



Reasoning About the Probabilistic Behavior of Classifiers

Guy Van den Broeck

CPAIOR Master Class - Jul 5, 2021

The AI Dilemma

Pure Logic

Pure Learning

The AI Dilemma

Pure Logic

- Slow thinking: deliberative, cognitive, model-based, extrapolation
- Amazing achievements until this day
- "Pure logic is brittle" noise, uncertainty, incomplete knowledge, ...



Pure Learning

The AI Dilemma

Pure Logic

- Fast thinking: instinctive, perceptive, model-free, interpolation
- Amazing achievements recently
- "Pure learning is brittle"

bias, algorithmic fairness, interpretability, explainability, adversarial attacks, unknown unknowns, calibration, verification, missing features, missing labels, data efficiency, shift in distribution, general robustness and safety fails to incorporate a sensible model of the world



Pure Learning

Pure Logic Probabilistic World Models Pure Learning A New Synthesis of Learning and Reasoning

• "Pure learning is brittle"

bias, **algorithmic fairness**, interpretability, **explainability**, adversarial attacks, unknown unknowns, calibration, **verification**, **missing features**, missing labels, data efficiency, shift in distribution, general robustness and safety

fails to incorporate a sensible model of the world

Outline

- 1. Theoretical motivation *Tractability of SHAP explanations* [AAAI'21]
- 2. Tractable reasoning about classifier behavior
Reasoning about missing features
Latent fair decisions[NeurIPS'19]
[AAAI'21]
[IJCAI'21]Probabilistic sufficient explanations[IJCAI'21]
- 3. Practical neuro-symbolic verification *Learning monotonic neural networks* [NeurIPS'20]

Outline

1. Theoretical motivation *Tractability of SHAP explanations*

[AAAI'21]

with Anton Lykov, Maximilian Schleich, Dan Suciu

Motivation: Explainable AI



What are SHAP explanations?

Feature-Based Attribution Score

- How much does ith feature influence F(x)?
- Based on Shapley values from Game Theory

Benefits

- Model-agnostic
- Intuitive
- Successfully applied in practice





Computing SHAP Explanations

Intuition:

- Assume a total order π of the features
- Compute effect on **E**[F] of presenting one feature at a time following π

Example:

- Assume $\pi = [X1, X2, ..., Xn]$
- Contribution of X2 w.r.t. π

$$c_{\pi}(X2) = \mathbf{E}[F \mid X1, X2] - \mathbf{E}[F \mid X1]$$

SHAP-score for X2:

Average contribution of X2 over all possible permutations

$$SHAP_{F,\mathbf{x}}(X2) = rac{1}{n!}\sum_{\pi}c_{\pi}(X2)$$

The Challenge

Various algorithms proposed to compute SHAP explanations:

approximately, exactly, efficiently, ..., for different machine learning models

There is considerable confusion about the tractability of computing SHAP explanations

- Are the exact algorithms exact, correct, and efficient?
- Are the approximations needed?

Example: TreeSHAP [ICML 2017]

How can we clear this up?



The Main Actors

1. The machine learning model class for function F

Linear regression, decision and regression trees, random forests, additive tree ensembles, logistic regression, neural nets with sigmoid activation functions, naive Bayes classifiers, factorization machines, regression circuits, logistic circuits, Boolean functions in d-DNNF, binary decision diagrams, bounded treewidth Boolean functions in CNF, Boolean functions in CNF or DNF, and arbitrary functions

2. The data distribution Pr to compute $\mathbf{E}[\mathbf{F}|\mathbf{y}] = \sum_{\mathbf{x}} \mathbf{Pr}(\mathbf{x}|\mathbf{y}) \mathbf{F}(\mathbf{x})$

Fully-factorized distributions





Empirical data distribution



Graphical models (naive Bayes)

Fully-factorized distributions



Key result:

- For any classifier F, the following problems have the same complexity:
 - Computing SHAP explanations of F
 - Computing the expectation **E** of F

Expectations **E** are efficient to compute for

- linear regression
- decision trees, random forests, additive tree ensembles
- Boolean functions in d-DNNF form, bounded-treewidth CNF
- ... and more

therefore

SHAP explanations are efficient to compute on those same models!

Fully-factorized distributions



Key result:

- For any classifier F, the following problems have the same complexity:
 - Computing SHAP explanations of F
 - Computing the expectation **E** of F

We prove that expectations **E** are **#P-hard** to compute for

- logistic regression
- naive Bayes classifiers
- neural networks with sigmoid activations
- Boolean functions in CNF or DNF

therefore

SHAP explanations are #P-hard to compute on those same models!

Intuition: Expectation of Logistic Regression

Consider the <u>number partitioning</u> problem for {1,2,3,2}

- {1,3} and {2,2} partition the set into subsets with the same sum
- Counting such partitions is **#P-hard**

Consider the logistic regression model:

F(X) = sigmoid(1000 X1 + 2000 X2 + 3000 X3 + 2000 X4 - 4500)

- $\mathbf{x} = [1,1,0,1]$ and $\mathbf{x'} = [0,0,1,0]$ correspond to non-partitions: $F(\mathbf{x}) \approx 1$ and $F(\mathbf{x'}) \approx 0$
- Under a uniform distribution $E[F] \approx 0.5$
- $\mathbf{x} = [1,0,1,0]$ and $\mathbf{x}' = [0,1,0,1]$ correspond to partitions: $F(\mathbf{x}) = F(\mathbf{x}') \approx 0$
- Missing probability mass 0.5 **E**[F] tells us how many partitions there are
- Computing **E**[F] is **#P-hard**

Going Beyond Fully-Factorized Distributions

Idea: the real world is not fully-factorized: features depend on each other

Consider the simplest case:

- 1. Simplest possible classifier: F(X) = X1
- 2. Simplest tractable distribution: naive Bayes





SHAP explanations are NP-hard to compute for all probabilistic graphical models, even all tractable probabilistic models, even on simple function classes

Trivial function classes do not make SHAP tractable...

Empirical Distributions



<u>Idea</u>: Properties of distributions are often estimated on sampled data. *Perhaps the empirical data distribution is easier to work with?*

The # of possible worlds is limited by the number of rows (samples) in data

Computing **SHAP** is **#**P-hard in the size of the empirical distribution.

The problem that TreeSHAP is trying to solve efficiently is in fact **#P-hard**

Summary of Contributions

	Distribution Pr					
Predictive Model F	Fully Factorized	Naive-Bayes	Empirical			
Linear regression Regression circuits Factorization machines	Tractable	Intractable	Intractable			
Decision Tree Random Forest,Boosted Tree	Tractable	Intractable	Intractable			
Boolean functions in d-DNNF, BDD, Bounded treewidth CNF	Tractable	Intractable	Intractable			
Logistic regression Logistic circuits, Naive Bayes	Intractable	Intractable	Intractable			
Neural Networks with sigmoid activation	Intractable	Intractable	Intractable			

- Proved connections between SHAP and the expectation of classifiers
- ... and more theoretical insights of independent interest

Then how can we reason about the behavior of classifiers under a non-trivial feature distribution?



Outline

- 1. Theoretical motivation *Tractability of SHAP explanations* [AAAI'21]
- 2. Tractable reasoning about classifier behavior





The Alphabet Soup of probabilistic models



Intractable and tractable models



a unifying framework for tractable models



Input nodes are tractable (simple) distributions, e.g., univariate gaussian or indicator p(X=1) = [X=1]



Product nodes are factorizations $\prod_{c \in in(n)} p_c(\mathbf{x})$



Sum nodes are mixture models $\sum_{c\in \mathsf{in}(n)} \theta_{n,c} \operatorname{p}_c(\mathbf{x})$

Feedforward $p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$



Feedforward $p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$



Feedforward $p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$



Why are these tractable models?

Let's compute a marginal probability
$$\int p(\mathbf{x}) d\mathbf{x}$$
.

Smoothness + decomposability = tractable MAR

If $m{p}(\mathbf{x}) = \sum_i w_i m{p}_i(\mathbf{x})$, (smoothness):

$$\int \mathbf{p}(\mathbf{x}) d\mathbf{x} = \int \sum_{i} w_{i} \mathbf{p}_{i}(\mathbf{x}) d\mathbf{x} =$$
$$= \sum_{i} w_{i} \int \mathbf{p}_{i}(\mathbf{x}) d\mathbf{x}$$

 \Rightarrow integrals are "pushed down" to children



Smoothness + decomposability = tractable MAR

If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (decomposability):

$$\int \int \int \mathbf{p}(\mathbf{x}, \mathbf{y}, \mathbf{z}) d\mathbf{x} d\mathbf{y} d\mathbf{z} =$$
$$= \int \int \int \int \mathbf{p}(\mathbf{x}) \mathbf{p}(\mathbf{y}) \mathbf{p}(\mathbf{z}) d\mathbf{x} d\mathbf{y} d\mathbf{z} =$$
$$= \int \mathbf{p}(\mathbf{x}) d\mathbf{x} \int \mathbf{p}(\mathbf{y}) d\mathbf{y} \int \mathbf{p}(\mathbf{z}) d\mathbf{z}$$



 \Rightarrow integrals decompose into easier ones

Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

inear in circuit size!

E.g. to compute $p(x_2, x_4)$: leafs over X_1 and X_3 output $\mathbf{Z}_i = \int p(x_i) dx_i$ for normalized leaf distributions: 1.0

leafs over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)





Expressive models without compromises

How expressive are probabilistic circuits?

density estimation benchmarks

dataset	best circuit	BN	MADE	VAE	dataset	best circuit	BN	MADE	VAE
nltcs	-5.99	-6.02	-6.04	-5.99	dna	-79.88	-80.65	-82.77	-94.56
msnbc	-6.04	-6.04	-6.06	-6.09	kosarek	-10.52	-10.83	-	-10.64
kdd	-2.12	-2.19	-2.07	-2.12	msweb	-9.62	-9.70	-9.59	-9.73
plants	-11.84	-12.65	-12.32	-12.34	book	-33.82	-36.41	-33.95	-33.19
audio	-39.39	-40.50	-38.95	-38.67	movie	-50.34	-54.37	-48.7	-47.43
jester	-51.29	-51.07	-52.23	-51.54	webkb	-149.20	-157.43	-149.59	-146.9
netflix	-55.71	-57.02	-55.16	-54.73	cr52	-81.87	-87.56	-82.80	-81.33
accidents	-26.89	-26.32	-26.42	-29.11	c20ng	-151.02	-158.95	-153.18	-146.9
retail	-10.72	-10.87	-10.81	-10.83	bbc	-229.21	-257.86	-242.40	-240.94
pumbs*	-22.15	-21.72	-22.3	-25.16	ad	-14.00	-18.35	-13.65	-18.81





Want to learn more?

Tutorial (3h)

Inference

Learning

Theory

Representations

Probabilistic Circuits

Antonio Vergari University of California, Los Angeles

Robert Peharz TU Eindhoven YooJung Choi University of California, Los Angeles

Guy Van den Broeck University of California, Los Angeles

September 14th, 2020 - Ghent, Belgium - ECML-PKDD 2020

▶ ▶| ◄) 0:00 / 3:02:46

https://youtu.be/2RAG5-L9R70

Overview Paper (80p)

	A U	Probabilistic Circuits: Inifying Framework for Tractable Probabilistic Models	*
Yo	oJu	ng Choi	
Ar	ntoni	o Vergari	
Gu Co Un Los	1y V mpute iversi s Ang	an den Broeck er Science Department ty of California eles, CA, USA	
Co	onte	ats	
1	Intr	oduction	3
2	Pro	babilistic Inference: Models, Queries, and Tractability	4
	2.1	Probabilistic Models	5
	2.2	Probabilistic Queries	6
	2.3 2.4	Properties of Tractable Probabilistic Models	9

http://starai.cs.ucla.edu/papers/ProbCirc20.pdf

Training PCs in Julia with Juice.jl

Training maximum likelihood parameters of probabilistic circuits

julia> using ProbabilisticCircuits; julia> data, structure = load(...); julia> num_examples(data) 17,412 julia> num_edges(structure) 270,448 julia> @btime estimate_parameters(structure , data); 63 ms

Juice-jl / Probabi	listicCircuits.jl	Unwatch + 5	Unstar 21 V Fork 4			
> Code ① Issues	12 11 Pull requests () Actions	Projects	Wiki			
⁹ master +	Go to file Add file	• 🛓 Code •	About \$			
khosravipasha som	e docs 🚃 🗙 2	3 days ago 🕚 452	Probabilistic Circuits from the Juice library			
.github/workflows	Install TagBot as a GitHub Action	7 months ago	probabilistic-circuits probabilistic-reasoning			
docs	some doos	23 days ago				
src	Add utility function for save_as_dot (#13)	3 months ago	tractable-models			
test 1	Add required test dependencies (#8)	3 months ago	Releases Releases Nov			
.gitignore	docs auto build	6 months ago				
travis.yml	fix notifications travis	6 months ago				
Artifacts.toml	fix density estimation hash	8 months ago				
LICENSE	Initial commit	14 months ago				
Project.toml	version bump	2 months ago				
README.md	add stable badge	3 months ago				
README_DEV.md	add release instructions	3 months ago				
			Packages			

Custom SIMD and CUDA kernels to parallelize over layers and training examples.

https://github.com/Juice-jl/

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- 1. Theoretical motivation *Tractability of SHAP explanations* [AAAI'21]
- 2. Tractable reasoning about classifier behavior **Reasoning about missing features** [NeurIPS'19] with Pasha Khosravi, YooJung Choi, Yitao Liang, Antonio Vergari

Prediction with Missing Features



Test with missing features

Expected Predictions

Consider **all possible complete inputs** and **reason** about the *expected* behavior of the classifier

$$\mathbb{E}_{\mathbf{X}^m \sim p(\mathbf{X}^m | \mathbf{X}^o)} \begin{bmatrix} f(\mathbf{X}^m \mathbf{X}^o) \end{bmatrix} \qquad \begin{array}{c} \mathbf{x}^o = \text{observed features} \\ \mathbf{x}^m = \text{missing features} \end{array}$$

How can this be tractable for a complex feature distribution?

- feature distribution is a probabilistic circuits
- classifier is a compatible regression circuit

Recursion that "breaks down" the computation

Expectation of function m w.r.t. dist. n?

Solve subproblems: (1,3), (1,4), (2,3), (2,4)



Probabilistic Circuits for Missing Data



[Khosravi et al. IJCAI19, NeurIPS20, Artemiss20]

ADV inference in Julia with Juice.jl

using ProbabilisticCircuits

- pc = load_prob_circuit(zoo_psdd_file("insurance.psdd"));
- rc = load_logistic_circuit(zoo_lc_file("insurance.circuit"), 1);

Is the predictive model biased by gender?

```
groups = make_observations([["male"], ["female"]])
exps, _ = Expectation(pc, rc, groups);
println("Female : \$ $(exps[2])");
println("Male : \$ $(exps[1])");
println("Diff : \$ $(exps[2] - exps[1])");
Female : $ 14170.125469335406
Male : $ 13196.548926381849
Diff : $ 973.5765429535568
```

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Model-Based Algorithmic Fairness: FairPC

Learn classifier given

- features S and X
- training labels/decisions D

Group fairness by demographic parity:

Fair decision D_f should be independent of the sensitive attribute S

Discover the **latent fair decision** D_f by learning a PC.



[Choi et al. AAAI21]

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Local Explanation Approaches

Model agnostic: (e.g. LIME, SHAP, Anchors)

- Treat classifier as black box
- Evaluate on sampled perturbations
 - Often ignores feature distribution (in favor of perturbation distribution)
 - Evaluate on impossible or low likelihood instances
- Can be fooled! [Slack et al., 2020; Dimanov et al., 2020]
- Might produce over-confident results [Ignatiev et al.]
- Very generally applicable
- No guarantees



Local Explanation Approaches

Logical explanations:

(e.g, sufficient reasons, abduction, prime implicants)

- Give formal guarantees with 100% certainty
- Ensure minimality
- Hard to compute

(e.g., reduce MNIST from 784 to 64 pixels)

- Ignores feature distribution (it is irrelevant!)
- Lead to complex explanations
 To give a guarantee with 100% certainty, one needs to know almost all of the pixels...



Probabilistic Sufficient Explanations

Explanation is a subset of features, s.t.

1. The explanation is "probabilistically sufficient"

Under the feature distribution, given the explanation, the classifier is likely to make the observed prediction.

- => Strong probabilistic guarantees
- 2. It is minimal and "simple"

Probabilistic Sufficiency Criteria

Same Decision Probability

$$\mathsf{SDP}_{\mathcal{C},\mathbf{x}}(\mathbf{z}) = \mathbb{E}_{\mathbf{m} \sim \Pr(\mathbf{M}|\mathbf{z})} \llbracket \mathcal{C}(\mathbf{zm}) = \mathcal{C}(\mathbf{x}) \rrbracket$$

C(.) is a threshold-based classifier, output is + or -

Similar criteria used in Anchors.

Logical Reasoning approaches require SDP=1.

Hard to calculate (PP^PP-hard on Bayesian networks, NP-hard on Naive Bayes)

Probabilistic Sufficiency Criteria

Expected Prediction

$$\mathsf{EP}(\mathbf{z}) = \mathbb{E}_{\mathbf{m} \sim \Pr(\mathbf{M}|\mathbf{z})} f(\mathbf{zm})$$

f(.) is a probabilistic classifier, output is a class probability or log-probability

Expected Prediction is tractable to compute for

- 1. Logistic regression with conformant Naive Bayes
- 2. Decision trees w.r.t. PC
- 3. Discriminative circuits w.r.t. PC
- 4. Feature distribution and classifier defined by same PC

Probabilistic Sufficient Explanation

Want to maximize the **expected prediction** while keeping explanations **simple**.

$$SE_k(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{z} \subseteq \mathbf{x}} EP(\mathbf{z}) \quad \text{s.t. } |\mathbf{z}| \le k$$

To also achieve **minimality**, we can choose the most likely ones.

$$\mathsf{MLSE}_k(\mathbf{x}) = \underset{\mathbf{z} \in \mathsf{SE}_k(\mathbf{x})}{\operatorname{argmax}} \operatorname{Pr}(\mathbf{z})$$

Correctly Classified Examples

Binary classification: 3 vs 5

Used decision forest classifier and probabilistic circuit feature distribution

Beam search - keep top b explanation candidates for each size

Sort by expected prediction, break ties by feature probability



Misclassified Examples

Binary classification: 3 vs 5

Used decision forest classifier and probabilistic circuit feature distribution

Beam search - keep top b explanation candidates for each size

Sort by expected prediction, break ties by feature probability



Comparison with Anchors on MNIST (784 pixels)

Method	$ \mathrm{EP}_\mathcal{O}(\mathbf{z}) $	$\text{SDP}_{\mathcal{C},\mathbf{x}}(\mathbf{z})$	$\log P(\mathbf{z})$
Anchors	0.75 ± 0.37	0.66 ± 0.08	-3.29 ± 0.88
MLSE _s	1.57 ± 0.29	0.86 ± 0.05	-3.05 ± 0.65
$MLSE_{10}$	3.11 ± 0.23	0.99 ± 0.01	-6.98 ± 1.37
MLSE ₂₀	3.60 ± 0.15	1.00 ± 0.00	-9.90 ± 2.14
MLSE ₃₀	3.75 ± 0.13	1.00 ± 0.00	-11.77 ± 2.88

- For same size of explanation
 - SE has more realistic explanations (higher marginal likelihood P(z))
 - SE has stronger guarantees (higher expected log-odds and SDP)
- For >10 pixels
 - SE are almost logical explanations (around 100% SDP)
 - Yet they remain `simple`: small and with high marginal likelihood

Explanation Complexity vs Sufficiency Constraints



- Simple explanations (high likelihood) give strong probabilistic guarantees (EP)
- Steep around 0 and 1: making guarantees even slightly probabilistic will lead to significant simplification of the explanations

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[AAAI'21]
- 3. Practical neuro-symbolic verification *Learning monotonic neural networks* [NeurIPS'20] with Aishwarya Sivaraman, Golnoosh Farnadi, Todd Millstein

Predict Loan Amount





Neural Network Model: Increasing income can decrease the approved loan amount

Monotonicity (Prior Knowledge): Increasing income should increase the approved loan amount

Counterexamples



$$\exists x, y \; x \leq y \implies f(x) > f(y)$$

Computed using SMT(LRA)

Maximal counterexamples (largest violation) using OMT

Counterexample-Guided Predictions



Monotonic Envelope:

- Replace each prediction by its maximal counterexample
- Envelope construction is online (during prediction)
- Guarantees monotonic predictions for any ReLU neural net
- Works for high-dimensional input
- Works for multiple monotonic features

Counterexample-Guided Learning

How to use monotonicity to improve model quality? "Monotonicity as inductive bias"



Counterexample-Guided Monotonicity Enforced Training (COMET)

Table 4: Monotonicity is an effective inductive bias. COMET outperforms Min-Max networks on all datasets. COMET outperforms DLN in regression datasets and achieves similar results in classification datasets.

Dataset	Features	Min-Max	DLN	Сомет	Dataset	Features	Min-Max	DLN	Сомет
Auto- MPG	Weight Displ. W,D W,D,HP	9.91 ± 1.20 11.78 ± 2.20 11.60 ± 0.54 10.14 ± 1.54	16.77 ± 2.57 16.67 ± 2.25 16.56 ± 2.27 13.34 ± 2.42	8.92±2.93 9.11±2.25 8.89±2.29 8.81±1.81	Heart	Trestbps Chol. T,C	0.75 ± 0.04 0.75 ± 0.04 0.75 ± 0.04	$\begin{array}{c} 0.85{\pm}0.02\\ 0.85{\pm}0.04\\ \textbf{0.86{\pm}0.02}\end{array}$	$\begin{array}{c} 0.86{\pm}0.03\\ 0.87{\pm}0.03\\ 0.86{\pm}0.03\end{array}$
Boston	Rooms Crime	30.88 ± 13.78 25.89 ± 2.47	$15.93{\pm}1.40\\12.06{\pm}1.44$	11.54±2.55 11.07±2.99	Adult	Cap. Gain Hours	0.77 0.73	0.84 0.85	0.84 0.84

Our Contributions

- Counterexample-guided algorithm that guarantees monotonicity at prediction time for an arbitrary ReLU neural network
- Counterexample-guided algorithm to incorporate monotonicity as an inductive bias during training
- Outperforms state-of-the-art monotonic learners in regression and classification tasks
- Counterexample-guided learning when used in conjunction with envelope **improves accuracy and provides provable guarantees**



"Pure learning is brittle"

bias, **algorithmic fairness**, interpretability, **explainability**, adversarial attacks, unknown unknowns, calibration, **verification**, **missing features**, missing labels, data efficiency, shift in distribution, general robustness and safety

We need to incorporate a sensible probabilistic/logic model of the world

Thanks

This was the work of many wonderful students/postdoc/collaborators!

References: http://starai.cs.ucla.edu/publications/