## Automated Reasoning for Explainable al

Joao Marques-Silva

ANITI, Univ. Toulouse, France

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## A disclaimer

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



Quantification \& CEGAR (QBF, QMaxSAT, etc.)

Function Synthesis (Min DNF cover, ...)

Optimization (MaxSAT, MinSAT, PBO, WBO, etc.)


Propositional Encodings, Backbones, Autarkies, Minimal models, etc.

## Enumeration

 (MUSes, MCSes, etc.)Proof Systems
(DRMaxSAT, etc.)
Primes, Abduction,
DLs, etc.

## A disclaimer - new area of research, since 2018...

Quantification \& CEGAR (QBF, QMaxSAT, etc.)

Function Synthesis

(Min DNF cover, ...)

Model Checking, Synthesizing Invariants, ATPG, Reconfiguration

Enumeration (MUSes, MCSes, etc.)

Proof Systems
(DRMaxSAT, etc.)
Primes, Abduction,
DLs, etc.
Explainability \& Interpretability in ML

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Quantification \& CEGAR
Function Synthesis

Inconsistency (MUS, MCS, etc.)
(QBF, QMaxSAT, etc.)
(Min DNF cover, ...)

Model Checking, Synthesizing Invariants, ATPG, Reconfiguration

Propositional Encodings, Backbones, Autarkies, Minimal models, etc.

Primes, Abduction, DLs, etc.


Proof Systems
(DRMaxSAT, etc.)

Optimization (MaxSAT, MinSAT, PBO, WBO, etc.)


## Recent \& ongoing ML successes


(0) DeepMind $\because$ AlphaGo

AlphaGo Zero \& Alpha Zero

Image \& Speech Recognition
ILSVRC top-5 Error on ImageNet



## 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

Original image


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


Benign

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.


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) |
| :---: | :---: | :---: | :---: | :---: | :---: |
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## Also, some ML models are interpretable

$$
\begin{array}{l|l}
\hline \text { decision|rule lists|sets } & \text { if } \neg \text { Meeting then Hike } \\
\text { decision trees; ... } & \text { if } \neg \text { Vacation then } \neg \text { Hike }
\end{array}
$$

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## But other ML models are not (interpretable)...



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## But other ML models are not (interpretable)...



## But other ML models are not (interpretable)...



## 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?


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## Machine Learning System



This is a cat.

Current Explanation

This is a cat:

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


XAI Explanation

## Why XAI?

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

 of 27 April 2016on 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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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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A new bill would force companies to check their algorithms for bias

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## Explainable Artificial Intelligence (XAI)



David Gunning
DARPA/I2O
Program Update November 2017

## Why XAI?


In order to only improve their robust- the council $\substack{\text { on the } \\ \text { move }}$ we must not only develop ways to make ness, ${ }^{5}$ but also develop, In te. Intelligi- tron ion en gus the free
European Union regulation their reasoning ins spot AI that makes and a "right bility will help us sporisutional drift or Bypecomanem mistakes due to mentations of goals mpanies to check their



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 when AI errs.

DARPA

## XAI \& EU guidelines

## Ethics guidelines for trustworthy Al

Following the publication of the draft ethics guidelines in December 2018 to which more than 500 comments were received, the independent expert group presents today their ethics guidelines for trustworthy artificial intelligence.

About Artificial intelligence

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## XAI \& the principle of explicability


$\square$

European Commission > Strategy > Digital Single Market > Reports an

## Digital Single Market

REPORT/CATi f explicability maintaining users' trus openly commun information, a decision what combinationd and
The principle of exp foulding and maspose of Al sys ffected. Without surputput or dec as ablack box a aditability and
 transparent, the capable to those directly model has g possible. These cability measures le.g. contested. An explantributed to tha circumstances, may be fundamenal onences if that output is erroup presents today their

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Blog posts
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\section*{XAI \& the principle of explicability}

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European Commission > Strategy > Digital Single Market > Reports an
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News

\section*{Today's talk}

\section*{Goals: Overview our work at intersection of AR \& ML}
- Part \#1: Learning interpretable models (brief)
- Additional detail in our IJCAl'18 \& IJCAR'18 papers
- Part \#2: Rigorous explanations for black-box models
- Additional detail in our AAAl'19 paper
- Part \#3: Assessing heuristic explanations (brief)
- Additional detail in our SAT'19 \& CoRR'19 papers
- Part \#4: Relating explanations with adversarial examples (brief)
- Additional detail in our NIPS'19 paper

\section*{Part 1}

\section*{Learning Interpretable ML Models}

\section*{Outline}

Background

\section*{Decision Sets}

A Word on Decision Trees

\section*{Classification problems I}
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- Binary features: \(\mathcal{F}=\left\{f_{1}, \ldots, f_{k}\right\}\)
- Literals: \(f_{r}\) and \(\neg f_{r}\)

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- Feature space: \(\mathcal{U} \triangleq \prod_{r=1}^{K}\left\{f_{r}, \neg f_{r}\right\}\)
- Binary classification: \(\mathcal{C}=\left\{c_{0}=0, c_{1}=1\right\}\)
- \(\mathcal{E}\) partitioned into \(\mathcal{E}^{-}\)and \(\mathcal{E}^{+}\)

\section*{Classification problems II}
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\end{tabular}
- \(e_{q} \in \mathcal{E}\) represented as a 2-tuple \(\left(\pi_{q}, \varsigma_{q}\right)\)
- \(\pi_{q} \in \mathcal{U}\) : literals associated with the example
- \(\varsigma_{q} \in\{0,1\}\) is the class of example

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- A literal \(l_{r}\) on a feature \(f_{r}, l_{r} \in\left\{f_{r}, \neg f_{r}\right\}\), 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

\section*{Example}
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\end{tabular}
- Binary features: \(\mathcal{F}=\left\{f_{1}, f_{2}, f_{3}, f_{4}\right\}\)
- \(f_{1} \triangleq V, f_{2} \triangleq C, f_{3} \triangleq M\), and \(f_{4} \triangleq E\)
- \(e_{1}\) is represented by the 2-tuple \(\left(\pi_{1}, \varsigma_{1}\right)\),
- \(\pi_{1}=(\neg \mathrm{V}, \neg \mathrm{C}, \mathrm{M}, \neg \mathrm{E})\)
- \(\varsigma_{1}=0\)
- Literals V, C, \(\neg \mathrm{M}\) and E discriminate \(e_{1}\)
\(\cdot \mathcal{U}=\{\mathrm{V}, \neg \mathrm{V}\} \times\{\mathrm{C}, \neg \mathrm{C}\} \times\{\mathrm{M}, \neg \mathrm{M}\} \times\{\mathrm{E}, \neg \mathrm{E}\}\)

\section*{Goal of explainable classification - our take}

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

\section*{Outline}

\section*{Background}

Decision Sets

A Word on Decision Trees

\section*{Itemsets \& decision sets}
- Given \(\mathcal{F}\), an itemset \(\pi\) is an element of \(\mathcal{I} \triangleq \prod_{r=1}^{K}\left\{f_{r}, \neg f_{r}, \mathfrak{u}\right\}\)
- u represents a don't care value

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- A rule is a 2 -tuple ( \(\pi, \varsigma\) ), with itemset \(\pi \in \mathcal{I}\), and class \(\varsigma \in \mathcal{C}\) Rule ( \(\pi, \varsigma\) ) interpreted as:
IF all specified literals in \(\pi\) are true, THEN pick class \(\varsigma\)

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IF all specified literals in \(\pi\) are true, THEN pick class \(\varsigma\)
- A decision set \(\mathbb{S}\) 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 \(\mathbb{S}\)
- Default rule is optional and used only when other rules do not apply on some feature space point

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\end{tabular}
- Rule 1: \(\left((\mathfrak{u}, \mathfrak{u}, \neg \mathrm{M}, \mathfrak{u}), \mathrm{c}_{1}\right)\)
- Meaning: if \(\neg\) Meeting then Hike
- Rule 2: (( \(\left.\neg \vee, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_{0}\right)\)
- Meaning: if \(\neg\) Vacation then \(\neg\) Hike

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- Rule 2: (( \(\left.\neg \vee, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_{0}\right)\)
- Meaning: if \(\neg\) Vacation then \(\neg\) Hike
- Default rule: \(\left(\emptyset, c_{0}\right)\)
- Meaning: if all other rules do not apply, then pick \(\neg\) Hike

\section*{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 \(\pi_{2}[r]=f_{r}\)

\section*{Issue with unordered rules - overlap}
- Itemsets \(\pi_{1}, \pi_{2} \in \mathcal{I}\) clash, \(\pi_{1} \cap \pi_{2}=\emptyset\), if for some coordinate \(r\) :
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- Two rules \(r_{1}=\left(\pi_{1}, \varsigma_{1}\right)\) and \(r_{2}=\left(\pi_{2}, \varsigma_{2}\right)\) overlap if \(\pi_{1}\) and \(\pi_{2}\) do not clash, i.e.
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\pi_{1} \cap \pi_{2} \neq \emptyset
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- Can be restricted to some set, e.g. \(\mathcal{E}\)

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- Forms of overlap:
- \(\oplus\) : overall where rules agree in prediction
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- Can be restricted to some set, e.g. \(\mathcal{E}\)
- Forms of overlap:
- \(\oplus\) : overall where rules agree in prediction
- \(\ominus\) : overlap where rules disagree in prediction
- Our goal:

Minimize number of rules in decision set, and provide guarantees in terms of overlap, namely \(\ominus\)-overlap

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\begin{tabular}{|c|c|c|c|c||c|}
\hline Ex. & Vacation (V) & Concert (C) & Meeting (M) & Expo (E) & Hike (H) \\
\hline \hline\(e_{1}\) & 0 & 0 & 1 & 0 & 0 \\
\hline\(e_{2}\) & 1 & 0 & 0 & 0 & 1 \\
\hline\(e_{3}\) & 0 & 0 & 1 & 1 & 0 \\
\hline\(e_{4}\) & 1 & 0 & 0 & 1 & 1 \\
\hline\(e_{5}\) & 0 & 1 & 1 & 0 & 0 \\
\hline\(e_{6}\) & 0 & 1 & 1 & 1 & 0 \\
\hline\(e_{7}\) & 1 & 1 & 0 & 1 & 1 \\
\hline
\end{tabular}
- Decision set:
\[
\left\{\left((\neg V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_{0}\right),\left((\mathfrak{u}, \mathfrak{u}, \neg M, \mathfrak{u}), c_{1}\right)\right\}
\]
- No \(\mathcal{E}^{\ominus \text {-overlap }}\)

\section*{Example}
\begin{tabular}{|c|c|c|c|c||c|}
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\end{tabular}
- Decision set:
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\]
- No \(\mathcal{E}^{\ominus}\)-overlap
- But, there exists overlap in feature space
- \(\ominus\)-overlap for \((\neg \mathrm{V}, \neg \mathrm{C}, \neg \mathrm{M}, \neg \mathrm{E}) \in \mathcal{U} \backslash \mathcal{E}\)

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- Decision set:
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- But, there exists overlap in feature space
- \(\ominus\)-overlap for \((\neg \mathrm{V}, \neg \mathrm{C}, \neg \mathrm{M}, \neg \mathrm{E}) \in \mathcal{U} \backslash \mathcal{E}\)
- However, there exists no \(\mathcal{U}^{\ominus}\)-overlap for decision set:
\[
\left\{\left((V, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_{1}\right),\left((\neg \vee, \mathfrak{u}, \mathfrak{u}, \mathfrak{u}), c_{0}\right)\right\}
\]

\section*{Succinct explanations}
- 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

\section*{Stating our goals}
- Assumptions:
- Represent \(\mathcal{E}^{-}\)with Boolean function \(E^{0}\)
- True for each example \(\mathcal{E}^{-}\)
- Represent \(\mathcal{E}^{+}\)with Boolean function \(E^{1}\)
- True for each example \(\mathcal{E}^{+}\)
- Also, let \(E^{0} \wedge E^{1} \vDash \perp\)

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- Represent \(\mathcal{E}^{+}\)with Boolean function \(E^{1}\)
- True for each example \(\mathcal{E}^{+}\)
- Also, let \(E^{0} \wedge E^{1} \vDash \perp\)
- 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 \(E^{1} \vDash F^{1}\)


\section*{An ideal model - MinDS 0}
- \(\mathrm{MinDS}_{0}\) :

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. \(F^{1} \leftrightarrow F^{0} \vDash \perp\)
- No \(\mathcal{U}^{\ominus}\)-overlap

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- Obs: MinDS \(_{0}\) ensures succinct explanations
- Computes \(F^{0}\) and \(F^{1}\) (i.e. no negation) and no default rule

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- No \(\mathcal{U}^{\ominus}\)-overlap
- Obs: MinDS \(0_{0}\) ensures succinct explanations
- Computes \(F^{0}\) and \(F^{1}\) (i.e. no negation) and no default rule
- Complexity-wise:
- \(M_{i n D S} \in \Sigma_{2}^{P}\)
- A conjecture: MinDSo hard for \(\Sigma_{2}^{P}\)

\section*{Curbing our expectations I}
- MinDS 4 : Minimize \(F^{0}\), given \(F^{1} \equiv E^{1}\) constant, and such that
1. \(E^{0} \vDash F^{0}\)
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- No succinct explanations for \(F^{1}\)

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- No \(\ominus\)-overlap;
- No succinct explanations for \(F^{1}\)
- \(\mathrm{MinDS}_{3}\) : Same as \(\mathrm{MinDS}_{4}\), but target \(F^{1}\) given \(F^{0} \equiv E^{0}\) constant
- Also, no \(\ominus\)-overlap;
- No succinct explanations for \(F^{0}\)

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- MinDS \(_{4}\) : Minimize \(F^{0}\), given \(F^{1} \equiv E^{1}\) constant, and such that
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- \(\mathrm{MinDS}_{3}\) : Same as \(\mathrm{MinDS}_{4}\), 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. \(E^{0} \vDash F^{0}\)
2. \(E^{1} \vDash F^{1}\)
3. \(F^{0} \wedge E^{1} \vDash \perp\)
4. \(F^{1} \wedge E^{0} \vDash \perp\)
- Also, no \(\mathcal{E}^{\ominus}\)-overlap; but \((\mathcal{U} \backslash \mathcal{E})^{\ominus}\)-overlap may exist
- All explanations succinct

\section*{Curbing our expectations II}
- MinDS \({ }_{1}\) : Minimize both \(F^{0}\) and \(F^{1}\), such that
1. \(E^{0} \vDash F^{0}\)
2. \(E^{1} \vDash F^{1}\)
3. \(F^{1} \wedge F^{0} \vDash \perp\)
- No \(\mathcal{U}^{\ominus}\)-overlap
- Default rule may be required for points in \(\mathcal{U} \backslash \mathcal{E}\)
- And, default rule explanations not succinct

\section*{Curbing our expectations II}
- MinDS \(1_{1}\) : Minimize both \(F^{0}\) and \(F^{1}\), such that
1. \(E^{0} \vDash F^{0}\)
2. \(E^{1} \vDash F^{1}\)
3. \(F^{1} \wedge F^{0} \vDash \perp\)
- No \(\mathcal{U}^{\ominus}\)-overlap
- Default rule may be required for points in \(\mathcal{U} \backslash \mathcal{E}\)
- And, default rule explanations not succinct
- Complexity-wise:
- Decision formulations of MinDS \(_{1}, \mathrm{MinDS}_{2}, \mathrm{MinDS}_{3}, \mathrm{MinDS} S_{4}\) are complete for NP
- In principle, could be solved with MaxSAT
- But no closed MaxSAT models for now

\section*{Experimental setup \& initial results}
- 49 datasets from the PMLB repository
- Assessment of MinDS \(1, M_{1}\) DS \(_{2}\) 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
- 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 600 s and memout of 10 GB

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\begin{tabular}{cccccccc}
\hline MP92 & MP92+SBP & MinDS \(_{2}\) & MinDS \(_{2}+\) SBP & MinDS & MinDS \(_{1}+\) SBP & IDS-supp0.2 & IDS-supp0.5 \\
\hline 42 & 45 & 42 & 45 & 6 & 6 & 0 & 2 \\
\hline
\end{tabular}

\section*{Outline}

\section*{Background}

\section*{Decision Sets}

A Word on Decision Trees

\section*{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
\begin{tabular}{|c|c|c|c|c|c|}
\hline SAT & Weather & Mouse & Cancer & Car & Income \\
\hline \hline DT2* & 27 K & 3.5 M & 92 G & 842 M & 354 G \\
DT1 & 190 K & 1.2 M & 5.2 M & 4.1 M & 1.2 G \\
\hline
\end{tabular}
- Several recent alternative proposals
- At least one outperforms our approach

\section*{Part 2}

Computing Rigorous Explanations

\section*{Our approach}
\begin{tabular}{|c|c|c|c|}
\hline Component & Representation & Notes \\
\hline
\end{tabular}

\section*{Relating with abduction}

What we know
\(\mathcal{C} \wedge \mathcal{F} \vDash \mathcal{E}\)

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& Hypotheses & \(\mathcal{C}\) \\
Propositional & Theory & \(\mathcal{F}\) \\
Abduction & Manifestation & \(\mathcal{E}\) \\
Goal & Find \(\mathcal{C}_{m} \subseteq \mathcal{C}\), s.t. & \(\mathcal{C}_{m} \wedge \mathcal{F} \not \models \perp \wedge \mathcal{C}_{m} \wedge \mathcal{F} \vDash \mathcal{E}\)
\end{tabular}

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\end{tabular}
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But, & \(\mathcal{C}_{m} \wedge \mathcal{F} \not \models \perp\) is tautology \\
And, & \(\mathcal{C}_{m} \wedge \mathcal{F} \vDash \mathcal{E}\) iff \(\mathcal{C}_{m} \vDash \mathcal{F} \rightarrow \mathcal{E}\) \\
Thus, & \(\mathcal{C}_{m}\) is prime implicant of \(\mathcal{F} \rightarrow \mathcal{E}\)
\end{tabular}

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

\section*{Relating with abduction}
What we know
\(\mathcal{C} \wedge \mathcal{F} \vDash \mathcal{E}\)


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

\section*{Computing one subset-minimal explanation}
```

Input: formula }\mathcal{F}\mathrm{ , input cube }\mathcal{C}\mathrm{ , prediction }\mathcal{E
Output: Subset-minimal explanation }\mp@subsup{\mathcal{C}}{m}{}\subseteq\mathcal{C
begin
for l }\in\mathcal{C}
if Entails(\mathcal{C}\{l},\mathcal{F}->\mathcal{E}):
\mathcal { C } \leftarrow \mathcal { C } \ \{ l \}
return }\mathcal{C
end

```

\section*{Computing one subset-minimal explanation}

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 \((\mathcal{C} \backslash\{l\}, \mathcal{F} \rightarrow \mathcal{E})\) : \(\mathcal{C} \leftarrow \mathcal{C} \backslash\{l\}\)
return \(\mathcal{C}\)
end


\section*{Computing one cardinality-minimal explanation}
```

Input: formula \mathcal{F}, input cube \mathcal{C}}\mathrm{ , prediction }\mathcal{E
Output: Cardinality-minimal explanation }\mp@subsup{\mathcal{C}}{m}{}\subseteq\mathcal{C
\Gamma \leftarrow \emptyset
while true do
\mathcal{C}
// Implicit hitting set dualization
if Entails(\mathcal{C}
return }\mp@subsup{\mathcal{C}}{m}{
else:
\mu\leftarrowGetAssignment()
\mathcal{C}
\Gamma\leftarrow\Gamma\cup\mathcal{C}
end

```

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Input: formula \(\mathcal{F}\), input cube \(\mathcal{C}\), prediction \(\mathcal{E}\)
Output: Cardinality-minimal explanation \(\mathcal{C}_{m} \subseteq \mathcal{C}\)
\(\Gamma \leftarrow \emptyset\)
while true do
\(\mathcal{C}_{m} \leftarrow\) MinimumHS \((\Gamma)\)
// Implicit hitting set dualization
if Entails \(\left(\mathcal{C}_{m}, \mathcal{F} \rightarrow \mathcal{E}\right)\) : return \(\mathcal{C}_{m}\)
else:
\(\mu \leftarrow\) GetAssignment()
\(\mathcal{C}_{T} \leftarrow\) PickFalseLits \(\left(\mathcal{C} \backslash \mathcal{C}_{m}, \mu\right)\)
\(\Gamma \leftarrow \Gamma \cup \mathcal{C}_{T}\)
end


\section*{Encodings NNs}

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

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\begin{tabular}{ccc} 
Input & Hidden & Output \\
layer & layer & layer
\end{tabular}
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- Compute output \(\mathbf{y}\) given \(\mathbf{x}^{\prime}\) and activation function
- Each unit uses a ReLU activation function

\section*{Encoding NNs using MILP}

Computation for a NN ReLU block:
\[
\begin{aligned}
& \mathbf{x}^{\prime}=\mathbf{A} \cdot \mathbf{x}+\mathbf{b} \\
& \mathbf{y}=\max \left(\mathbf{x}^{\prime}, \mathbf{0}\right)
\end{aligned}
\]

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\end{aligned}
\]

Encoding each block:
\[
\begin{aligned}
& \sum_{j=1}^{n} a_{i, j} x_{j}+b_{i}=y_{i}-s_{i} \\
& z_{i}=1 \rightarrow y_{i} \leq 0 \\
& z_{i}=0 \rightarrow s_{i} \leq 0 \\
& y_{i} \geq 0, s_{i} \geq 0, z_{i} \in\{0,1\}
\end{aligned}
\]

\section*{Sample of experimental results}
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline \multirow[t]{2}{*}{Dataset} & & & \multicolumn{3}{|r|}{Minimal explanation} & \multicolumn{3}{|l|}{Minimum explanation} \\
\hline & & & size & SMT (s) & MILP (s) & size & SMT (s) & MILP (s) \\
\hline \multirow{3}{*}{australian} & \multirow{3}{*}{(14)} & m & 1 & 0.03 & 0.05 & - & - & - \\
\hline & & a & 8.79 & 1.38 & 0.33 & - & - & - \\
\hline & & M & 14 & 17.00 & 1.43 & - & - & - \\
\hline \multirow{3}{*}{backache} & \multirow{3}{*}{(32)} & m & 13 & 0.13 & 0.14 & - & - & - \\
\hline & & a & 19.28 & 5.08 & 0.85 & - & - & - \\
\hline & & M & 26 & 22.21 & 2.75 & - & - & - \\
\hline \multirow{3}{*}{breast-cancer} & \multirow{3}{*}{(9)} & m & 3 & 0.02 & 0.04 & 3 & 0.02 & 0.03 \\
\hline & & a & 5.15 & 0.65 & 0.20 & 4.86 & 2.18 & 0.41 \\
\hline & & M & 9 & 6.11 & 0.41 & 9 & 24.80 & 1.81 \\
\hline \multirow{3}{*}{cleve} & \multirow{3}{*}{(13)} & m & 4 & 0.05 & 0.07 & 4 & - & 0.07 \\
\hline & & a & 8.62 & 3.32 & 0.32 & 7.89 & - & 5.14 \\
\hline & & M & 13 & 60.74 & 0.60 & 13 & - & 39.06 \\
\hline \multirow{3}{*}{hepatitis} & \multirow{3}{*}{(19)} & m & 6 & 0.02 & 0.04 & 4 & 0.01 & 0.04 \\
\hline & & a & 11.42 & 0.07 & 0.06 & 9.39 & 4.07 & 2.89 \\
\hline & & M & 19 & 0.26 & 0.20 & 19 & 27.05 & 22.23 \\
\hline \multirow{3}{*}{voting} & \multirow{3}{*}{(16)} & m & 3 & 0.01 & 0.02 & 3 & 0.01 & 0.02 \\
\hline & & a & 4.56 & 0.04 & 0.13 & 3.46 & 0.3 & 0.25 \\
\hline & & M & 11 & 0.10 & 0.37 & 11 & 1.25 & 1.77 \\
\hline \multirow{3}{*}{spect} & \multirow{3}{*}{(22)} & m & 3 & 0.02 & 0.02 & 3 & 0.02 & 0.04 \\
\hline & & a & 7.31 & 0.13 & 0.07 & 6.44 & 1.61 & 0.67 \\
\hline & & M & 20 & 0.88 & 0.29 & 20 & 8.97 & 10.73 \\
\hline
\end{tabular}

\section*{Part 3}

\section*{Assessing Heuristic Explanations}

\section*{Computing heuristic explanations}
- Many (highly visible) heuristic explanation approaches:
- LIME
- SHAP
- Anchor

\section*{Computing heuristic explanations}
- Many (highly visible) heuristic explanation approaches:
- LIME
- SHAP
- Anchor
- Q: How to assess the quality of heuristic explanations?

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

\section*{Approach}
- Learn ML model
- Focused on boosted trees obtained with XGBoost

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\section*{Approach}
- Learn ML model
- Focused on boosted trees obtained with XGBoost
- 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

\section*{An example - zoo dataset}

- Example instance:

IF \(\quad\) (animal_name \(=\) pitviper) \(\wedge \neg\) hair \(\wedge \neg\) feathers \(\wedge\) eggs \(\wedge \neg\) milk \(\wedge\) \(\neg\) airborne \(\wedge \neg\) aquatic \(\wedge\) predator \(\wedge \neg\) toothed \(\wedge\) backbone \(\wedge\) breathes \(\wedge\) venomous \(\wedge \neg\) fins \(\wedge(\) legs \(=0) \wedge\) tail \(\wedge \neg\) domestic \(\wedge \neg\) catsize
THEN (class = reptile)

\section*{An example - zoo dataset}

- Explanation obtained with Anchor

IF \(\quad \neg\) hair \(\wedge \neg\) milk \(\wedge \neg\) toothed \(\wedge \neg\) fins
THEN (class \(=\) reptile)

\section*{An example - zoo dataset}

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

IF \(\quad(\) animal_name \(=\) toad \() \wedge \neg\) hair \(\wedge \neg\) feathers \(\wedge\) eggs \(\wedge \neg\) milk \(\wedge\) \(\neg\) airborne \(\wedge \neg\) aquatic \(\wedge \neg\) predator \(\wedge \neg\) toothed \(\wedge\) backbone \(\wedge\) breathes \(\wedge\) \(\neg\) venomous \(\wedge \neg\) fins \(\wedge(\) legs \(=4) \wedge \neg\) tail \(\wedge \neg\) domestic \(\wedge \neg\) catsize
THEN (class = amphibian)

\section*{Some results}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline \multirow{3}{*}{Dataset} & \multirow{3}{*}{(\# unique)} & \multicolumn{6}{|c|}{Explanations} \\
\hline & & \multicolumn{2}{|l|}{optimistic} & \multicolumn{2}{|l|}{pessimistic} & \multicolumn{2}{|l|}{realistic} \\
\hline & & LIME & Anchor & LIME & Anchor & LIME & Anchor \\
\hline adult & (5579) & 61.3\% & 80.5\% & 7.9\% & 1.6\% & 30.8\% & 17.9\% \\
\hline lending & (4414) & 24.0\% & 3.0\% & 0.4\% & 0.0\% & 75.6\% & 97.0\% \\
\hline recidivism & (3696) & 94.1\% & 99.4\% & 4.6\% & 0.4\% & 1.3\% & 0.2\% \\
\hline compas & (778) & 71.9\% & 84.4\% & 20.6\% & 1.7\% & 7.5\% & 13.9\% \\
\hline german & (1000) & 85.3\% & 99.7\% & 14.6\% & 0.2\% & 0.1 \% & 0.1 \% \\
\hline
\end{tabular}

\section*{Some results}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline \multirow{3}{*}{Dataset} & \multirow{3}{*}{(\# unique)} & \multicolumn{6}{|c|}{Explanations} \\
\hline & & \multicolumn{2}{|l|}{optimistic} & \multicolumn{2}{|l|}{pessimistic} & \multicolumn{2}{|l|}{realistic} \\
\hline & & LIME & Anchor & LIME & Anchor & LIME & Anchor \\
\hline adult & (5579) & 61.3\% & 80.5\% & 7.9\% & 1.6\% & 30.8\% & 17.9\% \\
\hline lending & (4414) & 24.0\% & 3.0\% & 0.4\% & 0.0\% & 75.6\% & 97.0\% \\
\hline recidivism & (3696) & 94.1\% & 99.4\% & 4.6\% & 0.4\% & 1.3\% & 0.2\% \\
\hline compas & (778) & 71.9\% & 84.4\% & 20.6\% & 1.7\% & 7.5\% & 13.9\% \\
\hline german & (1000) & 85.3\% & 99.7\% & 14.6\% & 0.2\% & 0.1 \% & 0.1 \% \\
\hline
\end{tabular}

How often are local explanations consistent with prediction?

\section*{Approach}
- 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

\section*{Preliminary results}

- Anchor often claims \(\approx 99 \%\) precision

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\section*{Part 4}

\section*{Explanations vs. Adversarial Examples}
- Vast body of work on computing explanations (XPs)
- Mostly heuristic approaches, with recent rigorous solutions
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- The work exploits hitting set duality, first studied in model-based diagnosis

\section*{A well-known example}
[RN10]
\begin{tabular}{|c|c|c|c|c|c|c|c|c|c|c|c|}
\hline \multirow[b]{2}{*}{Example} & \multicolumn{10}{|c|}{Input Attributes} & \multirow[t]{2}{*}{Goal WillWait} \\
\hline & Alt & Bar & Fri & Hun & Pat & Price & Rain & Res & Type & Est & \\
\hline \(\chi_{1}\) & Yes & No & No & Yes & Some & \$\$\$ & No & Yes & French & 0-10 & \(y_{1}=\mathrm{Yes}\) \\
\hline \(x_{2}\) & Yes & No & No & Yes & Full & \$ & No & No & Thai & 30-60 & \(y_{2}=\mathrm{No}\) \\
\hline \(\chi_{3}\) & No & Yes & No & No & Some & \$ & No & No & Burger & 0-10 & \(y_{3}=\mathrm{Yes}\) \\
\hline \(x_{4}\) & Yes & No & Yes & Yes & Full & \$ & Yes & No & Thai & 10-30 & \(y_{4}=\mathrm{Yes}\) \\
\hline \(x_{5}\) & Yes & No & Yes & No & Full & \$\$\$ & No & Yes & French & >60 & \(y_{5}=\mathrm{No}\) \\
\hline \(\chi_{6}\) & No & Yes & No & Yes & Some & \$\$ & Yes & Yes & Italian & 0-10 & \(y_{6}=\mathrm{Yes}\) \\
\hline \(x_{7}\) & No & Yes & No & No & None & \$ & Yes & No & Burger & 0-10 & \(y_{7}=\mathrm{No}\) \\
\hline \(x_{8}\) & No & No & No & Yes & Some & \$\$ & Yes & Yes & Thai & 0-10 & \(y_{8}=\mathrm{Yes}\) \\
\hline \(\chi_{9}\) & No & Yes & Yes & No & Full & \$ & Yes & No & Burger & >60 & \(y_{9}=\mathrm{No}\) \\
\hline \(\chi_{10}\) & Yes & Yes & Yes & Yes & Full & \$\$\$ & No & Yes & Italian & 10-30 & \(y_{10}=\mathrm{No}_{0}\) \\
\hline \(\mathrm{x}_{11}\) & No & No & No & No & None & \$ & No & No & Thai & 0-10 & \(y_{11}=\mathrm{N}_{0}\) \\
\hline \(\chi_{12}\) & Yes & Yes & Yes & Yes & Full & \$ & No & No & Burger & 30-60 & \(\mathrm{y}_{12}=\mathrm{Yes}\) \\
\hline
\end{tabular}

\section*{A well-known example (Cont.)}
- 10 features:
\(\{\mathrm{A}(\) Iternate \(), \mathrm{B}(\) ar ), W(eekend), H(ungry), Pa (trons), \(\operatorname{Pr}(\) ice \(), \operatorname{Ra}(\) in), \(\operatorname{Re}(\) serv.), T (ype), E(stim.) \(\}\)
- Example instance ( \(x_{1}\), with outcome \(\left.y_{1}=Y e s\right)\) :
\[
\{\mathrm{A}, \neg \mathrm{~B}, \neg \mathrm{~W}, \mathrm{H},(\mathrm{~Pa}=\text { Some }),(\operatorname{Pr}=\$ \$ \$), \neg \mathrm{Ra}, \mathrm{Re},(\mathrm{~T}=\text { French }),(\mathrm{E}=0-10)\}
\]
- A possible decision set (obtained with some off-the-shelf tool, \& function*):
\[
\begin{array}{lll}
\text { IF } & (\mathrm{Pa}=\text { Some }) \wedge \neg(\mathrm{E}=>60) & \text { THEN } \\
\text { IF } & (\text { Wait }=Y \mathrm{Yes}) \\
\text { IF } & \neg \neg(\operatorname{Pr}=\$ \$ \$) \wedge \neg(\mathrm{E}=>60) & \text { THEN } \\
\text { (Wait }=\mathrm{Yes}) \\
\text { IF } & \text { TH } \wedge \neg(\mathrm{Pa}=\text { Some }) & \text { THEN }  \tag{R5}\\
\text { IF } & (\mathrm{E}=>60) & \text { THEN } \\
\text { (Wait }=\mathrm{No}) \\
\text { IF } & \neg(\mathrm{Pa}=\text { Some }) \wedge(\operatorname{Pr}=\$ \$ \$) & \text { THEN } \\
(\text { Wait }=\mathrm{No})
\end{array}
\]

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

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A literal \(\tau_{i}\) breaks a set of literals \(\mathcal{S}\) (each denoting a different feature) if \(\mathcal{S}\) contains a literal inconsistent with \(\tau_{i}\)

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(\mathrm{Pa}=\text { Some }) \wedge \neg(\mathrm{E}=>60)
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\]
- XP \(\mathcal{S}_{1}=\{(\mathrm{Pa}=\) Some \(), \neg(\mathrm{E}=>60)\}\) breaks CEx \(\mathcal{S}_{2}=\{\neg(\mathrm{Pa}=\) Some \(),(\operatorname{Pr}=\$ \$ \$)\}\) and vice-versa

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1. Relationship between XPs with CEx's:
- Each XP breaks every CEx
- Each CEx breaks every XP
\(\therefore\) XPS can be computed from all CEx's (by HSD) and vice-versa
2. Given instance \(\mathcal{I}\), an AE can be computed from closest CEX

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

\section*{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)
- Results for NNs and for BTs
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- 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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