Imperial College London

Explainability

- The right to an explanation
- Classical Interpretability and Partial Dependence Plots
- An overview of XAI techniques
- Are all explanations causal?

Linearity and additivity are the basis of classic XAI

```
In [1]: import pandas as pd
import shap
import sklearn

In [10]: # the classic diabetes dataset from https://www4.stat.ncsu.edu/~boos/var.select/diabetes.html
    X,y = shap.datasets.diabetes()

# a simple linear model
lreg = sklearn.linear_model.LinearRegression()
lreg.fit(X, y)
```

Linearity and additivity are the basis of classic XAI

```
In [14]: print("Model coefficients:\n")
    for i in range(X.shape[1]):
        print(X.columns[i], "=", lreg.coef_[i].round(4))

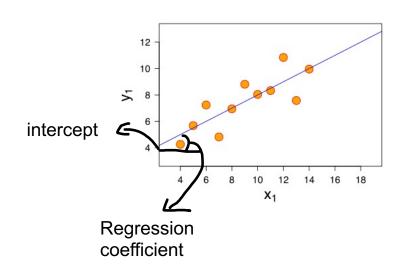
Model coefficients:

    age = -10.0122
    sex = -239.8191
    bmi = 519.8398
    bp = 324.3904
    s1 = -792.1842
    s2 = 476.7458
    s3 = 101.0446
    s4 = 177.0642
```

Linearity and additivity are the basis of classic XAI

$$y_i = \beta_0 + \sum_{j=1}^n \beta_j X_{ij}$$

```
In [40]: lreg.predict(np.array(X.loc[0]).reshape(1,-1))
Out[40]: array([206.11706979])
In [44]: np.sum(lreg.coef_*X.loc[0]) + lreg.intercept_
Out[44]: 206.11706978709228
```



Applicable Mathematics

Even linear regression requires careful interpretation

```
print("Model coefficients:\n")
for i in range(X.shape[1]):
    print(X.columns[i], "=", lreg.coef_[i].round(4))

Model coefficients:

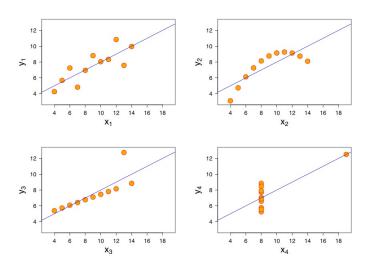
age = -10.0122
sex = -239.8191
bmi = 519.8398
bp = 324.3904
s1 = -792.1842
s2 = 476.7458
s3 = 101.0446
s4 = 177.0642
s5 = 751.2793
s6 = 67.6254
```

Sign reversal can sometimes occur in linear regression when removing one variable from a multivariable regression

```
lreg no s1 = sklearn.linear model.LinearRegression()
  X \text{ no } s1 = X.drop('s1', 1)
  lreg no s1.fit(X no s1, y)
  print("Model coefficients (removing BMI):\n")
  for i in range(X no s1.shape[1]):
      print(X no s1.columns[i], "=", lreg no s1.coef [i].round(4))
  Model coefficients (removing BMI):
  age = -7.9167
  sex = -234.1587
  bmi = 528.5262
  bp = 319.7704
\Rightarrow s2 = -143.2835
 3 = -250.5987
  s4 = 70.4507
  s5 = 461.8402
  s6 = 69.126
```

Even linear regression requires careful interpretation

- Explanations of the model's predictions do not necessarily explain the phenomenon itself.
- Checks of model assumptions are necessary in addition to checks of predictive accuracy for purposes of explainability / interpretability
- Robustness / stability is another key concern: communicated explanations should be qualitatively robust (e.g., top 5 most important drivers, signs, etc.) or, if not, supported by an explanation why not



Known as the Anscombe quartet, this selection of small datasets shows how the same line of best fit appears in 4 different situations

In tabular data, explainability involves four elements

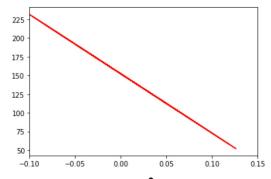
- Magnitude of feature importance
- Direction or shape of feature importance
- Interaction between features
- Confidence in feature importance

- Shap values
- Partial Dependence plots

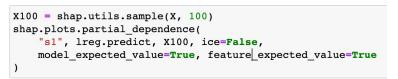
Partial dependence plots

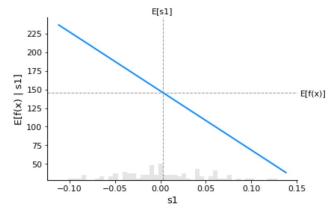
```
plt.plot(
    X100['s1'],
    lreg.coef_[4]*X100['s1'] + lreg.intercept_,
    color='red')
plt.xlim([-0.1,0.15])
```

(-0.1, 0.15)



$$p_2(\xi) = \hat{\beta}_2 \xi + \beta_0$$



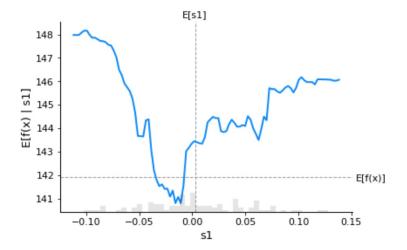


$$p_2(\xi) = \frac{1}{n} \sum_{i=1}^n f(x_{i1}, \xi, x_{i3}, \dots)$$

Partial dependence plots

$$p_2(\xi) = \frac{1}{n} \sum_{i=1}^n f(x_{i1}, \xi, x_{i3}, \dots)$$

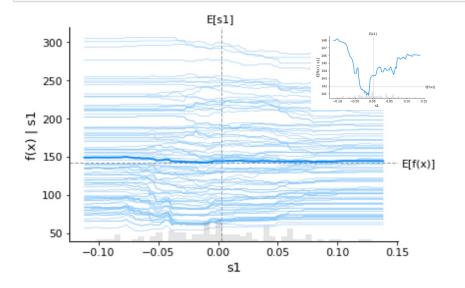
```
# a random forest
rf = sklearn.ensemble.RandomForestRegressor()
rf.fit(X, y)
shap.plots.partial_dependence(
    "s1", rf.predict, X100, ice=False,
    model_expected_value=True, feature_expected_value=True
)
```



Individual Conditional Expectation (ICE) plots

$$p_2(\xi) = \frac{1}{n} \sum_{i=1}^n f(x_{i1}, \xi, x_{i3}, \dots)$$

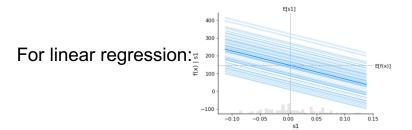
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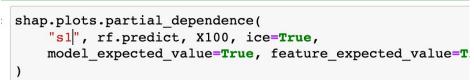


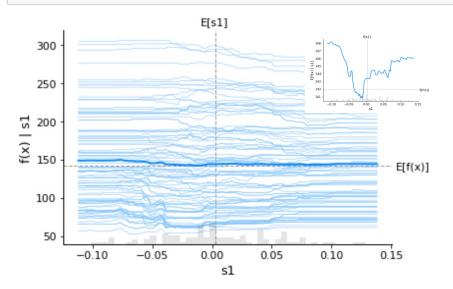
Applicable Mathematics

Individual Conditional Expectation (ICE) plots

$$p_2(\xi) = \frac{1}{n} \sum_{i=1}^n f(x_{i1}, \xi, x_{i3}, \dots)$$







Imperial College London Summary

- Classical interpretability relied on some mathematical properties like linearity and additivity.
- It produced explanations by way of assigning properties to individual features like "magnitude of effect", "direction of effect", "interactions between features", and "confidence".
- Even simple methods like linear regression can however be misleading and require care.
- Modern XAI techniques attempt to offer similar "explanations" to classical methods by generalizing the concept of an "effect" through methods like partial dependence plots.
- Familiarity with these tools is an absolute must-have in the work of a practicing data scientist