Business 4720 - Class 19

Interpretable Machine Learning – Explainable AI

Joerg Evermann

Faculty of Business Administration
Memorial University of Newfoundland
jevermann@mun.ca

This Class

What You Will Learn:

- Introduction to Interpetability and Explainability
- Model specific and Model agnostic methods
- Global explainability
- Local explainability

Based On

Molnar, Christoph: *Interpretable Machine Learning* (2023)

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

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Additional Materials

SciKit Learn

A machine learning framework for Python that also provides some interpretable ML functions.

`https://scikit-learn.org/stable/user_guide.html`

LIME

A Python package to compute Local Interpretable Model Explanations (a local model-agnostic method).

`https://github.com/marcotcr/lime`

SHAP

A Python package to compute Shapley Additive Explanations (a local model-agnostic interpretation method).

`https://shap.readthedocs.io/en/latest/`

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Tools

Install required Python packages:

```
pip install statsmodels matplotlib scikit-learn \
    PyALE lime shap
```

Importance of Interpretability

Human understanding of how the AI works and arrives at its results (decisions, predictions, . . .)

- Curiosity
- Human learning
- Human sensemaking of events and phenomena
- Knowledge extraction for scientific progress
- Safety and compliance assessment
- Reliability and robustness evaluation
- Identify knowledge limits
- Auditability
- Bias detection & ensuring fairness
- Trust and acceptance
- Debugging & failure analysis
- Legal obligations ("right to explanation")

Model Interpretability

Distinctions

- Intrinsic $\leftrightarrow$ Post-hoc
- Local $\leftrightarrow$ Global

Intrinsically Interpretable Models

Algorithm	Linear	Monotone	Interaction
Linear regression	Yes	Yes	No
Logistic regression	No	Yes	No
Decision trees	No	Some	Yes
RuleFit	Yes	No	Yes
Naive Bayes	No	Yes	No
k-NN	No	No	No

Source:

`https://christophm.github.io/interpretable-ml-book/simple.html`

Linear Regression

```r
# Load the bike rental data set
d <- read.csv('https://evermann.ca/busi4720/bike.csv')
# Perform the regression and summarize results
summary(lm(cnt~season+temp, data=d))
```

Results:

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   3151.02     169.35  18.606  < 2e-16 ***
seasonSPRING  -494.15     163.28  -3.026  0.00256 **
seasonSUMMER  -852.68     209.82  -4.064 5.35e-05 ***
seasonWINTER -1342.87     164.59  -8.159 1.49e-15 ***
temp           132.79      11.02  12.046  < 2e-16 ***
---
Residual standard error: 1433 on 726 degrees of freedom
Multiple R-squared: 0.4558, Adjusted R-squared: 0.4528
```

Linear Regression

- **Algorithmic transparency**: The ordinary least squares loss function is clear and intuitive; provides optimality guarantees
- **Coefficients** β
  - An increase of one unit of a predictor increases the prediction by β, *assuming all other predictors remain the same* ("ceteris paribus")
  - Switching from the reference category (see "contrasts") to another category increases the prediction by β, *assuming all other predictors remain the same* ("ceteris paribus")
  - **Intercept** is the predicted value when all other predictors are 0. Is this reasonable?
- R^2 is the amount of explained variance; model weights should only be interpreted when R^2 reasonable size.
- **Relative feature importance** is given by the $t = \frac{\hat{\beta}}{SE(\hat{\beta})}$ statistic.

Linear Regression

Dimension reduction to improve interpretability:

- Manual feature selection, e.g. based on effect size
- Automatic feature selection (forwards or backwards)
- Regression with PCA components
- Penalized regression with LASSO

Be aware of bias-variance trade-off with all of these.

Decision Trees

Decision Tree Types

- Regression trees
- Classification trees

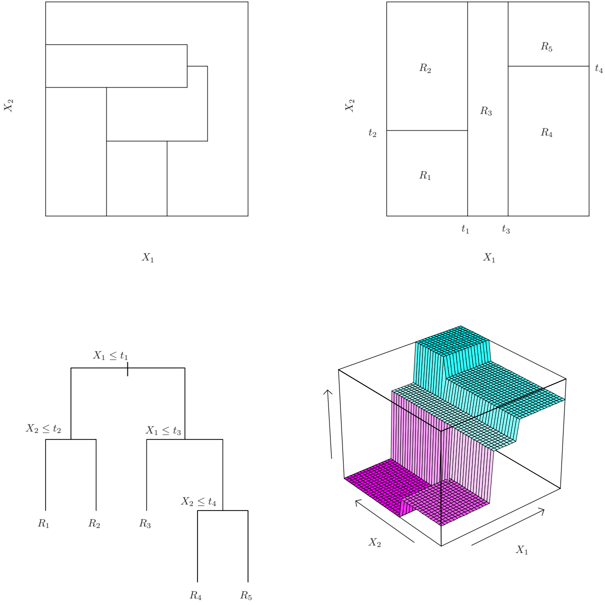
Strengths

- Intrinsically interpretable and visualizable
- Individual predictions explained by path through tree
- Captures feature interactions
- No need to transform features

Weaknesses

- Unstable (high variance)
- Tend to overfit
- Predictions are piecewise constant

Regression Trees



Source: ISLR2
Figure 8.3

Regression Trees

1. Recursively divide the predictor space into J distinct and non-overlapping regions $R_1, R_2, \ldots, R_j$
   - For every predictor j and split point s define regions

     $$R_1(j,s) = \{X | X_j < s\} \quad \text{and} \quad R_2(j,s) = \{X | X_j \geq s\}$$

   - Choose j and s to minimize variance in each region:

     $$\sum_{i: x_i \in R_1(j,s)} (y_i - \bar{y}_{R_1})^2 + \sum_{i: x_i \in R_2(j,s)} (y_i - \bar{y}_{R_2})^2$$

2. For every observation that falls into region R_j, prediction is the mean of the targets of training observations in R_j

Regression Trees

Prepare data:

```
import matplotlib.pyplot as plt
import pandas as pd
d=pd.read_csv('https://evermann.ca/busi4720/bike.csv')
x=d[['temp', 'hum']]
y=d['cnt']
```

Fit unpruned tree:

```
from sklearn.tree import DecisionTreeRegressor
regr = DecisionTreeRegressor()
regr.fit(x, y)
```

Print the MSE:

```
from sklearn.metrics import mean_squared_error
mean_squared_error(regr.predict(x), y)
```

Print the tree:

```
import sklearn
print (sklearn.tree.export_text(regr, \
    feature_names=x.columns))
```

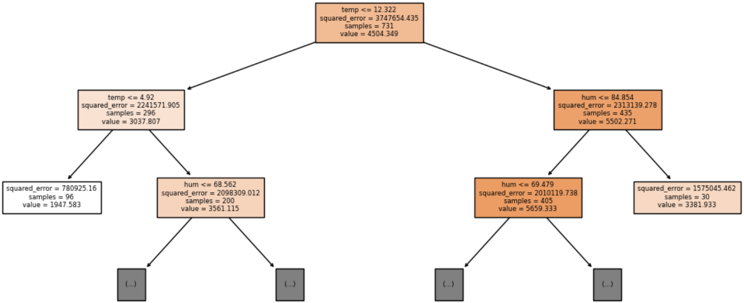
Plot the tree:

```
sklearn.tree.plot_tree(regr,
    max_depth=2, feature_names=x.columns,
    filled=True, fontsize=6)
plt.show()
```

Early stopping can prevent overfitting and maintain interpretability:

```
regr = DecisionTreeRegressor(max_depth=3)
regr = DecisionTreeRegressor(min_samples_leaf=10)
regr = DecisionTreeRegressor(max_leaf_nodes=8)
```

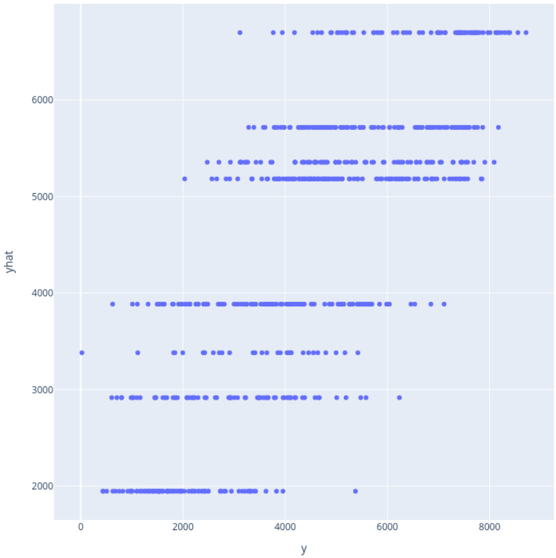
Regression Trees



Plot fitted versus true values:

```
import plotly.express as px
px.scatter(pd.DataFrame([y, regr.predict(x)], \
    index=['y', 'yhat']).transpose() \
        ,x='y', y='yhat').show()
```

Regression Trees



Hands-On Exercises

Fit regression trees to the bike dataset on the previous slides. Calculate the MSE, print the decision rules, and plot predicted versus true values as you vary:

- **max_depth**: choose values 1, 3, 5, 7
- **min_samples_leaf**: choose values 1, 5, 10, 20
- **max_leaf_nodes**: choose values 2, 8, 16, 32

How does the training MSE change? What can you observe from the plots of predicted versus true values?

Classification Trees

- Instead of mean, predict most common class in leaf node.
- Instead of MSE, use **Gini index** G (node purity) to determine splits:

$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

- Instead of Gini index, use **Entropy** H as loss functions to determine splits:

$$H = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

- Tree pruning using classification error rate

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Further reading:

https://scikit-learn.org/stable/modules/tree.html

https://scikit-learn.org/stable/auto_examples/tree/plot_unveil_tree_structure.html

https://scikit-learn.org/stable/auto_examples/tree/plot_cost_complexity_pruning.html

Global Model Agnostic Methods

- **Partial dependence plot (PDP)**
- **Individual conditional expectation (ICE) curves**
- **Accumulated local effects plot (ALE)**
- Feature interaction
- Functional decomposition
- **Permutation feature importance**
- **Global surrogate models**
- Prototypes

Partial Dependence Plot (PDP)

Marginal effect of one or a few features X_S on the outcome, marginalized (i.e. sum weighted by probability) over all other (complement) features X_C.

$$\hat{f}_S(X_S) = \mathbb{E}_{X_c}\left[\hat{f}(X_S, X_C))\right] = \int \hat{f}(X_S, X_C)p(X_C)dX_c$$

Estimated from sample data as:

$$\hat{f}_S(X_S) = \frac{1}{n}\sum_{i=1}^{n}\hat{f}(X_S, X_C^{(i)})$$

Shows how the *average* prediction changes when the focal predictor is changed (assuming feature independence).

Partial Dependence Plot (PDP)

Read the data set:

```
import pandas as pd
d=pd.read_csv('https://evermann.ca/busi4720/bike.csv')
x=d[['temp', 'hum']]
y=d[['cnt']]
```

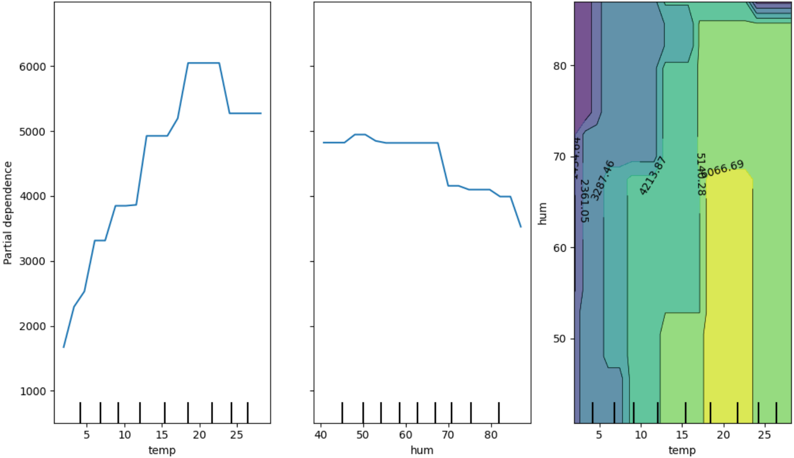
Fit a regression tree:

```
from sklearn.tree import DecisionTreeRegressor
regr = DecisionTreeRegressor(max_depth=5).fit(x, y)
```

Show the PDP:

```
import matplotlib.pyplot as plt
from sklearn.inspection import PartialDependenceDisplay
PartialDependenceDisplay \
    .from_estimator(regr, x, [0, 1, (0,1)],
        grid_resolution=20)
plt.show()
```

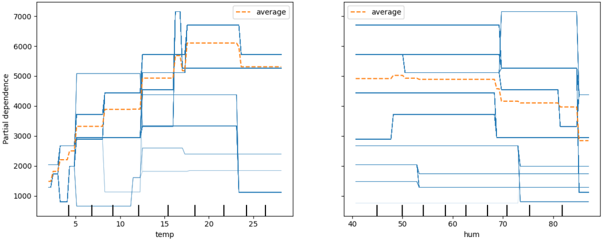
Partial Dependence Plot (PDP)



Individual Conditional Expectation (ICE) Plot

- Instead of the average effect of a feature, shows PDP for individual samples
- Identify individual **outlier** cases or **heterogeneous data**

```
PartialDependenceDisplay \
    .from_estimator(regr, x, [0, 1], kind='both')
```



(Individual samples overlaid due to piece-wise constant regression)

Accumulated Local Effects (ALE) Plot

- Effects computed for a grid of intervals (a ”local window”) (instead of the entire domain, as in PDP)
- Does not construct unrealistic feature combinations
- Overcomes the problem of correlated features in PDP
- Focuses on difference in predictions

$$\hat{\tilde{f}}_{j,ALE}(X) = \sum_{k=1}^{k_j(x)} \frac{1}{n_j(k)} \sum_{i:x_j^{(i)} \in N_j(k)} \left[\hat{f}(z_{k,j}, x_j^{(i)}) - \hat{f}(z_{k-1,j}, x_j^{(i)})\right]$$

- Difference of predictions (in sq brackets) is *local* to ”neighbourhood” $N_j(k)$ of feature j around observation k
- Outer sum *accumulates* the local effects

Centering the effects to mean 0:

$$\hat{f}_{j,ALE}(x) = \hat{\tilde{f}}_{j,ALE}(x) - \frac{1}{n} \sum_{i=1}^{n} \hat{\tilde{f}}_{j,ALE}(x_j^{(i)})$$

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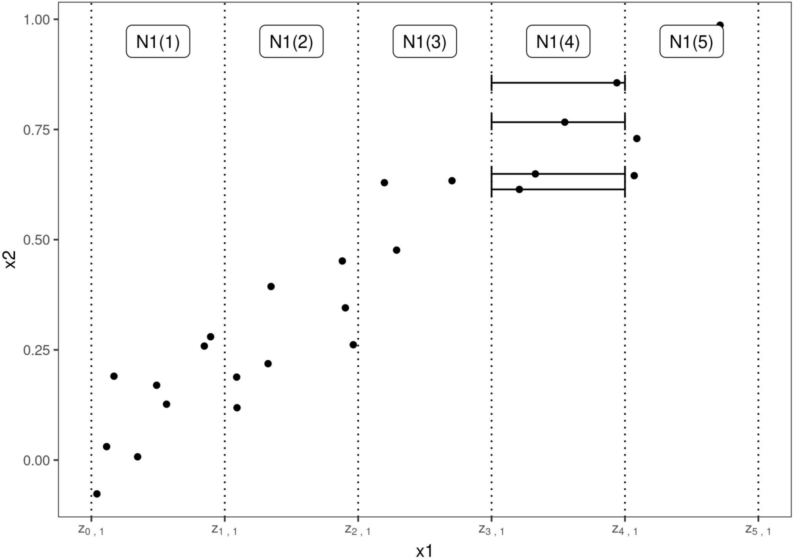
ALE Plots



Source: Molnar, Fig. 8.7

Accumulated Local Effects (ALE) Plot

Train model:

```
from sklearn.tree import DecisionTreeRegressor
regr=DecisionTreeRegressor(min_samples_leaf=10).fit(x,y)
```

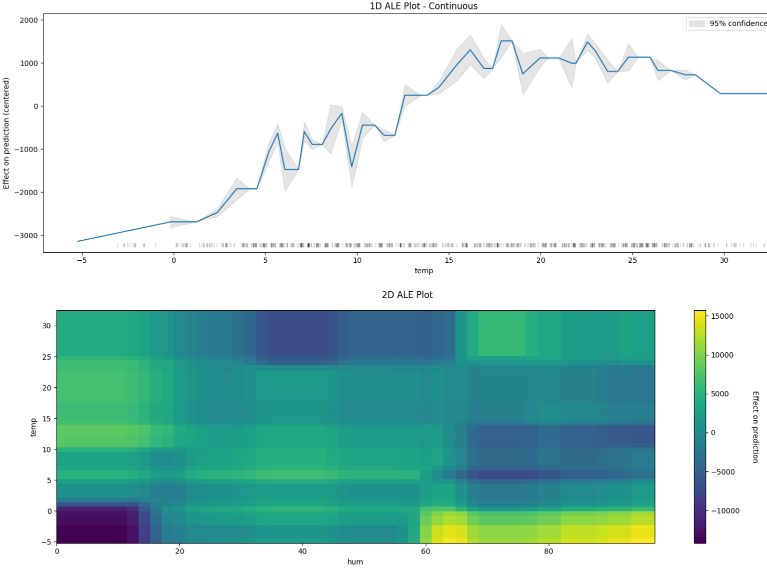
Construct the ALE and plot:

```
import matplotlib.pyplot as plt
from PyALE import ale
ale_effects = ale(X=x, model=regr, \
    feature=['temp'], grid_size=50, include_CI=True)
plt.show()
```

2D feature interactions:

```
ale_effects = ale(X=x, model=regr, \
    feature=['temp', 'hum'], grid_size=50)
plt.show()
```

Accumulated Local Effects (ALE) Plot



Permutation Feature Importance

Intuition

Calculate the increase in a model's prediction error when permuting a feature

1. Estimate model error on original data $e^{\text{orig}} = L(y, \hat{f}(X))$
2. For each feature j:
   - For each repetition k in $1 \cdots K$:
     - Generate $X^{\text{perm}}_{j,k}$ by permuting ("randomly shuffling") values of feature j
     - Estimate $e^{\text{perm}}_{j,k} = L(y, \hat{f}(X^{\text{perm}}_{j,k}))$
   - Calculate permutation feature importance as $i_j = e^{\text{orig}} - \frac{1}{K} \sum_k^K e^{\text{perm}}_{j,k}$

Calculate Permutation Feature Importance on *test* data

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Permutation Feature Importance

Prepare data:

```
import pandas as pd
d=pd.read_csv('https://evermann.ca/busi4720/bike.csv')
x=pd.get_dummies(d.drop(['yr','days_since_2011'],axis=1))
y=x.pop('cnt')
```

Train model:

```
from sklearn.tree import DecisionTreeRegressor
regr=DecisionTreeRegressor(min_samples_leaf=10).fit(x,y)
```

Calculate permutation feature importance and sort them:

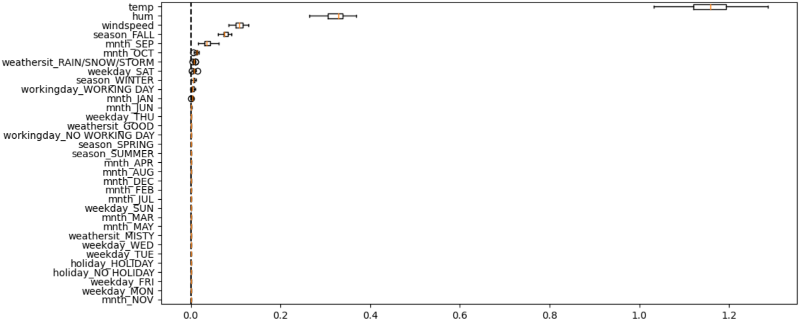
```
from sklearn.inspection import permutation_importance
r = permutation_importance(regr, x, y, n_repeats=30)
r_idx = r.importances_mean.argsort()
```

Permutation Feature Importance

Produce a nice plot of sorted feature importance:

```
import matplotlib.pyplot as plt
fig, ax = plt.subplots()
ax.boxplot(
    r.importances[r_idx].T,
    vert=False,
    labels=x.columns[r_idx])
ax.axvline(x=0, color="k", linestyle="--")
plt.show()
```

Permutation Feature Importance



Uncertainty due to multiple permutations (parameter `n_repeats`)

Global Surrogate Models

Intuition

Predict the predictions of a complex ”black box” model using an intrinsically interpretable model.

Example ”black box” model:

```
from sklearn.neural_network import MLPRegressor
regr = MLPRegressor((4, 2,), max_iter=10000)
regr.fit(x, y)
preds = regr.predict(x)
```

Interpretable, linear model to explain predictions:

```
from statsmodels.api import OLS
OLS(preds, x).fit().summary()
```

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Global Model Agnostic Methods – Summary

PDP/ICE	
Intuitive Clear interpretation Easy to implement	Limited number of features Assumes feature independence
ALE	
Unbiased for correlated features Clear interpretation Faster to compute than PDP	Local interpretation only ALE may differ from linear coefficients No ICE curves Unstable for large number of intervals
PFI	
Clear interpretation Concise, global measure Does not require retraining Takes into account all interactions	Linked to model error Requires access to true targets May be biased for correlated features
Global Surrogate Models	
Flexible Intuitive R-squared measure for fit	Conclusions about model, not data Unclear cut-off for goodness of fit

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Local Interpretable Model-Agnostic Explanations

Idea

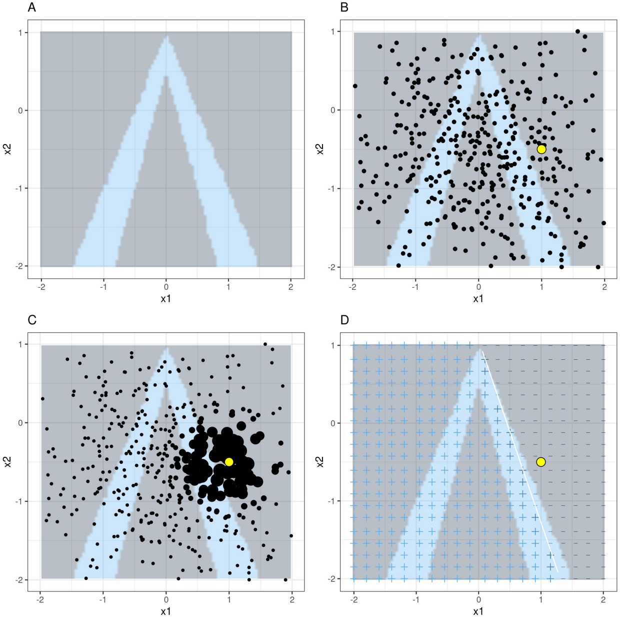
1. Choose an instance x of interest,
2. Sample instances around it, weight by distance kernel π_g,
3. Construct local interpretable model g
   - Minimize discrepancy $\mathcal{L}$ between g and black-box model f
   - Penalize by model complexity $\Omega(g)$

$$\xi(x) = \underset{g \in G}{\operatorname{argmin}} \ \mathcal{L}(f, g, \pi_x) + \Omega(g)$$

Method

1. Sample instances z_i' around x' (interpretable version of x)
2. Traing interpretable model on features z_i', targets $f(z_i)$ and weights $\pi_x(z_i)$ (z_i is the original version of z_i')

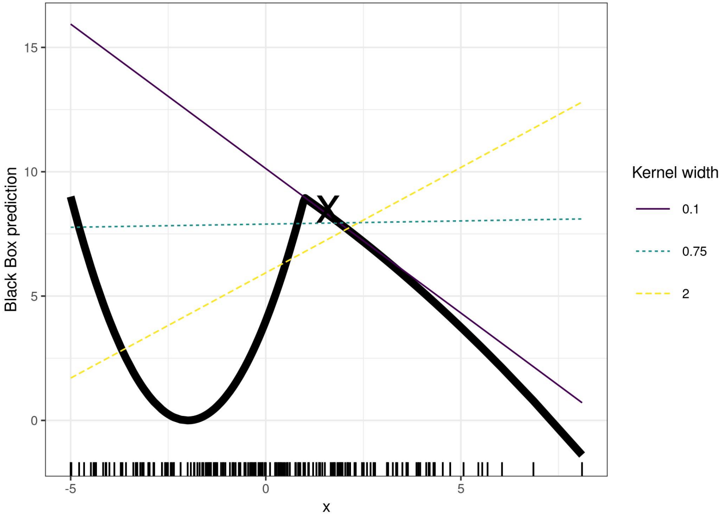
LIME – Example



Source: Molnar
Figure 9.5

LIME – Example

- Weight function π is often an exponential smoothing kernel
- Kernel width is critical determinant of explanation



Source: Molnar Figure 9.6

LIME – Example

Using a deep decision tree as ”black box”:

```
import sklearn.tree
dt = sklearn.tree.DecisionTreeClassifier(max_depth=8)
dt.fit(x, y)
```

Create the explainer:

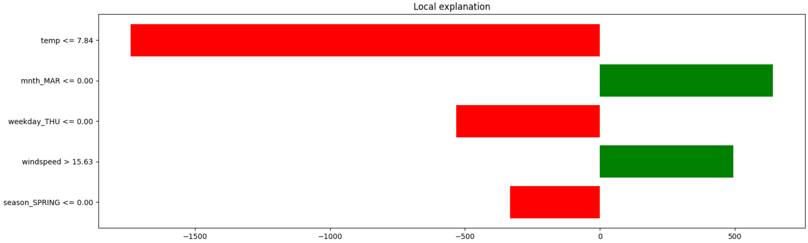
```
import lime, lime.lime_tabular
from sklearn.linear_model import Ridge

explainer = lime.lime_tabular.LimeTabularExplainer(
    x.to_numpy(),
    feature_names=x.columns,
    discretize_continuous = True,
    mode='regression',
    verbose=True)
```

LIME – Example

Explain instance number 5:

```
exp = explainer.explain_instance(
    x.to_numpy()[7],
    dt.predict,
    num_features=5,
    num_samples=1000,
    distance_metric='euclidean')
exp.as_list()
exp.as_pyplot_figure().show()
```



LIME for Images

LIME explanations for label ”bagel” and ”strawberries”:

Molnar, Figure 9.8

Python Examples:

https://github.com/marcotcr/lime

Paper:

https://arxiv.org/abs/1602.04938

Shapley Values

Motivation

How much does *feature value* x_j contribute to the overall prediction compared to the average prediction?

Game Theory

- Players cooperate in a coalition and receive a certain profit from this cooperation.
- Method for assigning payouts to players depending on their contribution to the total payout.

Shapley Values

$$\phi_i(v) = \frac{1}{n} \sum_{S \subseteq N \setminus \{i\}} \binom{n-1}{|S|}^{-1} [v(S \cup \{i\}) - v(S)]$$

- $v(S \cup \{i\}) - v(S)$: marginal contribution of player i to coalition of players S
- $\binom{n-1}{|S|}$: number of possible ways to form a coalition of size $|S|$ of the set $N \setminus \{i\}$ of $n-1$ players (set N without player i)

Shapley Value

Fairness Properties

- **Efficiency**: Contributions add up to total value
- **Symmetry**: If two players contribute equally to all possible coalitions, they have the same Shapley value
- **Dummy**: A player that does not contribute at all has a Shapley value of 0
- **Additivity**: For a game with combined payouts $v + w$, the Shapley values of players are $\phi^{(v)} + \phi^{(w)}$

Shapley Values in Interpretable ML

- Players are feature values
- Coalitions are combinations of feature values
- Presence in a coalition means we know the value
- Absence from a coalition means we don't know the value
  $\Rightarrow$ integrate/marginalize over all values of all features not in coalition S

$$v_x(S) = \int \cdots \int_{\mathbb{R}} \hat{f}(x_1, \ldots, x_p) d\mathbb{P}_{x \notin S} - E_x(\hat{f}(X))$$

- Expensive to compute $\Rightarrow$ in practice, approximation by sampling and permuting values (can make for unrealistic instances when features are correlated)

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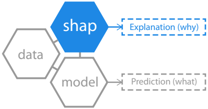
Shapley Additive Explanations (SHAP)



Paper

https://arxiv.org/abs/1705.07874

Documentation (Intro and Examples)

https://shap.readthedocs.io/en/latest/index.html

Python Code and Tutorials

https://github.com/shap/shap

SHAP Example

Fit a simple regression model to the California housing dataset:

```python
import sklearn
import shap

X, y = shap.datasets.california(n_points=1000)
model = sklearn.linear_model.LinearRegression()
model.fit(X, y)
```

Compute the SHAP values:

```python
X100 = shap.utils.sample(X, 100)
explainer = shap.Explainer(model.predict, X100)
shap_values = explainer(X)
```

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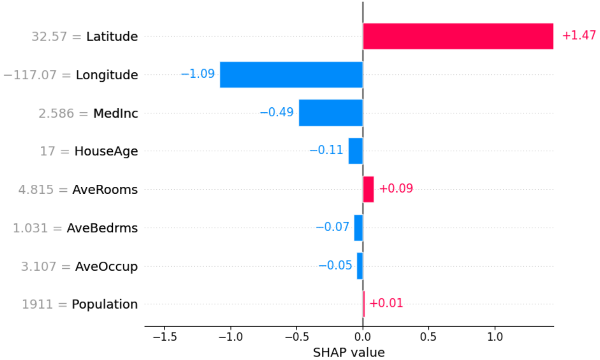
SHAP Example

The **barplot** shows the importance of feature values for an individual prediction:

```
shap.plots.bar(shap_values[20])
```



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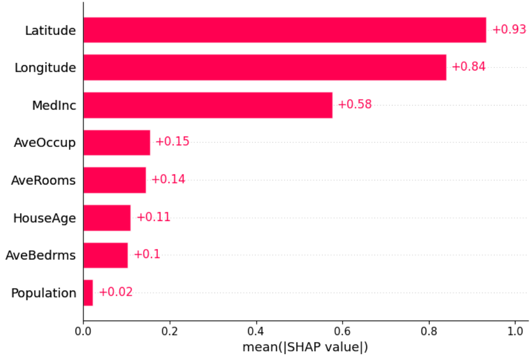
SHAP Example

The **barplot** can also show the importance of a feature by averaging over all instances (and their feature values):

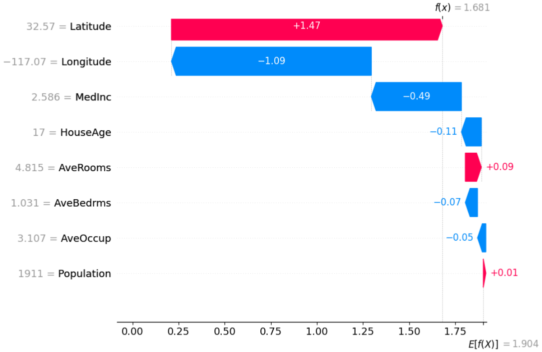
```
shap.plots.bar(shap_values)
```



SHAP Example

Waterfall plots explain how feature values combine to produce an individual prediction:

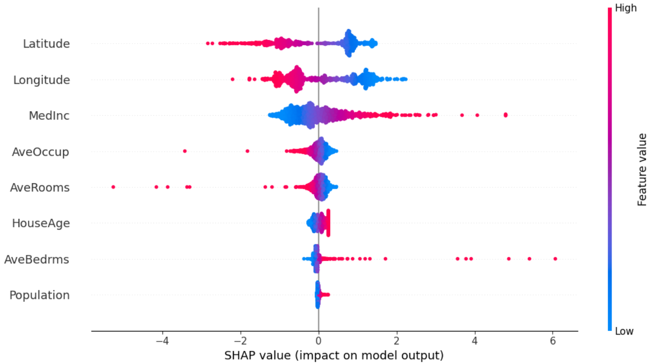
```
sha.plots.waterfall(shap_values[20], max_display=14)
```



SHAP Example

Beeswarm plots explain all feature values for all instances (represented by a dot):

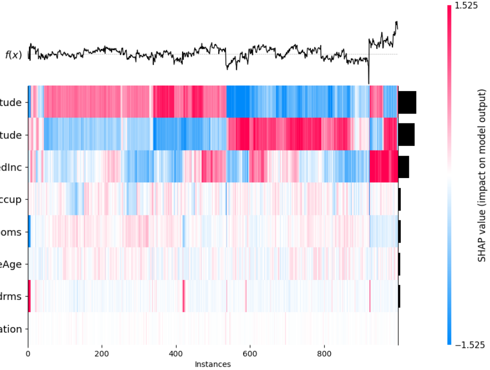
```
shap.plots.beeswarm(shap_values)
```



SHAP Example

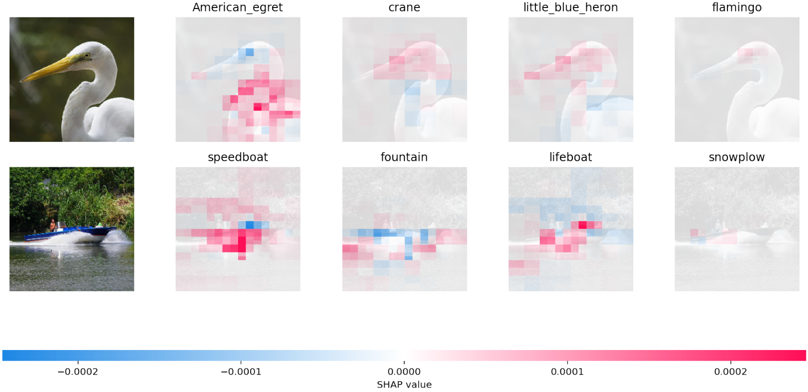
The **heatmap** shows SHAP values of feature values for all instances, and shows model prediction and global feature importance in rugs:

```
shap.plots.heatmap(shap_values)
```



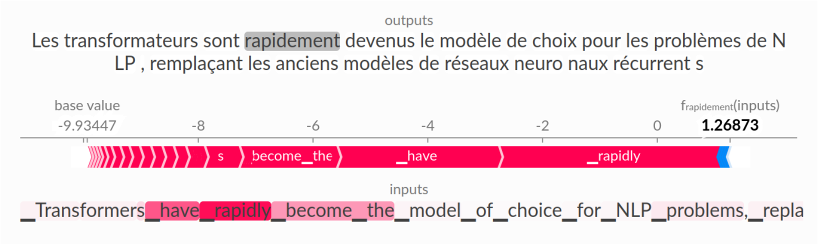
SHAP for Image Classification

- Presence/absence of features/pixels by masking parts of an image:



Source: `https://github.com/shap` (MIT License)

SHAP for Text Classification



Source: `https://shap.readthedocs.io/en/latest/text_examples.html` (MIT License)