Ex10.ShapleyValues

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1 10th exercise: Interpretable Machine Learning by means of Shapley Values

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- Date: 08.08.2023

GENERAL NOTE 1: Please make sure you are reading the entire notebook, since it contains a lot of information on your tasks (e.g. regarding the set of certain paramaters or a specific computational trick), and the written mark downs as well as comments contain a lot of information on how things work together as a whole.
GENERAL NOTE 2: * Please, when commenting source code, just use English language only. * When describing an observation please use English language, too. * This applies to all exercises throughout this course.

1.0.1 DESCRIPTION:

Before using Shapley values to explain complicated models, it is helpful to understand how they work for simple models.

In this respect the example in this notebook computes a model for the titanic data set (downloaded from Kaggle) and uses its outputs for explanation of feature importance using SHAP deepexplainer. In addition, several different visualization techniques (plots) for Shapley values are going to be demonstrated.

For a description of the features please refer to Kaggle Titanic data set.

1.0.2 TASKS:

The tasks that you need to work on within this notebook are always indicated below as bullet points. If a task is more challenging and consists of several steps, this is indicated as well. Make sure you have worked down the task list and commented your doings. This should be done by using markdown. Make sure you don't forget to specify your name and your matriculation number in the notebook.

YOUR TASKS in this exercise are as follows: 1. import the notebook to Google Colab or use your local machine. 2. make sure you specified you name and your matriculation number in the header below my name and date. * set the date too and remove mine. 3. read the entire notebook carefully * add comments whereever you feel it necessary for better understanding * run the notebook for the first time. 4. Develop a CNN for image classification and adapt the Shapley Value idea to that model. Comment your entire code.

1.1 Imports

Import all necessary python utilities.

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout
from tensorflow.keras import optimizers
import os
%matplotlib inline
import shap
import warnings
warnings.filterwarnings('ignore')
```

```
2023-12-17 18:54:24.257431: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: SSE4.1 SSE4.2 AVX AVX2 AVX_VNNI FMA, in
other operations, rebuild TensorFlow with the appropriate compiler flags.
```

1.2 load build-in dataset

take the titanic data set

[2]:
```
train_data = pd.read_csv('data/titanic/train.csv', index_col=0)
test_data = pd.read_csv('data/titanic/test.csv', index_col=0)
train_data.head()
```

[2]:
```
             Survived  Pclass  \
PassengerId
1                   0       3
```

```
2                      1        1
3                      1        3
4                      1        1
5                      0        3

                                                                  Name     Sex   Age  \
PassengerId
1                                              Braund, Mr. Owen Harris    male  22.0
2            Cumings, Mrs. John Bradley (Florence Briggs Th…  female  38.0
3                                               Heikkinen, Miss. Laina  female  26.0
4                 Futrelle, Mrs. Jacques Heath (Lily May Peel)  female  35.0
5                                             Allen, Mr. William Henry    male  35.0

             SibSp  Parch            Ticket     Fare Cabin Embarked
PassengerId
1                1      0         A/5 21171   7.2500   NaN        S
2                1      0          PC 17599  71.2833   C85        C
3                0      0  STON/O2. 3101282   7.9250   NaN        S
4                1      0            113803  53.1000  C123        S
5                0      0            373450   8.0500   NaN        S
```

1.3 Preprocessing

Since the titanic data is a raw data set there is a need to preprocess it by dropping unnecessary columns, handling missing data, converting categorical features to numeric features and conducting one-hot encoding.

[3]:
```
def data_preprocessing(df):

    df = df.drop(columns=['Name', 'Ticket', 'Cabin'])

    # fill na
    df[['Age']] = df[['Age']].fillna(value=df[['Age']].mean())
    df[['Embarked']] = df[['Embarked']].fillna(value=df['Embarked'].
 ↪value_counts().idxmax())
    df[['Fare']] = df[['Fare']].fillna(value=df[['Fare']].mean())

    # encode categorical features into numeric
    df['Sex'] = df['Sex'].map( {'female': 1, 'male': 0} ).astype(int)

    # one-hot encoding
    embarked_one_hot = pd.get_dummies(df['Embarked'], prefix='Embarked')

    df = df.drop('Embarked', axis=1)
    df = df.join(embarked_one_hot)

    return df
```

[4]:
```python
# training data processing
train_data = data_preprocessing(train_data)
train_data.isnull().sum()

# create data for training
x_train = train_data.drop(['Survived'], axis=1).values

# Check testing data
test_data.isnull().sum()

# normalize training data
scale = StandardScaler()
x_train = scale.fit_transform(x_train)

# prepare y_train
y_train = train_data['Survived'].values

# preprocess testing data
test_data = data_preprocessing(test_data)
x_test = test_data.values.astype(float)

# normalize testing data
x_test = scale.transform(x_test)

# Check testing data
test_data.isnull().sum()
```

[4]:
```
Pclass        0
Sex           0
Age           0
SibSp         0
Parch         0
Fare          0
Embarked_C    0
Embarked_Q    0
Embarked_S    0
dtype: int64
```

1.3.1 Build a simple vanilla ANN, compile and fit the model.

[5]:
```python
x_train.min()
```

[5]:
```
-2.2531554887793948
```

[6]:
```python
model = Sequential()
model.add(Dense(32, input_dim=x_train.shape[1], activation='relu'))
model.add(Dropout(0.25))
```

```python
model.add(Dense(128, activation='relu'))
model.add(Dropout(0.25))
model.add(Dense(32, activation='relu'))
model.add(Dropout(0.25))
model.add(Dense(8, activation='relu'))
model.add(Dropout(0.25))
model.add(Dense(2, activation='softmax'))

# compile model
model.compile(loss='sparse_categorical_crossentropy', optimizer = 'adam',
 ↪metrics = ['accuracy'])

# fit model
model.fit(x_train, y_train, epochs=100, batch_size=64)
```

```
Epoch 1/100

2023-12-17 18:54:25.286567: I
tensorflow/core/common_runtime/process_util.cc:146] Creating new thread pool
with default inter op setting: 2. Tune using inter_op_parallelism_threads for
best performance.

14/14 [==============================] - 1s 4ms/step - loss: 0.6752 - accuracy:
0.5567
Epoch 2/100
14/14 [==============================] - 0s 4ms/step - loss: 0.6237 - accuracy:
0.6420
Epoch 3/100
14/14 [==============================] - 0s 3ms/step - loss: 0.5842 - accuracy:
0.7183
Epoch 4/100
14/14 [==============================] - 0s 3ms/step - loss: 0.5637 - accuracy:
0.7542
Epoch 5/100
14/14 [==============================] - 0s 3ms/step - loss: 0.5593 - accuracy:
0.7306
Epoch 6/100
14/14 [==============================] - 0s 3ms/step - loss: 0.5264 - accuracy:
0.7688
Epoch 7/100
14/14 [==============================] - 0s 4ms/step - loss: 0.5187 - accuracy:
0.7654
Epoch 8/100
14/14 [==============================] - 0s 3ms/step - loss: 0.5085 - accuracy:
0.7744
Epoch 9/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4845 - accuracy:
0.7924
```

```
Epoch 10/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4888 - accuracy:
0.7969
Epoch 11/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4788 - accuracy:
0.7924
Epoch 12/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4670 - accuracy:
0.8148
Epoch 13/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4774 - accuracy:
0.8036
Epoch 14/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4603 - accuracy:
0.8058
Epoch 15/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4862 - accuracy:
0.7890
Epoch 16/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4647 - accuracy:
0.7924
Epoch 17/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4760 - accuracy:
0.8013
Epoch 18/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4648 - accuracy:
0.8171
Epoch 19/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4659 - accuracy:
0.8126
Epoch 20/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4520 - accuracy:
0.8047
Epoch 21/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4471 - accuracy:
0.7957
Epoch 22/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4527 - accuracy:
0.8171
Epoch 23/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4594 - accuracy:
0.8171
Epoch 24/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4528 - accuracy:
0.8114
Epoch 25/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4336 - accuracy:
0.8260
```

```
Epoch 26/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4513 - accuracy:
0.8081
Epoch 27/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4523 - accuracy:
0.8025
Epoch 28/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4265 - accuracy:
0.8182
Epoch 29/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4243 - accuracy:
0.8193
Epoch 30/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4402 - accuracy:
0.8193
Epoch 31/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4212 - accuracy:
0.8272
Epoch 32/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4321 - accuracy:
0.8238
Epoch 33/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4186 - accuracy:
0.8294
Epoch 34/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4401 - accuracy:
0.8148
Epoch 35/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4378 - accuracy:
0.8249
Epoch 36/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4271 - accuracy:
0.8092
Epoch 37/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4473 - accuracy:
0.8148
Epoch 38/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4349 - accuracy:
0.8126
Epoch 39/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4205 - accuracy:
0.8395
Epoch 40/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4253 - accuracy:
0.8272
Epoch 41/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4065 - accuracy:
0.8249
```

```
Epoch 42/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4265 - accuracy:
0.8249
Epoch 43/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4212 - accuracy:
0.8272
Epoch 44/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4356 - accuracy:
0.8227
Epoch 45/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4322 - accuracy:
0.8159
Epoch 46/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4255 - accuracy:
0.8159
Epoch 47/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4068 - accuracy:
0.8350
Epoch 48/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4249 - accuracy:
0.8260
Epoch 49/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4201 - accuracy:
0.8272
Epoch 50/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4292 - accuracy:
0.8294
Epoch 51/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4181 - accuracy:
0.8328
Epoch 52/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4280 - accuracy:
0.8249
Epoch 53/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4096 - accuracy:
0.8350
Epoch 54/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4329 - accuracy:
0.8215
Epoch 55/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4169 - accuracy:
0.8316
Epoch 56/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4218 - accuracy:
0.8339
Epoch 57/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4164 - accuracy:
0.8294
```

```
Epoch 58/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4156 - accuracy:
0.8193
Epoch 59/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4166 - accuracy:
0.8238
Epoch 60/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4107 - accuracy:
0.8350
Epoch 61/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4257 - accuracy:
0.8249
Epoch 62/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4169 - accuracy:
0.8260
Epoch 63/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4144 - accuracy:
0.8272
Epoch 64/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4288 - accuracy:
0.8159
Epoch 65/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4108 - accuracy:
0.8361
Epoch 66/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4134 - accuracy:
0.8384
Epoch 67/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4113 - accuracy:
0.8159
Epoch 68/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4148 - accuracy:
0.8305
Epoch 69/100
14/14 [==============================] - 0s 4ms/step - loss: 0.4045 - accuracy:
0.8339
Epoch 70/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4059 - accuracy:
0.8249
Epoch 71/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4012 - accuracy:
0.8384
Epoch 72/100
14/14 [==============================] - 0s 4ms/step - loss: 0.3966 - accuracy:
0.8373
Epoch 73/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4041 - accuracy:
0.8294
```

```
Epoch 74/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3935 - accuracy:
0.8316
Epoch 75/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3958 - accuracy:
0.8339
Epoch 76/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3987 - accuracy:
0.8305
Epoch 77/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4016 - accuracy:
0.8361
Epoch 78/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4089 - accuracy:
0.8238
Epoch 79/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4010 - accuracy:
0.8361
Epoch 80/100
14/14 [==============================] - 0s 2ms/step - loss: 0.3986 - accuracy:
0.8474
Epoch 81/100
14/14 [==============================] - 0s 2ms/step - loss: 0.3953 - accuracy:
0.8451
Epoch 82/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4090 - accuracy:
0.8373
Epoch 83/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3940 - accuracy:
0.8339
Epoch 84/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4160 - accuracy:
0.8328
Epoch 85/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4001 - accuracy:
0.8328
Epoch 86/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4087 - accuracy:
0.8316
Epoch 87/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3859 - accuracy:
0.8294
Epoch 88/100
14/14 [==============================] - 0s 4ms/step - loss: 0.3965 - accuracy:
0.8339
Epoch 89/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4016 - accuracy:
0.8249
```

```
Epoch 90/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3931 - accuracy:
0.8429
Epoch 91/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3955 - accuracy:
0.8316
Epoch 92/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4028 - accuracy:
0.8283
Epoch 93/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4025 - accuracy:
0.8272
Epoch 94/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3942 - accuracy:
0.8272
Epoch 95/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4003 - accuracy:
0.8361
Epoch 96/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4067 - accuracy:
0.8294
Epoch 97/100
14/14 [==============================] - 0s 3ms/step - loss: 0.3887 - accuracy:
0.8418
Epoch 98/100
14/14 [==============================] - 0s 3ms/step - loss: 0.4127 - accuracy:
0.8238
Epoch 99/100
14/14 [==============================] - 0s 4ms/step - loss: 0.3902 - accuracy:
0.8384
Epoch 100/100
14/14 [==============================] - 0s 2ms/step - loss: 0.4056 - accuracy:
0.8260
```

[6]:
```
<keras.callbacks.History at 0x7fd6301ecad0>
```

1.3.2 Now, compute the Shapley values

[7]:
```
explainer = shap.DeepExplainer(model, x_train)
shap_values = explainer.shap_values(x_test)
shap_values
```

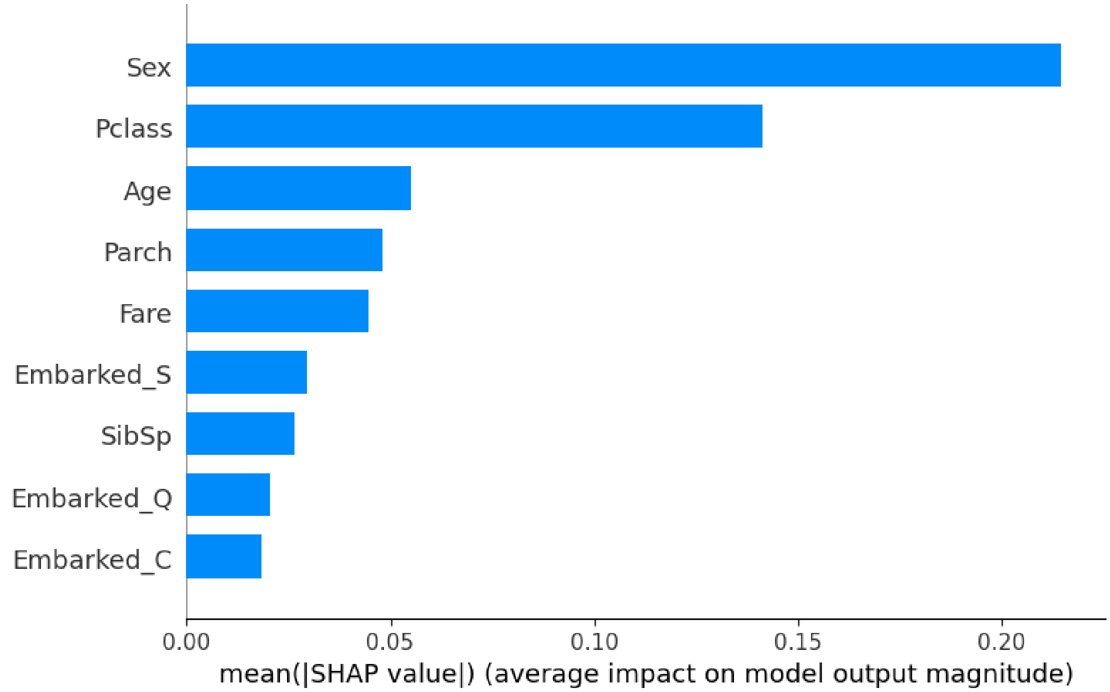
[7]:
```
[array([[ 0.05423852,  0.16233373,  0.02318682, …, -0.01188713,
          0.09136899, -0.0240086 ],
        [ 0.08069721, -0.14925867,  0.01674546, …, -0.00640352,
          0.0053753 ,  0.00919172],
        [ 0.01615058,  0.17092327,  0.07174964, …, -0.01181307,
```

```
        0.07219895, -0.01138471],
      ...,
      [ 0.07629597,  0.14646589,  0.0486063 , ..., -0.00848231,
       -0.00962658,  0.01267262],
      [ 0.07843381,  0.13353008, -0.01019708, ..., -0.00594252,
       -0.00379308,  0.01300846],
      [ 0.08700448,  0.10869418,  0.02990497, ...,  0.00152962,
       -0.01709231, -0.08912024]]),
array([[-0.05423852, -0.16233373, -0.02318682, ...,  0.01188712,
       -0.09136898,  0.0240086 ],
      [-0.0806972 ,  0.14925867, -0.01674545, ...,  0.00640352,
       -0.0053753 , -0.00919172],
      [-0.01615058, -0.17092327, -0.07174964, ...,  0.01181307,
       -0.07219895,  0.01138472],
      ...,
      [-0.07629597, -0.1464659 , -0.04860629, ...,  0.00848231,
        0.00962658, -0.01267262],
      [-0.0784338 , -0.13353007,  0.01019705, ...,  0.00594252,
        0.00379308, -0.01300846],
      [-0.08700449, -0.10869418, -0.02990497, ..., -0.00152962,
        0.01709231,  0.08912024]])]
```

1.3.3 Shapley values interpretation

Global interpretation method The summary plot shows the most important features and the magnitude of their impact on the model. It is the global interpretation.

[8]:
```
shap.summary_plot(shap_values[0], plot_type = 'bar', feature_names = test_data.
 ↪columns)
```



Local Interpretation methods

Force plot The force plot is great for seeing where the “output value” fits in relation to the “base value”. Further, it is possible to observe which features have a positive (red) or negative (blue) impact on the prediction and in addition the magnitude of the impact.

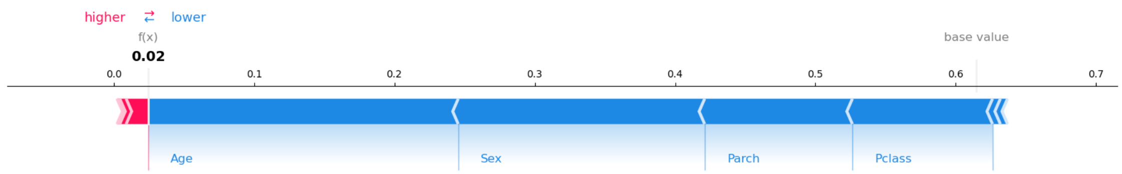
[9]:
```
shap.initjs()
```

```
<IPython.core.display.HTML object>
```

[10]:
```
i = 250
print(model.predict(x_test[i:i+1]))
print(test_data.iloc[i])
shap.force_plot(explainer.expected_value[0].numpy(), shap_values[0][i],␣
↪features = test_data.columns, matplotlib=True)
```

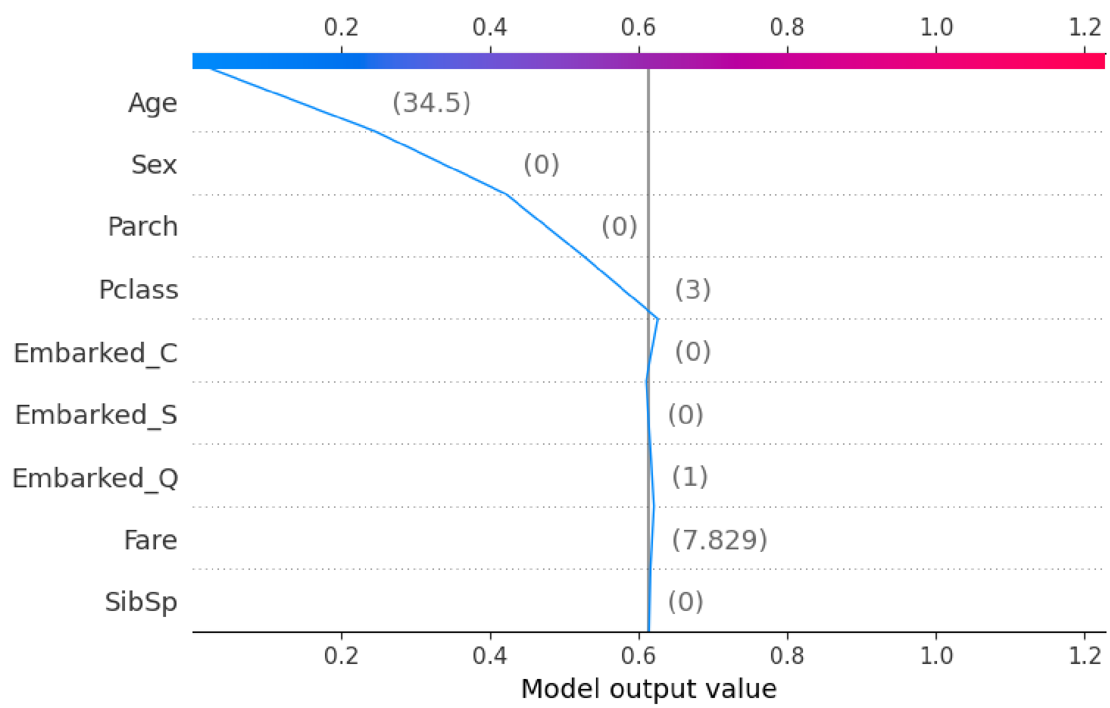
```
1/1 [==============================] - 0s 53ms/step
[[0.02461495 0.97538507]]
Pclass            2
Sex               1
Age            0.92
SibSp             1
Parch             2
Fare          27.75
Embarked_C    False
```

```
Embarked_Q     False
Embarked_S      True
Name: 1142, dtype: object
```



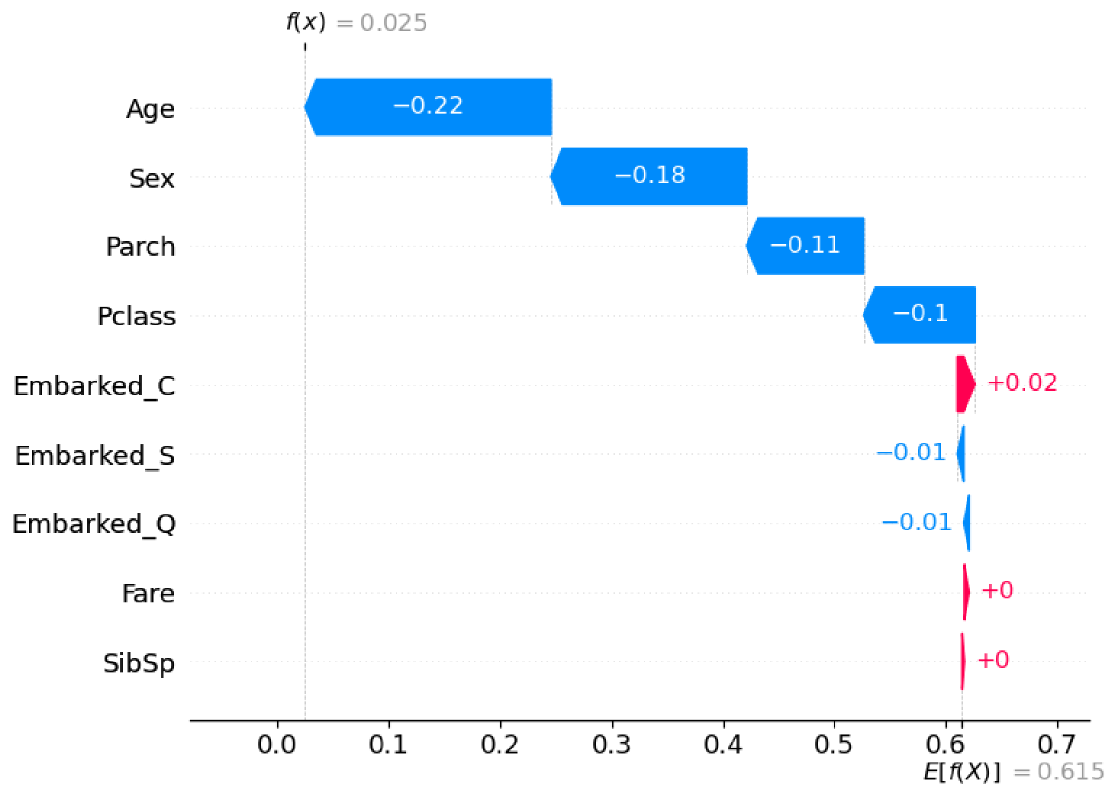
Decision plot The decision plot enables to observe the amplitude of each change taken by a sample for the values of the displayed features.

```
[11]: shap.decision_plot(explainer.expected_value[0].numpy(), shap_values[0][i],
      ↪features = test_data.iloc[0,:],
                         feature_names = test_data.columns.tolist())
```



Waterfall plot The waterfall plot allows for seeing the amplitude and the nature of the impact of a feature. It also allows for seeing the order of importance of the features and the values taken by each feature for the sample.

```
[12]: shap.plots._waterfall.waterfall_legacy(explainer.expected_value[0].numpy(),␣
      ↪shap_values[0][i],
                                          feature_names = test_data.columns)
```



1.4 Try to compute shap values on my own

First try to understand the library: Code below is copied and simplyfied

```
[14]: import tensorflow as tf

      def phi_symbolic(i):
          """ Get the SHAP value computation graph for a given model output.
          """

          @tf.function
          def grad_graph(shap_rAnD):
              phase = tf.keras.backend.learning_phase()
              tf.keras.backend.set_learning_phase(0)

              with tf.GradientTape(watch_accessed_variables=False) as tape:
                  tape.watch(shap_rAnD)
                  out = explainer.model(shap_rAnD)
```

```
            if explainer.multi_output:
                out = out[:,i]

        explainer._init_between_tensors(out.op, shap_rAnD)
        x_grad = tape.gradient(out, shap_rAnD)
        tf.keras.backend.set_learning_phase(phase)
        return x_grad

    explainer.phi_symbolics[i] = grad_graph

    return explainer.phi_symbolics[i]


def shap_values(X, ranked_outputs=None, output_rank_order="max", check_additivity=True):
    # check if we have multiple inputs
    if isinstance(X, list) and len(X) != 1:
        raise ValueError("Expected a single tensor as model input!")
    elif not isinstance(X, list):
        X = [X]
    assert len(explainer.model_inputs) == len(X), "Number of model inputs (%d) does not match the number given (%d)!" % (len(explainer.model_inputs), len(X))

    # compute the attributions
    output_phis = []
    phis = np.zeros_like(X[0])
    for j in range(X[0].shape[0]):
        bg_data = explainer.data

        tiled_X = [np.tile(X[0][j, :], (bg_data[0].shape[0], 1))]

        joint_input = [np.concatenate([tiled_X[0], bg_data[0]], 0)]

        # run attribution computation graph
        sample_phis = explainer.run(phi_symbolic(0), explainer.model_inputs, joint_input)

        # assign the attributions to the right part of the output arrays
        phis[j] = (sample_phis[0][bg_data[0].shape[0]:] * (X[0][j] - bg_data[0])).mean(0)

    return phis


explainer = shap.DeepExplainer(model, x_train).explainer
shap_val = shap_values(x_test)
```

```
WARNING:tensorflow:5 out of the last 5 calls to <function
phi_symbolic.<locals>.grad_graph at 0x7fd5d4051120> triggered tf.function
retracing. Tracing is expensive and the excessive number of tracings could be
due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with
different shapes, (3) passing Python objects instead of tensors. For (1), please
define your @tf.function outside of the loop. For (2), @tf.function has
reduce_retracing=True option that can avoid unnecessary retracing. For (3),
please refer to https://www.tensorflow.org/guide/function#controlling_retracing
and https://www.tensorflow.org/api_docs/python/tf/function for  more details.
WARNING:tensorflow:6 out of the last 6 calls to <function
phi_symbolic.<locals>.grad_graph at 0x7fd5d41c3b00> triggered tf.function
retracing. Tracing is expensive and the excessive number of tracings could be
due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with
different shapes, (3) passing Python objects instead of tensors. For (1), please
define your @tf.function outside of the loop. For (2), @tf.function has
reduce_retracing=True option that can avoid unnecessary retracing. For (3),
please refer to https://www.tensorflow.org/guide/function#controlling_retracing
and https://www.tensorflow.org/api_docs/python/tf/function for  more details.
```

[15]:
```
np.abs(shap_val).mean(axis=0)
```

[15]:
```
array([0.14129085, 0.21470557, 0.05518179, 0.02627479, 0.04811384,
       0.04451882, 0.01838769, 0.02057474, 0.02948183])
```

[117]:
```
# https://christophm.github.io/interpretable-ml-book/shapley.html
def get_permutations(x, z, feat_idx):
    assert x.shape == z.shape
    l = list(range(x.shape[1]))
    l.remove(feat_idx)
    ll = np.random.permutation(l)
    ll = np.insert(ll, feat_idx, feat_idx)
    x_pls_j = np.append(x[:, ll[:feat_idx+1]], z[:, ll[feat_idx+1:]], axis=1)
    x_mns_j = np.append(x[:, ll[:feat_idx]], z[:, ll[feat_idx:]], axis=1)
    return x_pls_j, x_mns_j

get_permutations(np.array([[5, 6, 7, 8]]), np.array([[1, 2, 3, 4]]), 1)
```

[117]:
```
(array([[5, 6, 4, 3]]), array([[5, 2, 4, 3]]))
```

[186]:
```
def compute_shap_values(feat_idx):
    x = x_train[np.random.choice(x_train.shape[0], 500, replace=False), :] #␣
 ↪randomly choose rows from x_train
    z = np.tile(x_test[0], (500, 1)) # choose songle sample from x_test
    x_plus_j, x_minus_j = get_permutations(x, z, feat_idx)
    diff = model.predict(x_plus_j) - model.predict(x_minus_j)
    return np.mean(diff, axis=0)
```

```
compute_shap_values(0)
```

```
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
```

[186]:
```
array([-0.03168424,  0.03168413], dtype=float32)
```

[233]:
```
svs = []
for _ in range(10):
    svs.append(compute_shap_values(1))
```

```
16/16 [==============================] - 0s 6ms/step
16/16 [==============================] - 0s 7ms/step
16/16 [==============================] - 0s 5ms/step
16/16 [==============================] - 0s 3ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 5ms/step
16/16 [==============================] - 0s 5ms/step
16/16 [==============================] - 0s 5ms/step
16/16 [==============================] - 0s 3ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 1ms/step
16/16 [==============================] - 0s 5ms/step
16/16 [==============================] - 0s 3ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
16/16 [==============================] - 0s 2ms/step
```

[234]:
```
np.mean(np.vstack(svs), axis=0)
```

[234]:
```
array([-0.15415852,  0.15415852], dtype=float32)
```

[185]:
```
# These are the shaply values computed by library
explainer = shap.DeepExplainer(model, x_train)
shap_values = explainer.shap_values(x_test[0:1])
shap_values
```

[185]:
```
[array([[ 0.05423852,  0.16233373,  0.02318682, -0.00345705, -0.0208473 ,
          0.03038135, -0.01188713,  0.09136899, -0.0240086 ]]),
 array([[-0.05423852, -0.16233373, -0.02318682,  0.00345705,  0.0208473 ,
         -0.03038135,  0.01188712, -0.09136898,  0.0240086 ]])]
```

1.5 Result

Self computed shaply values pretty close to the ones computes with the shap library Library gets to 0.16 for the second feature, my computation is at 0.15

Trying to understand what happens inside the library is though very hard to understand

1.6 Image Classification with shapley as explainer

[235]:
```
# read the data

train_df = pd.read_csv("data/fashion-mnist_train.csv")
x_train = train_df.values[:, :-1]
y_train = train_df.values[:, 0]
x_train.shape, y_train.shape
```

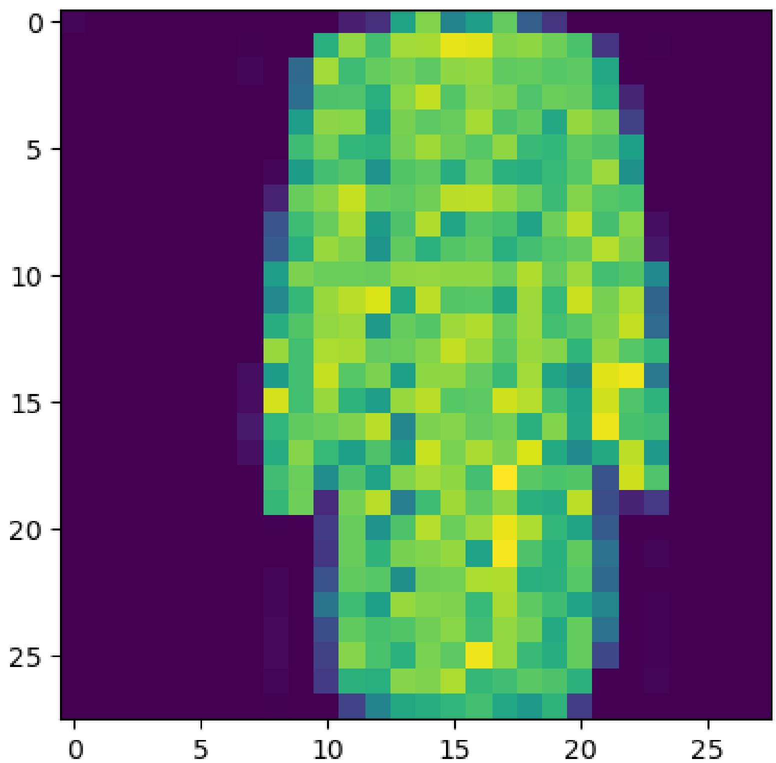
[235]:
```
((60000, 784), (60000,))
```

[236]:
```
# reshape into image format
x_train = x_train.reshape(-1,  28, 28, 1) / 255
x_train.shape
```

[236]:
```
(60000, 28, 28, 1)
```

[237]:
```
plt.imshow(x_train[200,  :, :, 0])
```

[237]:
```
<matplotlib.image.AxesImage at 0x7fd5c1af71d0>
```



[238]:
```
# read and prepare test and validation data

xtest_data = pd.read_csv("data/fashion-mnist_test.csv").values[:, :-1].
 ↪reshape(-1, 28, 28, 1)
ytest_data = pd.read_csv("data/fashion-mnist_test.csv").values[:, 0]

x_test = xtest_data[:5000] / 255
x_val = xtest_data[5000:] / 255
y_test = ytest_data[:5000]
y_val = ytest_data[5000:]
y_val, y_test
```

[238]: (array([1, 2, 4, …, 8, 8, 1]), array([0, 1, 2, …, 2, 6, 9]))

[239]:
```
# One hot encoding

y_train = np.eye(10)[y_train]
y_test = np.eye(10)[y_test]
y_val = np.eye(10)[y_val]
```

[240]:
```
from keras.layers import Conv2D,MaxPooling2D,Flatten,Dropout
from keras.optimizers import Adam
```

```
model = Sequential()

model = Sequential()
model.add(Conv2D(32, kernel_size=(3, 3), activation="relu", input_shape=(28,␣
↪28, 1)))
model.add(Conv2D(64, (3, 3), activation="relu"))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Dropout(0.25))
model.add(Flatten())
model.add(Dense(128, activation="relu"))
model.add(Dropout(0.5))
model.add(Dense(10, activation="softmax"))

model.compile(optimizer=Adam(lr=0.001), loss="categorical_crossentropy",␣
↪metrics=["accuracy"])
```

[241]:
```
history = model.fit(x_train, y_train, batch_size=128, epochs=12,␣
↪validation_data=(x_val, y_val))
```

```
Epoch 1/12
469/469 [==============================] - 73s 155ms/step - loss: 0.5354 -
accuracy: 0.8078 - val_loss: 0.3147 - val_accuracy: 0.8924
Epoch 2/12
469/469 [==============================] - 82s 175ms/step - loss: 0.3495 -
accuracy: 0.8746 - val_loss: 0.2651 - val_accuracy: 0.9082
Epoch 3/12
469/469 [==============================] - 78s 166ms/step - loss: 0.3018 -
accuracy: 0.8918 - val_loss: 0.2476 - val_accuracy: 0.9114
Epoch 4/12
469/469 [==============================] - 77s 164ms/step - loss: 0.2709 -
accuracy: 0.9025 - val_loss: 0.2348 - val_accuracy: 0.9148
Epoch 5/12
469/469 [==============================] - 77s 165ms/step - loss: 0.2485 -
accuracy: 0.9099 - val_loss: 0.2180 - val_accuracy: 0.9210
Epoch 6/12
469/469 [==============================] - 77s 164ms/step - loss: 0.2276 -
accuracy: 0.9173 - val_loss: 0.2242 - val_accuracy: 0.9198
Epoch 7/12
469/469 [==============================] - 77s 165ms/step - loss: 0.2077 -
accuracy: 0.9230 - val_loss: 0.2054 - val_accuracy: 0.9246
Epoch 8/12
469/469 [==============================] - 79s 168ms/step - loss: 0.1947 -
accuracy: 0.9280 - val_loss: 0.2007 - val_accuracy: 0.9272
Epoch 9/12
469/469 [==============================] - 74s 159ms/step - loss: 0.1806 -
accuracy: 0.9330 - val_loss: 0.2026 - val_accuracy: 0.9282
```

```
Epoch 10/12
469/469 [==============================] - 76s 163ms/step - loss: 0.1672 -
accuracy: 0.9384 - val_loss: 0.2000 - val_accuracy: 0.9304
Epoch 11/12
469/469 [==============================] - 78s 166ms/step - loss: 0.1576 -
accuracy: 0.9411 - val_loss: 0.1980 - val_accuracy: 0.9324
Epoch 12/12
469/469 [==============================] - 79s 168ms/step - loss: 0.1456 -
accuracy: 0.9457 - val_loss: 0.1932 - val_accuracy: 0.9336
```

[242]:
```
# test data is more or less balanced --> I'm going to got with accuracy as␣
↪model measure instead of f1
np.sum(y_test, axis=0)
```

[242]:
```
array([502., 490., 490., 507., 506., 490., 519., 471., 508., 517.])
```

[243]:
```
# predict and transform back to numeric values
performance = np.argmax(model.predict(x_test), axis=1) == np.argmax(y_test,␣
↪axis=1)
```

```
157/157 [==============================] - 6s 37ms/step
```

[244]:
```
np.count_nonzero(performance) / len(performance)
```

[244]:
```
0.9326
```

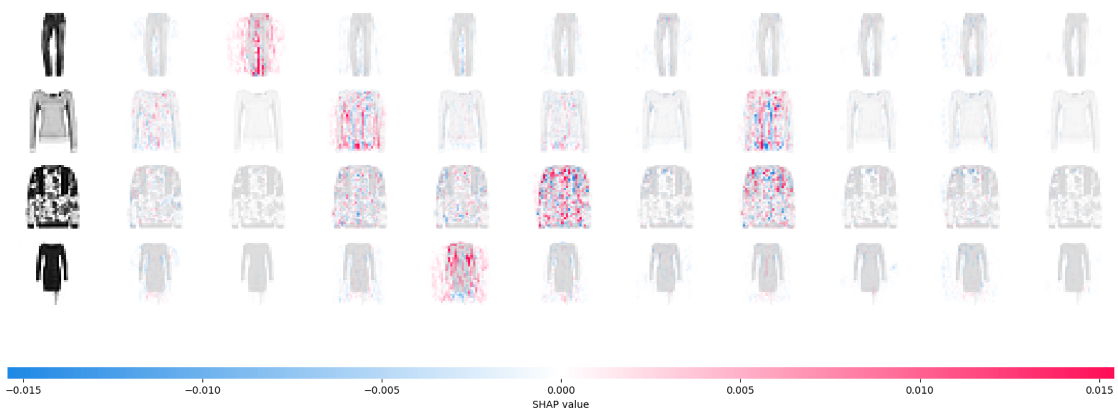
[245]:
```
samples = x_train[np.random.choice(x_train.shape[0], 100, replace=False)]
```

[246]:
```
import shap

# select a set of background examples to take an expectation over
background = x_train[np.random.choice(x_train.shape[0], 100, replace=False)]

# explain predictions of the model on three images
e = shap.DeepExplainer(model, background)
# ...or pass tensors directly
# e = shap.DeepExplainer((model.layers[0].input, model.layers[-1].output),␣
↪background)
shap_values = e.shap_values(x_test[1:5])
```

```
WARNING:tensorflow:5 out of the last 425 calls to <function
TFDeep.phi_symbolic.<locals>.grad_graph at 0x7fd5bbb9e8e0> triggered tf.function
retracing. Tracing is expensive and the excessive number of tracings could be
due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with
different shapes, (3) passing Python objects instead of tensors. For (1), please
define your @tf.function outside of the loop. For (2), @tf.function has
reduce_retracing=True option that can avoid unnecessary retracing. For (3),
please refer to https://www.tensorflow.org/guide/function#controlling_retracing
```

```
and https://www.tensorflow.org/api_docs/python/tf/function for  more details.
WARNING:tensorflow:5 out of the last 11 calls to <function
TFDeep.phi_symbolic.<locals>.grad_graph at 0x7fd5bbb9e340> triggered tf.function
retracing. Tracing is expensive and the excessive number of tracings could be
due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with
different shapes, (3) passing Python objects instead of tensors. For (1), please
define your @tf.function outside of the loop. For (2), @tf.function has
reduce_retracing=True option that can avoid unnecessary retracing. For (3),
please refer to https://www.tensorflow.org/guide/function#controlling_retracing
and https://www.tensorflow.org/api_docs/python/tf/function for  more details.
```

[247]:
```
shap.image_plot(shap_values, -x_test[1:5])
```



[ ]:
```

```