A logical approach to model interpretability

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Motivation

- A growing interest in developing methods to explain predictions made by machine learning models
- This has led to the development of several notions of explanation
- Instead of struggling with the increasing number of such notions, one can developed a declarative query language for interpretability task

A call for an interpretability query language

- Several interpretability notions have been studied independently
- Interpretability admits no silver bullet; different contexts require different notions
- Interpretability may require combining different notions; it is better to think of it as an interactive process

A call for an interpretability query language

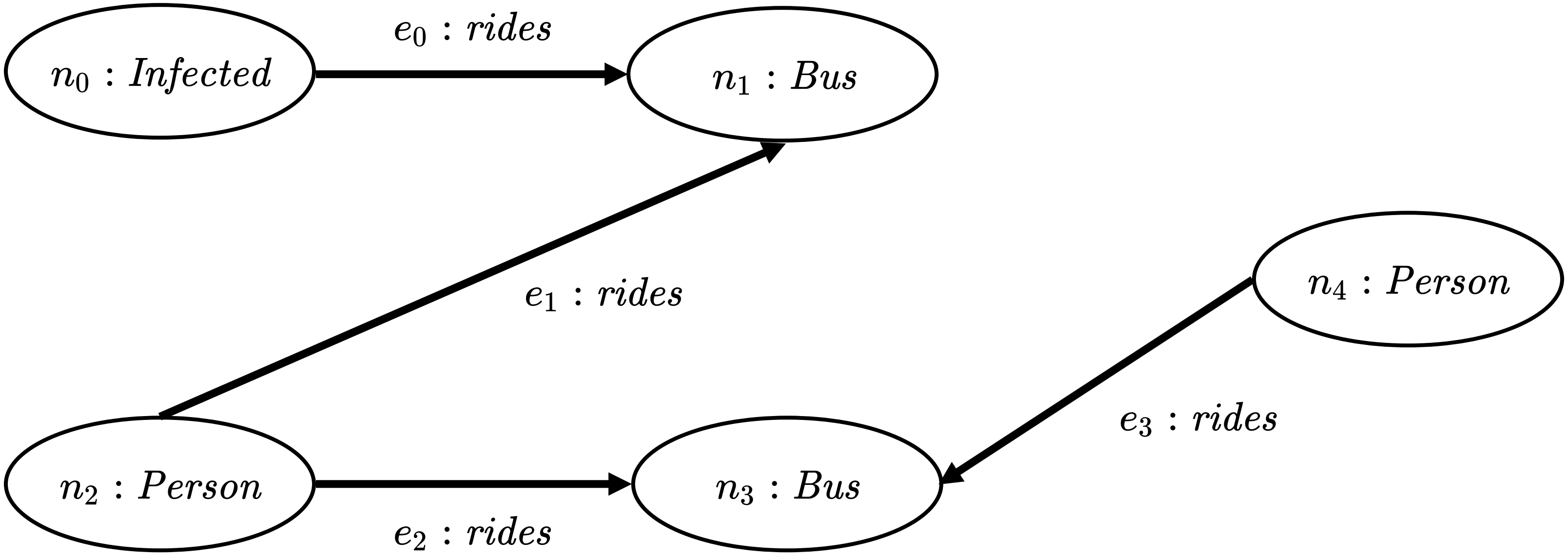
- This naturally suggests the possibility of interpretability query languages
- These languages should de declarative, and should allow to express a wide variety of queries
- This gives control to the end-user to tailor interpretability queries to their particular needs

Our goal is to develop such an interpretability query language

Basic ingredients: classification models are represented as **labeled graphs**, and **first-order logic** is used as query language

A brief remainder: extracting paths in a labeled graph

$$Person/rides/Bus/rides^{-}/Infected$$



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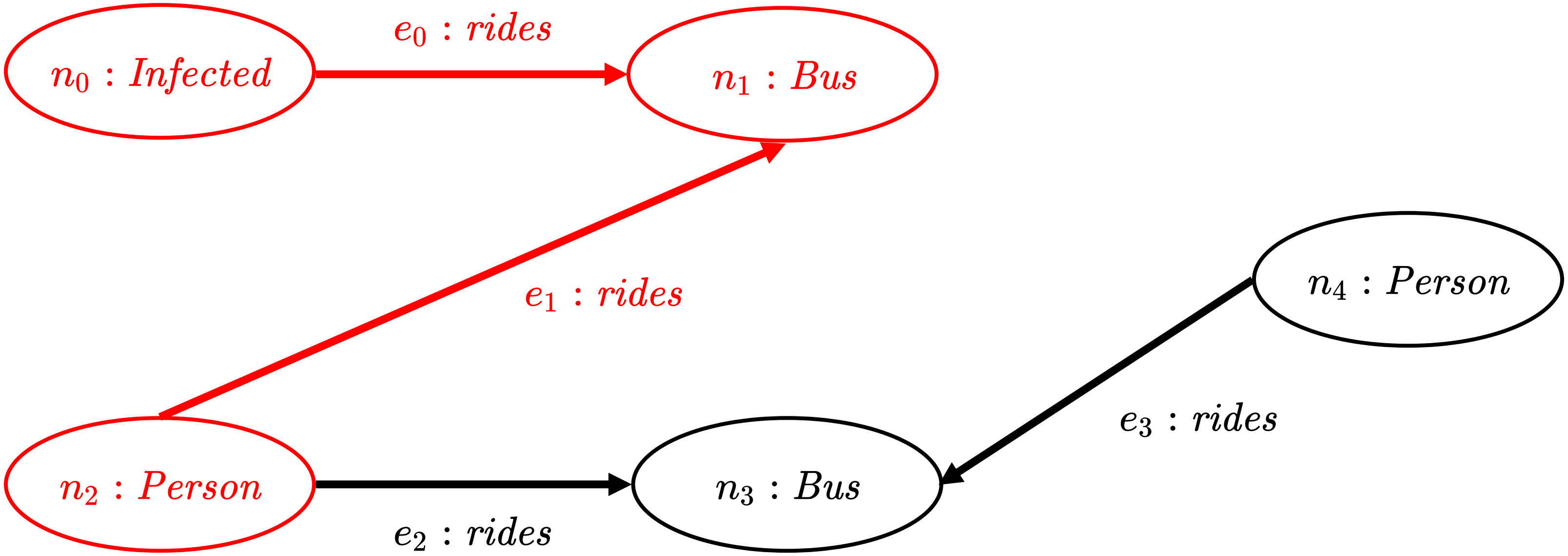

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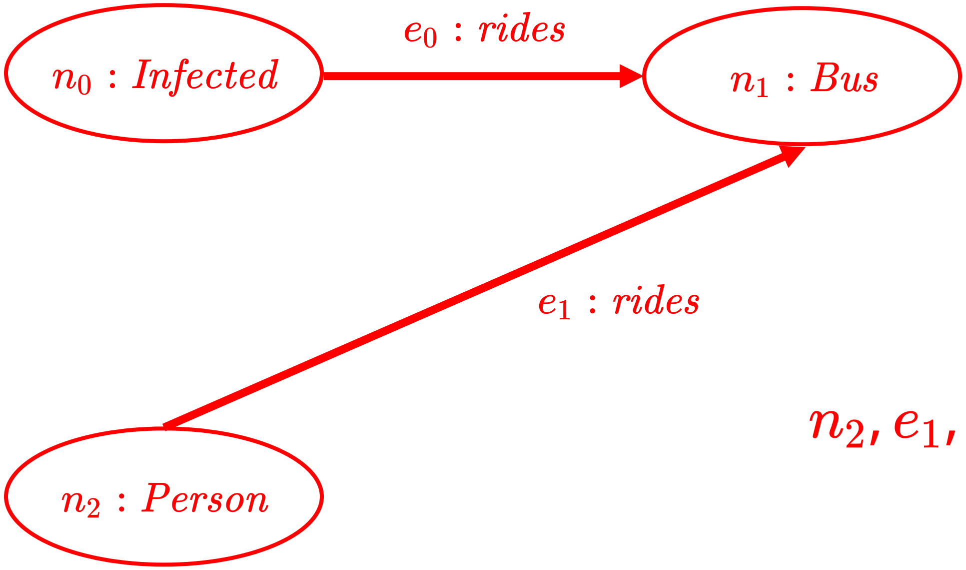
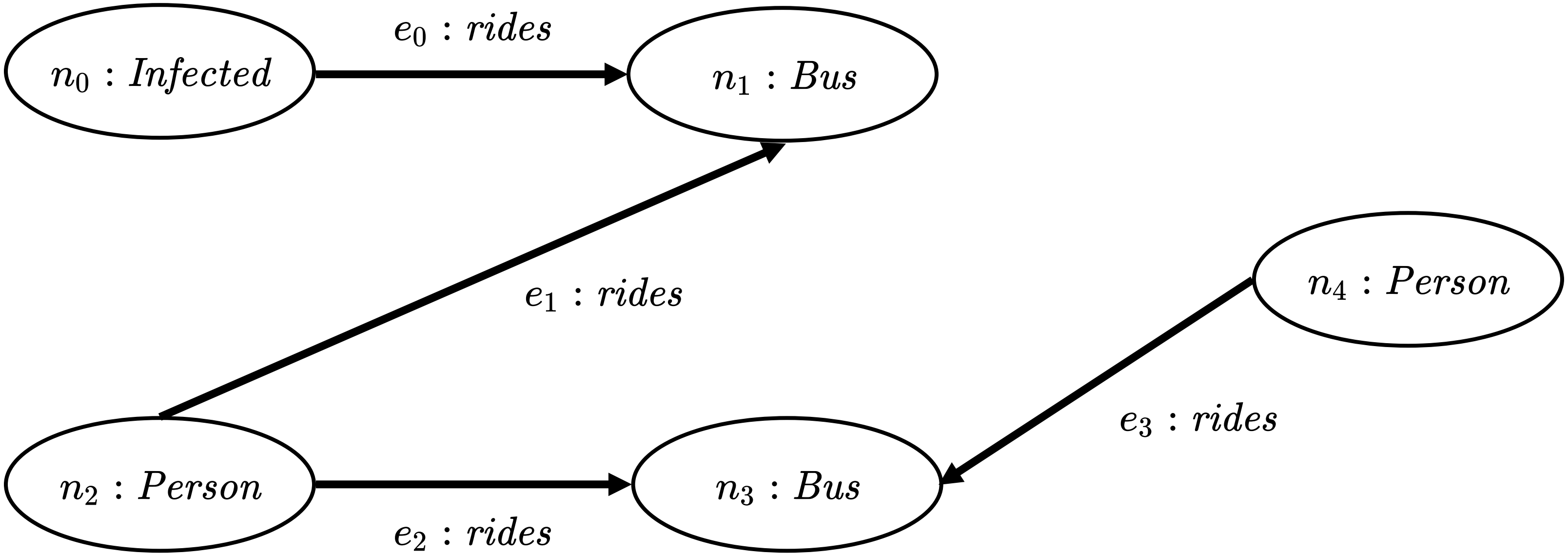


$$n_2, e_1, n_1, e_0, n_0$$

A brief remainder: extracting paths in a labeled graph

$$Person(x) \wedge rides(x, y) \wedge Bus(y) \wedge rides(z, y) \wedge Infected(z)$$



An interpretability query language

We start by focusing on a simple but widely used model

- **Decision trees** are widely used, in particular because they are considered *readily* interpretable models
- The main ingredients of our logical approach are already present in this case

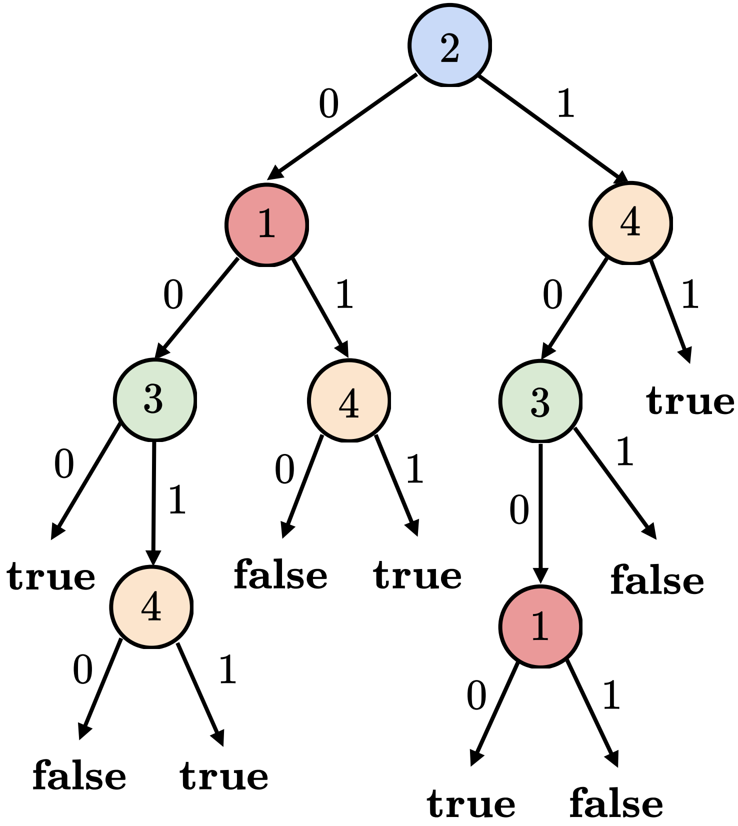
A classification model:

$$\mathcal{M} : \{0,1\}^n \to \{0,1\}$$

- The dimension of $\mathcal{M}$ is n, and each $i \in \{1, \ldots, n\}$ is called a feature
- $\mathbf{e} \in \{0,1\}^n$ is an instance
- $\mathcal{M}$ accepts $\mathbf{e}$ if $\mathcal{M}(\mathbf{e}) = 1$, otherwise $\mathcal{M}$ rejects $\mathbf{e}$

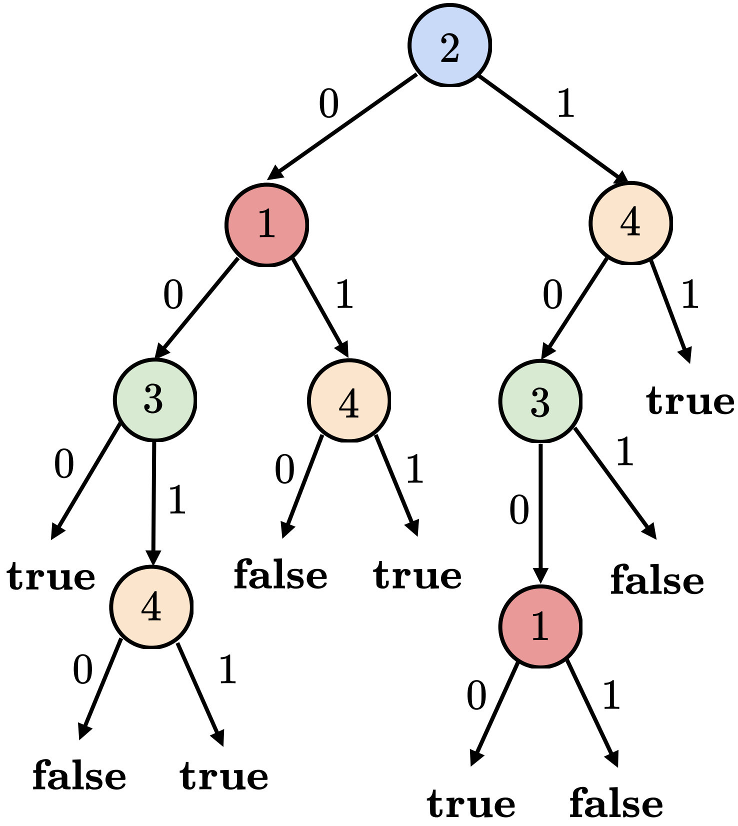
A decision tree $\mathcal{T}$ of dimension n

- Each internal node is labeled with a feature $i \in \{1, \ldots, n\}$, and has two outgoing edges labeled 0 and 1
- Each leaf is labeled $\mathbf{true}$ or $\mathbf{false}$
- No two nodes on a path from the root to a leaf have the same label



A decision tree $\mathcal{T}$ of dimension n

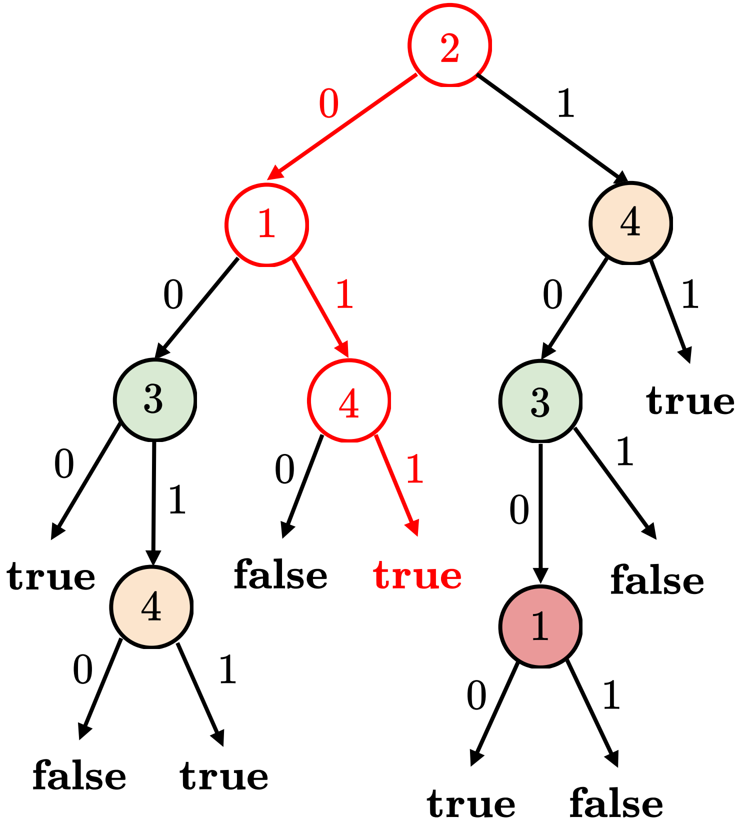
- Every instance $\mathbf{e}$ defines a unique path $n_1, e_1, n_2, \ldots, e_{k-1}, n_k$ from the root to a leaf
- $\mathcal{T}(\mathbf{e}) = 1$ if the label n_k is **true**



A decision tree $\mathcal{T}$ of dimension n

- Every instance $\mathbf{e}$ defines a unique path $n_1, e_1, n_2, \ldots, e_{k-1}, n_k$ from the root to a leaf
- $\mathcal{T}(\mathbf{e}) = 1$ if the label n_k is $\mathbf{true}$

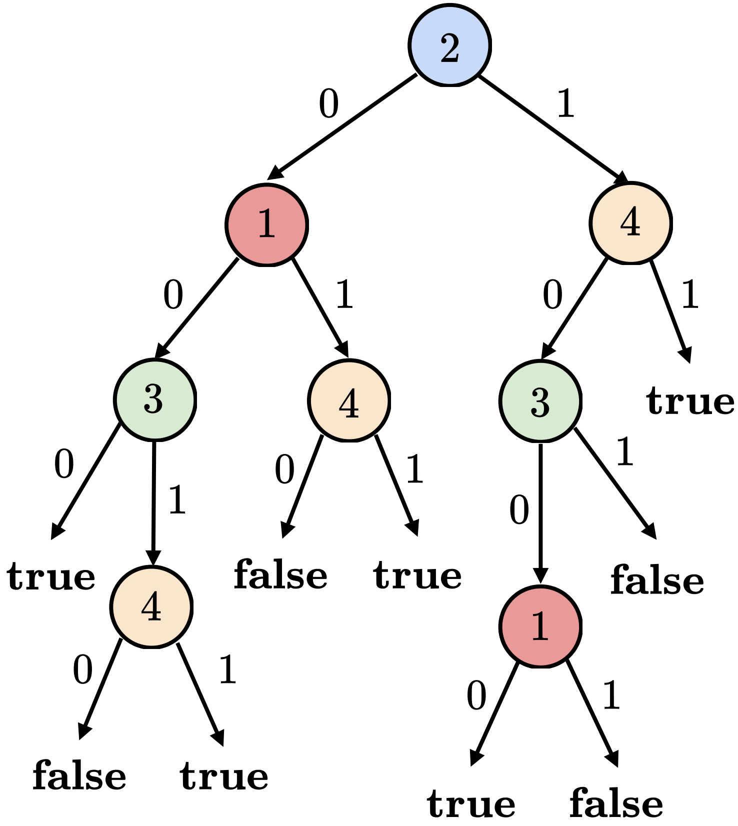
$\mathcal{T}(\mathbf{e_1}) = 1$ for instance $\mathbf{e_1} = (1, 0, 1, 1)$



The evaluation of a model as a query

Is $\mathcal{T}(\mathbf{e_1}) = 1$ for instance $\mathbf{e_1} = (1, 0, 1, 0)$?

$$\left(1/1 + 2/0 + 3/1 + 4/0\right)^* / \mathbf{true}$$



But our problem is to explain the output of a model

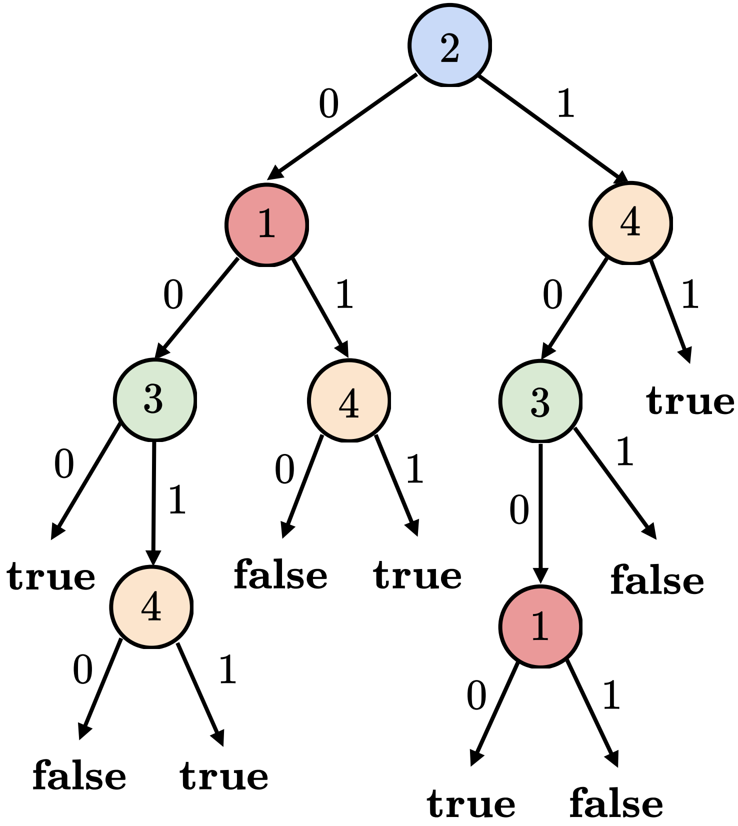
- What are interesting notions of explanation?
- What notions have been studied? What notions are used in practice?
- Can these notions be expressed as queries over decision trees?

But our problem is to explain the output of a model

Is there a completion of $2 \mapsto 0$ that is classified positively?

$$\big(1/(0+1) + \color{red}{2/0} + 3/(0+1) + 4/(0+1)\big)^*/\mathbf{true}$$

Are all the completions of $2 \mapsto 0$ classified positively?

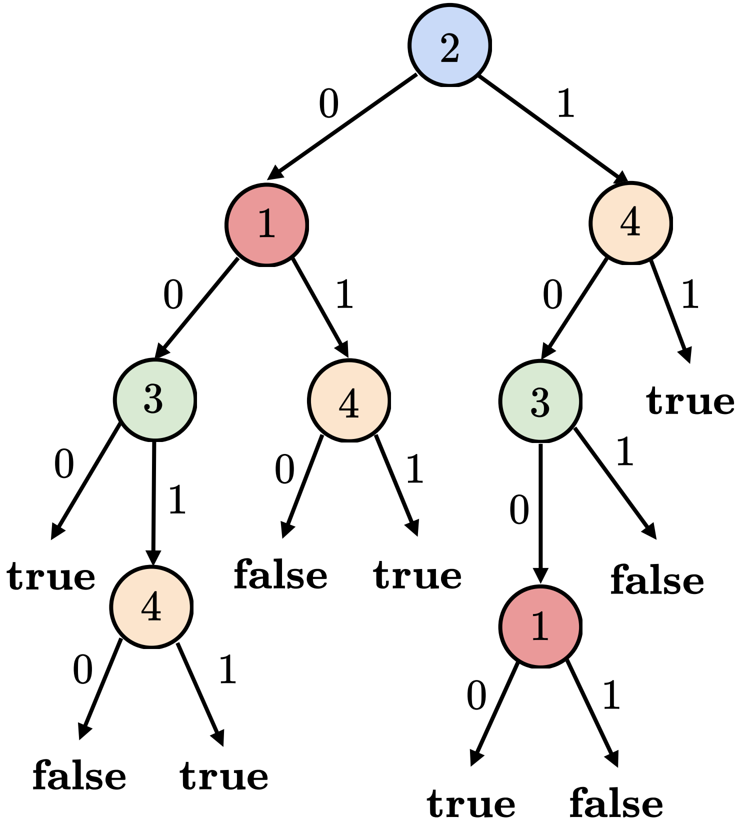


Notions of explanation: sufficient reason

$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1, 1, 1, 1)$

The value of feature 3 is not needed to obtain this result

- $\{1, 2, 4\}$ is a *sufficient reason*

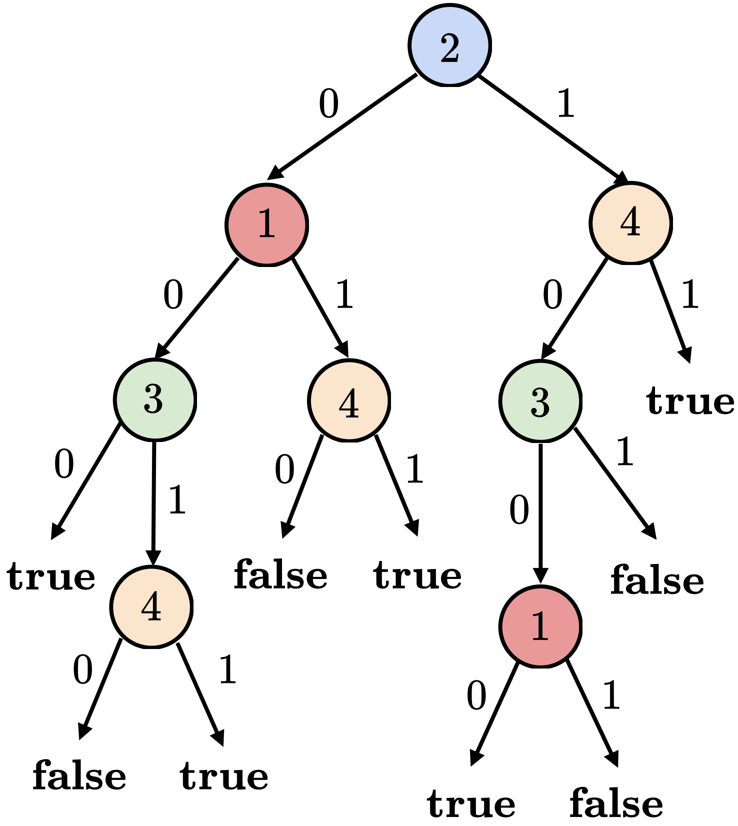


Notions of explanation: minimal sufficient reason

$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1, 1, 1, 1)$

The value of features 1 and 3 are not needed to obtain this result

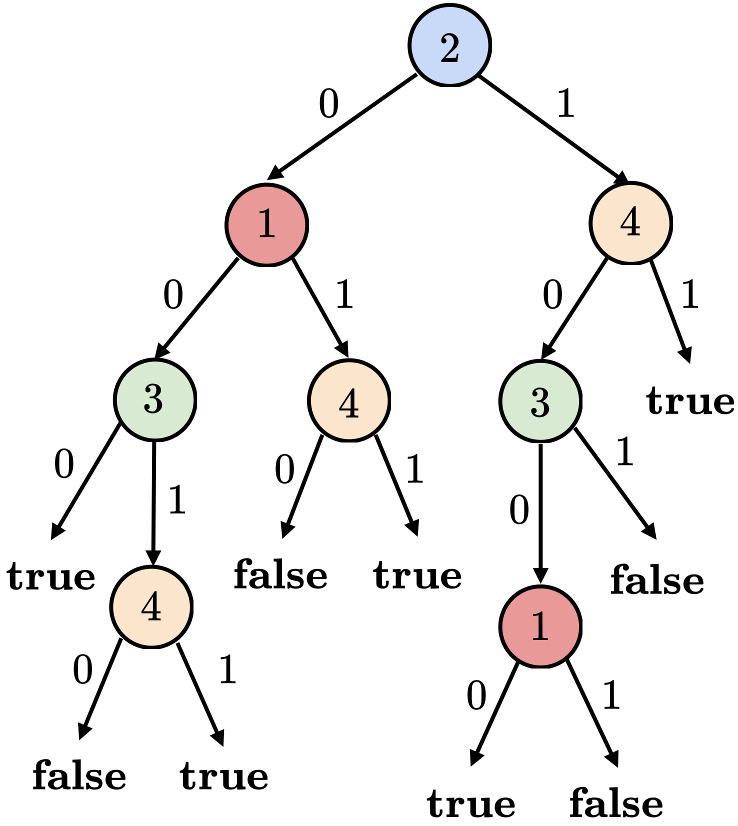
- $\{2, 4\}$ is a *minimal sufficient reason*



Notions of explanation: relevant feature set

If the values of features $\{1, 3, 4\}$ are fixed, then the output of the model is fixed

The output of the model depends only on these features

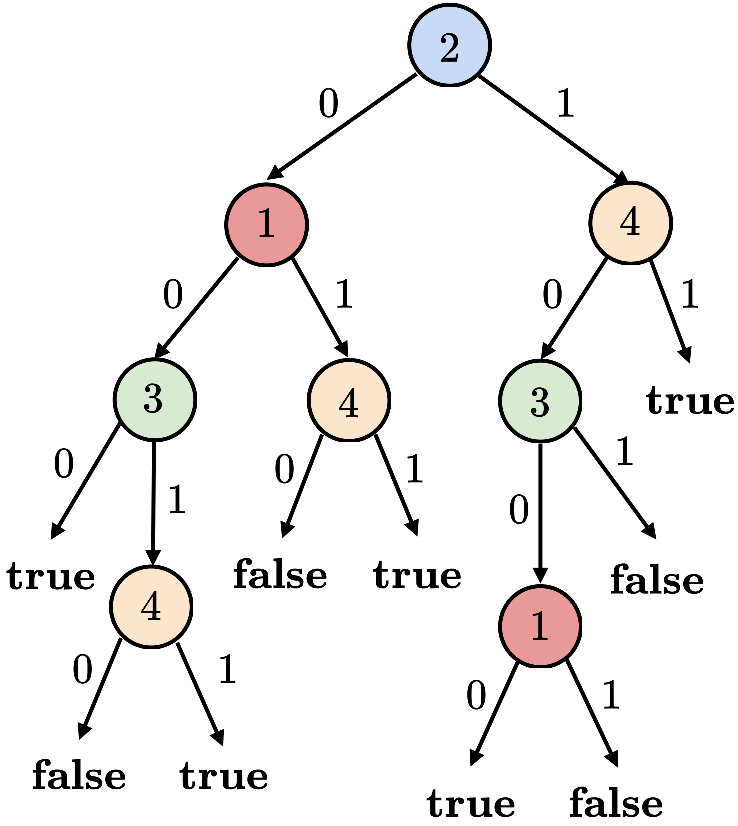


Notions of explanation: relevant feature set

If the values of features $\{1, 3, 4\}$ are fixed, then the output of the model is fixed

If $\mathbf{e}[1] = \mathbf{e}[3] = \mathbf{e}[4] = 0$:

$\mathcal{T}(\mathbf{e}) = 1$

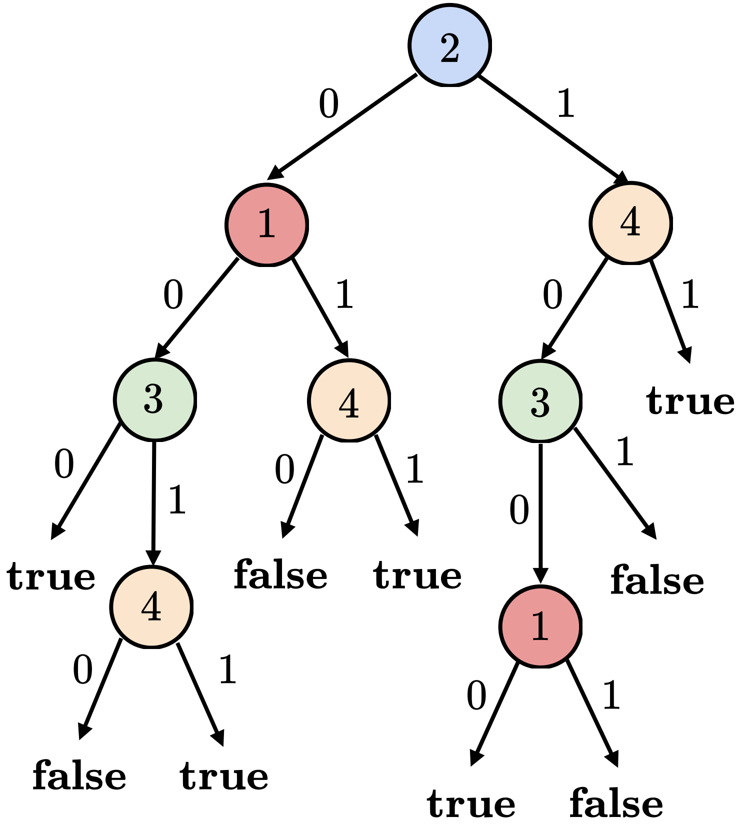


Notions of explanation: relevant feature set

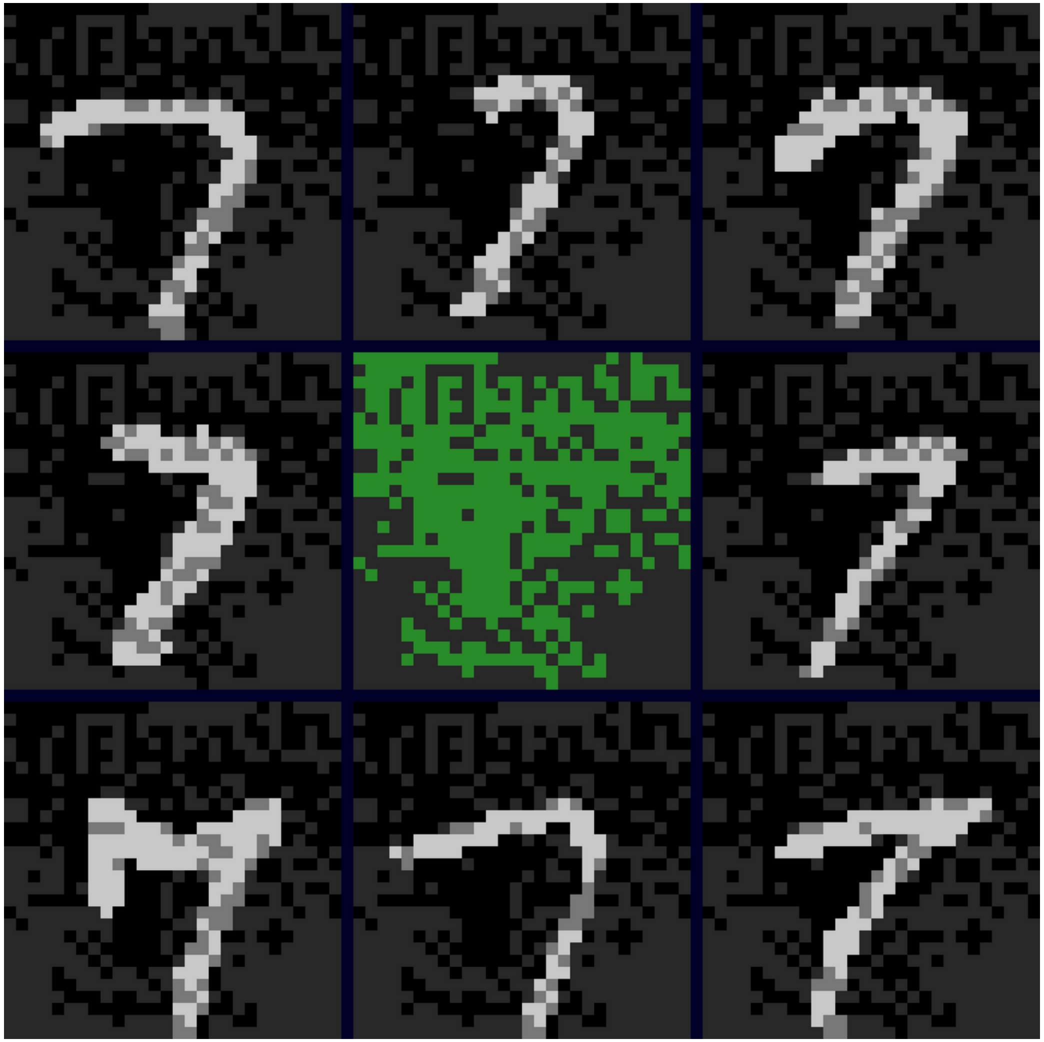
If the values of features $\{1, 3, 4\}$ are fixed, then the output of the model is fixed

If $\mathbf{e}[1] = \mathbf{e}[3] = 1$ and $\mathbf{e}[4] = 0$:

$$\mathcal{T}(\mathbf{e}) = 0$$



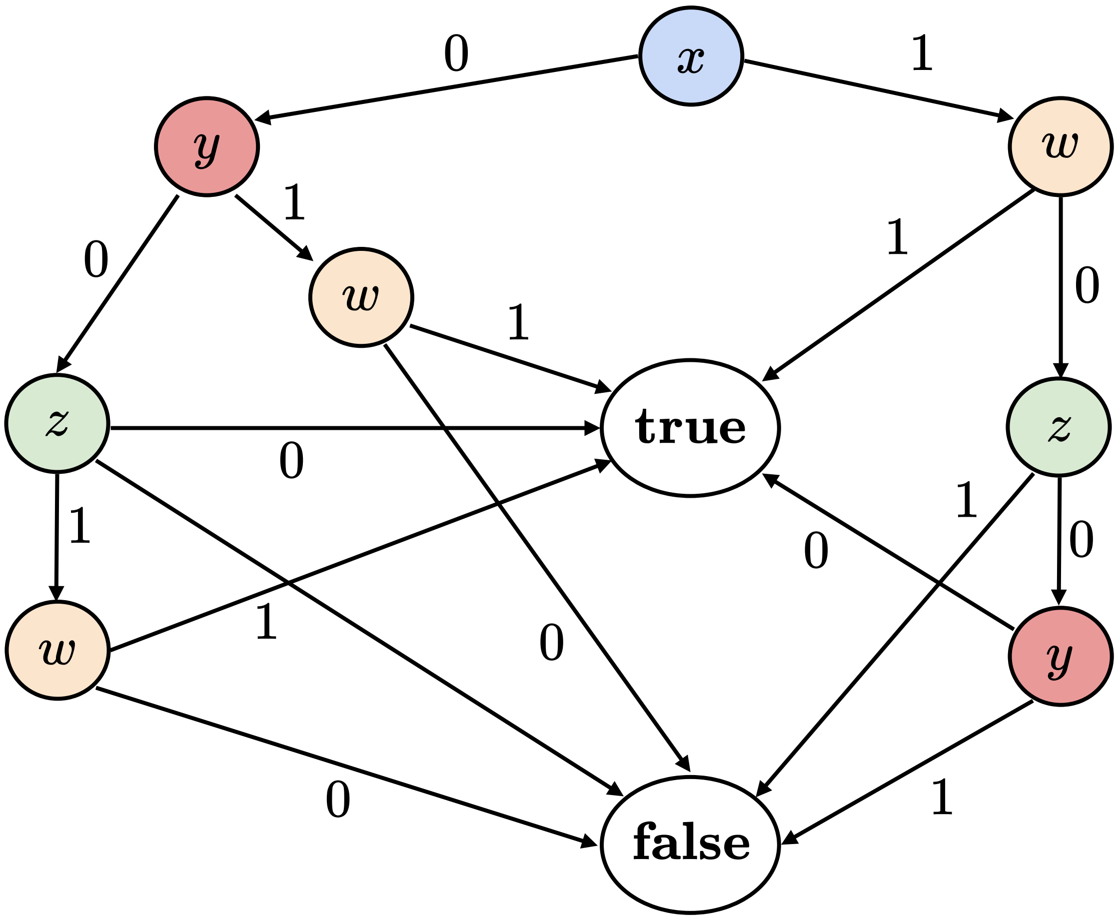
MNIST: relevant feature set



Can these queries be expressed in a graph query language?

- How do we express the previous interpretability queries?
- Is there a common framework for them?
- Is there a *natural* framework based on labeled graphs?

Can these queries be expressed in a graph query language?



Binary decision diagrams (BDDs)

- OBDDs
- FBDDs

A first attempt: FOIL

First-order logic defined on a suitable vocabulary to describe classification models

Key notion: partial instance $\mathbf{e} \in \{0, 1, \perp\}^n$ of dimensión n

$\mathbf{e}_1$ is subsumed by $\mathbf{e}_2$ if $\mathbf{e}_1, \mathbf{e}_2$ are partial instances such that for every $i \in \{1, \ldots, n\}$, if $\mathbf{e}_1[i] \neq \perp$, then $\mathbf{e}_1[i] = \mathbf{e}_2[i]$

$$(1, \perp, 0, \perp) \ \subseteq \ (1, 0, 0, \perp) \ \subseteq \ (1, 0, 0, 1)$$

A first attempt: FOIL

First-order logic defined on a suitable vocabulary to describe classification models: $\{\mathrm{Pos}, \subseteq\}$

A model $\mathcal{M}$ of dimensión n is represented as a structure $\mathfrak{A}_{\mathcal{M}}$:

- The domain of $\mathfrak{A}_{\mathcal{M}}$ is $\{0, 1, \perp\}^n$
- $\mathrm{Pos}(\mathbf{e})$ holds if $\mathbf{e}$ is an instance such that $\mathcal{M}(\mathbf{e}) = 1$
- $\mathbf{e}_1 \subseteq \mathbf{e}_2$ holds if $\mathbf{e}_1, \mathbf{e}_2$ are partial instances such that $\mathbf{e}_1$ is subsumed by $\mathbf{e}_2$

The semantics of FOIL

Given a **FOIL** formula $\Phi(x_1, x_2, \ldots, x_k)$, a classification model $\mathcal{M}$ of dimensión n, and instances $\mathbf{e}_1$, $\mathbf{e}_2$, ..., $\mathbf{e}_k$

$$\mathcal{M} \models \Phi(\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k)$$

$$\iff$$

$$\mathfrak{A}_{\mathcal{M}} \models \Phi(\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k)$$

(in the usual sense)

Some examples

$$\text{Full}(x) \;=\; \forall y\,(x \subseteq y \to x = y)$$

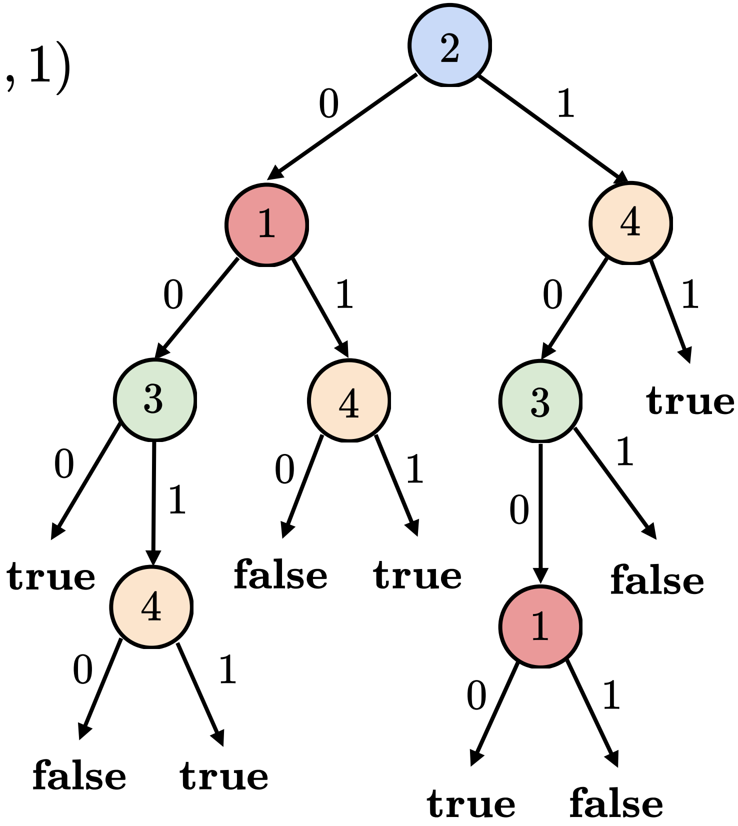
$$\text{AllPos}(x) \;=\; \forall y\,\big((x \subseteq y \wedge \text{Full}(y)) \to \text{Pos}(y)\big)$$

$$\text{AllNeg}(x) \;=\; \forall y\,\big((x \subseteq y \wedge \text{Full}(y)) \to \neg\text{Pos}(y)\big)$$

Notions of explanation: sufficient reason

$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1,1,1,1)$, and $\mathbf{e}_1 = (1,1,\bot,1)$ is a sufficient reason for this

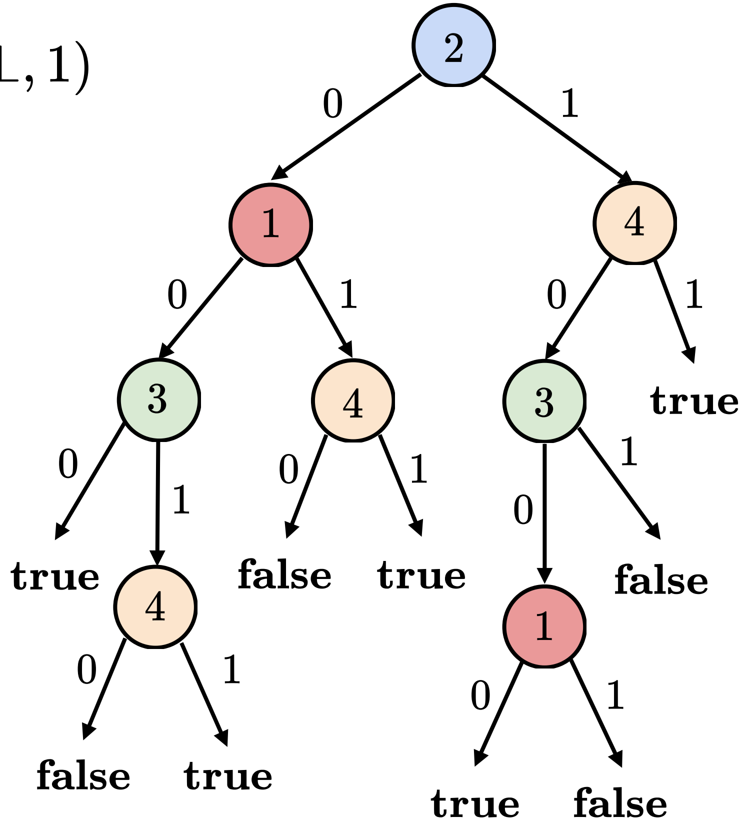
$$\mathcal{T} \models \mathrm{SR}(\mathbf{e}, \mathbf{e}_1)$$



$$\begin{aligned}\mathrm{SR}(x,y) \;=\; & \mathrm{Full}(x) \wedge y \subseteq x \wedge \\ & (\mathrm{Pos}(x) \rightarrow \mathrm{AllPos}(y)) \wedge \\ & (\neg\mathrm{Pos}(x) \rightarrow \mathrm{AllNeg}(y))\end{aligned}$$

Notions of explanation: minimal sufficient reason

$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1, 1, 1, 1)$, and $\mathbf{e}_2 = (\bot, 1, \bot, 1)$ is a minimal sufficient reason for this

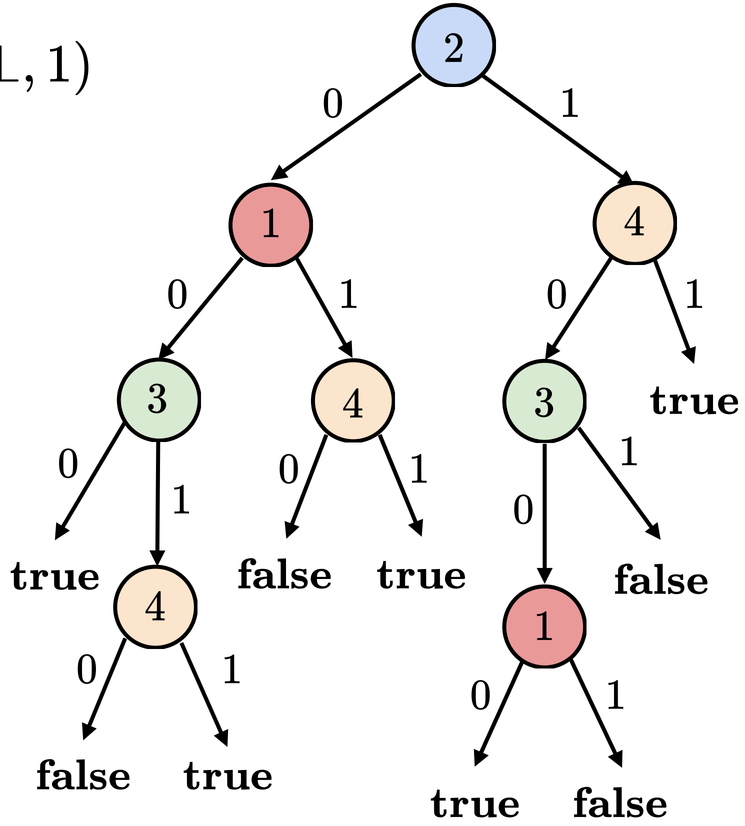


Notions of explanation: minimal sufficient reason

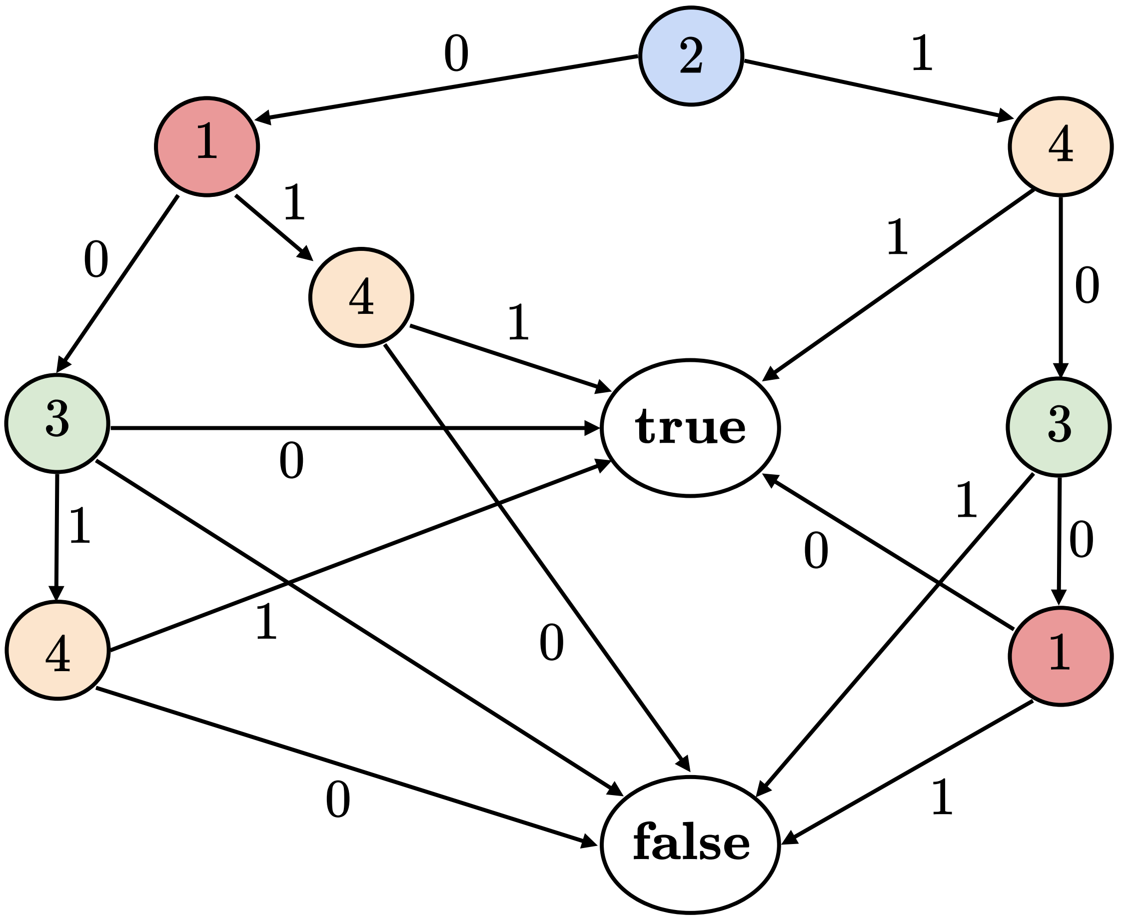
$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1,1,1,1)$, and $\mathbf{e}_2 = (\bot, 1, \bot, 1)$
is a minimal sufficient reason for this

$$\mathcal{T} \models \text{MinimalSR}(\mathbf{e}, \mathbf{e}_2)$$

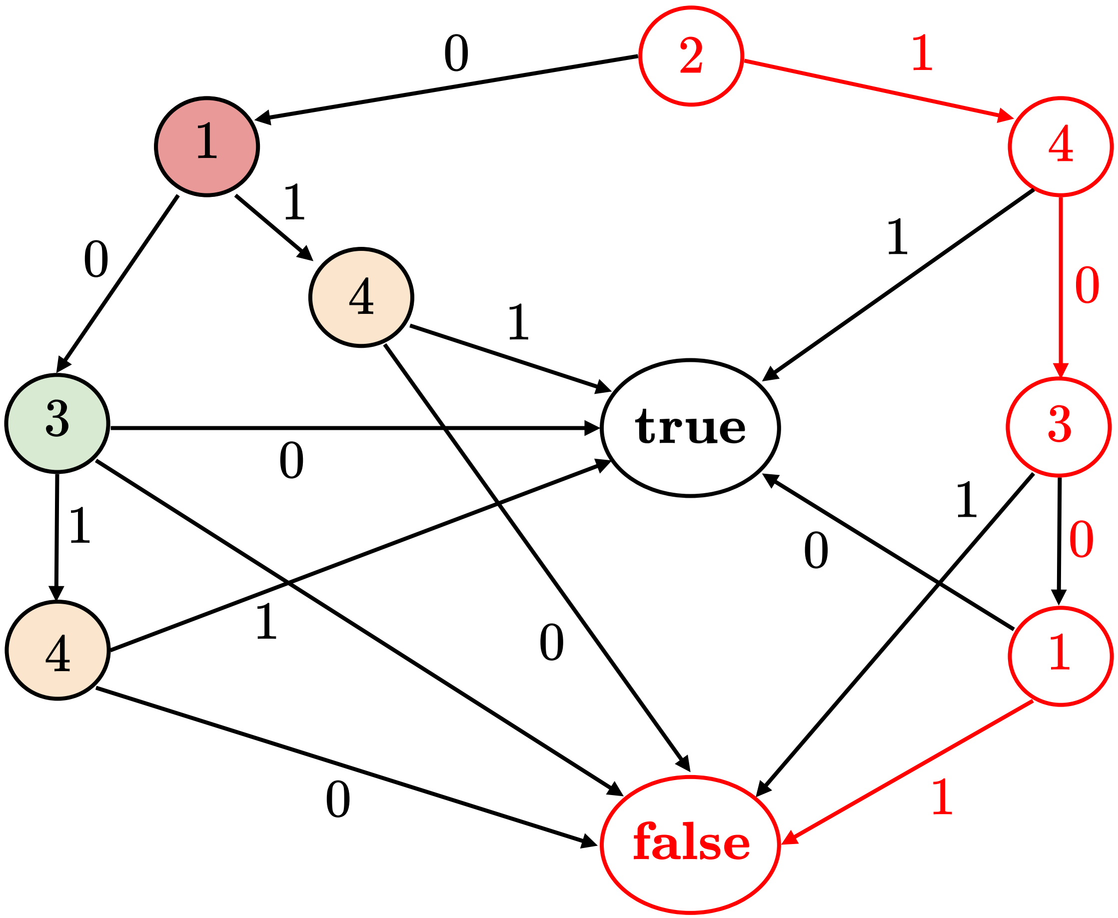
$$\text{MinimalSR}(x, y) \;=\; \text{SR}(x, y) \wedge$$
$$\forall z \left((\text{SR}(x, z) \wedge z \subseteq y) \to z = y \right)$$



FOIL is a graph query language

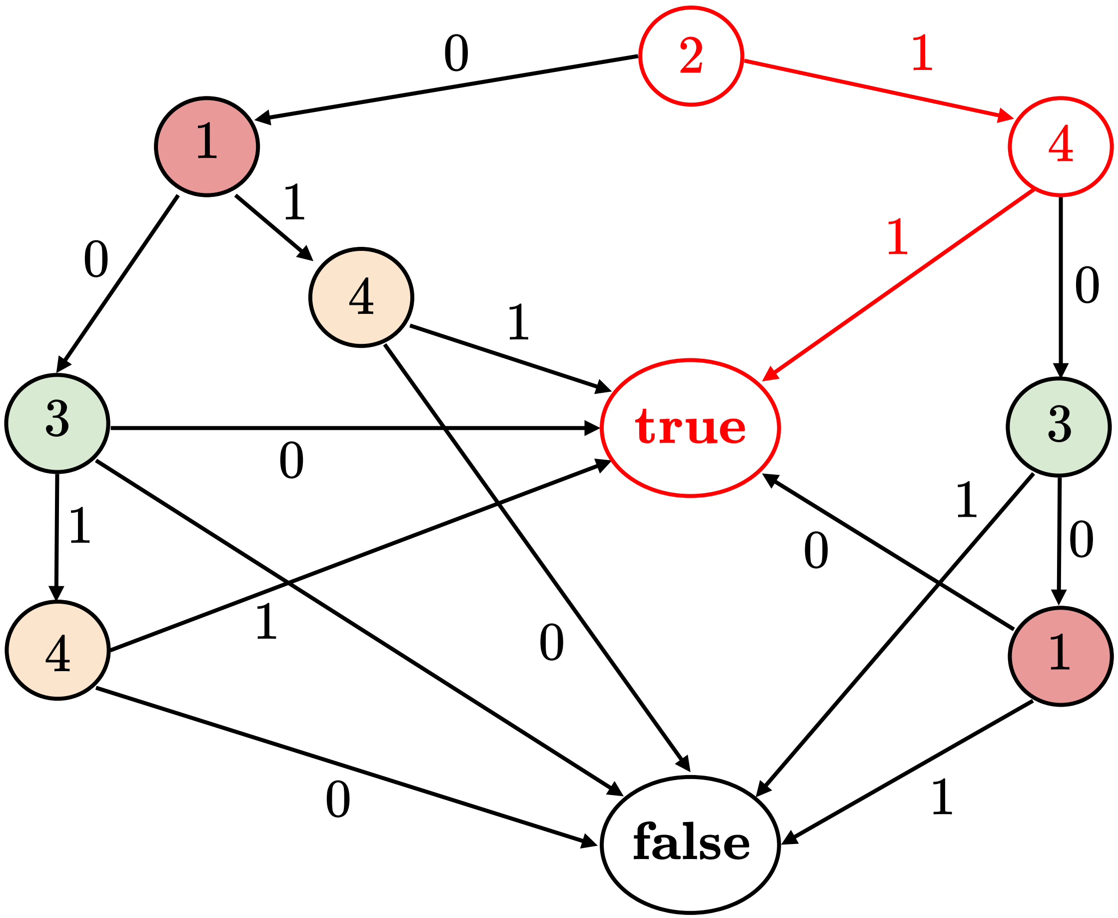


FOIL is a graph query language

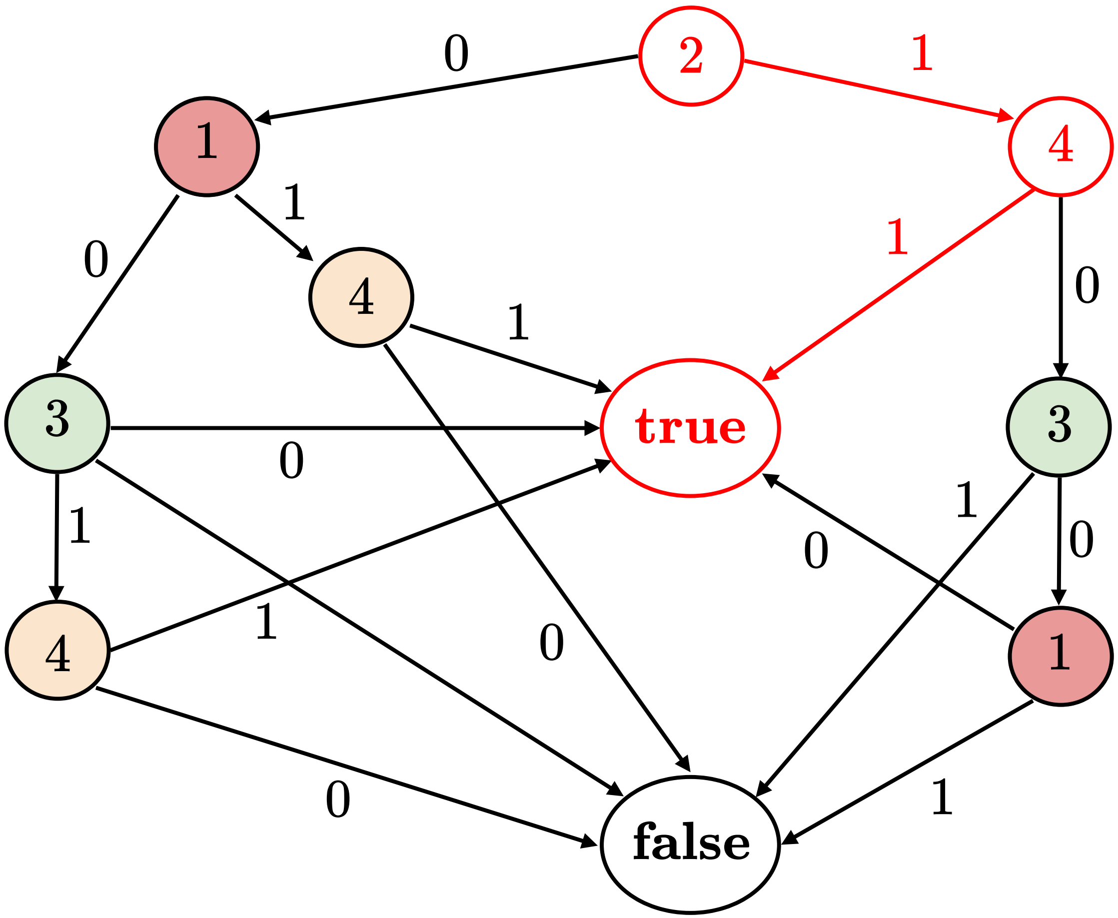


This path represents the instance $(1, 1, 0, 0)$

FOIL is a graph query language



FOIL is a graph query language



This path represents the partial instance $(\perp, 1, \perp, 1)$

Expressiveness and complexity of FOIL

- What notions of explanation can be expressed in **FOIL**?
- What notions of explanation cannot be expressed in **FOIL**?
- What is the complexity of the evaluation problem for **FOIL**?

The evaluation problem for FOIL

We consider the data complexity of the problem, so fix a **FOIL** formula $\Phi(x_1, \ldots, x_k)$

$\mathbf{Eval(\Phi)}$:

- **Input:** decision tree $\mathcal{T}$ of dimension n and partial instances $\mathbf{e}_1, \ldots, \mathbf{e}_k$ of dimension n
- **Output:** yes if $\mathcal{T} \models \Phi(\mathbf{e}_1, \ldots, \mathbf{e}_k)$, and no otherwise

The evaluation problem for FOIL

$\mathcal{T} \models \Phi(\mathbf{e}_1, \ldots, \mathbf{e}_k)$ if and ony if $\mathfrak{A}_{\mathcal{T}} \models \Phi(\mathbf{e}_1, \ldots, \mathbf{e}_k)$

But $\mathfrak{A}_{\mathcal{T}}$ could be of exponential size in the size of $\mathcal{T}$

- $\mathfrak{A}_{\mathcal{T}}$ should not be materialized to check whether $\mathcal{T} \models \Phi(\mathbf{e}_1, \ldots, \mathbf{e}_k)$
- $\mathfrak{A}_{\mathcal{T}}$ is used only to define the semantics of **FOIL**

Bad news ...

Theorem:

1. For every **FOIL** formula Φ, there exists $k \geq 0$ such that $\mathrm{Eval}(\Phi)$ is in Σ_k^{P}
2. For every $k \geq 0$, there exists a **FOIL** formula Φ such that $\mathrm{Eval}(\Phi)$ is Σ_k^{P}-hard

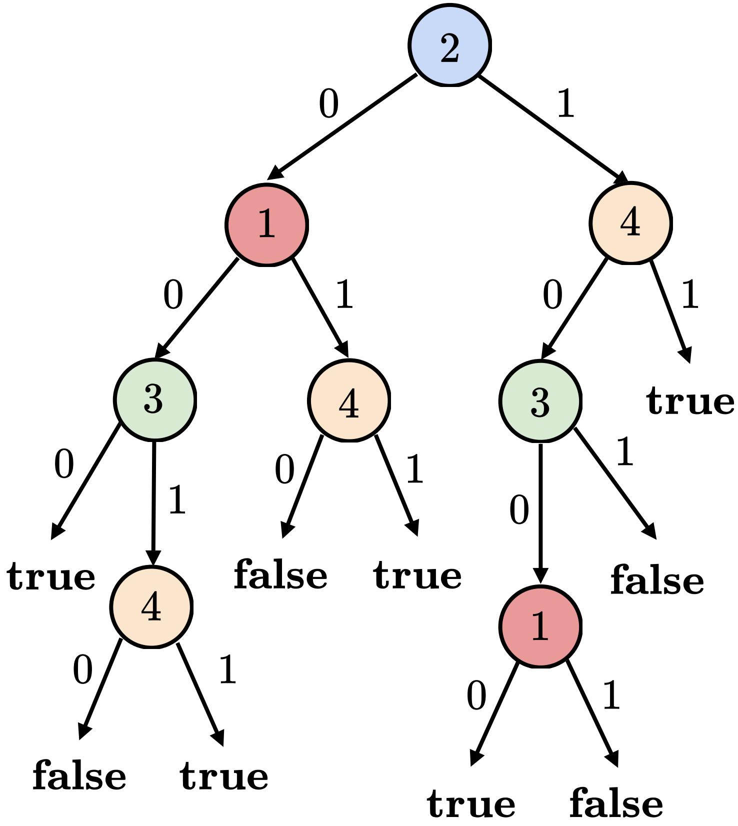
More bad news …

$\mathcal{T}(\mathbf{e}) = 1$ for $\mathbf{e} = (1, 1, 1, 1)$

$\{2, 4\}$ is a minimum sufficient reason for $\mathbf{e}$ over $\mathcal{T}$

- There is no sufficient reason for $\mathbf{e}$ over $\mathcal{T}$ with a smaller number of features

$\mathbf{e}_2 = (\bot, 1, \bot, 1)$ is a minimum sufficient reason for $\mathbf{e}$ over $\mathcal{T}$



More bad news ...

Theorem:

There is no **FOIL** formula $\mathrm{MinimumSR}(x, y)$ such that, for every decision tree $\mathcal{T}$, instance $\mathbf{e}_1$ and partial instance $\mathbf{e}_2$:

$$\mathcal{T} \models \mathrm{MinimumSR}(\mathbf{e}_1, \mathbf{e}_2)$$

$$\iff$$

$\mathbf{e}_2$ is a minimum sufficient reason for $\mathbf{e}_1$ over $\mathcal{T}$

How do we overcome these limitations?

- We use first-order logic, over a larger vocabulary but with some syntactic restrictions
- We continue using some common notions for graphs
- Our goal is to find languages with polynomial or even NP data complexity, since the latter allows the use of SAT solvers

The StratiFOILed Logic

StratiFOILed is a model-specific interpretability query language

- Specifically designed for decision trees

The logic **StratiFOILed** is defined by considering three layers

The StratiFOILed Logic

All the notions of explanation discussed in this talk can be expressed in **StratiFOILed**

- $\text{SR}(x, y)$, $\text{MinimalSR}(x, y)$, $\text{MinimumSR}(x, y)$, $\text{FRS}(x)$, $\text{MinimalFRS}(x)$, $\text{MinimumFRS}(x)$

$\text{Eval}(\Phi)$ can be solved with a fixed number of calls to a SAT solver, for each **StratiFOILed** formula Φ

Implementation based on SAT solvers

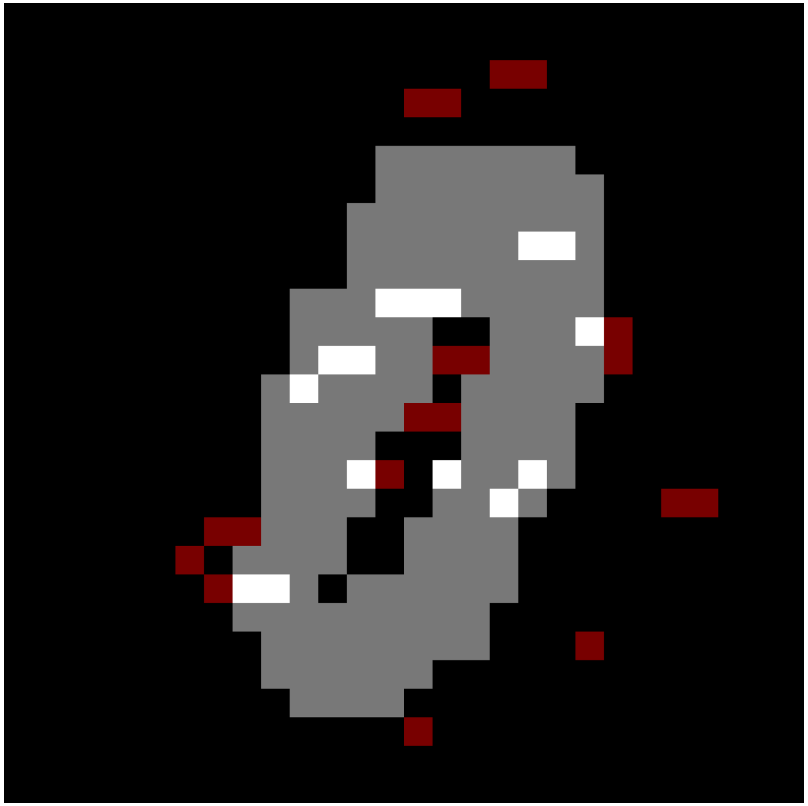
Any SAT solver can be used

Given the complexity of the evaluation problem for **StratiFOILed**, we use:

- **YalSAT:** to find a truth assignment that satisfies a propositional formula
- **Kissat:** to prove that a propositional formula is not satisfiable

MNIST: sufficient reason

$\mathbf{e}$



$\alpha(x, z) = \exists y\,(\mathrm{SR}(x, y) \wedge \mathrm{LEL}(y, z))$

Evaluate whether $\alpha(\mathbf{e}, \mathbf{u}_{730})$ holds

$\mathbf{u}_{730} \in \{0, 1, \perp\}^{784}$ satisfies that $|\{i \in \{1, \ldots, 784\} \mid \mathbf{u}_{730}[i] = \perp\}| = 730$

Concluding remarks

StratiFOILed is a model-specific interpretability query language

- How can the definition of **StratiFOILed** be extended to OBDDs and FBDDs?

Concluding remarks

FOIL is a model-agnostic interpretability query language

- The evaluation problem for some fragments of **FOIL** can be solved in polynomial time for decision trees and OBDDs
- What is an appropriate fragment of **FOIL** to be evaluated using SAT solvers?
- What is an appropriate interpretability query language for FBDDs that is based on **FOIL**?

Concluding remarks

How can probabilities be incorporated into this framework?

- A probability distribution on the possible values of features, and a probabilistic classifier

Probabilistic circuits seem to be the right model for this

- A natural and robust generalization of Boolean circuits, with many well-understood properties

Thanks!

Backup slides

The StratiFOILed Logic

The logic **StratiFOILed** is defined by considering three layers

1. Atomic formulas
2. Guarded formulas
3. The formulas from **StratiFOILed** itself

The first layer

$\subseteq$ can be considered as a *syntactic* predicate, it does not refer to the models

We need another predicate like that. Given partial instances $\mathbf{e}_1, \mathbf{e}_2$ of dimension n:

$\mathbf{LEL}(\mathbf{e}_1, \mathbf{e}_2)$ holds

if and only if

$$|\{i \in \{1, \dots n\} \mid \mathbf{e}_1[i] = \bot\}| \geq |\{i \in \{1, \dots n\} \mid \mathbf{e}_1[i] = \bot\}|$$

Why do we need another syntactic predicate?

$$\begin{aligned}\mathrm{MinimumSR}(x,y) \;=\; & \mathrm{SR}(x,y) \wedge \\ & \forall z \left((\mathrm{SR}(x,z) \wedge \mathrm{LEL}(z,y)) \rightarrow \mathrm{LEL}(y,z) \right)\end{aligned}$$

How many more predicates do we need to include?

Atomic formulas

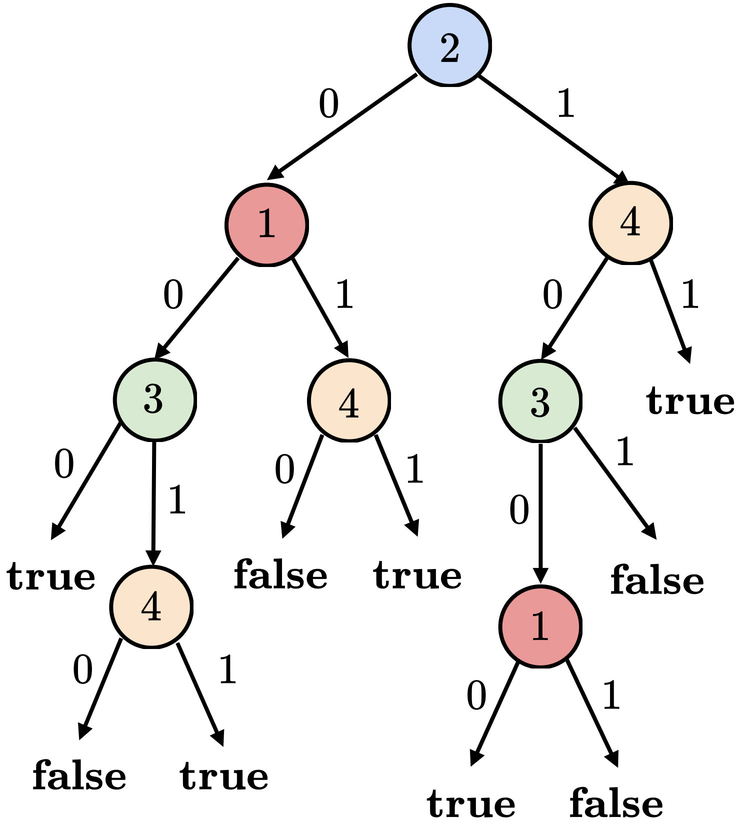
All the syntactic predicates needed in our formalism can be expressed as first-order queries over $\{\subseteq, \mathrm{LEL}\}$

Theorem: if Φ is a first-order formula defined over $\{\subseteq, \mathrm{LEL}\}$, then $\mathrm{Eval}(\Phi)$ can be solved in polynomial time

Atomic formulas of StratiFOILed: the set of first-order formulas defined over $\{\subseteq, \mathrm{LEL}\}$

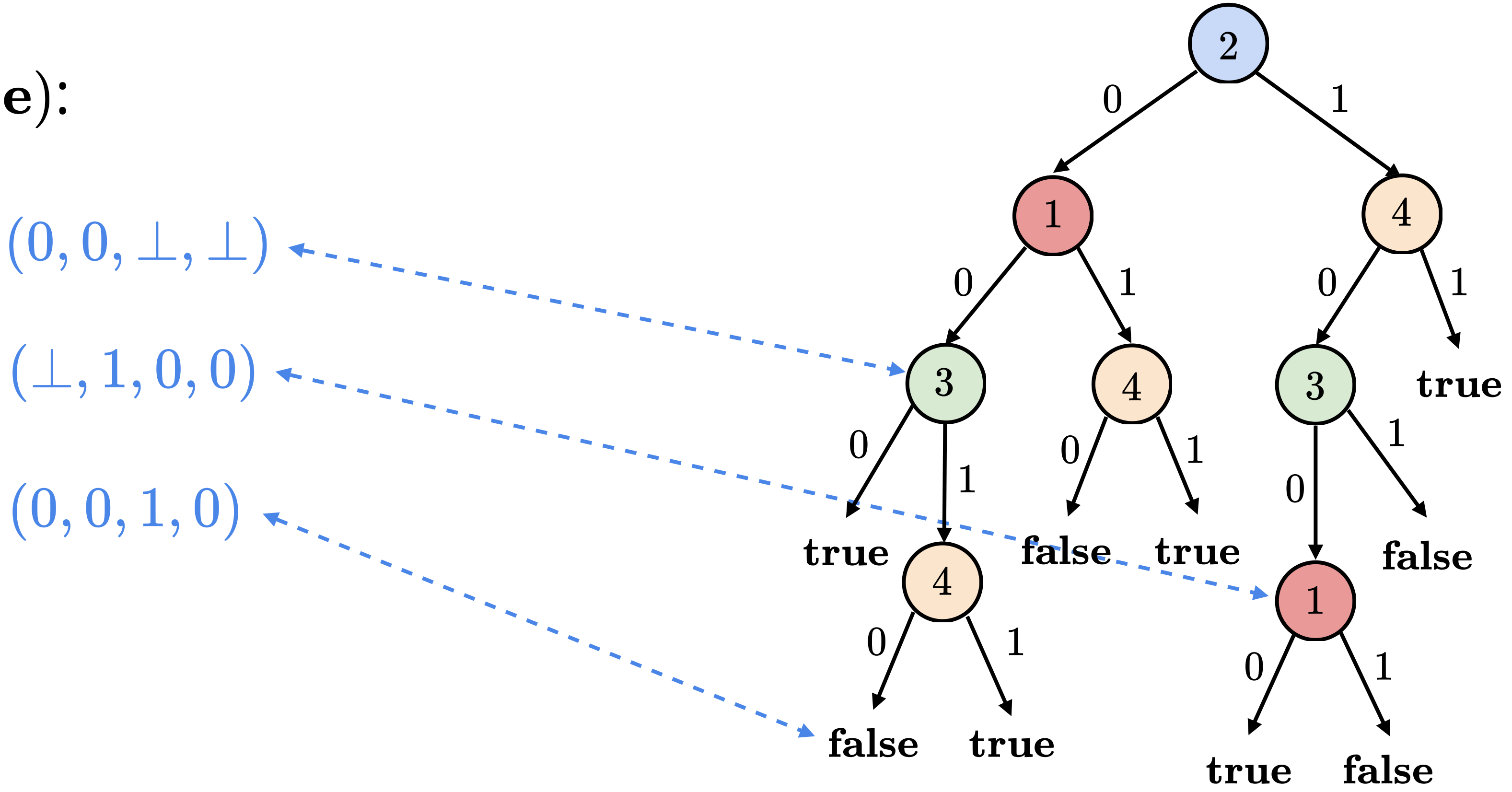
The second layer

Node($\mathbf{e}$):



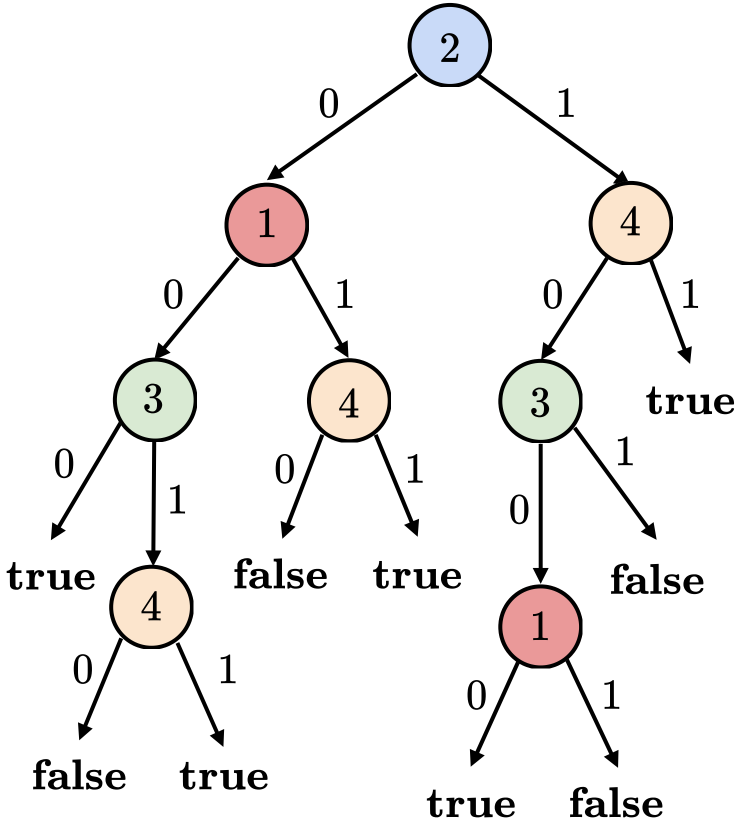
The second layer

Node($\mathbf{e}$):



The second layer

PosLeaf($\mathbf{e}$):

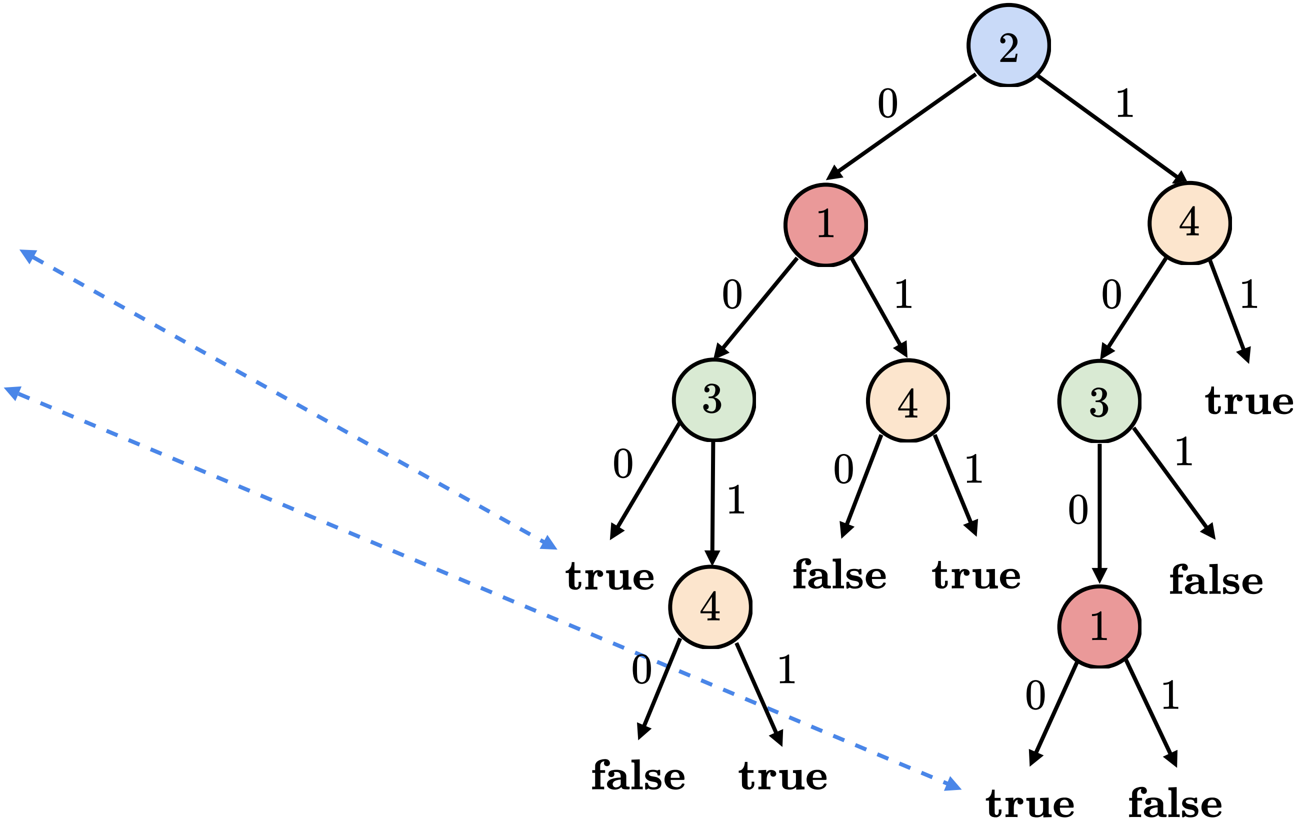


The second layer

PosLeaf($\mathbf{e}$):

$(0, 0, 0, \perp)$

$(0, 1, 0, 0)$



Guarded formulas

1. Each atomic formula is a guarded formula
2. Boolean combinations of guarded formulas are guarded formulas
3. If Φ is a guarded formula, then so are

$$\exists x\ (\mathrm{Node}(x) \wedge \Phi) \qquad \forall x\ (\mathrm{Node}(x) \rightarrow \Phi)$$

$$\exists x\ (\mathrm{PosLeaf}(x) \wedge \Phi) \qquad \forall x\ (\mathrm{PosLeaf}(x) \rightarrow \Phi)$$

An example of a guarded formula

$$
\begin{aligned}
\mathrm{FRS}(x) \; = \; & \forall y \, \big[\mathrm{Node}(y) \to (\mathrm{AllPos}(y) \; \to \\
& \quad \forall z \, (\mathrm{Node}(z) \to (\mathrm{AllNeg}(z) \to \\
& \qquad \neg \exists w \, (\mathrm{Suf}(x, w) \land \mathrm{Cons}(w, y) \land \mathrm{Cons}(w, z)))))\big]
\end{aligned}
$$

guarded formula

An example of a guarded formula

$$\mathrm{FRS}(x) \;=\; \forall y \left[\mathrm{Node}(y) \to (\mathrm{AllPos}(y) \;\to\; \forall z\,(\mathrm{Node}(z) \to (\mathrm{AllNeg}(z) \to \neg\exists w\,(\mathrm{Suf}(x,w) \wedge \mathrm{Cons}(w,y) \wedge \mathrm{Cons}(w,z)))))\right]$$

guarded formula (annotation on $\forall z\,(\mathrm{Node}(z) \to$)

An example of a guarded formula

$$\mathrm{FRS}(x) \; = \; \forall y \left[\mathrm{Node}(y) \rightarrow (\mathrm{AllPos}(y) \; \rightarrow \right.$$
$$\forall z \, (\mathrm{Node}(z) \rightarrow (\mathrm{AllNeg}(z) \rightarrow$$
$$\left. \neg \exists w \, (\mathrm{Suf}(x, w) \wedge \mathrm{Cons}(w, y) \wedge \mathrm{Cons}(w, z))))) \right]$$

atomic formulas

An example of a guarded formula

$$\mathrm{FRS}(x) \;=\; \forall y \left[\mathrm{Node}(y) \to (\mathrm{AllPos}(y) \;\to \right.$$

$$\forall z \,(\mathrm{Node}(z) \to (\mathrm{AllNeg}(z) \to$$

$$\left. \neg\exists w \,(\mathrm{Suf}(x,w) \wedge \mathrm{Cons}(w,y) \wedge \mathrm{Cons}(w,z))))) \right]$$

atomic formula

The third layer: StratiFOILed

1. Each guarded formula is a **StratiFOILed** formula
2. If Φ is a guarded formula, then $\exists x_1 \cdots \exists x_k \, \Phi$ and $\forall x_1 \cdots \forall x_k \, \Phi$ are **StratiFOILed** formulas
3. Boolean combinations of **StratiFOILed** formulas are **StratiFOILed** formulas

Examples of StratiFOILed formulas

$\mathrm{SR}(x,y)$, $\mathrm{MinimalSR}(x,y)$, $\mathrm{MinimumSR}(x,y)$ can be expressed as **StratiFOILed** formulas

$$\begin{aligned}\mathrm{FRS}(x) \;=\; \forall y \,\big[\mathrm{Node}(y) \to (\mathrm{AllPos}(y) \;\to \\ \forall z\,(\mathrm{Node}(z) \to (\mathrm{AllNeg}(z) \to \\ \neg\exists w\,(\mathrm{Suf}(x,w) \wedge \mathrm{Cons}(w,y) \wedge \mathrm{Cons}(w,z)))))\big]\end{aligned}$$

$\mathrm{MinimalFRS}(x)$, $\mathrm{MinimumFRS}(x)$ can be expressed as a **StratiFOILed** formulas

The evaluation problem for StratiFOILed

BH: Boolean Hierarchy over NP

Theorem:

1. For each **StratiFOILed** formula Φ, there exists $k \geq 1$ such that $\mathrm{Eval}(\Phi)$ is in BH_k
2. For every $k \geq 1$, there exists a **StratiFOILed** formula Φ such that $\mathrm{Eval}(\Phi)$ is in BH_k-hard