

Tuel efficiency Prediction

Provided with the classic <u>Auto MPG</u> dataset, we will predict the **fuel efficiency** of the late-1970s and early 1980s automobiles, leveraging features such as cylinders, displacement, horsepower, weight, etc.

It is a very small dataset and there are only a few features. We will first build a linear model and a neural network, evaluate their performances, and then leverage an auto-machine learning (AutoML) library called <u>TPOT</u> to see how it can be used to search over many ML model acchitectures.

Learning Objectives

By the end of this session, you will be able to

- understand the core building blocks of a neural network
- understand what dense and activation layers do
- build, train, and evaluate neural networks
- perform AutoML to search for optimal tree-based pipeline for a regression task

Note: <u>State of Data Science and Machine Learning 2021</u> by Kaggle shows that the most commonly used algorithms were linear and logtistic regressions, followed closely by decision trees, random forests, and gradient boosting machines (are you surprised?). Multilayer perceptron, or artificial neural networks are not yet the popular tools for tabular/structured data; see more technical reasons in papers: <u>Deep Neural Networks and Tabular Data: A Survey, Tabular Data: Deep Learning is Not All You Need</u>. For this assignment, the main purpose is for you to get familiar with the basic building blocks in constructing neural networks before we dive into more specialized neural network architectures.

IMPORTANT

You only need to run the following cells if you're completing the assignment in Google Collab. If you've already installed these libraries locally, you can skip installing these libraries.

```
# Connect colab to your Google Drive
from google.colab import drive
drive.mount('/content/drive')
    Mounted at /content/drive
!pip install -q seaborn ## Use seaborn for pairplot
!pip install -q tpot # Use TPOT for automl
                                             87 kB 3.3 MB/s
                                           192.9 MB 70 kB/s
                                         139 kB 56.0 MB/s
      Building wheel for stopit (setup.py) ... done
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
# Make NumPy printouts easier to read.
np.set_printoptions(precision=3, suppress=True)
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers
print(tf.__version__)
    2.8.2
```

→ Task 1 - Data: Auto MPG dataset

1. The dataset is available from the <u>UCI Machine Learning Repository</u>. First download and import the dataset using pandas:

```
url = 'http://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data
column_names = [
   'MPG', 'Cylinders', 'Displacement', 'Horsepower', 'Weight',
   'Acceleration', 'Model Year', 'Origin'
```

dataset.tail()

		MPG	Cylinders	Displacement	Horsepower	Weight	Acceleration	Model Year	(
3	393	27.0	4	140.0	86.0	2790.0	15.6	82	
3	394	44.0	4	97.0	52.0	2130.0	24.6	82	
3	395	32.0	4	135.0	84.0	2295.0	11.6	82	
3	396	28.0	4	120.0	79.0	2625.0	18.6	82	
3	397	31.0	4	119.0	82.0	2720.0	19.4	82	

2. The dataset contains a few unknown values, we drop those rows to keep this initial tutorial simple. Use pd.DataFrame.dropna():

```
dataset = dataset.dropna()
```

3. The "origin" column is categorical, not numeric. So the next step is to one-hot encode the values in the column with <u>pd.get_dummies</u>.

```
dataset['Origin'] = dataset['Origin'].replace({1: 'USA', 2: 'Europe', 3: 'Japan'})
dataset = pd.get_dummies(dataset, columns=['Origin'], prefix='', prefix_sep='')
dataset.tail()
```

	MPG	Cylinders	Displacement	Horsepower	Weight	Acceleration	Model Year	I
393	27.0	4	140.0	86.0	2790.0	15.6	82	
394	44.0	4	97.0	52.0	2130.0	24.6	82	
395	32.0	4	135.0	84.0	2295.0	11.6	82	
396	28.0	4	120.0	79.0	2625.0	18.6	82	
397	31.0	4	119.0	82.0	2720.0	19.4	82	

4. Split the data into training and test sets. To reduce the module importing overhead, instead of sklearn.model_selection.train_test_split(), use pd.DataFrame.sample() to save 80% of the data aside to train dataset, set the random state to be 0 for reproducibility.

Then use pd.DataFrame.drop() to obtain the test_dataset.

```
train_dataset = dataset.sample(frac=0.8, random_state=0)
test_dataset = dataset.drop(train_dataset.index)
```

5. Review the pairwise relationships of a few pairs of columns from the training set.

The top row suggests that the fuel efficiency (MPG) is a function of all the other parameters. The other rows indicate they are functions of each other.

```
sns.pairplot(train_dataset[['MPG', 'Cylinders', 'Displacement', 'Weight']], diag_kind=
```



Let's also check the overall statistics. Note how each feature covers a very different range:

train_dataset.describe().transpose()

	count	mean	std	min	25%	50%	75%	max
MPG	314.0	23.310510	7.728652	10.0	17.00	22.0	28.95	46.6
Cylinders	314.0	5.477707	1.699788	3.0	4.00	4.0	8.00	8.0
Displacement	314.0	195.318471	104.331589	68.0	105.50	151.0	265.75	455.0
Horsepower	314.0	104.869427	38.096214	46.0	76.25	94.5	128.00	225.0
Weight	314.0	2990.251592	843.898596	1649.0	2256.50	2822.5	3608.00	5140.0
Acceleration	314.0	15.559236	2.789230	8.0	13.80	15.5	17.20	24.8
Model Year	314.0	75.898089	3.675642	70.0	73.00	76.0	79.00	82.0
Europe	314.0	0.178344	0.383413	0.0	0.00	0.0	0.00	1.0
Japan	314.0	0.197452	0.398712	0.0	0.00	0.0	0.00	1.0
USA	314.0	0.624204	0.485101	0.0	0.00	1.0	1.00	1.0
📆		I	2	I	.8	28 8-	1 1	\

5. Split features from labels

Separate the target value—the "label"—from the features. This label is the value that you will train the model to predict.

train features

	Cylinders	Displacement	Horsepower	Weight	Acceleration	Model Year	Europe
146	4	90.0	75.0	2125.0	14.5	74	(
282	4	140.0	88.0	2890.0	17.3	79	(
69	8	350.0	160.0	4456.0	13.5	72	(
378	4	105.0	63.0	2125.0	14.7	82	(
331	4	97.0	67.0	2145.0	18.0	80	(
281	6	200.0	85.0	2990.0	18.2	79	(
229	8	400.0	180.0	4220.0	11.1	77	(
150	4	108.0	93.0	2391.0	15.5	74	(

Task 2 - Normalization Layer

314 rows × 9 columns

It is good practice to normalize features that use different scales and ranges. Although a model *might* converge without feature normalization, normalization makes training much more stable.

Similar to scikit-learn, tensorflow.keras offers a list of <u>preprocessing layers</u> so that you can build and export models that are truly end-to-end.

1. The Normalization layer (<u>tf.keras.layers.Normalization</u> is a clean and simple way to add feature normalization into your model. The first step is to create the layer:

```
normalizer = tf.keras.layers.Normalization(axis=-1)
```

2. Then, fit the state of the preprocessing layer to the data by calling Normalization.adapt:

```
normalizer.adapt(np.array(train_features))
```

We can see the feature mean and variance are stored in the layer:

```
print(f'feature mean: {normalizer.mean.numpy().squeeze()}\n')
print(f'feature variance: {normalizer.variance.numpy().squeeze()}')

feature mean: [ 5.478 195.318 104.869 2990.252 15.559 75.898 0.178 0.624]
```

```
feature variance: [ 2.88 10850.413 1446.699 709896.9 7.755 13 0.147 0.158 0.235]
```

When the layer is called, it returns the input data, with each feature independently normalized:

→ Task 3 - Linear regression ✓

Before building a deep neural network model, start with linear regression using all the features.

Training a model with tf.keras typically starts by defining the model architecture. Use a tf.keras.Sequential model, which represents a sequence of steps.

There are two steps in this multivariate linear regression model:

- Normalize all the input features using the tf.keras.layers.Normalization preprocessing layer. You have defined this ealier as normalizer.
- Apply a linear transformation (y = mx + b where m is a matrix and b is a vector.) to produce 1 output using a linear layer ($\underline{\mathsf{tf.keras.layers.Dense}}$).

The number of *inputs* can either be set by the <code>input_shape</code> argument, or automatically when the model is run for the first time.

1. Build the Keras Sequential model:

```
linear_model = tf.keras.Sequential([
    normalizer,
    tf.keras.layers.Dense(1)
])
```

linear_model.summary()

Model: "sequential"

```
Layer (type)

Output Shape

Param #

normalization (Normalizatio (None, 9) 19

n)

dense (Dense) (None, 1) 10

Total params: 29

Trainable params: 10

Non-trainable params: 19
```

2. This model will predict 'MPG' from all features in train_features. Run the untrained model on the first 10 data points / rows using Model.predict(). The output won't be good, but notice that it has the expected shape of (10, 1):

3. When you call the model, its weight matrices will be built—check that the kernel weights (the m in y = mx + b) have a shape of (9, 1):

```
linear model.layers[1].kernel
```

4. Once the model is built, configure the training procedure using the Keras Model.compile method. The most important arguments to compile are the loss and the optimizer, since these define what will be optimized and how (using the tf.keras.optimizers.Adam).

Here's a list of built-in loss functions in <u>tf.keras.losses</u>. For regression tasks, <u>common loss functions</u> include mean squared error (MSE) and mean absolute error (MAE). Here, MAE is preferred such that the model is more robust against outliers.

For optimizers, gradient descent (check this video <u>Gradient Descent, Step-by-Step</u> for a refresher) is the preferred way to optimize neural networks and many other machine learning algorithms. Read <u>an overview of graident descent optimizer algorithms</u> for several popular gradient descent algorithms. Here, we use the popular <u>tf.keras.optimizers.Adam</u>, and set the learning rate at 0.1 for faster learning.

```
linear_model.compile(
    optimizer = tf.keras.optimizers.Adam(learning_rate=0.1),
    loss = tf.keras.losses.MeanAbsoluteError()
    )
```

5. Use Keras Model.fit to execute the training for 100 epochs, set the verbose to 0 to suppress logging and keep 20% of the data for validation:

```
%%time
# history = linear_model.fit(train_features.astype("float32") , train_labels.astype("float32") , train_labels.astype("float32") , train_labels.astype("float32") , epochs=1
CPU times: user 4.01 s, sys: 220 ms, total: 4.23 s
Wall time: 3.99 s
```

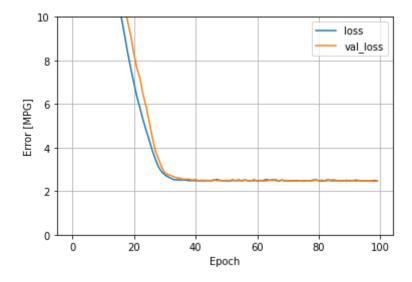
6. Visualize the model's training progress using the stats stored in the history object:

```
hist = pd.DataFrame(history.history)
hist['epoch'] = history.epoch
hist.tail()
```

```
loss val_loss
                           epoch
     95 2.473868
                   2.473518
                                95
     96 2.471930
                   2.453896
                               96
def plot_loss(history):
  plt.plot(history.history['loss'], label='loss')
 plt.plot(history.history['val_loss'], label='val_loss')
 plt.ylim([0, 10])
 plt.xlabel('Epoch')
 plt.ylabel('Error [MPG]')
 plt.legend()
 plt.grid(True)
```

Use plot_loss(history) provided to visualize the progression in loss function for training and validation data sets.

```
plot_loss(history)
```



7. Collect the results on the test set for later using Model.evaluate().

→ Task 4 - Regression with a deep neural network (DNN)

You just implemented a linear model for multiple inputs. Now, you are ready to implement multiple-input DNN models.

The code is very similar except the model is expanded to include some "hidden" **non-linear** layers. The name "hidden" here just means not directly connected to the inputs or outputs.

- The normalization layer, as before (with normalizer for a multiple-input model).
- Two hidden, non-linear, <u>Dense</u> layers with the ReLU (relu) activation function nonlinearity. One way is to set parameter activation inside <u>Dense</u> Set the number of neurons at each layer to be 64.
- A linear Dense single-output layer.
- 1. Include the model and compile method in the build and compile model function below.

2. Create a DNN model with normalizer (defined earlier) as the normalization layer:

```
dnn model = build and compile model(normalizer)
```

3. Inspect the model using Model.summary(). This model has quite a few more trainable parameters than the linear models:

```
Model.summary()

Model: "sequential_1"

Layer (type) Output Shape Param #
```

4. Train the model with Keras Model.fit:

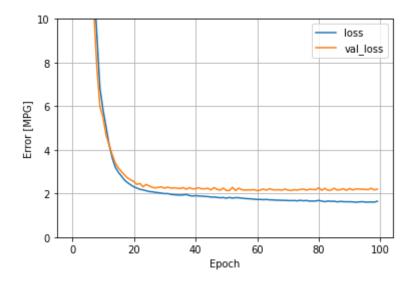
Non-trainable params: 19

```
%%time
history = dnn_model.fit(
    train_features,
    train_labels,
    validation_split=0.2,
    verbose=0, epochs=100)

CPU times: user 4.34 s, sys: 233 ms, total: 4.58 s
Wall time: 5.63 s
```

5. Visualize the model's training progress using the stats stored in the history object.

plot_loss(history)



Do you think the DNN model is overfitting? What gives away?

YOUR ANSWER HERE

6. Let's save the results for later comparison.

```
test_results['dnn_model'] = dnn_model.evaluate(test_features, test_labels, verbose=0)
```




1. Since both models have been trained, we can review their test set performance:

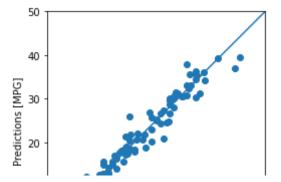
```
pd.DataFrame(test results, index=['Mean absolute error [MPG]']).T
```

	Mean	absolute	error	[MPG]
linear_model			2.	514709
dnn model			1.0	654161

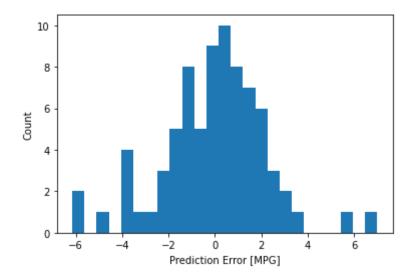
These results match the validation error observed during training.

2. We can now make predictions with the dnn model on the test set using Keras Model.predict and review the loss. Use .flatten().

```
test predictions = dnn model.predict(test features).flatten()
a = plt.axes(aspect='equal')
plt.scatter(test labels, test predictions)
plt.xlabel('True Values [MPG]')
plt.ylabel('Predictions [MPG]')
lims = [0, 50]
plt.xlim(lims)
plt.ylim(lims)
= plt.plot(lims, lims)
```



3. It appears that the model predicts reasonably well. Now, check the error distribution:



4. Save it for later use with Model.save:

```
dnn_model.save('dnn_model')
```

5. Reload the model with Model.load_model; it gives identical output:

```
reloaded = tf.keras.models.load_model('dnn_model')

test_results['reloaded'] = reloaded.evaluate(
    test_features, test_labels, verbose=0)

pd.DataFrame(test_results, index=['Mean absolute error [MPG]']).T
```

	Mean	absolute	error	[MPG]
linear_model			2.	514709
dnn_model			1.0	654161
reloaded			1.0	654161

Task 6 - Nonlinearity

We mentioned that the relu activation function introduce non-linearity; let's visualize it. Yet there are six numerical features and 1 categorical features, it is impossible to plot all the dimensions on a 2D plot; we need to simplify/isolate it.

Note: in this task, code is provided; the focus in on understanding.

1. We focus on the relationship between feature Displacement and target MPG.

To do so, create a new dataset of the same size as train_features, but all other features are set at their median values; then set the Displacement between 0 and 500.

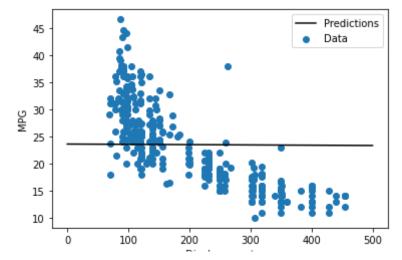
```
fake = np.outer(np.ones(train_features.shape[0]), train_features.median())
fake = pd.DataFrame(fake, columns = train_features.columns)
fake.Displacement = np.linspace(0, 500, train_features.shape[0])
```

2. Create a plotting function to a) visualize real values between <code>Displacement</code> and <code>MPG</code> from the training dataset in scatter plot b) overlay the predicted MPG from Displacement varying from 0 to 500, but holding all other features constant.

```
def plot_displacement(x, y):
   plt.scatter(train_features['Displacement'], train_labels, label='Data')
   plt.plot(x, y, color='k', label='Predictions')
   plt.xlabel('Displacement')
   plt.ylabel('MPG')
   plt.legend()
```

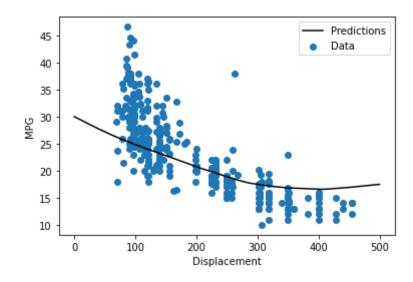
3. Visualize predicted MPG using the linear model.

```
plot displacement(fake.Displacement, linear model(fake))
```



4. Visualize predicted MPG using the neural network model. Do you see an improvement/non-linearity from the linear model?

plot_displacement(fake.Displacement, dnn_model.predict(fake))



- 5. What are the other activation functions? Check the list of <u>activations</u>.
 Optional. Modify the DNN model with a different activation function, and fit it on the data; does it perform better?
- 6. Overfitting is a common problem for DNN models, how should we deal with it? Check <u>Regularizers</u> on tf.keras. Any other techiniques that are invented for neural networks?

Task 7 - AutoML with TPOT

1. Instantiate and train a TPOT auto-ML regressor.

The parameters are set fairly arbitrarily (if time permits, you shall experiment with different sets of parameters after reading <u>what each parameter does</u>). Use these parameter values:

```
generations: 10
population_size: 40
scoring: negative mean absolute error; read more in scoring functions in TPOT
verbosity: 2 (so you can see each generation's performance)
```

The final line with create a Python script <code>tpot_products_pipeline.py</code> with the code to create the optimal model found by TPOT.

440/440 [07:41<00:00, 1.15s/pipel

2. Examine the model pipeline that TPOT regressor offers. If you see any model, function, or class that are not familiar, look them up!

Note: There is randomness to the way the TPOT searches, so it's possible you won't have exactly the same result as your classmate.

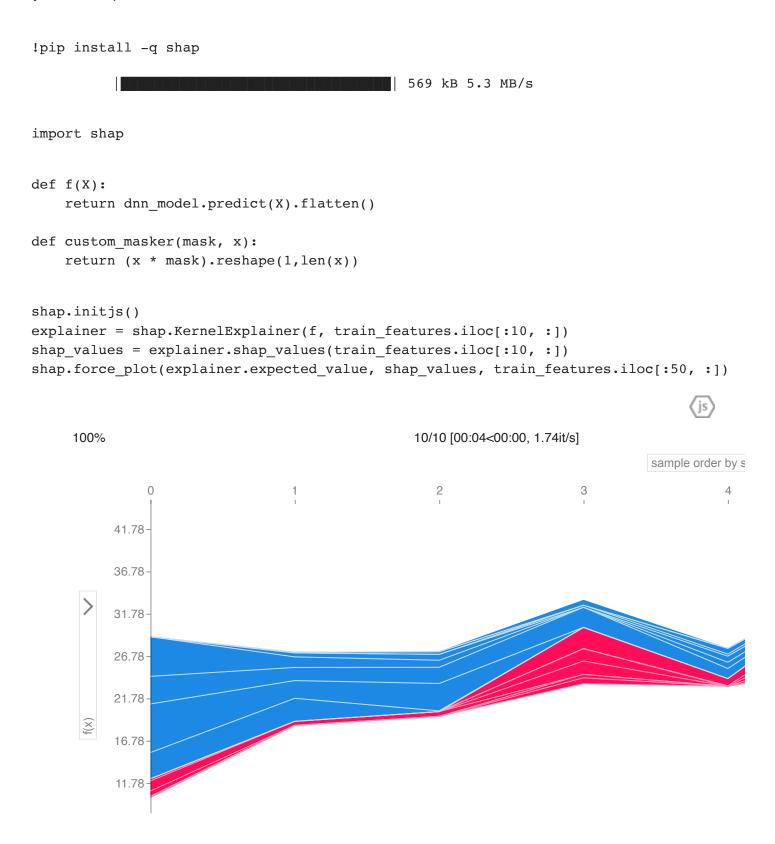
```
GENELACION J - CULLENC DESC INCELNAL CV SCOLE: -1.24/70171V170707
cat tpot mpg pipeline.py
    import numpy as np
    import pandas as pd
    from sklearn.ensemble import ExtraTreesRegressor
    from sklearn.linear model import RidgeCV
    from sklearn.model selection import train test split
    from sklearn.pipeline import make_pipeline, make_union
    from tpot.builtins import StackingEstimator
    from tpot.export_utils import set_param_recursive
    # NOTE: Make sure that the outcome column is labeled 'target' in the data file
    tpot_data = pd.read_csv('PATH/TO/DATA/FILE', sep='COLUMN_SEPARATOR', dtype=np.flc
    features = tpot data.drop('target', axis=1)
    training features, testing features, training target, testing target = \
                 train_test_split(features, tpot_data['target'], random_state=42)
    # Average CV score on the training set was: -1.247981910198969
    exported pipeline = make pipeline(
        StackingEstimator(estimator=ExtraTreesRegressor(bootstrap=True, max_features:
        RidgeCV()
    # Fix random state for all the steps in exported pipeline
    set param recursive(exported pipeline.steps, 'random state', 42)
    exported pipeline.fit(training features, training target)
    results = exported pipeline.predict(testing features)
```

3. Optional: Take the appropriate lines (e.g., updating path to data and the variable names) from tpot_mpg_pipeline.py to build a model on our training set and make predictions on the test set. Save the predictions as y_pred, and compute appropriate evaluation metric. You may find that for this simple data set, the nueral network we built outperforms the tree-based model, yet note it is not a conclusion that we can be generalized for all tabular data.

Task 8 - Model Explainability

Last week, we introduced model explainability with SHAP and will continue to incorporate it as part our model output this week. You can use the <u>Kernal Explainer</u> for explainability of both the Neural Networks and the TPOT classifier.

NOTE: If you're using Collab to complete this assignment, please run the following cell - otherwise you can skip it.



What is Normalization and how does Normalization make training a model more stable?

The goal of normalization is to change the values of numeric columns in the dataset to use a common scale, without distorting differences in the ranges of values or losing information. The difference in scal eof certain columns when analyzing data can cause problems when you attempt to combine the values as features during modeling. Normalization avoids these problems by creating new values that maintain the general distribution and ratios in the source data, while keeping values within a scale applied across all numeric columns used in the model.

What are loss and optimizer functions and how do they work?

While training the deep learning model, we need to modify each epoch's weights and minimize the loss function. An optimizer is a function or an algorithm that modifies the attributes of the neural network, such as weights and learning rate. Thus, it helps in reducing the overall loss and improve the accuracy.

Loss functions are helpful to train a neural network. Given an input and a target, they calculate the loss, i.e difference between output and target variable.

What is Gradient Descent and how does it work?

Gradient Descent calcultes gradient for the whole dataset and updates values in direction opposite to the gradients until we find a local minima. Stochastic Gradient Descent performs a parameter update for each training example unlike normal Gradient Descent which performs only one update. Thus it is much faster. Gradient Decent algorithms can further be improved by tuning important parametes like momentum, learning rate etc.

What is an activation function?

The activation function defines the output of a neuron / node given an input or set of input (output of multiple neurons). It's the mimic of the stimulation of a biological neuron.

The output of the activation function to the next layer (in shallow neural network: input layer and output layer, and in deep network to the next hidden layer) is called forward propagation (information propagation). It's considered as a non linearity transformation of a neural network.

What are the outputs of the following activation functions: ReLU, Softmax Tanh, Sigmoid

- In tanh function the drawback we saw in sigmoid function is addressed (not entirely), here the only difference with sigmoid function is the curve is symetric across the origin with values ranging from -1 to 1. Tanh help to solve non zero centered problem of sigmoid function. Tanh squashes a real-valued number to the range [-1, 1]. It's non-linear too.
- Sigmoid functions are used in machine learning for logistic regression and basic neural network implementations and they are the introductory activation units. But for advanced

Neural Network Sigmoid functions are not preferred due to various drawbacks (vanishing gradient problem). It is one of the most used activation function for beginners in Machine Learning and Data Science when starting out. It is a very simple which takes a real value as input and gives probability that 's always between 0 or 1. It looks like 'S' shape.

- A Rectified Linear Unit (A unit employing the rectifier is also called a rectified linear unit ReLU) has output 0 if the input is less than 0, and raw output otherwise. That is, if the input is greater than 0, the output is equal to the input. The operation of ReLU is closer to the way our biological neurons work. ReLU is non-linear and has the advantage of not having any backpropagation errors unlike the sigmoid function, also for larger Neural Networks, the speed of building models based off on ReLU is very fast opposed to using Sigmoids. This is most popular activation function which is used in hidden layer of NN. It's not linear and provides the same benefits as Sigmoid but with better performance.
- Softmax maps output to a [0,1] range but also maps each output in such a way that the total sum is 1. The output of Softmax is therefore a probability distribution. The softmax function is often used in the final layer of a neural network-based classifier. Such networks are commonly trained under a log loss (or cross-entropy) regime, giving a non-linear variant of multinomial logistic regression. Generally, we use the function at last layer of neural network which calculates the probabilities distribution of the event over 'n' different events. The main advantage of the function is able to handle multiple classes.

What is the TPOT algorithm and how does it work?

TPOT is an open-source library for performing AutoML in Python. It makes use of the popular Scikit-Learn machine learning library for data transforms and machine learning algorithms and uses a Genetic Programming stochastic global search procedure to efficiently discover a top-performing model pipeline for a given dataset.

TPOT uses a tree-based structure to represent a model pipeline for a predictive modeling problem, including data preparation and modeling algorithms and model hyperparameters.

An optimization procedure is then performed to find a tree structure that performs best for a given dataset. Specifically, a genetic programming algorithm, designed to perform a stochastic global optimization on programs represented as trees.

What does TPOT stand for?

TPOT (Tree-based Pipeline Optimization Tool) is an AutoML tool specifically designed for the efficient construction of optimal pipelines through genetic programming. TPOT is and open source library and makes use of scikit-learn components for data transformation, feature decomposition, feature selection and model selection

Double-click (or enter) to edit

Task 9 - Taking it to the Next Level!

Let's take our models and make a model comparison demo like we did last week, but this time you're taking the lead!

- 1. Save your training dataset as a CSV file so that it can be used in the Streamlit app.
- 2. Build a results DataFrame and save it as a CSV so that it can be used in the Streamlit app.
- 3. In Tab 1 Raw Data:
- Display your training dataset in a Streamlit DataFrame (st.DataFrame).
- Build 1-2 interactive Plotly visualizations that explore the dataset (correlations, scatterplot, etc.)
- 2. In Tab 2 Model Results:
- Display your performance metrics appropriately using 2-3 metrics for model comparison.
- 3. In Tab 3 Model Explainability:
- Make local and global explainability plots to compare two models at a time side-by-side.

Here is a good example if how to create some different explainability plots using Plotly.

Additional Resources

- <u>Tensorflow playground</u> for an interactive experience to understand how nueral networkds work.
- An Introduction to Deep Learning for Tabular Data covers embeddings for categorical variables.
- <u>Imbalanced classification: credit card fraud detection</u> demonstrates using class_weight to handle imbalanced classification problems.

Acknowledgement and Copyright

Acknowledgement

This notebook is adapted from tensorflow/keras tuorial - regression

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