



# **Tractability and Optimization of Shap-Score Computation for Explainable Al**

Leopoldo Bertossi

Dagstuhl, January 2024

www.scs.carleton.ca/~bertossi

(日) (部) (目) (日) 크

• Bank client **e** = (john, 18, plumber, 70K, harlem, ...)

As an entity represented as a record of values for features Name, Age, Activity, Income, ...

• Bank client **e** = (john, 18, plumber, 70K, harlem, ...)

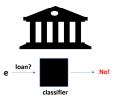
As an entity represented as a record of values for features Name, Age, Activity, Income, ...

• e requests a loan from a bank that uses a classifier

• Bank client **e** = (john, 18, plumber, 70K, harlem, ...)

As an entity represented as a record of values for features Name, Age, Activity, Income, ...

• e requests a loan from a bank that uses a classifier

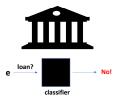


• Bank client  $\mathbf{e} = \langle \mathsf{john}, 18, \mathsf{plumber}, 70\mathsf{K}, \mathsf{harlem}, \ldots \rangle$ 

As an entity represented as a record of values for features Name, Age, Activity, Income, ...

• e requests a loan from a bank that uses a classifier

• The client asks *Why*?



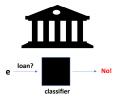
• Bank client  $\mathbf{e} = \langle \mathsf{john}, 18, \mathsf{plumber}, 70\mathsf{K}, \mathsf{harlem}, \ldots \rangle$ 

As an entity represented as a record of values for features Name, Age, Activity, Income, ...

• e requests a loan from a bank that uses a classifier

- The client asks *Why*?
- What kind of *explanation*? How?

From what?



• Explanations come in different forms

- Explanations come in different forms
- Some of them are *causal explanations*, some are *explanation scores* a.k.a. *attribution scores*

- Explanations come in different forms
- Some of them are *causal explanations*, some are *explanation scores* a.k.a. *attribution scores*
- They are sometimes related
  - E.g. actual causality leads to responsibility scores

- Explanations come in different forms
- Some of them are *causal explanations*, some are *explanation scores* a.k.a. *attribution scores*
- They are sometimes related

E.g. actual causality leads to responsibility scores

• Large part of our recent research is about the use of causality, and score definition and computation

In data management and machine learning

- Explanations come in different forms
- Some of them are *causal explanations*, some are *explanation scores* a.k.a. *attribution scores*
- They are sometimes related

E.g. actual causality leads to responsibility scores

 Large part of our recent research is about the use of causality, and score definition and computation

In data management and machine learning

- Some of them (in data management or ML)
  - Responsibility (in its original and generalized versions)
  - The Causal Effect score
  - The Shapley value (as Shap in ML)

(ロ) (同) (E) (E) (E) (0)(0)

• Based on the general Shapley value

- Based on the general Shapley value
- Set of players  ${\mathcal F}$  contain features, relative to classified entity  ${\boldsymbol e}$

- Based on the general Shapley value
- Set of players  ${\mathcal F}$  contain features, relative to classified entity  ${\bf e}$
- We need an appropriate e-dependent game function that maps (sub)sets of players to real numbers

- Based on the general Shapley value
- Set of players  ${\mathcal F}$  contain features, relative to classified entity  ${\boldsymbol e}$
- We need an appropriate e-dependent game function that maps (sub)sets of players to real numbers
- For  $S \subseteq \mathcal{F}$ , and  $\mathbf{e}_S$  the projection of  $\mathbf{e}$  on S:  $\mathcal{G}_{\mathbf{e}}(S) := \mathbb{E}(L(\mathbf{e}') \mid \mathbf{e}' \in \mathcal{E} \& \mathbf{e}'_S = \mathbf{e}_S)$

- Based on the general Shapley value
- Set of players  ${\mathcal F}$  contain features, relative to classified entity  ${\boldsymbol e}$
- We need an appropriate e-dependent game function that maps (sub)sets of players to real numbers
- For  $S \subseteq \mathcal{F}$ , and  $\mathbf{e}_S$  the projection of  $\mathbf{e}$  on S:  $\mathcal{G}_{\mathbf{e}}(S) := \mathbb{E}(L(\mathbf{e}') \mid \mathbf{e}' \in \mathcal{E} \& \mathbf{e}'_S = \mathbf{e}_S)$
- For a feature  $F^{\star} \in \mathcal{F}$ , compute:  $Shap(\mathcal{F}, \mathcal{G}_{e}, F^{\star})$

$$\sum_{S\subseteq \mathcal{F}\setminus\{F^{\star}\}} \frac{|S|!(|\mathcal{F}|-|S|-1)!}{|\mathcal{F}|!} [\underbrace{\mathbb{E}(L(\mathbf{e}'|\mathbf{e}'_{S\cup\{F^{\star}\}}=\mathbf{e}_{S\cup\{F^{\star}\}})}_{\mathcal{G}_{\mathbf{e}}(S\cup\{F^{\star}\})} - \underbrace{\mathbb{E}(L(\mathbf{e}')|\mathbf{e}'_{S}=\mathbf{e}_{S})}_{\mathcal{G}_{\mathbf{e}}(S)}]$$

- Based on the general Shapley value
- Set of players  $\mathcal F$  contain features, relative to classified entity  ${\bf e}$
- We need an appropriate e-dependent game function that maps (sub)sets of players to real numbers
- For  $S \subseteq \mathcal{F}$ , and  $\mathbf{e}_S$  the projection of  $\mathbf{e}$  on S:  $\mathcal{G}_{\mathbf{e}}(S) := \mathbb{E}(L(\mathbf{e}') \mid \mathbf{e}' \in \mathcal{E} \& \mathbf{e}'_S = \mathbf{e}_S)$
- For a feature  $F^{\star} \in \mathcal{F}$ , compute:  $Shap(\mathcal{F}, \mathcal{G}_{e}, F^{\star})$

$$\sum_{S\subseteq \mathcal{F}\setminus\{F^{\star}\}} \frac{|S|!(|\mathcal{F}|-|S|-1)!}{|\mathcal{F}|!} [\underbrace{\mathbb{E}(L(\mathbf{e}'|\mathbf{e}'_{S\cup\{F^{\star}\}}=\mathbf{e}_{S\cup\{F^{\star}\}})}_{\mathcal{G}_{\mathbf{e}}(S\cup\{F^{\star}\})} - \underbrace{\mathbb{E}(L(\mathbf{e}')|\mathbf{e}'_{S}=\mathbf{e}_{S})}_{\mathcal{G}_{\mathbf{e}}(S)}]$$

• Shap score has become popular

(Lee & Lundberg, 2017)

- Based on the general Shapley value
- Set of players  ${\mathcal F}$  contain features, relative to classified entity  ${\boldsymbol e}$
- We need an appropriate e-dependent game function that maps (sub)sets of players to real numbers
- For  $S \subseteq \mathcal{F}$ , and  $\mathbf{e}_S$  the projection of  $\mathbf{e}$  on S:

$$\mathcal{G}_{\mathbf{e}}(S) := \mathbb{E}(L(\mathbf{e}') \mid \mathbf{e}' \in \mathcal{E} \& \mathbf{e}'_S = \mathbf{e}_S)$$

• For a feature  $F^{\star} \in \mathcal{F}$ , compute:  $Shap(\mathcal{F}, \mathcal{G}_{e}, F^{\star})$ 

$$\sum_{S\subseteq \mathcal{F}\setminus\{F^{\star}\}} \frac{|S|!(|\mathcal{F}|-|S|-1)!}{|\mathcal{F}|!} [\underbrace{\mathbb{E}(L(\mathbf{e}'|\mathbf{e}'_{S\cup\{F^{\star}\}}=\mathbf{e}_{S\cup\{F^{\star}\}})}_{\mathcal{G}_{\mathbf{e}}(S\cup\{F^{\star}\})} - \underbrace{\mathbb{E}(L(\mathbf{e}')|\mathbf{e}'_{S}=\mathbf{e}_{S})}_{\mathcal{G}_{\mathbf{e}}(S)}]$$

• *Shap* score has become popular

(Lee & Lundberg, 2017)

◆□ ▶ ◆□ ▶ ◆ □ ▶ ◆ □ ▶ ● □ ● ● ● ●

• Assumes a probability distribution on entity population

Shap computation is #P-hard in general

Shap computation is #P-hard in general

• Can we do better with an open-box classifier?





Exploiting its elements and internal structure?

Shap computation is #P-hard in general

• Can we do better with an open-box classifier?





Exploiting its elements and internal structure?

• What if we have a decision tree, or a random forest, or a Boolean circuit?

Shap computation is #P-hard in general

• Can we do better with an open-box classifier?





Exploiting its elements and internal structure?

- What if we have a decision tree, or a random forest, or a Boolean circuit?
- Can we compute Shap in polynomial time?

#### **Tractability for BC-Classifiers**

• We investigated this problem in detail<sup>1</sup>

<sup>&</sup>lt;sup>1</sup>Arenas, Bertossi, Barcelo, Monet; AAAI'21; JMLR'23

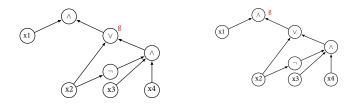
### **Tractability for BC-Classifiers**

- We investigated this problem in detail<sup>1</sup>
- <u>Theorem:</u> Shap can be computed in polynomial time for dDBCs under the uniform distribution

<sup>&</sup>lt;sup>1</sup>Arenas, Bertossi, Barcelo, Monet; AAAI'21; JMLR'23

#### **Tractability for BC-Classifiers**

- We investigated this problem in detail<sup>1</sup>
- <u>Theorem:</u> Shap can be computed in polynomial time for dDBCs under the uniform distribution
- Can be extended to a product distribution on  $\mathcal{E} = \{0, 1\}^N$



<sup>&</sup>lt;sup>1</sup>Arenas, Bertossi, Barcelo, Monet; AAAI'21; JMLR'23

• <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for

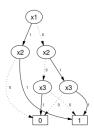
- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)

- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

Compatible variable orders along full paths

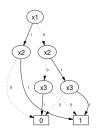
Compact representation of Boolean formulas



- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

Compatible variable orders along full paths

Compact representation of Boolean formulas



- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

Compatible variable orders along full paths

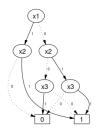
Compact representation of Boolean formulas

- Deterministic-decomposable negation normal-form (dDNNFs) As dDBC, with negations affecting only input variables

- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

Compatible variable orders along full paths

Compact representation of Boolean formulas

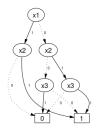


- Deterministic-decomposable negation normal-form (dDNNFs) As dDBC, with negations affecting only input variables
- All the latter relevant in Knowledge Compilation

- <u>Corollary</u>: Via polynomial time transformations, under the uniform and product distributions, *Shap* can be computed in polynomial time for
  - Decision trees (and random forests)
  - Ordered binary decision diagrams (OBDDs)

Compatible variable orders along full paths

Compact representation of Boolean formulas



- Deterministic-decomposable negation normal-form (dDNNFs) As dDBC, with negations affecting only input variables
- All the latter relevant in Knowledge Compilation
- An optimized efficient algorithm for *Shap* computation can be applied to any of these

## Shap on Neural Networks

• Binary Neural Networks (BNNs) are commonly considered black-box models

## Shap on Neural Networks

- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex

## Shap on Neural Networks

- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex
- Better try to compile the BNN into an open-box BC where *Shap* can be computed efficiently

- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex
- Better try to compile the BNN into an open-box BC where *Shap* can be computed efficiently
- We have experimented with Shap computation with a black-box BNN and with its compilation into a dDBC<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>Bertossi, Leon; JELIA'23

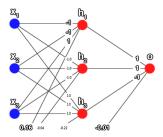
- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex
- Better try to compile the BNN into an open-box BC where *Shap* can be computed efficiently
- We have experimented with Shap computation with a black-box BNN and with its compilation into a dDBC<sup>2</sup>
- Even if the compilation is not entirely of polynomial time, it may be worth performing this one-time computation

- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex
- Better try to compile the BNN into an open-box BC where *Shap* can be computed efficiently
- We have experimented with Shap computation with a black-box BNN and with its compilation into a dDBC<sup>2</sup>
- Even if the compilation is not entirely of polynomial time, it may be worth performing this one-time computation
- Particularly if the target dDBC will be used multiple times, as is the case for explanations

<sup>&</sup>lt;sup>2</sup>Bertossi, Leon; JELIA'23

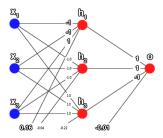
- Binary Neural Networks (BNNs) are commonly considered black-box models
- Naively computing Shap on a BNN is bound to be complex
- Better try to compile the BNN into an open-box BC where *Shap* can be computed efficiently
- We have experimented with Shap computation with a black-box BNN and with its compilation into a dDBC<sup>2</sup>
- Even if the compilation is not entirely of polynomial time, it may be worth performing this one-time computation
- Particularly if the target dDBC will be used multiple times, as is the case for explanations
- We illustrate the approach by means of an example

<sup>&</sup>lt;sup>2</sup>Bertossi, Leon; JELIA'23



$$\begin{array}{lll} \phi_g(\bar{i}) & = & sp(\bar{w}_g \bullet \bar{i} + b_g) \\ & := & \left\{ \begin{array}{ll} 1 & \text{if } \bar{w}_g \bullet \bar{i} + b_g \geq 0, \\ -1 & \text{otherwise}, \end{array} \right. \end{array}$$

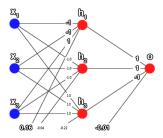
<ロト < 回 ト < 巨 ト < 巨 ト < 巨 ト ミ の < で 9/13



$$\begin{split} \phi_g(\bar{i}) &= sp(\bar{w}_g \bullet \bar{i} + b_g) \\ &:= \begin{cases} 1 & \text{if } \bar{w}_g \bullet \bar{i} + b_g \geq 0, \\ -1 & \text{otherwise}, \end{cases} \end{split}$$

 The BNN is described by a propositional formula, which is further transformed and optimized into CNF

$$\begin{array}{l} \longleftrightarrow (-[(x_3 \wedge (x_2 \vee x_1)) \vee (x_2 \wedge x_1)] \wedge \\ ([(-x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)] \vee \\ (x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)])) \vee \\ ([(-x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)] \wedge \\ ((x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)]). \end{array}$$



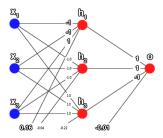
$$\begin{array}{lll} \phi_{\mathcal{G}}(\bar{i}) & = & sp(\bar{w}_{\mathcal{G}} \bullet \bar{i} + b_{\mathcal{G}}) \\ & := & \left\{ \begin{array}{ll} 1 & \text{if } \bar{w}_{\mathcal{G}} \bullet \bar{i} + b_{\mathcal{G}} \geq 0, \\ -1 & \text{otherwise}, \end{array} \right. \end{array}$$

 The BNN is described o <
by a propositional
formula, which is further
transformed and
optimized into CNF

$$\begin{array}{l} \longrightarrow (-[(x_3 \land (x_2 \lor x_1)) \lor (x_2 \land x_1)] \land \\ ([(-x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)] \lor \\ [(x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)])) \lor \\ ([(-x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)] \land \\ [(x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)]). \end{array}$$

• Done using always CNFs and keeping them "short" ...

(room for optimizations)



$$\begin{array}{lll} \phi_{\mathcal{G}}(\bar{i}) & = & sp(\bar{w}_{\mathcal{G}} \bullet \bar{i} + b_{\mathcal{G}}) \\ & := & \left\{ \begin{array}{ll} 1 & \text{if } \bar{w}_{\mathcal{G}} \bullet \bar{i} + b_{\mathcal{G}} \geq 0, \\ -1 & \text{otherwise}, \end{array} \right. \end{array}$$

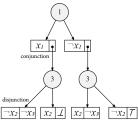
 The BNN is described or by a propositional formula, which is further transformed and optimized into CNF

$$\begin{array}{l} \longmapsto (-[(x_3 \land (x_2 \lor x_1)) \lor (x_2 \land x_1)] \land \\ ([(-x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)] \lor \\ [(x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)])) \lor \\ ([(-x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)] \land \\ [(x_3 \land (-x_2 \lor -x_1)) \lor (-x_2 \land -x_1)]). \end{array}$$

• Done using always CNFs and keeping them "short" ... (room for optimizations)

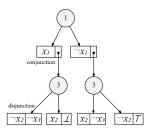
• In CNF: 
$$o \leftrightarrow (-x_1 \vee -x_2) \wedge (-x_1 \vee -x_3) \wedge (-x_2 \vee -x_3)$$





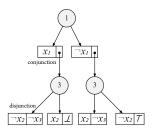
- The CNF is transformed into an SDD It succinctly represents the CNF
- The expensive compilation step

But upper-bounded by an exponential only in the tree-width of the CNF



- The CNF is transformed into an SDD It succinctly represents the CNF
- The expensive compilation step

But upper-bounded by an exponential only in the tree-width of the CNF



イロト イヨト イヨト イヨト

10/13

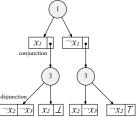
TW of the associated undirected graph: an edge between variables if together in a clause

A measure of how close it is to a tree (In example, graph is clique, TW is #vars -1 =2)

- The CNF is transformed into an SDD It succinctly represents the CNF
- The expensive compilation step

But upper-bounded by an exponential only in the tree-width of the CNF

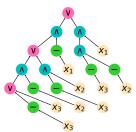
disjunction  $\chi_2$ 



TW of the associated undirected graph: an edge between variables if together in a clause

A measure of how close it is to a tree (In example, graph is clique, TW is #vars -1 = 2)

 The SDD is easily transformed into a dDBC



イロト イヨト イヨト イヨト

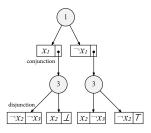
- The CNF is transformed into an SDD It succinctly represents the CNF
- The expensive compilation step

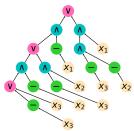
But upper-bounded by an exponential only in the tree-width of the CNF

TW of the associated undirected graph: an edge between variables if together in a clause

A measure of how close it is to a tree (In example, graph is clique, TW is #vars -1 =2)

- The SDD is easily transformed into a dDBC
- On it Shap is computed, possibly multiple times





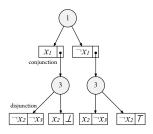
- The CNF is transformed into an SDD It succinctly represents the CNF
- The expensive compilation step

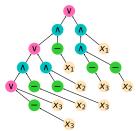
But upper-bounded by an exponential only in the tree-width of the CNF

TW of the associated undirected graph: an edge between variables if together in a clause

A measure of how close it is to a tree (In example, graph is clique, TW is #vars -1 =2)

- The SDD is easily transformed into a dDBC
- On it Shap is computed, possibly multiple times
- With considerable efficiency gain





イロト 不同 とうほう 不同 とう

• In our experiments, we used a BNN with 14 gates

- In our experiments, we used a BNN with 14 gates
- It was compiled into a dDBC with 18,670 nodes

- In our experiments, we used a BNN with 14 gates
- It was compiled into a dDBC with 18,670 nodes

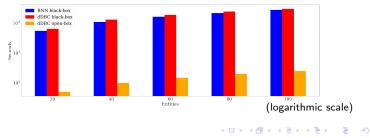
• A one-time computation that fully replaces the BNN

- In our experiments, we used a BNN with 14 gates
- It was compiled into a dDBC with 18,670 nodes

- A one-time computation that fully replaces the BNN
- We compared *Shap* computation time for black-box BNN, open-box dDBC, and black-box dDBC

- In our experiments, we used a BNN with 14 gates
- It was compiled into a dDBC with 18,670 nodes

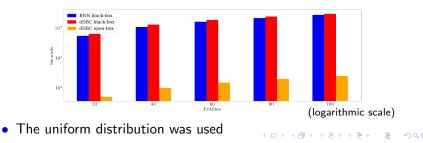
- A one-time computation that fully replaces the BNN
- We compared *Shap* computation time for black-box BNN, open-box dDBC, and black-box dDBC
- Total time for computing *all Shap scores for all entities*, with increasing numbers of them



- In our experiments, we used a BNN with 14 gates
- It was compiled into a dDBC with 18,670 nodes

11/13

- A one-time computation that fully replaces the BNN
- We compared *Shap* computation time for black-box BNN, open-box dDBC, and black-box dDBC
- Total time for computing *all Shap scores for all entities*, with increasing numbers of them



### **Some Research Directions**

• The above results on *Shap* computation hold under the uniform and product distributions

The latter imposes independence among features

### **Some Research Directions**

• The above results on *Shap* computation hold under the uniform and product distributions

The latter imposes independence among features

- Other distributions have been considered for  ${\it Shap}$  and other scores
- The empirical and product-empirical distributions
- They naturally arise when no more information available about the distribution

### **Some Research Directions**

• The above results on *Shap* computation hold under the uniform and product distributions

The latter imposes independence among features

- Other distributions have been considered for  ${\it Shap}$  and other scores
- The empirical and product-empirical distributions
- They naturally arise when no more information available about the distribution
- How far can we go with other distributions?
- Do we still have an efficient algorithm?

• Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

• Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

Imposing or using explicit and additional domain semantics or domain knowledge is relevant to explore • Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

Imposing or using explicit and additional domain semantics or domain knowledge is relevant to explore

Can we modify *Shap*'s definition and computation accordingly?

Or the probability distribution?

 Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

Imposing or using explicit and additional domain semantics or domain knowledge is relevant to explore

Can we modify *Shap*'s definition and computation accordingly?

Or the probability distribution?

• Shapley values satisfy desirable properties for general coalition game theory

 Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

Imposing or using explicit and additional domain semantics or domain knowledge is relevant to explore

Can we modify *Shap*'s definition and computation accordingly?

Or the probability distribution?

• Shapley values satisfy desirable properties for general coalition game theory

Existing scores have been criticized or under-explored in terms of general properties

 Explanation scores commonly use the classifier plus a probability distribution over the underlying entity population

Imposing or using explicit and additional domain semantics or domain knowledge is relevant to explore

Can we modify *Shap*'s definition and computation accordingly?

Or the probability distribution?

• Shapley values satisfy desirable properties for general coalition game theory

Existing scores have been criticized or under-explored in terms of general properties

Specific general and expected properties for Explanations Scores (in AI)?