

Project Report

Introduction to the domain:

Malware is a worldwide pandemic. It is designed to damage computer systems without the knowledge of the owner using the system. Software's from reputable vendors also contain malicious code that affects the system or leaks information's to remote servers. Malware includes computer viruses, spyware, dishonest ad-ware, rootkits, Trojans, etc.

Malicious software disrupts IT and computer processes and in extreme cases can delete, steal or complete breakdown of the corporate network or the loss of business-critical data.

Following can be the impacts of malware on business:

- Attack sites and disable services
- Identity Theft/Identity Spoofing
- Affect network performance or complete breakdown of the corporate network
- Steal sensitive information
- Control over the applications running in your systems
- Hardware Failure

According to security firm Kaspersky Lab reports, cybercriminals do not steal just data. They also stole up to \$1 billion from 100 different financial institutions across the U.S., Germany, Russia, Ukraine, and China over the past two years.

According to Coveware Q2 Ransomware Marketplace Report "Ransomware Attacks Costs Nearly Triple in 2019 to over \$36K per Attack".

According to the FBI's Internet Crime Complaint Center, ransomware--malicious programs that infect a computer or network and hold data hostage until a ransom is paid--has cost companies \$18 million in the past 15 months.

The problem statement:

In the current world scenario, the internet has become a huge part of everyone's lives, with millions and millions of data packets being downloaded and uploaded each day. With such a huge transfer rate, it becomes very easy for some to sneak in just one unit of data, capable of massive destruction of an application, a whole system, or the entire network.

One may never find out if the file one is about to download contains malware or not. With one download containing so many files, it is nearly impossible to physically find out if a file contains a malware or not.

Thankfully, this job has been made easier by Machine Learning algorithms. Using appropriate datasets, a machine learning model can be trained to understand certain parameters of data, and can then predict if a particular file contains malware or not.

Proposed Solution:

Every time the user downloads something, before running/opening/executing it, the user can pass it through a trained ML model, which will predict if the data contains malware or not. If it does, the user can delete the file right away, avoiding any damage to the system. If it does not have any malware, the user can safely open/run the file.

Libraries/modules imported:

- os
- sklearn
- boto3
- sagemaker
- numpy
- pandas
- sklearn.feature_extraction and sklearn.preprocessing
- itertools

Data Analysis, Cleaning and Preprocessing:

After importing all the necessary libraries, pandas' info() function is executed on the data, to see how many columns are there in the data, along with the number of entries in each columns. If the number of entries do not match in the columns, it implies there are Null values present.

```
In [3]: 1 df_Csv.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 50181 entries, 0 to 50180
Data columns (total 28 columns):
BaseOfCode          50181 non-null int64
BaseOfData          50181 non-null int64
Characteristics      50181 non-null int64
DllCharacteristics  50181 non-null int64
Entropy             50181 non-null float64
FileAlignment       50181 non-null int64
FirstSeenDate       50181 non-null object
Identify            35958 non-null object
ImageBase           50181 non-null int64
ImportedDlls        50181 non-null object
ImportedSymbols     50181 non-null object
Label               50181 non-null int64
Machine             50181 non-null int64
Magic               50181 non-null int64
NumberOfRvaAndSizes 50181 non-null int64
NumberOfSections    50181 non-null int64
NumberOfSymbols     50181 non-null int64
PE_TYPE             50181 non-null int64
PointerToSymbolTable 50181 non-null int64
SHA1                50181 non-null object
Size                50181 non-null int64
SizeOfCode          50181 non-null int64
SizeOfHeaders       50181 non-null int64
SizeOfImage         50181 non-null int64
SizeOfInitializedData 50181 non-null int64
SizeOfOptionalHeader 50181 non-null int64
SizeOfUninitializedData 50181 non-null int64
TimeStampStamp      50181 non-null int64
dtypes: float64(1), int64(22), object(5)
memory usage: 10.7+ MB
```

As seen, there are 28 columns, each having a different meaning. Nearly all of them have 50181 entries, but one column: 'Identify'. It has way too less entries (35958). Since it's an Identification type, filling this column's NaNs does not make sense. If we are to drop those rows having the NaN's it would mean a loss of 50,181-35,958 = 14,223 rows, which will lead to too large a loss of relevant data. Hence, that column will be dropped. Let us now have a 'first glance' at the data. (all the columns not visible here)

BaseOfCode	BaseOfData	Characteristics	DllCharacteristics	Entropy	FileAlignment	FirstSeen	Identify	ImageBase	ImportedDlls	ImportedSymbols	Label	Machine	Magic	NumberOfRvaAndSizes	NumberOfSections	NumberOfSymbols	PE_TYPE	PointerToSymbolTable	SHA1	Size	SizeOfCode	SizeOfData	SizeOfHeaders	SizeOfImage
4096	69632	783	0	5.981249	512	01-01-70	powerbas	4194304	comdlg32.printdlga	g	0	332	267	16	5	0	267	0	b0068836e	76288	64855	1024		
4096	1851392	783	0	6.081747	512	01-01-70		4194304	comctl32.imagelist_i	g	0	332	267	16	6	0	267	0	5741708cc	2558464	1843888	1024	2	
4096	40960	783	0	5.586422	512	01-01-70		4194304	comdlg32.getopenfil	g	0	332	267	16	9	0	267	0	507fe5d82	178688	33792	1024	33	
1359872	2138112	783	0	7.969464	512	01-01-70	upx 2.93	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	e51a7811c	806816	778240	4096	2	
4096	40960	783	32768	7.9999	512	01-01-70		4194304	advapi32.cregcloseke		0	332	267	16	7	0	267	0	0e046d999	50689096	35840	1024		
192512	245760	783	0	7.328245	512	01-01-70	upx v0.89	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	19de4645c	76800	53248	4096		
8192	61440	33166	0	6.257786	512	01-01-70		4194304	kernel32.dgetstringty		0	332	267	16	5	0	267	0	f6e045232	69660	52224	1024		
4096	40960	775	0	5.308237	512	03-01-70		4194304	lua53.dll.klua_callm		0	332	267	16	9	1574	267	75264	56e362bc3	110146	34304	1024		
4096	40960	775	0	5.256822	512	03-01-70		4194304	lua53.dll.klua_callm		0	332	267	16	9	1542	267	73728	01a8b85f2	107962	34304	1024		
4096	131072	775	0	5.909817	512	04-01-70		4194304	kernel32.ddeletcriti		0	332	267	16	9	2226	267	194560	1bad4f17d	246187	123392	1024		
4096	262144	783	0	6.233885	512	04-01-70		4194304	kernel32.dclosehandl		0	332	267	16	7	0	267	0	8a1b8284c	315904	257536	1024		
524288	921600	259	0	7.994843	512	06-01-70	upx -> vvv	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	d5a4e36ef	5767600	397312	4096	1	
532480	937984	259	0	7.993068	512	06-01-70	upx -> vvv	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	41081871c	4934008	405504	4096	1	
614400	1093632	259	0	7.950715	512	07-01-70	upx -> vvv	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	12a5489dd	3188880	479232	4096	1	
614400	1093632	259	0	7.95329	512	07-01-70	upx -> vvv	4194304	kernel32.dloadlibrary		0	332	267	16	3	0	267	0	f5867990c	3309048	479232	4096	1	
65536	131072	33166	0	7.956131	512	15-02-76	borland cl	4194304	kernel32.dlstrenla	lst	0	332	267	16	6	0	267	0	7bd53b19c	778356	23040	1024		
4096	34975744	782	0	6.478057	512	28-05-80		4194304	advapi32.ccopysid cr		0	332	267	16	12	0	267	0	f15fa12bb	49366808	34969088	1024	49	
4096	40960	783	32768	7.992968	512	16-07-84		4194304	advapi32.cregcloseke		0	332	267	16	7	0	267	0	0ff72230a	2253360	34816	1024		
4096	40506	33167	32768	7.995115	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	eaeef116aa	11415344	37888	1024		
4096	40506	33167	32768	7.998887	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	7cb4c3c0e	5122240	40448	1024		
4096	40506	33167	32768	7.992212	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	62d99928c	1704035	40448	1024		
4096	40506	33167	32768	7.999957	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	587e1e47c	48232863	37888	1024		
4096	40506	33167	32768	7.957969	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	30a0d3b3f	657424	40448	1024		
4096	40506	33167	32768	7.999077	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	99ab5e41c	30941112	40448	1024		
4096	40506	33167	32768	7.988488	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	ac7417f36	5125196	37888	1024		
4096	40506	33167	32768	7.985504	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	d9cd7474c	3515824	37888	1024		
4096	40506	33167	32768	7.974753	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	d8e8d4d4c	856481	40448	1024		
4096	40506	33167	32768	7.999804	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	d8ef34bce	14462573	40448	1024		
4096	40506	33167	32768	7.999999	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	0b41190dc	66382626	40448	1024		
4096	45056	33167	32768	7.957253	512	19-06-92	borland de	4194304	kernel32.ddeletcriti		0	332	267	16	8	0	267	0	c73ae03b1c	854558	37888	1024		

Though one cannot comprehend the data at first glance, it can be seen that there are a few columns with redundant values, all along. (except 'Label' of course, that's important). Columns like Magic, File Alignment, SizeOfOptionalHeader, PE_TYPE are some. If they have only one value, they will not help our model in understanding the generality of the data better. It is better to have these columns removed. Also, the column SHA1 has serial-like values, i.e. they are a mixture of numbers and characters, and it makes no sense to find out any pattern in that data. It is better to have this column removed as well.

```
: 1 df_Csv = df_Csv.drop(columns=['SHA1', 'FirstSeenDate', 'Identify', 'PE_TYPE', 'SizeOfOptionalHeader', 'Magic'])
```

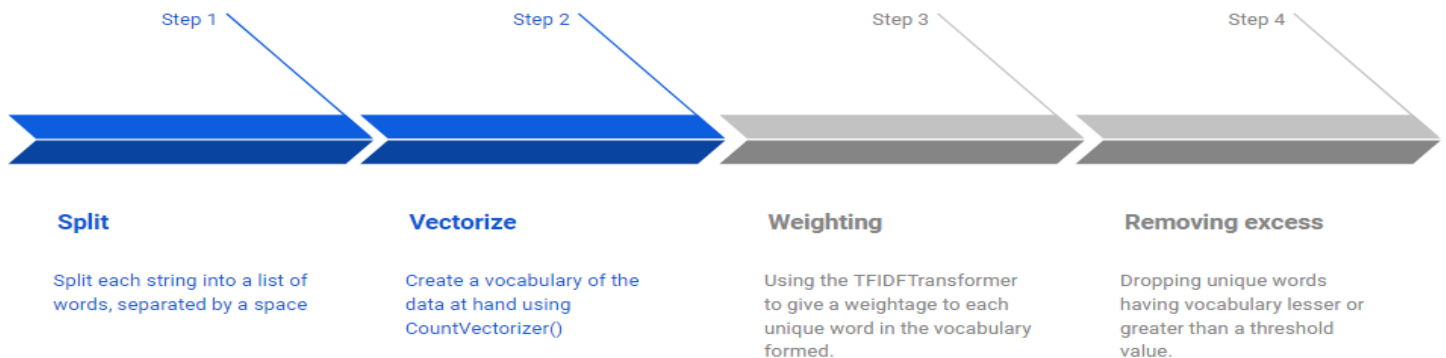
Now that the columns which would hinder the data analytics have been removed, let's move on to processing and analysing the remaining data. Taking a look at the output of the info() function once again, it is observed that:

Though most of the remaining columns now have numerical values, columns 'ImportedDlls' and

'ImportedSymbols' having data type 'object', meaning they contain strings.

DLLs: DLL is a dynamic link library file format used for holding multiple codes and procedures for Windows programs. DLL files were created so that multiple programs could use their information at the same time, aiding memory conservation. It also allows the user to edit the coding of multiple applications at once, without changing the applications themselves. [<https://whatis.techtarget.com/fileformat/DLL-Dynamic-link-library-file>]

These columns hold data which will significantly contribute to the analysis of the data, as seen by the definition of DLLs. Hence it is necessary to convert the data stored here to a form which is easily understood by the model. The following plan will be used for conversion of both the columns:



To decide the threshold value in step 4, we use the sparsity of the data as a decision parameter as well.

Sparsity: In a database, sparsity and density describe the number of cells in a table that are empty (sparsity) and that contain information (density), though sparse cells are not always technically empty—they often contain a “0” digit. Tables and databases are the sum total of their sparse and dense cells.[

<https://www.quora.com/What-is-a-clear-explanation-of-data-sparsity>]

Mathematically, sparsity is calculated as:

$$\text{Sparsity}(S) = \frac{\text{number of non – zero entries in data}}{\text{number of rows of data} * \text{number of columns of data}}$$

```
In [40]: 1 cvec = CountVectorizer(stop_words='english', min_df=0.001, max_df=0.8, ngram_range=(1,1), token_pattern = '[a-zA-Z0-9$&+;=?
2 cvec.fit(df_Csv.ImportedDlls)
3 list(islice(cvec.vocabulary_.items(), 20))
4 len(cvec.vocabulary_)

Out[40]: 235
```

```
In [41]: 1 cvec_counts = cvec.transform(df_Csv.ImportedDlls)
2 print('sparse matrix shape:', cvec_counts.shape)
3 print('nonzero count:', cvec_counts.nnz)
4 print('sparsity: %.2f%%' % (100.0 * cvec_counts.nnz / (cvec_counts.shape[0] * cvec_counts.shape[1])))

sparse matrix shape: (50143, 235)
nonzero count: 407391
sparsity: 3.46%
```

For column 'ImportedDLLs'

```
In [45]: 1 cvec = CountVectorizer(stop_words='english', min_df=0.005, max_df=0.9, ngram_range=(1,1))
2 cvec.fit(df_Csv.ImportedSymbols)
3 list(islice(cvec.vocabulary_.items(), 20))
4 len(cvec.vocabulary_)

Out[45]: 1935
```

```
In [46]: 1 cvec_counts = cvec.transform(df_Csv.ImportedSymbols)
2 print('sparse matrix shape:', cvec_counts.shape)
3 print('nonzero count:', cvec_counts.nnz)
4 print('sparsity: %.2f%%' % (100.0 * cvec_counts.nnz / (cvec_counts.shape[0] * cvec_counts.shape[1])))

sparse matrix shape: (50143, 1935)
nonzero count: 8174793
sparsity: 8.43%
```

For column 'ImportedSymbols'

It is important to keep the sparsity of the dataset as low as possible, in order to maintain a good dataset.

Keeping in mind the sparsity and the amount of data to be maintained later, we set the limits of the Vectorizer as (0.001,0.8) for Imported DLLs, and (0.05,0.9) for Imported Symbols. The arranged words in the vocabulary of each column is seen in the notebook.

Once separation of the string into words is done, we need to convert it into a form that the model understands, i.e. in numerical format. In order to do that,

- Create a new dataframe, with the columns as the words of the vocabulary.
- For every row entry in the original dataframe:
 - See each element of the list in the column 'ImportedDLLs'
 - If the element matches with a column in the new dataframe (<element> == <column name>), then under that column put 1 (in the new dataframe), else put a
- Repeat the same for column 'ImportedSymbols'

Thus, we would have successfully converted the data into a numerical form. Currently, we have 3 dataframes:

- df_Csv, the original dataframe
- df2, the dataframe created for 'ImportedDLLs'
- df3, the dataframe created for 'ImportedSymbols'

The three dataframes are to be combined as one as the last step of pre-processing the data for our machine learning models.

Using pandas' concat function, we can combine the three dataframes, and convert the resultant dataframe into a new csv, called 'final.csv', which has the pre-processed data, ready to be sent to the model.

Note: Due to some internal problem in AWS, the pre-processing was done locally, and the Jupyter Notebook's code was copied into this notebook, and 'final.csv' was physically uploaded to the S3 bucket and the notebook instance. Since the final part of the pre-processing takes really long, re-executing that code cell would be impractical. The file, 'final.csv' is of size 400+Mb. All further coding has been continued in the AWS notebook instance, the second notebook.

Now that we have completed our pre-processing, we can move on to the model selection, training and tuning.

Dataset Splitting:

As the data is now processed, it should be split up into its training and testing sets. A threshold of 30% was decided to separate the training and the testing set, i.e. the testing set will be 30% of the original dataset, and the training set will be the remaining, i.e. 70% of the original dataset. Of this 70%, we will again split the data into training and validation sets. We will use 20% of the training set obtained above, as the validation set. Then, we will upload the sets our S3 bucket.

Model Selection:

In the second Jupyter Notebook, 4 models were chosen for comparison:

- Decision Tree Classifier
- AdaBoost Classifier
- Random Forest Classifier
- XGBoost Classifier

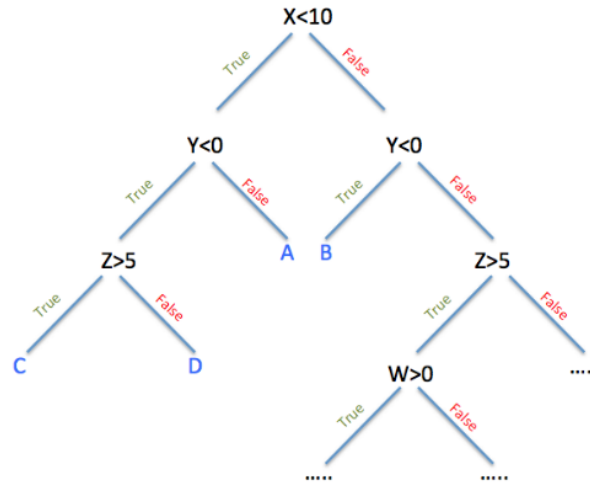
The above 4 models will be compared to one another on a part of the pre-processed data.

About the models:

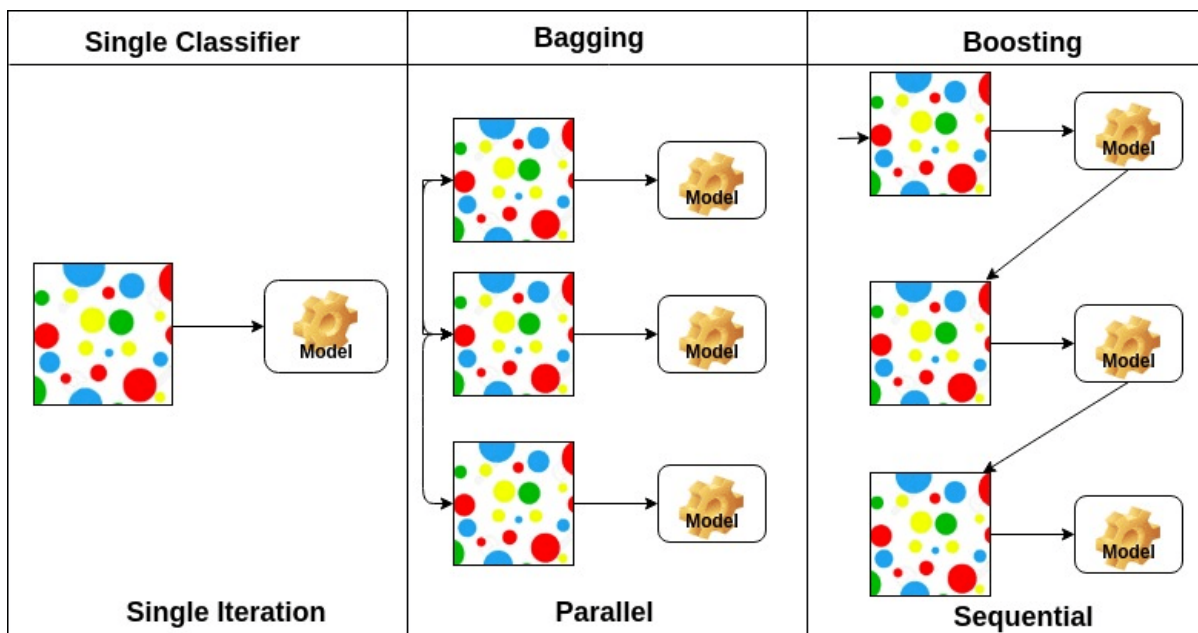
A **Decision Tree** is a simple representation for classifying examples. It is a Supervised Machine Learning where the data is continuously split according to a certain parameter.

Decision Tree consists of:

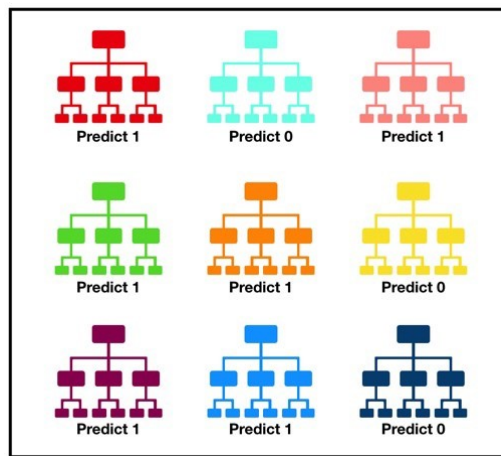
- Nodes: Test for the value of a certain attribute.
- Edges/ Branch: Correspond to the outcome of a test and connect to the next node or leaf.
- Leaf nodes: Terminal nodes that predict the outcome (represent class labels or class distribution).



An **AdaBoost Classifier** is a meta-estimator that begins by fitting a classifier on the original dataset and then fits additional copies of the classifier on the same dataset but where the weights of incorrectly classified instances are adjusted such that subsequent classifiers focus more on difficult cases.



A **random forest** is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if `bootstrap=True`



XGBoost is an optimized distributed gradient boosting library designed to be highly efficient, flexible and portable. It implements machine learning algorithms under the Gradient Boosting framework. XGBoost provides a parallel tree boosting (also known as GBDT, GBM) that solve many data science problems in a fast and accurate way. The same code runs on major distributed environment (Hadoop, SGE, MPI) and can solve problems beyond billions of examples



The Comparison:

The comparison could not be done on the Sagemaker Notebook, as the 'xgboost' module could not be imported for the comparison the way it was done locally. Hence, an html report of the local notebook has been uploaded along with the files, so that one may see the output of the execution done locally. A pipeline was made to train the models, one by one on 3 parts of the dataset, having 1%, 10% and 100% of the data.

Naturally, the data had been split into training and testing sets, with 30% of the data being kept as the testing data. The models were allowed to fit on the data, with certain factors being noted and stored in a dictionary named 'result'. We then compare the different values among all 4 models in the 'result', and decide which model will be further tuned and hyper-parameters will be set.


```

In [ ]: 1 from sklearn.metrics import fbeta_score, accuracy_score
        2 from time import time
        3 def train_predict(learner, sample_size, X_train, y_train, X_test, y_test):
        4     '''
        5     inputs:
        6     - learner: the learning algorithm to be trained and predicted on
        7     - sample_size: the size of samples (number) to be drawn from training set
        8     - X_train: features training set
        9     - y_train: income training set
       10     - X_test: features testing set
       11     - y_test: income testing set
       12     ...
       13
       14     results = {}
       15
       16     start = time() # Get start time
       17     learner.fit(X_train[:sample_size], y_train[:sample_size])
       18     end = time() # Get end time
       19     results['train_time'] = end-start
       20     start = time() # Get start time
       21     predictions_test = learner.predict(X_test)
       22     predictions_train = learner.predict(X_train[:300])
       23     end = time() # Get end time
       24     results['pred_time'] = end-start
       25     results['acc_train'] = accuracy_score(y_train[:300], predictions_train)
       26     results['acc_test'] = accuracy_score(y_test, predictions_test)
       27     results['f_train'] = fbeta_score(y_train[:300], predictions_train, beta=0.01)
       28     results['f_test'] = fbeta_score(y_test, predictions_test, beta=0.01)
       29     return results

```

For each model, the following factors have been taken into consideration:

- Prediction time: The amount of time taken by the model to generate an output, measured from the moment the model was created.
- Accuracy on training set: Shows how well the model has learnt from the training set
- Accuracy on testing set: Shows how well the model can apply its knowledge to the testing set.
- F-score on training: Shows the precision of the model on the training set
- F-score on testing: Shows the precision of the model on the testing set

It should be noted, that the accuracy of the training set and the f-score on the training being more than their corresponding scores on the testing set indicate overfitting of the model. The model should ideally perform better on the testing set, which means that it has got the patterns of the data, rather than learning the data itself.

The following is the result of the comparison. Cases 1,2,3 are on 1%, 10% and 100% of the data respectively:

-----case 1-----	-----case 2-----	-----case 3-----
DecisionTreeClassifier	DecisionTreeClassifier	DecisionTreeClassifier
Training time: 0.2520310878753662	Training time: 0.27184438705444336	Training time: 7.098905086517334
Prediction time: 0.21492242813110352	Prediction time: 0.12193489074707031	Prediction time: 0.15091276168823242
Accuracy Score: train 1.0	Accuracy Score: train 1.0	Accuracy Score: train 1.0
Accuracy Score: test 0.8974853645556147	Accuracy Score: test 0.9439861628525812	Accuracy Score: test 0.9753858435337945
Fscore : train 1.0	Fscore : train 1.0	Fscore : train 1.0
Fscore : test 0.915014269776282	Fscore : test 0.9496265932613658	Fscore : test 0.9787504104711272
AdaBoostClassifier	AdaBoostClassifier	AdaBoostClassifier
Training time: 0.6650574207305908	Training time: 1.8499319553375244	Training time: 28.6019926071167
Prediction time: 8.689386367797852	Prediction time: 1.6690373420715332	Prediction time: 1.6130716800689697
Accuracy Score: train 0.9833333333333333	Accuracy Score: train 0.94	Accuracy Score: train 0.92
Accuracy Score: test 0.8929616817456094	Accuracy Score: test 0.9337413517828632	Accuracy Score: test 0.9456492815327302
Fscore : train 0.98224910186443	Fscore : train 0.9518060822760106	Fscore : train 0.933733814891023
Fscore : test 0.8984199975638543	Fscore : test 0.9441414971664508	Fscore : test 0.9572152081963373
RandomForestClassifier	RandomForestClassifier	RandomForestClassifier
Training time: 0.11994600296020508	Training time: 0.19388937950134277	Training time: 2.7414186000823975
Prediction time: 0.17587995529174805	Prediction time: 0.1739184856414795	Prediction time: 0.17987632751464844
Accuracy Score: train 0.9933333333333333	Accuracy Score: train 1.0	Accuracy Score: train 1.0
Accuracy Score: test 0.9098589675359233	Accuracy Score: test 0.939196381053752	Accuracy Score: test 0.9700638637573177
Fscore : train 0.9940476190476191	Fscore : train 1.0	Fscore : train 1.0
Fscore : test 0.9243721074950858	Fscore : test 0.9521408953858418	Fscore : test 0.975558585510146
XGBClassifier	XGBClassifier	XGBClassifier
Training time: 5.440302848815918	Training time: 34.03155255317688	Training time: 359.3747401237488
Prediction time: 2.8927595615386963	Prediction time: 2.4855659008026123	Prediction time: 2.603517770767212
Accuracy Score: train 0.9966666666666667	Accuracy Score: train 0.9566666666666667	Accuracy Score: train 0.9533333333333334
Accuracy Score: test 0.9348722724853645	Accuracy Score: test 0.9589542309739223	Accuracy Score: test 0.966138903672166
Fscore : train 0.994083428392917	Fscore : train 0.9640712790569571	Fscore : train 0.9529422974670738
Fscore : test 0.9389723835449842	Fscore : test 0.9659403613360804	Fscore : test 0.9705610825498041

Observing the outputs obtained above, we can see that the Random Forest Classifier would prove a really good fit, as suggested in papers. However, currently it's a little overfitting. The XGBClassifier, on the other hand, takes significantly more time in training, but does a better job than the Random Forest Classifier at preventing overfitting. Observing the Adaboost Classifier, we may see that it also does not overfit. However, it gets beat by the XGBoost Classifier at all the scores. The Decision Tree Classifier heavily overfits.

Thus, we will use the XGBoost classifier as our model to train and tune.

Testing Metrics:

Although accuracy may be a good measure, we might want to observe the confusion matrix:

		Actual Values	
		Positive (1)	Negative (0)
Predicted Values	Positive (1)	TP is malware, predicted malware	FP is malware, predicted goodwill
	Negative (0)	FN not malware, predicted malware	TN not malware, predicted goodwill

In our case, accuracy will not be the best metric. Though we can afford having False Negatives (hey, the model's playing it safe), we cannot have any False Positives at all.

Hence, a good testing metric would be the Recall value of the model, over its precision.

We can check the f-beta score of the model, beta being set to a value close to 1. The testing metric would be the **f-beta score**.

Historical model for comparison(benchmark):

It has been found through a paper (included in the repository) that the Random Forest Classifier has been expected to be the best model, with around 97% accuracy. However, it was not compared to the XGBoost Classifier.

Hence, a goal of this project would be to test if a tuned XGBoost Classifier can do better than the Random Forest, using the same dataset. Also, as mentioned, the f-beta score will be used to see the true applicability of the model.

The XGBoost Classifier:

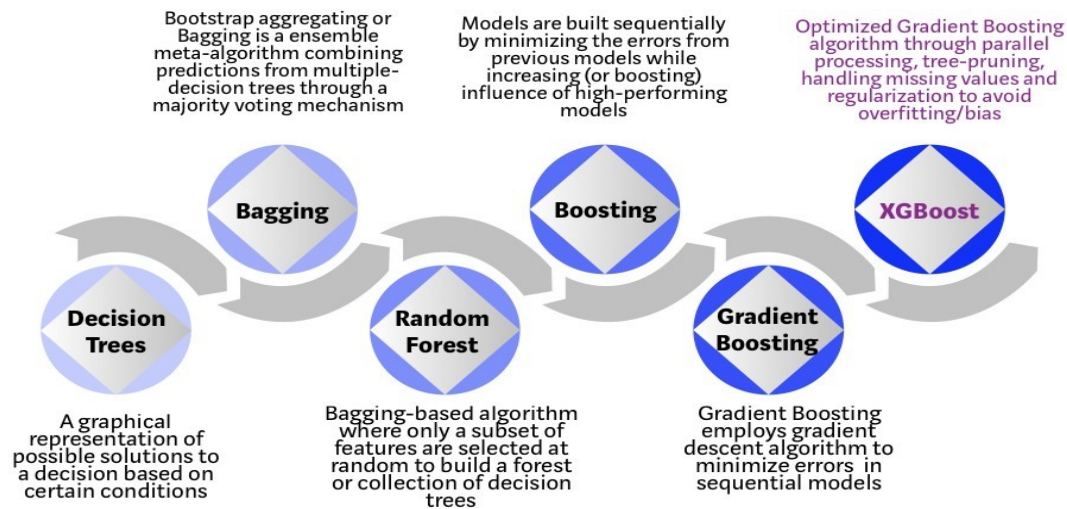
As seen in the blog [<https://towardsdatascience.com/https-medium-com-vishalmorde-xgboost-algorithm-long-she-may-rein-edd9f99be63d>],

XGBoost is a decision-tree-based ensemble Machine Learning algorithm that uses a gradient boosting framework. In prediction problems involving unstructured data (images, text, etc.) artificial neural networks tend to outperform all other algorithms or frameworks. However, when it comes to small-to-medium structured/tabular data, decision tree-based algorithms are considered best-in-class right now.

In the figure is the history of tree-based algorithms over the years.

The XGBoost library implements the gradient boosting decision tree algorithm. This algorithm goes by lots of different names such as gradient boosting, multiple additive regression trees, stochastic gradient boosting or gradient boosting machines. Boosting is an ensemble technique where new models are added to correct the errors made by existing models. Models are added sequentially until no further improvements can be made. A popular example is the AdaBoost algorithm that weights data points that are hard to predict. Gradient boosting is an approach where new models are created that predict the residuals or errors of prior models and then added together to make the final prediction. It is called gradient boosting because it uses a gradient descent algorithm to minimize the loss when adding new models.

[<https://machinelearningmastery.com/gentle-introduction-xgboost-applied-machine-learning/>]



Features of the XGBoost Classifier:

- **Regularization:** XGBoost has an option to penalize complex models through both L1 and L2 regularization. Regularization helps in preventing overfitting
- **Handling sparse data:** Missing values or data processing steps like one-hot encoding make data sparse. XGBoost incorporates a sparsity-aware split finding algorithm to handle different types of sparsity patterns in the data
- **Weighted quantile sketch:** Most existing tree based algorithms can find the split points when the data points are of equal weights (using quantile sketch algorithm). However, they are not equipped to handle weighted data. XGBoost has a distributed weighted quantile sketch algorithm to effectively handle weighted data
- **Block structure for parallel learning:** For faster computing, XGBoost can make use of multiple cores on the CPU. This is possible because of a block structure in its system design. Data is sorted and stored in in-memory units called blocks. Unlike other algorithms, this enables the data layout to be reused by subsequent iterations, instead of computing it again. This feature also serves useful for steps like split finding and column sub-sampling
- **Cache awareness:** In XGBoost, non-continuous memory access is required to get the gradient statistics by row index. Hence, XGBoost has been designed to make optimal use of hardware. This is done by allocating internal buffers in each thread, where the gradient statistics can be stored
- **Out-of-core computing:** This feature optimizes the available disk space and maximizes its usage when handling huge datasets that do not fit into memory

Model Training and Tuning:

Since we are using Sagemaker, we will need to define the model in a different style than earlier. We will need to use Sagemaker's estimator function to define the model, setting relevant parameters.

```
In [5]: from sklearn.model_selection import train_test_split
X_train,X_test,y_train,y_test = train_test_split(X, y, test_size=0.3, random_state=42)

print("Testing set has {} samples.".format(X_test.shape[0]))
X_train,X_val,y_train,y_val = train_test_split(X_train, y_train, test_size=0.2, random_state=42)
print("Training set has {} samples.".format(X_train.shape[0]))
print("Validation set has {} samples.".format(X_val.shape[0]))
```

```
Testing set has 15032 samples.
Training set has 28058 samples.
Validation set has 7015 samples.
```

```
In [6]: X_test.to_csv('test.csv',header = False, index = False)
pd.concat([y_val,X_val],axis =1).to_csv('validation.csv',header=False, index=False)
pd.concat([y_train,X_train],axis =1).to_csv('train.csv',header = False, index = False)
```

```
In [8]: prefix = 'malware-detection'
test_location = session.upload_data('test.csv',key_prefix = prefix)
val_location = session.upload_data('validation.csv',key_prefix = prefix)
train_location = session.upload_data('train.csv',key_prefix = prefix)
```

First, let us split the data into training, testing and validation sets, and save them in 3 different csv's, 'train.csv', 'test.csv', 'validation.csv'

After saving them as 3 different csv's, we upload the data into the s3 bucket, in the folder 'malware-detection'.

Now, to define the XGBoost model. Before we define it, let us understand the meaning of the parameters.

According to the AWS documentation (attached with the notebook):

- **max_depth**: Maximum depth of a tree. Increasing this value makes the model more complex and likely to be overfit. 0 indicates no limit. A limit is required when grow_policy=depth-wise.
- **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.
- **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.
- **subsample**: Subsample ratio of the training instance. Setting it to 0.5 means that XGBoost randomly collects half of the data instances to grow trees. This prevents overfitting.
- **gamma**: Minimum loss reduction required to make a further partition on a leaf node of the tree. The

Amazon S3 > sagemaker-ap-south-1-812709844112 > malware-detection

sagemaker-ap-south-1-812709844112

Overview

Q Type a prefix and press Enter to search. Press ESC to clear.

Upload Create folder Download Actions

Asia Pacific (Mumbai)

Viewing 1 to 3

<input type="checkbox"/> Name	Last modified	Size	Storage class
<input type="checkbox"/> test.csv	Mar 15, 2020 3:24:24 PM GMT+0530	126.1 MB	Standard
<input type="checkbox"/> train.csv	Mar 15, 2020 3:24:26 PM GMT+0530	235.4 MB	Standard
<input type="checkbox"/> validation.csv	Mar 15, 2020 3:24:25 PM GMT+0530	58.9 MB	Standard

Viewing 1 to 3

larger, the more conservative the algorithm is.

- **early_stopping_rounds:** The model trains until the validation score stops improving. Validation error needs to decrease at least every `early_stopping_rounds` to continue training. Amazon SageMaker hosting uses the best model for inference.

The XGBoost Classifier has a lot more hyperparameters, we will use only the ones mentioned above.

```
container = get_image_uri(session.boto_region_name, 'xgboost')
xgb = sagemaker.estimator.Estimator(container,
                                    role,
                                    train_instance_count = 1,
                                    train_instance_type = 'ml.m4.xlarge',
                                    output_path = 's3://{}/{}'.format(session.default_bucket(), prefix),
                                    sagemaker_session = session)
```

WARNING:root:There is a more up to date SageMaker XGBoost image. To use the newer image, please set 'repo_version'='0.90-1'. For example:
`get_image_uri(region, 'xgboost', '0.90-1').`

```
xgb.set_hyperparameters(max_depth = 5,
                        eta = 0.2,
                        gamma = 4,
                        min_child_weight = 6,
                        subsample = 0.8,
                        objective = 'reg:linear',
                        early_stopping_rounds = 10,
                        num_round = 200)
```

Now, we define the Hyperparameter Tuner, and start finding the best model, using the training and validation set. We will now get the data to be fed into the models using sagemaker's `s3_input()` function.

```
s3_input_train = sagemaker.s3_input(s3_data=train_location, content_type = 'csv')
s3_input_validation = sagemaker.s3_input(s3_data=val_location, content_type = 'csv')
```

```
#xgb.fit({'train':s3_input_train, 'validation':s3_input_validation})
from sagemaker.tuner import IntegerParameter, ContinuousParameter, HyperparameterTuner
xgb_hyperparameter_tuner = HyperparameterTuner(estimator = xgb,
                                                objective_metric_name = 'validation:rmse', #precision
                                                objective_type = 'Minimize',
                                                max_jobs = 30,
                                                max_parallel_jobs = 3,
                                                hyperparameter_ranges = {
                                                    'max_depth':IntegerParameter(3,12),
                                                    'eta':ContinuousParameter(0.05,0.5),
                                                    'min_child_weight':IntegerParameter(2,8),
                                                    'subsample':ContinuousParameter(0.5,0.9),
                                                    'gamma':ContinuousParameter(0,10)
                                                }
                                                )
```

```
xgb_hyperparameter_tuner.fit({'train':s3_input_train, 'validation':s3_input_validation})
```

```
xgb_hyperparameter_tuner.wait()
```

Then, we define our Hyperparameter Tuner, we set the ranges for:

- max_depth as a set of Integers, from 3 to 12
- eta as a set of floating numbers from 0.05 to 0.5
- min_child_weight as a set of Integers from 2 to 8
- subsample as a set of floating numbers from 0.5 to 0.9
- gamma as a set of floating numbers from 0 to 10

We have set 30 models to train, 3 executing at a time. We set the objective of the model to decrease as much 'root mean squared error' as possible, using the validation set as reference. Once we set them to fit, we wait for the 30 training jobs to finish. Since we have that many models, it takes quite some time to finish. Once it finishes, we attach it to the estimator, and generate the optimised model's predictions.

```
: #seeing the best tuner:
xgb_hyperparameter_tuner.best_training_job()

: 'xgboost-200315-1213-019-3ee3ccc4'
```

This is the best out of 30 different models we had set to run. Now, to use this estimator to predict.

Using a bit of Jupyter notebook magic, we'll fetch a local copy the output of the optimized estimator, and compare with the labels of the testing set.

Then, we'll see the accuracy score and the f-beta score, and find out if the XGBoost Classifier can beat the said record made by the Random Forest Classifier (97% accuracy).

```
!aws s3 cp --recursive $xgb_transform.output_path $'../output'
```

download: s3://sagemaker-ap-south-1-812709844112/xgboost-200315-1213-019-3ee3ccc4-2020-03-15-13-57-45-224/test.csv.out to ../output/test.csv.out

```
y_pred = pd.read_csv('../output/test.csv.out', header = None)
```

```
for i in range(len(y_pred)):
    y_pred[0][i] = np.abs(np.round(y_pred[0][i]))
```

```
from sklearn.metrics import accuracy_score
print("Accuracy of the model: ", accuracy_score(y_test, y_pred))
```

Accuracy of the model: 0.9860298030867483

```
from sklearn.metrics import fbeta_score
print(fbeta_score(y_test, y_pred, beta = 0.01))
```

0.9897990767381056

We have achieved an **accuracy of 98.6%** using XGBoost Classifier, with an **f-beta score of 0.98**.

Inference:

Thus, the tuned XGBoost Classifier seems a good fit as a model for spam prediction, better than the Random Forest Classifier. The optimized model has an accuracy score better than the Random Forest Classifier, and a very good f-beta score, indicating that it is capable of properly functioning as a good Malware Classifier, preventing as many false positives as possible.

However, the following factors must be taken into account:

- The columns dropped right before analysis might have held relevant data, which might affect the model's decisions.
- The hyperparameter tuning jobs could have produced a better model than the one achieved.
- The columns we have right now, might not be enough data to predict on new files. Unless we have enough info on a new file, we cannot make an accurate prediction.

In the future, this model could be deployed using AWS, or could be integrated into a website and deployed, as a malware detector.

However, it might not be ready for a real-world application, where data unknown to us could be provided, which might prove an essential factor in deciding whether a file contains malware or not.

But, if we get as much data as in the way the model has been trained, it would do a good job at correctly classifying files. The vocabulary of the DLLs and Imported Symbols is currently limited. However, that pre-processing can be easily done-over and the model re-trained, making it possible to use in the future.

The model built currently is pretty robust, and can handle different types of cases with ease. The only lagging factor is the one mentioned above, but the model can always be retrained and redeployed, with the new vocabulary it has learnt from.

Major Challenges faced:

Though I had a pretty clear idea on what was to be followed in the project, there were certain difficulties that needed to be overcome. Though they have been managed for now, a better implementation of the solutions will always be present.

- Finding/Choosing the dataset: It was a little difficult to get the dataset used currently, as it is not easily available. Moreover, given the big number of columns, understanding the meaning behind each required intense research, to decide whether a column's value could be a key factor or not.
- Pre-processing the 2 'string' type problems: Deciding the size of the vocabulary for the DLLs and Symbols proved difficult, as one needed to keep the sparsity and the size of the data for training. Following that, the python code written to encode the values into the dataframe takes too much time, as it has to go through each cell of about 50,000x 2,000 cells of data. The current time complexity of the code is $O(n^3)$, and could use optimization
- Deciding between Neural Networks and XGBoost: It was a tough time deciding whether the model to be trained and tuned should be the XGBoost Classifier or a Neural Network. I finally came to the decision to use XGBoost, as NNs take up a lot of space and computing time. Also, this project could also serve to show the evolution of tree-based algorithms, The Random Forest Classifier being one of them.
- AWS Compatibilities: There were difficulties in transferring the project from a local python notebook to an AWS notebook instance. One must keep in mind the difference of libraries and modules available while working on both, locally and on AWS. For instance, the xgboost module not running in the notebook, despite installing it through the terminal of the Jupyter Notebook through pip and conda. Also, one must keep in mind the type of instance of the notebook to be used. Due to heavy calculations, the default instance 'ml.t2.medium' could function properly, and often ran out of memory. It had to be upgraded to 'ml.t2.xlarge' for a smooth flow of execution.