In [1]:
```
import pandas as pd
from fastai.tabular.all import *
from fastai.data.transforms import IndexSplitter
```

Gradient Boosting Machines - Forecasting Stic Sales

Introduction

After learning about **ensembles of decision trees** as an approach to modelling tabular data, I'v decided to have another shot at the Forecasting Sticker Sales Kaggle competition.

While I initially approached the problem with **deep learning** and scored in the top % of pre I want to see if I can improve on this by taking a different approach.

In my last notebook I uncovered **random forests** which is one approach of ensembling decision However, there is another area of ensembling I wish to learn more about, called **gradient boost machines (GBMs)**.

Since I've already gone into detail in my previous notebook about how decision trees are made a ensembling is, I will be focusing on *building* that knowledge. I won't go into detail about when to **ensembles of decision trees** vs **deep learning**.

Furthermore, I've selected a **regression** problem for this project, as I practiced a **classification** when learning random forests.

The first thing to establish is the key differences between **random forests** and **GBMs**.

Where random forests utilise **bagging** (training each model on a different data subset and avera GBMs use **boosting**, where models are 'added'. Each new decision tree correct the errors made previous models and the final prediction is the the weighted sum of all the predictions from all the models. Each decision tree in the ensemble is referred to as an **estimator**.

GBMs can generally perform better than random forests, but they are more complicated to imple

- They require some fussing with hyperparamaters.
- They are prone to overfitting as each tree is not independent of the others.
- They are rely on sequential training, which is slower, whereas random forests can utilise par training (as they are independent trees).

So, a good approach would be to start with a random forest, then try a GBM. We will do that her description for random forests will be brief as we have already gone into detail about this previou

Data Engineering

Let's start with our data.

In [2]:
```
```

```
df = pd.read_csv('train.csv')
df.isnull().sum()
```

Out[2]:

id	
date	
country	
store	
product	
num_sold	

dtype: int

We will drop training rows missing the independent variable to focus on learning the concept of C

Normally, with features missing values (there are none here) we would fill numerical features wit mean/median/mode and categorical features with a placeholder like 'Unknown' as the fact that d missing can still be useful information to train a model.

In [3]:
```
df.dropna(axis=0, inplace=True)
df
```

Out[3]:

id	date	country	store	product	num
-	-	Canada	Discount Stickers	Kaggle	
-	-	Canada	Discount Stickers	Kaggle Tiers	
-	-	Canada	Discount Stickers	Kerneler	
-	-	Canada	Discount Stickers	Kerneler Dark Mode	
-	-	Canada	Stickers for Less	Holographic Goose	
...	...	...	...	...	...
-	-	Singapore	Premium Sticker Mart	Holographic Goose	
-	-	Singapore	Premium Sticker Mart	Kaggle	
-	-	Singapore	Premium Sticker Mart	Kaggle Tiers	
-	-	Singapore	Premium Sticker Mart	Kerneler	
-	-	Singapore	Premium Sticker Mart	Kerneler Dark Mode	

rows × columns

Now, we will perform much of the same **feature engineering** as the deep learning approach. Sir based models are robust to non-normality, log transformations will not be used in this approach predictors; however, we will perform a log transformation on the `num_sold` column as our pred are highly skewed with a long right tail (shown in the last notebook).

As previously discussed, OHE is generally not needed for tree-based approaches.

In [4]:
```
%%capture
df['num_sold'] = np.log1p(df['num_sold'])

# extract useful features from date
add_datepart(df, 'date')

# drop unneeded columns
df.drop('id', axis=1, inplace=True)
```

Now, we can define a training and validation set. Since we are working with data over time, we w the end of the df and use this as our **validation set**.

I am going to be using a new techinque I recently learn for this, defined by `TabularPandas`. `TabularPandas` sits on top of a pandas df and is provided by `fastai`. This class modifies d place and runs transformations when data is passed in, rather than lazily as data is accessed.

In [5]:
```
procs = [Categorify, FillMissing]
```

These two transformations are not strictly necessary on this dataset as we have no missing valu predictor columns. However, `FillMissing` is a `TabularProc` (much like a `Transform` i pandas) that replaces missing values with median values. `Categorify` is a new feature that i `True` for any row where the value was missing (as missing values can hold valuable informatic training). We will pass the `TabularProc`s when creating our training and validation sets.

In [6]:
```
cond = df.Year<2016
train_idx, valid_idx = np.where(cond)[0], np.where(~cond)[0]
splits = (list(train_idx),list(valid_idx))
```

`where()` is a useful function returning indices of all True values.

We also want to define our **categorical** and **continuous** variables before creating our `TabularPandas`. While we did this manually last time, we can actually benefit from the `fast` function `cont_cat_split` that can automtically infer the variable type.

In [7]:
```
cont, cat = cont_cat_split(df, dep_var="num_sold")
cont, cat
```

Out[7]:
```
(['Week', 'Day', 'Dayofyear', 'Elapsed'],
 ['country',
  'store',
  'product',
  'Year',
  'Month',
  'Dayofweek',
  'Is_month_end',
  'Is_month_start',
  'Is_quarter_end',
  'Is_quarter_start',
  'Is_year_end',
  'Is_year_start'])
```

Now we are ready for our `TabularPandas`!

In [8]:
```
data = TabularPandas(df, procs, cat, cont, y_names="num_sold", splits=spl
len(data.train), len(data.valid)
```

Out[8]:
```
(189492, 31767)
```

Random Forest

Making the Model

Let's build a random forest! While I have previously discussed in-depth how **random forests** wo now using a random forest for a **regression** task for the first time.

How does the decision tree predict a continuous value?

Each decision tree will output a numerical value for a data point, which is the mean of the target the training samples in the leaf node where the data point falls.

But how does the model decide where to make the split at each binary split?

The model will calculate and minimise the **variance** also known as **minimizing impurity**. Just lil classification task, the model will see how similar the targets of each data point are for each pos split. Instead of just comparing if they are the same or different though, it will use a formula calle **weighted average variance**. This basically means that values that are closer together will have **impurity** and this split will be prioritised.

This explains how a decision tree performs a regression task as opposed to a classification task.

In [9]:
```
from sklearn.ensemble import RandomForestRegressor

rf = RandomForestRegressor(n_jobs=-1, # no of jobs to run in parallel, -1
                           n_estimators=100, # no trees
                           max_features=0.5, # no of columns to sample at
                           min_samples_leaf=3, # min number of data point
                           max_samples=0.75, # how many rows to sample fo
                           oob_score=True) # we use oob to claculate the

rf.fit(data.train.xs, data.train.y)
y_pred = rf.predict(data.valid.xs)
```

Now that we have our predictions, let's evaluate them using **mean absolute percentage error** (which is the defined metric for this Kaggle competition.

In [10]:
```
import numpy as np

def mape(y_actual, y_pred, epsilon=1e-10):
  y_actual = np.array(y_actual)
  y_pred = np.array(y_pred)

  mape = np.mean(np.abs((y_actual - y_pred) / (y_actual + epsilon)))
  return mape

mape(data.valid.y, y_pred)
```

Out[10]:
```
0.01948954560857891
```

Out-of-bag Error

At this point, we're going to find a new way of measuring the prediciton error on the trainin set, b only the calculation of a row's error trees where that rows was not included in the training.

Since every tree is trained on a different random subset of rows, we can imagine that every tree own validation set, which is the rows that were not selected for that tree's training. The predictior calculated on these remaining rows is called the **out-of-bag (OOB) error**.

This is useful if we don't have much data (so perhaps not useful here), as we can see whether o generalises without needing to separate data for a validation set.

This is why when training the model we activated the parameter `oob_score`.

In [12]:
```
mape(rf.oob_prediction_, data.train.y)
```

Out[12]:
```
0.008896529053385985
```

We can see that the out-of-bag error is much lower than our validation set error - since OOB san still part of the overall training set, they are not entirely independent of the training process, maki optimistic (but nevertheless useful) performance estimate.

Submitting Predictions

At this point, I'm going to make some predictions on the test dataset and submit to Kaggle, just t where we are at!

I ran into some issues here, as the data pipeline for the model requires a `TabularPandas`. Si appears this class was designed for neural networks with fastai - which inherintly hold informatio the data formatting - I can't seem to find a way to add a test set to my pre-exisiting `TabularPa` object. The code below is a bit messy, and the test_data is stored in `.train`. If anyone has a b way of approaching this, I would love to know!

In [13]:
```
%%capture
test_df = pd.read_csv('test.csv')
add_datepart(test_df, 'date')

test_data = TabularPandas(test_df, procs, cat, cont)

test_df['num_sold'] = rf.predict(test_data.train.xs)
test_df['num_sold'] = np.expm1(test_df['num_sold'])
sub_df = test_df[['id', 'num_sold']]

sub_df.to_csv('submission.csv', index=False)
```

So, after submitting the results of our predictions on the test data, we were scoring a MAPE of . ! This is not a bad prediction considering our deep learning result was sitting around th optimisation!

Gradient Boosting Machine

Making the Model

I can now try out the `GradientBoostingRegressor` also provided by sklearn.

In [14]:
```
from sklearn.ensemble import GradientBoostingRegressor

gbm = GradientBoostingRegressor(
    n_estimators = 100,
    learning_rate=1,
    max_depth=20,
    min_samples_split=2,
```

```
    min_samples_leaf=3
)

gbm.fit(data.train.xs, data.train.y)

y_pred = gbm.predict(data.valid.xs)

mape(data.valid.y, y_pred)
```

Out[14]: 0.02168047853938121

As you can see above, the model requires a lot more playing around with hyperparameters and took significantly longer to train.

The **learning rate** in a GBM is used to scale the contribution of each new weak decision tree to model. A smaller learning rate means smaller updates to the model, while a larger learning rate larger updates to the model. You use the learning rate in GBMs much like you would in a NN - yo want the value to big or too small.

Submitting Predictions

In [15]:
```
%%capture
test_df = pd.read_csv('test.csv')
add_datepart(test_df, 'date')

test_data = TabularPandas(test_df, procs, cat, cont)

test_df['num_sold'] = rf.predict(test_data.train.xs)
test_df['num_sold'] = np.expm1(test_df['num_sold'])
sub_df = test_df[['id', 'num_sold']]

sub_df.to_csv('submission2.csv', index=False)
```

I used the model on the test set (as above) and after playing around with the hyperparameters I to get a MAPE value of . , slightly worse than the random forest.

While we weren't able to improve on the result generated by our NN in the competition, there is useful information we can derive from our **ensembles of decision trees**.

Prediction Confidence

Another useful piece of information we can derive from an ensemble of decision trees is the star deviation of the predictions across trees.

While the mean will provide the estimate, the standard deviation will provide **the confidence**, as show if each tree agrees with the others or not. A low standard deviation indicates high confiden whereas a high standard deviation represents a low confidence.

This would be useful if you were making critical decisions based on the model - if the model was confident in its prediction it might make you think twice before doing something rash.

We will use Numpy to make this prediction, as it is optimised to work with large matrices.

- `gbm.estimators_` is a list of all `DecisionTreeRegressor`s that makes u gradient boosting machine.
- `tree` is a list containing the `DecisionTreeRegressor` at position and the data t position .
- `data.valid.xs.to_numpy()` takes our `TabularPandas` of all validation feeatures a converts it to a numpy array
- We calculate each decision tree's prediction of each data point in the validation set, returnin a list of predictions using `predict()`.

In [27]:
```
preds = np.stack([tree[0].predict(data.valid.xs.to_numpy()) for tree in g
preds.shape
```

Out[27]:
```
(100, 31767)
```

Now that we have tree's predictions of , data points, we can stack thos predictions and calculate the standard deviation across the th axis (i.e., the axis containing decision trees).

In [25]:
```
preds_std = preds.std(0)
preds_std.max(), preds_std.min()
```

Out[25]:
```
(0.41395298975817885, 0.0023943965717917568)
```

We can see the value of this calculation by comparing the highest standard deviation and the lo there is a big difference between the model's level of confidence (. %). This would be ve important to gauge if using the model to predict a piece of data.

Feature Importance

We can also use the **ensembles of decision trees** to determine how much each feature contrib the improvement of the model. Scikit-learn has a great feature to help us calculate that.

In [29]:
```
df.columns
```

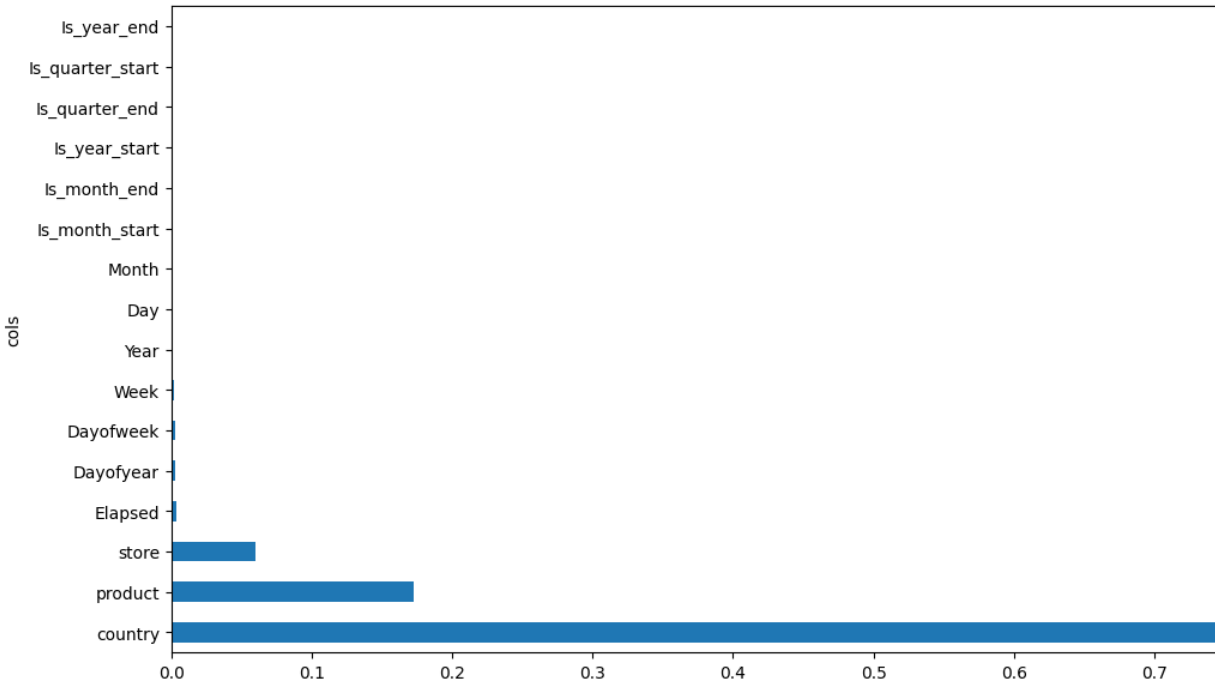
Out[29]:
```
Index(['country', 'store', 'product', 'num_sold', 'Year', 'Month', 'Week',
       'Day', 'Dayofweek', 'Dayofyear', 'Is_month_end', 'Is_month_start',
       'Is_quarter_end', 'Is_quarter_start', 'Is_year_end', 'Is_year_start',
       'Elapsed'],
      dtype='object')
```

In [38]:
```
pd.options.display.float_format = '{:.3f}'.format # prevent scientific no
fi = pd.DataFrame({'cols':cat+cont, 'imp':gbm.feature_importances_}).sort
```

Now, we can plot this data.

In [39]:
```
fi.plot('cols','imp','barh', figsize=(12,7), legend=False)
```

Out[39]:
```
<Axes: ylabel='cols'>
```



This is a really interesting discovery. Essentially, only features actually contribute to our de tree's performance:

- `country`
- `product`
- `store`

These are the three features we didn't play around with at all. This indicates that either the date not a useful indicator of sales, or that we've done a poor job of feature engineering it.

Since the purpose of this notebook is to work on understanding **ensembles of decision trees**, I further into improving the model. But this does give us valuable insight into the power of this mod technique. If we were working with thousands and thousands of features, this would be a very ea to immediately eliminate unhelpful features.

Remove Low-importance Variables

Let's get rid of the low-importance variables (those with a feature performance < .) and s it affects the model's performance.

In [40]:
```
to_keep = fi[fi.imp>=0.01].cols
len(to_keep)
```

Out[40]: 3

Now, we will retrain the model.

In [56]:
```
xs_imp = data.train.xs[to_keep]
valid_xs_imp = data.valid.xs[to_keep]
gbm2 = GradientBoostingRegressor(
    n_estimators = 100,
    learning_rate=1,
    max_depth=20,
```

```
    min_samples_split=2,
    min_samples_leaf=3
)

gbm2.fit(xs_imp, data.train.y)

y_pred = gbm2.predict(valid_xs_imp)

mape(data.valid.y, y_pred)
```

Out[56]: 0.03336315076930216

That trained in less then a second and our MAPE has barely changed!

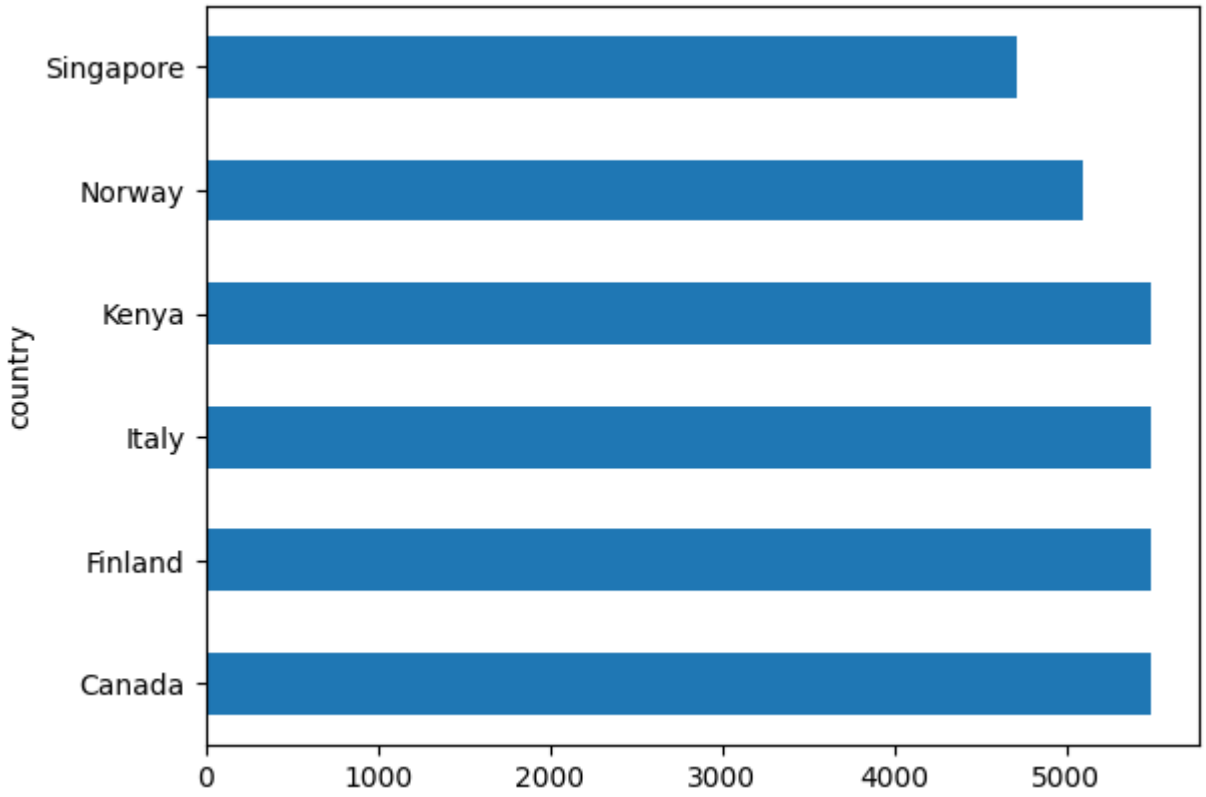
Partial Dependence

Partial dependence measures the relationship between a subset of input features and the pred outcome of a model. We can use partial dependence to understand the relationship between ou predictors and sticker sales.

Let's start by looking at the count of values per category.

In [57]:
```
p = valid_xs_imp['country'].value_counts().plot.barh()
c = data.classes['country'][1:] # position 0 is for null values, we have
plt.yticks(range(len(c)), c)
```

Out[57]:
```
([<matplotlib.axis.YTick at 0x7edfdeba4c50>,
  <matplotlib.axis.YTick at 0x7edfdeb451d0>,
  <matplotlib.axis.YTick at 0x7edfdf2449d0>,
  <matplotlib.axis.YTick at 0x7edfdf247010>,
  <matplotlib.axis.YTick at 0x7edfdf2a1490>,
  <matplotlib.axis.YTick at 0x7edfdf2a1650>],
 [Text(0, 0, 'Canada'),
  Text(0, 1, 'Finland'),
  Text(0, 2, 'Italy'),
  Text(0, 3, 'Kenya'),
  Text(0, 4, 'Norway'),
  Text(0, 5, 'Singapore')])
```



We are going to just calculate the partial dependence on our most predictive feature.

Partial dependence plots answer the question: if a row varied on nothing other than the feature question, how would it impact the dependent variable? What we do, is replace every single value `country` column with `Canada` then take the average over all the auctions. We repeat for `Fi` `Italy`, and so forth.

In [64]:
```
c
```

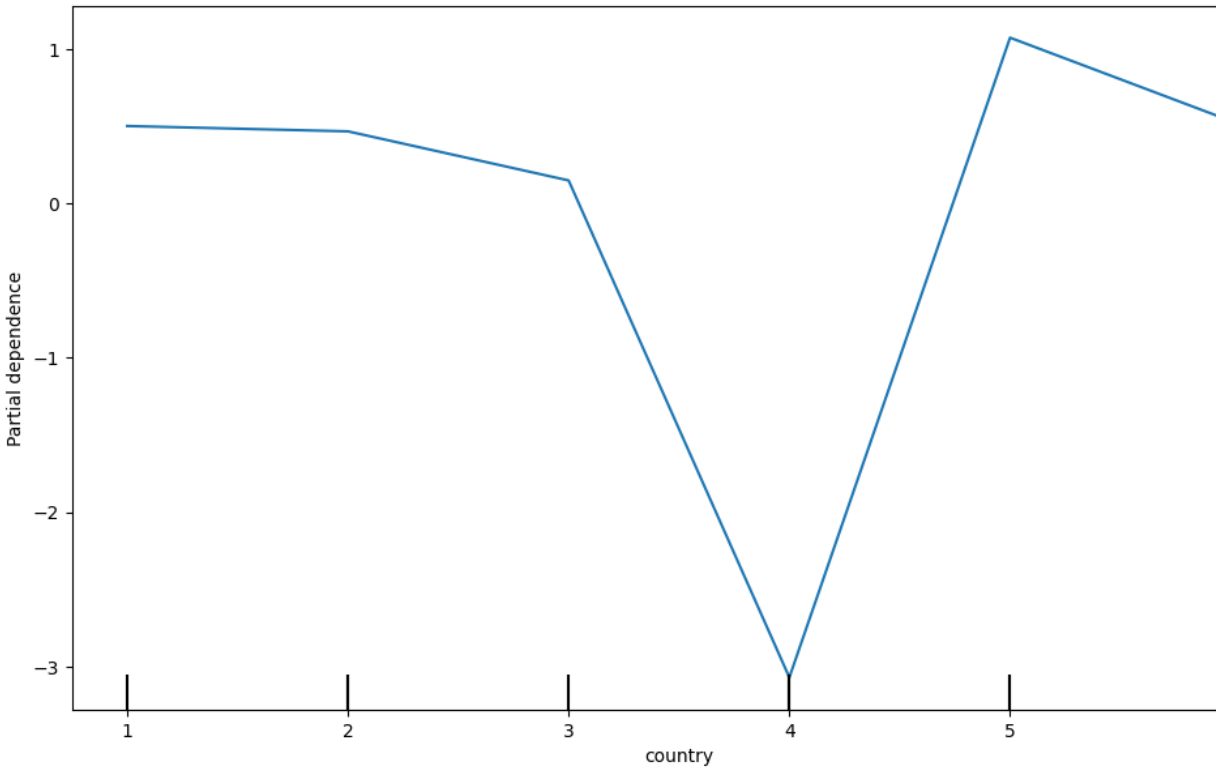
Out[64]:
```
(#6) ['Canada','Finland','Italy','Kenya','Norway','Singapore']
```

In [82]:
```
from sklearn.inspection import PartialDependenceDisplay

fig, ax = plt.subplots(figsize=(12, 7))

PartialDependenceDisplay.from_estimator(gbm2, valid_xs_imp, ['country'],

plt.show()
```



This is very insightful - it is essentially telling us that sales from `5`, which corresponds to `Norw` results in a much higher number of sales. Alternatively, sales from `4`, corresponding to `Kenya` in a much lower level of sales.

Waterfall Charts

Another useful piece of information we can derive from ensembles of decision trees, is what the important factors are in making a prediction for a particular row of data.

We can use the `waterfallcharts` library to understand this.

Let's say we are looking at a particular data entry that has predicted a really high number of sale want to understand why it's been predicted as having a really high number of sales. So, we take of data an put it through the decision tree. At each level of the decision tree, we what the increas decrease in the prediction is.

While technically you can perform this on GBM, it makes more sense to perform it on a **random** Random forests consist of single decision trees that can be independently interpreted, where as build cumulatively, so we can't just pass our prediction through a single **estimator** (or decision tr we will use our random forest model to visualise the **waterfall chart**.

Let's start by installing dependencies.

In [91]:
```
%%capture
!pip install treeinterpreter
!pip install waterfallcharts
```

Now, we can take the first row of validation data.

In [109…
```
row = data.valid.xs.iloc[:1]
```

In [110…
```
from treeinterpreter import treeinterpreter
from waterfall_chart import plot as waterfall

pred, bias, cont = treeinterpreter.predict(rf, row.values)
```

- `pred` represents the prediction the random forest makes.
- `bias` is the starting point, as **the decision tree begins with a certain base prediction**. I
  regression model, this is the average value of the target variable across all training data.
- `cont` is what is interesting to us. It tells us the total change in prediction due to each of the
  independent variables. This means `cont.sum()` is the models final prediction.

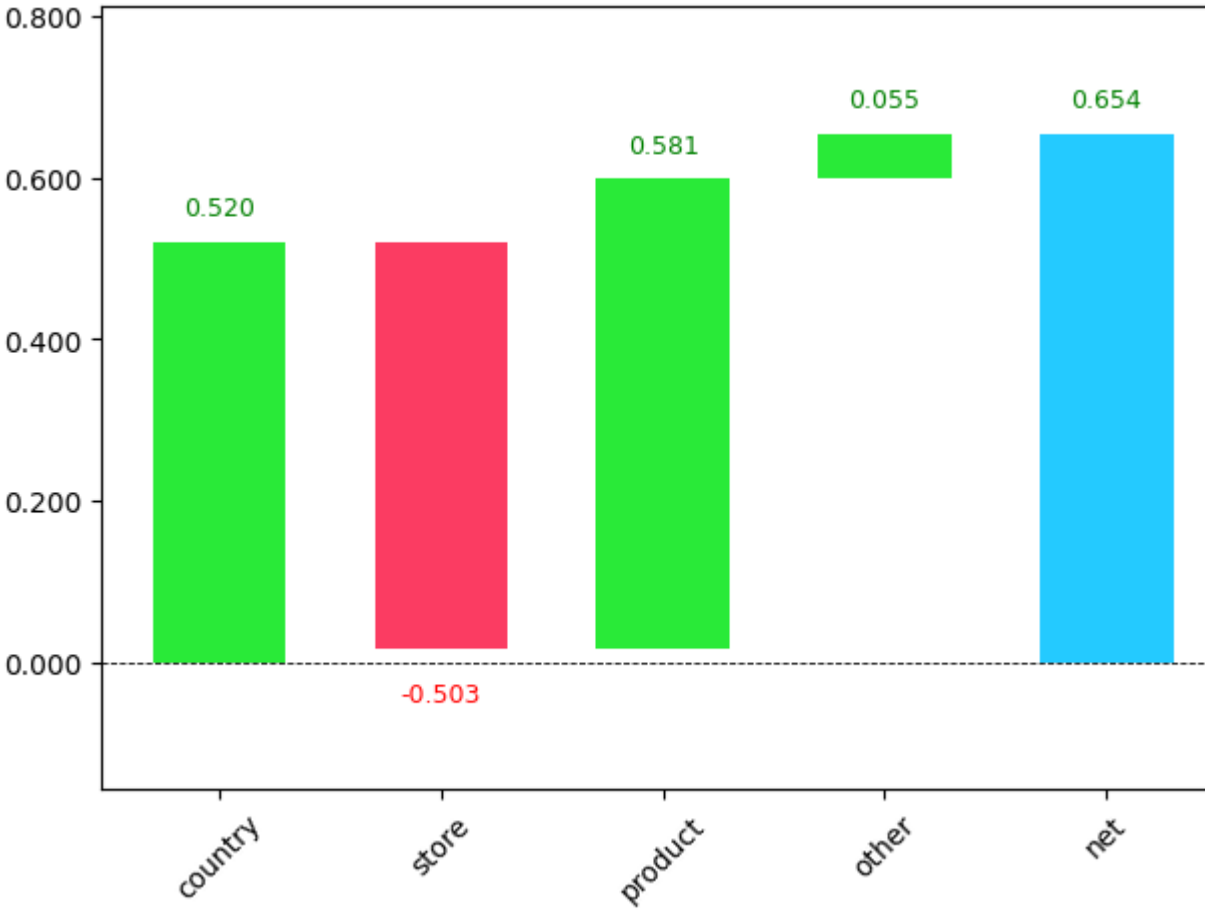
In [111…
```
cont, cont.sum()
```

Out[111…
```
array([[ 5.20224816e-01, -5.02621247e-01,  5.81039838e-01,
        -9.40199112e-04,  2.81878830e-04, -1.56760420e-02,
        -5.35762845e-04,  1.24408894e-04,  0.00000000e+00,
         0.00000000e+00,  0.00000000e+00,  9.40642754e-04,
         4.52863830e-02, -4.27637887e-04,  5.81439979e-03,
         2.04699338e-02]])
```

In [114…
```
waterfall(data.valid.xs.columns, # list of column names
          cont.flatten(), # it's current 2 dimensional, so we flatten it
          threshold=0.08, # if a value is too small, don't inclde it
          rotation_value=45, # rotate the x axis titles
          formatting='{:,.3f}')
```

```
/usr/local/lib/python3.11/dist-packages/waterfall_chart.py:141: FutureWarning
Series.__getitem__ treating keys as positions is deprecated. In a future vers
integer keys will always be treated as labels (consistent with DataFrame beha
To access a value by position, use `ser.iloc[pos]`
  y = y_height[loop] + row['amount']
/usr/local/lib/python3.11/dist-packages/waterfall_chart.py:139: FutureWarning
Series.__getitem__ treating keys as positions is deprecated. In a future vers
integer keys will always be treated as labels (consistent with DataFrame beha
To access a value by position, use `ser.iloc[pos]`
  y = y_height[loop]
```

Out[114…
```
<module 'matplotlib.pyplot' from '/usr/local/lib/python3.11/dist-packages/
matplotlib/pyplot.py'>
```



Look at this valuable information! We can see that the `country` value and `product` value in its prediction by a substantial amount, while `store` decreased it.

The y-axis unit is the same as `num_sales`, which we took a log transformation of at the start. final prediction of the model would be `exp1(0.654)`.

This information is more useful in **production** rather than **model development**.

Limitations and Considerations

These are some limitations discussed in Chapter of the textbook which I've reduced for my understanding.

Data Leakage

This is not a consideration only for ensembles of decision trees but for **all types of modelling**.

Data leakage occurs when information from outside the training data set 'leaks' to train the mode leading to overfitting.

The example given in the textbook revolves around a competition to predict which researchers w recieve a grant. The information that was given included info about the researchers and their res model was built performing with % accuracy.

The reason it turned out, was data leakage. One identifier column showed that the information w missing in this column **whenever** the university had rejected the grant. If using the model in prac information would obviously **not be available** - hence, data leakage.

How do we detect it?

- Check whether the accuracy is **too good to be true**.
- Look for important predictors that **don't make sense in practice**.
- Look for partial dependence plot results that **don't make sense in practice**.

Extrapolation

An issue with ensembles of decision trees is that they struggle with **extrapolation**.

A decision tree simply predicts the average value of the rows in a leaf. Therefore, a decision tree extension random forests and GBMs can never predict values outside the range of the training d can be problematic for data where there is a trend over time, such as inflation (or sticker sales!) wish to make predictions for a future time - the predictions will be systematically too low.

This problem extends beyond time as **ensembles of decision trees** are not able to extrapolate of types of data they have seen in a more general sense. So, we need to make sure our **validati does not contain out-of-domain data**.

Our dataset, which has only a few useful features, is not going to be suitable for a demonstration However, it is important to note that we can use random forests to **predict whether a row is in t validation set or the training set**. Then, we can get feature importance of this new random fore

If certain features have high importance, it indicates that they contain information that varies grea between the two datasets (hence, why the model uses it in its predictions). Oftentimes, removing values can impove accuracy and make the dataset more resilient, easier to maintain and easier understand. It will help the model generalise on the data, reducing overfitting.

What we are identifying here is called **domain shift**, which is where the distribution of data in the set differs from the distribution of data in real-world data.

Sometimes, it's also useful to remove really old data which contains patterns which may no longe useful. This applies more-so to temporal data, but is a useful paradigm - sometimes a subset of can produce better results. Bigger isn't always better.

Conclusion

Before I wrap up this notebook, there's one more important discussion. We've talked about ense decision trees BUT, what if we ensembled a **neural network** and a **random forest**? This is actu valid technique that can "add a nice little boost to any models that you have built." We don't do th the neural network is in a separate notebook. However, you can easily do this, by converting the rank- tensor prediction to a rank- Numpy array and taking the mean of the two prediction

This notebook has been a great insight into **ensembles of decision trees** as well as the useful information they can provide. Thank you to the textbook for its valuable content which I used to r notebook!