AUTOMATED REASONING FOR EXPLAINABLE AI

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A disclaimer

A disclaimer - recent & not so recent work...



A disclaimer – new area of research, since 2018...



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Recent & ongoing ML successes



https://en.wikipedia.org/wiki/Waymo

Image & Speech Recognition







AlphaGo Zero & Alpha Zero



http://gradientscience.org/intro_adversarial/

But ML models are brittle — adversarial examples



Goodfellow et al., ICLR'15

But ML models are brittle — adversarial examples



Goodfellow et al., ICLR'15



Eykholt et al'18

Aung et al'17

But ML models are brittle — adversarial examples



Adversarial examples can be very problematic



Dermatoscopic image of a benign melanocytic nevus, along with the diagnostic probability computed by a deep neural network.



Malignant

Model confidence

Adversarial noise



Perturbation computed by a common adversarial attack technique.

Adversarial example

=



Combined image of nevus and attack perturbation and the diagnostic probabilities from the same deep neural network.



Benign Malignant

Model confidence Finlayson et al., Nature 2019

Also, some ML models are interpretable

decision|rule lists|sets decision trees; ...

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
<i>e</i> ₁	0	0	1	0	0
<i>e</i> ₂	1	0	0	0	1
e ₃	0	0	1	1	0
e ₄	1	0	0	1	1
е5	0	1	1	0	0
e ₆	0	1	1	1	0
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Also, some ML models are interpretable

decision|rule lists|sets decision trees; ... if ¬Meeting then Hike if ¬Vacation then ¬Hike

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e7	1	1	0	1	1







Why does the NN predict a cat?





ML meets AR

ML meets AR



"Combining machine learning with logic is the challenge of the day"

M. Vardi, MLmFM'18 Summit

ML meets AR - a challenge for the next decade?



ML meets AR - a challenge for the next decade?



ML meets AR - a challenge for the next decade?



What is eXplainable AI (XAI)?



This is a cat.

Current Explanation

This is a cat:

- It has fur, whiskers, and claws.
- It has this feature:





XAI Explanation

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REGULATION (EU) 2016/679 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL

of 27 April 2016

on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation)

(Text with EEA relevance)

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European Union regulations on algorithmic decision-making and a "right to explanation"

Bryce Goodman,1* Seth Flaxman,2

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■ We summarize the potential impact that the European Union's new General Data Protection Regulation will have on the routine use of machine-learning algorithms. Slated to take effect as law across the European Union in 2018, it will place restrictions on automated individual decision making (that is, algorithms that make decisions based on user-level predictors) that "significantly affect" users. When put into practice, the law may also effectively create a right to explanation, whereby a user can ask for an explanation of an algorithmic decision that significantly affects them. We argue that while this law may pose large challenges for industry, it highlights opportunities for computer scientists to take the lead in designing algorithms and evaluation frameworks that avoid discrimination and enable explanation.

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European Union regulations on algorithmic decision-making and a "right to explanation" A new bill would force companies to check their algorithms for bias

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XAI & EU guidelines



XAI & the principle of explicability



XAI & the principle of explicability



& tens of recent papers!

Goals: Overview our work at intersection of AR & ML

 Part #1: Learning interpretable models (brief) Additional detail in our IJCAI'18 & IJCAR'18 papers 	[IPNM18, NIPM18]	
 Part #2: Rigorous explanations for black-box models Additional detail in our AAAI'19 paper 	[INM19a]	
 Part #3: Assessing heuristic explanations (brief) Additional detail in our SAT'19 & CoRR'19 papers 	[NSM ⁺ 19, INM19b]	
 Part #4: Relating explanations with adversarial examples Additional detail in our NIPS'19 paper 	(brief) [INMS19]	

Part 1

Learning Interpretable ML Models

Background

Decision Sets

A Word on Decision Trees

Classification problems I

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
<i>e</i> ₁	0	0	1	0	0
e_2	1	0	0	0	1
e ₃	0	0	1	1	0
e_4	1	0	0	1	1
e_5	0	1	1	0	0
e ₆	0	1	1	1	0
e7	1	1	0	1	1

• Training data (or **examples**/instances): $\mathcal{E} = \{e_1, \dots, e_M\}$

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- Training data (or **examples**/instances): $\mathcal{E} = \{e_1, \dots, e_M\}$
- Binary **features**: $\mathcal{F} = \{f_1, \ldots, f_K\}$
 - Literals: f_r and $\neg f_r$

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- Binary **features**: $\mathcal{F} = \{f_1, \ldots, f_K\}$
 - Literals: f_r and $\neg f_r$
- Feature space: $\mathcal{U} \triangleq \prod_{r=1}^{K} \{f_r, \neg f_r\}$
- Binary classification: $C = \{c_0 = 0, c_1 = 1\}$
 - \mathcal{E} partitioned into \mathcal{E}^- and \mathcal{E}^+

Classification problems II

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
e1	0	0	1	0	0
e2	1	0	0	0	1
e ₃	0	0	1	1	0
e4	1	0	0	1	1
e5	0	1	1	0	0
e ₆	0	1	1	1	0
e7	1	1	0	1	1

- $e_q \in \mathcal{E}$ represented as a 2-tuple (π_q, ς_q)
 - $\pi_q \in \mathcal{U}$: literals associated with the example
 - $\varsigma_q \in \{0,1\}$ is the class of example

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 - $\pi_q \in \mathcal{U}$: literals associated with the example
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- A literal l_r on a feature f_r , $l_r \in \{f_r, \neg f_r\}$, discriminates an example e_q if $\pi_q[r] = \neg l_r$
 - I.e. feature *r* takes the value **opposite** to the value in the tuple of literals of the example

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- Binary features: $\mathcal{F} = \{f_1, f_2, f_3, f_4\}$
 - $\cdot f_1 \triangleq V, f_2 \triangleq C, f_3 \triangleq M, and f_4 \triangleq E$
- \cdot e_1 is represented by the 2-tuple (π_1,ς_1) ,
 - $\pi_1 = (\neg V, \neg C, M, \neg E)$
 - $\varsigma_1 = 0$
- Literals V, C, \neg M and E discriminate e_1
- $\boldsymbol{\cdot} \ \mathcal{U} = \{V, \neg V\} \times \{C, \neg C\} \times \{M, \neg M\} \times \{E, \neg E\}$

Given training data, **learn set of DNFs** that correctly classify that data, perform suitably well on unseen data, and offer human-understandable explanations for the predictions made Background

Decision Sets

A Word on Decision Trees

- Given \mathcal{F} , an **itemset** π is an element of $\mathcal{I} \triangleq \prod_{r=1}^{k} \{f_r, \neg f_r, \mathfrak{u}\}$
 - **u** represents a don't care value

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- A **rule** is a 2-tuple (π, ς) , with itemset $\pi \in \mathcal{I}$, and class $\varsigma \in \mathcal{C}$ Rule (π, ς) interpreted as:

IF all specified literals in π are true, THEN pick class ς

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IF all specified literals in π are true, THEN pick class ς

- A decision set \$ is a finite set of rules unordered
- A rule of the form $\mathfrak{D} \triangleq (\emptyset,\varsigma)$ denotes the **default rule** of a decision set \$
 - Default rule is **optional** and used **only** when other rules do not apply on some feature space point

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
<i>e</i> ₁	0	0	1	0	0
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e4	1	0	0	1	1
e5	0	1	1	0	0
e ₆	0	1	1	1	0
e7	1	1	0	1	1

- Rule 1: $((\mathfrak{u}, \mathfrak{u}, \neg \mathsf{M}, \mathfrak{u}), c_1)$
 - Meaning: **if** ¬Meeting **then** Hike
- Rule 2: $((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_0)$
 - Meaning: if ¬Vacation then ¬Hike

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
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- Rule 1: $((\mathfrak{u},\mathfrak{u},\neg\mathsf{M},\mathfrak{u}),c_1)$
 - \cdot Meaning: if $\neg \text{Meeting then}$ Hike
- Rule 2: $((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_0)$
 - Meaning: if ¬Vacation then ¬Hike
- Default rule: (\emptyset, c_0)
 - $\cdot\,$ Meaning: if all other rules do not apply, then pick $\neg \text{Hike}\,$

Issue with unordered rules

- Itemsets $\pi_1, \pi_2 \in \mathcal{I}$ clash, $\pi_1 \cap \pi_2 = \emptyset$, if for some coordinate *r*:
 - $\pi_1[r] = f_r$ and $\pi_2[r] = \neg f_r$, or $\pi_1[r] = \neg f_r$ and $\pi_2[r] = f_r$

Issue with unordered rules - overlap

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 - $\pi_1[r] = f_r$ and $\pi_2[r] = \neg f_r$, or $\pi_1[r] = \neg f_r$ and $\pi_2[r] = f_r$
- Two rules $r_1 = (\pi_1, \varsigma_1)$ and $r_2 = (\pi_2, \varsigma_2)$ overlap if π_1 and π_2 do not clash, i.e.

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 \cdot Can be restricted to some set, e.g. ${\cal E}$

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 $\pi_1 \cap \pi_2 \neq \emptyset$

- \cdot Can be restricted to some set, e.g. ${\cal E}$
- Forms of overlap:
 - \cdot \oplus : overall where rules agree in prediction
 - $\cdot \ominus$: overlap where rules **disagree** in prediction

Issue with unordered rules - overlap

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- \cdot Can be restricted to some set, e.g. ${\cal E}$
- Forms of overlap:
 - \cdot \oplus : overall where rules agree in prediction
 - ⊖: overlap where rules **disagree** in prediction
- Our goal:

Minimize number of rules in decision set, and provide guarantees in terms of overlap, namely $\ominus\text{-}overlap$

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e7	1	1	0	1	1

• Decision set:

 $\{((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), C_0), ((\mathfrak{u}, \mathfrak{u}, \neg M, \mathfrak{u}), C_1)\}$

• No \mathcal{E}^{\ominus} -overlap

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
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• Decision set:

 $\{((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), C_0), ((\mathfrak{u}, \mathfrak{u}, \neg M, \mathfrak{u}), C_1)\}$

- No \mathcal{E}^{\ominus} -overlap
- But, there exists overlap in feature space
 - $\cdot \, \ominus \text{-overlap for } (\neg V, \neg C, \neg M, \neg E) \in \mathcal{U} \setminus \mathcal{E}$

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
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• Decision set:

 $\{((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_0), ((\mathfrak{u}, \mathfrak{u}, \neg M, \mathfrak{u}), c_1)\}$

- No \mathcal{E}^{\ominus} -overlap
- But, there exists overlap in feature space
 - $\cdot \ \ominus \text{-overlap for } (\neg V, \neg C, \neg M, \neg E) \in \mathcal{U} \setminus \mathcal{E}$
- However, there exists no \mathcal{U}^{\ominus} -overlap for decision set:

 $\{((\forall,\mathfrak{u},\mathfrak{u},\mathfrak{u},\mathfrak{u}),\mathit{C_1}),((\neg\forall,\mathfrak{u},\mathfrak{u},\mathfrak{u}),\mathit{C_0})\}$

- If a rule fires, the set of literals represents the **explanation** for the predicted class
 - Explanation is **succinct** : **only** the literals in the rule used; independent of example
- For the default class, **must** pick one **falsified** literal in **every** rule that predicts a different class
 - Explanation is **not succinct** : explanation depends on **each** example
- **Obs: Uninteresting** to predict *c*₁ as **negation** of *c*₀ (and vice-versa)
 - Explanations also **not** succinct

Stating our goals

- Assumptions:
 - Represent \mathcal{E}^- with Boolean function \mathcal{E}^0
 - + True for each example \mathcal{E}^-
 - Represent \mathcal{E}^+ with Boolean function E^1
 - + True for each example \mathcal{E}^+
 - Also, let $E^0 \wedge E^1 \vDash \bot$

Stating our goals

- Assumptions:
 - Represent \mathcal{E}^- with Boolean function E^0
 - \cdot True for each example \mathcal{E}^-
 - Represent \mathcal{E}^+ with Boolean function E^1
 - + True for each example \mathcal{E}^+
 - + Also, let $E^0 \wedge E^1 \vDash \bot$
- DNF functions to compute:
 - F^0 for predicting c_0 , while **ensuring** $E^0 \vDash F^0$
 - F^1 for predicting c_1 , while ensuring $E^1 \vDash F^1$



• MinDS₀:

Find the smallest DNF representations of Boolean functions F^0 and F^1 , measured in the number of terms, such that:

- 1. $E^0 \models F^0$ 2. $E^1 \models F^1$ 3. $F^1 \leftrightarrow F^0 \models \bot$
- · No \mathcal{U}^{\ominus} -overlap

• MinDS₀:

Find the smallest DNF representations of Boolean functions *F*⁰ and *F*¹, measured in the number of terms, such that:

- 1. $E^0 \vDash F^0$ 2. $E^1 \vDash F^1$ 3. $F^1 \leftrightarrow F^0 \vDash \bot$
- · No \mathcal{U}^{\ominus} -overlap
- Obs: MinDS₀ ensures succinct explanations
 - Computes F^0 and F^1 (i.e. **no** negation) and **no** default rule

• $MinDS_0$:

Find the smallest DNF representations of Boolean functions F^0 and F^1 , measured in the number of terms, such that:

- 1. $E^0 \vDash F^0$ 2. $E^1 \vDash F^1$ 3. $F^1 \leftrightarrow F^0 \vDash \bot$
- · No \mathcal{U}^{\ominus} -overlap
- Obs: MinDS₀ ensures succinct explanations
 - Computes F^0 and F^1 (i.e. **no** negation) and **no** default rule
- Complexity-wise:
 - $MinDS_0 \in \Sigma_2^P$
 - + A conjecture: MinDS_0 hard for Σ_2^{P}

(from late 2017)

Curbing our expectations I

- MinDS₄: Minimize F^0 , given $F^1 \equiv E^1$ constant, and such that
 - 1. $E^0 \models F^0$
 - 2. $F^0 \wedge E^1 \vDash \bot$
 - No \ominus -overlap;
 - No succinct explanations for *F*¹

Curbing our expectations I

- MinDS₄: Minimize F^0 , given $F^1 \equiv E^1$ constant, and such that
 - 1. $E^0 \models F^0$
 - 2. $F^0 \wedge E^1 \vDash \bot$
 - · No \ominus -overlap;
 - No succinct explanations for F^1
- MinDS₃: Same as MinDS₄, but target F^1 given $F^0 \equiv E^0$ constant
 - · Also, no \ominus -overlap;
 - No succinct explanations for F^0

Curbing our expectations I

- MinDS₄: Minimize F^0 , given $F^1 \equiv E^1$ constant, and such that
 - 1. $E^0 \models F^0$
 - 2. $F^0 \wedge E^1 \vDash \bot$
 - · No \ominus -overlap;
 - No succinct explanations for F^1
- MinDS₃: Same as MinDS₄, but target F^1 given $F^0 \equiv E^0$ constant
 - · Also, no \ominus -overlap;
 - No succinct explanations for F^0
- $MinDS_2$: Minimize both F^0 and F^1 , such that
 - 1. $E^0 \models F^0$
 - 2. $E^1 \vDash F^1$
 - 3. $F^0 \wedge E^1 \vDash \bot$
 - 4. $F^1 \wedge E^0 \vDash \bot$
 - · Also, no \mathcal{E}^{\ominus} -overlap; but $(\mathcal{U}\setminus\mathcal{E})^{\ominus}$ -overlap may exist
 - All explanations succinct

Curbing our expectations II

• $MinDS_1$: Minimize both F^0 and F^1 , such that

- 1. $E^0 \models F^0$
- 2. $E^1 \models F^1$
- 3. $F^1 \wedge F^0 \vDash \bot$
- No \mathcal{U}^{\ominus} -overlap
- + Default rule may be required for points in $\mathcal{U} \setminus \mathcal{E}$
- $\cdot\,$ And, default rule explanations not succinct

Curbing our expectations II

• $MinDS_1$: Minimize both F^0 and F^1 , such that

- 1. $E^0 \models F^0$
- 2. $E^1 \models F^1$
- 3. $F^1 \wedge F^0 \vDash \bot$
- · No \mathcal{U}^{\ominus} -overlap
- + Default rule may be required for points in $\mathcal{U} \setminus \mathcal{E}$
- And, default rule explanations not succinct

- Complexity-wise:
 - Decision formulations of MinDS₁, MinDS₂, MinDS₃, MinDS₄ are complete for NP
 - In principle, could be solved with MaxSAT
 - But no closed MaxSAT models for now

Experimental setup & initial results

- 49 datasets from the PMLB repository
- Assessment of MinDS1, MinDS2 and MP92, w/ and w/o SBPs
 - A basic model MP92 developed in the 90s
 - We devised SBPs for the MinDS and the MP92 models
- $\cdot\,$ Comparison with (state of the art) IDS
 - Heuristic approach, using smooth local search
 - Default settings & additional settings
- All experiments on an Intel Xeon E5-2630 2.60GHz processor with 64GB of memory, running Ubuntu Linux
 - Timeout of 600s and memout of 10GB

[KKRR92]

[LBL16]

Experimental setup & initial results

- 49 datasets from the PMLB repository
- Assessment of MinDS1, MinDS2 and MP92, w/ and w/o SBPs
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MP92	MP92+SBP	$MinDS_2$	$MinDS_2 + SBP$	$MinDS_1$	$MinDS_1 + SBP$	IDS-supp0.2	IDS-supp0.5
42	45	42	45	6	6	0	2

[KKRR92]

LBL16]

Background

Decision Sets

A Word on Decision Trees

Propositional encodings for DTs

- Proposed tight encoding for computing smallest decision tree
 - Encoding also serves to **pick** the structure of the binary tree
- Encoding much tighter (and more general) than earlier work

SAT	Weather	Mouse	Cancer	Car	Income
DT2*	27K	3.5M	92G	842M	354G
DT1	190K	1.2M	5.2M	4.1M	1.2G

- Several recent alternative proposals
 - $\cdot\,$ At least one outperforms our approach

[VZ19, HRS19, VNP+19]

[VNP+19]

[BHO09]

Part 2

Computing Rigorous Explanations

Component	Representation	Notes
	С	Conjunction of literals, i.e. cube
	F	Model encoding, e.g. SAT/SMT/CP/ILP/FOL
Cat	ε	Predicted class, i.e. literal
What we know

 $\mathcal{C}\wedge\mathcal{F}\vDash\mathcal{E}$

What we know		$\mathcal{C}\wedge\mathcal{F}\vDash\mathcal{E}$		
Propositional Abduction	Hypotheses	С		
	Theory	${\cal F}$		
	Manifestation	${\cal E}$		
Goal	Find $\mathcal{C}_m \subseteq \mathcal{C}$, s.t.	$\mathcal{C}_m \land \mathcal{F} \nvDash \perp \land \mathcal{C}_m \land \mathcal{F} \vDash \mathcal{E}$		

What we know	C ,	$\land \mathcal{F} \vDash \mathcal{E}$
Propositional Abduction	Hypotheses Theory Manifestation	C F E
Goal	Find $\mathcal{C}_m \subseteq \mathcal{C}$, s.t.	$\mathcal{C}_m \land \mathcal{F} \nvDash \bot \land \mathcal{C}_m \land \mathcal{F} \vDash \mathcal{E}$
But, And, Thus,	$\mathcal{C}_m \land \mathcal{F} \nvDash \perp$ is tautology $\mathcal{C}_m \land \mathcal{F} \vDash \mathcal{E}$ iff $\mathcal{C}_m \vDash \mathcal{F} \rightarrow \mathcal{C}_m$ is prime implicant of	\mathcal{E} of $\mathcal{F} ightarrow \mathcal{E}$

What we know	$\mathcal{C}\wedge\mathcal{F}Dash\mathcal{E}$	
Propositional Abduction	Hypotheses Theory Manifestation	С <i>F</i> Е
Goal	Find $\mathcal{C}_m \subseteq \mathcal{C}$, s.t.	$\mathcal{C}_m \land \mathcal{F} \nvDash \bot \land \mathcal{C}_m \land \mathcal{F} \vDash \mathcal{E}$
But, And, Thus,	$\mathcal{C}_m \land \mathcal{F} \nvDash \bot \text{ is tautology}$ $\mathcal{C}_m \land \mathcal{F} \vDash \mathcal{E} \text{ iff } \mathcal{C}_m \vDash \mathcal{F} \to \mathcal{E}$ $\mathcal{C}_m \text{ is prime implicant of } \mathcal{F} \to \mathcal{E}$	ε

We can compute subset-/cardinality-minimal (prime) implicants

What we know	$\mathcal{C}\wedge\mathcal{F}$ =	= <i>E</i>		
Propositional Abduction	Hypotheses Theory	C F	Obs: For any instance tent with C_m , and give model \mathcal{F} , the prediction	consis- ven the on is $\mathcal E$!
Goal	Manifestation Find $\mathcal{C}_m \subseteq \mathcal{C}$, s.t.	${\cal E}$ ${\cal C}_m \wedge .$	$\mathcal{F} \nvDash \stackrel{!}{\rightharpoonup} \wedge \mathcal{C}_m \wedge \mathcal{F} \vDash \mathcal{E}$	
But, And, Thus,	$C_m \land \mathcal{F} \nvDash \bot \text{ is tautology}$ $C_m \land \mathcal{F} \vDash \mathcal{E} \text{ iff } C_m \vDash \mathcal{F} \to \mathcal{E}$ $C_m \text{ is prime implicant of \mathcal{F} \to \mathcal{F}$	$\rightarrow \mathcal{E}$		

We can compute **subset**-/**cardinality**-minimal (prime) implicants - **i.e. explanations!**

```
Input: formula \mathcal{F}, input cube \mathcal{C}, prediction \mathcal{E}
Output: Subset-minimal explanation \mathcal{C}_m \subseteq \mathcal{C}
begin
for l \in \mathcal{C}:
if Entails(\mathcal{C} \setminus \{l\}, \mathcal{F} \to \mathcal{E}):
\mathcal{C} \leftarrow \mathcal{C} \setminus \{l\}
return \mathcal{C}
end
```

```
Input: formula \mathcal{F}, input cube \mathcal{C}, prediction \mathcal{E}
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```
Input: formula \mathcal{F}, input cube \mathcal{C}, prediction \mathcal{E}
Output: Cardinality-minimal explanation C_m \subseteq C
\Gamma \leftarrow \emptyset
while true do
      \mathcal{C}_m \leftarrow \mathsf{MinimumHS}(\Gamma)
      if Entails(\mathcal{C}_m, \mathcal{F} \to \mathcal{E}) :
             return C_m
      else:
            \mu \leftarrow \text{GetAssignment}()
            C_T \leftarrow \mathsf{PickFalseLits}(\mathcal{C} \setminus \mathcal{C}_m, \mu)
            \Gamma \leftarrow \Gamma \cup \mathcal{C}_{\mathcal{T}}
end
```

// Implicit hitting set dualization

```
Input: formula \mathcal{F}, input cube \mathcal{C}, prediction \mathcal{E}
Output: Cardinality-minimal explanation C_m \subseteq C
\Gamma \leftarrow \emptyset
while true do
     \mathcal{C}_m \leftarrow \mathsf{MinimumHS}(\Gamma)
                                                                                                  // Implicit hitting set dualization
      if Entails(\mathcal{C}_m, \mathcal{F} \to \mathcal{E}) :
            return C_m
      else:
            \mu \leftarrow \text{GetAssignment}()
           \mathcal{C}_{T} \leftarrow \mathsf{PickFalseLits}(\mathcal{C} \setminus \mathcal{C}_{m}, \mu)
            \Gamma \leftarrow \Gamma \cup \mathcal{C}_{\mathcal{T}}
end
                                                                                                                        Computes
                                                                                                                         smallest
```

prime

Encodings NNs



- Each layer (except first) viewed as a **block**
 - + Compute \mathbf{x}' given input \mathbf{x} , weights matrix \mathbf{A} , and bias vector \mathbf{b}
 - + Compute output $\mathbf y$ given $\mathbf x'$ and activation function

Encodings NNs



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 - + Compute \mathbf{x}' given input \mathbf{x} , weights matrix \mathbf{A} , and bias vector \mathbf{b}
 - + Compute output \mathbf{y} given \mathbf{x}' and activation function
- $\cdot\,$ Each unit uses a ReLU activation function

[NH10]

Encoding NNs using MILP

Computation for a NN ReLU **block**:

 $\mathbf{x}' = \mathbf{A} \cdot \mathbf{x} + \mathbf{b}$ $\mathbf{y} = \max(\mathbf{x}', \mathbf{0})$

Encoding NNs using MILP

Computation for a NN ReLU **block**:

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Encoding each **block**:

$$\sum_{j=1}^{n} a_{i,j} x_j + b_i = y_i - s_i$$

$$z_i = 1 \to y_i \le 0$$

$$z_i = 0 \to s_i \le 0$$

$$y_i \ge 0, s_i \ge 0, z_i \in \{0, 1\}$$

Simpler encodings exist, but not as effective

[KBD+17]

Sample of experimental results

Dataset			Min	imal expla	nation	Minimum explanation		
			size	SMT (s)	MILP (s)	size	SMT (s)	MILP (s)
australian	(14)	m a M	$\begin{smallmatrix}&1\\8.79\\14\end{smallmatrix}$	$0.03 \\ 1.38 \\ 17.00$	$0.05 \\ 0.33 \\ 1.43$	 		 _
backache	(32)	m a M	$\begin{array}{r}13\\19.28\\26\end{array}$	$0.13 \\ 5.08 \\ 22.21$	$0.14 \\ 0.85 \\ 2.75$			
breast-cancer	(9)	m a M	$\begin{array}{c}3\\5.15\\9\end{array}$	$0.02 \\ 0.65 \\ 6.11$	$0.04 \\ 0.20 \\ 0.41$	$\begin{smallmatrix}&3\\4.86\\&9\end{smallmatrix}$	$0.02 \\ 2.18 \\ 24.80$	$0.03 \\ 0.41 \\ 1.81$
cleve	(13)	m a M	$\begin{array}{c} 4\\ 8.62\\ 13 \end{array}$	$0.05 \\ 3.32 \\ 60.74$	$0.07 \\ 0.32 \\ 0.60$	4 7.89 13		$0.07 \\ 5.14 \\ 39.06$
hepatitis	(19)	m a M		$0.02 \\ 0.07 \\ 0.26$	$0.04 \\ 0.06 \\ 0.20$	$\begin{array}{r}4\\9.39\\19\end{array}$	$0.01 \\ 4.07 \\ 27.05$	$0.04 \\ 2.89 \\ 22.23$
voting	(16)	m a M	$\begin{array}{c}3\\4.56\\11\end{array}$	$0.01 \\ 0.04 \\ 0.10$	$0.02 \\ 0.13 \\ 0.37$	$\begin{array}{c}3\\3.46\\11\end{array}$	$0.01 \\ 0.3 \\ 1.25$	$0.02 \\ 0.25 \\ 1.77$
spect	(22)	m a M	$3 \\ 7.31 \\ 20$	$0.02 \\ 0.13 \\ 0.88$	$0.02 \\ 0.07 \\ 0.29$	$\begin{array}{c}3\\6.44\\20\end{array}$	$0.02 \\ 1.61 \\ 8.97$	$0.04 \\ 0.67 \\ 10.73$

Part 3

Assessing Heuristic Explanations

• Many (highly visible) heuristic explanation approaches:

•	LIME	[RSG16]
•	SHAP	[LL17]
•	Anchor	[RSG18]

• Many (highly visible) heuristic explanation approaches:

•	LIME	[RSG16]
•	SHAP	[L17]
•	Anchor	[RSG18]
•		

• Q: How to assess the quality of heuristic explanations?

What is the **global** quality of heuristic explanations in light of computed **local** explanations?

- Learn ML model
 - $\cdot\,$ Focused on boosted trees obtained with XGBoost

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 - 2. It it holds but has redundant literals (i.e. it's pessimistic), then refine it

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- Compute local explanation for some instance
- Use our abduction-based approach to assess whether local explanation holds globally, and
 - 1. If it does **not** (i.e. it's **optimistic**), then **fix** it
 - 2. It it holds but has redundant literals (i.e. it's pessimistic), then refine it
 - 3. Otherwise, report the local explanation as a global explanation

An example - zoo dataset



An example – zoo dataset



- Example instance:

An example - zoo dataset



• Explanation obtained with Anchor

[RSG18

IF \neg hair $\land \neg$ milk $\land \neg$ toothed $\land \neg$ finsTHEN(class = reptile)

An example – zoo dataset



• But, explanation incorrectly holds on another instance (from training data)

		Explanations						
Dataset	(# unique)	optir	optimistic		pessimistic		realistic	
		LIME	Anchor	LIME	Anchor	LIME	Anchor	
adult	(5579)	61.3%	80.5%	7.9%	1.6%	30.8%	17.9%	
lending	(4414)	24.0%	3.0%	0.4%	0.0%	75.6%	97.0%	
recidivism	(3696)	94.1%	99.4%	4.6%	0.4%	1.3 %	0.2%	
compas	(778)	71.9%	84.4%	20.6%	1.7 %	7.5%	13.9 %	
german	(1000)	85.3%	99.7%	14.6%	0.2%	0.1 %	0.1 %	

		Explanations						
Dataset	(# unique)	optin	optimistic		pessimistic		realistic	
		LIME	Anchor	LIME	Anchor	LIME	Anchor	
adult	(5579)	61.3%	80.5%	7.9%	1.6%	30.8%	17.9%	
lending	(4414)	24.0%	3.0%	0.4%	0.0%	75.6%	97.0%	
recidivism	(3696)	94.1%	99.4%	4.6%	0.4%	1.3 %	0.2%	
compas	(778)	71.9%	84.4%	20.6%	1.7 %	7.5%	13.9 %	
german	(1000)	85.3%	99.7%	14.6%	0.2%	0.1 %	0.1 %	



How often are local explanations consistent with prediction?

- Exploit ML model with SAT-based encoding
 - In our case: used binarized neural networks (BNNs)

• Compute local explanations with Anchor (similar results with LIME or SHAP)

• Use (approximate) model counter to assess how often explanation is consistent with prediction

Preliminary results



• Anchor often claims $\approx 99\%$ precision

Preliminary results



• Anchor often claims \approx 99% precision; out results demonstrate otherwise

Part 4

Explanations vs. Adversarial Examples
- Vast body of work on computing explanations (XPs)
 - \cdot Mostly heuristic approaches, with recent rigorous solutions

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- \cdot Vast body of work on coping with adversarial examples (AEs)
 - $\cdot\,$ Both heuristic and rigorous approaches

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- \cdot We recently proposed a (first) link between XPs and AEs

[INMS19]

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 - Both heuristic and rigorous approaches
- Can XPs and AEs be somehow related?
 - Recent work observed that some connection existed, but formal connection has been elusive
- We recently proposed a (first) link between XPs and AEs
 - The work exploits hitting set duality, first studied in model-based diagnosis

Evamplo	Input Attributes										
Example	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Туре	Est	WillWait
<i>X</i> ₁	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0-10	$y_1 = Yes$
X_2	Yes	No	No	Yes	Full	\$	No	No	Thai	30-60	$y_2 = No$
X ₃	No	Yes	No	No	Some	\$	No	No	Burger	0-10	$y_3 = Yes$
X_4	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	$y_4 = Yes$
X_5	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	$y_5 = No$
X ₆	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0-10	$y_6 = Yes$
X_7	No	Yes	No	No	None	\$	Yes	No	Burger	0-10	$y_7 = No$
X8	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0-10	$y_8 = Yes$
X_9	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	$y_9 = No$
X10	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10-30	$y_{10} = No$
X ₁₁	No	No	No	No	None	\$	No	No	Thai	0-10	$y_{11} = No$
X_{12}	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30-60	$y_{12} = $ Yes

A well-known example (Cont.)

• 10 features:

{A(lternate), B(ar), W(eekend), H(ungry), Pa(trons), Pr(ice), Ra(in), Re(serv.), T(ype), E(stim.)}

• Example instance (x_1 , with outcome $y_1 =$ Yes):

 $\{A, \neg B, \neg W, H, (Pa = Some), (Pr = \$\$), \neg Ra, Re, (T = French), (E = 0-10)\}$

• A possible decision set (obtained with some off-the-shelf tool, & <u>function</u>*):

IF	$(Pa = Some) \land \neg(E = >60)$	THEN	(Wait = Yes)	(R1)
IF	$W \land \neg(Pr = \$\$\$) \land \neg(E = >60)$	THEN	(Wait = Yes)	(R2)
IF	$\neg W \land \neg(Pa = Some)$	THEN	(Wait = No)	(R3)
IF	(E = >60)	THEN	(Wait = No)	(R4)
IF	$\neg(Pa = Some) \land (Pr = \$\$)$	THEN	(Wait = No)	(R5)

Counterexamples & breaks

A subset-minimal set C of literals is a counterexample (CEx) to a prediction π , if $C \models (\mathcal{M} \rightarrow \rho)$, with $\rho \in \mathbb{K} \land \rho \neq \pi$

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• Breaks:

A literal τ_i breaks a set of literals S (each denoting a different feature) if S contains a literal inconsistent with τ_i

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- Back to the example, consider prediction (Wait = Yes):
 - Using (R1) (and assuming a consistent instance), an explanation is:

 $(Pa = Some) \land \neg(E = >60)$

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 \cdot Due to (R5), a counterexample is:

 $\neg(Pa = Some) \land (Pr = \$\$)$

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 - Using (R1) (and assuming a consistent instance), an explanation is:

 $(Pa = Some) \land \neg(E = >60)$

• Due to (R5), a counterexample is:

$$\neg$$
(Pa = Some) \land (Pr = \$\$\$)

• XP $S_1 = \{(Pa = Some), \neg(E = >60)\}$ breaks CEx $S_2 = \{\neg(Pa = Some), (Pr = \$\$\}\}$ and vice-versa

1. Relationship between XPs with CEx's:

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 - Each XP breaks every CEx

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 - \therefore XPs can be computed from all CEx's (by HSD) and vice-versa

- 1. Relationship between XPs with CEx's:
 - Each XP breaks every CEx
 - Each CEx breaks every XP
 - : XPs can be computed from all CEx's (by HSD) and vice-versa

2. Given instance \mathcal{I}_{r} an AE can be computed from closest CEx

- Restaurant dataset
- ML model is decision set (shown earlier)
- Prediction is (Wait = Yes)
- Global explanations:
 - 1. (Pa = Some) $\land \neg(E = >60)$
 - 2. $W \land \neg(Pr = \$\$) \land \neg(E = >60)$
- Counterexamples:
 - 1. $\neg W \land \neg (Pa = Some)$
 - 2. (E = >60)
 - 3. $\neg(Pa = Some) \land (Pr = \$\$)$
- The XP's break the CEx's and vice-versa

Conclusions & roadmap

- Glimpse of work on learning interpretable ML models (using SAT)
 - Smallest decision trees & decision sets
- New approach for finding explanations of black-box models by computing prime implicants (using ILP&SMT)
 - $\cdot\,$ Results for ${\rm NNs}$ and for ${\rm BTs}$
- Hitting set duality between explanations and counterexamples
 - $\cdot\,$ Can compute CEx's from XP's and AEs from CEx's

Conclusions & roadmap

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- Hitting set duality between explanations and counterexamples
 - $\cdot\,$ Can compute CEx's from XP's and AEs from CEx's
- Our remit @ ANITI:

To explain, to verify & to learn ML models

with guarantees of **rigor**, by using AR tools & techniques

Questions?





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