different feature engineering

```
xgb.set_hyperparameters(objective='reg:linear',
                        num_round=100,
                        booster='gbtree',
                        eta=0.2,
                        max_depth=5,
                        min_child_weight=6,
                        verbose=1,
                        gamma=4,
                        subsample=0.7,
                        early_stopping_rounds=10,
                        scale_pos_weight=8,)
```

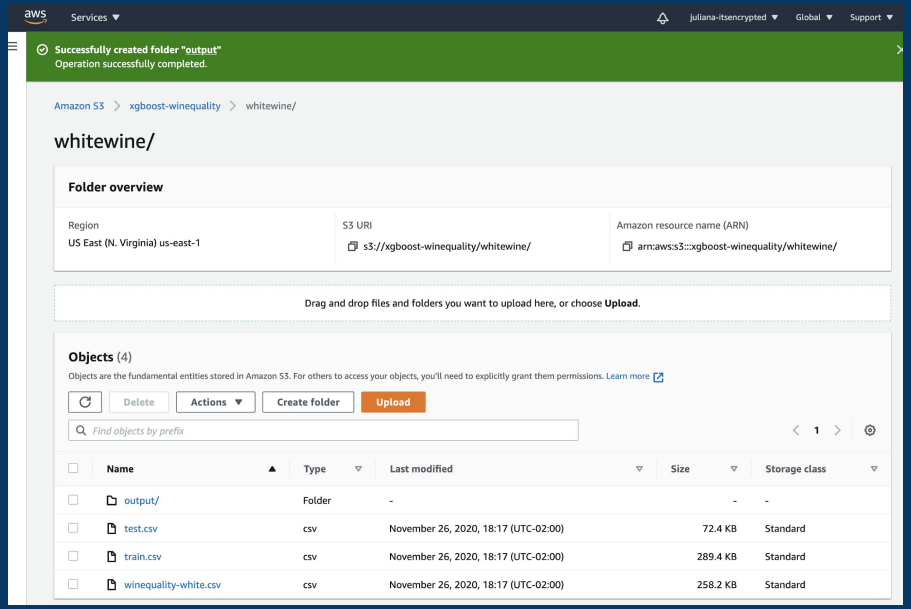




Hyperparameters

Key	Value
num_round	10
objective	reg:linear
scale_pos_weight	1

Uploading train/test data into an S3 bucket



SageMaker - Training Model

Setting the Hyperparameters

xgb.set_hyperparameters(objective='reg:linear', num_round=100, booster=gbtree, eta=0.3, max_depth=6, min_child_weight=1.0, scale_pos_weight=1, eval_metric=rmse)

Hyperparameters

Key	Value
eta	0.2
gamma	4
max_depth	5
min_child_weight	6
num_round	50
objective	reg:linear
silent	0
subsample	0.7

```
xgb.set_hyperparameters(objective='reg:linear',
                        num_round=100,
                        booster='gbtree',
                        eta=0.2,
                        max_depth=5,
                        min_child_weight=6,
                        verbose=1,
                        gamma=4,
                        subsample=0.7,
                        early_stopping_rounds=10,
                        scale_pos_weight=8,)
```

Hyperparameters

- ***eta***: Step size shrinkage used in updates to prevent overfitting. After each boosting step, you can directly get the weights of new features. The eta parameter actually shrinks the feature weights to make the boosting process more conservative.
- ***alpha***: L1 regularization term on weights. Increasing this value makes models more conservative.
- ***min_child_weight***: Minimum sum of instance weight (hessian) needed in a child. If the tree partition step results in a leaf node with the sum of instance weight less than min_child_weight, the building process gives up further partitioning. In linear regression models, this simply corresponds to a minimum number of instances needed in each node. The larger the algorithm, the more conservative it is.
- ***max_depth***: Maximum depth of a tree. Increasing this value makes the model more complex and likely to be overfitted.

XGBoost algorithm has dozens of hyperparameters and we need to pick the right values for those hyperparameters in order to achieve the desired model training results. Since each hyperparameter setting can lead to the best result depends on the dataset as well, it is almost impossible to pick the best hyperparameter setting without searching for it, and a good search algorithm can search for the **best hyperparameter setting in an automated and effective way**.

I used SageMaker hyperparameter tuning to automate the searching process effectively. Specifically, we specify a range, or a list of possible values in the case of categorical hyperparameters, **for each of the hyperparameter that we plan to tune. SageMaker hyperparameter tuning will automatically launch multiple training jobs with different hyperparameter settings**, evaluate results of those training jobs based on a predefined "objective metric", and select the hyperparameter settings for future attempts based on previous results. For each hyperparameter tuning job, we I gave it a budget (max number of training jobs) and it completed once that many training jobs have been executed. (**max jobs =10**)

All this can be done using SageMaker Python SDK to set up and manage the hyperparameter tuning job. First, I configured the training jobs the hyperparameter tuning job will launch by initiating an estimator, which includes:

The container image for the algorithm (XGBoost)

```
container = get_image_uri(region, 'xgboost', repo_version='latest')
```

Configuration for the output of the training jobs

The values of static algorithm hyperparameters, those that are not specified will be given default values

The type and number of instances to use for the training jobs

ML Algorithm Tuning

Testing the AI Service

Testing the AI Service

Report the test accuracy / RMSE on the test dataset

Report several other performance metrics that might be relevant

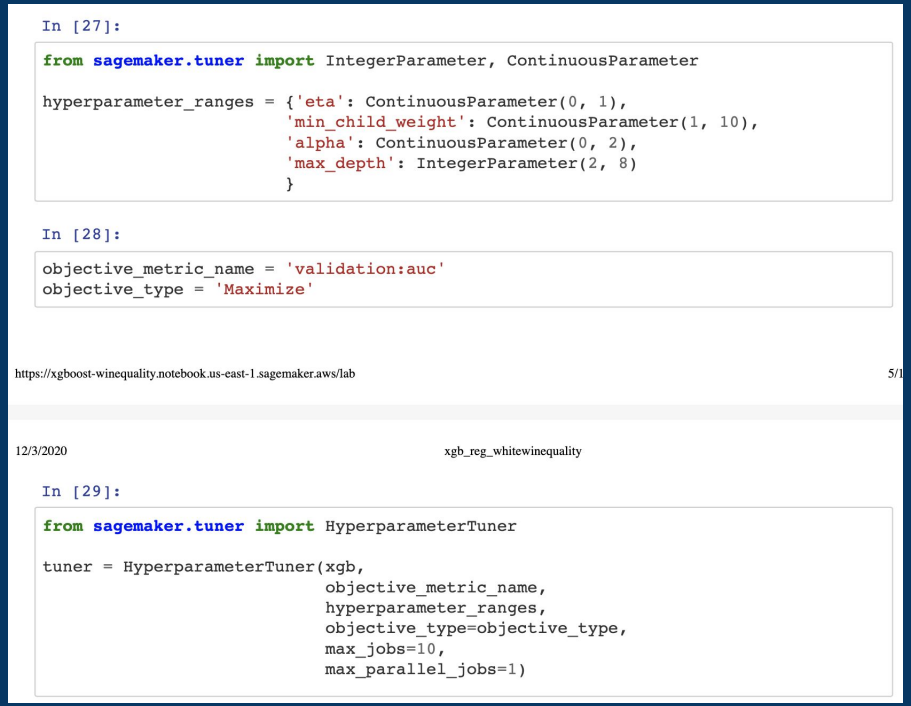
Add noise to the features of the test dataset and report the sensitivity of the algorithm to noise on different features

Model Tuning

Tuning resource configurations such as: Number of training jobs to run in total and how many training jobs can be run in parallel.

Next we'll specify the objective metric that we'd like to tune and its definition, which includes the regular expression (Regex) needed to extract that metric from the CloudWatch logs of the training job. Since we are using built-in **XGBoost algorithm** here, it **emits two predefined metrics: validation:auc and train:auc**, and **I initially elected to monitor validation:auc** but got error messages mentioning that it only worked for datasets with a mix of positive and negative numbers. Hence, my struggle to find another good objective metric.

In this case, we only need to specify the metric name and do not need to provide regex.



In [27]:

```
from sagemaker.tuner import IntegerParameter, ContinuousParameter

hyperparameter_ranges = {'eta': ContinuousParameter(0, 1),
                         'min_child_weight': ContinuousParameter(1, 10),
                         'alpha': ContinuousParameter(0, 2),
                         'max_depth': IntegerParameter(2, 8)
                         }
```

In [28]:

```
objective_metric_name = 'validation:auc'
objective_type = 'Maximize'
```

https://xgboost-winequality.notebook.us-east-1.sagemaker.aws/lab 5/1

12/3/2020 xgb_reg_whitewinequality

In [29]:

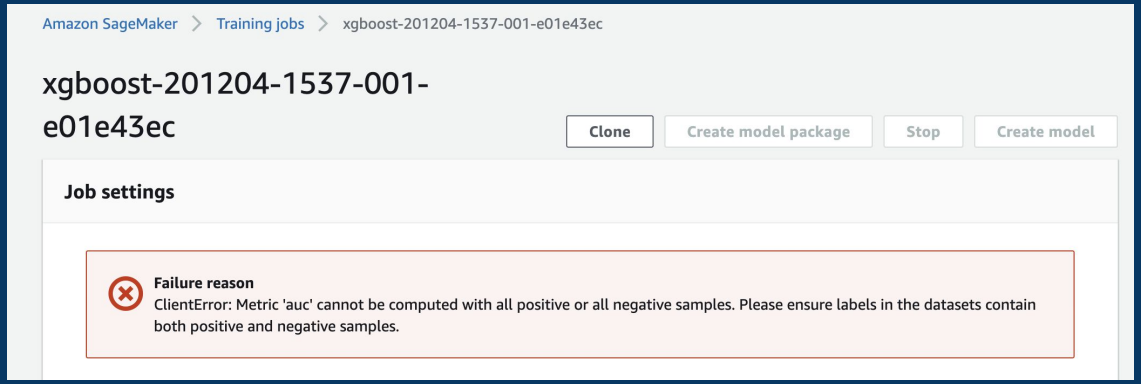
```
from sagemaker.tuner import HyperparameterTuner

tuner = HyperparameterTuner(xgb,
                            objective_metric_name,
                            hyperparameter_ranges,
                            objective_type=objective_type,
                            max_jobs=10,
                            max_parallel_jobs=1)
```

Attention If you bring your own algorithm, your algorithm emits metrics by itself. In that case, you'll need to add a MetricDefinition object here to define the format of those metrics through regex, so that SageMaker knows how to extract those metrics from your CloudWatch logs.

AWS Documentation for Model Tuning

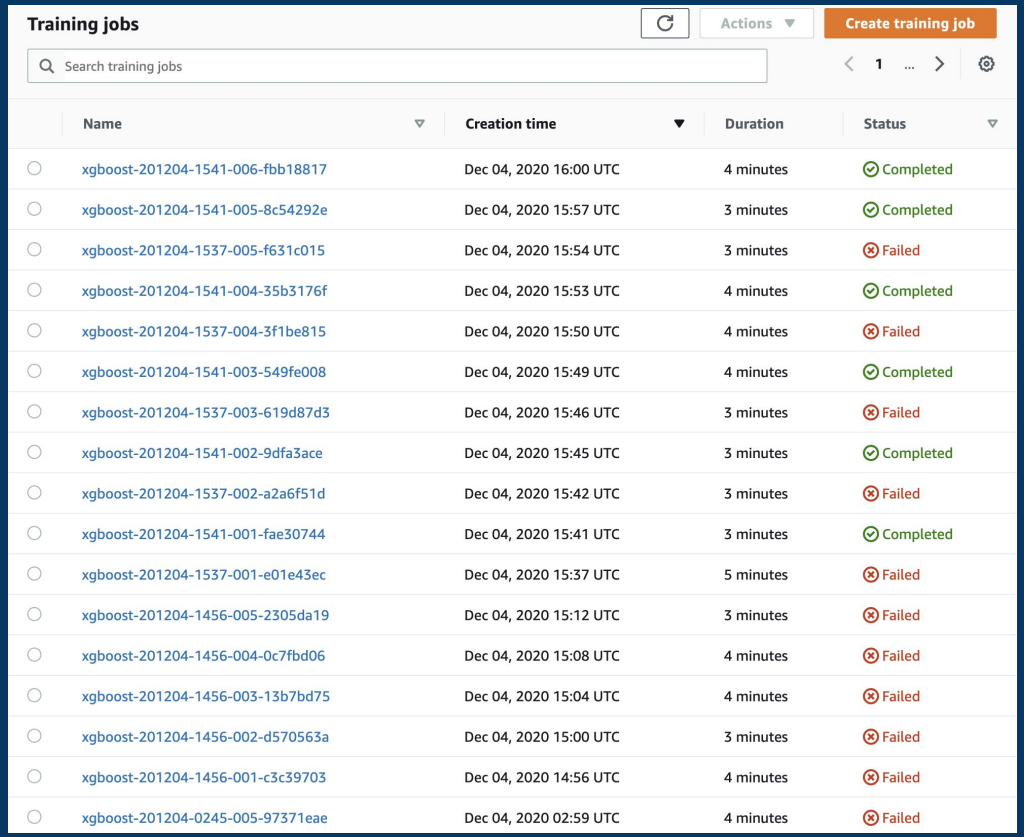
The following guide: https://docs.aws.amazon.com/sagemaker/latest/dg/xgboost-tuning.html allowed me to remember that **linear regression** requires **Root Mean Square Error (rmse)**; so, after many trial and errors I finally found the following error message:



which was causing the majority of the training jobs to fail. When I finally changed the model to tune itself automatically optimizing **validation:rmse** to the lowest amount (**objective_type: 'Minimize'**); I got successful training jobs marked as **completed**

The Hyperparameter Tuner actually looks to the model with the highest precision; in other words, where the square root mean error is the lowest.

Some light in the end of the tunnel



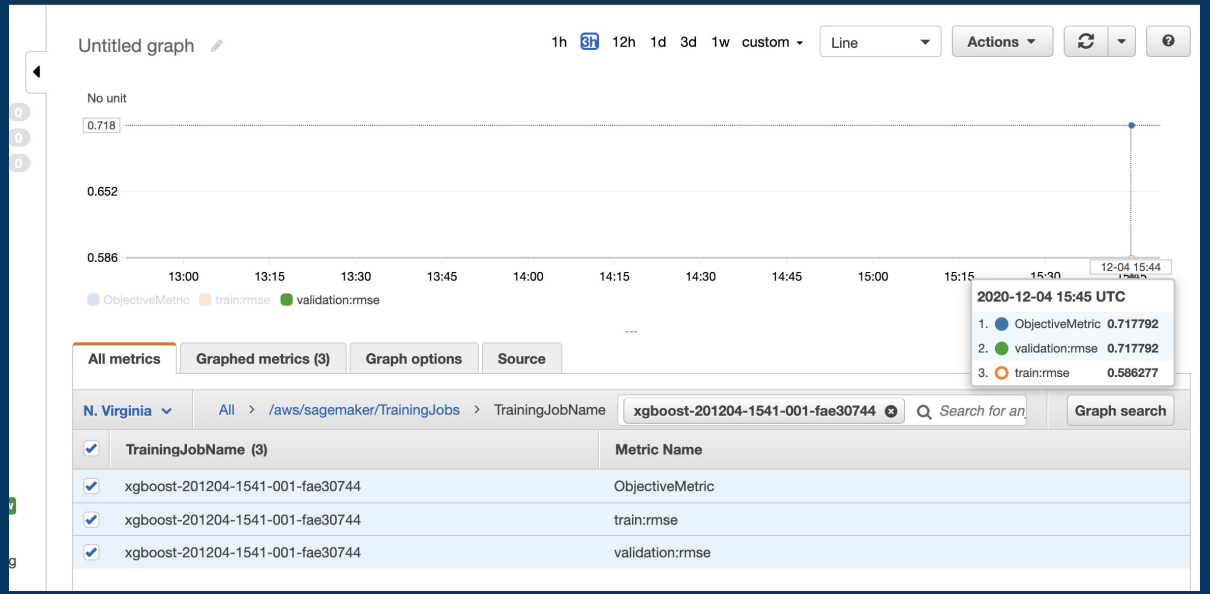
Automatic Model Tuning

Output data configuration

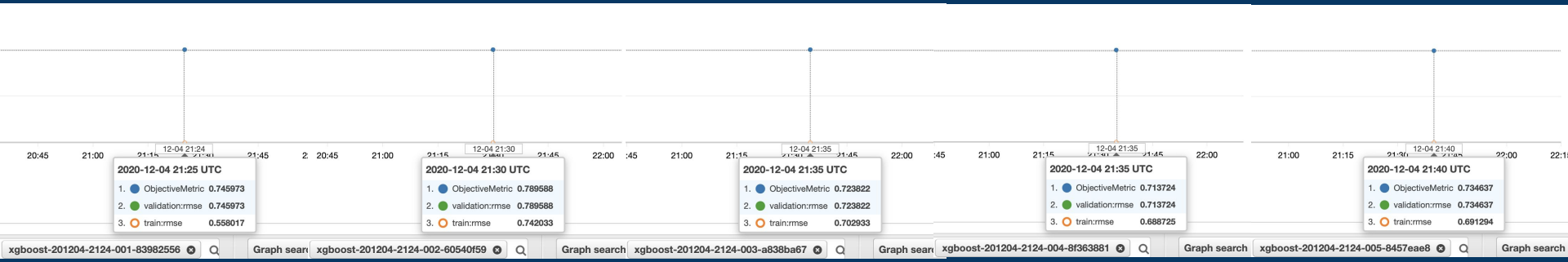
S3 output path	Output encryption key
s3://sagemaker-us-east-1-029754830265/sagemaker/xgboost-whitewinequality/output	-

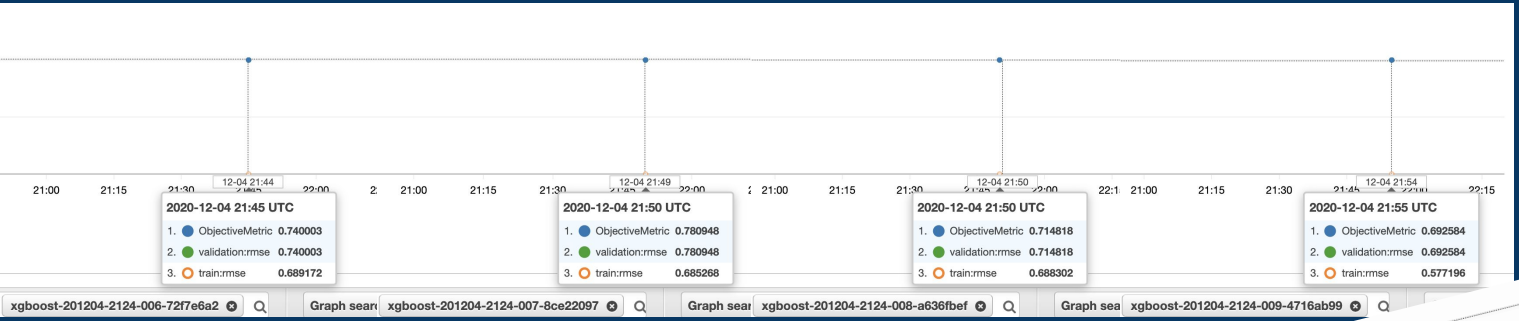
Hyperparameters

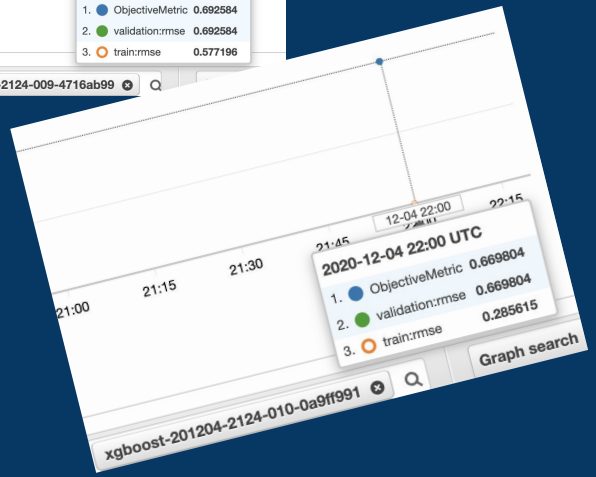
Key	Value
_tuning_objective_metric	validation:rmse
alpha	0.09892440128424873
booster	gbtree
early_stopping_rounds	10
eta	0.7077653378927984
gamma	4
max_depth	5
min_child_weight	7.105857974946885
num_round	100
objective	reg:linear
scale_pos_weight	8
subsample	0.7
verbose	1



Completed training jobs started to produce some good results back from hyperparameter tuning







https://docs.google.com/spreadsheets/d/1V85fvQ03RUSPNPoViaHaTMDVMTM2-oZHFo-k2SjwbKw/edit?usp=sharing

Endpoint creation

xgb_reg_whitewinequality.i

Code git

```
[ ]: tuner.fit({'train': s3_input_train, 'validation': s3_input_validation})
```

```
.....
```

```
[21]: sagemaker = boto3.Session().client(service_name='sagemaker')

# Get tuning job name
job_name = tuner.latest_tuning_job.job_name
print(job_name)

sagemaker.describe_hyper_parameter_tuning_job(
    HyperParameterTuningJobName=job_name)['HyperParameterTuningJobStatus']
```

```
xgboost-201204-2346
[21]: 'Completed'
```

```
[22]: # Deploying the best model
tuning_job_result = sagemaker.describe_hyper_parameter_tuning_job(HyperParameterTuningJobName=job_name)
best_model_name = tuning_job_result['BestTrainingJob']['TrainingJobName']
print(best_model_name)

import time
timestamp = time.strftime('%Y-%m-%d-%H-%M-%S', time.gmtime())
endpoint_name = best_model_name + '-ep-' + timestamp
print(endpoint_name)
```

```
xgboost-201204-2346-001-2df21373
xgboost-201204-2346-001-2df21373-ep-2020-12-05-13-17-34
```

```
[*]: tuner.deploy(initial_instance_count=1, instance_type='ml.m4.xlarge', endpoint_name=endpoint_name)
```

```
2020-12-04 23:50:08 Starting - Preparing the instances for training
2020-12-04 23:50:08 Downloading - Downloading input data
2020-12-04 23:50:08 Training - Training image download completed. Training in progress.
2020-12-04 23:50:08 Uploading - Uploading generated training model
2020-12-04 23:50:08 Completed - Training job completed
------
```

Testing 10 samples

```
[29]: #Predicting the first 10 samples with the best model
smrt = boto3.client('sagemaker-runtime')

# Predict samples from the validation set
payload = validation_data[:10].drop(['quality'], axis=1)
payload = payload.to_csv(header=False, index=False).rstrip()

print(payload)
```

```
6.4,0.22,0.56,14.5,0.055,27.0,159.0,0.998,2.98,0.4,9.1
6.4,0.23,0.33,1.15,0.044000000000000004,15.5,217.5,0.992,3.33,0.44,11.0
7.8,0.13,0.3,1.8,0.04,43.0,179.0,0.9955,3.43,0.41,9.0
5.8,0.17,0.34,1.8,0.045,96.0,170.0,0.99035,3.38,0.9,11.8
7.3,0.17,0.23,6.3,0.051,35.0,240.0,0.9963,3.36,0.54,10.0
6.3,0.28,0.24,8.45,0.031,32.0,172.0,0.9958,3.39,0.57,9.7
7.3,0.21,0.49,1.8,0.038,44.0,152.0,0.9912,3.32,0.44,12.6
7.0,0.15,0.28,14.7,0.051,29.0,149.0,0.99792,2.96,0.39,9.0
7.5,0.14,0.34,1.3,0.055,50.0,153.0,0.9945,3.29,0.8,9.6
5.8,0.25,0.24,13.3,0.044000000000000004,41.0,137.0,0.9972,3.34,0.42,9.5
```

```
[31]: response = smrt.invoke_endpoint(
    EndpointName=endpoint_name,
    Body=payload.encode('utf8'),
    ContentType='text/csv')

print(response['Body'].read())
```

```
b'5.73413085938,5.72361278534,6.14390325546,7.92762136459,5.81308412552,5.9978966713,7.02605772018,6.8381
0567856,5.9601764679,5.40178489685'
```

```
[ ]: #And last but not least, let's not run unecessary costs in the Cloud; so here's a handy script to delete
sagemaker.delete_endpoint(EndpointName=endpoint_name)
```

```
[ ]:
```

Publishing the Model

Publishing the Model

Publish the model on Github or AI Club Projects / Share with the class:
https://github.com/itsencrypted/xgboost_regression

Notebook details and execution:

https://drive.google.com/file/d/1hPCsFk9t_Gbu6K1XbrVJpThUxoG7G5wh/view?usp=sharing

Spreadsheet with hyperparameters/Training Models metrics:

https://docs.google.com/spreadsheets/d/1V85fvQ03RUSPNPoViaHaTMDVMTM2-oZHFo-k2SjwbKw/edit?usp=sharing

Publish code parts on Github and link to projects in AI Club

Write a Medium blog describing your projects with links to AI Club and Github

Special Thanks

My immense gratitude to the help and assistance of Sindhu Ghanta; our teacher at the AI Camp Full Stack AWS Sagemaker course for the knowledge shared and support with feature engineering.

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For all the material digged under: https://github.com/aws/amazon-sagemaker-examples and the new stable version of SageMaker Python SDK: https://sagemaker.readthedocs.io/en/stable/ and Julien Simon's Gitlab repo: https://gitlab.com/juliensimon/dlnotebooks

Without this support this project wouldn't be completed on time.

And a shoutout to all my colleagues and people interested in AI Camp courses: https://learn.xnextcon.com/ there are some great hands on courses there if you're interested in machine learning frameworks. I highly recommend!

And if you want to see more projects like this; and engage in Full Stack ML with AWS please visit:
https://aiclub.world/workshops https://aiclub.world/projects https://aiclub.world/news