Tractability and Optimization of Shap-Score Computation for Explainable AI

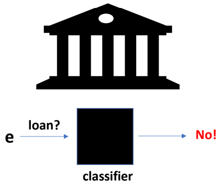
Leopoldo Bertossi

Explanations in Machine Learning

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

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

- $\mathbf{e}$ 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
- 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)

A Score-Based Approach: Responsibility

- Causality has been developed in AI for three decades or so
- In particular: Actual Causality
- Also the quantitative notion of Responsibility: a measure of causal contribution (the *Resp*-score)
- Both based on Counterfactual Interventions
- Hypothetical changes of values in a causal model to detect other changes

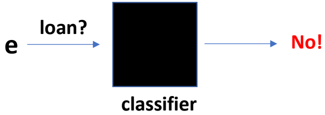
  "What would happen if we change ..."?

  By so doing identify actual causes
- Does the deletion of the DB tuple invalidates the query?
- Does a change of this feature value leads to label "Yes"?

- We have investigated actual causality and responsibility in data management and ML-based classification
- Semantics, computational mechanisms, intrinsic complexity, logic-based specifications, reasoning, etc.
- Assign numbers to, e.g., database tuples or features values to capture their causal, or, more generally, explanatory strength
- They can be applied without knowing "the internals" of a classifier Only input/output relation needed

  It can be a "black box", or treated as such (a complex NN)
- We have experimentally compared responsibility scores with other *local attribution scores*
  - *Shap*
  - *Ad hoc* scores, such as for FICO data on "open-box" model (connected logistic regressions)

- Simplified Case:



$$\mathbf{e} \;=\; \langle \text{john}, 18, \text{plumber}, 70\text{K}, \text{harlem}, \ldots \rangle \qquad \text{No}$$

- Counterfactual versions:

$$\mathbf{e}' \;=\; \langle \text{john}, 25, \text{plumber}, 70\text{K}, \text{harlem}, \ldots \rangle \qquad \text{Yes}$$

$$\mathbf{e}'' = \langle \text{john}, 18, \text{plumber}, 80\text{K}, \text{brooklyn}, \ldots \rangle \qquad \text{Yes}$$

- For the gist:

1. Value for feature Age is counterfactual cause with explanatory responsibility $\mathit{Resp}(\mathbf{e}, \text{Age}) = 1$

2. Value change Income := 80K needs an additional, minimum contingent change: $\Gamma = \{\text{Area} := \text{brooklin}\}$

   Income := 70K is actual cause with $\mathit{Resp}(\mathbf{e}, \text{Income}) = \frac{1}{1+|\Gamma|} = \frac{1}{2}$

The Generalized *Resp* Score

- For binary (two-valued) features the previous "definition" works fine (previous example is non-binary)
- Otherwise, there may be many values for a feature that do not change the label: original value not great explanation

  Similarly for features in a potential contingency set
- Better consider average labels obtained via counterfactual interventions

  Resp, our extended version of responsibility, will be expressed in terms of an expected value[1]

[1] Bertossi, Li, Schleich, Suciu,Vagena; SIGMOD Deem WS'20

- Pass from a local score (local for Γ and associated assignment $\bar{w}$)

$$Resp(\mathbf{e}, F^\star, \underline{\Gamma, \bar{w}}) := \frac{L(\mathbf{e}) - \mathbb{E}(\ L(\mathbf{e}') \mid F(\mathbf{e}') = \ F(\mathbf{e}^{\Gamma,\bar{w}}),\ \forall F \in (\mathcal{F} \smallsetminus \{F^\star\})\ )}{1 + |\Gamma|} \qquad (*)$$

  To global score, with "best" contingencies $(\Gamma, \bar{w})$

$$Resp(\mathbf{e}, F^\star) \ := \max_{\Gamma, \bar{w}:\ |\Gamma| \text{ is min. \& } (*) > 0} \ Resp(\mathbf{e}, F^\star, \Gamma, \bar{w})$$

  In particular with Γ of minimum size

- We are interested in maximum-score feature values

  Associated to minimum (cardinality) contingency sets

- Already with binary domains, *Resp* is intractable[2]

- Can we compute it faster when we have access to the internals?

  This kind of research was done for *Shap* (coming)

[2] Bertossi; TPLP'23

Coalition Games and the Shapley Value

- Usually *several tuples together* produce a query result
  And *several feature values* lead to a classification label
- Like players in a *coalition game* contributing, possibly differently, to a shared wealth-distribution function
- Apply standard measures used in game theory: the Shapley value of a player (as a measure of its contribution)
- The Shapley value is a established measure of contribution by players to a wealth function
- It emerges as the only measure enjoying certain properties
- We need a game (function) ...

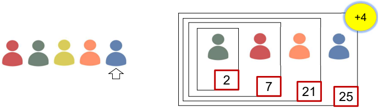
- Set of players D, and game function $\mathcal{G}: \mathcal{P}(D) \longrightarrow \mathbb{R}$
  ($\mathcal{P}(D)$ the power set of D)

- The Shapley value of player p among a set of players D:

$$Shapley(D, \mathcal{G}, p) := \sum_{S \subseteq D \setminus \{p\}} \frac{|S|!(|D| - |S| - 1)!}{|D|!} (\mathcal{G}(S \cup \{p\}) - \mathcal{G}(S))$$

- $|S|!(|D| - |S| - 1)!$ is number of permutations of D with all players in S coming first, then p, and then all the others

- Expected contribution of player p under all possible additions of p to a partial random sequence of players followed by a random sequence of the rest of the players



- For each application one defines an appropriate game function

- Shapley is difficult to compute

  Naive approach: exponentially many counterfactual combinations

- Actually, Shapley computation is #P-hard in general

- A complexity class of (possibly implicitly) computational counting problems

- Being #P-hard is evidence of difficulty: $\#SAT$ is #P-hard

  Counting satisfying assignments for a propositional formula

  At least as difficult as SAT

Shap Scores

- Based on the general Shapley value
- Set of players $\mathcal{F}$ contain features, relative to classified entity $\mathbf{e}$
- We need an appropriate $\mathbf{e}$-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: $\mathit{Shap}(\mathcal{F}, \mathcal{G}_{\mathbf{e}}, F^\star)$

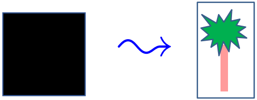
$$\sum_{S \subseteq \mathcal{F} \setminus \{F^\star\}} \frac{|S|!(|\mathcal{F}|-|S|-1)!}{|\mathcal{F}|!} [\underbrace{\mathbb{E}(L(\mathbf{e}'|\mathbf{e}'_{S \cup \{F^\star\}} = \mathbf{e}_{S \cup \{F^\star\}})}_{\mathcal{G}_{\mathbf{e}}(S \cup \{F^\star\})} - \underbrace{\mathbb{E}(L(\mathbf{e}')|\mathbf{e}'_S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

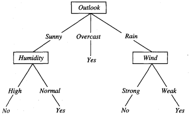
- *Shap* score has become popular (Lee & Lundberg, 2017)
- Assumes a probability distribution on entity population

- *Shap* may end up considering exponentially many combinations

  And multiple passes through the black-box classifier

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





  Exploiting its elements and internal structure?

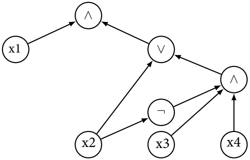
- What if we have a decision tree, or a random forest, or a Boolean circuit?

- Can we compute *Shap* in polynomial time?

Tractability for BC-Classifiers: Big Picture

- We investigated this problem in detail[3]
- Tractable and intractable cases, with algorithms for the former

  Investigated approximation algorithms
- Choosing the right abstraction (model) is crucial
- We considered Boolean-Circuit Classifiers (BCCs), i.e. propositional formulas with a (binary) output gate
- We had shown already that *Shap* is intractable for "Monotone 2CNF" classifiers under the product distribution (at most 2 variables per clause, and positive)
- So, it had to be a broad and interesting class of BCs



[3] Arenas, Bertossi, Barcelo, Monet; AAAI'21; JMLR'23

Shap for Boolean-Circuit Classifiers

- Features $F_i \in \mathcal{F},\ i = 1, \ldots, n, \quad Dom(F_i) = \{0, 1\}$,
  $\mathbf{e} \in \mathcal{E} := \{0,1\}^n, \quad L(\mathbf{e}) \in \{0,1\}$
- There is also a probability distribution P on $\mathcal{E}$
- For BC-classifier L: $\quad Shap(\mathcal{F}, G_{\mathbf{e}}, F^\star) \ =$

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

  Depends on $\mathbf{e}$ and L
- $SAT(L) := \{\mathbf{e}' \in \mathcal{E} \mid L(\mathbf{e}') = 1\} \qquad \#SAT(L) := |SAT(L)|$

  Counting the number of inputs that get label 1
- We established that *Shap* is at least as hard as model counting for the BC:

  Proposition: For the uniform distribution P^u, and $\mathbf{e} \in \mathcal{E}$

  $$\#SAT(L) \ = \ 2^{|\mathcal{F}|} \times (\ L(\mathbf{e}) - \sum_{i=1}^{n} Shap(\mathcal{F}, G_{\mathbf{e}}, F_i)\ )$$

- When $\#SAT(L)$ is hard for a Boolean classifier L, *Shap* is also hard

- Corollary: Computing *Shap* is $\#P$-hard for Boolean classifiers defined by Monotone 2DNF or Monotone 2CNF

  (Provan & Ball, 1983)

- Can we do better for other classes of binary classifiers?

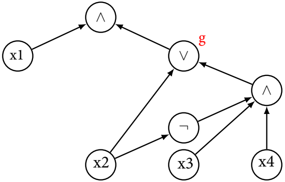
  Other classes of Boolean-circuit classifiers?

Deterministic and Decomposable BCs

- A Boolean circuit over set of variables X is a DAG $\mathcal{C}$ with:
  - Each input (source) node labeled with a variable or a constant in $\{0, 1\}$
  - Other nodes labeled with a gate in $\{\neg, \wedge, \vee\}$
  - Single sink node, O, the output
- For gate g of $\mathcal{C}$, $\mathcal{C}(g)$ is the induced subgraph containing gates on a path in $\mathcal{C}$ to g

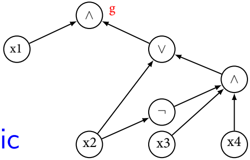
  $Var(g)$ is the set of variables of $\mathcal{C}(g)$

  $Var(g) = \{x2, x3, x4\}$



- $\mathcal{C}$ is deterministic if every $\vee$-gate g with input gates g_1, g_2: $\mathcal{C}(g_1)(\mathbf{e}) \neq \mathcal{C}(g_2)(\mathbf{e})$, for every $\mathbf{e}$

- $\mathcal{C}$ is decomposable if every $\wedge$-gate g with input gates g_1, g_2: $\mathit{Var}(g_1) \cap \mathit{Var}(g_2) = \emptyset$



- We concentrated on the class of deterministic and decomposable Boolean circuits (dDBCs)

- *Shap* computation in polynomial time not initially precluded

- A class of BCCs that includes -via efficient (knowledge) compilation- many interesting ones, syntactic and not ... (more coming)

Shap for dDBCs

- Proposition: For dDBCs $\mathcal{C}$, $\#SAT(\mathcal{C})$ can be computed in polynomial time ($\not\Longrightarrow$ the same for *Shap*)

  Idea: Bottom-up procedure that inductively computes $\#SAT(\mathcal{C}(g))$, for each gate g of $\mathcal{C}$

- To show that *Shap* can be computed efficiently for dDBCs, we need a detailed analysis

- We assume the uniform distribution for the moment

- Theorem: *Shap* can be computed in polynomial time for dDBCs under the uniform distribution

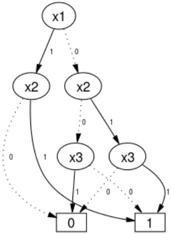
- It can be extended to any product distribution on $\mathcal{E}$

- Corollary: 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)

      $(\neg x_1 \wedge \neg x_2 \wedge \neg x_3) \vee (x_1 \wedge x_2) \vee (x_2 \wedge x_3)$

      Compatible variable orders along full paths

      Compact representation of Boolean formulas



    - Sentential decision diagrams (SDDs)

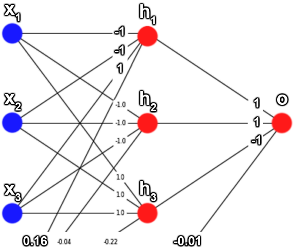
      Generalization of OBDDs
    - Deterministic-decomposable negation normal-form (dDNNFs)

      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
- 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[4]
- 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

[4] Bertossi, Leon; JELIA'23



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

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

$$\begin{aligned} o \longleftrightarrow\ & (-[(x_3 \wedge (x_2 \vee x_1)) \vee (x_2 \wedge x_1)] \wedge \\ & ([(-x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)] \vee \\ & [(x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)])) \vee \\ & ([(-x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)] \wedge \\ & [(x_3 \wedge (-x_2 \vee -x_1)) \vee (-x_2 \wedge -x_1)]). \end{aligned}$$

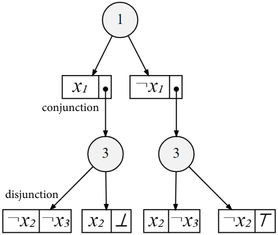
- Done using always CNFs and keeping them "short" ...

  (room for optimizations)

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

- The CNF is transformed into an SDD

  It succinctly represents the CNF

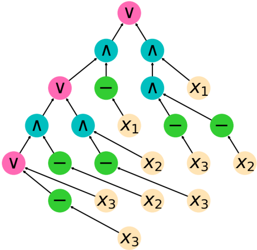


- The expensive compilation step

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

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

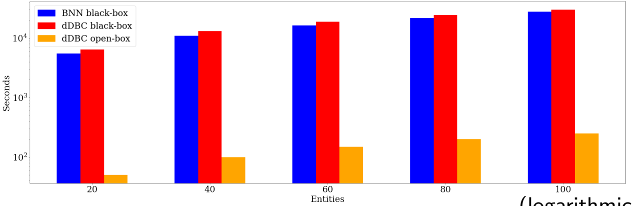
  A measure of how close it is to a tree
  (In example, graph is clique, TW is #vars -1 =2)



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

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

  (room for optimizations)
- 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



(logarithmic scale)

- The uniform distribution was used

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 *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

  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)?

- Features (in ML and in general) may be hierarchically ordered according to categorical dimensions

  address $\rightarrow$ neighborhood $\rightarrow$ *city* $\rightarrow \cdots$

  We may want to define and compute explanations (scores) at different levels of abstraction

  How to do this in a systematic way, possibly reusing results at different levels?

  Multi-dimensional explanations?

- There is a need for principled and sensible algorithms for explanation score aggregation

  At the individual level as in ~~(3)~~ or at the group level, e.g. categories of instances

  Hopefully guided by a declarative and flexible specifications (about what to aggregate and at which level)