Mudcard

- **What are we supposed to do if we find out model contains many very unimportant features when we run these tests, should we remove them and retrain the model without them? That seems like not the best option, also is it different for each type of model, i.e. you mentioned xgboost handling unimportant features well where as some models may not.**
  - Global importances usually just give you an idea of which features are important and you'd consult with a subject matter expert (if it is not you) to verify if the expected features are used.
  - If you use k nearest neighbors for example, removing unimportant features will likely improve model performance. If you use tree-based methods (like RF, XGB), I don't expect the model performance to change. So it kinda depends.
  - The safest thing to do is to train a new model after you remove the unimportant features and check how the model performance changes.
  - Yes, it's different for each type of model. Each model looks at the data differently. Linear models have one weight per feature, decision tree-based models use simple binary splits, SVMs use gaussian kernels to "smooth" the data out, k nearest neighbors look at nearby points, etc. So the different models have different properties based on how they learn and make predictions.
- **"There is a difference in performance between the not all scaled and all scaled in the class. Do we need to scale all the features before the training?**
  - The question is whether the difference is significant. :)
  - The difference is in the third decimal point (0.858 vs 0.857). If you recalculate the scores for a couple of different random states, you might find that the scores are well within +/- 1 standard deviation
  - Yes, you need to scale all the features before training. It's good practice and it ensures that you can use the weights of your linear model to measure feature importance.

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

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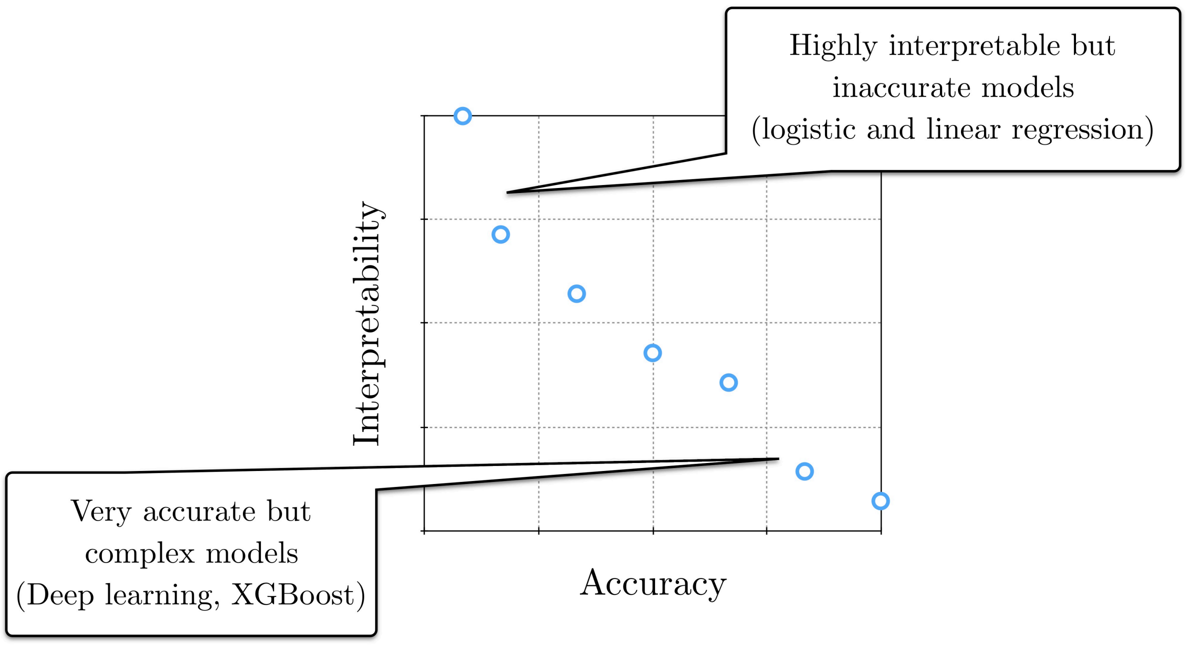
Motivation

- can we trust the model?
  - global feeature 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

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

Motivation



- local feature importance improves the interpretability of complex models
- check out this page for a good example

Local feature importance metrics

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- **Apply SHAP**
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SHAP values

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

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?

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?

How is it calculated?

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

- 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

How is it calculated?

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

- 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

Quiz 1

In [1]:
```
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
```

In [2]:
```
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-country']
    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)
```

```python
    # 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
```

In [3]:

```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_)
```

```
Fitting 4 folds for each of 16 candidates, totalling 64 fits
0.862906941031941
0.8667280822969445
{'randomforestclassifier__max_depth': 100, 'randomforestclassifier__min_samples_split': 64}
```

In [4]:

```python
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))
```

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

Explain a point

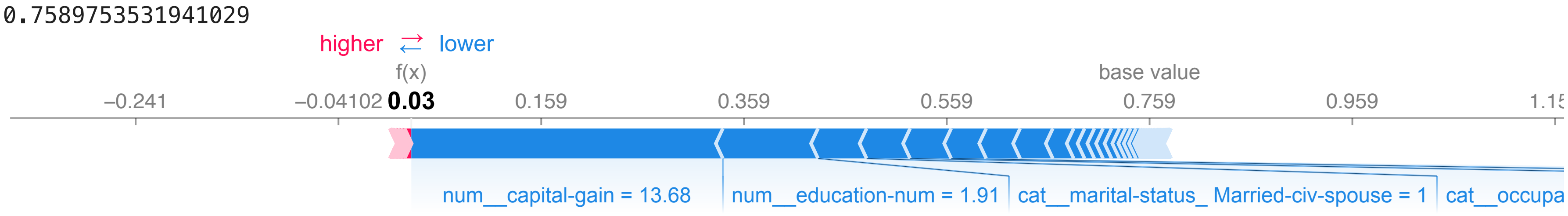
In [5]:

```python
index = 42 # the index of the point to explain
print(explainer.expected_value[0]) # we explain class 0 predictions! Change indices to 1 if you want to explain cla

shap.force_plot(explainer.expected_value[0], shap_values[index,:,0], features = X_test_transformed[index,:],feature
```

```
0.7589753531941029
```

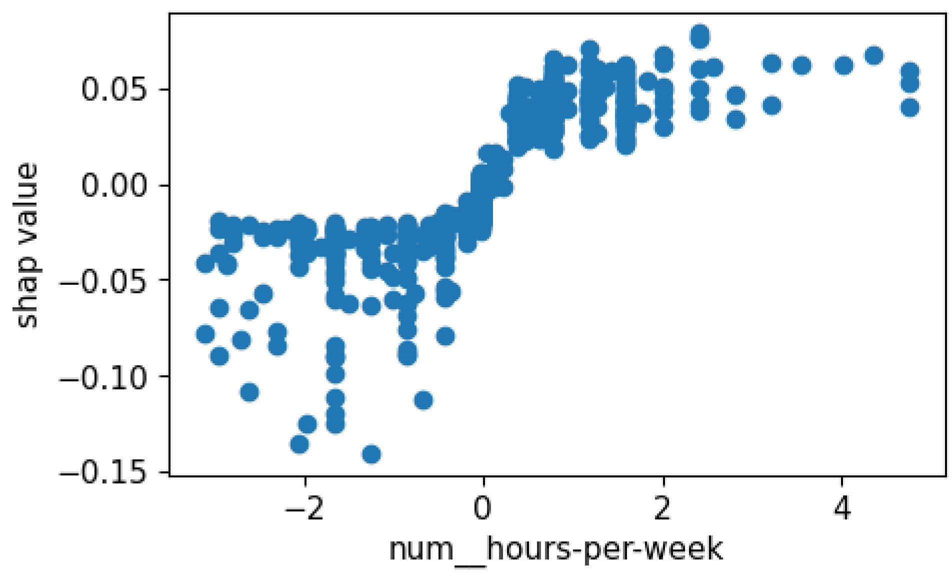
Out[5]:



Feature value vs. shap value

In [6]:

```python
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[:,indx,1])
plt.ylabel('shap value')
plt.xlabel(ftr)
plt.show()
```



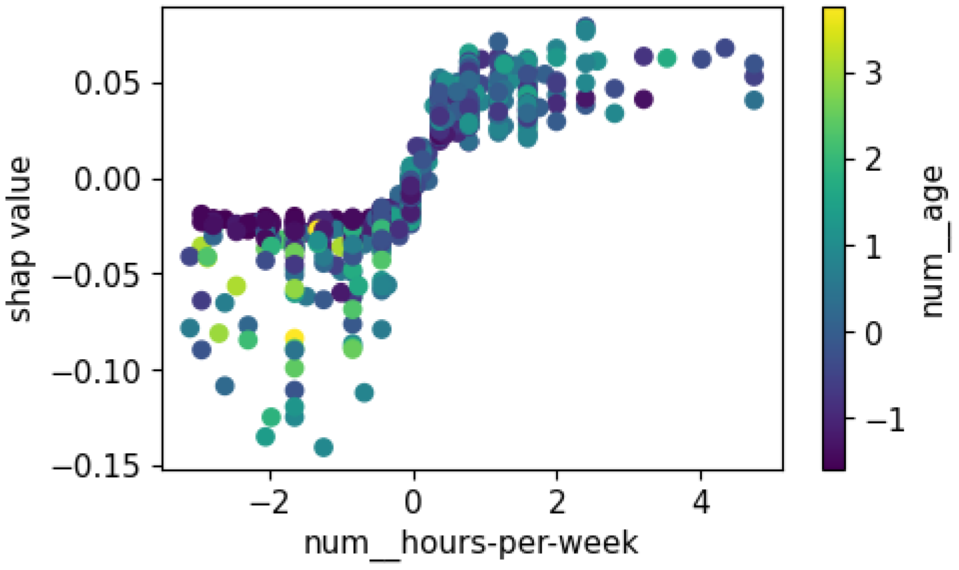
Dependence plot

In [7]:

```python
ftr1 = 'num__hours-per-week'
ftr2 = 'num__age'
indx1 = np.argwhere(feature_names==ftr1)
```

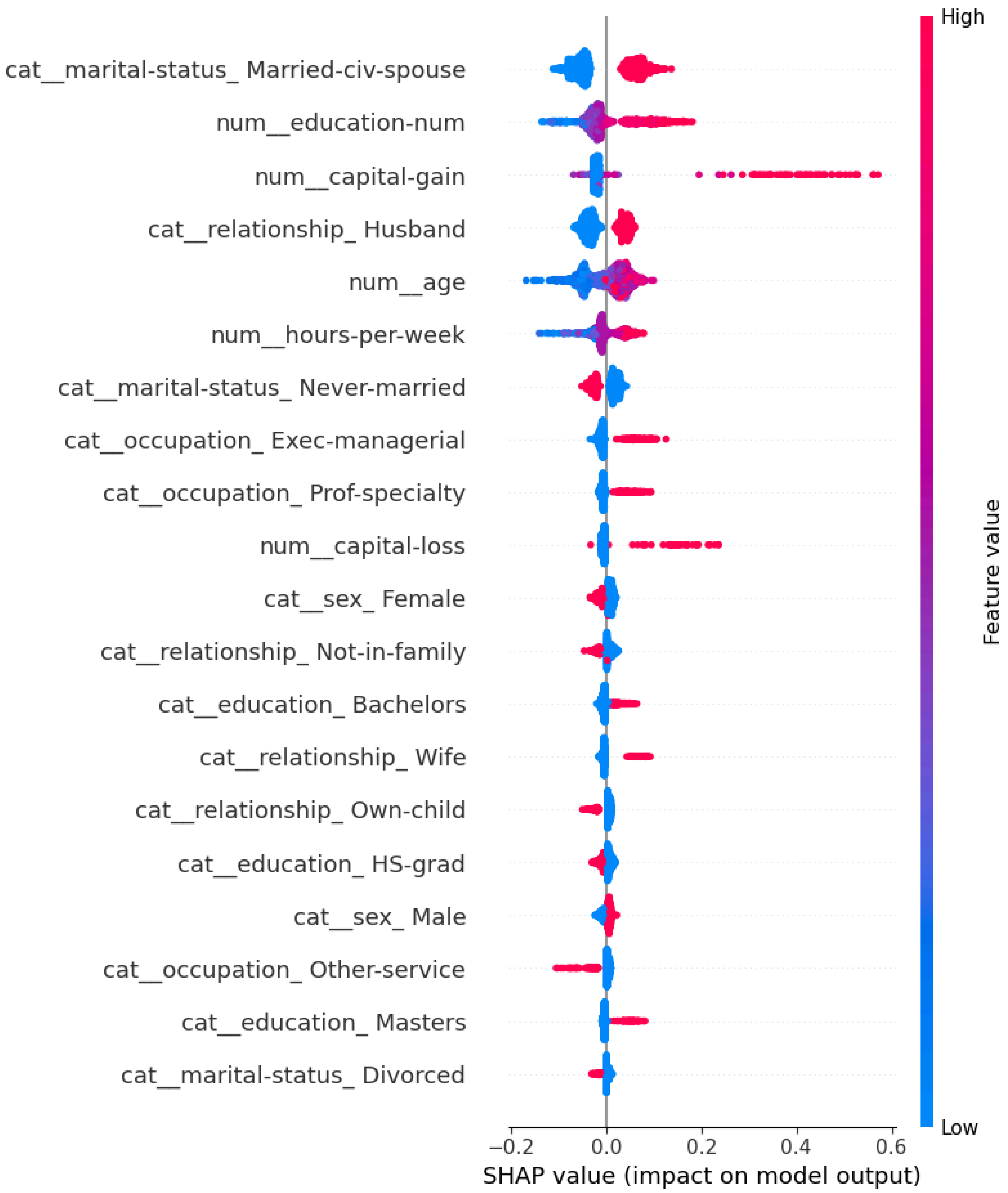
```
indx2 = np.argwhere(feature_names==ftr2)

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



It can also be used for global feature importance

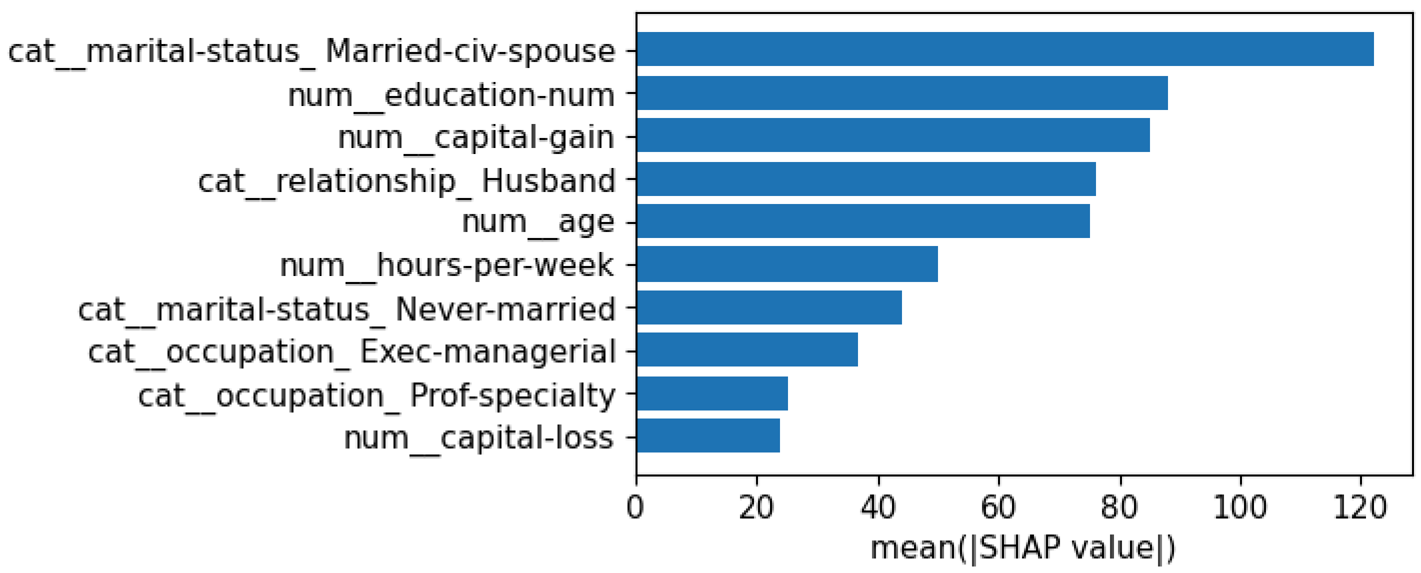
In [8]:
```
shap.summary_plot(shap_values[:,:,1], X_test_transformed[:1000],feature_names = feature_names)
```



In [9]:

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

plt.figure(figsize=(5,3))
plt.barh(feature_names[indcs[-10:]],shap_summary[indcs[-10:]])
plt.xlabel('mean(|SHAP value|)')
plt.show()
```



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

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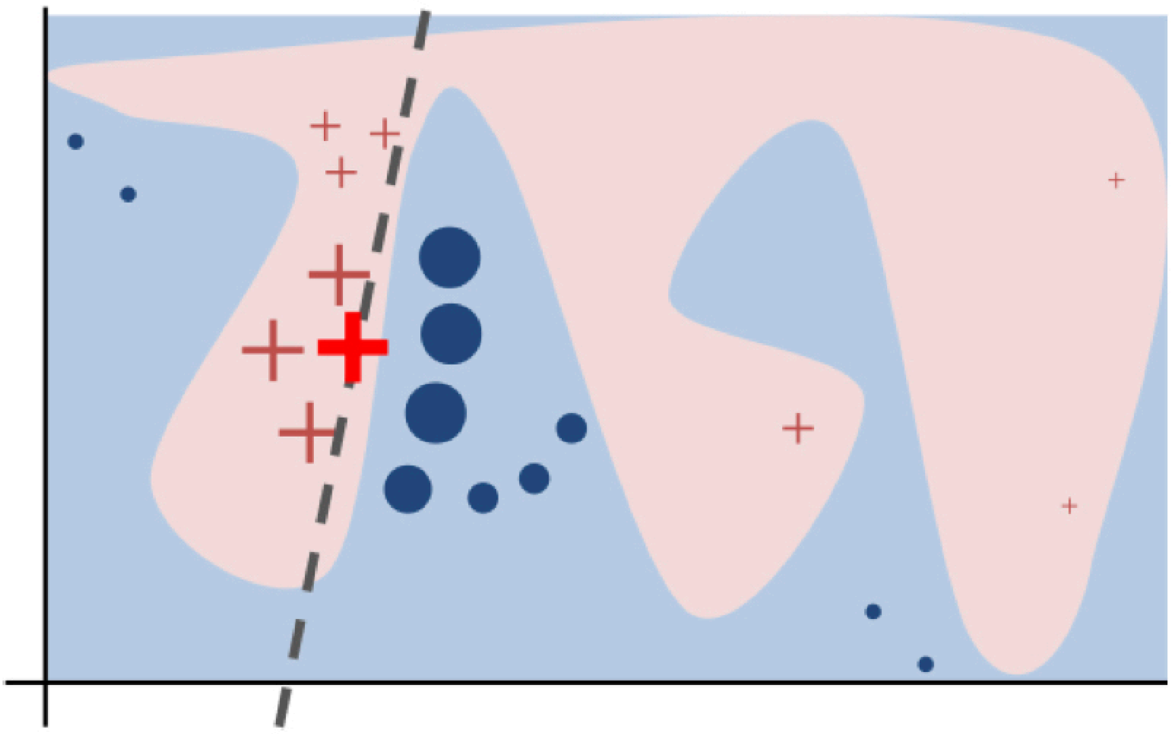
Locally Interpretable Model-agnostic Explanations

- 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

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



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

Online book recommendation!

"Interpretable Machine Learning" by Christoph Molnar

https://christophm.github.io/interpretable-ml-book/

Mudcard

```
In [ ]:
```