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How to interpret model prediction using interpretability tools on Azure Machine Learning?

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Session goals

- In this level 100 session, you will learn:
  - Why ML Interpretability is important,
  - An overview of SHAP, one of the most robust methods for ML Interpretability,
  - How to apply Azure Machine Learning Interpret tools for:
    - Regression use case – Tabular data,
    - Generic image classification use case,
  - Limitations of Azure Machine Learning Interpret tools.

Why ML Interpretability is important? What vs. Why?

- Modern ML techniques have enabled us to develop highly accurate models [the "What" question]
  - These generate very complex models which are often difficult to understand.
- For many high-stakes applications, understanding of these "black box" models are essential to gain the trust of stakeholders [the "Why" question]
  - This determines the success of the project, without which it is almost impossible to deploy these models into production.
- ML Interpretability addresses the trade-off between the "What" and the "Why"
  - Use complex model with high confidence.

What do we expect from a ML Interpretability tool?

From interpretably module, we will learn:

- Global point of view: From all the features in the model, which are most important.
- Local point of view: For any single prediction from a model, the marginal contribution of each feature in the data on that instance of prediction.

Why SHAP?

Here, we will learn about SHAP (**SH**apley **A**dditive **E**xplanation):

- Based on Shapley, from coalitional game theory,
- Mathematically very sound and robust,
- Provides both local and global explanation,
- Model agnostic,
- Can be applied to any type of data,
- Integrated within Azure Machine Learning Interpretability toolkit.

Intuition

For this data, this is “fit” from ML:

Black Box ML: $y = f(x_1, x_2)$

y	x_1	x_2
1	-1	1
14	1	4
1	2	-1
11	4	1
4	-1	2
-1	1	-1

Intuition

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How to break down the target between features?

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Black Box ML: $y = f(x_1, x_2)$

How to break down the target between features?

$$y = f(x_1, x_2) = 2x_1 + 3x_2$$

y	x_1	x_2	I_{x_1}	I_{x_2}
1	-1	1	-2	3
14	1	4	2	12
1	2	-1	4	-3
11	4	1	8	3
4	-1	2	-2	6
-1	1	-1	2	-3

Intuition

For this data, this is “fit” from ML:

Black Box ML: $y = f(x_1, x_2)$

How to break down the target between features?

$$y = f(x_1, x_2) = 2x_1 + 3x_2$$

- For instance i of the data (row i) the effect of $x_{1,i}$ on y_i is $2x_{1,i}$
- For instance i of the data (row i) the effect of $x_{2,i}$ on y_i is $3x_{2,i}$

y	x_1	x_2	I_{x_1}	I_{x_2}
1	-1	1	-2	3
14	1	4	2	12
1	2	-1	4	-3
11	4	1	8	3
4	-1	2	-2	6
-1	1	-1	2	-3

Intuition

- We know the "effect" of each feature for each instance of data.
- Which feature is "more" important?

y	x_1	x_2	I_{x_1}	I_{x_2}
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Local view: For some instances, x_1 has bigger impact and for others x_2 has bigger impact.

Intuition

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- Which feature is “more” important?

<u>Local view:</u> For some instances, x_1 has bigger impact and for others x_2 has bigger impact.

How about **<u>global view</u>**?

y	x_1	x_2	I_{x_1}	I_{x_2}
1	-1	1	-2	3
14	1	4	2	12
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Intuition

- We know the "effect" of each feature for each instance of data.
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How about **global view**?

y	x_1	x_2	I_{x_1}	I_{x_2}
1	-1	1	-2	3
14	1	4	2	12
1	2	-1	4	-3
11	4	1	8	3
4	-1	2	-2	6
-1	1	-1	2	-3

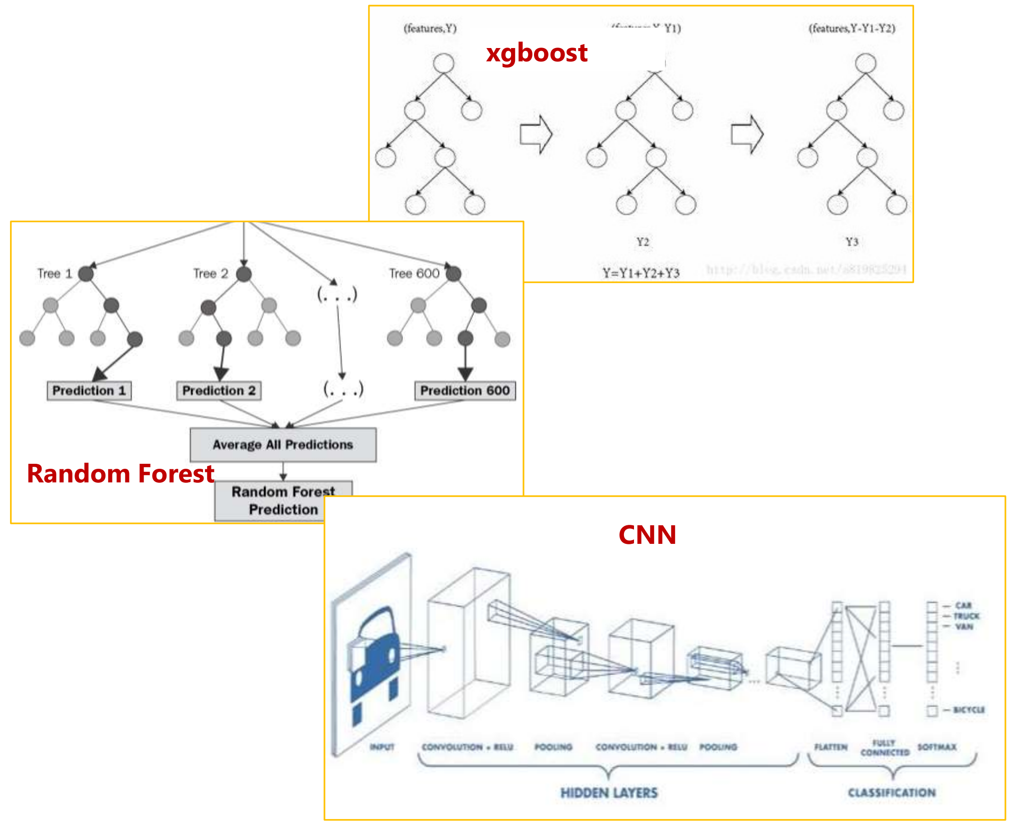
$$\mathrm{x}_{1,\mathrm{total}} = \frac{\sum \left|I_{x_{1,i}}\right|}{N} = \frac{20}{6} = 3.34$$

$$\mathrm{x}_{2,\mathrm{total}} = \frac{\sum \left|I_{x_{2,i}}\right|}{N} = \frac{30}{6} = 5$$

Globally, in this space, $-1 \leq x_1 \leq 4$ & $-1 \leq x_2 \leq 4$, x_2, comparing to x_1, is more important.

How about more complex models?

- How to answer these questions for a more complex ML model?
  - For any single prediction from a model, what is the **"fair"** contribution of each feature?
  - Which features in the model are more "important"?
- SHAP provides answers to both questions and "sheds light" on "black box" models.



Shapley Values

- The goal of SHAP is to explain the prediction of an instance, by computing the marginal contribution of each feature to the prediction.

- The SHAP explanation method computes Shapley values from coalitional game theory
  - The **feature** values of a data instance act as **players** in a coalition.
  - Shapley values tell us how to fairly distribute the "**payout**" (= the **prediction**) among all the features.

Target Space dim $N \times 1$

Feature Space dim $N \times M$

game	score	A	B	…	C
1	y_1	x_{11}	x_{12}	.	x_{1M}
2	y_2	x_{21}	x_{22}	.	x_{2M}
3	y_3	x_{31}	x_{32}	.	x_{3M}
4	y_4	x_{41}	x_{42}	.	x_{4M}
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
N	y_N	x_{N1}	x_{N2}	.	x_{NM}

Coalitional Game Theory

- Suppose we have a game with 3 players, A, B, C and they have scored Y for a given game,
- Supposed we have trained a model, F, to predict target, Y,
- Let's see how to estimate "marginal" contribution of player (i.e. feature) A to score (i.e. target) Y for game i, based on coalition game theory, **this is the Shapley value of A for instance i**

game	score	A	B	C
i	Y	$\boldsymbol{A}$	B	C

Coalitional Game Theory

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Coalition Exclude A	Target Estimation Exclude A
$\emptyset$	$\mathrm{F}(\emptyset)$
B	$\mathrm{F}(B)$
C	$\mathrm{F}(C)$
B, C	$\mathrm{F}(B, C)$

game	score	A	B	C
i	Y	$\boldsymbol{A}$	B	C

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game	score	A	B	C
i	Y	$\boldsymbol{A}$	B	C

Coalition Exclude A	Target Estimation Exclude A	Coalition Include A	Target Estimation Include A
$\emptyset$	$\mathrm{F}(\emptyset)$	A	$\mathrm{F}(A)$
B	$\mathrm{F}(B)$	A, B	$\mathrm{F}(A, B)$
C	$\mathrm{F}(C)$	A, C	$\mathrm{F}(A, C)$
B, C	$\mathrm{F}(B, C)$	A, B, C	$\mathrm{F}(A, B, C)$

Coalitional Game Theory

- Suppose we have a game with 3 players, A, B, C and they have scored Y for a given game,
- Supposed we have trained a model, F, to predict target, Y,
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game	score	A	B	C
i	Y	$\boldsymbol{A}$	B	C

Coalition Exclude A	Target Estimation Exclude A	Coalition Include A	Target Estimation Include A	Difference in Target Estimation
$\emptyset$	$\mathrm{F}(\emptyset)$	A	$\mathrm{F}(A)$	$\mathrm{F}(A) - \mathrm{F}(\emptyset)$
B	$\mathrm{F}(B)$	A, B	$\mathrm{F}(A, B)$	$\mathrm{F}(A, B) - \mathrm{F}(B)$
C	$\mathrm{F}(C)$	A, C	$\mathrm{F}(A, C)$	$\mathrm{F}(A, C) - \mathrm{F}(C)$
B, C	$\mathrm{F}(B, C)$	A, B, C	$\mathrm{F}(A, B, C)$	$\mathrm{F}(A, B, C) - \mathrm{F}(B, C)$

Coalitional Game Theory

game	score	A	B	C
i	Y	A	B	C

Coalition Exclude A	Target Estimation Exclude A	Coalition Include A	Target Estimation Include A	Difference in Target Estimation	weight
$\emptyset$	$\mathrm{F}(\emptyset)$	A	$\mathrm{F}(A)$	$\mathrm{F}(A) - \mathrm{F}(\emptyset)$	1/3
B	$\mathrm{F}(B)$	A, B	$\mathrm{F}(A, B)$	$\mathrm{F}(A, B) - \mathrm{F}(B)$	1/6
C	$\mathrm{F}(C)$	A, C	$\mathrm{F}(A, C)$	$\mathrm{F}(A, C) - \mathrm{F}(C)$	1/6
B, C	$\mathrm{F}(B, C)$	A, B, C	$\mathrm{F}(A, B, C)$	$\mathrm{F}(A, B, C) - \mathrm{F}(B, C)$	1/3

Shapley value of A for instance i is the weighted average of marginal contributions for all the coalitions:

$$\frac{|S|!\,(N-|S|-1)!}{N!}$$

$$\frac{1}{3}\big(\mathrm{F}(A) - \mathrm{F}(\emptyset)\big) + \frac{1}{6}\big(\mathrm{F}(A, B) - \mathrm{F}(B)\big) + \frac{1}{6}\big(\mathrm{F}(A, C) - \mathrm{F}(C)\big) + \frac{1}{3}\big(\mathrm{F}(A, B, C) - \mathrm{F}(B, C)\big)$$

Robustness

$$\varphi_i(v) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!\,(N - |S| - 1)!}{N!} (v(S \cup \{i\}) - v(S))$$

The Shapley value is the only method that meets the criteria for a “fair” payout for each player (feature):

- **Efficiency:** sum of the Shapley values for all features in each instance, equals to the total coalition value, i.e. difference between prediction, and expected value.
- **Symmetry:** all features have a fair chance to join the game, i.e. if two instances of a feature contribute equally to all possible collations, the Shapley values are the same.
- **Dummy:** if a feature has no contribution to any coalition, then the Shapley value of that feature is zero.
- **Additivity:** the combined Shapley values of any pair of games, is the sum of the Shapley values of each game, $\varphi(v + v') = \varphi(v) + \varphi(v')$

What about SHAP?

- The disadvantage of using Shapley values is that it is computationally very expensive,
  - For M features and N observation, to calculate the entire Shapley values "matrix", we have $\mathrm{N} \times 2^M$ possible coalitions.
  - Plus, the absence of a feature in each coalition must be "simulated" by drawing random instances.
- What SHAP brings to the table, is to address these issues.

Target Space
dim $N \times 1$

Feature Space
dim $N \times M$

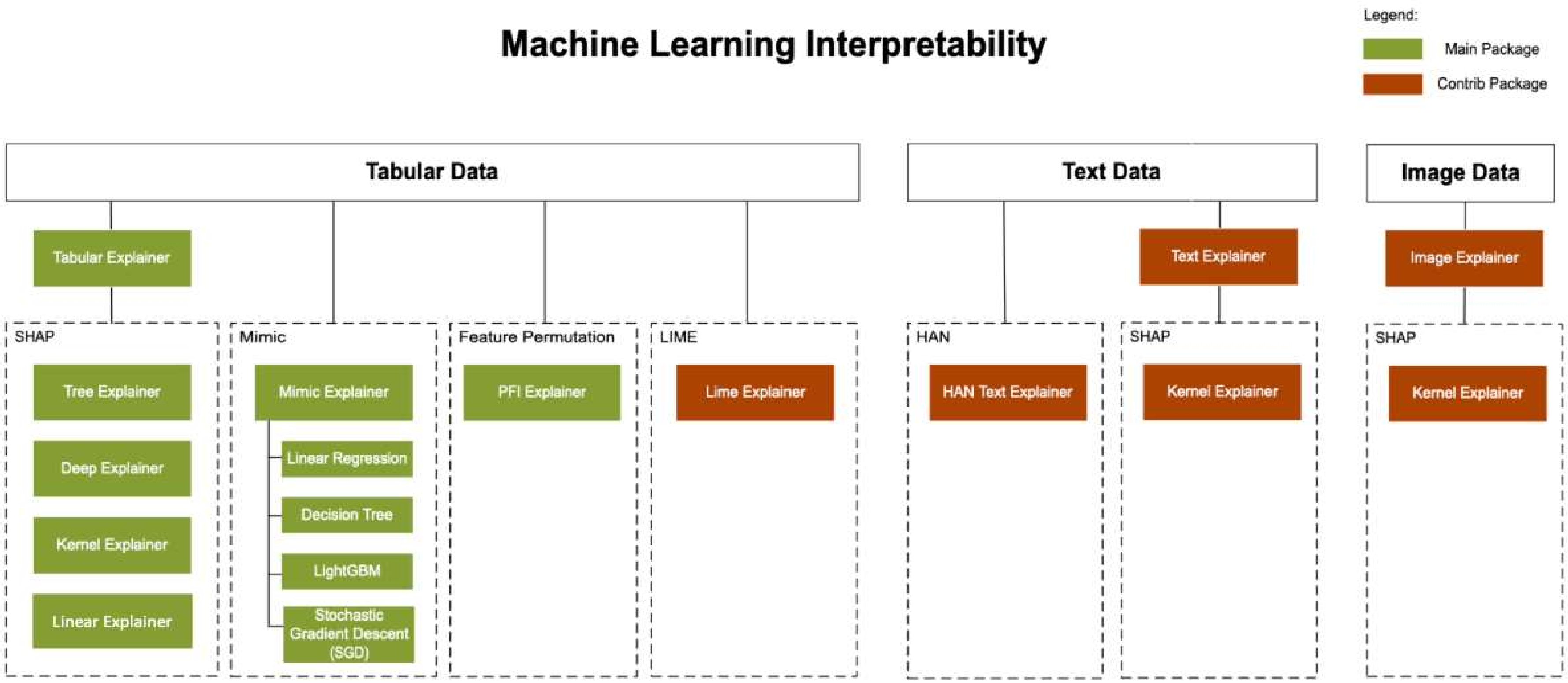
game	score	A	B	...	C
1	y_1	x_{11}	x_{12}	.	x_{1M}
2	y_2	x_{21}	x_{22}	.	x_{2M}
3	y_3	x_{31}	x_{32}	.	x_{3M}
4	y_4	x_{41}	x_{42}	.	x_{4M}
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
N	y_N	x_{N1}	x_{N2}	.	x_{NM}

How SHAP helps with computational overhead?

SHAP optimizes the number of coalitions based on different scenarios:

1. LinearExplainer:
   - For linear models.
2. TreeExplainer:
   - Tree-based models,
   - This relaxes the dependency to background data,
   - Reduces the complexity space from $O(TL2^M)$ to $O(TLD^2)$.
3. KernelExplainer:
   - Model agnostic,
   - Reduces the complexity space from 2^M to $2M + 2048$, based on weights in Shapley formula,
   - Missing features are simulated from background data.
4. DeepExplainer:
   - This is a high-speed approximation algorithm for SHAP values in deep learning models.

Azure Machine Learning-Interpret



Overview of different methods in AML-interpret

SHAP
- Both local and global interpretability
- Can be applied to any type of data
- Both model agnostic and model specific tools
- Provides marginal contribution of features to prediction of target
- Incorporates the interactions between features

Mimic
- Both local and global interpretability
- Model agnostic, based on global surrogate models
- Approximate explanation
- Applicable to tabular data
- Provides marginal contribution of features to prediction of target
- Incorporates the interactions between features

Feature permutation
- Provides global explanation
- Model agnostic
- Univariate model explanation
- Applicable to tabular data
- Provides explanation based on the effect of the feature on model performance

LIME
- Provide local interpretability
- Model agnostic
- Applicable to tabular and image data

Demo

Notebooks

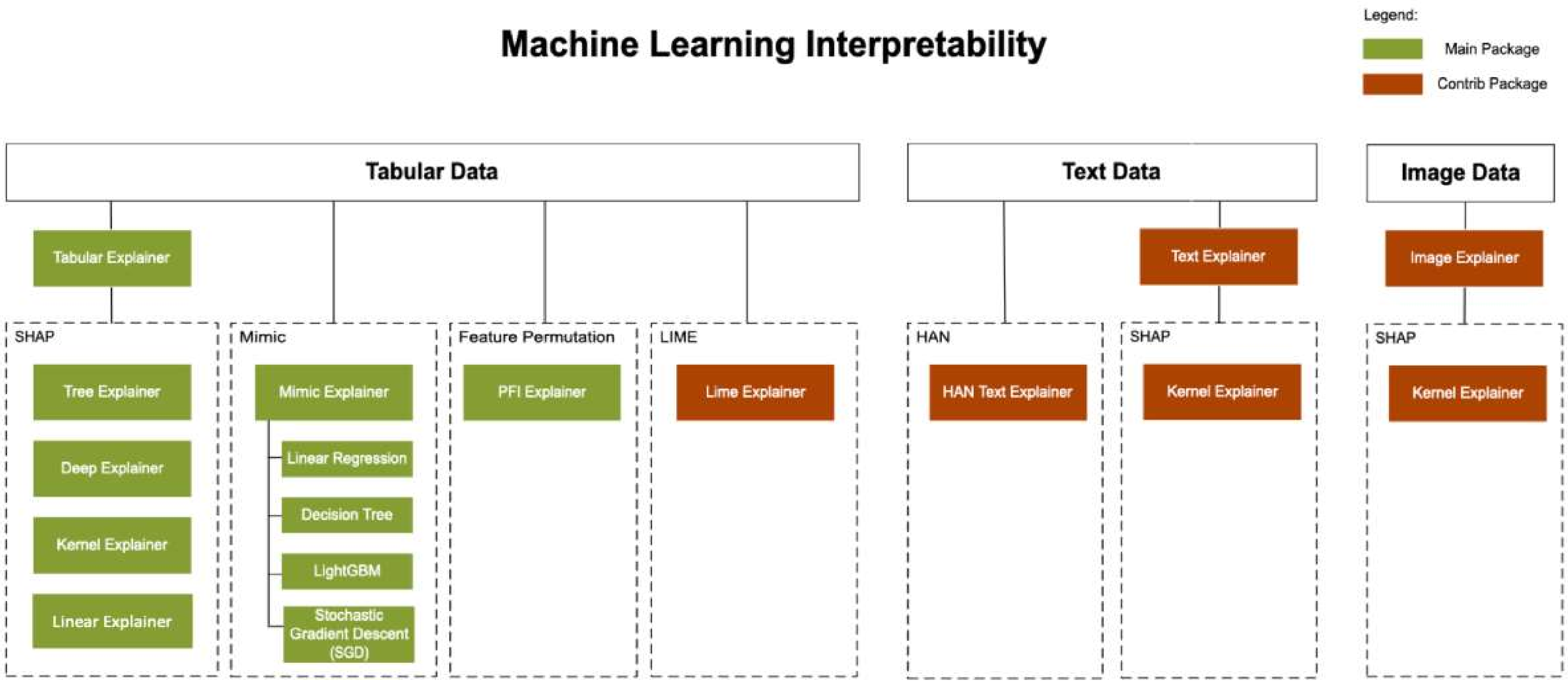
1. Regression use case using Azure ML Interpret
2. Image classification using Azure ML Interpret
3. ~~Image classification using OSS SHAP~~

Session Goals

- Why interpretability is important.
- SHAP, one of the most robust tools for ML interpretability:
  - is applicable to any type of model,
  - is applicable to any type of data,
  - provides both local and global interpretability.
- How to apply Azure Machine Learning Interpret tools for:
  - A regression use case,
  - A generic image classification use cases:
    - Explain on super-pixels from azureml toolkit,
- Limitations of Azure Machine Learning Interpret tools and work-arounds
- Notebooks are available for future reference
  https://github.com/microsoft/AML_Interpret_usecases

Reference 1
Reference 2

Azure Machine Learning-Interpret



Q&A

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