Rigorous Explanations for Machine Learning Models

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(joint work with A. Ignatiev and N. Narodytska)

University of Lisbon, Portugal

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Obergurgl, Austria

April 2019

Progress in automated reasoning

- Automated reasoners (AR):
  - SAT
  - ILP

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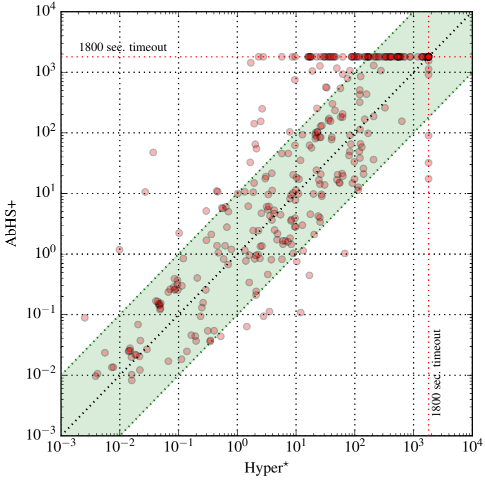
Propositional abduction



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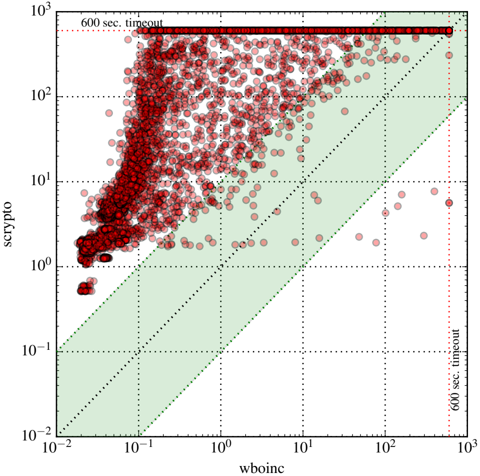
Model-based diagnosis



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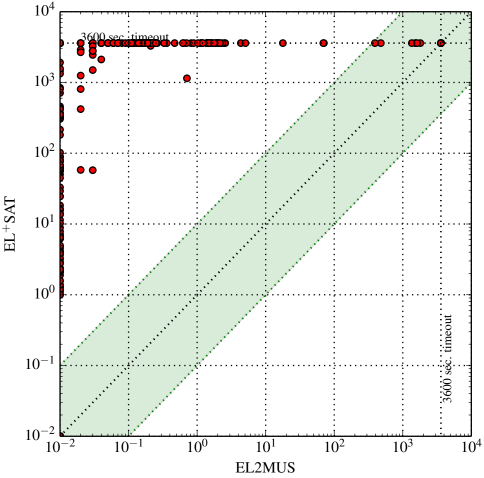
Axiom pinpointing for $\mathcal{EL}+$



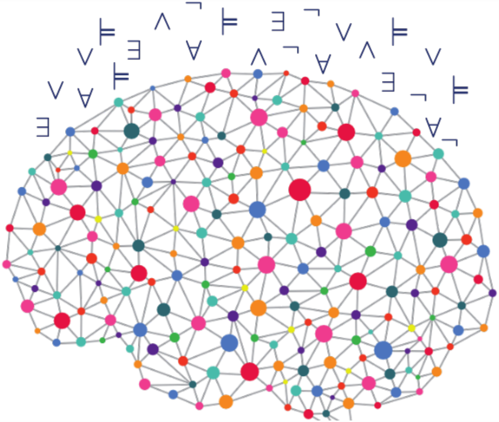
The question: how can AR improve ML's robustness?

Moshe Vardi

Machine learning and logic: Fast and slow thinking

ABSTRACT. There is a recent perception that computer science is undergoing a Kuhnian paradigm shift, with CS as a model-driven science being replaced as a data-driven science. I will argue that, in general new scientific theories refine old scientific theories, rather than replace them. Thus, data-driven CS and model-driven CS complement each other, just as fast thinking and slow thinking complement each other in human thinking, as explicated by Daniel Kahneman. I will then use automated vehicles as an example, where in recent years, car makers and tech companies have been racing to be the first to market. In this rush there has been little discussion of how to obtain scalable standardization of safety assurance, without which this technology will never be commercially deployable. Such assurance requires formal methods, and combining machine learning with logic is the challenge of the day.

M. Vardi, MLMFM'18 Summit



Machine learning vs. automated reasoning

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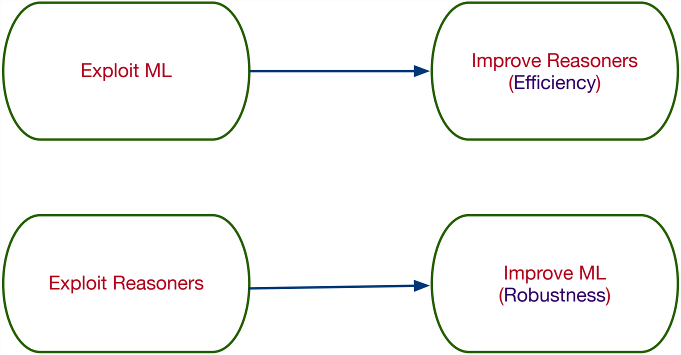

Our work ...

- Focus on classification problems

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- Globally correct (ie rigorous) **explanations** for predictions made

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- Globally correct (ie rigorous) **explanations** for predictions made

- Disclaimer: first inroads into ML & XAI;
  comments welcome

Outline

Successes & Pitfalls of ML

Explainable AI

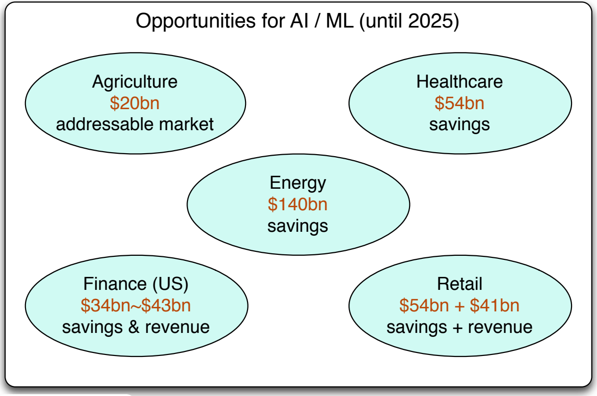
Explanations with Abductive Reasoning

Results

Some ML successes & expectations

- IBM Watson
- Deepmind AlphaGo
  - & AlphaZero
- Image Recognition
- Speech Recognition
- Financial Services
- Medical Diagnosis
- ...

Circa 2017



Source: Goldman-Sachs

Many more applications expected

source: Google

Many more applications expected

source: Google

source: Wikipedia

ⓒDARPA

But ML models are **brittle**

Eykholt et al'18

Aung et al'17

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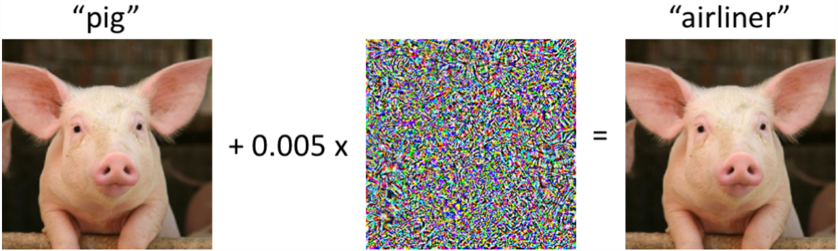

Source: http://gradientscience.org/intro_adversarial/

Also, some ML models are **interpretable**

decision|rule lists|sets
decision trees

Ex.	Vacation (V)	Concert (C)	Meeting (M)	Expo (E)	Hike (H)
e_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
e_7	1	1	0	1	1

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if $\neg$Meeting **then** Hike
if $\neg$Vacation **then** $\neg$Hike

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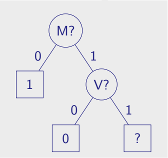
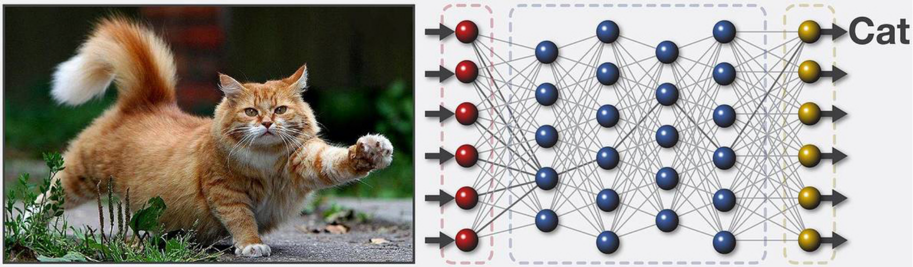


But other ML models are **not** (interpretable)...



ⓒ DARPA

Why does the NN predict a cat?

Sample of ongoing efforts

- **Verification of NNs**:
  - Sound vs. unsound vs. complete [M.P. Kumar, VMCAI'19]
  - E.g. Reluplex: dedicated reasoning within SMT solver

- **Explanations for non-interpretable (ie black-box) models**:
  - Until recently, most approaches heuristic-based

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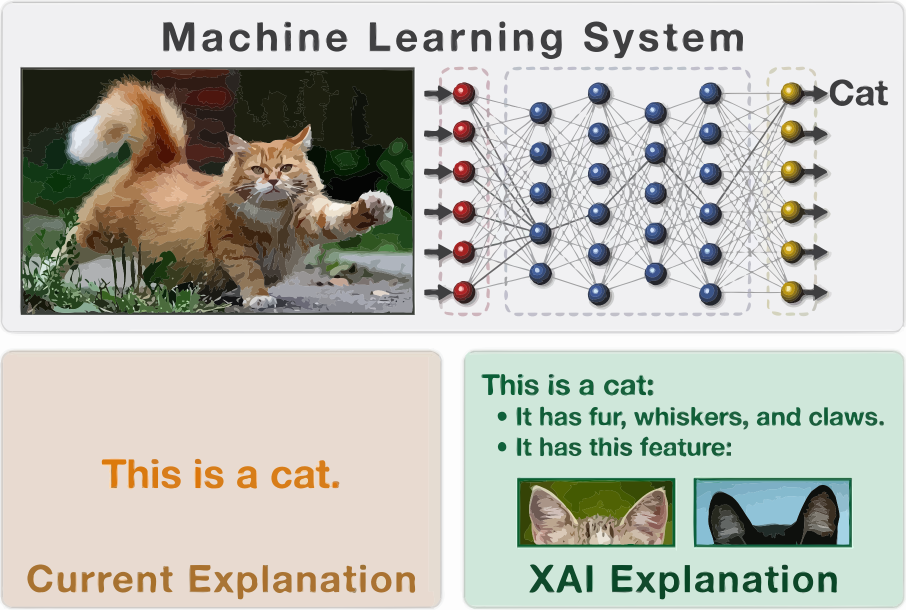

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Why XAI?

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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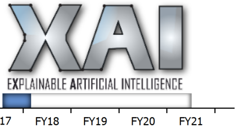
Explainable Artificial Intelligence (XAI)



David Gunning
DARPA/I2O
Program Update November 2017

Relevancy of XAI

MIT Technology Review

The Dark Secret at the Heart of AI
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April 11, 2017

THE WALL STREET JOURNAL. WSJ

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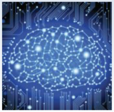

Entrepreneur

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Military EMBEDDED SYSTEMS

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Science AAAS

Relevancy of XAI & hundreds(?) of recent papers

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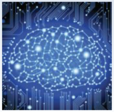

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Main challenge: **black-box models**

Heuristic approaches, e.g. **LIME** & **Anchor** [Guerreiro et al., KDD'16, AAAI'18]

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Recent efforts on **rigorous** approaches

- **Compilation**-based, e.g. for BNCs [Shih,Choi&Darwiche, IJCAI'18]
  - Issues with scalability
- **Abduction**-based, e.g. for NNs [Ignatiev,Narodytska,M.-S., AAAI'19]
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Some current challenges

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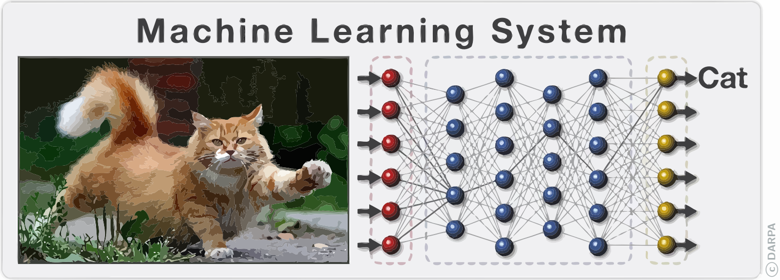
- For rigorous methods: scalability, scalability, scalability...

Outline

From ML model to logic



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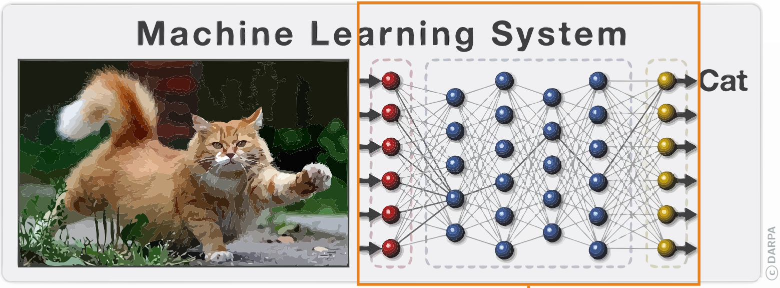
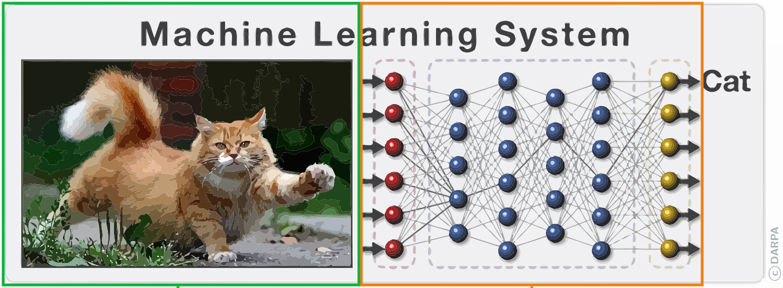


formula $\mathcal{F}$

From ML model to logic



cube $\mathcal{C}$

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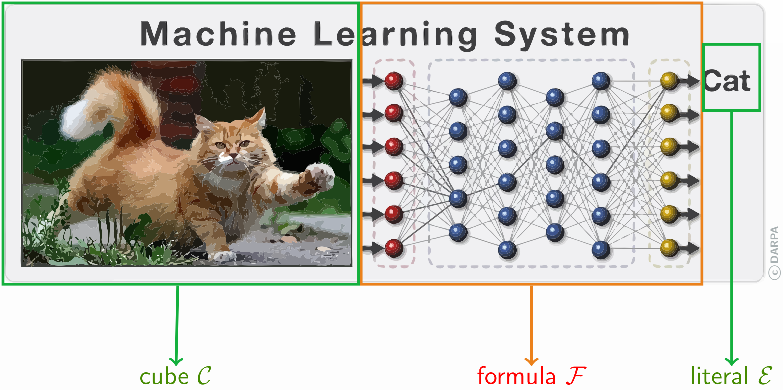

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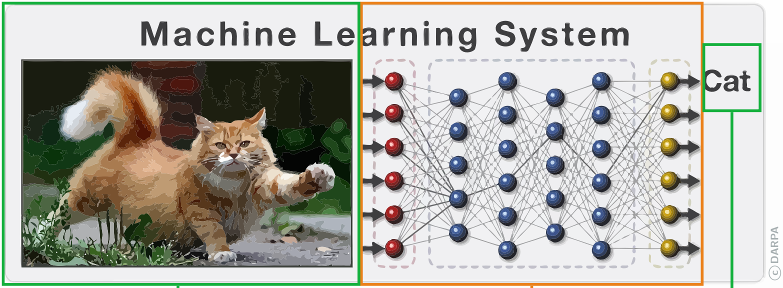
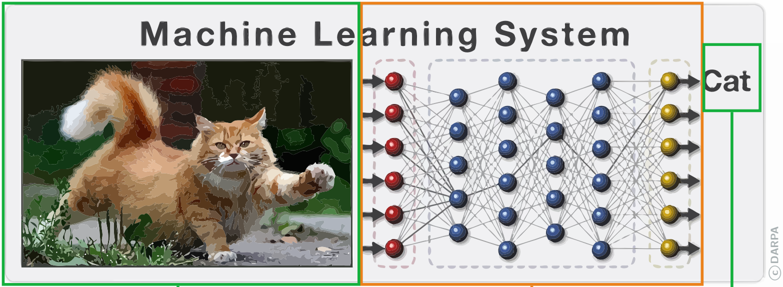


cube $\mathcal{C}$ formula $\mathcal{F}$ literal $\mathcal{E}$

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

From ML model to logic



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Must be able to encode ML model
E.g. SMT, ILP, etc.

Abductive explanations of ML models

given a **classifier** $\mathcal{F}$, a **cube** $\mathcal{C}$ and a **prediction** $\mathcal{E}$,

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and

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$\Downarrow$

iterative explanation procedure

Computing primes

1. $\mathcal{C}_m \wedge \mathcal{F} \not\models \bot$

Computing primes

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Computing primes

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2. $\mathcal{C}_m \wedge \mathcal{F} \models \mathcal{E}$

Computing primes

$$
\begin{array}{lccc}
\textbf{1.} & \mathcal{C}_m \wedge \mathcal{F} \not\models \bot & \textbf{—} & \textbf{tautology} \\
\textbf{2.} & \mathcal{C}_m \wedge \mathcal{F} \models \mathcal{E} & \Leftrightarrow & \mathcal{C}_m \models (\mathcal{F} \rightarrow \mathcal{E})
\end{array}
$$

Computing primes

1. $\mathcal{C}_m \wedge \mathcal{F} \not\models \bot$ — **tautology**

2. $\mathcal{C}_m \wedge \mathcal{F} \models \mathcal{E} \quad \Leftrightarrow \quad \mathcal{C}_m \models (\mathcal{F} \rightarrow \mathcal{E})$

$\Downarrow$

$\mathcal{C}_m$ is a **prime implicant** of $\mathcal{F} \rightarrow \mathcal{E}$

Computing one minimal explanation

- **One** subset-minimal explanation:

Input: $\mathcal{F}$ under $\mathcal{M}$, initial cube $\mathcal{C}$, prediction $\mathcal{E}$
Output: **Subset-minimal** explanation $\mathcal{C}_m$

```
begin
   for l ∈ C :
      if Entails(C \ {l}, F → E) :
         C ← C \ {l}
   return C
end
```

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- **One** cardinality-minimal explanation:
  - Harder than computing subset-minimal explanation
  - Exploit **implicit hitting set dualization**
  - Details in earlier papers

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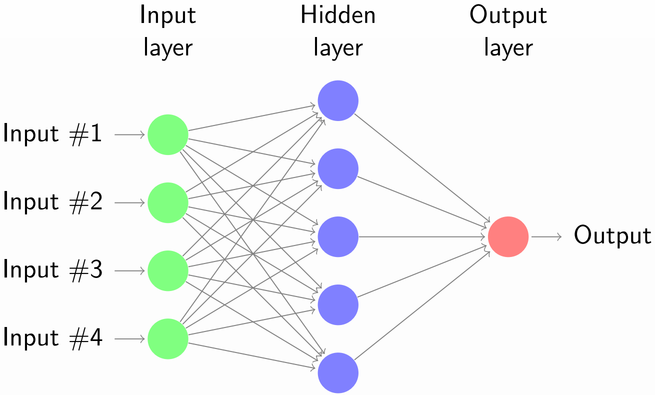
Encodings NNs



- 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

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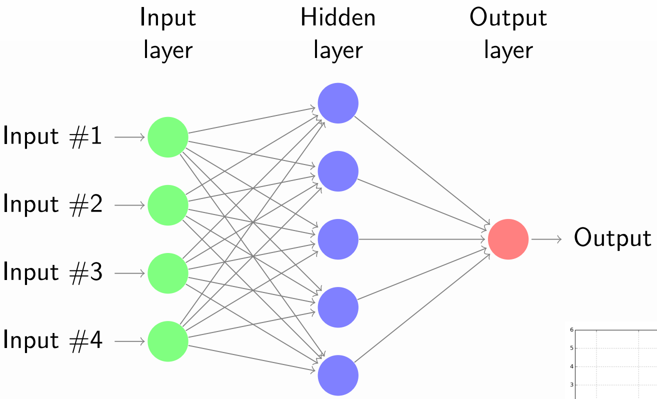

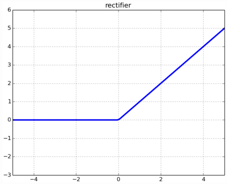

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- Each unit uses a ReLU activation function

Encoding NNs using MILP

Computation for a NN ReLU block:

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

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Block encoded as follows: [Fischetti&Jo, CJ'18]

$$\sum_{j=1}^{n} a_{i,j} x_j + b_i = y_i - s_i$$
$$z_i = 1 \rightarrow y_i \leq 0$$
$$z_i = 0 \rightarrow s_i \leq 0$$
$$y_i \geq 0, s_i \geq 0, z_i \in \{0, 1\}$$

– Simpler encodings not as effective [Katz et al. CAV'17]

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Experimental setup

- Implementation in Python
  - Supports SMT solvers through PySMT
    - Yices2 used
  - Supports CPLEX 12.8.0

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  - Supports CPLEX 12.8.0
- **ReLU-based** neural networks [Fischetti&Jo CJ'18]
  - One *hidden* layer with $i \in \{10, 15, 20\}$ neurons
  - Pick NN that achieves *good* accuracy

Experimental setup

- Implementation in Python
  - Supports SMT solvers through PySMT
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  - One *hidden* layer with $i \in \{10, 15, 20\}$ neurons
  - Pick NN that achieves *good* accuracy
- Benchmarks selected from:
  - **UCI** Machine Learning Repository
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  - **MNIST** Digits Database

Experimental setup

- Implementation in Python
  - Supports SMT solvers through PySMT
    - Yices2 used
  - Supports CPLEX 12.8.0
- **ReLU-based** neural networks [Fischetti&Jo CJ'18]
  - One *hidden* layer with $i \in \{10, 15, 20\}$ neurons
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- Benchmarks selected from:
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  - **MNIST** Digits Database
- Machine configuration:
  - Intel Core i7 2.8GHz, 8GByte
  - Time limit — 1800s
  - Memory limit — 4GByte

Sample of experimental results

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

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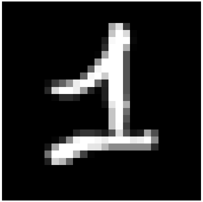
- `(    0 1 1 1   0 0       1 1 0  )` — **9 literals**

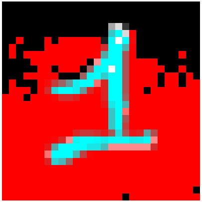
subset-minimal explanations computed by **our approach**:

- `(      1         0   0       0  )` — **4 literals**
- `(      1         0   0           )` — **3 literals**
- `(    0 1         0   0       0  )` — **5 literals**
- `(    0 1         0   0         1)` — **5 literals**

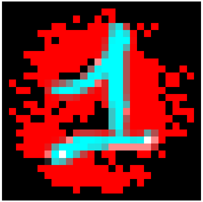
There are many explanations of different quality



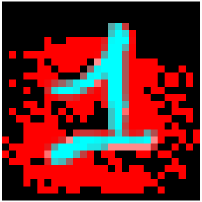
(a) digit 1



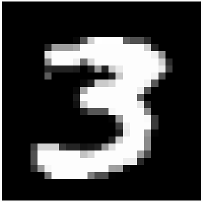
(b) simple expl.



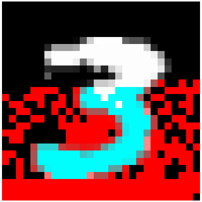
(c) central pixels



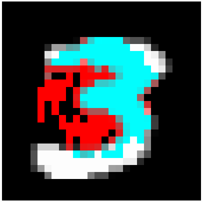
(d) light pixels



(a) digit 3



(b) simple expl.



(c) central pixels

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Outline

Successes & Pitfalls of ML

Explainable AI

Explanations with Abductive Reasoning

Results

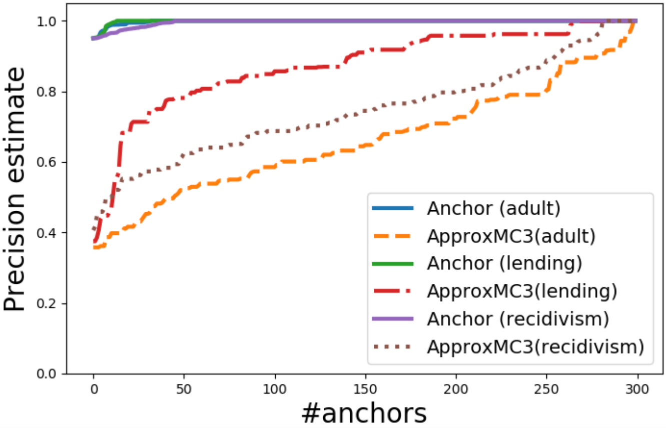
- Assessing Local Explanations – Recent Work

Assessing precision with model counting

- Evaluated Anchor [Guerreiro et al., AAAI18]
  - Anchor more accurate than LIME
  - Anchor computes accuracy estimate for each explanation

- Represented ML model as propositional formula
  - E.g. binarized NNs (BNNs)
  - Use (approximate) model counter to assess precision of ML model on explanation (anchor) computed by Anchor

Preliminary results



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

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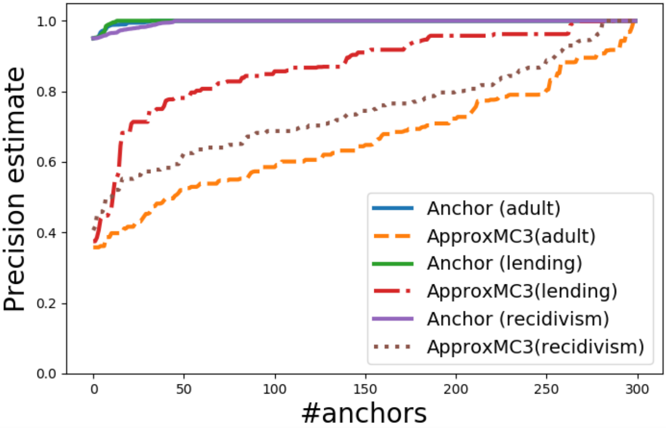

- Anchor often claims $\approx$ 99% precision; this cannot be confirmed

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- **Principled** approach to XAI

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- **Other** ML models?
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  - More advanced **reasoners**?
- Explanation **enumeration**? + **preferences**?

Questions?

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