Workshop: Introduction to Interpretability in ML

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Materials available at https://github.com/azsom/ODSC-East-2022

About me

- Born and raised in Hungary
- Astrophysics PhD at MPIA, Heidelberg, Germany
- Postdoctoral researcher at MIT (still in astrophysics at the time)
- Started at Brown in 2015 as a Data Scientist in CCV (Center for Computation and Visualization)
- Lead Data Scientist since 2017 at CCV
- Assistant Professor since summer of 2021 at the DSI

Data Science at AI+Training

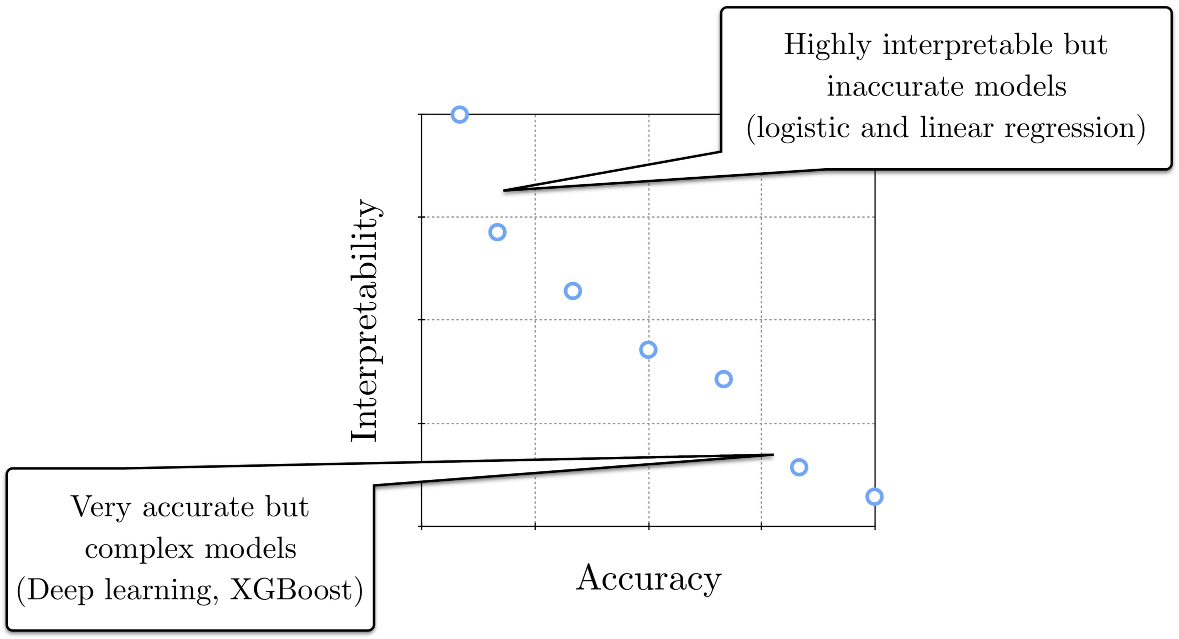
- Supervised Machine Learning Course Series - https://app.aiplus.training/courses/supervised-machine-learning-series
- 6 courses that walk through the main steps of developing an ML pipeline
- github repo available here: https://github.com/azsom/Supervised-Learning
- Week 7 of the ODSC ML Certification - https://aiplus.training/certificates/
- this workshop is based on course 6

Introduction to Interpretability in ML

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

- calculate global explanations using the coefficients of linear models
- perform permutation importance using any ML model
- use the SHAP package to calculate local explanations

Motivation: simple vs. complex models



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

Motivation: build trust in your model

- debugging ML models is tough
  - a model that runs without errors/warning is not necessarily correct
- model seems accurate but does it make predictions the way you expect it to be?
  - wolf vs. husky classifier
- model inspection is important
  - feature importance metrics measure useful they are at predicting the target variable
  - global: one score per feature, a vector of shape (1, n_features)
    - general overview over a larger sample size
  - local: one score per feature and point, an array of shape (n_samples, n_features)
    - explanation specific to each sample
- discuss the interpretability results with a subject matter expert
  - if they say something is surprising, you either
    - have a bug in your code (more likely),
    - you discovered something new which is exciting!

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Math recap

Linear regression:

$$f(X_i) = y_i' = \theta_0 + X_{i1}\theta_1 + X_{i2}\theta_2 + ... = \theta_0 + \sum_{j=1}^{m} \theta_j X_{ij},$$

Logistic regression:

$$f(X_i) = y_i' = \frac{1}{1+e^{-z}},$$

$$z = \theta_0 + \sum_{j=1}^{m} \theta_j x_{ij}$$

Here, y_i' is the prediction of the model for sample i using the X_i feature vector, and θ are coefficients.

What to do if you want to use the coefficients of your linear model as explanations

- **Look at the absolute value of the coefficients!**
  - a feature is important, if its coefficient's magnitude is large
  - doesn't matter if the coefficient is positive or negative
- **Standardize *ALL* features!**
  - most practitioners standarize the continuous features
  - but practicioners often forget to standarize the one-hot encoded or ordinal encoded features which is a mistake!
  - all features need to have the same mean and standard deviation if you want to use the coefficients to measure importance!

Simple ML pipeline

- we will use the diabetes dataset in this workshop
- https://www4.stat.ncsu.edu/~boos/var.select/diabetes.html
- "Ten baseline variables, age, sex, body mass index, average blood pressure, and six blood serum measurements were obtained for each of n = 442 diabetes patients, as well as the response of interest, a quantitative measure of disease progression one year after baseline."

In [1]:
```
# read in the dataset
import pandas as pd
```

```
df = pd.read_csv('data/diabetes.csv')
df.head()

y = df['Y']
X = df.loc[:, df.columns != 'Y']
print(y.head())
print(X.head())
```

```
0    151
1     75
2    141
3    206
4    135
Name: Y, dtype: int64
   AGE     SEX   BMI     BP   S1     S2    S3   S4      S5  S6
0   59    male  32.1  101.0  157   93.2  38.0  4.0  4.8598  87
1   48  female  21.6   87.0  183  103.2  70.0  3.0  3.8918  69
2   72    male  30.5   93.0  156   93.6  41.0  4.0  4.6728  85
3   24  female  25.3   84.0  198  131.4  40.0  5.0  4.8903  89
4   50  female  23.0  101.0  192  125.4  52.0  4.0  4.2905  80
```

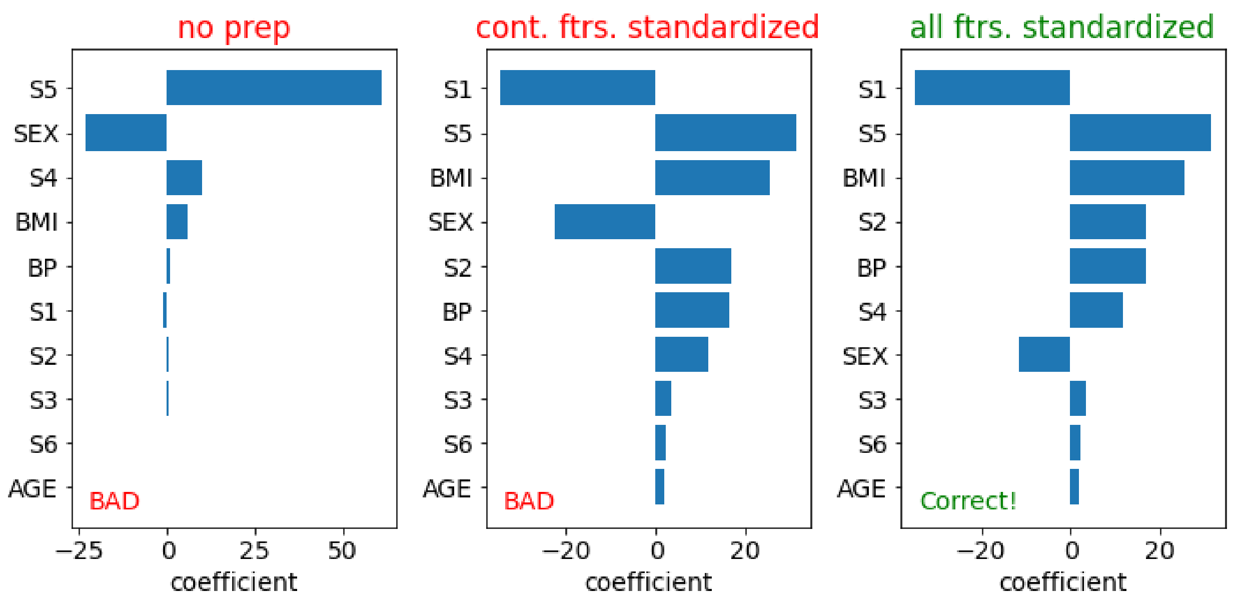
In [2]:
```
# our ML pipeline
def MLpipe_KFold_R2(X, y, preprocessor, ML_algo, param_grid,random_state):
    '''
    This function splits the data to other/test (80/20) and then applies KFold
    The RMSE is minimized in cross-validation.
    '''

    # split data to other/test 80/20, and the use KFold with 4 folds
    X_other, X_test, y_other, y_test = train_test_split(X, y, test_size=0.2, ra
    kf = KFold(n_splits=4, shuffle=True, random_state=random_state)

    # the sklearn pipeline
    if preprocessor == None:
        # no preprocessing
        pipe = Pipeline(steps=[('regressor', ML_algo)])
    else:
        pipe = Pipeline(steps=[('preprocessor', preprocessor),
                               ('regressor', ML_algo)])

    # loop through the hyperparameter combinations or use GridSearchCV
    grid = GridSearchCV(pipe, param_grid=param_grid,scoring='r2',
                        cv=kf, return_train_score=True)
    # for each combination, calculate the train and validation scores using the
    grid.fit(X_other, y_other)
    # find which hyperparameter combination gives the best validation score
    print(grid.best_params_)

    # calculate the test score
    test_score = grid.score(X_test,y_test)
    print(test_score)

    return grid.best_estimator_, test_score, (X_other, y_other), (X_test,y_test
```

In [3]:
```
# let's try three different preprocessing techniques and collect the model coe
from sklearn.linear_model import Ridge
from sklearn.pipeline import Pipeline
from sklearn.model_selection import ParameterGrid
from sklearn.model_selection import train_test_split
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import make_scorer
from sklearn.metrics import r2_score
from sklearn.preprocessing import StandardScaler, OrdinalEncoder
from sklearn.compose import ColumnTransformer

param_grid = {'regressor__alpha': [1e-3,1e-2,1e-1,1e0,1e1,1e2]}

num_ftrs = ['AGE', 'BMI', 'BP', 'S1', 'S2', 'S3', 'S4', 'S5', 'S6']
ord_ftrs = ['SEX']

# ordinal encoder
ordinal_transformer = Pipeline(steps=[
    ('ordinal', OrdinalEncoder())])
# standard scaler
numeric_transformer = Pipeline(steps=[
    ('scaler', StandardScaler())])

#
# ordinal encode SEX only!
#
preprocessor1 = ColumnTransformer(remainder = 'passthrough',
    transformers=[
        ('ord', ordinal_transformer, ord_ftrs)])

model, test_score, train_set, test_set = MLpipe_KFold_R2(X, y, preprocessor1, F
coefs_no_prep = model['regressor'].coef_
print(coefs_no_prep)

#
# ordinal encode SEX, and standardize continuous features
#
preprocessor2 = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, num_ftrs),
        ('ord', ordinal_transformer, ord_ftrs)])

model, test_score, train_set, test_set = MLpipe_KFold_R2(X, y, preprocessor2, F
coefs_some_prep = model['regressor'].coef_
print(coefs_some_prep)

#
# ordinal encode SEX, standardize continuous features, and standarize all featu
#
preprocessor3 = Pipeline(steps=[
    ('prep2', preprocessor2),
    ('scaler', StandardScaler())])

model, test_score, train_set, test_set = MLpipe_KFold_R2(X, y, preprocessor3, F
coefs_prep = model['regressor'].coef_
print(coefs_prep)
```

```
{'regressor__alpha': 1.0}
0.4520945451686046
[-22.80861461   0.14269511   5.90541998   1.19867986  -1.07900835
   0.62662466   0.3774738    9.77013169  60.79394666   0.21396887]
{'regressor__alpha': 1.0}
0.45418697357725524
[  1.79050083  25.75648091  16.71212465 -34.65085803  17.05080545
   3.3870545   11.71899321  31.39253301   2.45268588 -22.69228495]
{'regressor__alpha': 1.0}
0.4541465207069819
[  1.80734179  25.73269892  16.73429974 -34.67195409  17.05307485
   3.36991411  11.76426044  31.3783838    2.45813922 -11.44818951]
```

In [4]:

```python
import matplotlib.pyplot as plt
import numpy as np
plt.rcParams.update({'font.size': 14})

def plot_coefs(coefs,title,color,feature_names):
    feature_names = np.array(feature_names)
    sorted_indcs = np.argsort(np.abs(coefs))
    plt.barh(np.arange(10),coefs[sorted_indcs])
    plt.yticks(np.arange(10),feature_names[sorted_indcs])
    plt.xlabel('coefficient')
    plt.title(title,color=color)
    return

plt.figure(figsize=(10,5))

plt.subplot(1,3,1)
plot_coefs(coefs_no_prep,'no prep','r', ord_ftrs + num_ftrs)
plt.annotate('BAD',xy=(10,10),xycoords = 'axes points',color='r')

plt.subplot(1,3,2)
plot_coefs(coefs_some_prep,'cont. ftrs. standardized','r', num_ftrs + ord_ftrs)
plt.annotate('BAD',xy=(10,10),xycoords = 'axes points',color='r')

plt.subplot(1,3,3)
plot_coefs(coefs_prep,'all ftrs. standardized','g', num_ftrs + ord_ftrs)
plt.annotate('Correct!',xy=(10,10),xycoords = 'axes points',color='g')

plt.tight_layout()
plt.savefig('figures/coefs_comparison.png',dpi=300)
plt.show()
```



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Permutation feature importance

- model agnostic, you can use it with any supervised ML model
- steps:
    - train a model and calculate a test score :)
    - randomly shuffle a single feature in the test set
    - recalculate the test score with the shuffled data
    - model score worsens because the shuffling breaks the relationship between feature and target
    - the larger the difference, the more important the feature is

In [5]:
```
from sklearn.svm import SVR
param_grid = {'regressor__C': [0.01, 0.1, 1, 10, 100, 1000, 10000],
              'regressor__gamma': [1e-4, 1e-3, 0.01, 0.1, 1, 10, 100]}

model, test_score, train_set, test_set = MLpipe_KFold_R2(X, y, preprocessor3, S
```

```
{'regressor__C': 1000, 'regressor__gamma': 0.01}
0.5645801016038898
```

In [6]:
```
np.random.seed(42)

X_test = test_set[0]
y_test = test_set[1]
ftr_names = X_test.columns
```

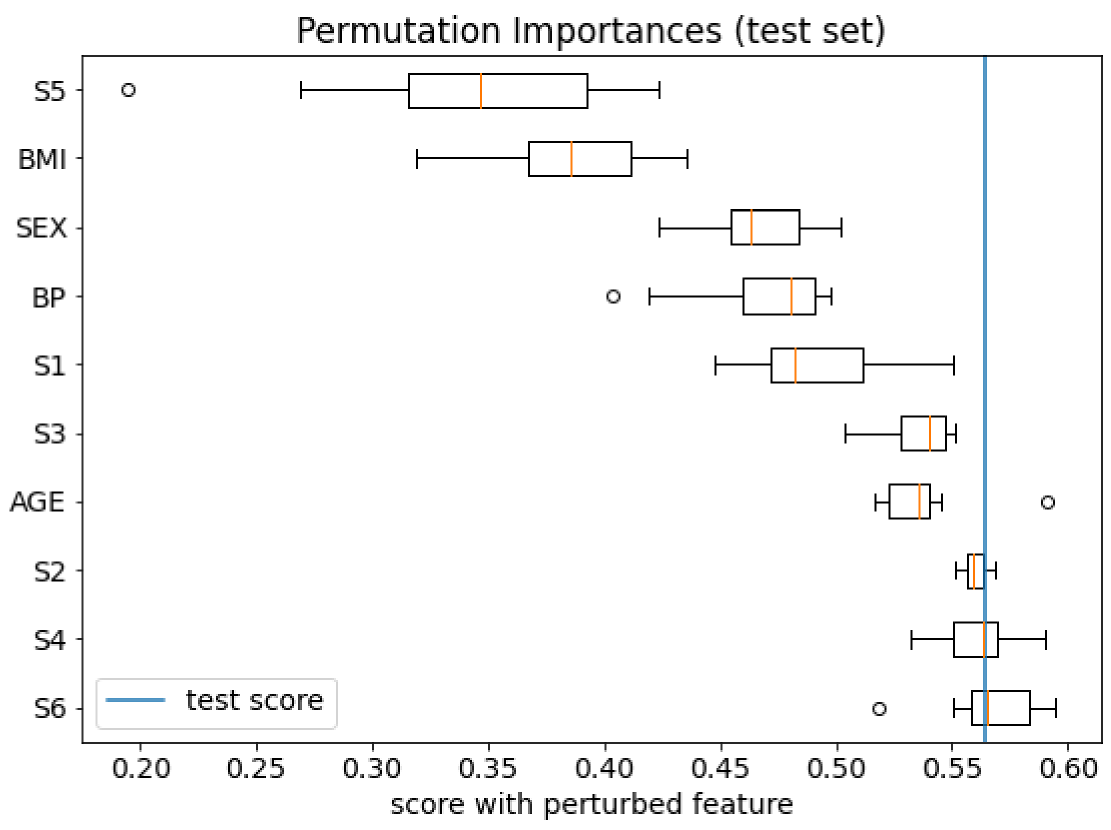
```
nr_runs = 10
scores = np.zeros([len(ftr_names),nr_runs])

print('test score = ',test_score)
# loop through the features
for i in range(len(ftr_names)):
    print('shuffling '+str(ftr_names[i]))
    r2_scores = []
    for j in range(nr_runs):
        X_test_shuffled = X_test.copy()
        X_test_shuffled[ftr_names[i]] = np.random.permutation(X_test[ftr_names[
        r2_scores.append(model.score(X_test_shuffled,y_test))
    print('   shuffled test score:',np.around(np.mean(r2_scores),3),'+/-',np.ar
    scores[i] = r2_scores
```

```
test score =  0.5645801016038898
shuffling AGE
   shuffled test score: 0.537 +/- 0.02
shuffling SEX
   shuffled test score: 0.467 +/- 0.021
shuffling BMI
   shuffled test score: 0.384 +/- 0.037
shuffling BP
   shuffled test score: 0.468 +/- 0.031
shuffling S1
   shuffled test score: 0.493 +/- 0.034
shuffling S2
   shuffled test score: 0.56 +/- 0.005
shuffling S3
   shuffled test score: 0.535 +/- 0.014
shuffling S4
   shuffled test score: 0.561 +/- 0.016
shuffling S5
   shuffled test score: 0.34 +/- 0.066
shuffling S6
   shuffled test score: 0.567 +/- 0.021
```

In [7]:

```
sorted_indcs = np.argsort(np.mean(scores,axis=1))[::-1]
plt.rcParams.update({'font.size': 14})
plt.figure(figsize=(8,6))
plt.boxplot(scores[sorted_indcs].T,labels=ftr_names[sorted_indcs],vert=False)
plt.axvline(test_score,label='test score')
plt.title("Permutation Importances (test set)")
plt.xlabel('score with perturbed feature')
plt.legend()
plt.tight_layout()
plt.show()
```



Check out sklearn's permutation importance!

https://scikit-learn.org/stable/modules/generated/sklearn.inspection.permutation_importance.html

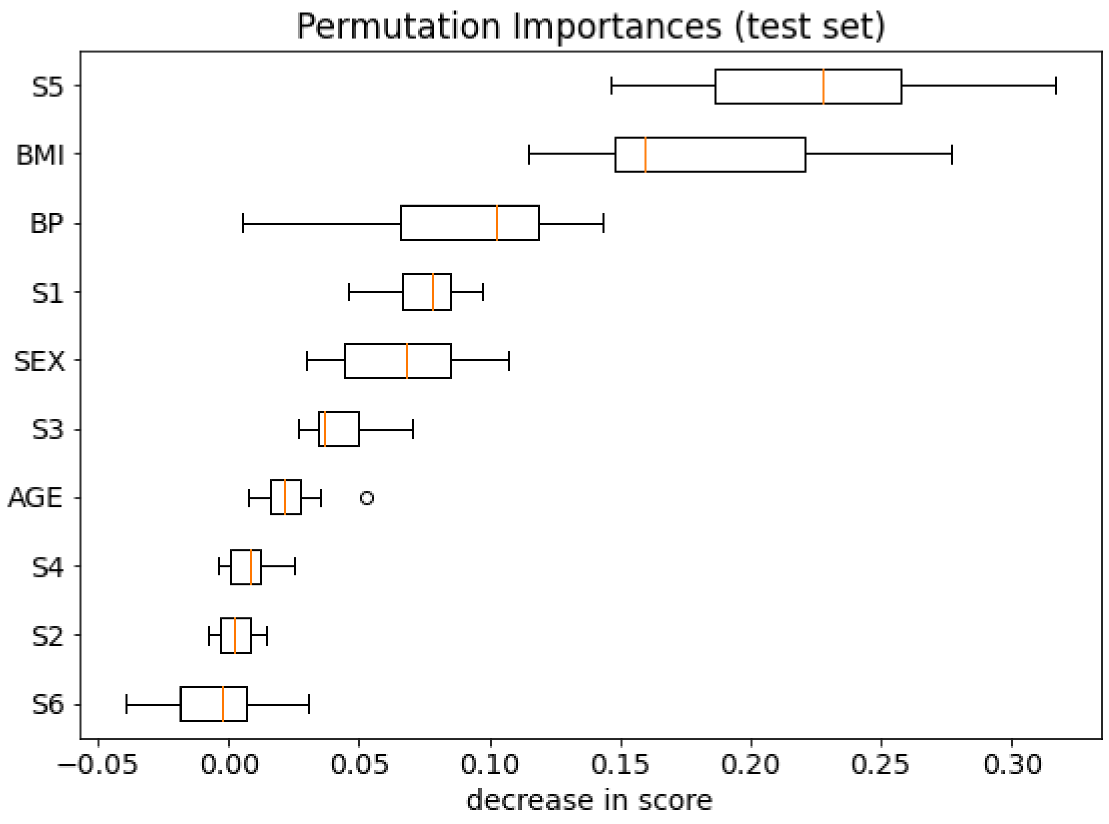
https://scikit-learn.org/stable/modules/permutation_importance.html#permutation-importance

In [8]:
```
from sklearn.inspection import permutation_importance

result = permutation_importance(model, X_test, y_test,n_repeats=10,random_state
ftr_names = X_test.columns

sorted_indcs = result.importances_mean.argsort()

plt.rcParams.update({'font.size': 14})
plt.figure(figsize=(8,6))
plt.boxplot(result.importances[sorted_indcs].T,labels=ftr_names[sorted_indcs],v
plt.title("Permutation Importances (test set)")
plt.xlabel('decrease in score')
plt.tight_layout()
plt.show()
```



Cons of permutation feature importance

- strongly correlated features
  - if one of the features is shuffled, the model can still use the other correlated feature
  - both features appear to be less important but they might actually be important
  - solution:
    - check the correlation matrix plot
    - remove all but one of the strongly correlated features
- no feature interactions
  - one feature might appear unimportant but combined with another feature could be important
  - solution:
    - permute two features to measure how important feature pairs are
    - this can be computationally expensive

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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

```
In [9]: import shap
        shap.initjs() # required for visualizations later on

        explainer = shap.KernelExplainer(model[1].predict,model[0].transform(train_set[
        # transform the test set
        X_test_transformed = model[0].transform(X_test)
        print(np.shape(X_test_transformed))
        # calculate shap values on the test
        shap_values = explainer.shap_values(X_test_transformed)
        print(np.shape(shap_values))
        ftr_names = num_ftrs + ord_ftrs
```

```
Using 353 background data samples could cause slower run times. Consider using
shap.sample(data, K) or shap.kmeans(data, K) to summarize the background as K
samples.
(89, 10)
  0%|          | 0/89 [00:00<?, ?it/s]
(89, 10)
```

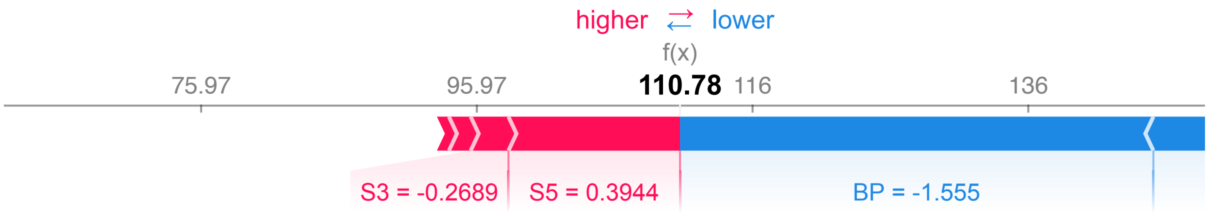
Explain a point

```
In [10]: ftr_names = np.array(num_ftrs + ord_ftrs)

         index = 1 # the index of the point to explain

         shap.force_plot(explainer.expected_value, shap_values[index,:], X_test_transfor
```

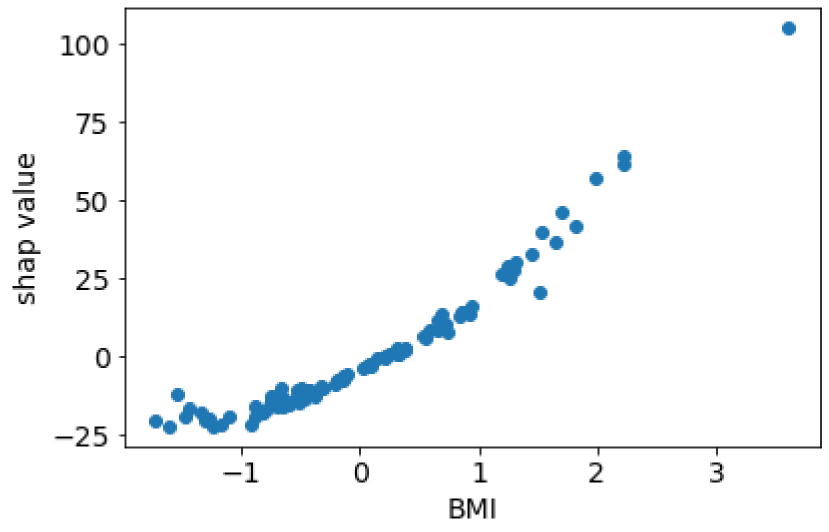
Out[10]:



Feature value vs. shap value

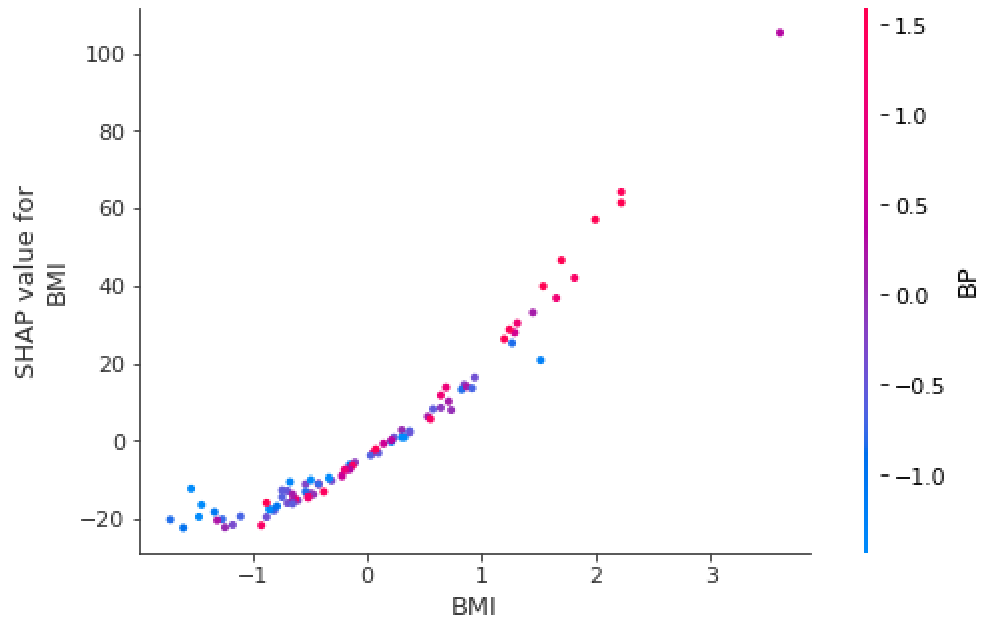
```
In [11]: ftr = 'BMI'
         indx = np.argwhere(ftr_names==ftr)

         plt.scatter(X_test_transformed[:,indx],shap_values[:,indx])
         plt.ylabel('shap value')
         plt.xlabel(ftr)
         plt.tight_layout()
         plt.show()
```



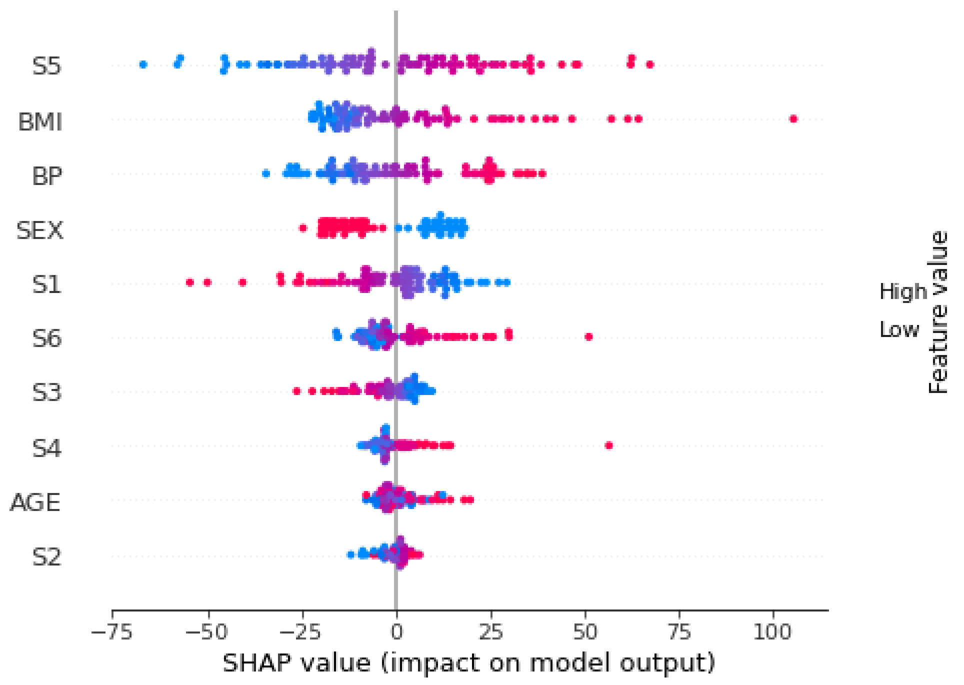
Dependence plot

```
In [12]: shap.dependence_plot('BMI', shap_values, X_test_transformed, feature_names=ftr_
```



It can also be used for global feature importance

```
In [13]: shap.summary_plot(shap_values, X_test_transformed,feature_names = ftr_names)
```



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 an approximation

Recap: Introduction to Interpretability in ML

By now, you can

- calculate global explanations using the coefficients of linear models
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Brown Data Science Master's Program

- if your company is looking to hire talented data scientists, reach out to me
- our students are looking for internships and full time positions!
- email: andras_zsom@brown.edu
- I'm also around tomorrow and until the early afternoon on Thursday