local

December 2, 2023

1 Mudcard

- **what exactly is gain using to determine the accuracy through each feature?**
  - check the description here
  - we don't need the exact definition of gain in this class but we cover it in more detail in DATA2060/CSCI1420

1.1 Local feature importance metrics

By the end of this module, you will be able to - Describe motivation behind local feature importance metrics - Apply SHAP - Describe LIME

1.2 Local feature importance metrics

By the end of this module, you will be able to - **Describe motivation behind local feature importance metrics** - Apply SHAP - Describe LIME

1.3 Motivation

- can we trust the model?
  - global feature importance: does the model make predictions based on reasonable features?
  - local feature importance: can we trust the model's prediction for one specific data point?
- global feature importance is often not enough especially when you work with human data
  - medical: the doctor needs to be able to explain the reasoning behind the model prediction to the patient
  - finance: customer wants to know why they were declined a loan/mortgage/credit card/etc

1.4 Global vs. local importance

- global: one value per feature, it is a vector of shape (n_{ftrs})
  - it describes how important each feature is generally
- local: one value per feature and data points, it is a 2D array with a shape of (n_{points}, n_{ftrs}) - the same shape as your feature matrix
  - it describes how important each feature is for predicting one particular data point

1.5 Motivation

- local feature importance improves the interpretability of complex models

- check out this page for a good example

1.6 Local feature importance metrics

By the end of this module, you will be able to - Describe motivation behind local feature importance metrics - **Apply SHAP** - Describe LIME

1.7 SHAP values

- one way to calculate local feature importances
- it is based on Shapely values from game theory
- read more here, here, and here

1.7.1 Cooperative game theory

- A set of m players in a coalition generate a surplus.
- Some players contribute more to the coalition than others (different bargaining powers).
- How important is each player to the coalition?
- How should the surplus be divided fairly amongst the players?

1.7.2 Cooperative game theory applied to feature attribution

- A set of m features in a model generate a prediction.
- Some features contribute more to the model than others (different predictive powers).
- How important is each feature to the model?
- How should the prediction be divided amongst the features?

1.8 How is it calculated?

1.8.1 $\Phi_i = \sum_{S \subseteq M \setminus i} \frac{|S|!(M-|S|-1)!}{M!}[f_x(S \cup i) - f_x(S)]$

- Φ_i - the contribution of feature i
- M - the number of features
- S - a set of features excluding i, a vector of 0s and 1s (0 if a feature is missing)
- $|S|$ - the number of features in S
- $f_x(S)$ - the prediction of the model with features S

This is the sum of how much feature i contribute to the prediction. The weight is related to combination theory – M choose |S|.

1.9 How is it calculated?

1.9.1 $\Phi_i = \sum_{S \subseteq M \setminus i} \frac{|S|!(M-|S|-1)!}{M!}[f_x(S \cup i) - f_x(S)]$

- the difference feature i makes in the prediction:
  - $f_x(S \cup i)$ - the prediction with feature i
  - $f_x(S)$ - the prediction without feature i
- loop through all possible ways a set of S features can be selected from the M features excluding i
- weight the contribution based on how many ways we can select $|S|$ features

2 Quiz 1

Let's calculate the weight term (in blue) of the shap equation. Let's assume we have 4 features and we want to calculate the shap value of one of them. Then M = 4, S can be [0,0,0], [1,0,0], [0,1,0],[0,0,1], [1,1,0], [1,0,1], [0,1,1], and [1,1,1]. What's |S| and the value of the blue term in each of these cases?

[1]:
```
import math

M = 4
S_list = [[0,0,0], [1,0,0], [0,1,0], [0,0,1], [1,1,0], [1,0,1], [0,1,1],␣
    ↪[1,1,1]]
for S in S_list:
    num_S = sum(S)
    print('|S| =', num_S)
    print('weight:', math.factorial(num_S) * math.factorial(M-num_S-1) / math.
    ↪factorial(M))
```

```
|S| = 0
weight: 0.25
|S| = 1
weight: 0.08333333333333333
|S| = 1
weight: 0.08333333333333333
|S| = 1
weight: 0.08333333333333333
|S| = 2
weight: 0.08333333333333333
|S| = 2
weight: 0.08333333333333333
|S| = 2
weight: 0.08333333333333333
|S| = 3
weight: 0.25
```

- if |S| = 0, then 0!*(4-1)!/4! = 1/4.
- if |S| = 1, then 1!*(4-1-1)!/4! = 2!/4! = 1/12.
- if |S| = 2, then 2!*(4-2-1)!/4! = 1/12.
- if |S| = 3, then 3!*(4-3-1)!/4! = 1/4.

Note that |S| = 0 and 3 only once, while |S| = 1 and 2 three times. 1* 1/4 + 3* 1/12 + 3* 1/12 + 1* 1/4 = 1 so the sum of the weights is 1.

[2]:
```
import numpy as np
import pandas as pd
import xgboost
from sklearn.ensemble import RandomForestClassifier
from sklearn.pipeline import make_pipeline
```

```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import train_test_split
from sklearn.model_selection import StratifiedKFold
from sklearn.preprocessing import StandardScaler
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import OneHotEncoder
import matplotlib.pylab as plt

df = pd.read_csv('data/adult_data.csv')
label = 'gross-income'
y = df[label]
df.drop(columns=[label],inplace=True)
X = df
ftr_names = X.columns
print(X.head())
print(y)
```

```
   age          workclass  fnlwgt   education  education-num  \
0   39          State-gov   77516   Bachelors             13
1   50   Self-emp-not-inc   83311   Bachelors             13
2   38            Private  215646     HS-grad              9
3   53            Private  234721        11th              7
4   28            Private  338409   Bachelors             13

        marital-status          occupation    relationship    race      sex  \
0        Never-married        Adm-clerical   Not-in-family   White     Male
1   Married-civ-spouse     Exec-managerial         Husband   White     Male
2             Divorced   Handlers-cleaners   Not-in-family   White     Male
3   Married-civ-spouse   Handlers-cleaners         Husband   Black     Male
4   Married-civ-spouse      Prof-specialty            Wife   Black   Female

   capital-gain  capital-loss  hours-per-week  native-country
0          2174             0              40   United-States
1             0             0              13   United-States
2             0             0              40   United-States
3             0             0              40   United-States
4             0             0              40            Cuba
0         <=50K
1         <=50K
2         <=50K
3         <=50K
4         <=50K
          …
32556     <=50K
32557      >50K
32558     <=50K
32559     <=50K
```

```
32560      >50K
Name: gross-income, Length: 32561, dtype: object
```

[3]:

```python
def ML_pipeline_kfold(X,y,random_state,n_folds):
    # create a test set
    X_other, X_test, y_other, y_test = train_test_split(X, y, test_size=0.2, random_state = random_state)
    # splitter for _other
    kf = StratifiedKFold(n_splits=n_folds,shuffle=True,random_state=random_state)
    # create the pipeline: preprocessor + supervised ML method
    cat_ftrs = ['workclass','education','marital-status','occupation','relationship','race','sex','native-
    cont_ftrs = ['age','fnlwgt','education-num','capital-gain','capital-loss','hours-per-week']
    # one-hot encoder
    categorical_transformer = Pipeline(steps=[
        ('onehot', OneHotEncoder(sparse_output=False,handle_unknown='ignore'))])
    # standard scaler
    numeric_transformer = Pipeline(steps=[
        ('scaler', StandardScaler())])
    preprocessor = ColumnTransformer(
        transformers=[
            ('num', numeric_transformer, cont_ftrs),
            ('cat', categorical_transformer, cat_ftrs)])
    pipe = make_pipeline(preprocessor,RandomForestClassifier(n_estimators = 100,random_state=random_state))
    # the parameter(s) we want to tune
    param_grid = {'randomforestclassifier__max_depth': [10,30,100,300],
                  'randomforestclassifier__min_samples_split': [16, 32, 64, 128]}
    # prepare gridsearch
    grid = GridSearchCV(pipe, param_grid=param_grid,cv=kf, return_train_score = True,n_jobs=-1,verbose=10)
    # do kfold CV on _other
    grid.fit(X_other, y_other)
    feature_names = grid.best_estimator_[0].get_feature_names_out()
    return grid, np.array(feature_names), X_test, y_test
```

[6]:

```python
grid, feature_names, X_test, y_test = ML_pipeline_kfold(X,y,42,4)
print(grid.best_score_)
print(grid.score(X_test,y_test))
print(grid.best_params_)
print(grid.best_estimator_)
```

```
Fitting 4 folds for each of 16 candidates, totalling 64 fits
0.862906941031941
0.8667280822969445
```

```
{'randomforestclassifier__max_depth': 100,
'randomforestclassifier__min_samples_split': 64}
Pipeline(steps=[('columntransformer',
                 ColumnTransformer(transformers=[('num',
                                                  Pipeline(steps=[('scaler',
StandardScaler())]),
                                                  ['age', 'fnlwgt',
                                                   'education-num',
                                                   'capital-gain',
                                                   'capital-loss',
                                                   'hours-per-week']),
                                                 ('cat',
                                                  Pipeline(steps=[('onehot',
OneHotEncoder(handle_unknown='ignore',
 sparse_output=False))]),
                                                  ['workclass', 'education',
                                                   'marital-status',
                                                   'occupation', 'relationship',
                                                   'race', 'sex',
                                                   'native-country'])])),
                ('randomforestclassifier',
                 RandomForestClassifier(max_depth=100, min_samples_split=64,
                                        random_state=42))])
```

[5]:
```
import shap
shap.initjs() # required for visualizations later on
# create the explainer object with the random forest model
explainer = shap.TreeExplainer(grid.best_estimator_[1])
# transform the test set
X_test_transformed = grid.best_estimator_[0].transform(X_test)
print(np.shape(X_test_transformed))
# calculate shap values on the first 1000 points in the test
shap_values = explainer.shap_values(X_test_transformed[:1000])
print(np.shape(shap_values))
```

```
Using `tqdm.autonotebook.tqdm` in notebook mode. Use `tqdm.tqdm` instead to
force console mode (e.g. in jupyter console)
```

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

```
(6513, 108)
(2, 1000, 108)
```

[7]:
```
print(grid.best_estimator_[0])
```

```
ColumnTransformer(transformers=[('num',
                                 Pipeline(steps=[('scaler', StandardScaler())]),
                                 ['age', 'fnlwgt', 'education-num',
                                  'capital-gain', 'capital-loss',
                                  'hours-per-week']),
```

```
                              ('cat',
                               Pipeline(steps=[('onehot',
OneHotEncoder(handle_unknown='ignore',
sparse_output=False))]),
                               ['workclass', 'education', 'marital-status',
                                'occupation', 'relationship', 'race', 'sex',
                                'native-country'])])
```

2.1 Explain a point

[10]:
```
explainer.expected_value
```

[10]:
```
array([0.75897535, 0.24102465])
```

[8]:
```
index = 42 # the index of the point to explain
print(explainer.expected_value[0]) # we explain class 0 predictions
shap.force_plot(explainer.expected_value[0], shap_values[0][index,:], features␣
 ↪= X_test_transformed[index,:],feature_names = feature_names)
```

```
0.7589753531941029
```

[8]:
```
<shap.plots._force.AdditiveForceVisualizer at 0x11815819350>
```

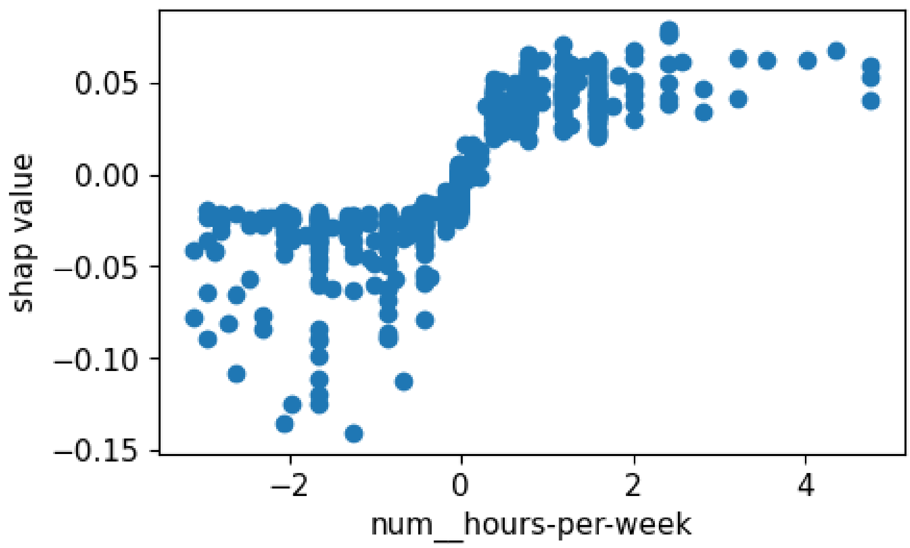
[11]:
```
index = 0 # the index of the point to explain
print(explainer.expected_value[0]) # we explain class 0 predictions
shap.force_plot(explainer.expected_value[0], shap_values[0][index,:], features␣
 ↪= X_test_transformed[index,:],feature_names = feature_names)
```

```
0.7589753531941029
```

[11]:
```
<shap.plots._force.AdditiveForceVisualizer at 0x11816eccb50>
```

2.2 Feature value vs. shap value

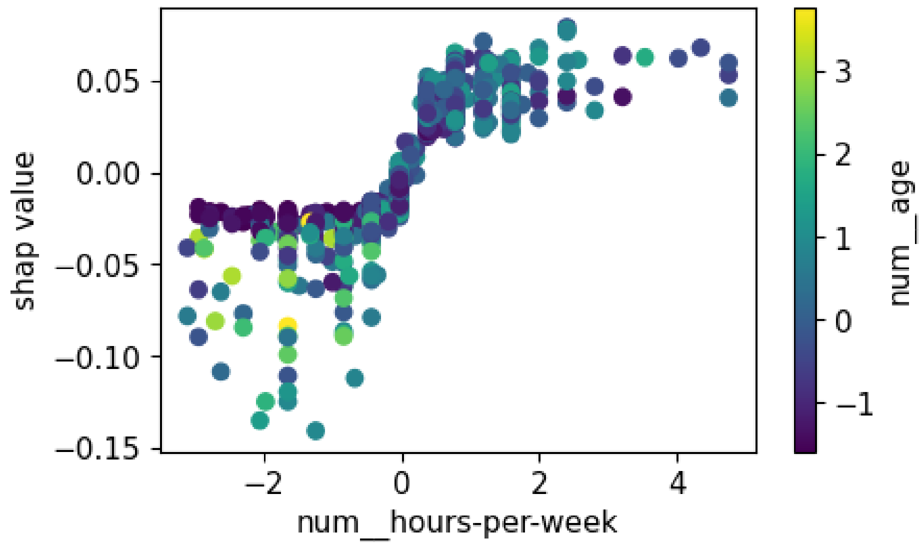
[16]:
```
import matplotlib
matplotlib.rcParams.update({'font.size': 11})
ftr = 'num__hours-per-week'
indx = np.argwhere(feature_names==ftr)
plt.figure(figsize=(5,3))
plt.scatter(X_test_transformed[:1000,indx],shap_values[1][:,indx])
plt.ylabel('shap value')
plt.xlabel(ftr)
plt.show()
```



2.3 Dependence plot

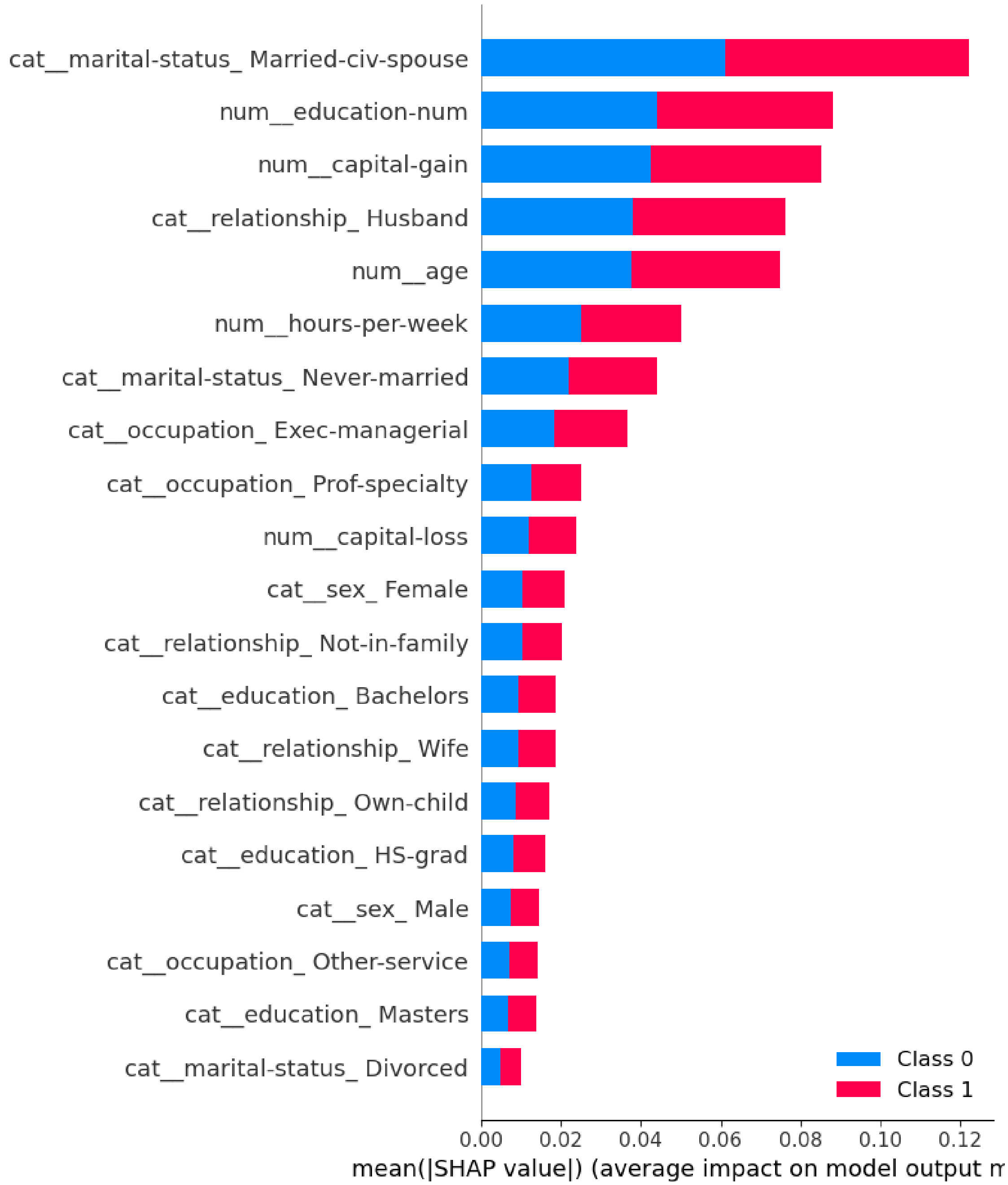
[17]:
```
ftr1 = 'num__hours-per-week'
ftr2 = 'num__age'
indx1 = np.argwhere(feature_names==ftr1)
indx2 = np.argwhere(feature_names==ftr2)

plt.figure(figsize=(5,3))
plt.scatter(X_test_transformed[:1000,indx1],shap_values[1][:
 ↪,indx1],c=X_test_transformed[:1000,indx2])
plt.ylabel('shap value')
plt.xlabel(ftr1)
plt.colorbar(label=ftr2)
plt.show()
```



2.4 It can also be used for global feature importance

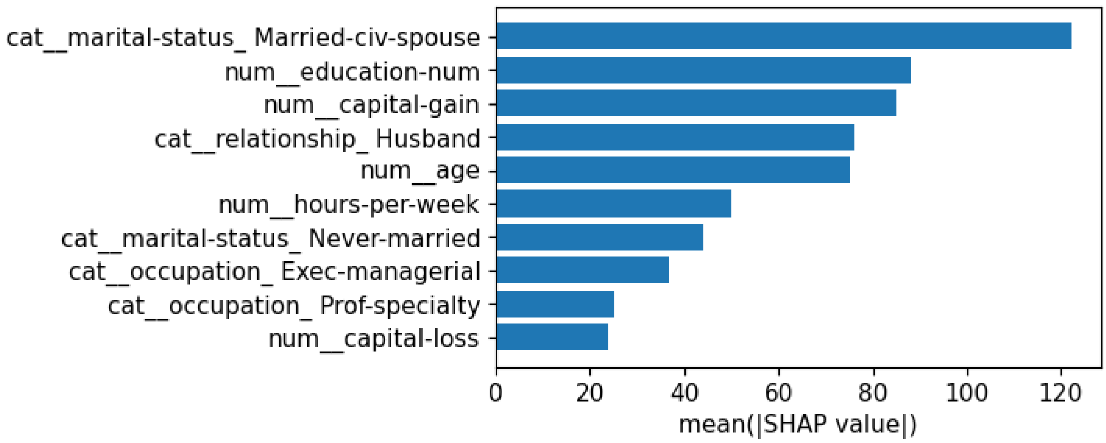
[18]:
```
shap.summary_plot(shap_values, X_test_transformed[:1000],feature_names =
  feature_names)
```



[19]:
```
shap_summary = np.sum(np.abs(shap_values[1]),axis=0)+np.sum(np.
↪abs(shap_values[0]),axis=0) # same shape as the number of features
indcs = np.argsort(shap_summary)
shap_summary[indcs]

plt.figure(figsize=(5,3))
plt.barh(feature_names[indcs[-10:]],shap_summary[indcs[-10:]])
```

```python
plt.xlabel('mean(|SHAP value|)')
plt.show()
```



2.5 SHAP cons

- it can be numerically expensive
  - an efficient shap method was developed for trees, see here
- how to estimate $f_x(S)$?
  - this is not trivial because models cannot change the number of features they use
  - usually the values of the dropped features are replaced with the mean or 0
  - this is approximate but no one came up with a better way

2.6 Local feature importance metrics

By the end of this module, you will be able to - Describe motivation behind local feature importance metrics - Apply SHAP - **Describe LIME**

2.7 Locally Interpretable Model-agnostic Explanations

- read about it here, here, and here
- classification and regression models can be complex and explaining the whole model is challenging
- let's focus on one point at a time
- generate an interpretable model (linear regression) in the local neighborhood of that one point
- study the coefficients of that model

2.8 LIME steps:

- select a data point you want to explain
- generate random samples
- weight the samples based on their distance from the data point of interest (exponential kernel)
- train a linear regression model (usually lasso) using the weighted samples

- study the local model around the point

2.9 Cons, the devil is in the details

- the random samples are not taken around the data point of interest
- how to define the half width of the kernel?
  - the explanation can be very sensitive to the kernel width
  - there is no good way to define/measure what a good kernel width is
- the distance measure treats each feature equally which can be problematic

3 Mudcard

[ ]:

```

```