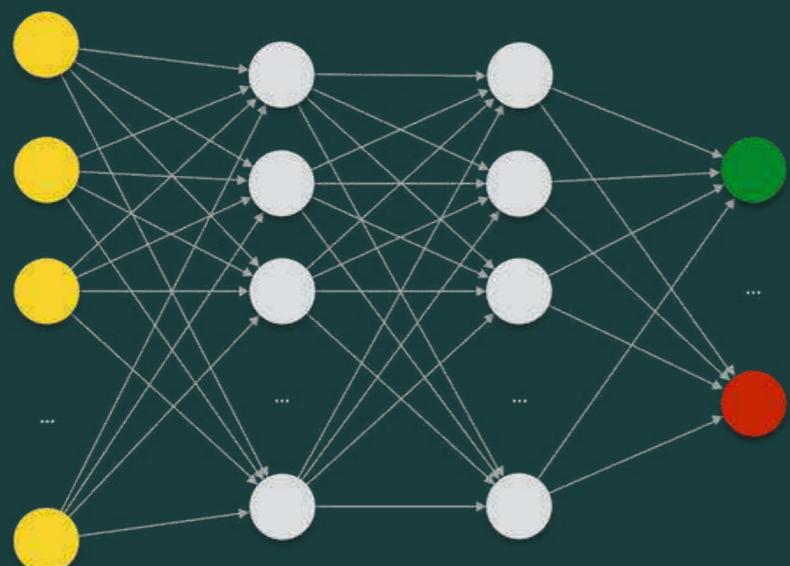


# Formal Methods for Machine Learning Pipelines

VTSA 2024



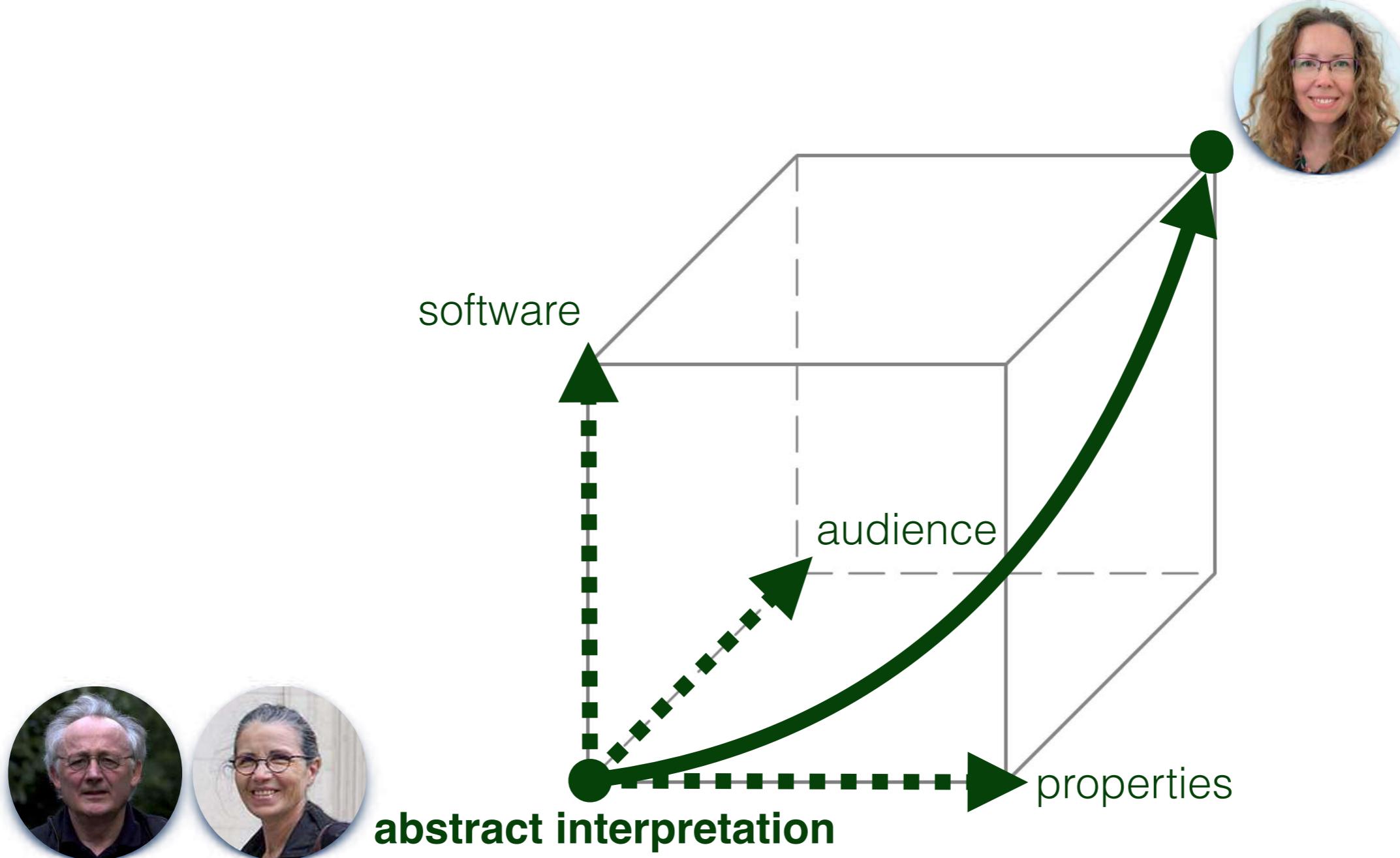
# Who am I?



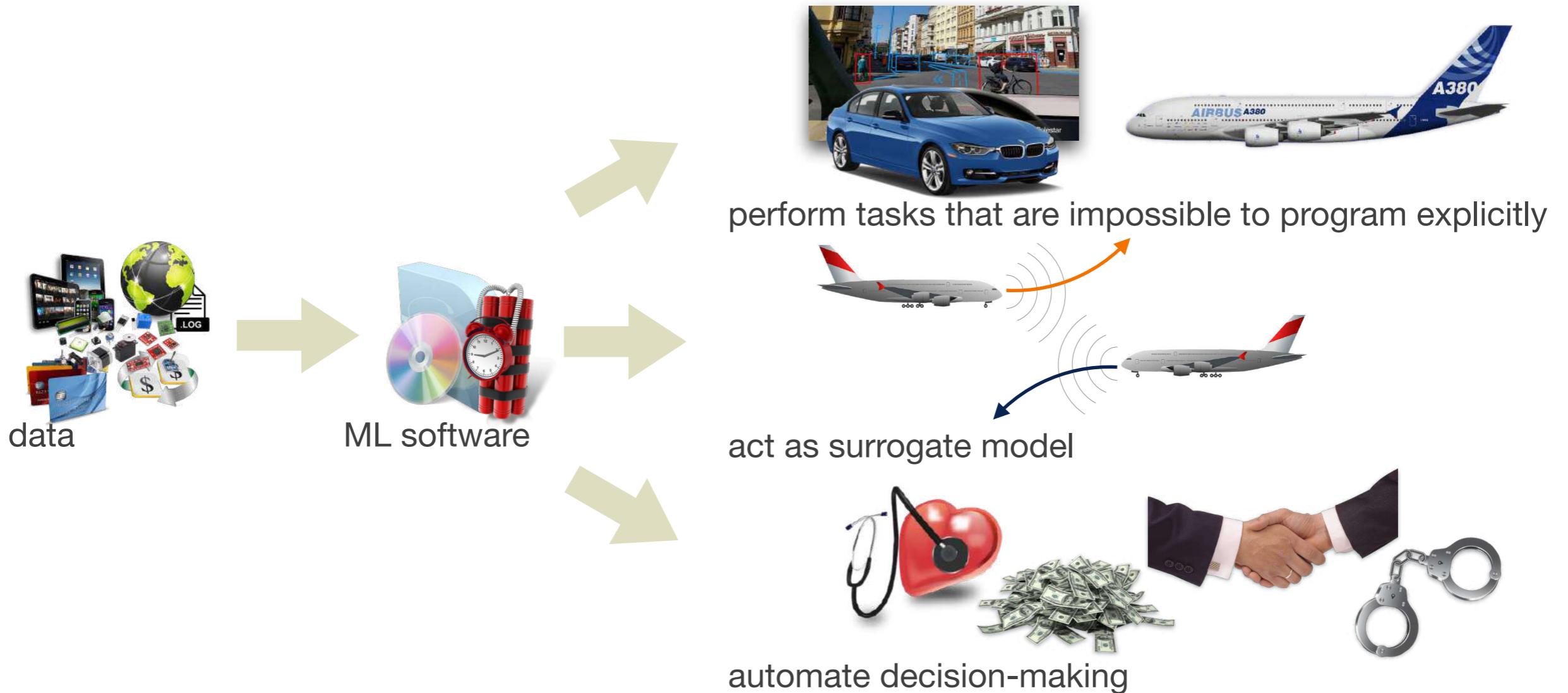
1987	Udine, Italie	
2006 - 2011	Università degli Studi di Udine	BSc, MSc
2011 - 2015	École Normale Supérieure	PhD
2015	NASA & Carnegie Mellon University	Internship
2015 - 2019	ETH Zurich	Postdoc
Since 2019	Inria	

BSc, MSc  
PhD  
Internship  
Postdoc

# What do I do?



# ML in High-Stakes Applications



# ML in High-Stakes Applications



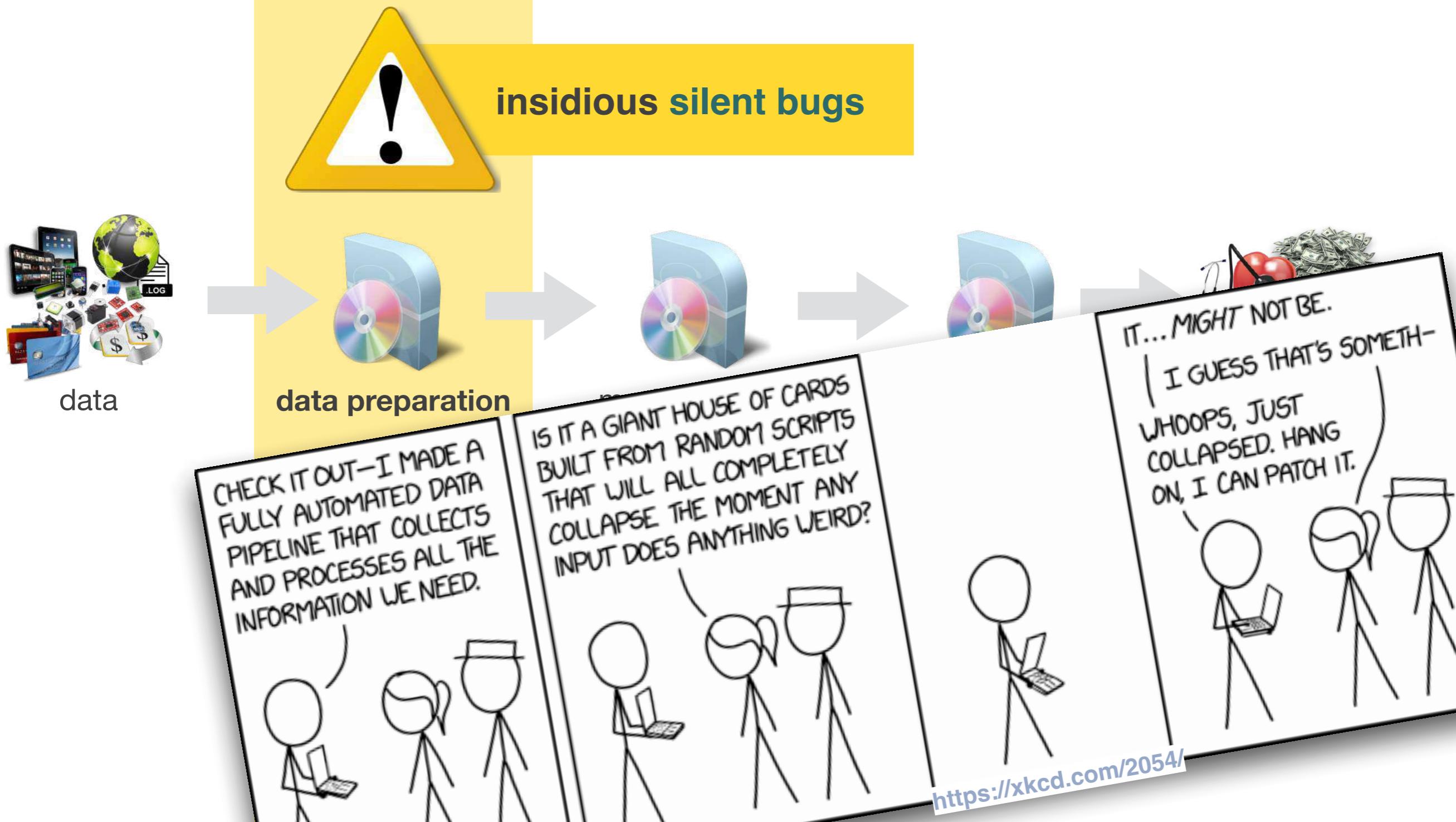
# Machine Learning Pipeline

## Machine Learning Development Process



# Machine Learning Pipeline

Data Preparation is **Fragile**



# Machine Learning Pipeline

Model Training is Highly Non-Deterministic

The image consists of two main parts. On the left is a white rectangular box containing a cartoon illustration. The cartoon shows a stick figure pouring data from a funnel labeled "DATA" into a large pile of mathematical symbols (matrices and vectors) on the ground. A second stick figure is shown stirring this pile with a large spoon. The text inside the box reads:

THIS IS YOUR MACHINE LEARNING SYSTEM?  
YUP! YOU POUR THE DATA INTO THIS BIG  
PILE OF LINEAR ALGEBRA, THEN COLLECT  
THE ANSWERS ON THE OTHER SIDE.  
WHAT IF THE ANSWERS ARE WRONG?  
JUST STIR THE PILE UNTIL  
THEY START LOOKING RIGHT.

Below the cartoon is the URL <https://xkcd.com/1838/>.

On the right is a yellow rectangular box containing a flowchart of a machine learning pipeline. It shows three stages: "model training" (represented by a blue CD icon), "model deployment" (another blue CD icon), and "predictions" (an icon of a handshake between a red heart and a stack of money). Arrows connect the stages. Below the flowchart is a yellow warning sign with an exclamation mark. To its right, the text reads:

no predictability and traceability

# Machine Learning Pipeline

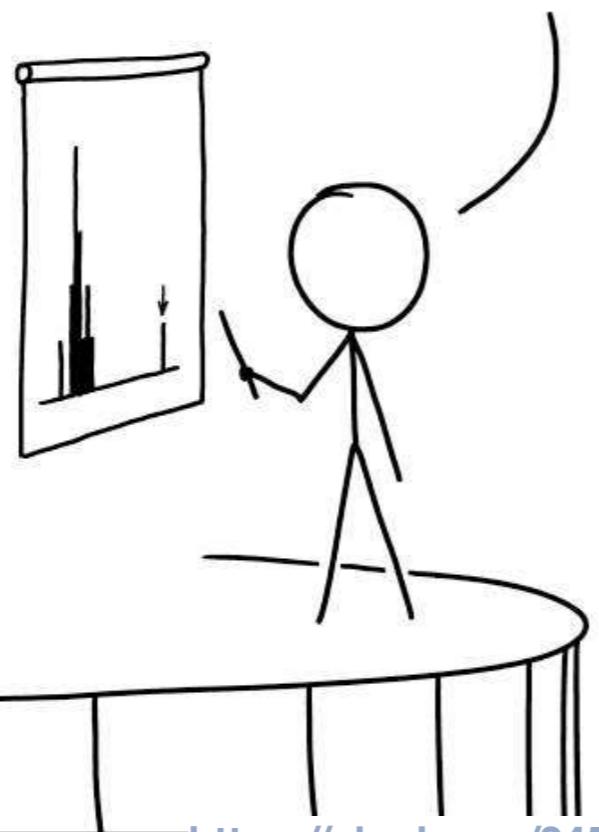
## Models Only Give Probabilistic Guarantees



data

DESPITE OUR GREAT RESEARCH RESULTS, SOME HAVE QUESTIONED OUR AI-BASED METHODOLOGY.

BUT WE TRAINED A CLASSIFIER ON A COLLECTION OF GOOD AND BAD METHODOLOGY SECTIONS, AND IT SAYS OURS IS FINE.



<https://xkcd.com/2451/>



model deployment



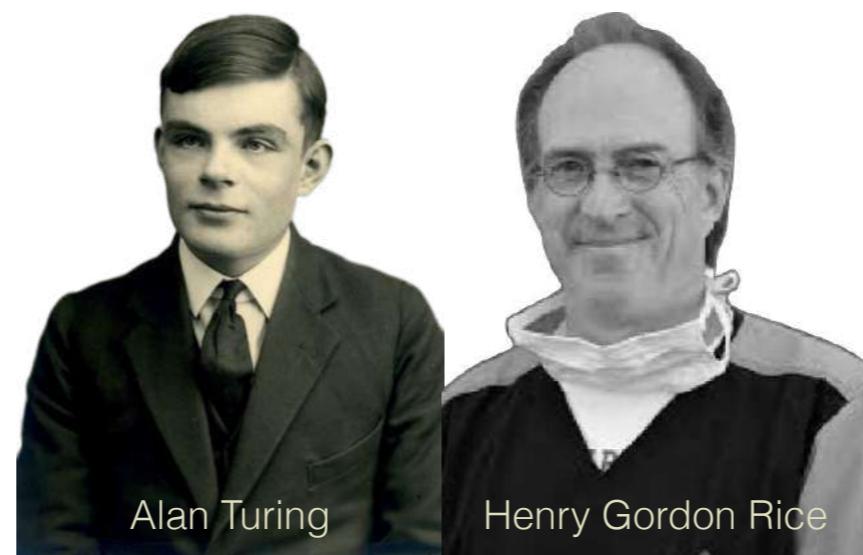
predictions

not sufficient for guaranteeing  
an acceptable failure rate  
under any circumstance



# Correctness Guarantees

A Mathematically Proven Hard Problem

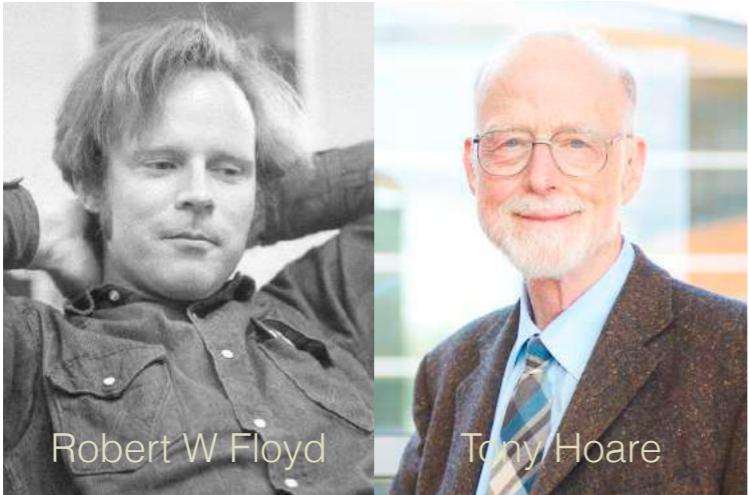


Alan Turing

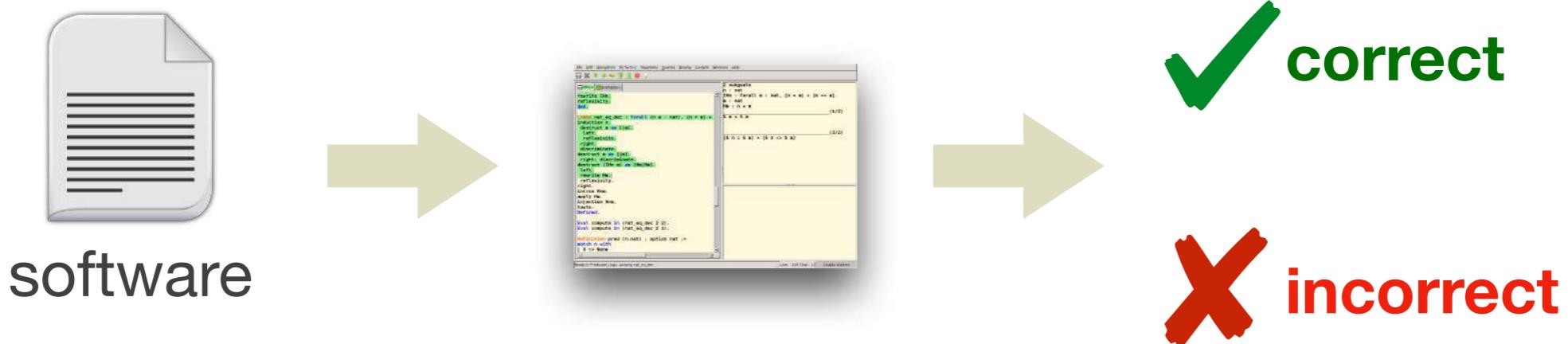
Henry Gordon Rice

# Formal Methods

## Deductive Verification

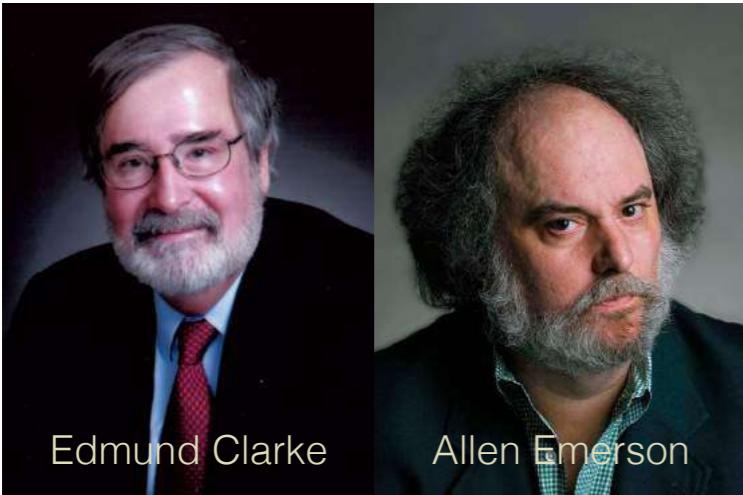


- extremely **expressive**
- **relies on the user** to guide the proof



# Formal Methods

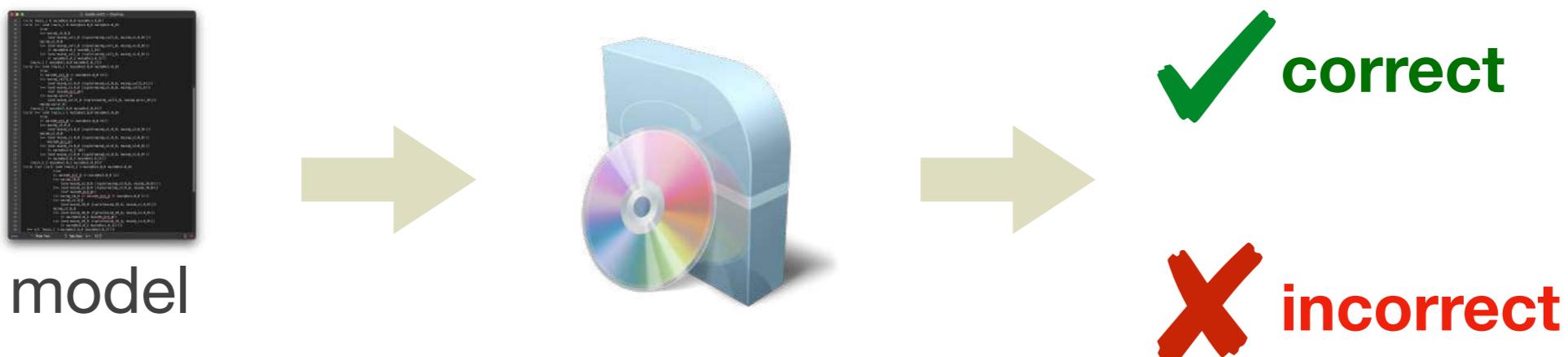
## Model Checking



Edmund Clarke

Allen Emerson

- analysis of a **model** of the software
- **sound and complete with respect to the model**

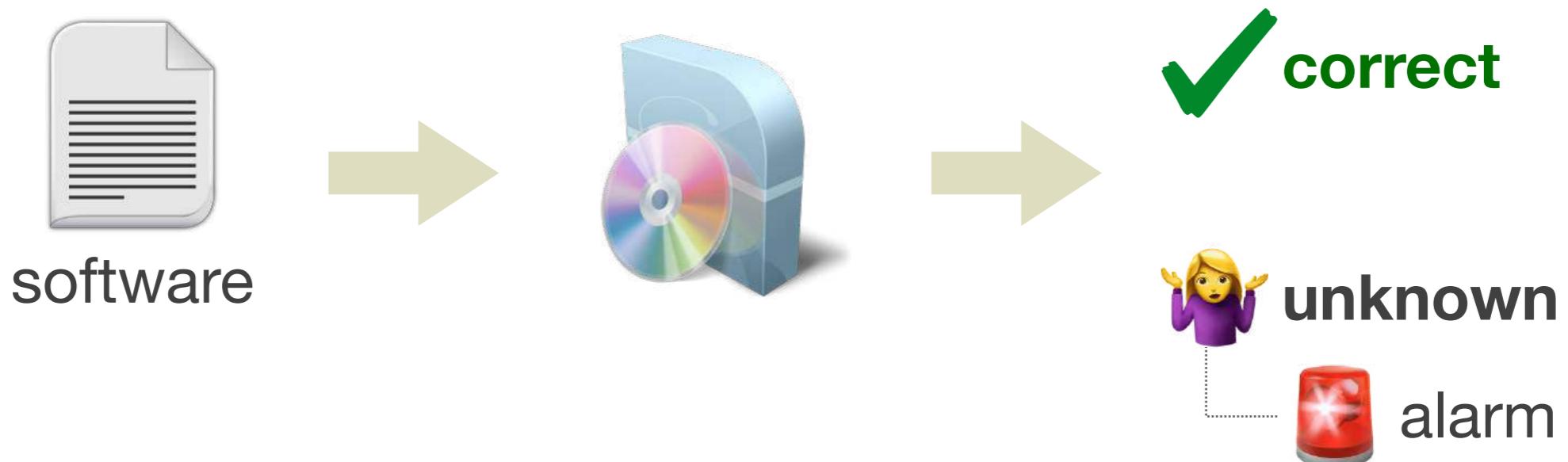


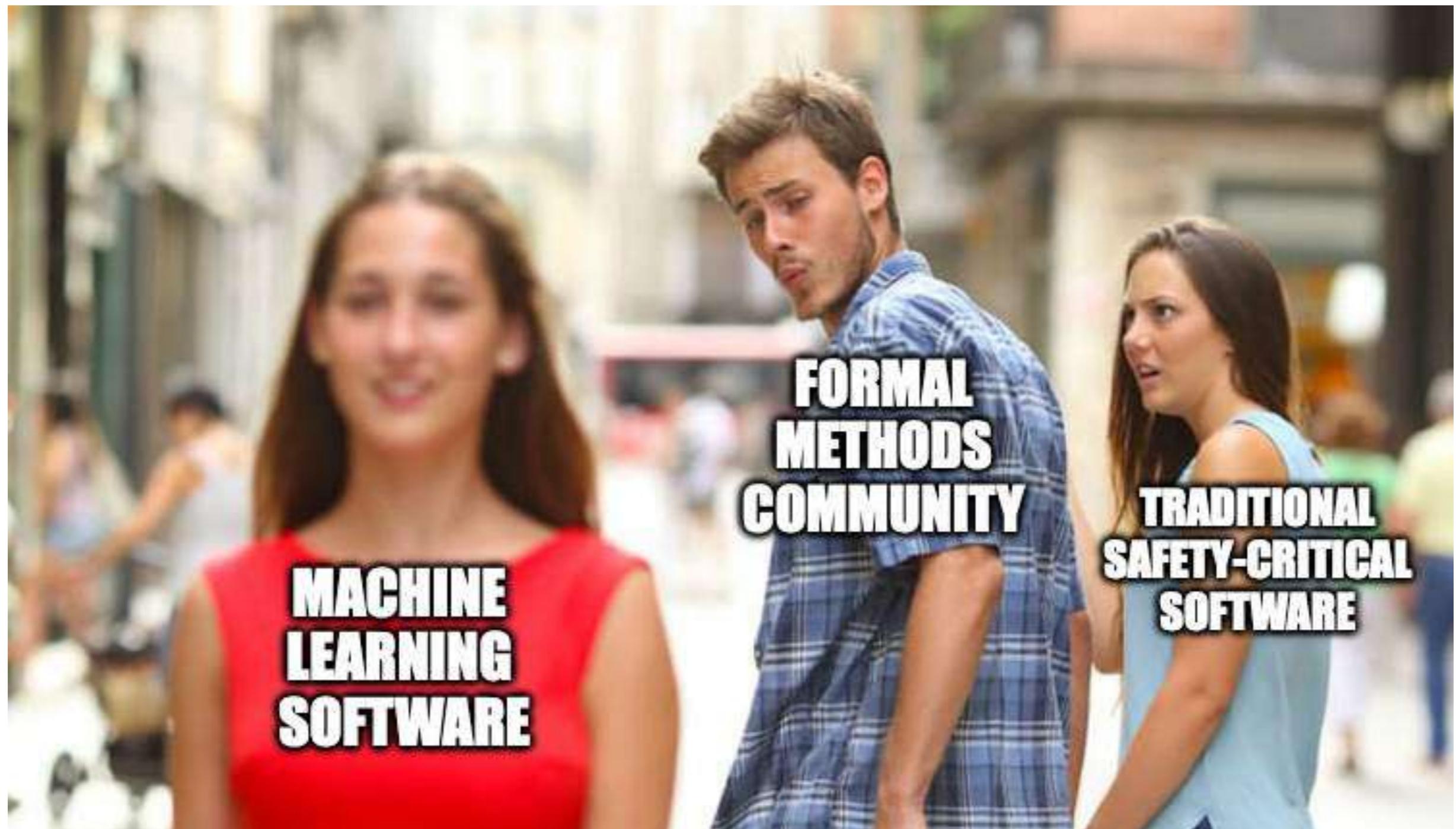
# Formal Methods

## Static Analysis by Abstract Interpretation



- analysis of the **source or object code**
- fully **automatic** and **sound** by construction
- generally **not complete**





COLLIMBE

# Formal Methods for ML



Robert W. Floyd

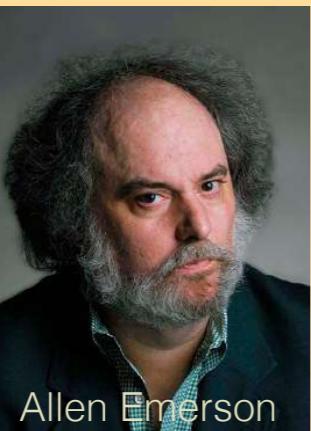


Tony Hoare

## Deductive Verification



Edmund Clarke



Allen Emerson

## Model Checking



Patrick Cousot

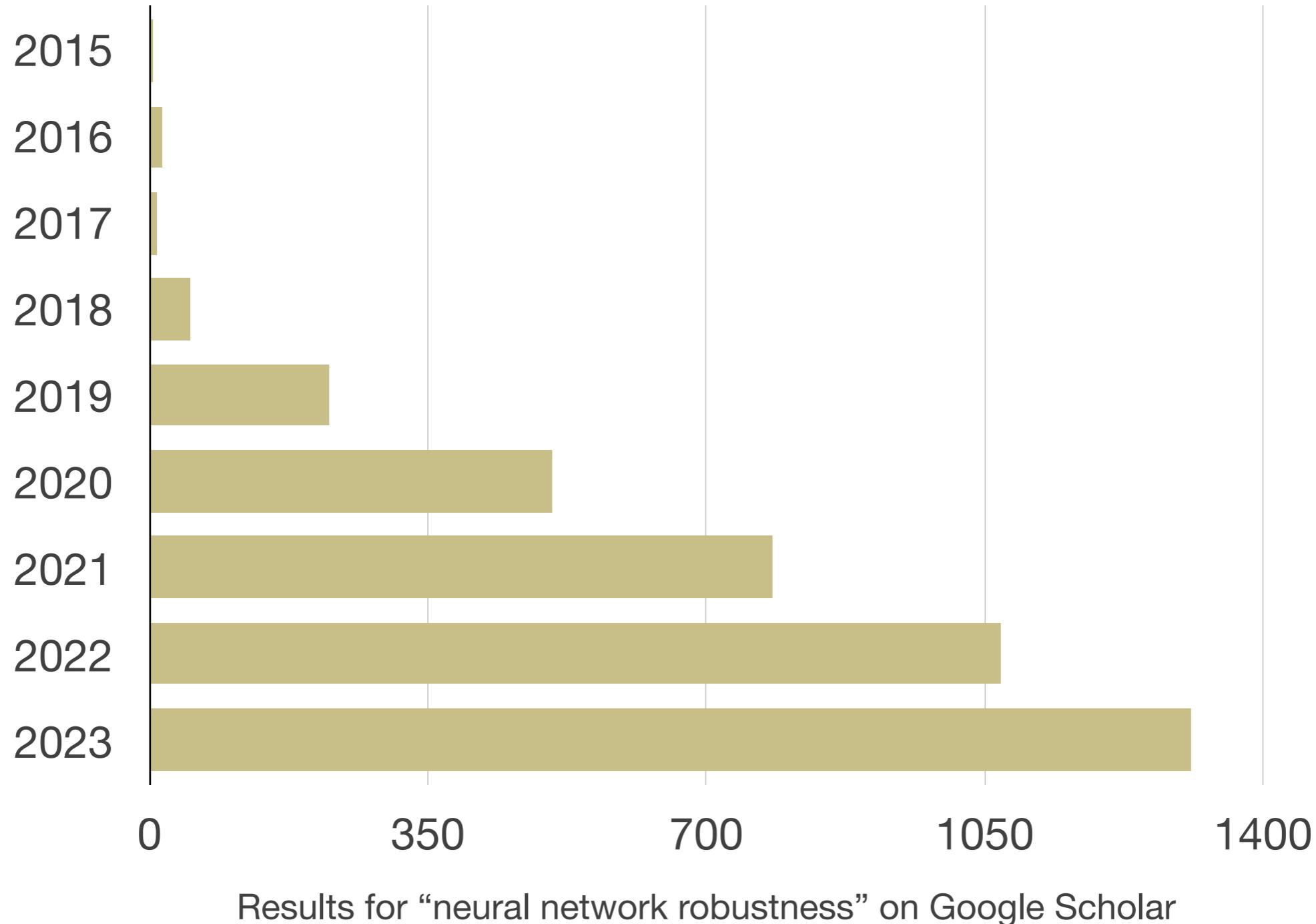


Radhia Cousot

## Static Analysis



# Formal Methods for ML



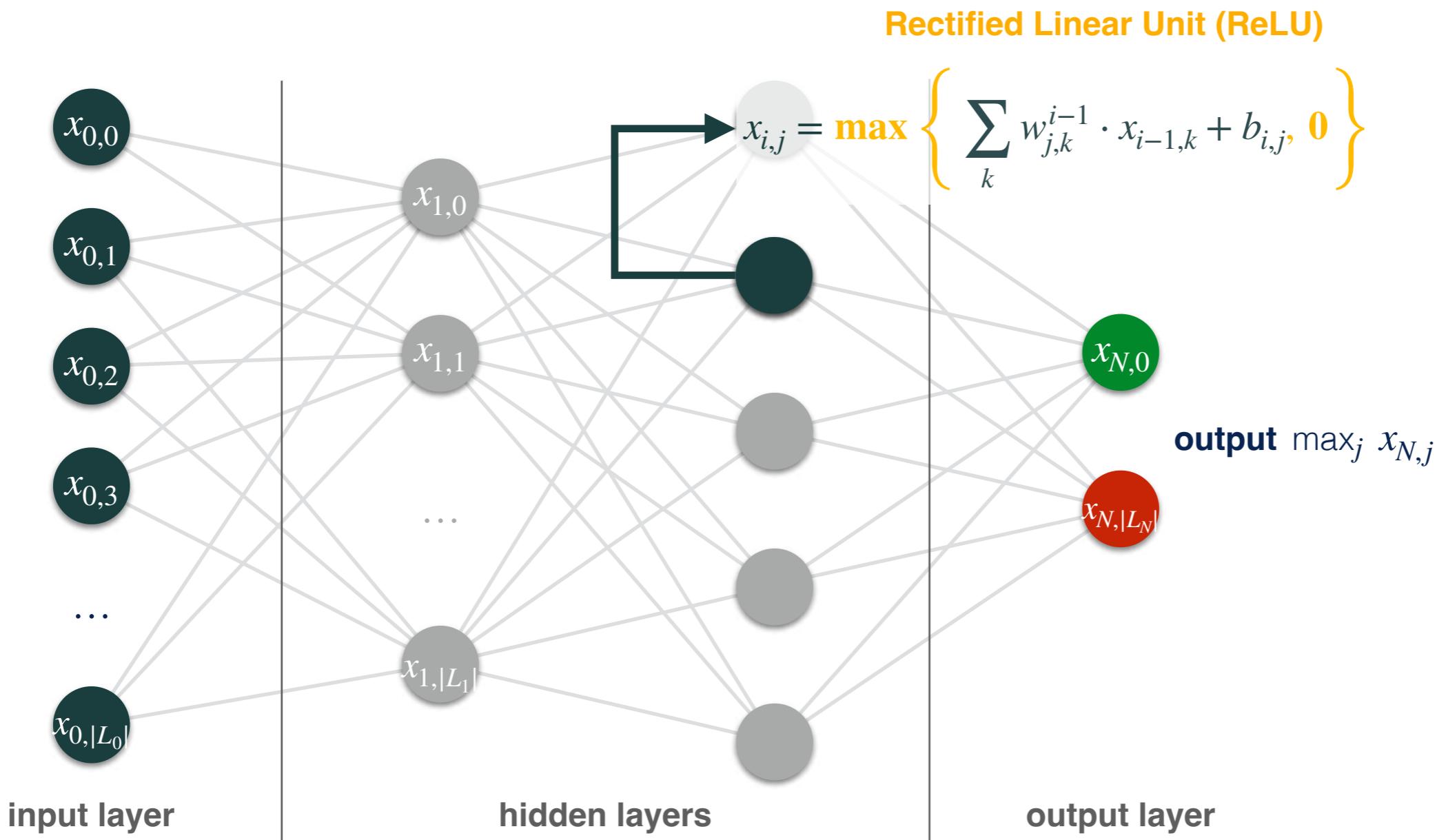
# Formal Methods for Trained Models



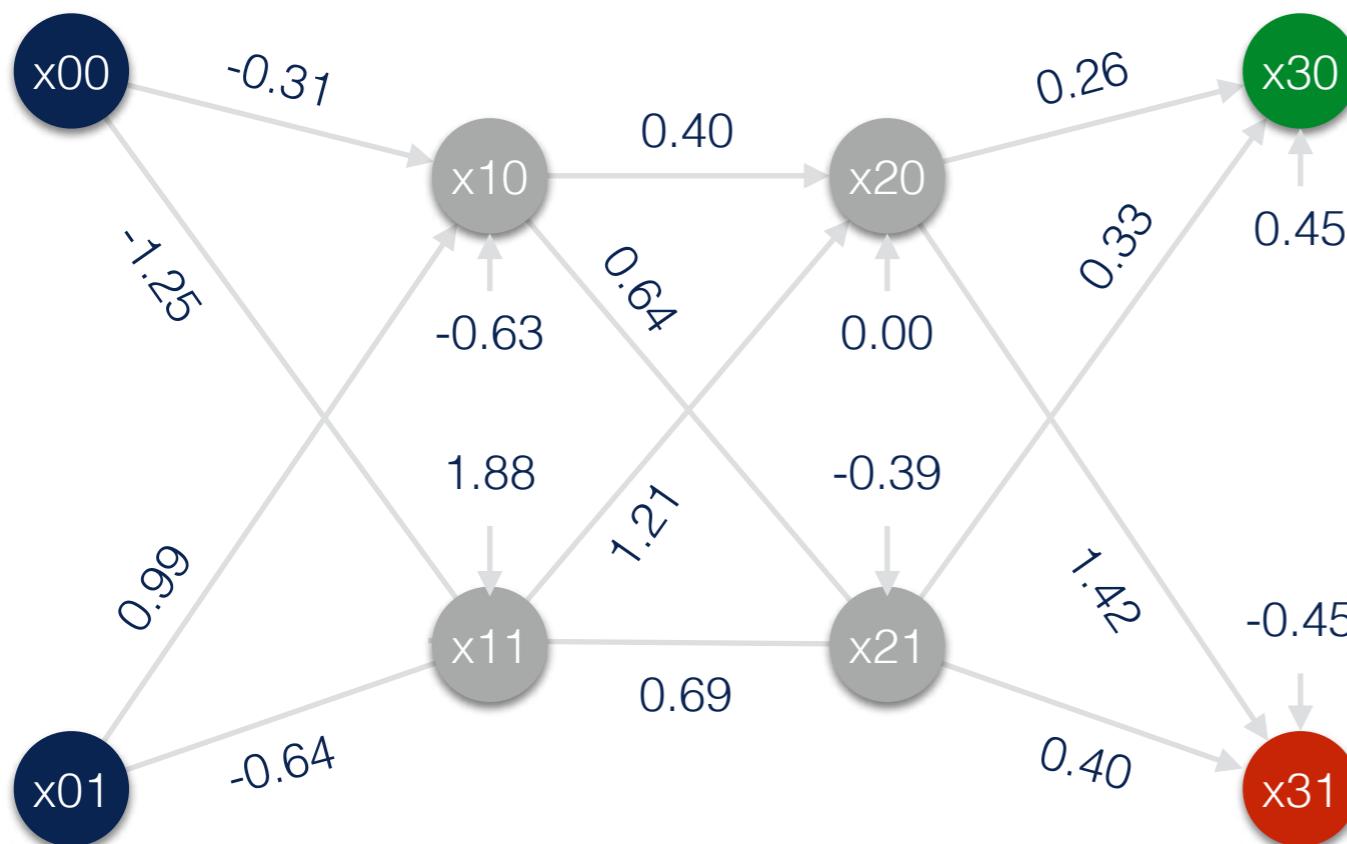
# Neural Networks

# Neural Networks

## Feed-Forward ReLU-Activated Neural Networks



# Neural Networks as Programs



```
x00 = input()
x01 = input()

x10 = -0.31 * x00 + 0.99 * x01 + (-0.63)
x11 = -1.25 * x00 + (-0.64) * x01 + 1.88

x10 = 0 if x10 < 0 else x10
x11 = 0 if x11 < 0 else x11

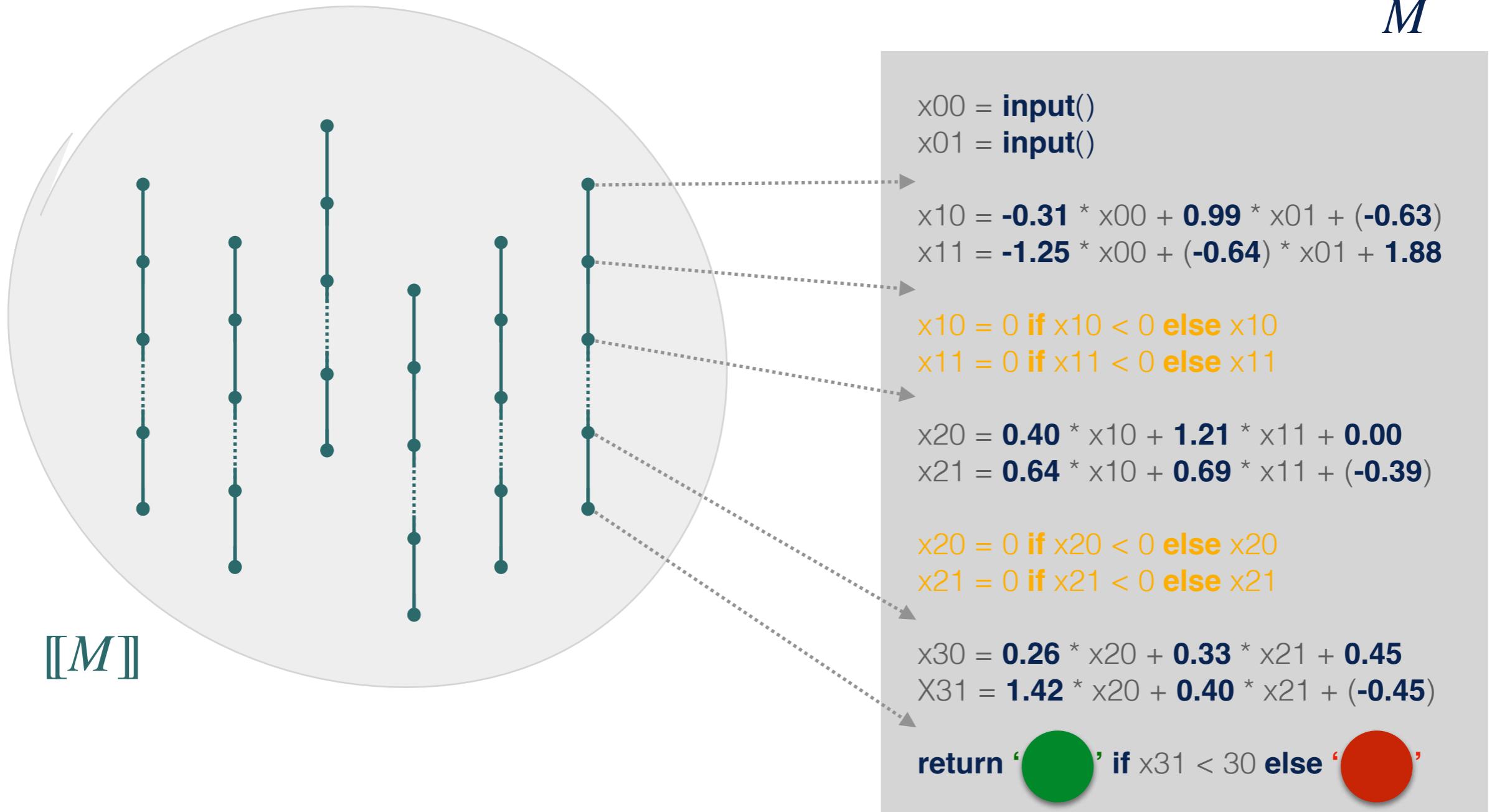
x20 = 0.40 * x10 + 1.21 * x11 + 0.00
x21 = 0.64 * x10 + 0.69 * x11 + (-0.39)

x20 = 0 if x20 < 0 else x20
x21 = 0 if x21 < 0 else x21

x30 = 0.26 * x20 + 0.33 * x21 + 0.45
x31 = 1.42 * x20 + 0.40 * x21 + (-0.45)

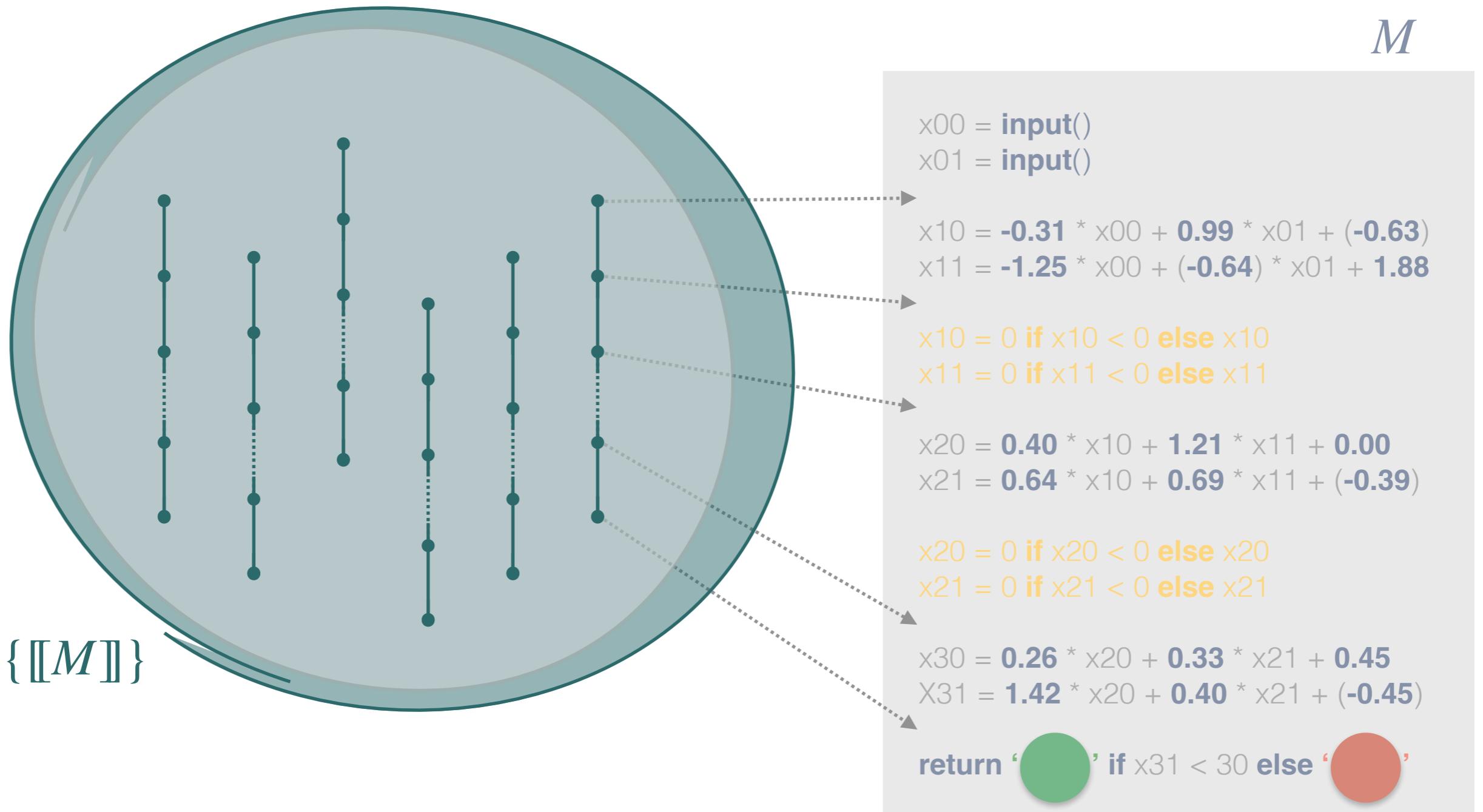
return 'green' if x31 < 30 else 'red'
```

# Maximal Trace Semantics



# Neural Network Verification

# Collecting Semantics



# Collecting Semantics

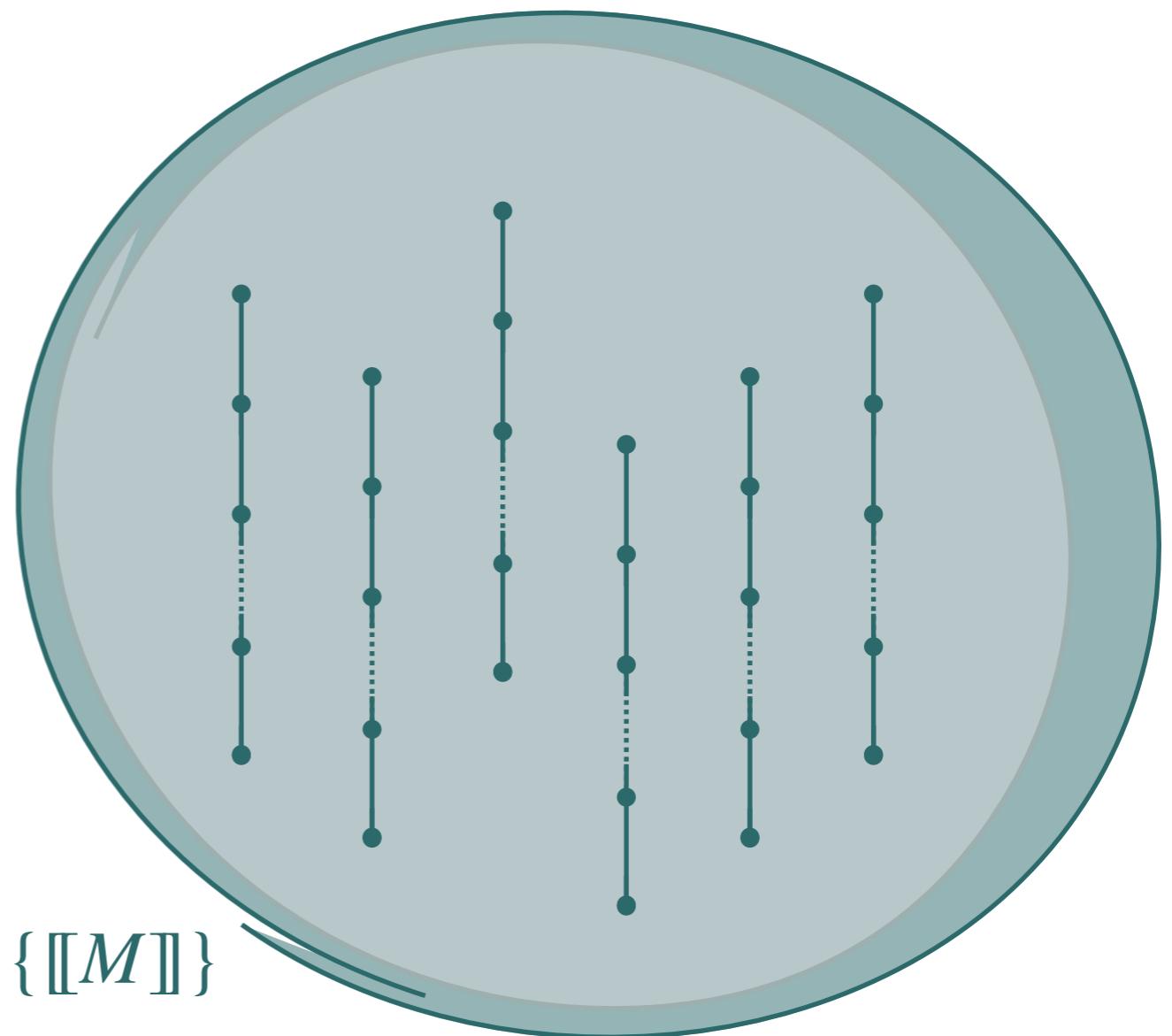
## Intuition

**Property (by extension): set of elements that have that property**

Property “being Jun Pang”

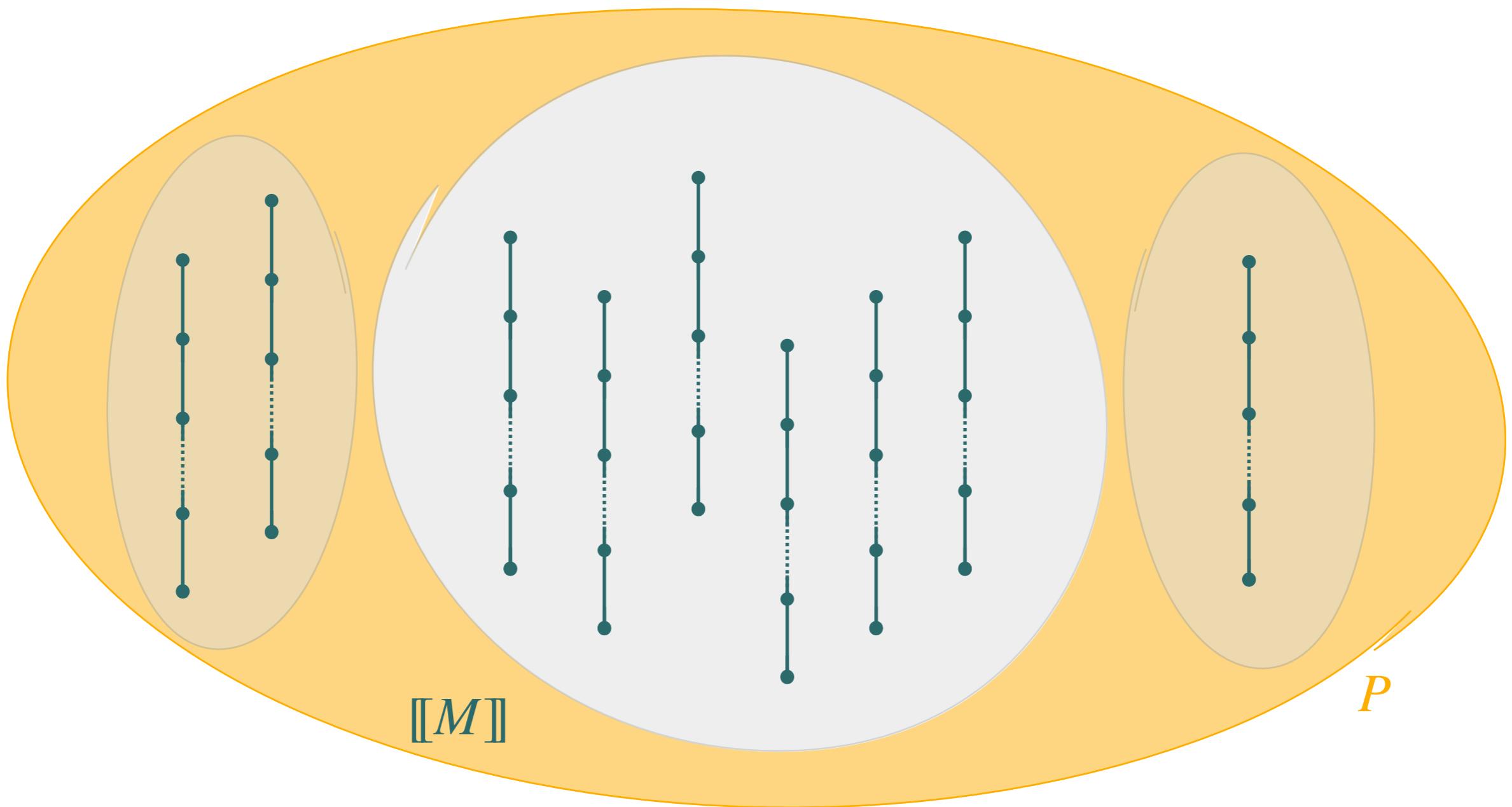


Property “being neural network M”



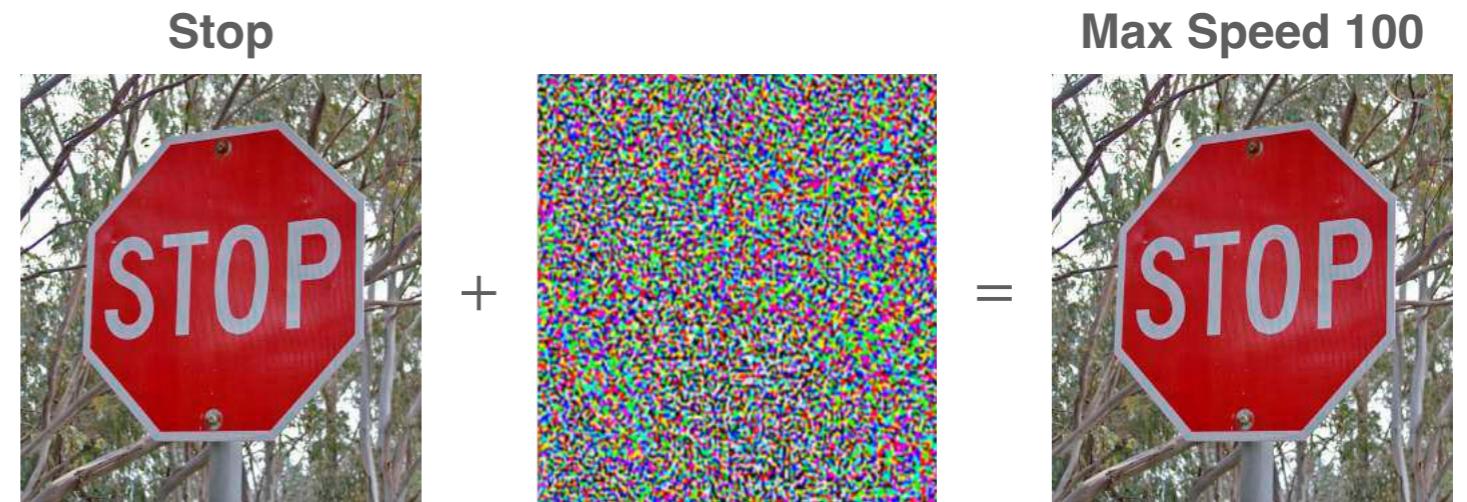
# Property Verification

$$\mathcal{M} \in P \Leftrightarrow \{\mathcal{M}\} \subseteq P$$



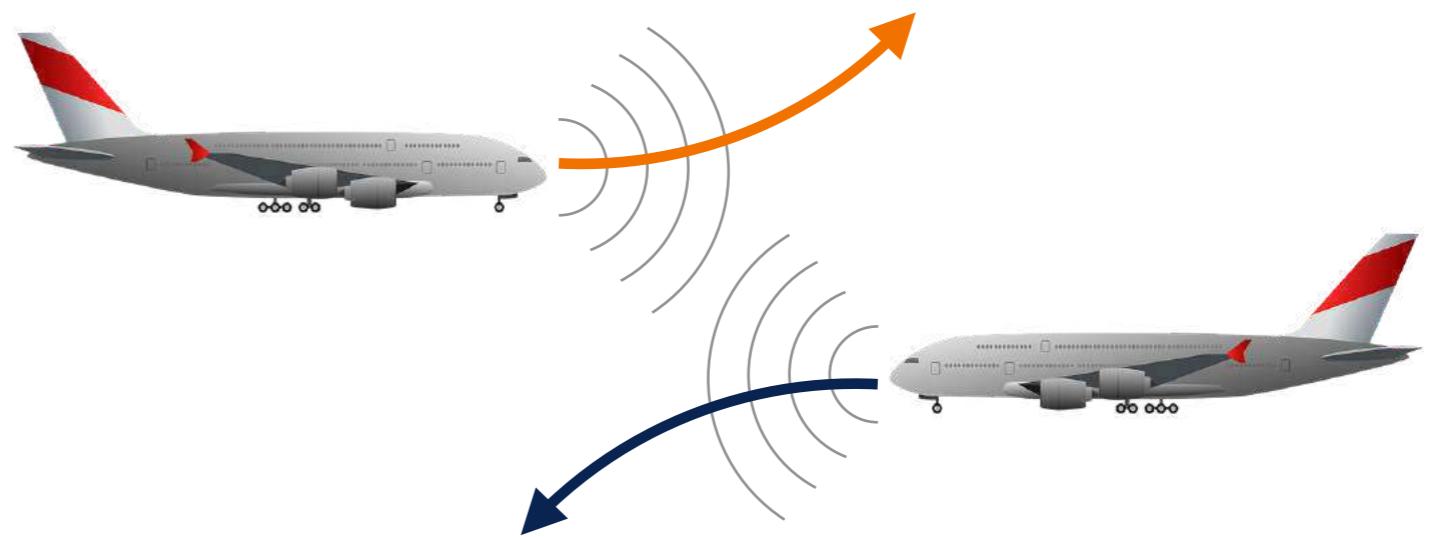
# Stability

Goal G3 in [Kurd03]



# Safety

Goal G4 in [Kurd03]

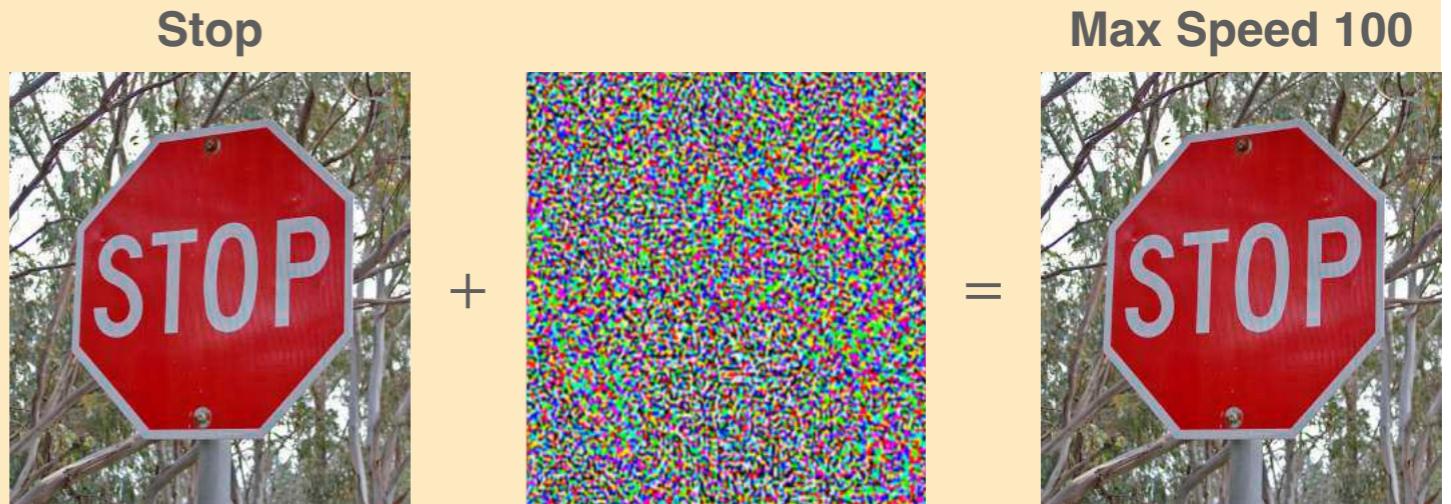


# Fairness



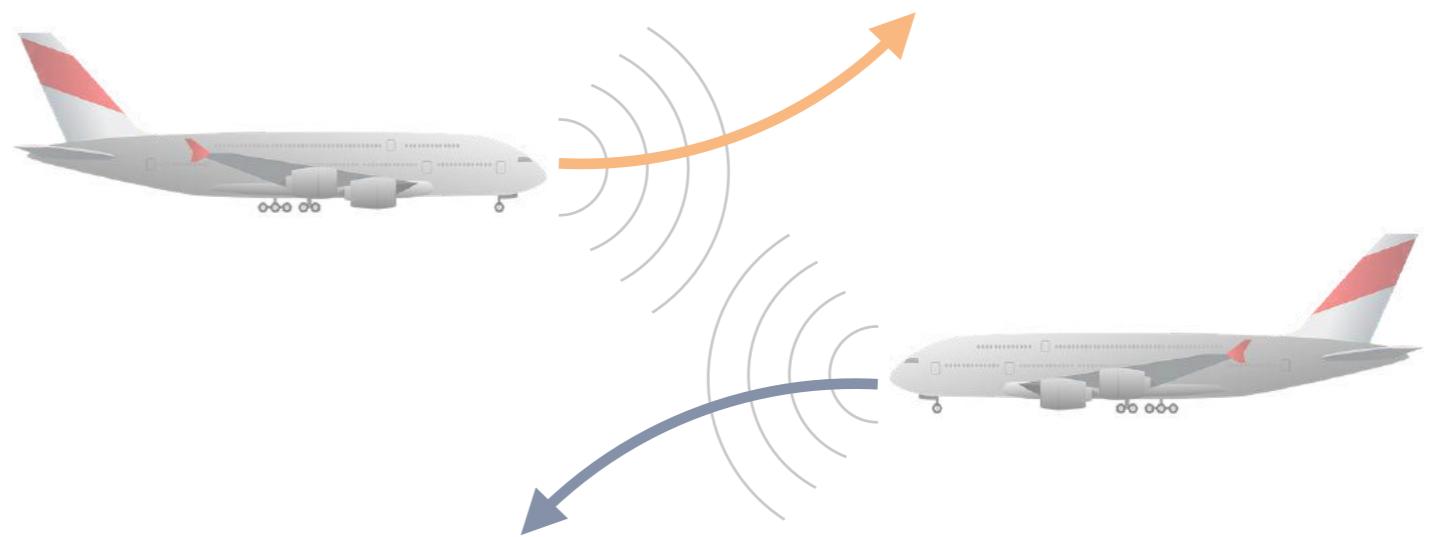
# Stability

Goal G3 in [Kurd03]

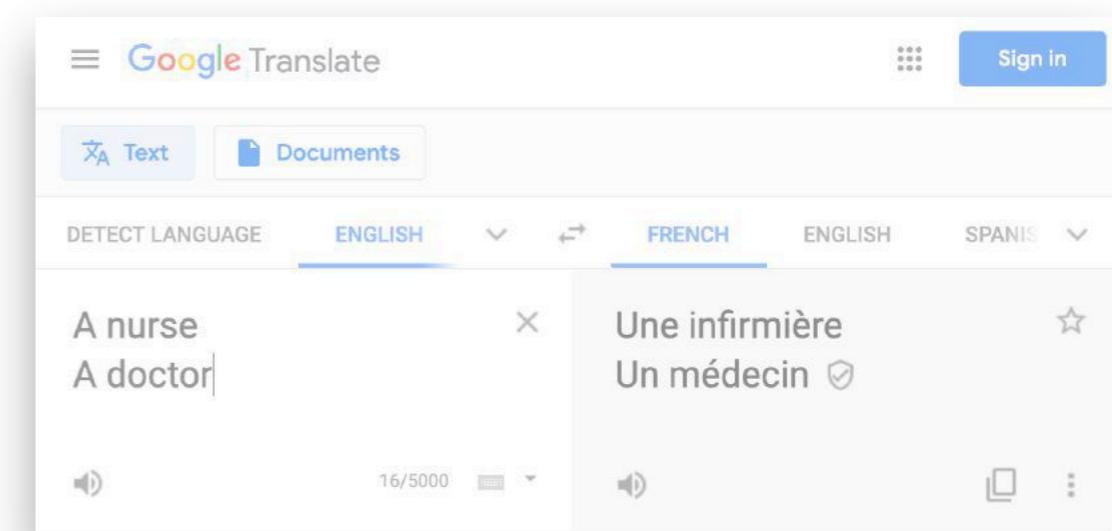


# Safety

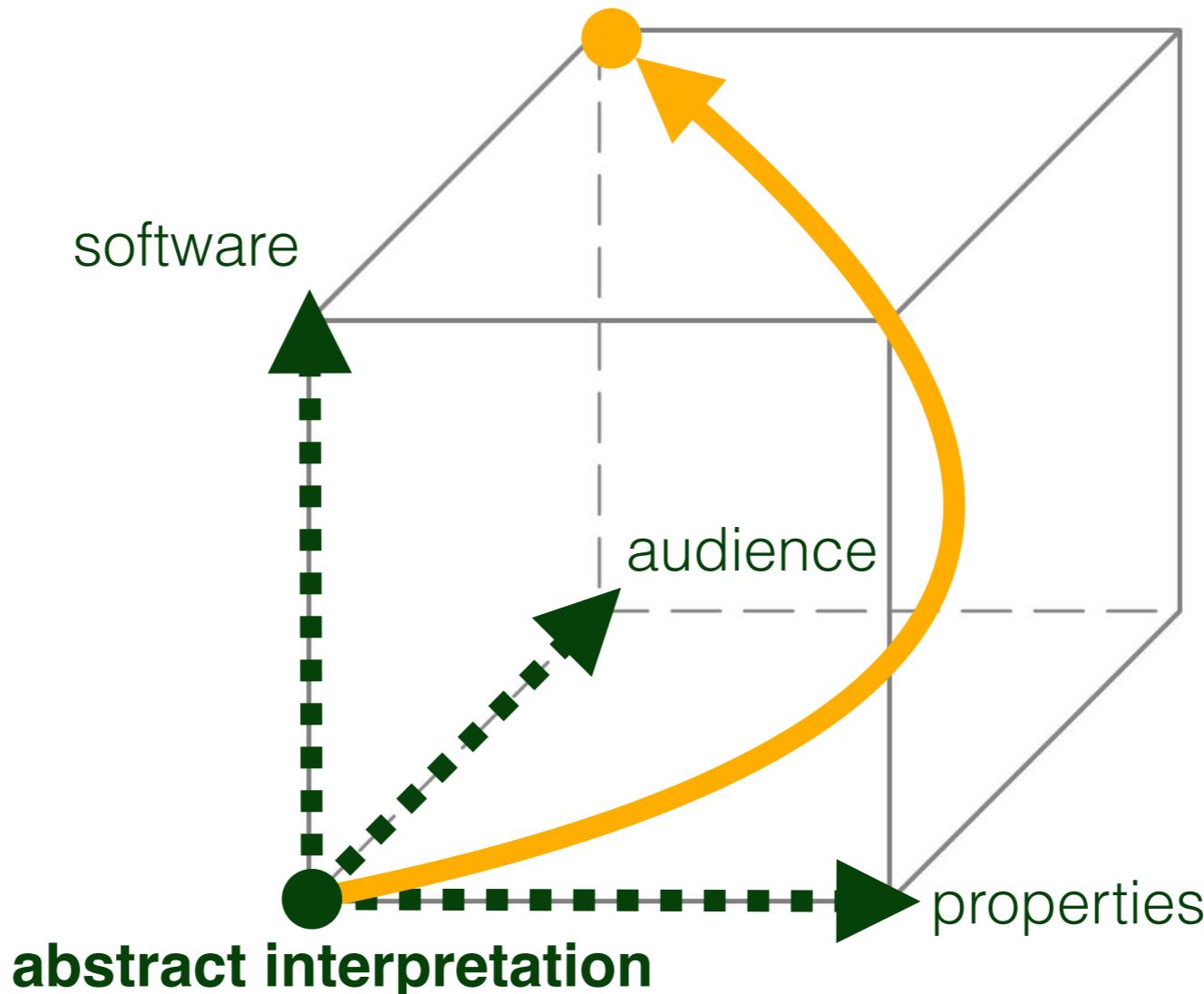
Goal G4 in [Kurd03]



# Fairness

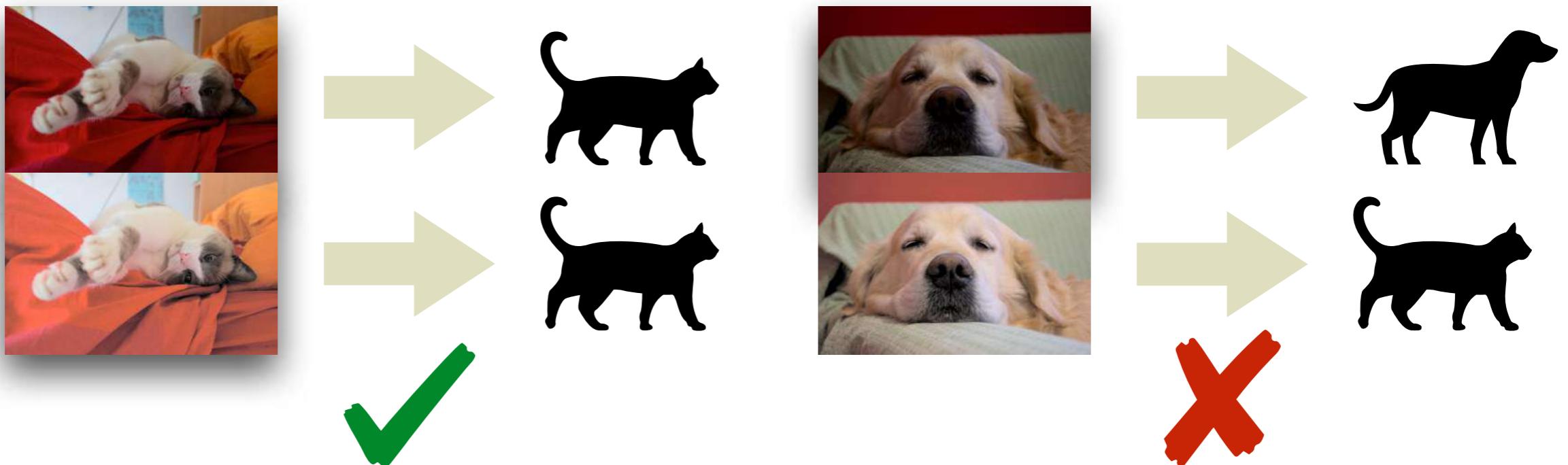
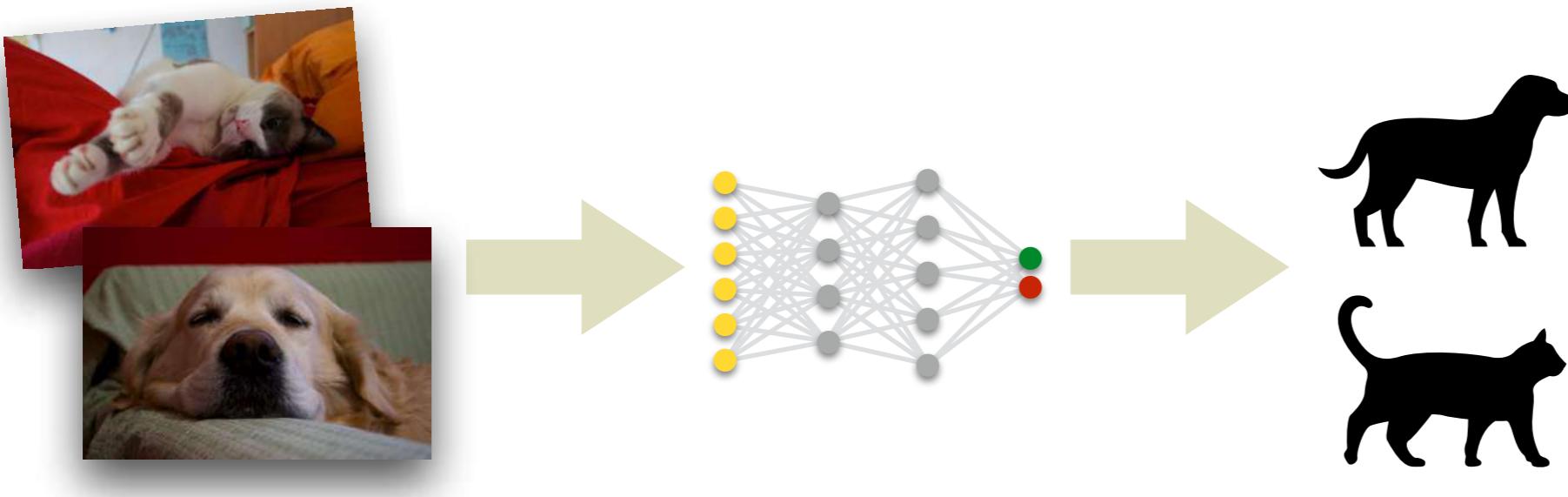


# Stability Verification



# Local Prediction Stability

Prediction is **Unaffected** by Input Perturbations



# Local Prediction Stability

## Distance-Based Perturbations

$$P_{\delta,\epsilon}(\mathbf{x}) \stackrel{\text{def}}{=} \{\mathbf{x}' \in \mathcal{R}^{|L_0|} \mid \delta(\mathbf{x}, \mathbf{x}') \leq \epsilon\}$$

Example ( $L_\infty$  distance):  $P_{\infty,\epsilon}(\mathbf{x}) \stackrel{\text{def}}{=} \{\mathbf{x}' \in \mathcal{R}^{|L_0|} \mid \max_i |\mathbf{x}_i - \mathbf{x}'_i| \leq \epsilon\}$

$$\mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \stackrel{\text{def}}{=} \{\llbracket M \rrbracket \mid \text{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(\llbracket M \rrbracket)\}$$

$\mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$  is the set of all neural networks  $M$  (or, rather, their semantics  $\llbracket M \rrbracket$ ) that are **stable** in the neighborhood  $P_{\delta,\epsilon}(\mathbf{x})$  of a given input  $\mathbf{x}$

$$\text{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(T) \stackrel{\text{def}}{=} \forall t, t' \in T: t_0 = \mathbf{x} \wedge t'_0 \in P_{\delta,\epsilon}(\mathbf{x}) \Rightarrow t_\omega = t'_\omega$$

### Theorem

$$M \models \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \Leftrightarrow \{\llbracket M \rrbracket\} \subseteq \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$$

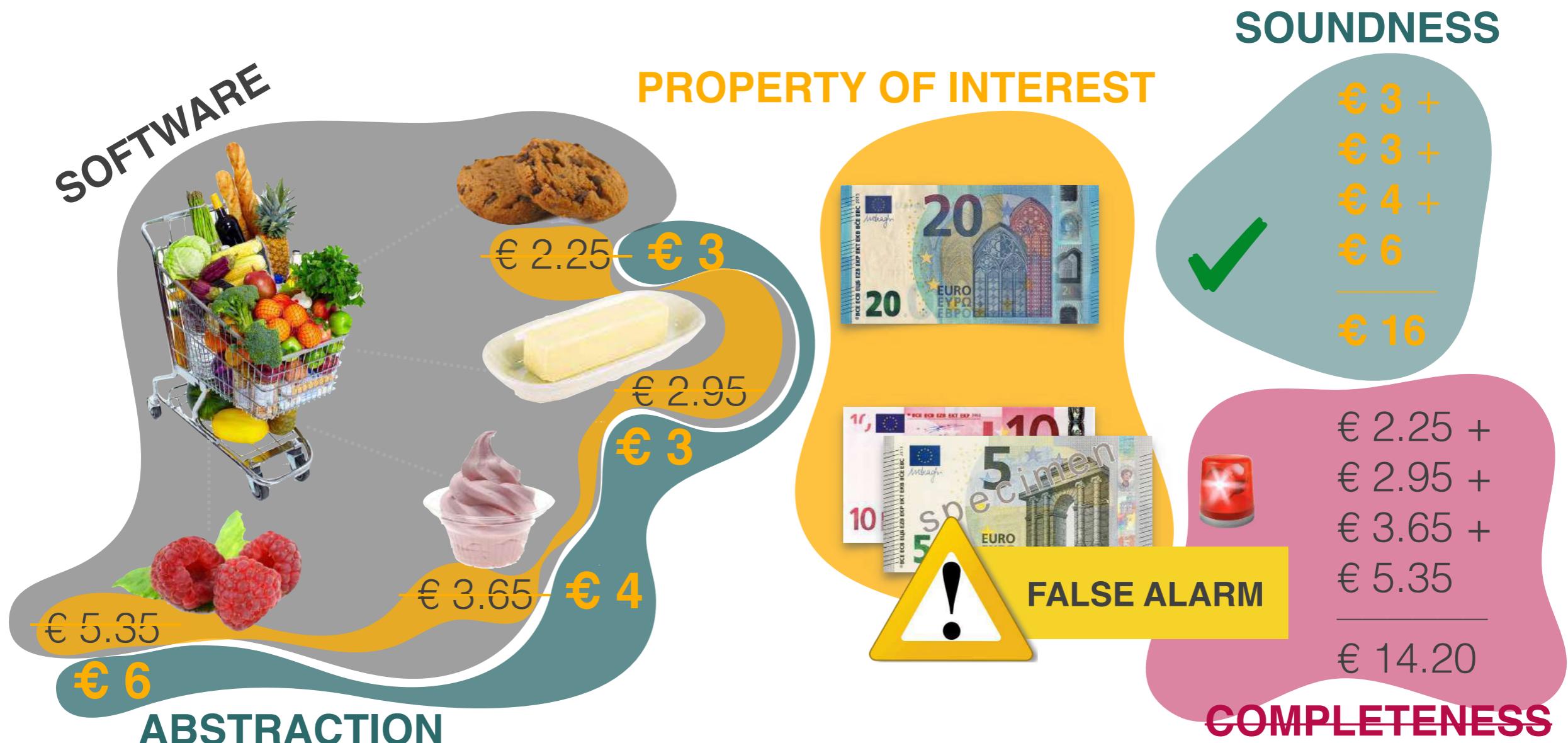
### Corollary

$$M \models \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \Leftrightarrow \llbracket M \rrbracket \subseteq \bigcup \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$$

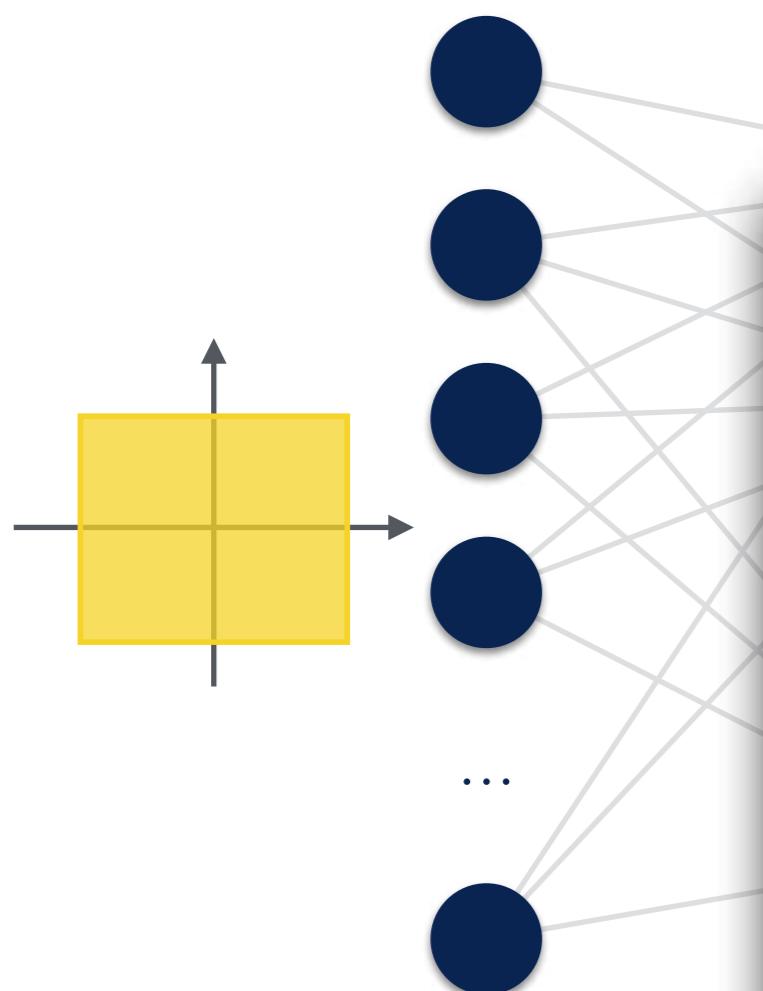
# Static Analysis Methods

# Abstract Interpretation

## Intuition



# Forward Analysis



- ① proceed **forwards from an abstraction** of all possible perturbations

## Local Prediction Stability

### Distance-Based Perturbations

$$P_{\delta,\epsilon}(\mathbf{x}) \stackrel{\text{def}}{=} \{\mathbf{x}' \in \mathcal{R}^{|L_0|} \mid \delta(\mathbf{x}, \mathbf{x}') \leq \epsilon\}$$

Example ( $L_\infty$  distance):  $P_{\infty,\epsilon}(\mathbf{x}) \stackrel{\text{def}}{=} \{\mathbf{x}' \in \mathcal{R}^{|L_0|} \mid \max_i |\mathbf{x}_i - \mathbf{x}'_i| \leq \epsilon\}$

$$\mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \stackrel{\text{def}}{=} \{\llbracket M \rrbracket \mid \text{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(\llbracket M \rrbracket)\}$$

$\mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$  is the set of all neural networks  $M$  (or, rather, their semantics  $\llbracket M \rrbracket$ ) that are **stable** in the neighborhood  $P_{\delta,\epsilon}(\mathbf{x})$  of a given input  $\mathbf{x}$

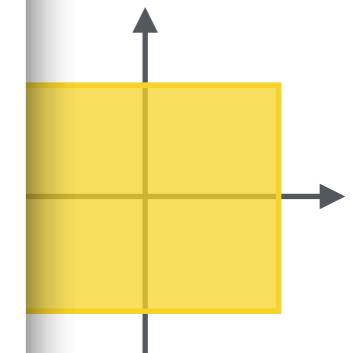
$$\text{STABLE}_{\mathbf{x}}^{\delta,\epsilon}(T) \stackrel{\text{def}}{=} \forall t, t' \in T: t'_0 = \mathbf{x} \wedge t_0 \in P_{\delta,\epsilon}(\mathbf{x}) \Rightarrow t_\omega = t'_\omega$$

Theorem	Corollary
$M \models \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \Leftrightarrow \{\llbracket M \rrbracket\} \subseteq \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$	$M \models \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \Leftrightarrow \llbracket M \rrbracket \subseteq \bigcup \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$

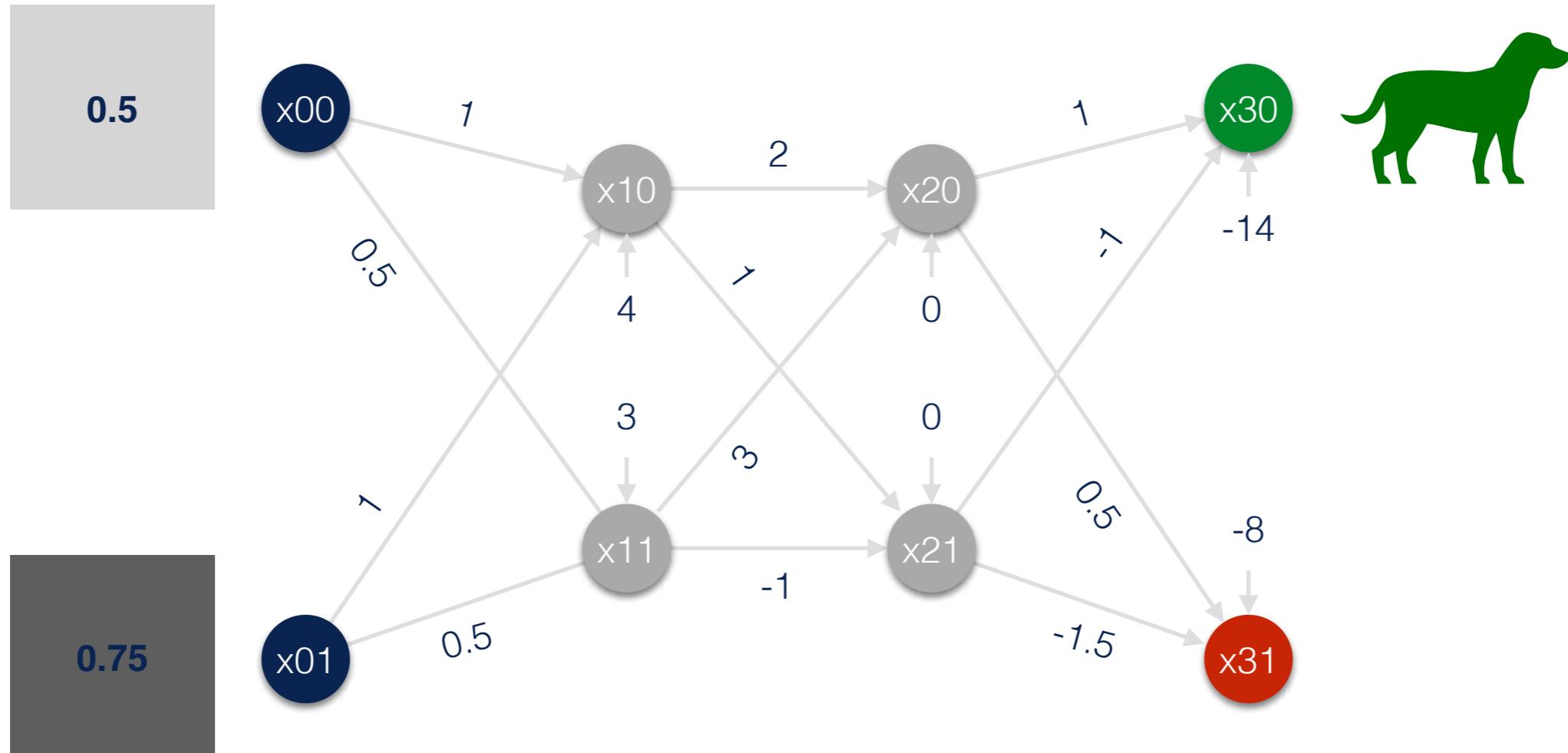
**Theorem**

$$\llbracket M \rrbracket \subseteq \llbracket M \rrbracket^\natural \subseteq \bigcup \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon} \Rightarrow M \models \mathcal{R}_{\mathbf{x}}^{\delta,\epsilon}$$

- ② check output for **inclusion** in **expected output**: included → **stable**  
otherwise → **alarm**



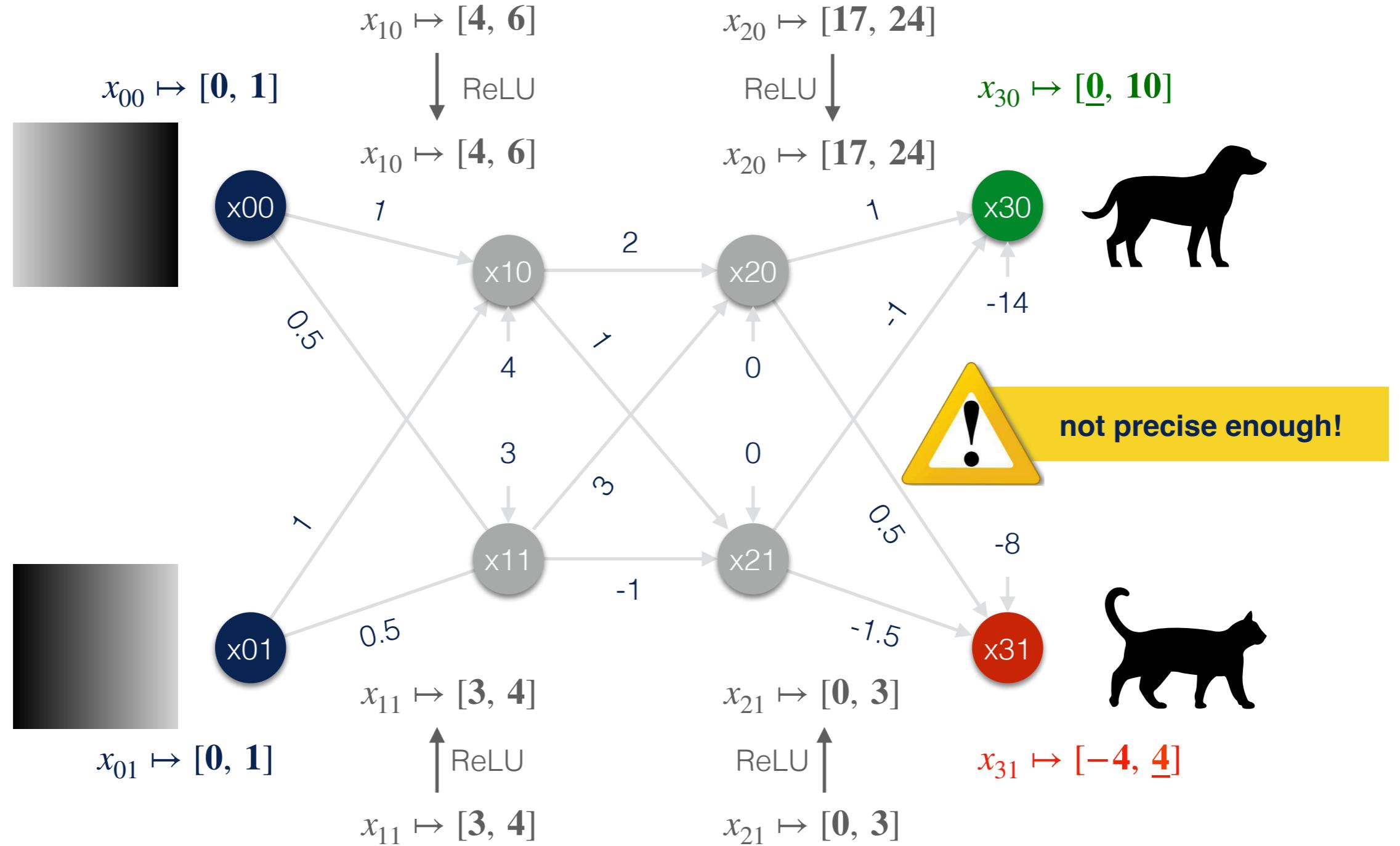
# Example



$$P(\langle 0.5, 0.75 \rangle) \stackrel{\text{def}}{=} \{ \mathbf{x} \in \mathcal{R} \times \mathcal{R} \mid 0 \leq x_0 \leq 1 \wedge 0 \leq x_1 \leq 1 \}$$

# Interval Abstraction

$$x_{i,j} \mapsto [a, b] \\ a, b \in \mathcal{R}$$



# Abstract Interpretation

## Improving Precision



# Interval Abstraction

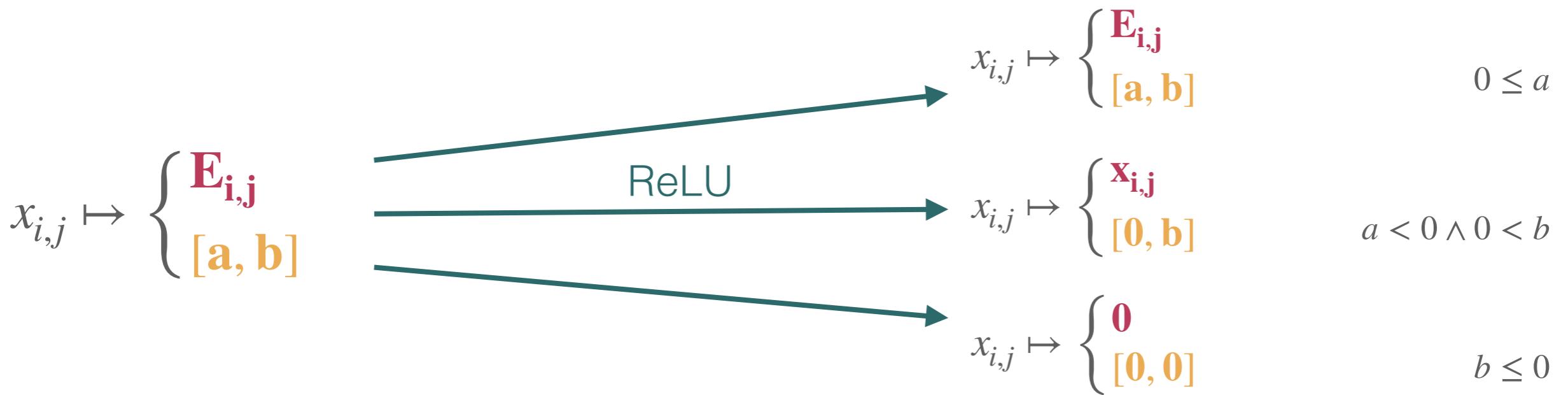


each neuron as a **linear combination** of the inputs and the previous ReLUs

## with Symbolic Constant Propagation [Li19]

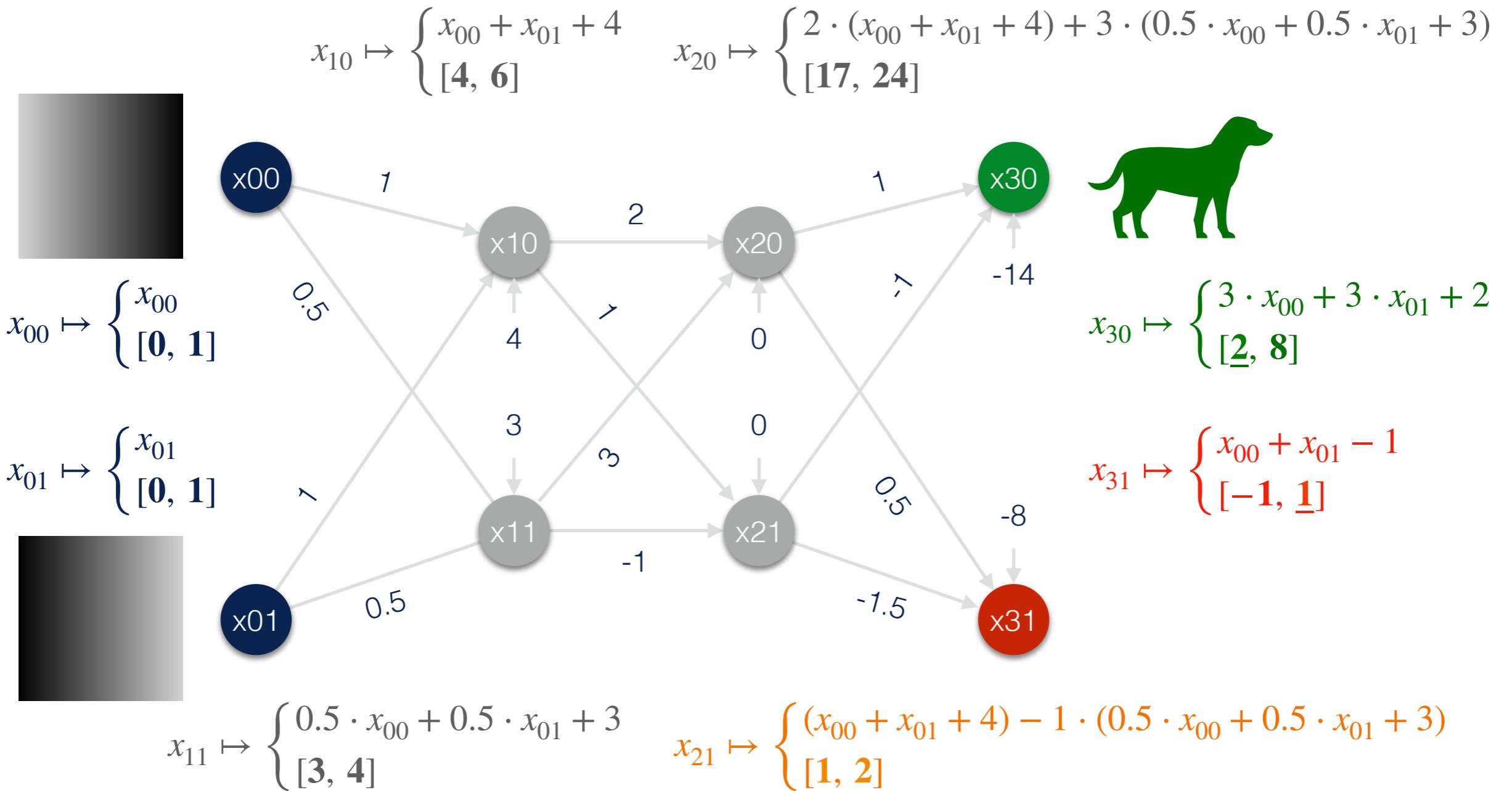
$$x_{i,j} \mapsto \begin{cases} \sum_{k=0}^{i-1} \mathbf{c}_k \cdot \mathbf{x}_k + \mathbf{c} & \mathbf{c}_k, \mathbf{c} \in \mathcal{R}^{|\mathbf{X}_k|} \\ [a, b] & a, b \in \mathcal{R} \end{cases}$$

$$\begin{array}{l} x_{i-1,0} \mapsto \mathbf{E}_{\mathbf{i}-1,0} \\ \dots \\ x_{i-1,j} \mapsto \mathbf{E}_{\mathbf{i}-1,j} \\ \dots \end{array} \xrightarrow{x_{i,j} = \sum_k w_{j,k}^{i-1} \cdot x_{i-1,k} + b_{i,j}} x_{i,j} \mapsto \sum_k w_{j,k}^{i-1} \cdot \mathbf{E}_{\mathbf{i}-1,k} + b_{i,j}$$



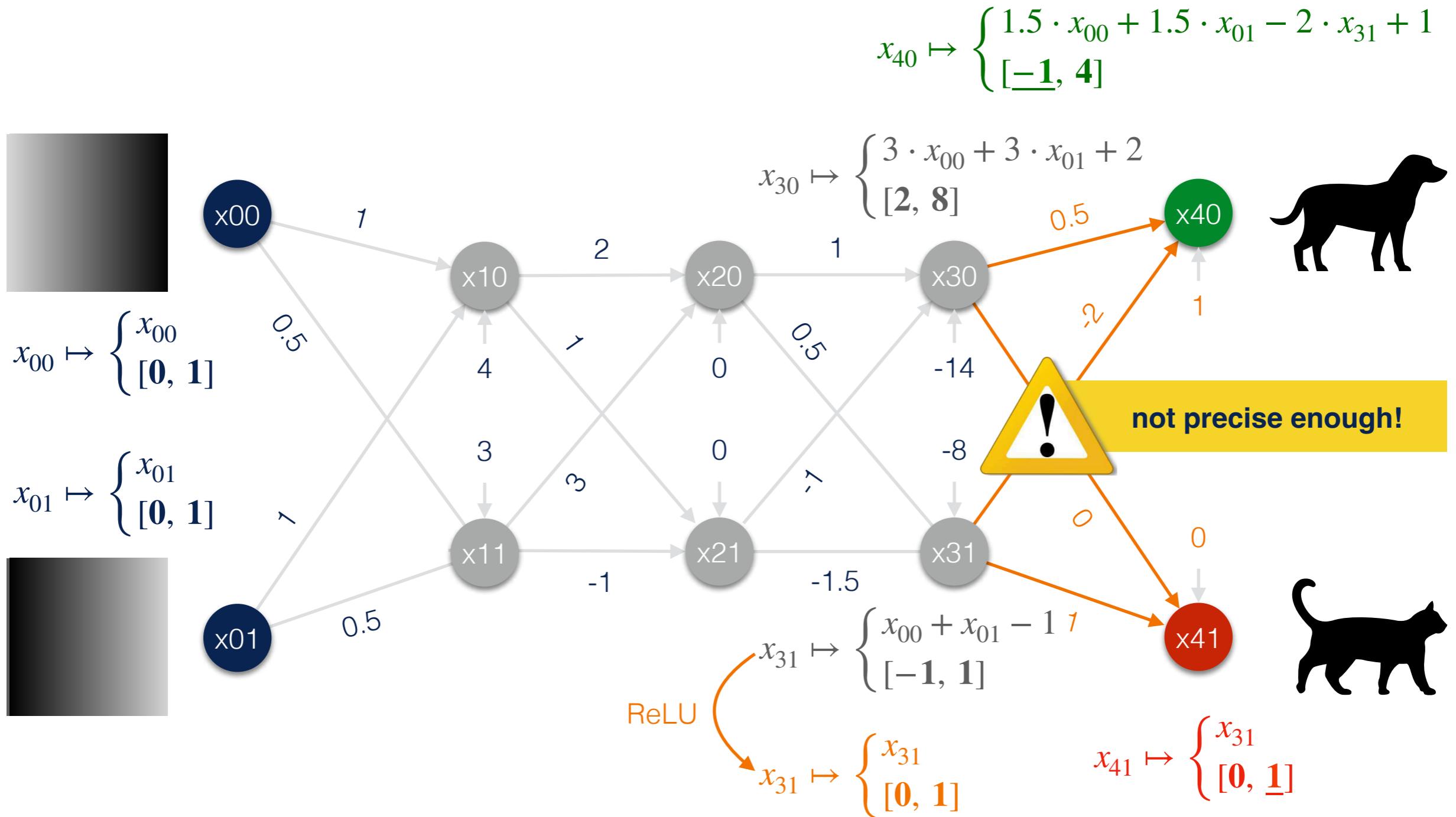
# Interval Abstraction

with Symbolic Constant Propagation [Li19]



# Interval Abstraction

with Symbolic Constant Propagation [Li19]

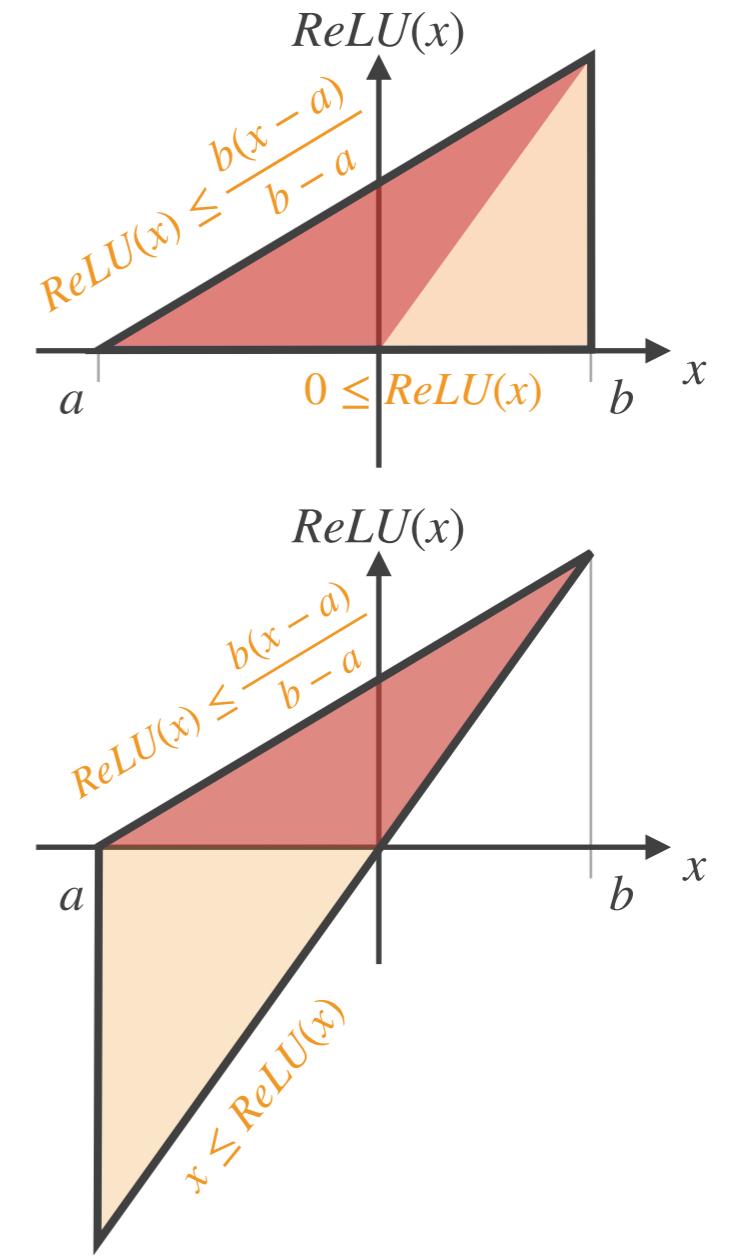
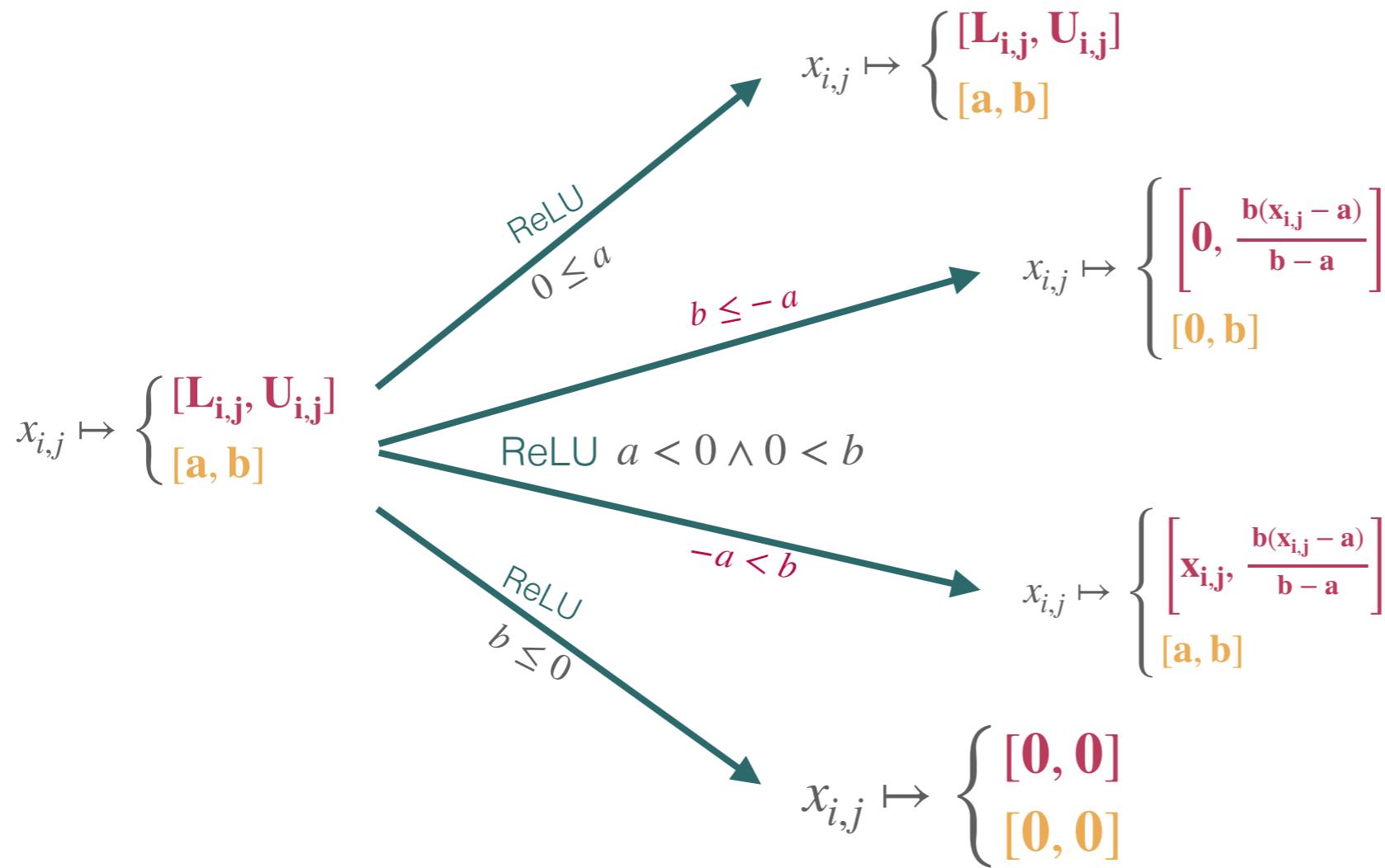


# DeepPoly

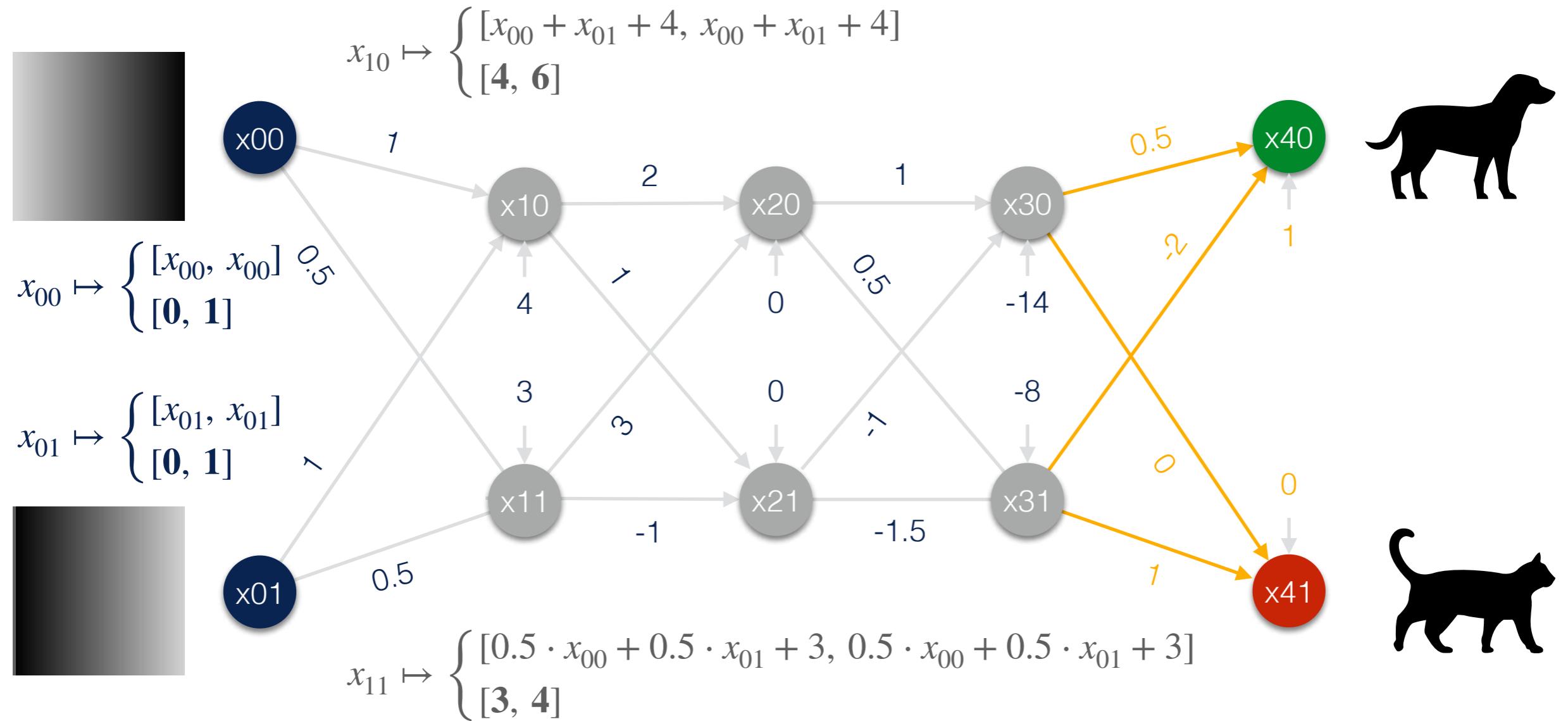
[Singh19]

 maintain symbolic lower- and upper-bounds for each neuron  
+ convex ReLU approximations

$$x_{i+1,j} \mapsto \begin{cases} [\sum_k c_{i,k} \cdot x_{i,k} + c, \sum_k d_{i,k} \cdot x_{i,k} + d] & c_{i,k}, c, d_{i,k}, d \in \mathcal{R} \\ [a, b] & a, b \in \mathcal{R} \end{cases}$$

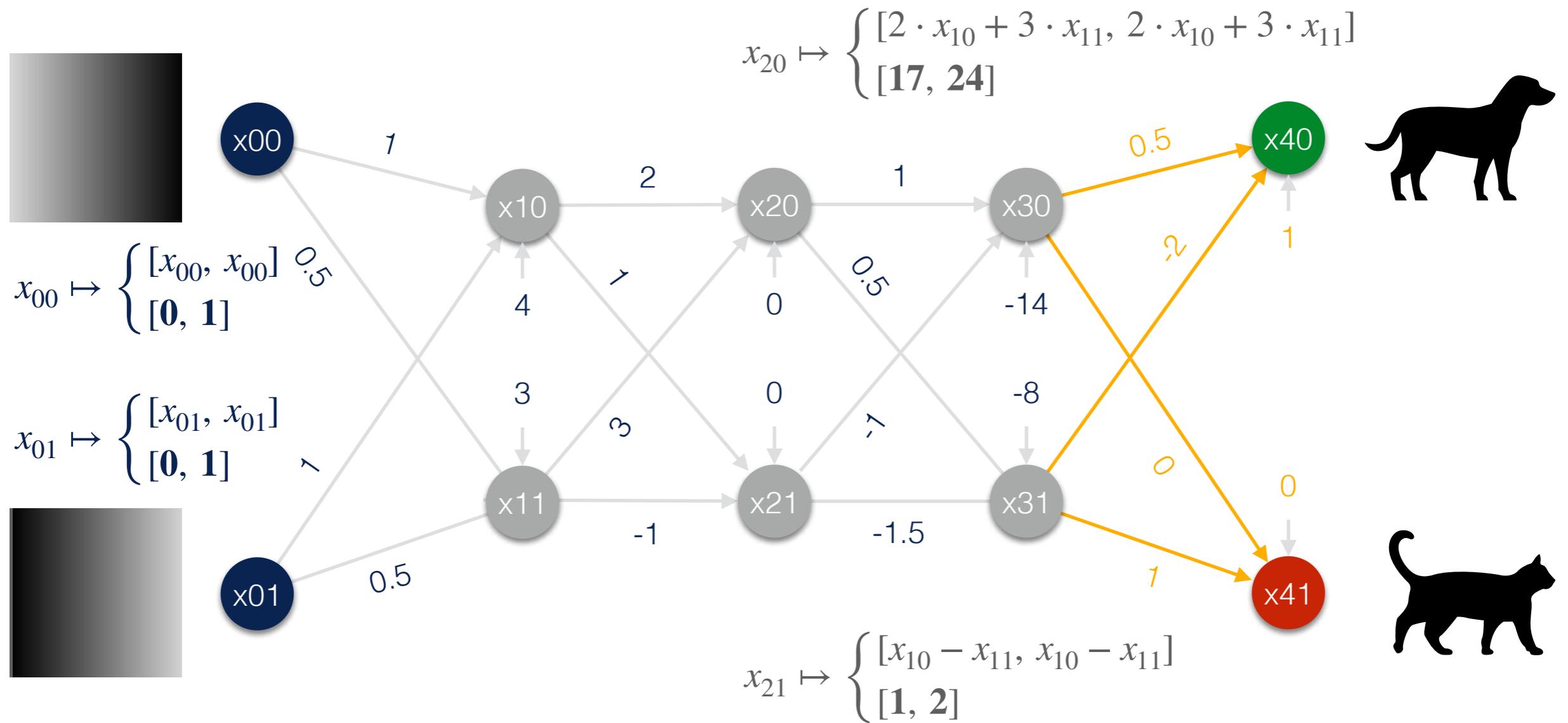


# DeepPoly [Singh19]

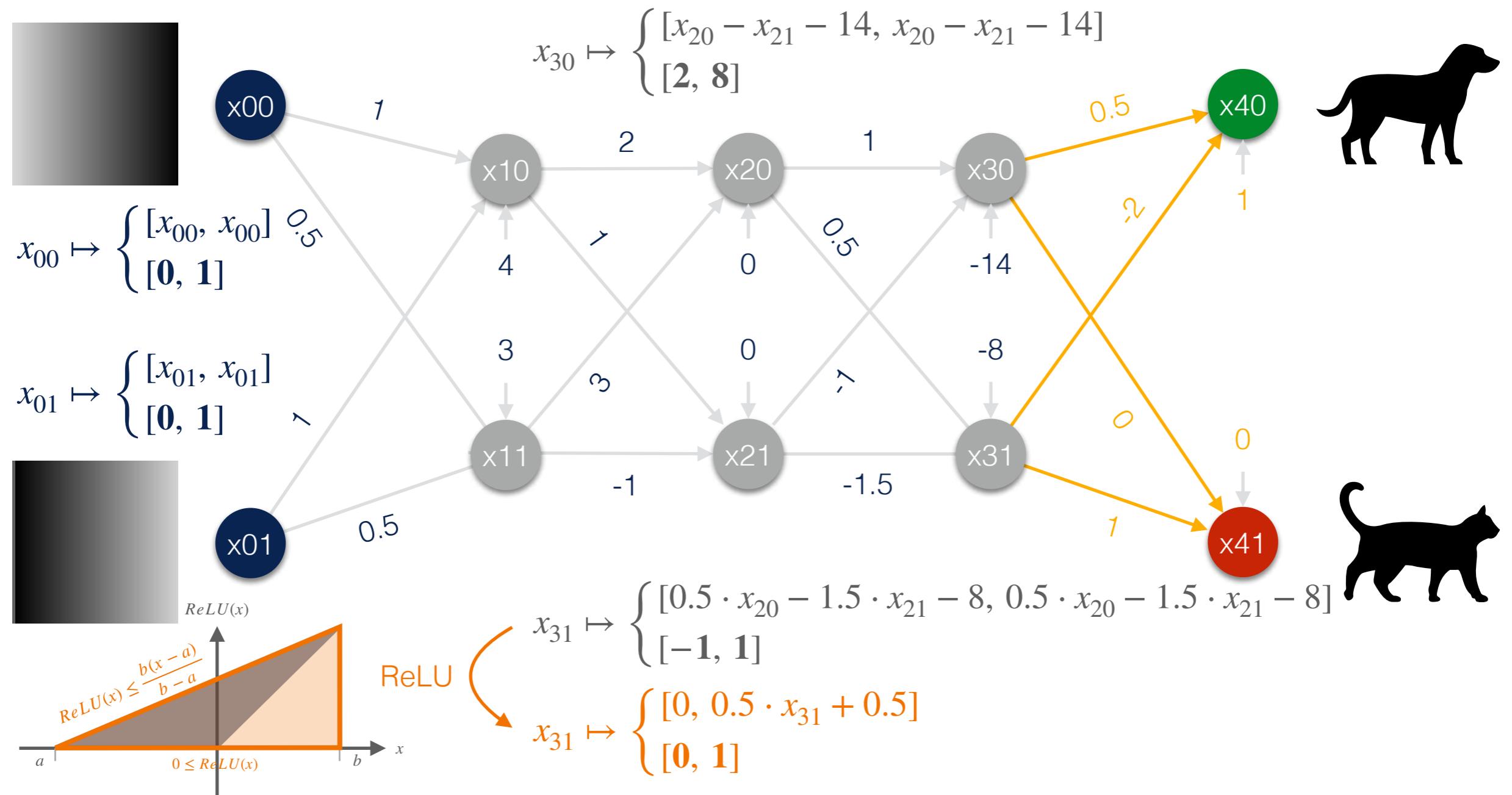


# DeepPoly

[Singh19]

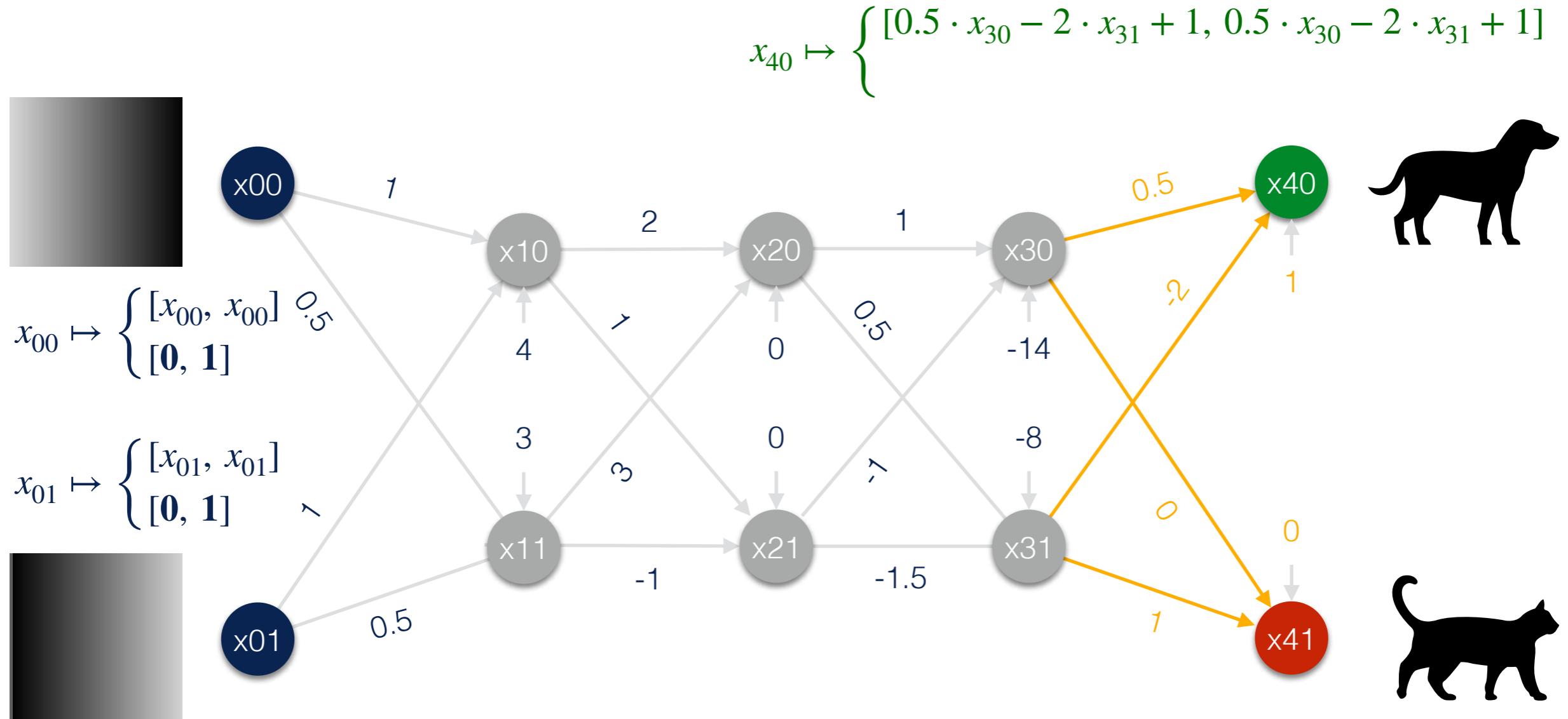


# DeepPoly [Singh19]



# DeepPoly

[Singh19]



# DeepPoly [Singh19]

## Back-Substitution

$$x_{00} \mapsto [0, 1]$$

$$x_{10} \mapsto \begin{cases} [x_{00} + x_{01} + 4, x_{00} + x_{01} + 4] \\ [4, 6] \end{cases}$$

$$x_{20} \mapsto \begin{cases} [2 \cdot x_{10} + 3 \cdot x_{11}, 2 \cdot x_{10} + 3 \cdot x_{11}] \\ [17, 24] \end{cases}$$

$$x_{30} \mapsto \begin{cases} [x_{20} - x_{21} - 14, x_{20} - x_{21} - 14] \\ [2, 8] \end{cases}$$

$$x_{01} \mapsto [0, 1]$$

$$x_{11} \mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3] \\ [3, 4] \end{cases}$$

$$x_{21} \mapsto \begin{cases} [x_{10} - x_{11}, x_{10} - x_{11}] \\ [1, 2] \end{cases}$$

$$x_{31} \mapsto \begin{cases} [0, 0.5 \cdot (0.5 \cdot x_{20} - 1.5 \cdot x_{21} - 8) + 0.5] \\ [0, 1] \end{cases}$$

$$x_{40} \mapsto \begin{cases} [0.5 \cdot x_{30} - 2 \cdot x_{31} + 1, 0.5 \cdot x_{30} - 2 \cdot x_{31} + 1] \end{cases}$$

$$\mapsto \begin{cases} [x_{21} + 1, 0.5 \cdot x_{20} - 0.5 \cdot x_{21} - 6] \end{cases}$$

$$\mapsto \begin{cases} [x_{10} - x_{11} + 1, 0.5 \cdot x_{10} + 2 \cdot x_{11} - 6] \end{cases}$$

$$\mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 2, 1.5 \cdot x_{00} + 1.5 \cdot x_{01} + 2] \\ [2, 5] \end{cases}$$

# DeepPoly [Singh19]

## Partial Back-Substitution

$$x_{00} \mapsto [0, 1]$$

$$x_{10} \mapsto \begin{cases} [x_{00} + x_{01} + 4, x_{00} + x_{01} + 4] \\ [4, 6] \end{cases}$$

$$x_{20} \mapsto \begin{cases} [2 \cdot x_{10} + 3 \cdot x_{11}, 2 \cdot x_{10} + 3 \cdot x_{11}] \\ [17, 24] \end{cases}$$

$$x_{30} \mapsto \begin{cases} [x_{20} - x_{21} - 14, x_{20} - x_{21} - 14] \\ [2, 8] \end{cases}$$

$$x_{40} \mapsto \begin{cases} [0.5 \cdot x_{30} - 2 \cdot x_{31} + 1, 0.5 \cdot x_{30} - 2 \cdot x_{31} + 1] \\ [\underline{0}, 5] \end{cases}$$

$$\mapsto \begin{cases} [x_{21} + 1, 0.5 \cdot x_{20} - 0.5 \cdot x_{21} - 6] \\ [2, \underline{5.5}] \end{cases}$$

$$\mapsto \begin{cases} [x_{10} - x_{11} + 1, 0.5 \cdot x_{10} + 2 \cdot x_{11} - 6] \\ [\underline{1}, 5] \end{cases}$$

$$\mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 2, 1.5 \cdot x_{00} + 1.5 \cdot x_{01} + 2] \\ [2, 5] \end{cases}$$

$$x_{01} \mapsto [0, 1]$$

$$x_{11} \mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3] \\ [3, 4] \end{cases}$$

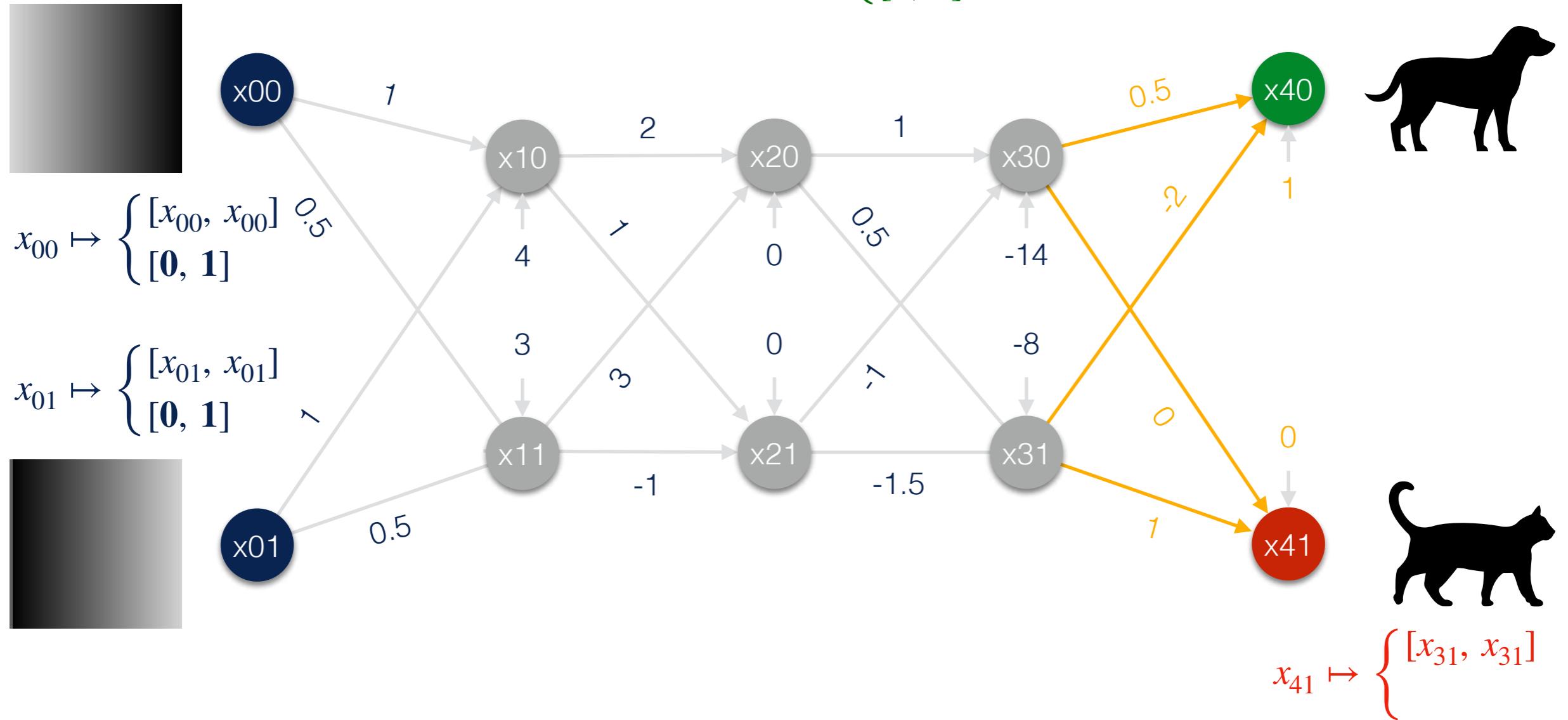
$$x_{21} \mapsto \begin{cases} [x_{10} - x_{11}, x_{10} - x_{11}] \\ [1, 2] \end{cases}$$

$$x_{31} \mapsto \begin{cases} [0, 0.5 \cdot (0.5 \cdot x_{20} - 1.5 \cdot x_{21} - 8) + 0.5] \\ [0, 1] \end{cases}$$

# DeepPoly

[Singh19]

$$x_{40} \mapsto \begin{cases} [0.5 \cdot x_{30} - 2 \cdot x_{31} + 1, 0.5 \cdot x_{30} - 2 \cdot x_{31} + 1] \\ [2, 5] \end{cases}$$



# DeepPoly [Singh19]

## Back-Substitution

$$x_{00} \mapsto [0, 1]$$

$$x_{10} \mapsto \begin{cases} [x_{00} + x_{01} + 4, x_{00} + x_{01} + 4] \\ [4, 6] \end{cases}$$

$$x_{20} \mapsto \begin{cases} [2 \cdot x_{10} + 3 \cdot x_{11}, 2 \cdot x_{10} + 3 \cdot x_{11}] \\ [17, 24] \end{cases}$$

$$x_{30} \mapsto \begin{cases} [x_{20} - x_{21} - 14, x_{20} - x_{21} - 14] \\ [2, 8] \end{cases}$$

$$\begin{aligned} x_{41} &\mapsto \begin{cases} [x_{31}, x_{31}] \\ \mapsto \begin{cases} [0, 0.25 \cdot x_{20} - 0.75 \cdot x_{21} - 3.5] \\ \mapsto \begin{cases} [0, -0.25 \cdot x_{10} + 1.5 \cdot x_{11} - 3.5] \\ \mapsto \begin{cases} [0, 0.5 \cdot x_{00} + 0.5 \cdot x_{01}] \\ [0, \underline{1}] \end{cases} \end{cases} \end{cases} \end{aligned}$$

$$x_{01} \mapsto [0, 1]$$

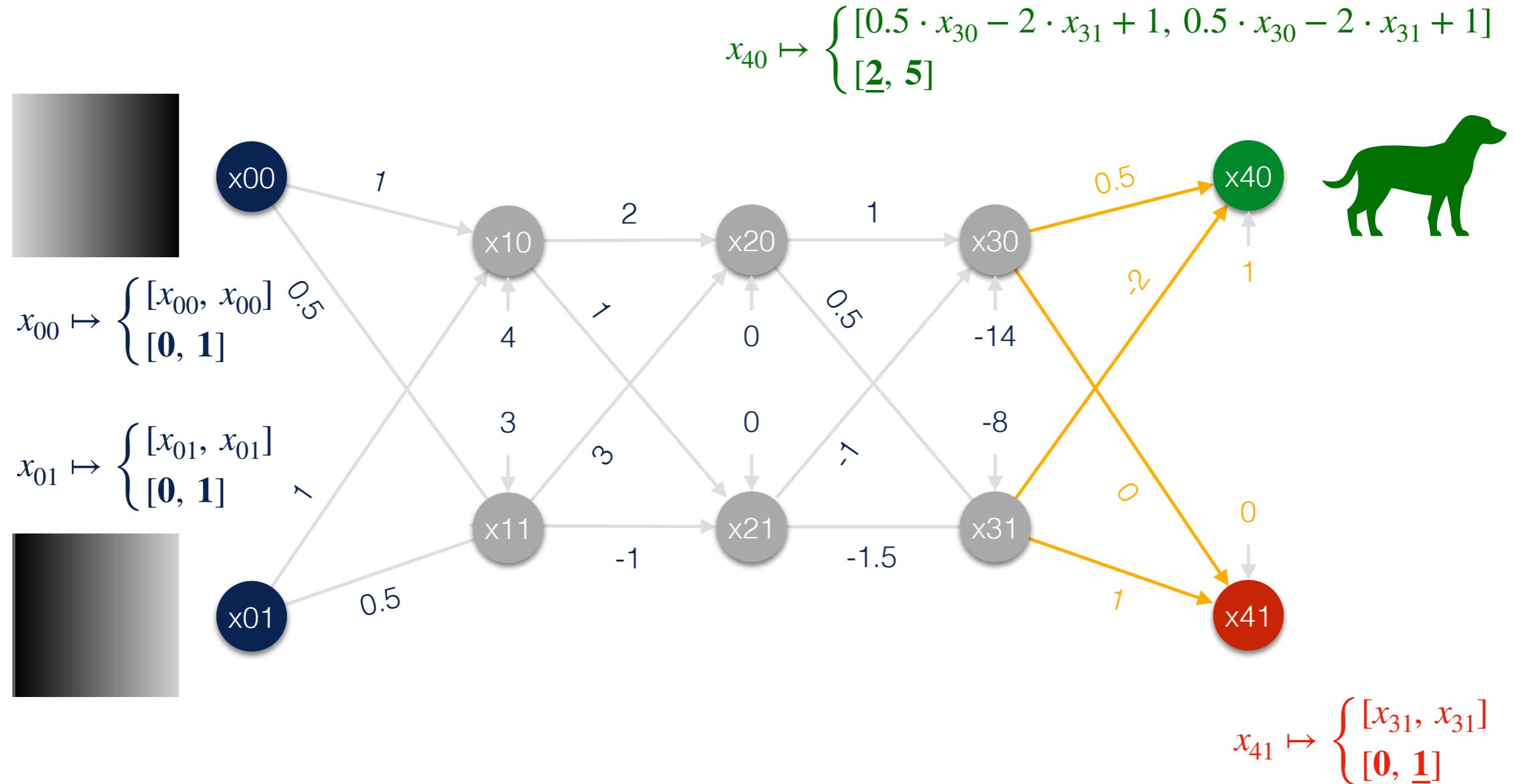
$$x_{11} \mapsto \begin{cases} [0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 3] \\ [3, 4] \end{cases}$$

$$x_{21} \mapsto \begin{cases} [x_{10} - x_{11}, x_{10} - x_{11}] \\ [1, 2] \end{cases}$$

$$x_{31} \mapsto \begin{cases} [0, 0.5 \cdot (0.5 \cdot x_{20} - 1.5 \cdot x_{21} - 8) + 0.5] \\ [0, 1] \end{cases}$$

# DeepPoly

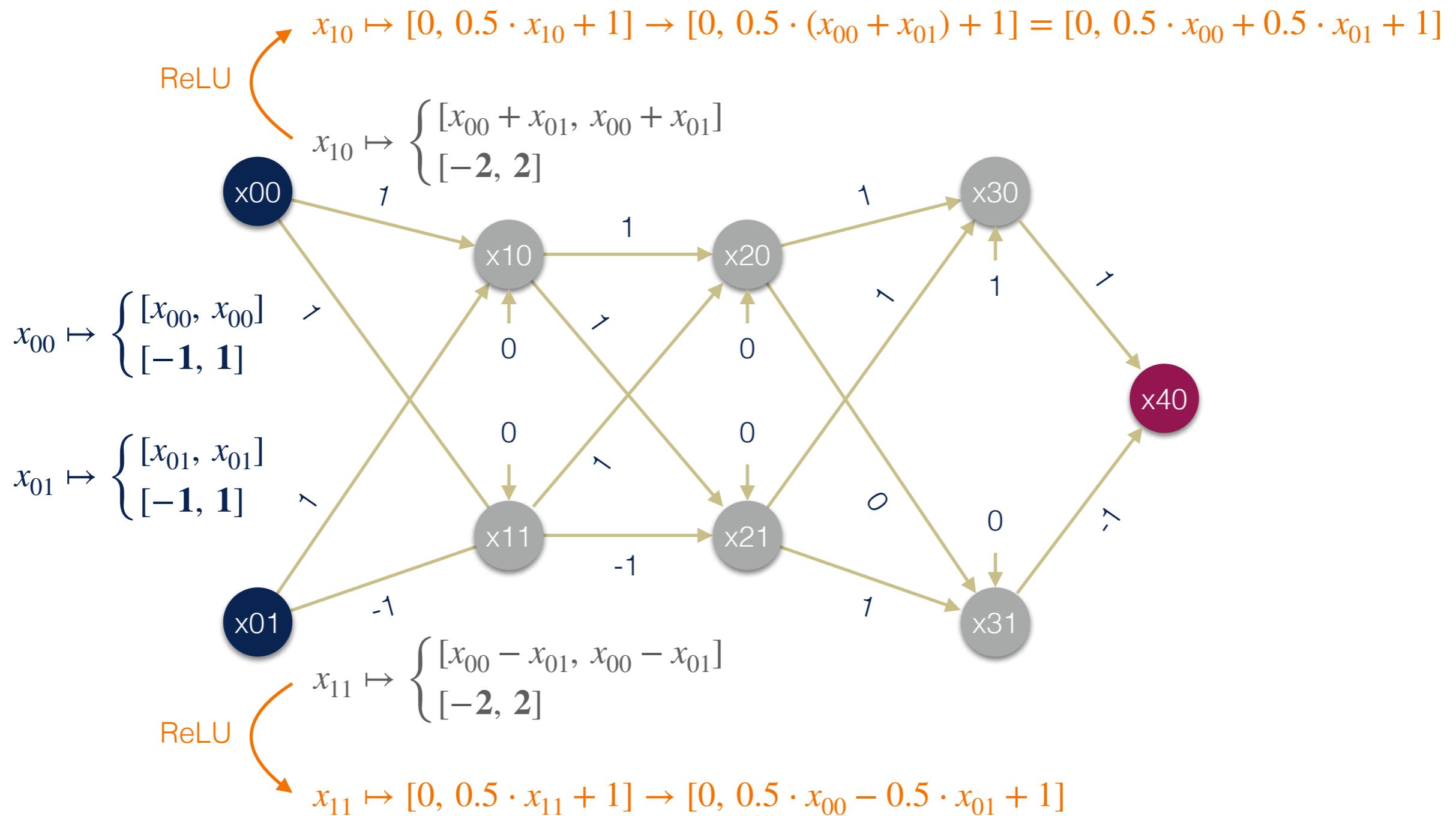
[Singh19]



# DeepPoly

[Singh19]

## Maintaining Symbolic Bounds wrt Inputs

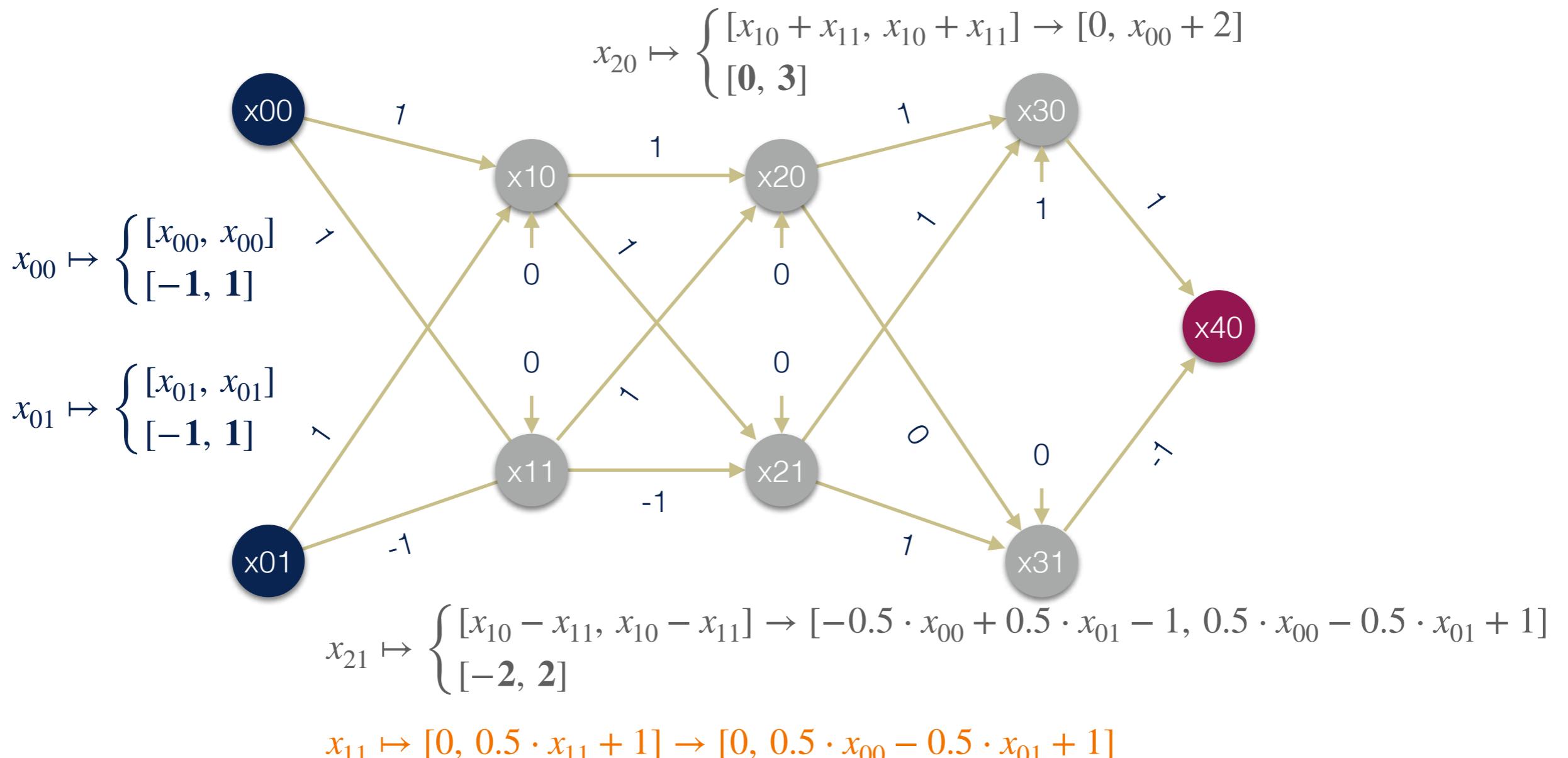


# DeepPoly

[Singh19]

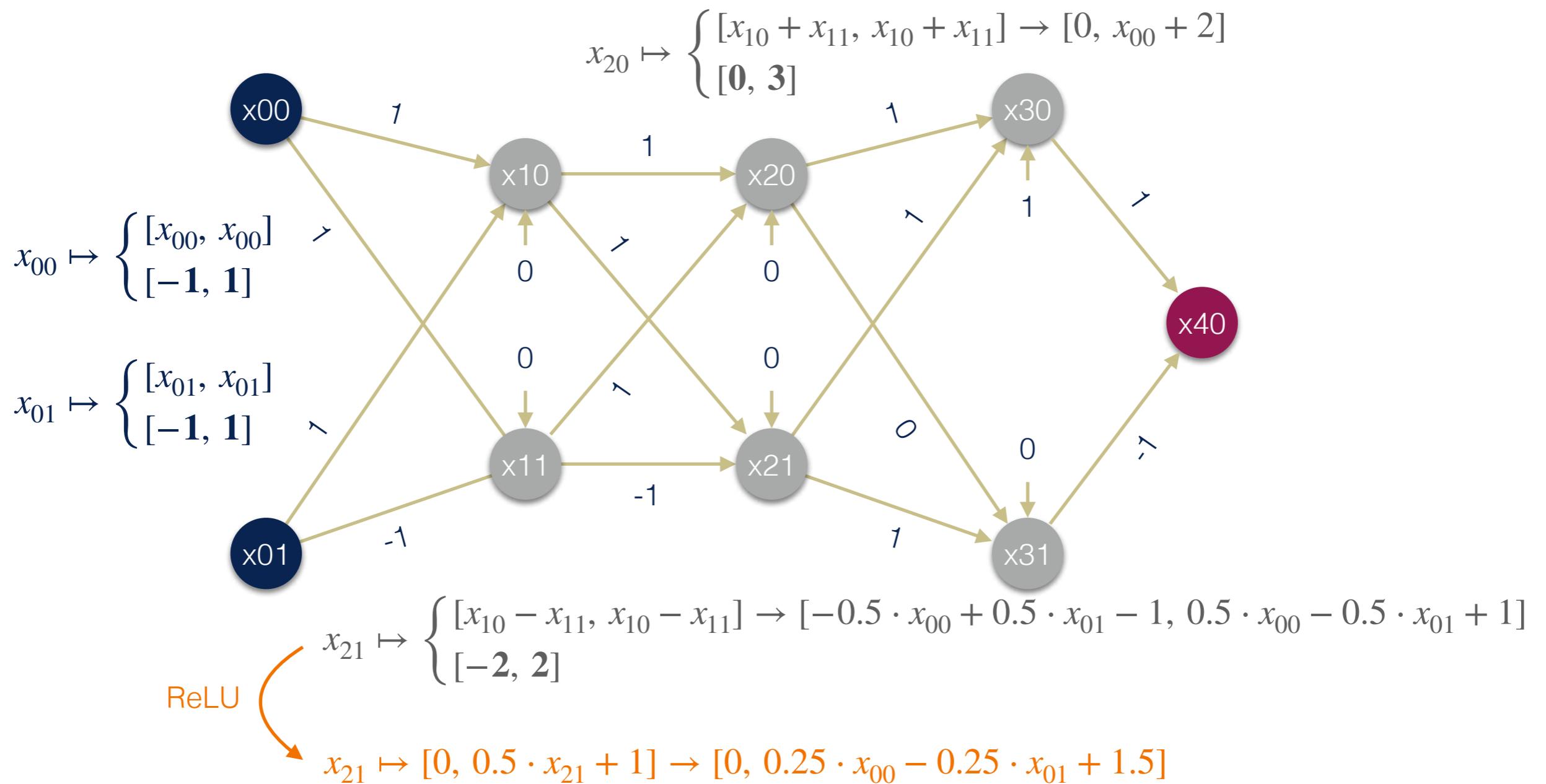
## Maintaining Symbolic Bounds wrt Inputs

$$x_{10} \mapsto [0, 0.5 \cdot x_{10} + 1] \rightarrow [0, 0.5 \cdot (x_{00} + x_{01}) + 1] = [0, 0.5 \cdot x_{00} + 0.5 \cdot x_{01} + 1]$$



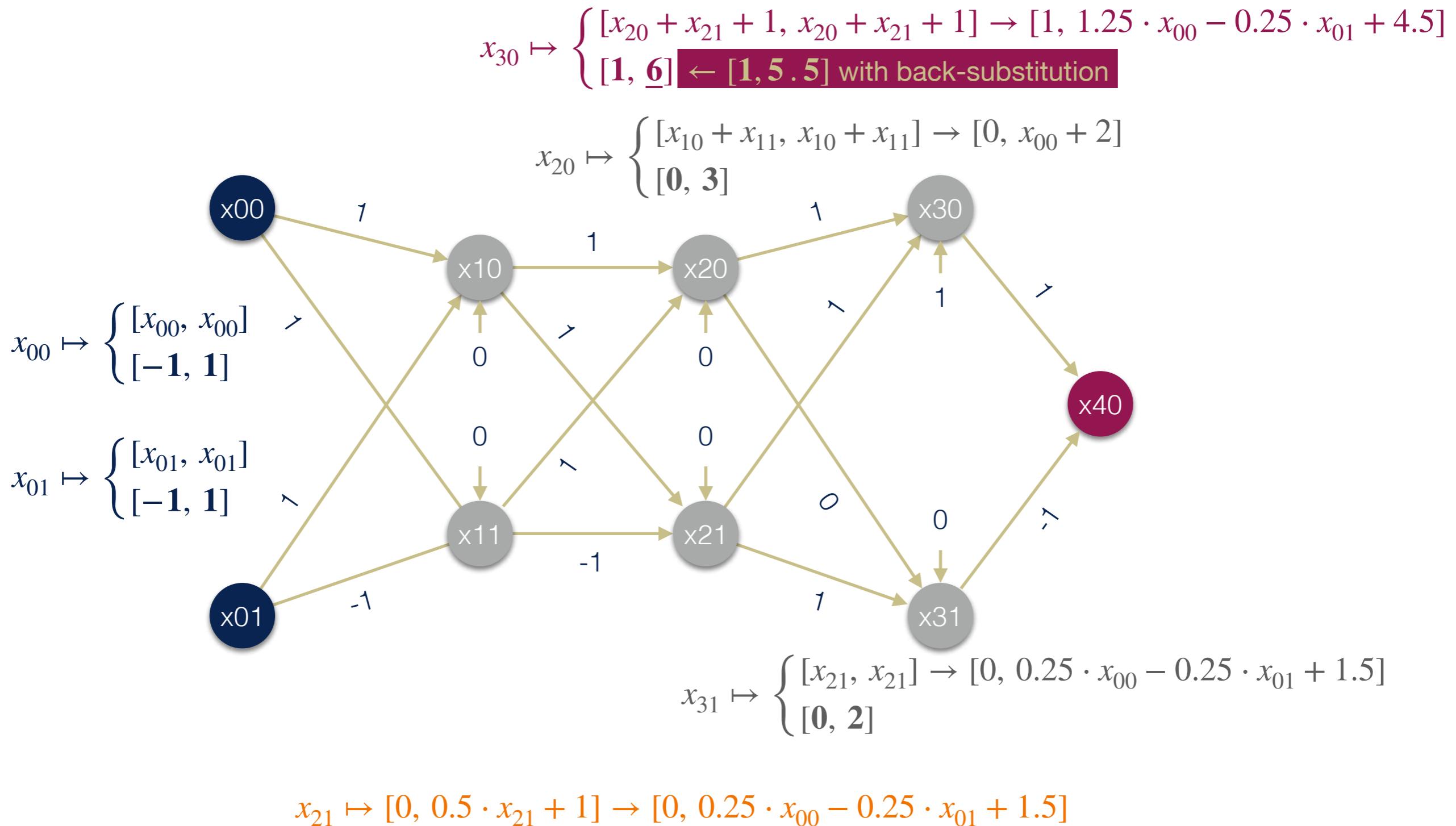
# DeepPoly [Singh19]

## Maintaining Symbolic Bounds wrt Inputs



# DeepPoly [Singh19]

## Maintaining Symbolic Bounds wrt Inputs

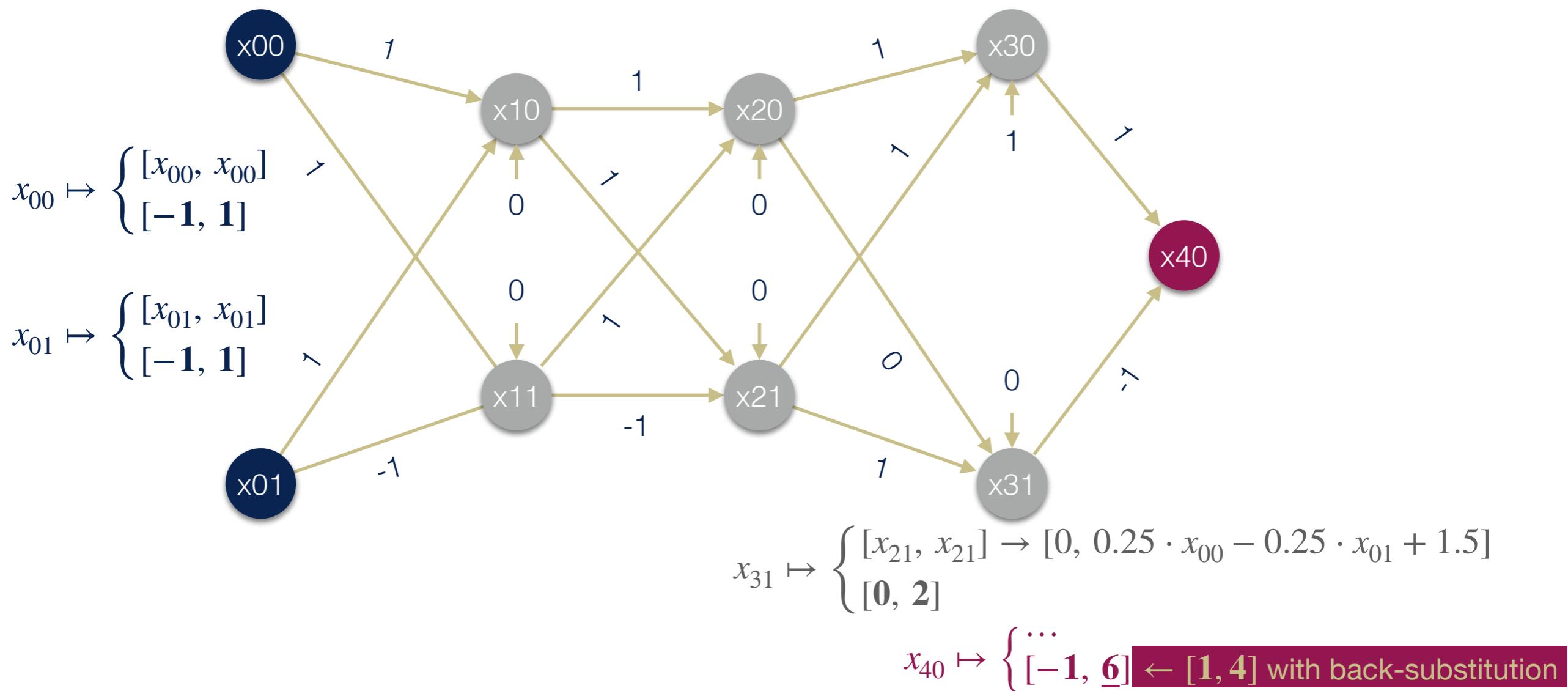


# DeepPoly

[Singh19]

## Maintaining Symbolic Bounds wrt Inputs

$$x_{30} \mapsto \begin{cases} [x_{20} + x_{21} + 1, x_{20} + x_{21} + 1] \rightarrow [1, 1.25 \cdot x_{00} - 0.25 \cdot x_{01} + 4.5] \\ [1, \underline{6}] \leftarrow [1, 5.5] \text{ with back-substitution} \end{cases}$$

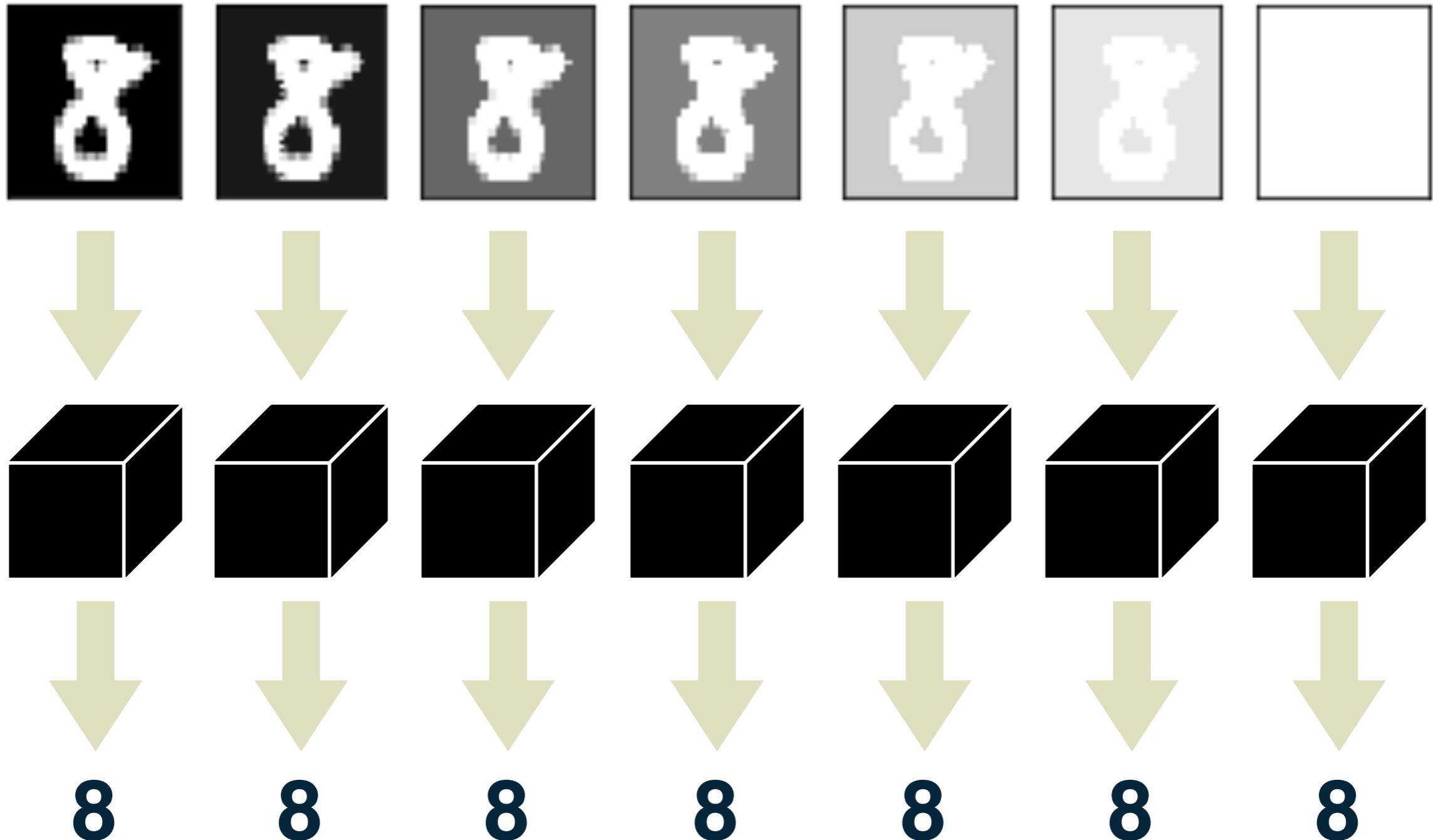


# Other Static Analysis Methods

- **T. Gehr, M. Mirman, D. Drachsler-Cohen, P. Tsankov, S. Chaudhuri, and M. Vechev.** *AI2: Safety and Robustness Certification of Neural Networks with Abstract Interpretation*. In S&P, 2018.  
**the first use of abstract interpretation for verifying neural networks**
- **G. Singh, T. Gehr, M. Mirman, M. Püschel, and M. Vechev.** *Fast and Effective Robustness Certification*. In NeurIPS, 2018.  
**a custom zonotope domain for certifying neural networks**
- **G. Singh, R. Ganvir, M. Püschel, and M. Vechev.** *Beyond the Single Neuron Convex Barrier for Neural Network Certification*. In NeurIPS, 2019.  
**a framework to jointly approximate k ReLU activations**
- **M. N. Müller, G. Makarchuk, G. Singh, M. Püschel, and M. Vechev.** *PRIMA: General and Precise Neural Network Certification via Scalable Convex Hull Approximations*. In POPL, 2022.  
**a multi-neuron abstraction via a convex-hull approximation algorithm**

# Local Prediction Stability

Not Enough!



# Local Explanation Stability

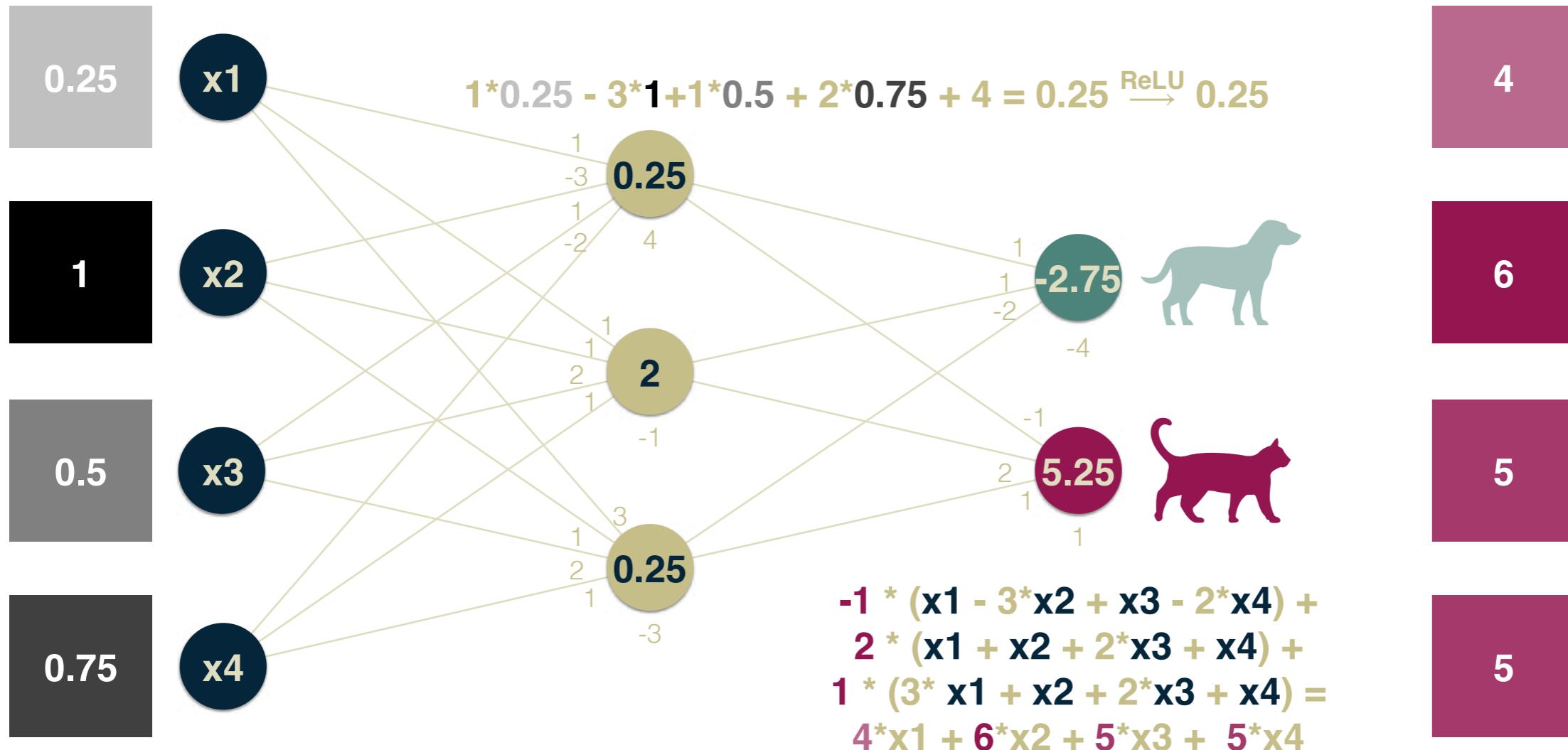
[Munakata23]

Input



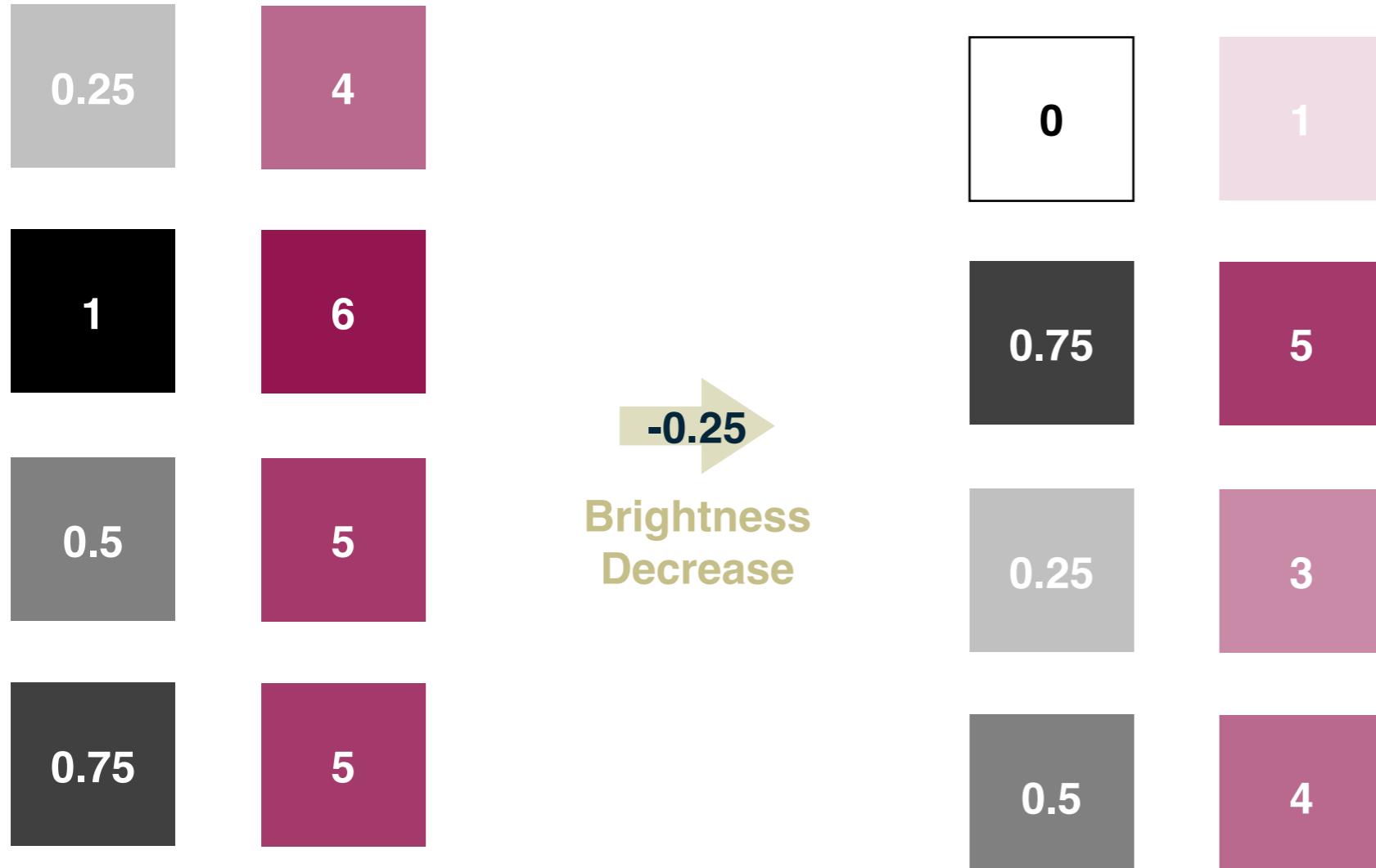
# Example

## Saliency Maps



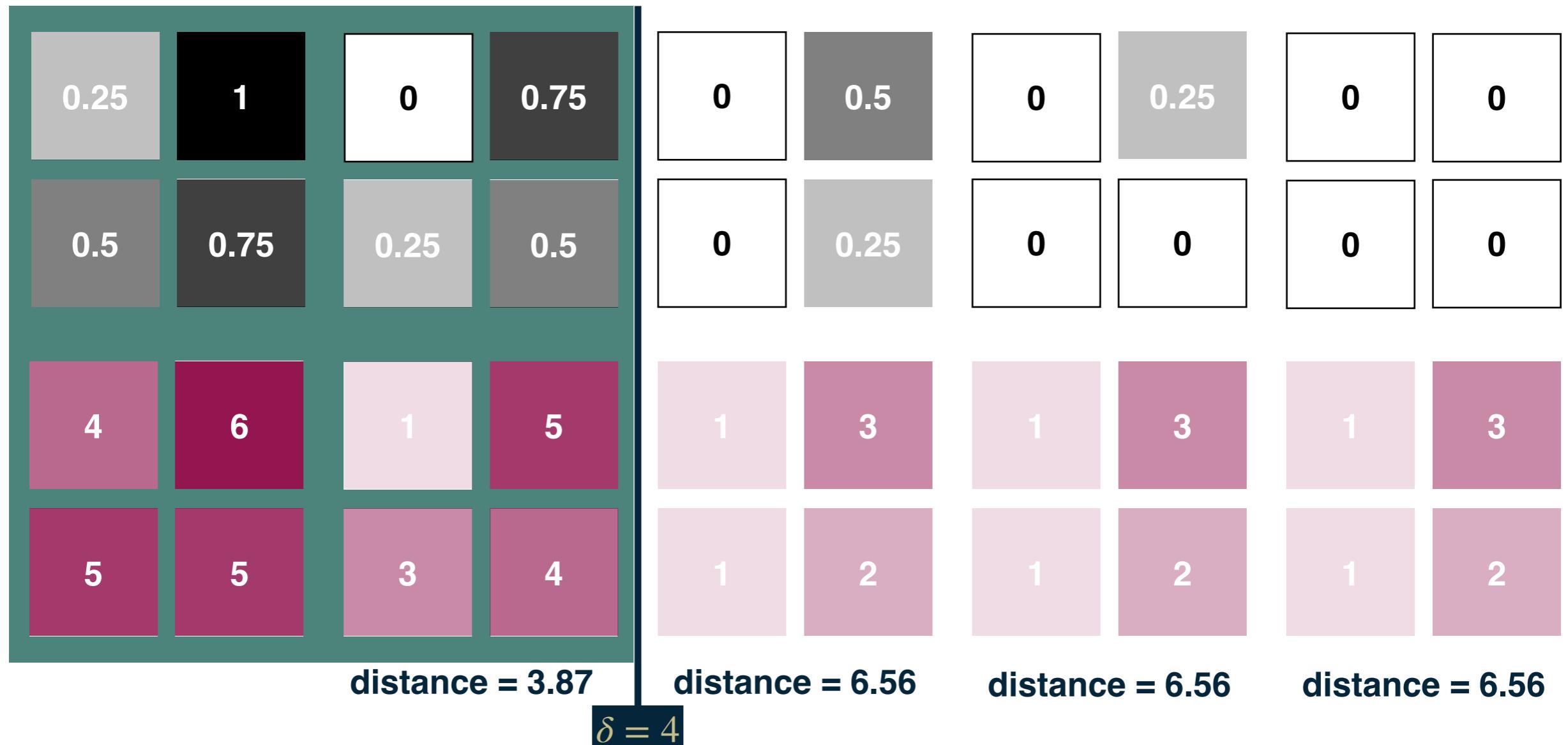
# Example

## Semantic Perturbations



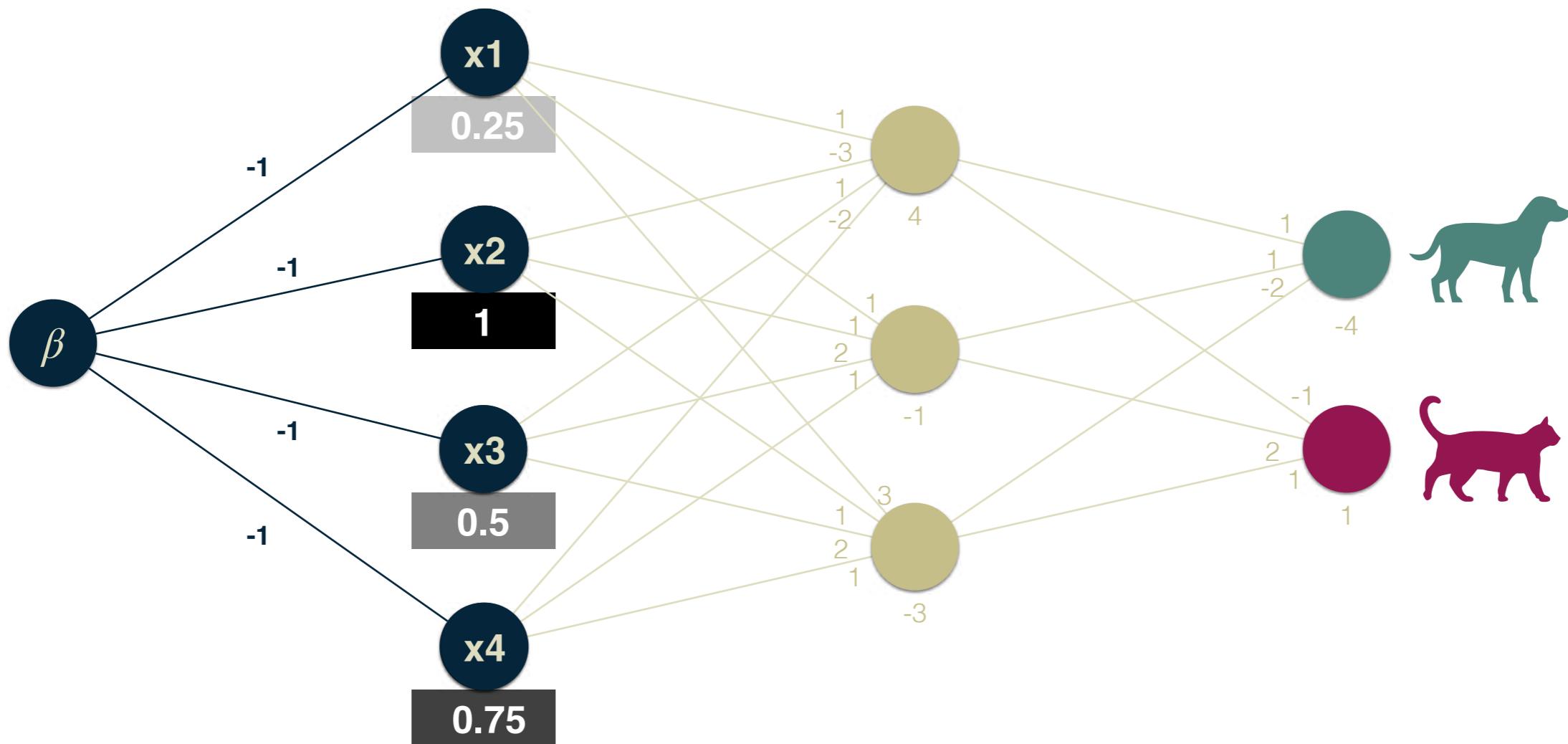
# Example

## Saliency Map Stability



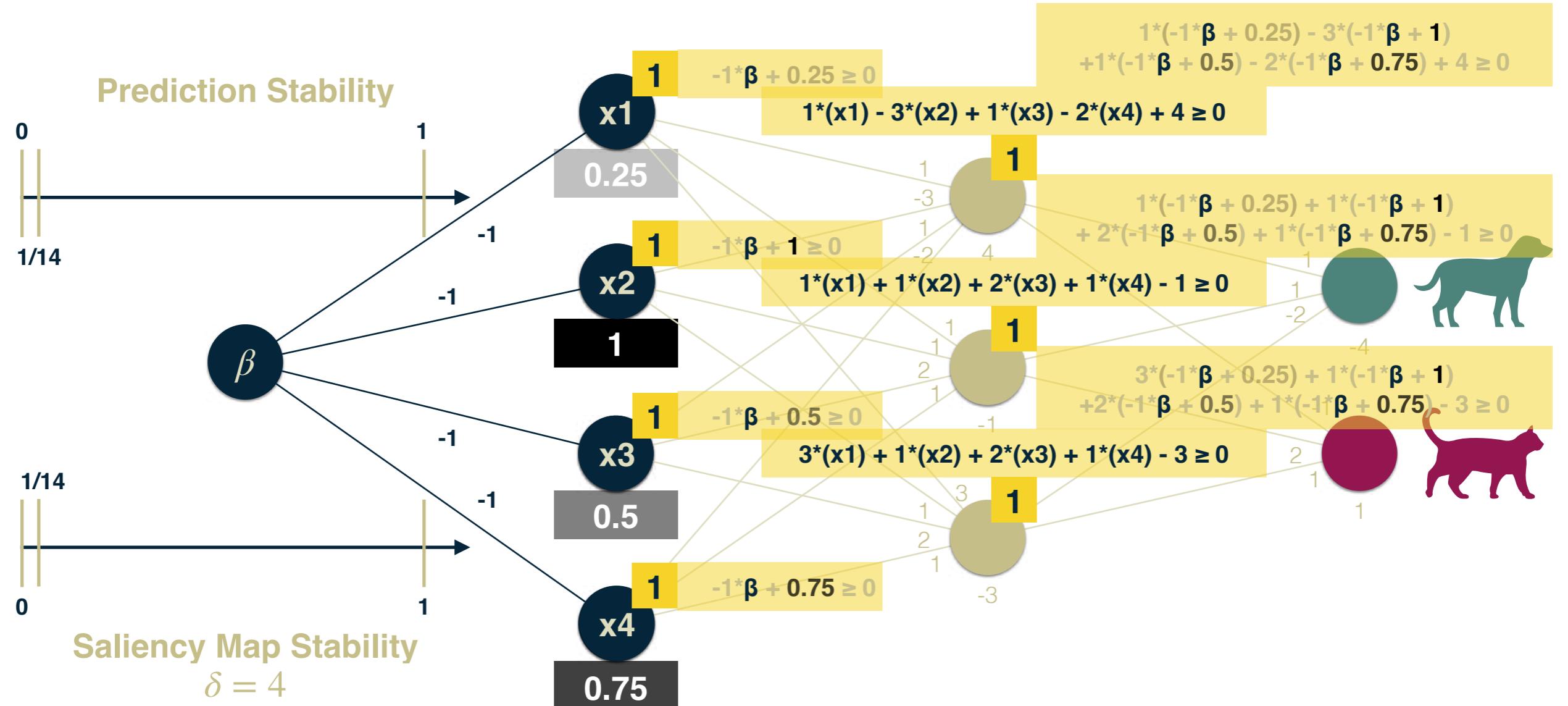
# Example

## Encoding Semantic Perturbations [Mohapatra20]



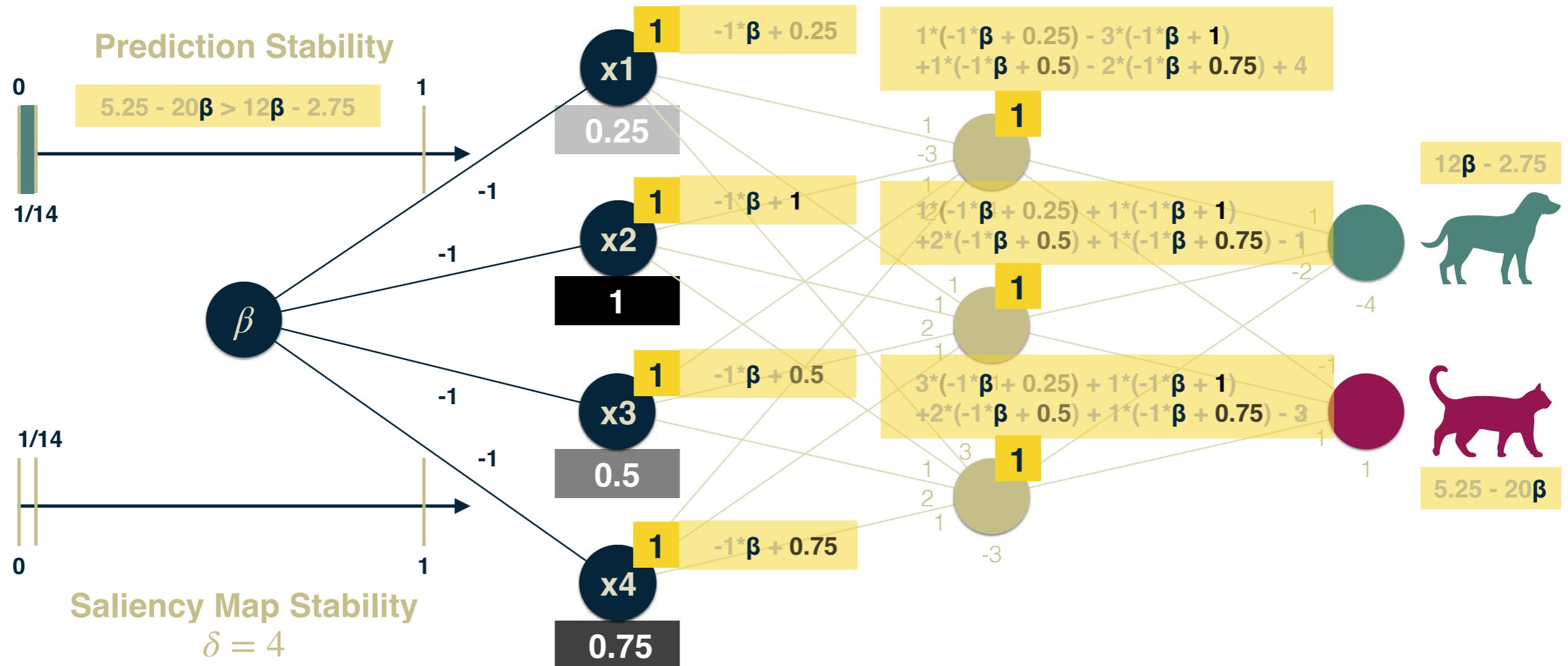
# Example

## Activation Patterns



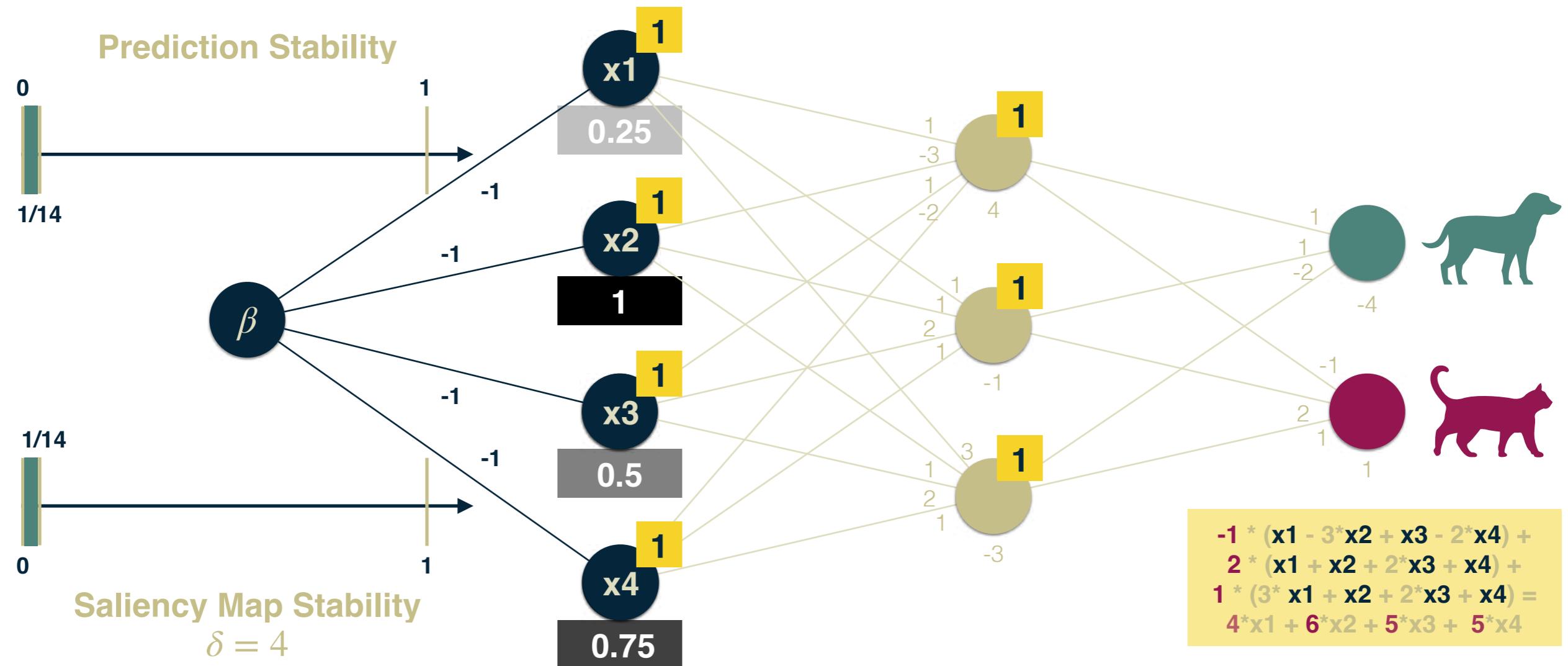
# Example

## Prediction Stability



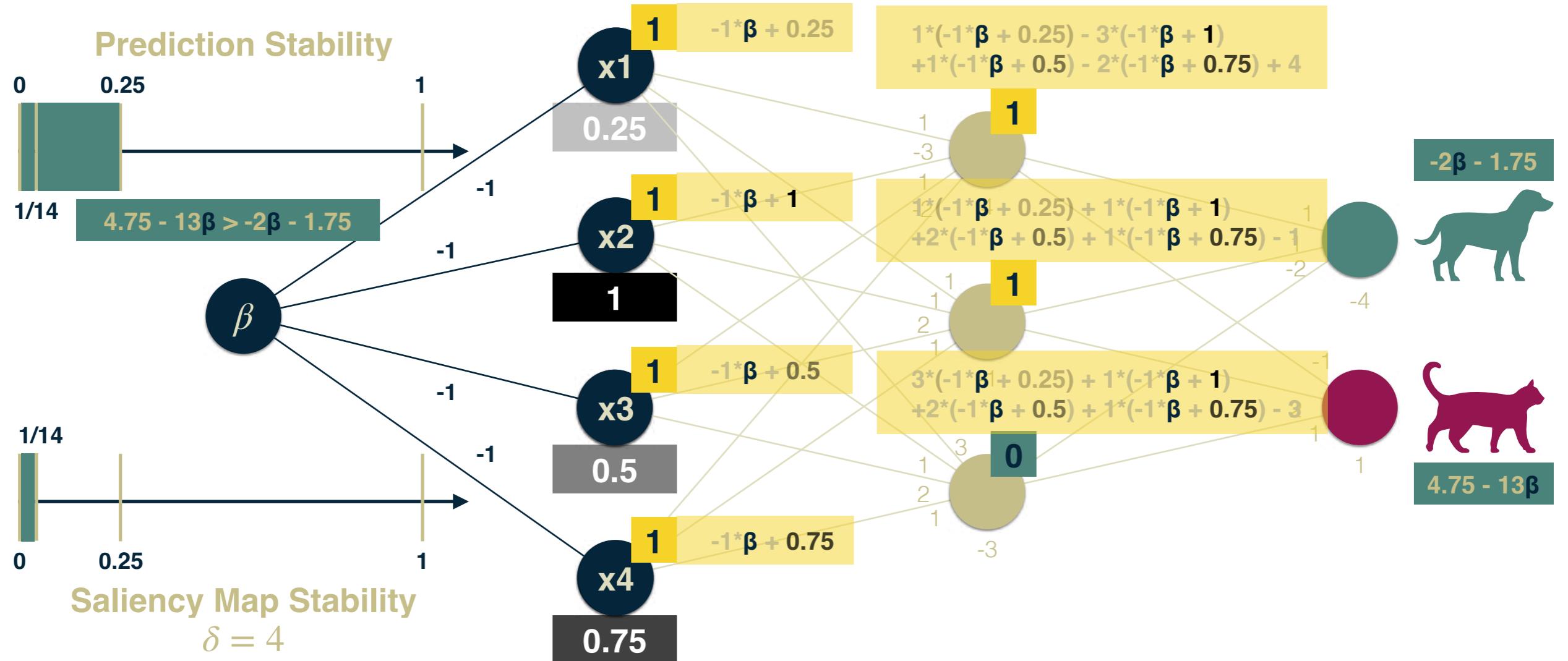
# Example

## Saliency Map Stability



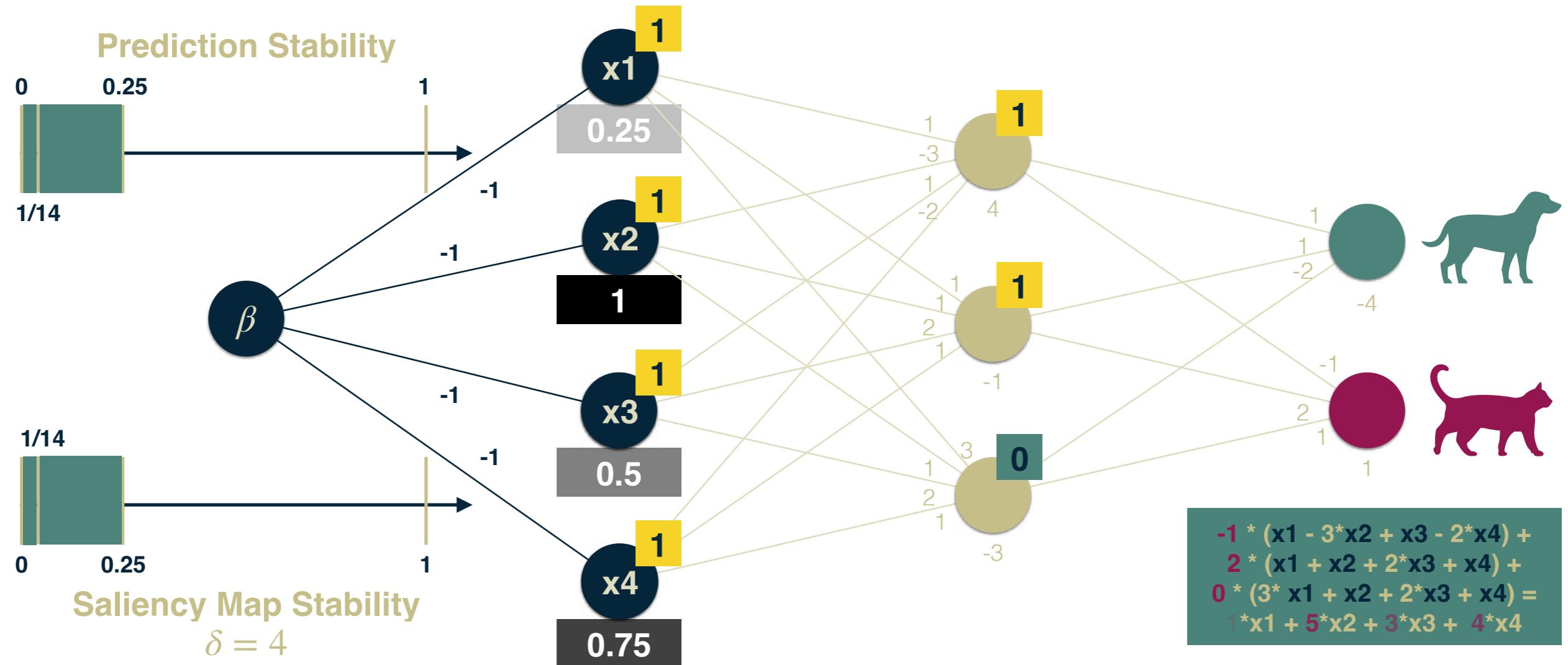
# Example

## Naïve Breadth-First Search



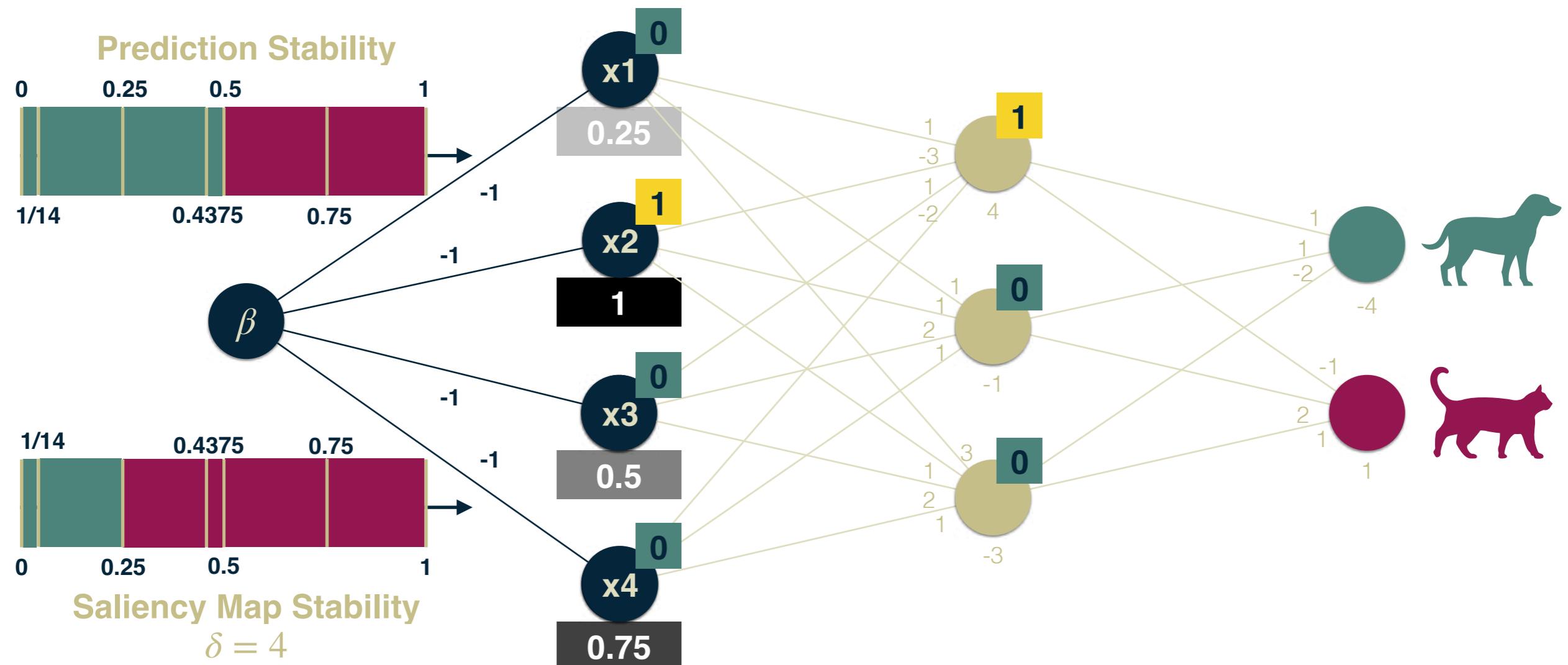
# Example

## Naïve Breadth-First Search



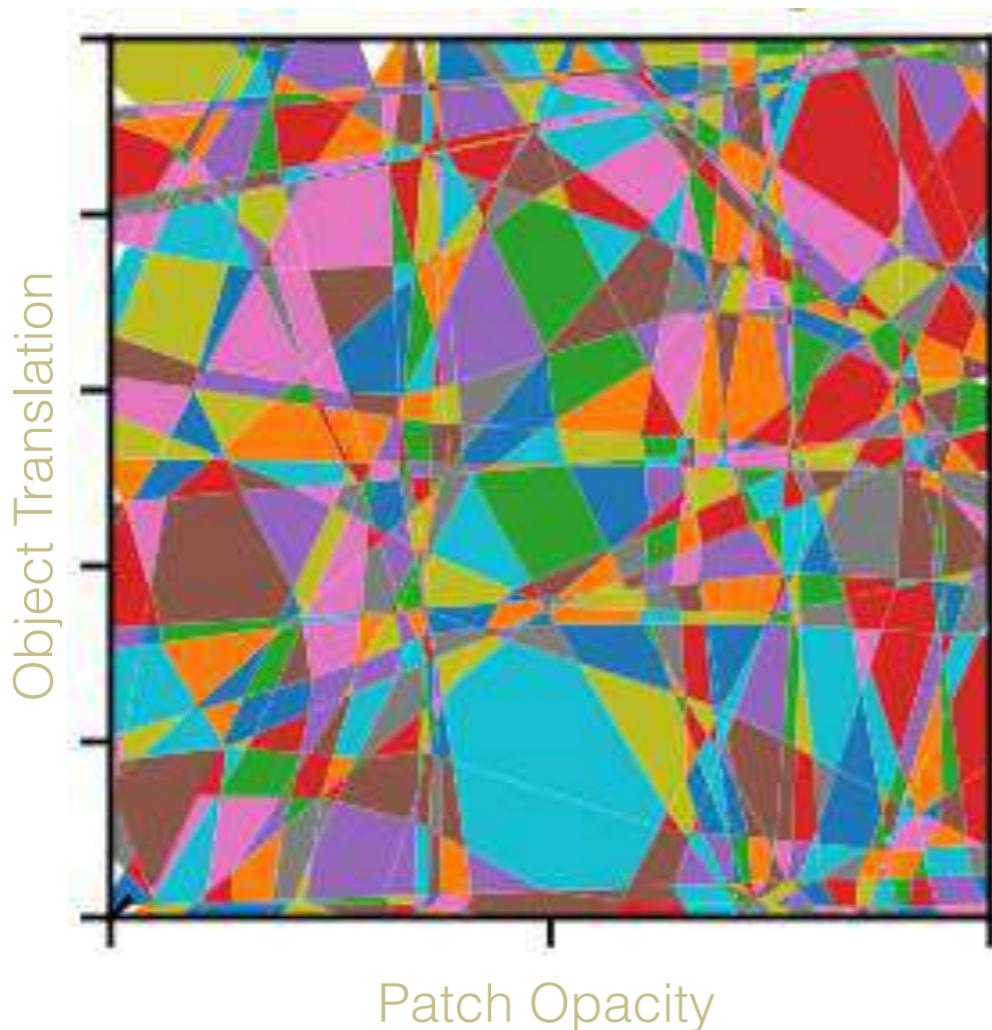
# Example

## Naïve Breadth-First Search



# Naïve Breadth-First Search

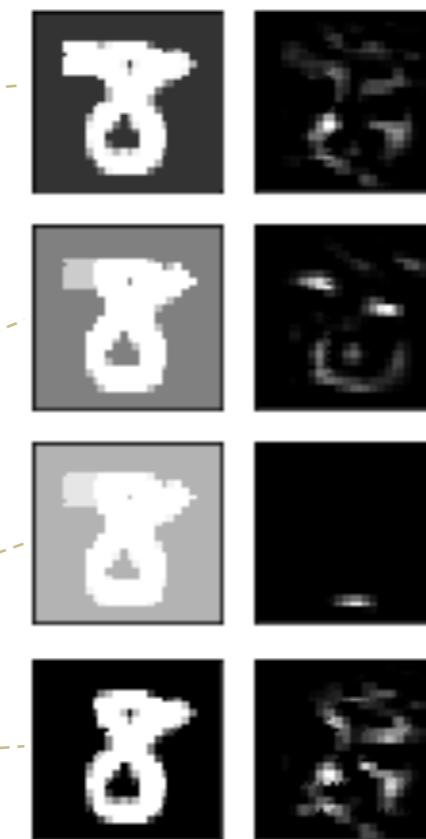
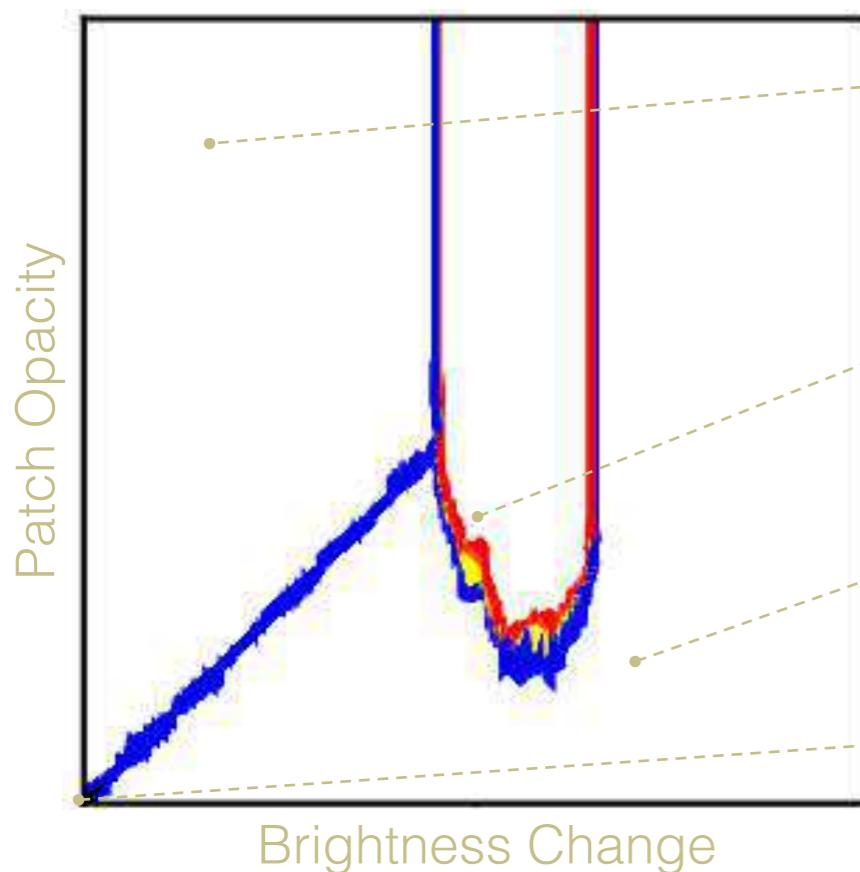
Too Many Activation Patterns!



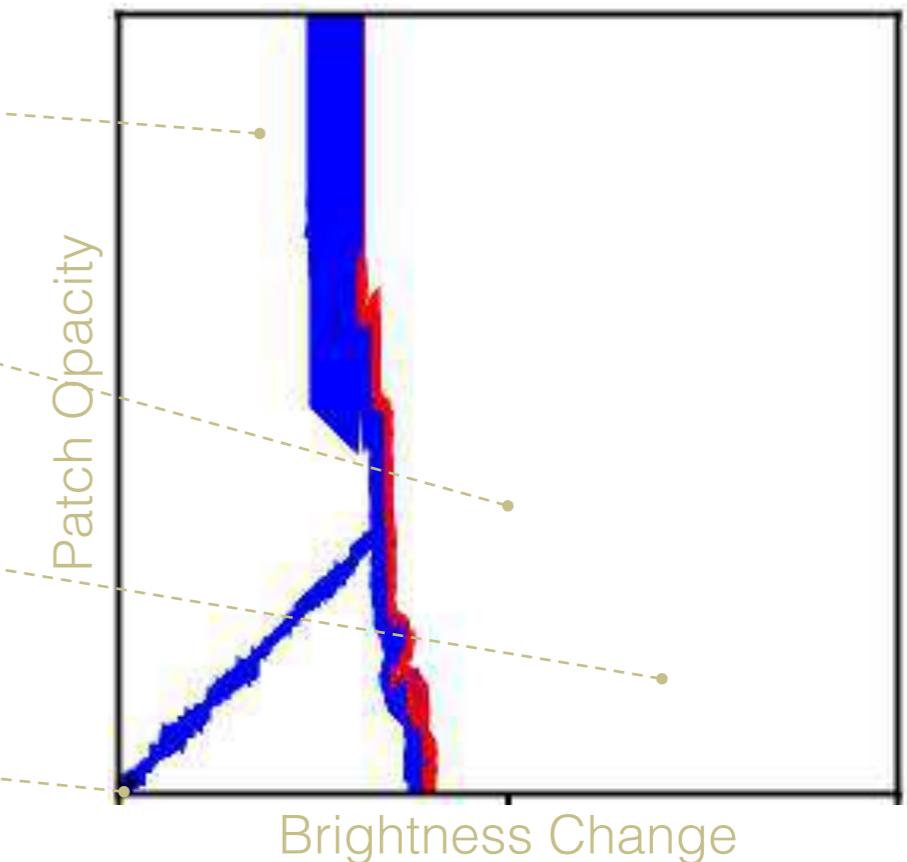
# Geometric Boundary Search

[Munakata23]

Prediction Stability

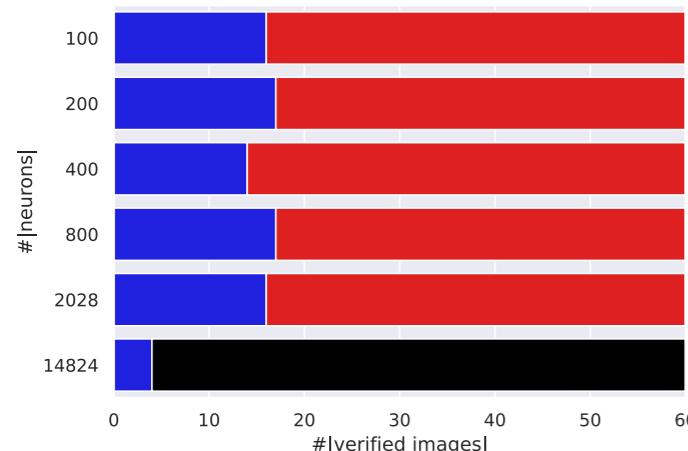


Saliency Map Stability

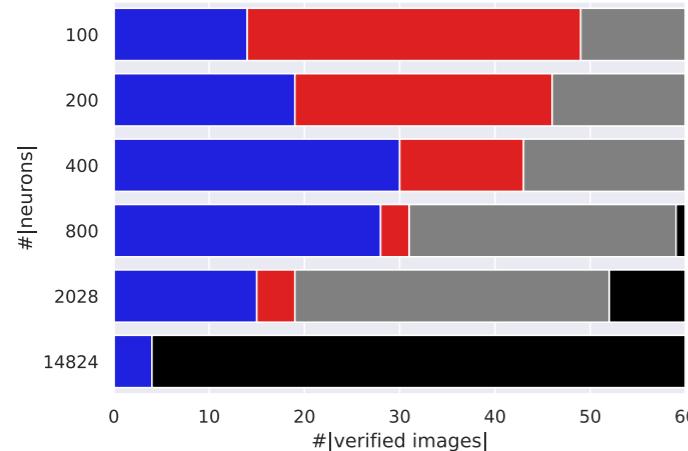


# Geometric Boundary Search

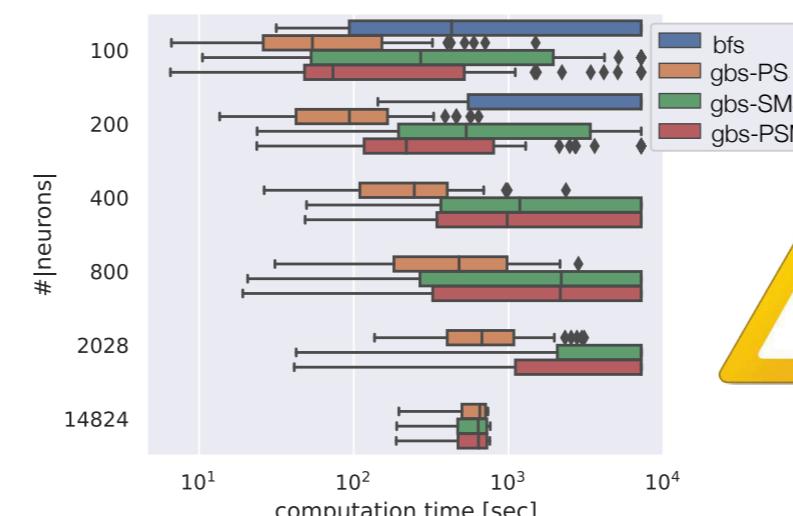
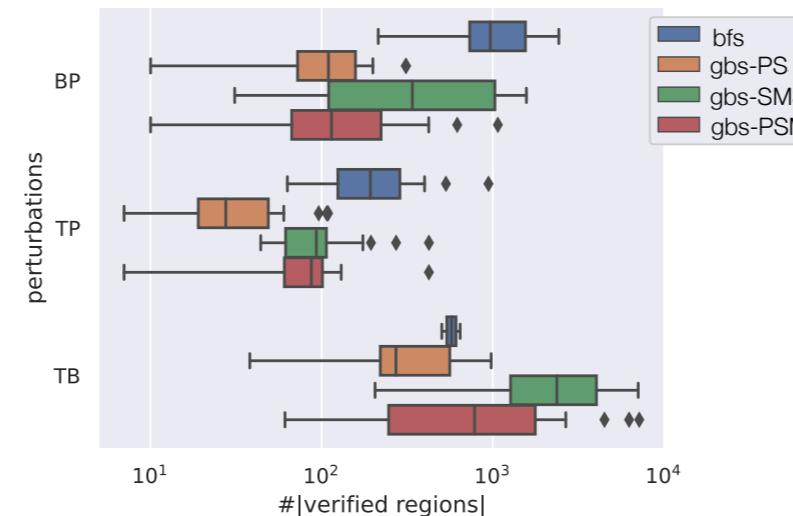
## Experimental Results



Prediction Stability (PS)



Saliency Map Stability (SMS)

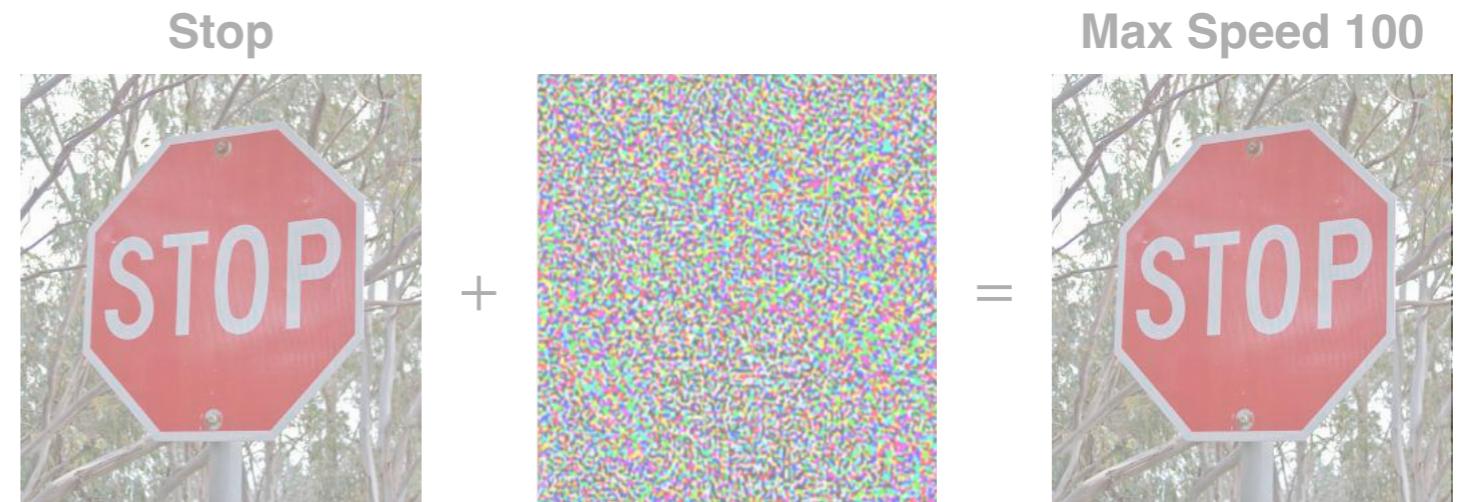


# Abstract (Boundary) Search



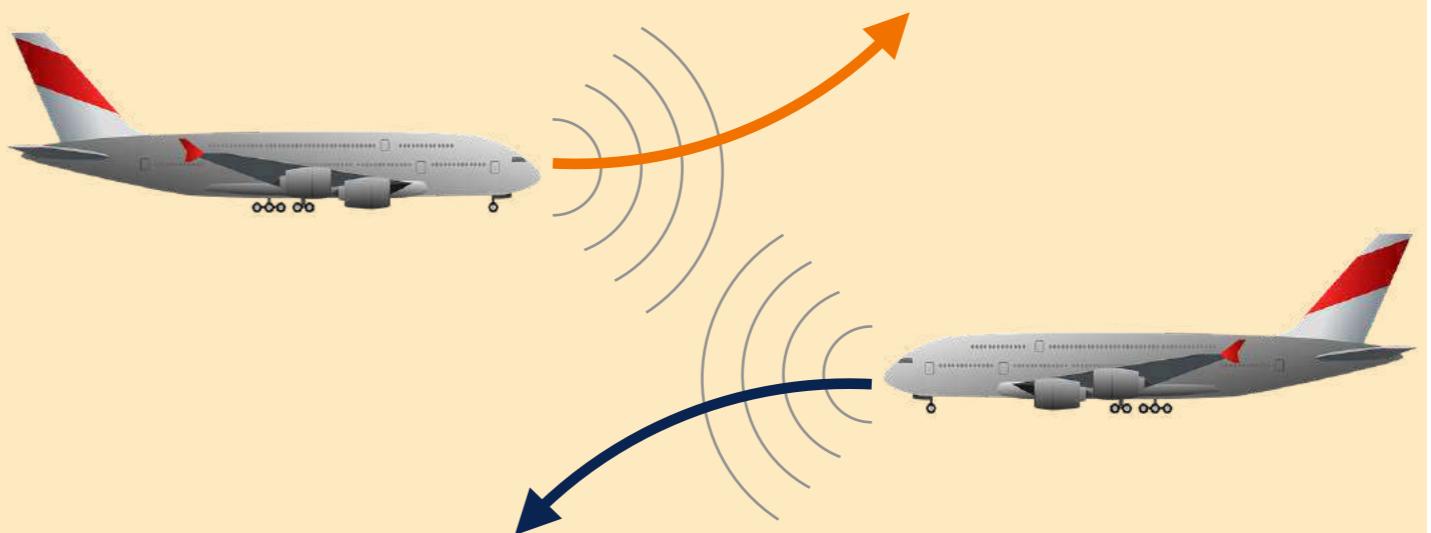
# Stability

Goal G3 in [Kurd03]



# Safety

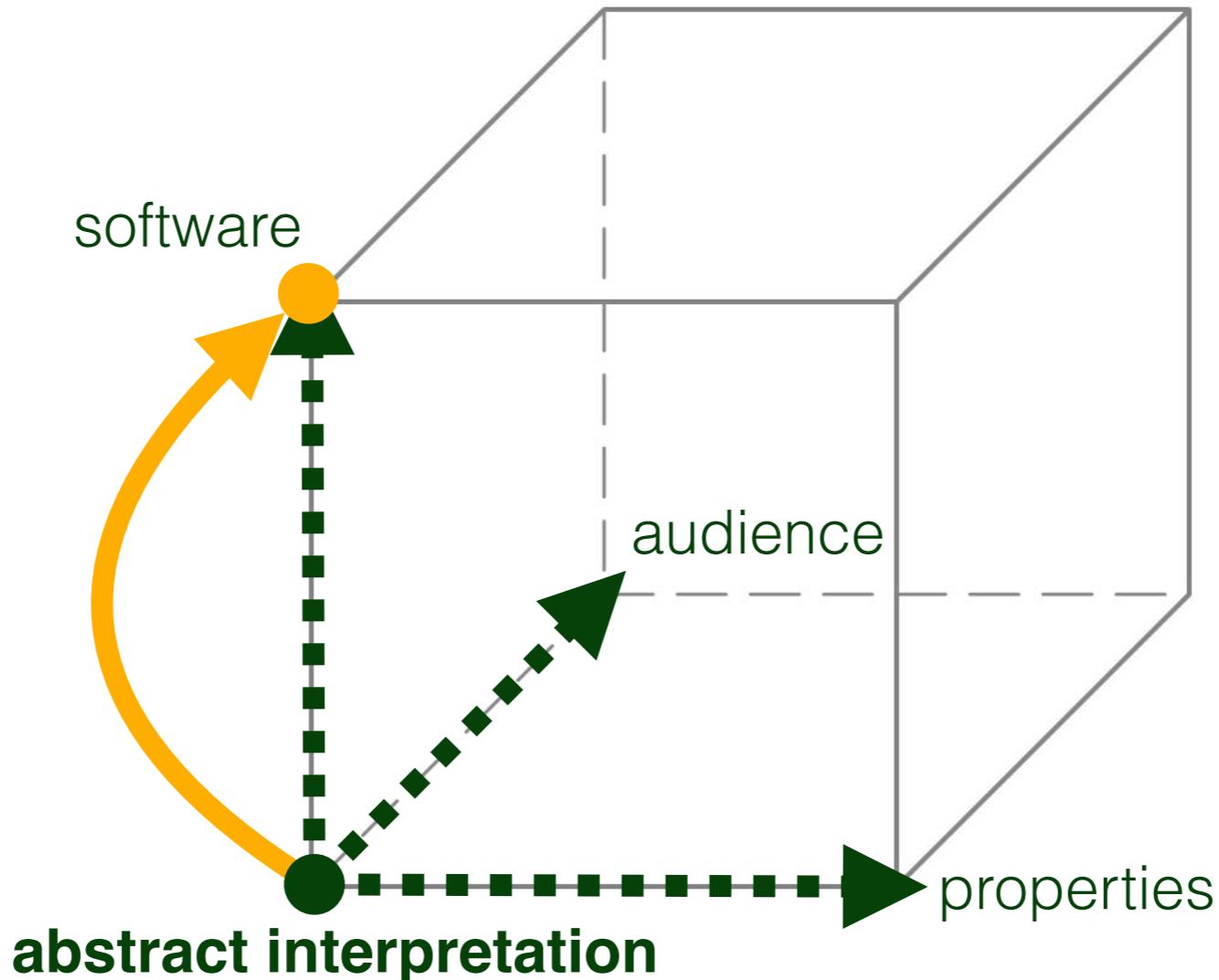
Goal G4 in [Kurd03]



# Fairness



# Safety Verification

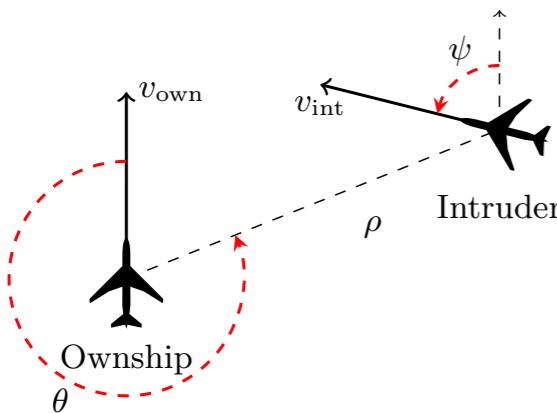


# ACAS Xu

[Julian16][Katz17]

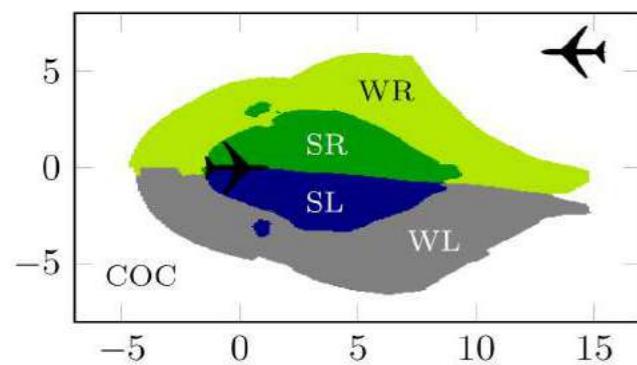
Airborne Collision Avoidance System for Unmanned Aircraft

implemented using 45 feed-forward fully-connected ReLU networks



## 5 input sensor measurements

- $\rho$ : distance from ownship to intruder
- $\theta$ : angle to intruder relative to ownship heading direction
- $\psi$ : heading angle to intruder relative to ownship heading direction
- $v_{own}$ : speed of ownship
- $v_{int}$ : speed of intruder



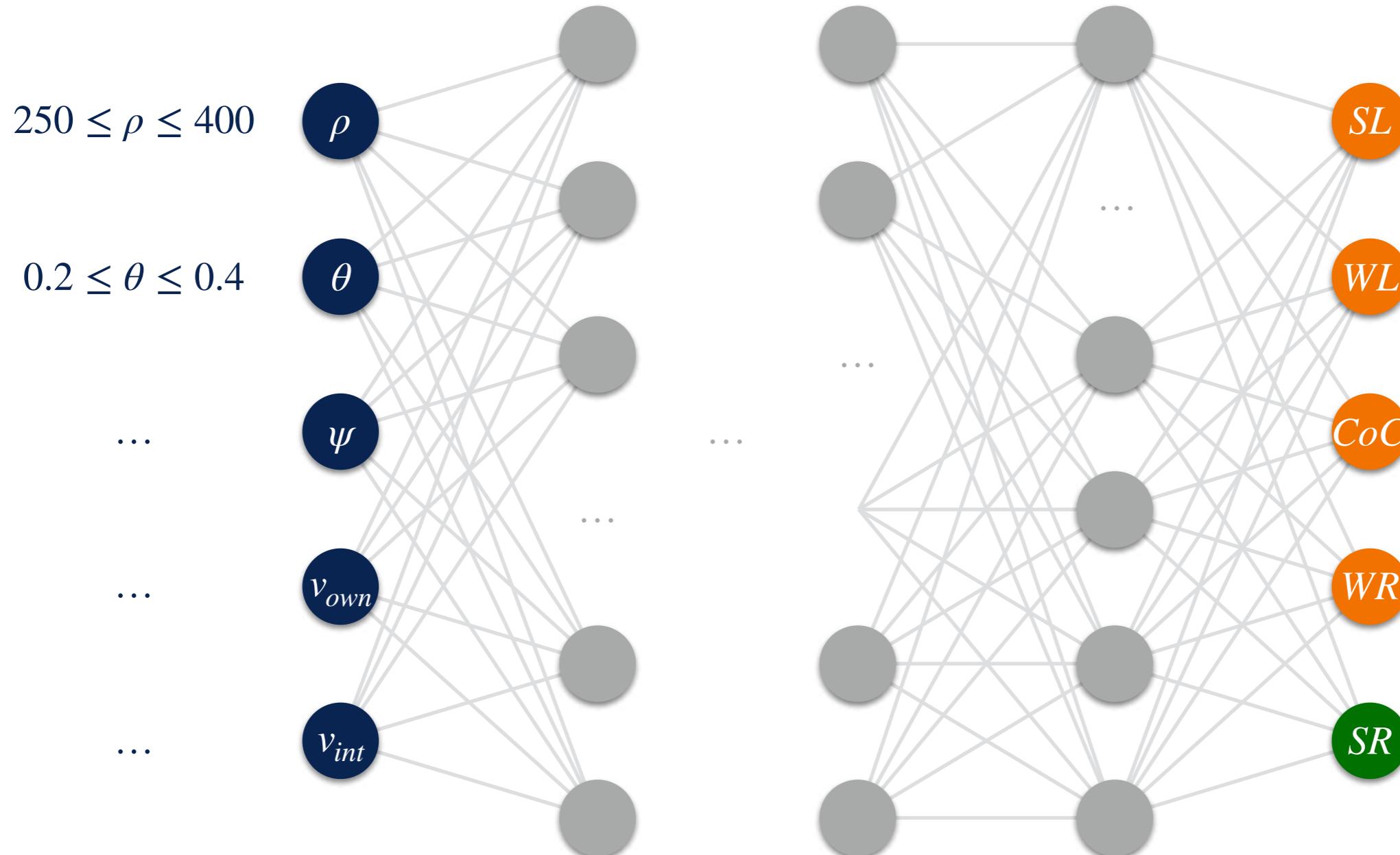
## 5 output horizontal advisories

- Strong Left
- Weak Left
- Clear of Conflict
- Weak Right
- Strong Right

# ACAS Xu Properties

[Katz17]

Example: “if intruder is **near** and approaching **from the left**, go **Strong Right**”



# Safety

## Input-Output Properties

**I**: input specification

**O**: output specification

$$\mathcal{S}_O^I \stackrel{\text{def}}{=} \{[M] \mid \text{SAFE}_O^I([M])\}$$

$\mathcal{S}_O^I$  is the set of all neural networks  $M$  (or, rather, their semantics  $[M]$ ) that **satisfy** the input and output specification **I** and **O**

$$\text{SAFE}_O^I([M]) \stackrel{\text{def}}{=} \forall t \in [M]: t_0 \models I \Rightarrow t_\omega \models O$$

### Theorem

$$M \models \mathcal{S}_O^I \Leftrightarrow \{[M]\} \subseteq \mathcal{S}_O^I$$

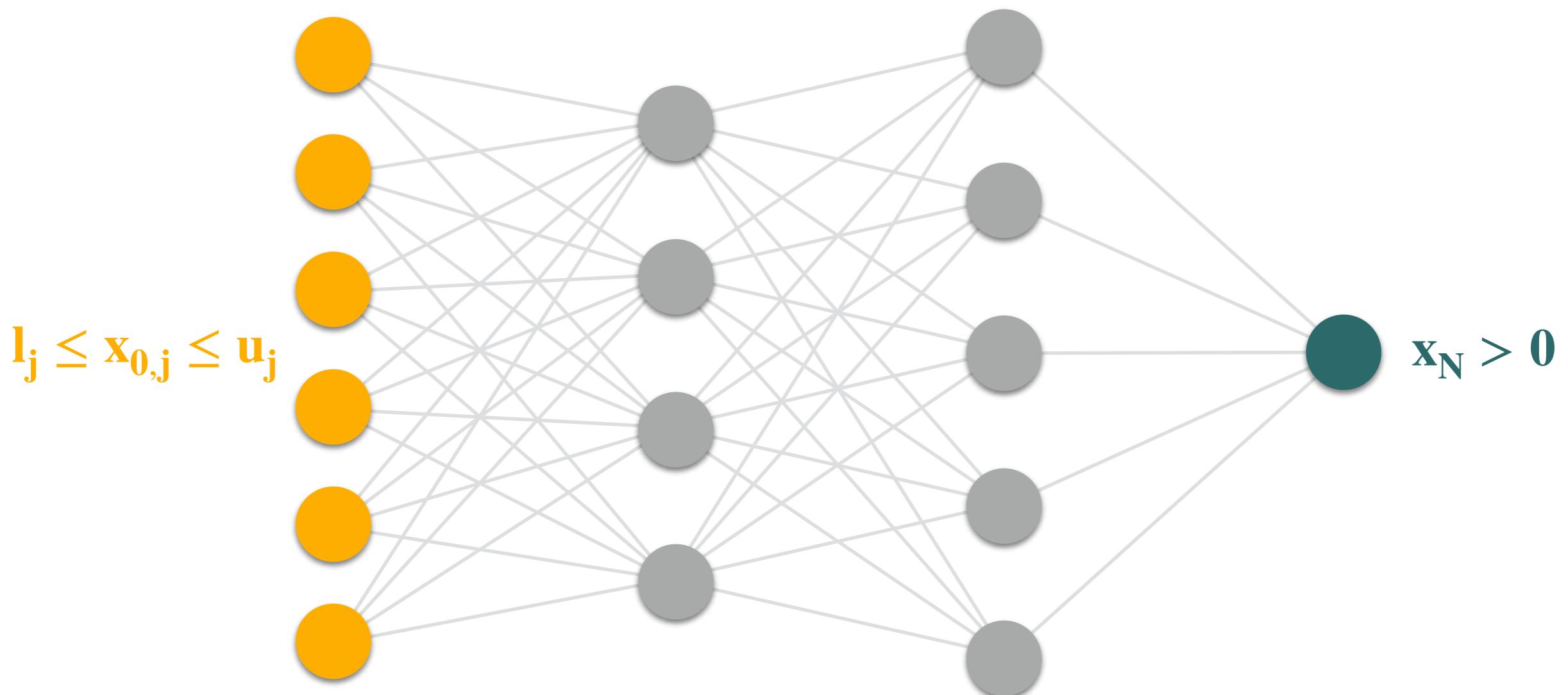
### Corollary

$$M \models \mathcal{S}_O^I \Leftrightarrow [M] \subseteq \bigcup \mathcal{S}_O^I$$

# Model Checking Methods

# Safety

## Example



# SMT-Based Methods

Verification Reduced to **Constraint Satisfiability**

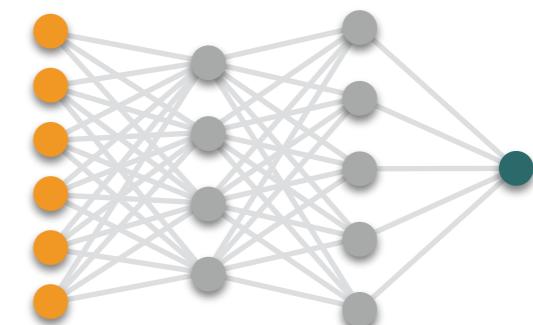
$$l_j \leq x_{0,j} \leq u_j$$

$$j \in \{0, \dots, |\mathbf{X}_0|\}$$

**input specification**

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \quad i \in \{0, \dots, n-1\}$$

$$x_{i,j} = \max\{0, \hat{x}_{i,j}\} \quad i \in \{1, \dots, n-1\}, \\ j \in \{0, \dots, |\mathbf{X}_i|\}$$



$$\mathbf{x}_N \leq \mathbf{0}$$

(negation of)  
**output specification**

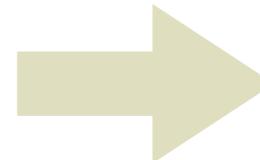
**satisfiable** → **counterexample**  
otherwise → **safe**

# Planet



use approximations to  
reduce the solution search space

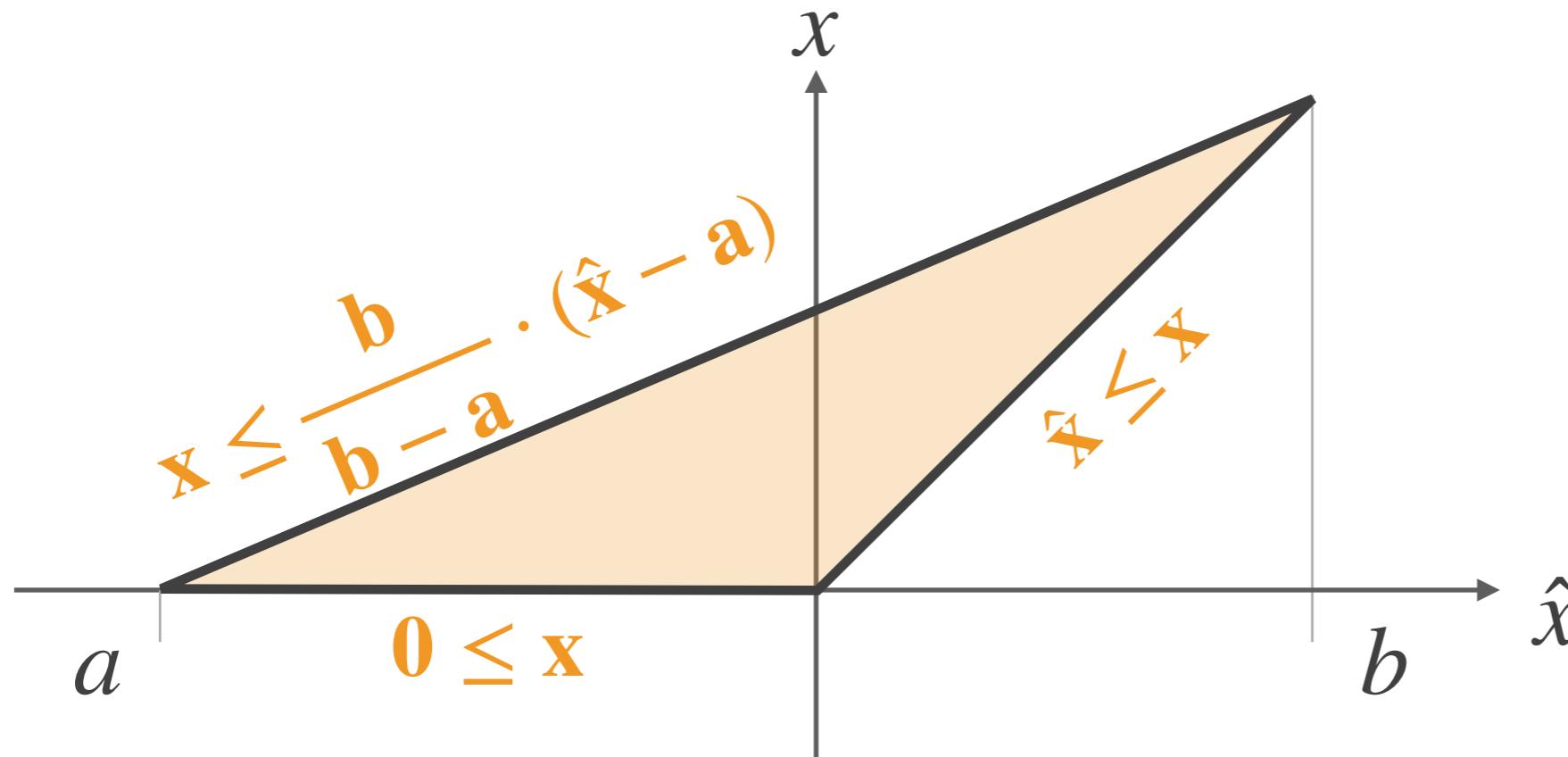
$$x_{i,j} = \max\{0, \hat{x}_{i,j}\}$$



$$0 \leq x_{i,j}$$

$$\hat{x}_{i,j} \leq x_{i,j}$$

$$x_{i,j} \leq \frac{b_{i,j}}{b_{i,j} - a_{i,j}} \cdot (\hat{x}_{i,j} - a_{i,j})$$

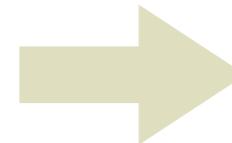


# Reluplex

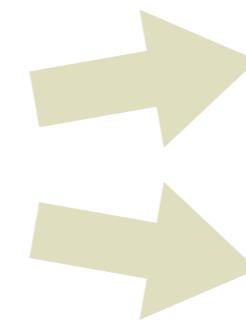


based on the **simplex algorithm**  
extended to support ReLUs

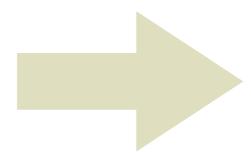
Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}_{ij}$
$\mathbf{x}_{ij}$	$v_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



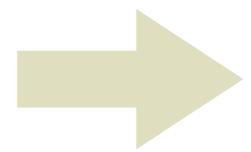
Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	$v_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	$\hat{v}'_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	0
...	...
$\mathbf{x}_N$	$v_N$



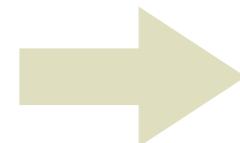
# Reluplex



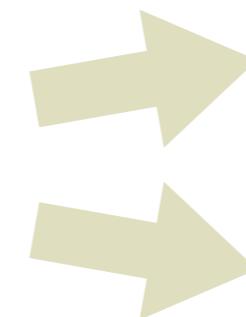
Follow-up Work

G. Katz et al. - The Marabou Framework for Verification and Analysis of Deep Neural Networks (CAV 2019)

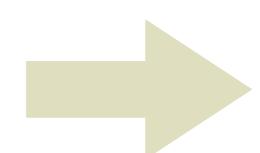
Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}_{ij}$
$\mathbf{x}_{ij}$	$v_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



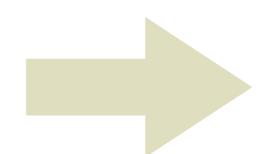
Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	$v_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	$v'_{ij}$
...	...
$\mathbf{x}_N$	$v_N$



Variable	Value
$\mathbf{x}_{00}$	$v_{00}$
...	...
$\hat{\mathbf{x}}_{ij}$	$\hat{v}'_{ij}$
$\mathbf{x}_{ij}$	0
...	...
$\mathbf{x}_N$	$v_N$



# Other SMT-Based Methods

- L. Pulina and A. Tacchella. *An Abstraction-Refinement Approach to Verification of Artificial Neural Networks*. In CAV, 2010.  
the **first formal verification method for neural networks**
- O. Bastani, Y. Ioannou, L. Lampropoulos, D. Vytiniotis, A. Nori, and A. Criminisi. *Measuring Neural Net Robustness with Constraints*. In NeurIPS, 2016.  
an approach for finding the **nearest adversarial example according to the  $L_\infty$  distance**
- X. Huang, M. Kwiatkowska, S. Wang, and M. Wu. *Safety Verification of Deep Neural Networks*. In CAV, 2017.  
an approach for proving **local robustness to adversarial perturbations**
- N. Narodytska, S. Kasiviswanathan, L. Ryzhyk, M. Sagiv, and T. Walsh. *Verifying Properties of Binarized Deep Neural Networks*. In AAAI, 2018.  
C. H. Cheng, G. Nührenberg, C. H. Huang, and H. Ruess. *Verification of Binarized Neural Networks via Inter-Neuron Factoring*. In VSTTE, 2018.  
approaches focusing on **binarized neural networks**

# MILP-Based Methods

Verification Reduced to Mixed Integer Linear Program

$$l_j \leq x_{0,j} \leq u_j$$

$$j \in \{0, \dots, |\mathbf{X}_0| \}$$

input specification

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \quad i \in \{0, \dots, n-1\}$$

$$x_{i,j} = \delta_{i,j} \cdot \hat{x}_{i,j}$$

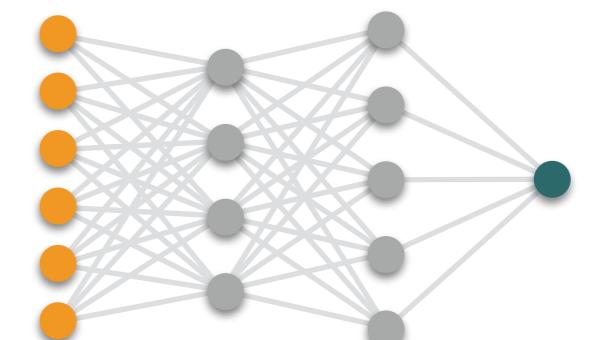
$$\delta_{i,j} \in \{0, 1\}$$

$$\delta_{i,j} = 1 \Rightarrow \hat{x}_{i,j} \geq 0$$

$$i \in \{1, \dots, n-1\}$$

$$\delta_{i,j} = 0 \Rightarrow \hat{x}_{i,j} < 0$$

$$j \in \{0, \dots, |\mathbf{X}_i| \}$$



$$\min \mathbf{x}_N$$

objective function

$\min \mathbf{x}_N \leq 0 \rightarrow \text{X counterexample}$   
otherwise  $\rightarrow \checkmark \text{safe}$

# MILP-Based Methods

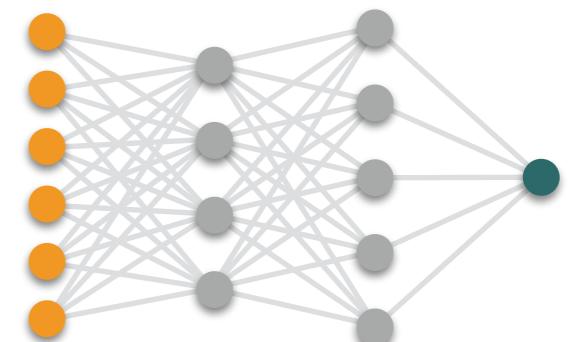
## Bounded Encoding with Symmetric Bounds

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|X_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \quad i \in \{0, \dots, n-1\}$$

$$0 \leq x_{i,j} \leq \mathbf{M}_{i,j} \cdot \delta_{i,j} \quad \delta_{i,j} \in \{0, 1\}$$

$$\hat{x}_{i,j} \leq x_{i,j} \leq \hat{x}_{i,j} - \mathbf{M}_{i,j} \cdot (1 - \delta_{i,j}) \quad i \in \{1, \dots, n-1\}$$

$$\mathbf{M}_{i,j} = \max\{-\mathbf{l}_i, \mathbf{u}_i\} \quad j \in \{0, \dots, |X_i|\}$$



# Sherlock

## Output Range Analysis



use local search to  
speed up the MILP solver

$$l_j \leq x_{0,j} \leq u_j$$

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|X_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j}$$

$$0 \leq x_{i,j} \leq M_{i,j} \cdot \delta_{i,j}$$

$$\hat{x}_{i,j} \leq x_{i,j} \leq \hat{x}_{i,j} - M_{i,j} \cdot (1 - \delta_{i,j})$$

$$M_{i,j} = \max\{-l_i, u_i\}$$

$$x_N < \hat{L}$$



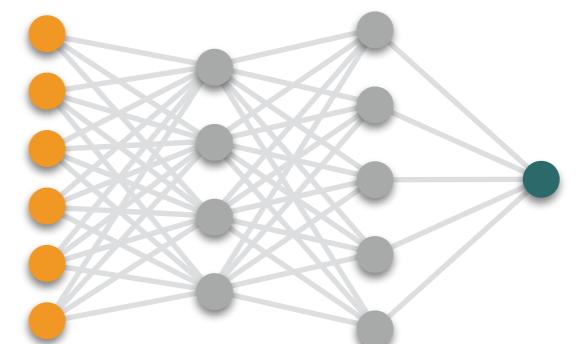
find another input  $\hat{X}$   
such that  $\hat{L} \leq x_N$

# MILP-Based Methods

## Bounded Encoding with Asymmetric Bounds

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|X_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \quad i \in \{0, \dots, n-1\}$$

$$0 \leq x_{i,j} \leq \mathbf{u}_{i,j} \cdot \delta_{i,j} \quad \delta_{i,j} \in \{0, 1\}$$
$$\hat{x}_{i,j} \leq x_{i,j} \leq \hat{x}_{i,j} - \mathbf{l}_{i,j} \cdot (1 - \delta_{i,j}) \quad i \in \{1, \dots, n-1\}$$
$$j \in \{0, \dots, |X_i|\}$$



# MIPVerify

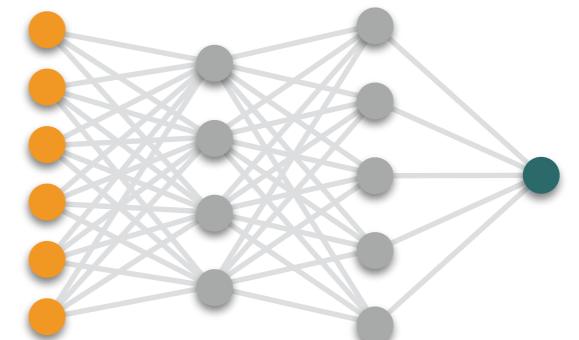
## Finding Nearest Adversarial Example

$$\min_{\mathbf{X}'} \mathbf{d}(\mathbf{X}, \mathbf{X}')$$

$$\hat{x}_{i+1,j} = \sum_{k=0}^{|\mathbf{X}_i|} w_{j,k}^i \cdot x_{i,k} + b_{i,j} \quad i \in \{0, \dots, n-1\}$$

$$0 \leq x_{i,j} \leq \mathbf{u}_{i,j} \cdot \delta_{i,j} \quad \delta_{i,j} \in \{0, 1\}$$
$$\hat{x}_{i,j} \leq x_{i,j} \leq \hat{x}_{i,j} - \mathbf{l}_{i,j} \cdot (1 - \delta_{i,j}) \quad i \in \{1, \dots, n-1\}$$
$$j \in \{0, \dots, |\mathbf{X}_i|\}$$

$$\mathbf{x}_N \neq \mathbf{0}$$

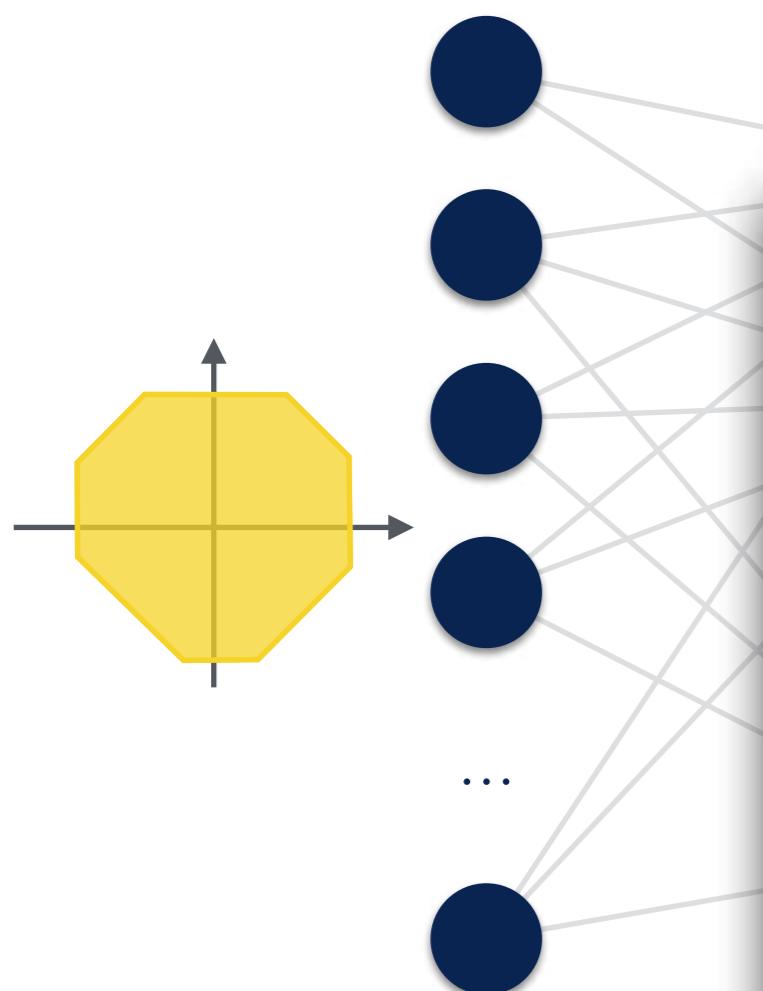


# Other MILP-Based Methods

- R. Bunel, I. Turkaslan, P. H. S. Torr, P. Kohli, and M. P. Kumar. *A Unified View of Piecewise Linear Neural Network Verification*. In NeurIPS, 2018.  
a **unifying verification framework** for **piecewise-linear ReLU neural networks**
- C.-H. Cheng, G. Nührenberg, and H. Ruess. *Maximum Resilience of Artificial Neural Networks*. In ATVA, 2017.  
an approach for finding a **lower bound on robustness** to **adversarial perturbations**
- M. Fischetti and J. Jo. *Deep Neural Networks and Mixed Integer Linear Optimization*. 2018.  
an approach for **feature visualization** and **building adversarial examples**

# Static Analysis Methods

# Forward Analysis



- ① proceed **forwards from an abstraction** of the input specification **I**

## Safety

### Input-Output Properties

**I:** input specification

**O:** output specification

$$\mathcal{S}_O^I \stackrel{\text{def}}{=} \{[\![M]\!] \in \mathcal{P}(\Sigma^*) \mid \text{SAFE}_O^I([\![M]\!])\}$$

$\mathcal{S}_O^I$  is the set of all neural networks  $M$  (or, rather, their semantics  $[\![M]\!]$ ) that **satisfy** the input and output specification **I** and **O**

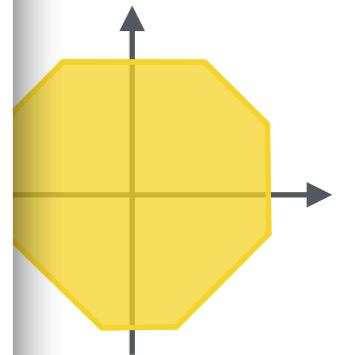
$$\text{SAFE}_O^I([\![M]\!]) \stackrel{\text{def}}{=} \forall t \in [\![M]\!]: t_0 \models \mathbf{I} \Rightarrow t_\omega \models \mathbf{O}$$

Theorem	Corollary
$M \models \mathcal{S}_O^I \Leftrightarrow \{[\![M]\!]\} \subseteq \mathcal{S}_O^I$	$M \models \mathcal{S}_O^I \Leftrightarrow [\![M]\!] \subseteq \bigcup \mathcal{S}_O^I$

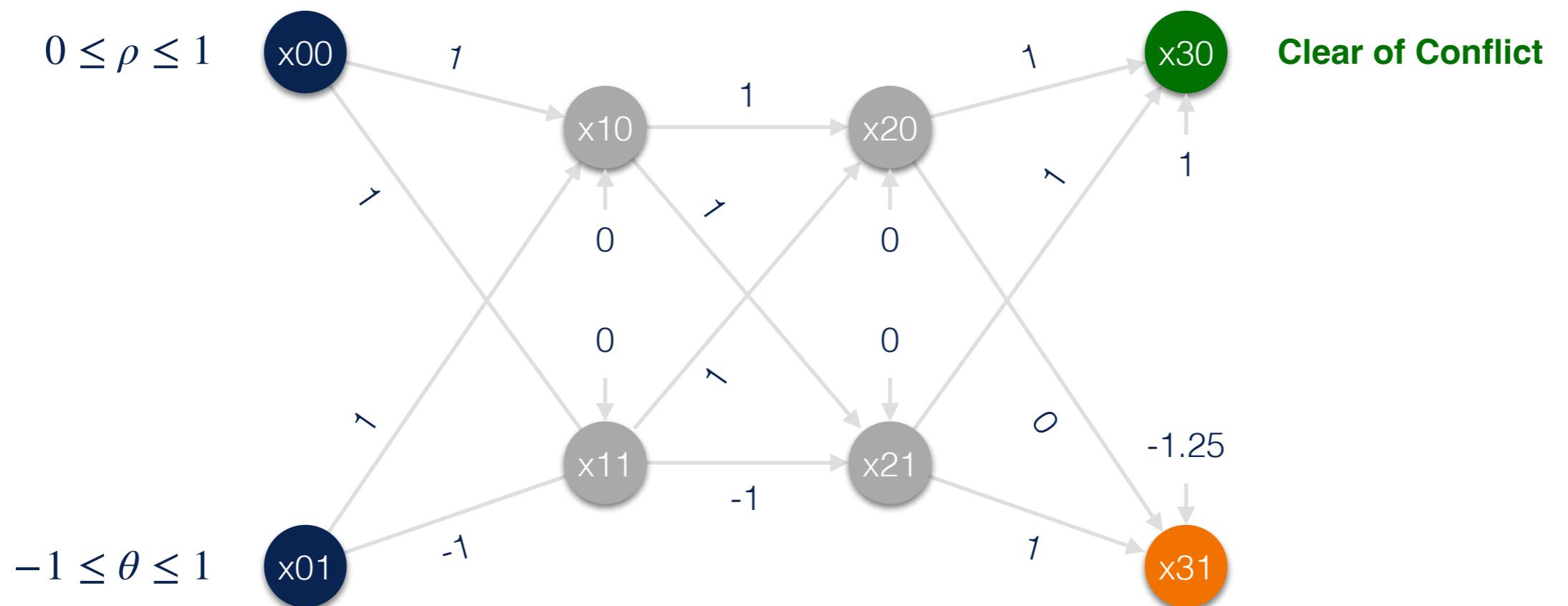
**Theorem**

$$[\![M]\!] \subseteq [\![M]\!]^\natural \subseteq \bigcup \mathcal{S}_O^I \Rightarrow M \models \mathcal{S}_O^I$$

- ② check output for **inclusion** in **output specification O**:  
included → **safe**  
otherwise → **alarm**

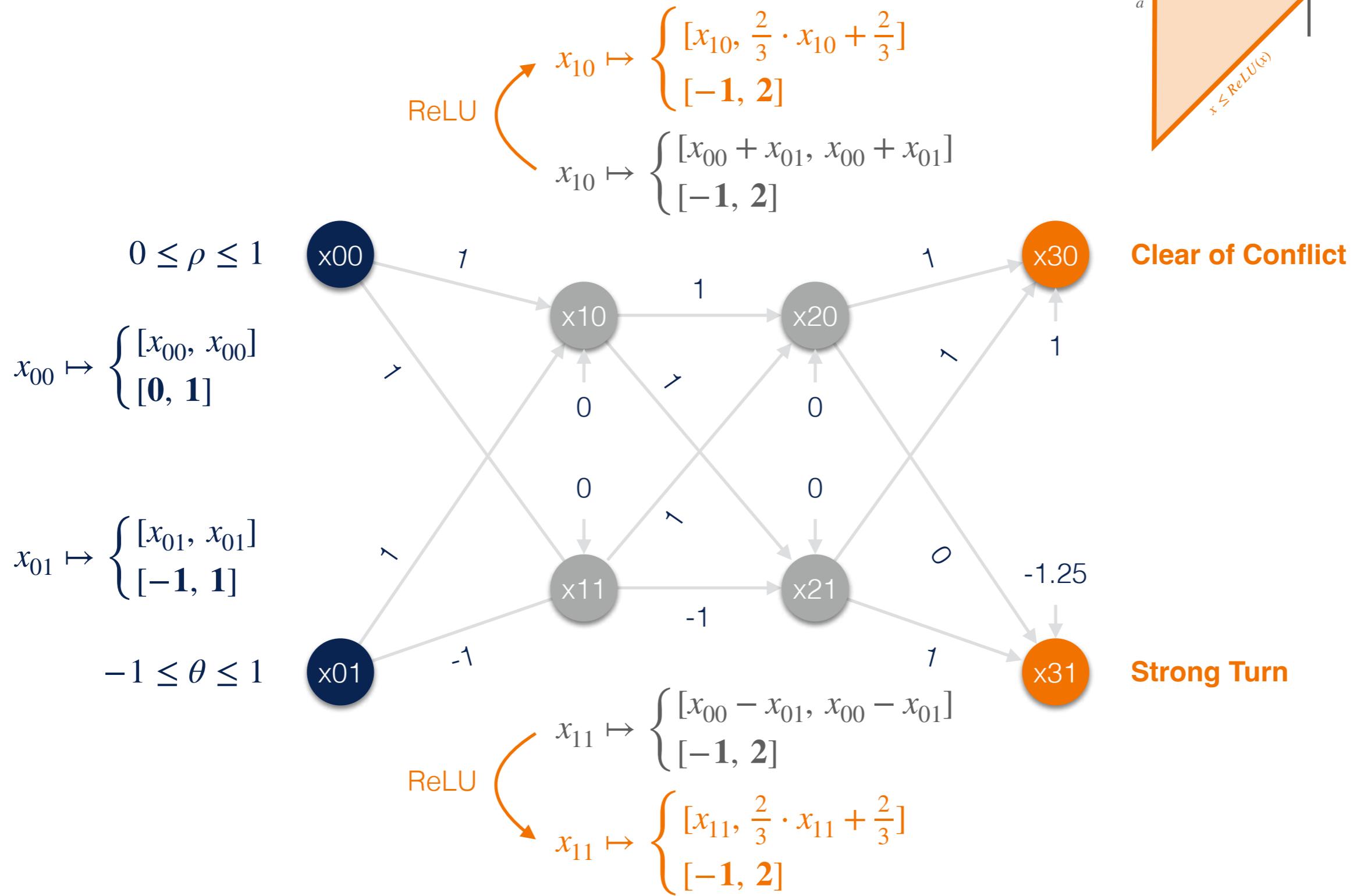
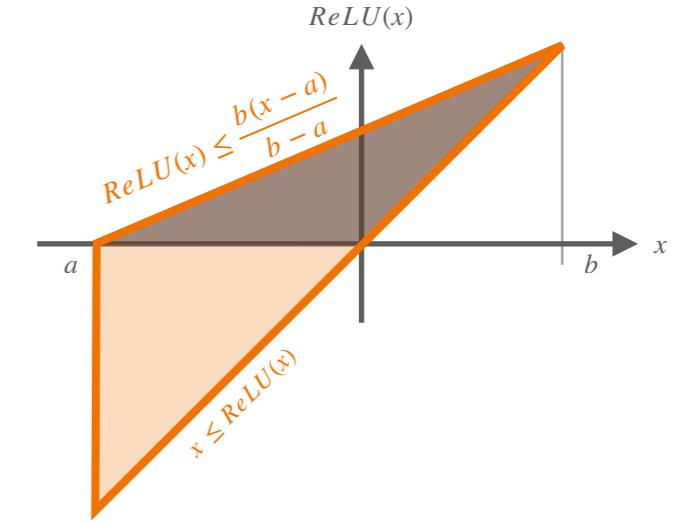


# Example



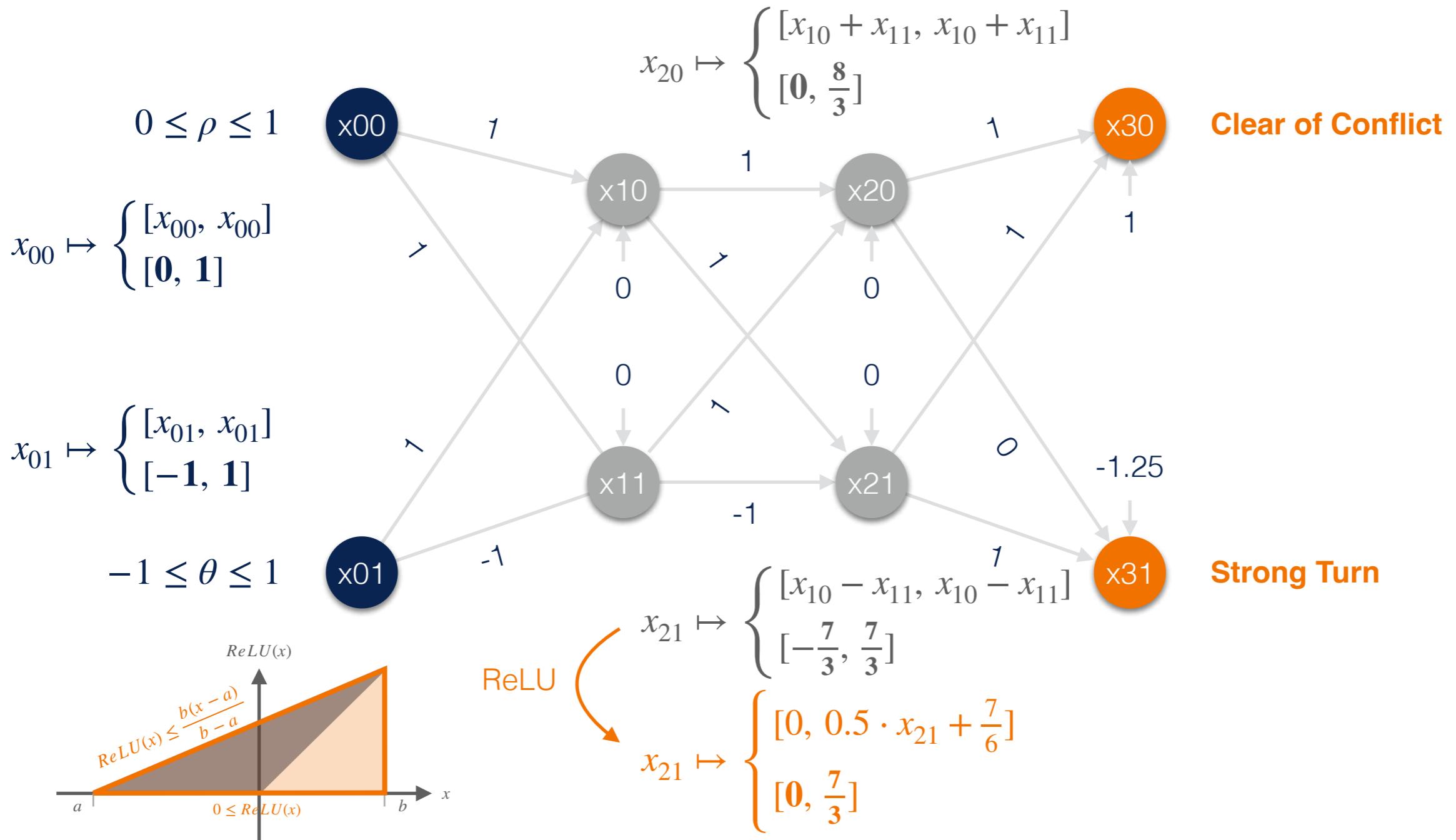
# DeepPoly

[Singh19]



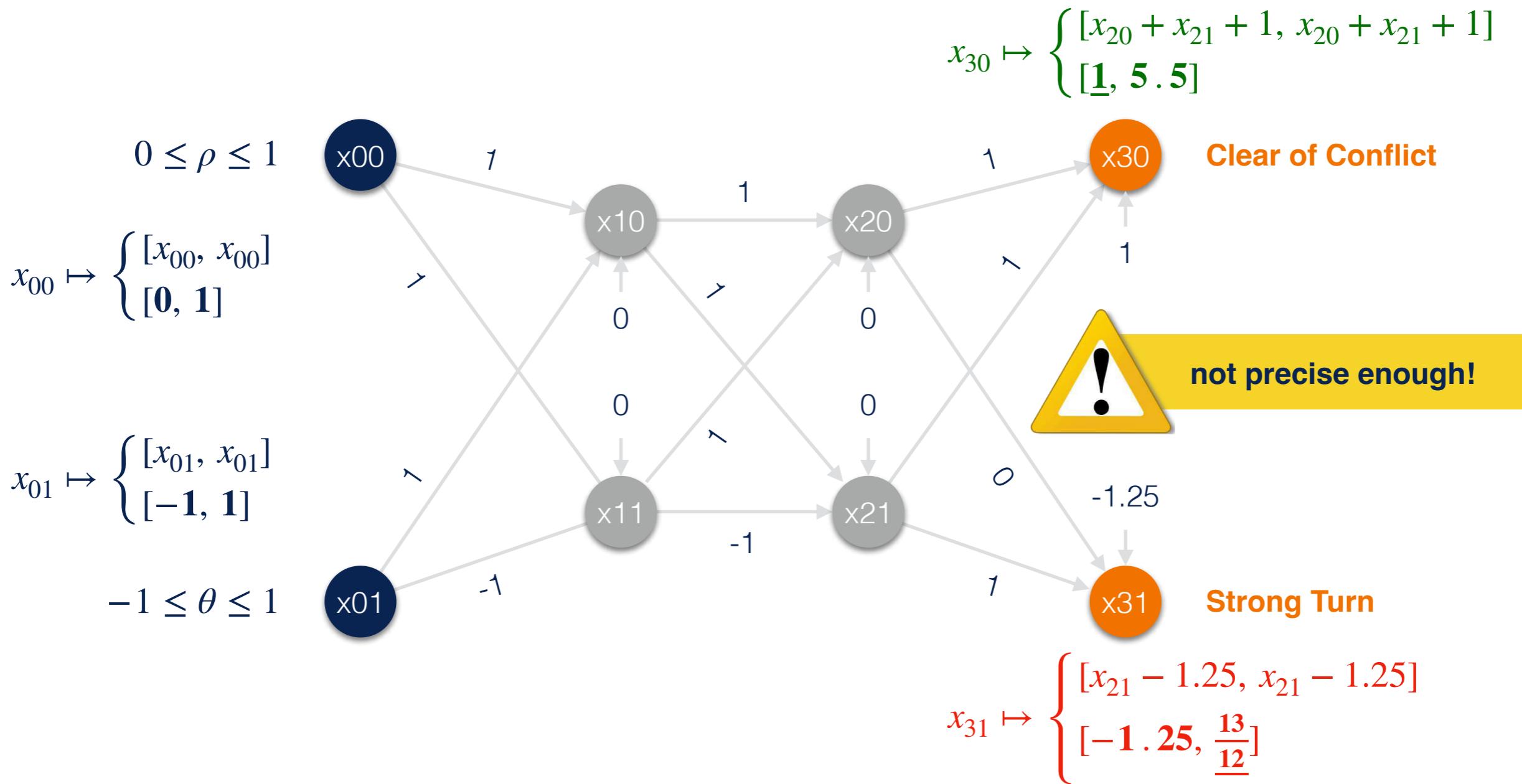
# DeepPoly

[Singh19]



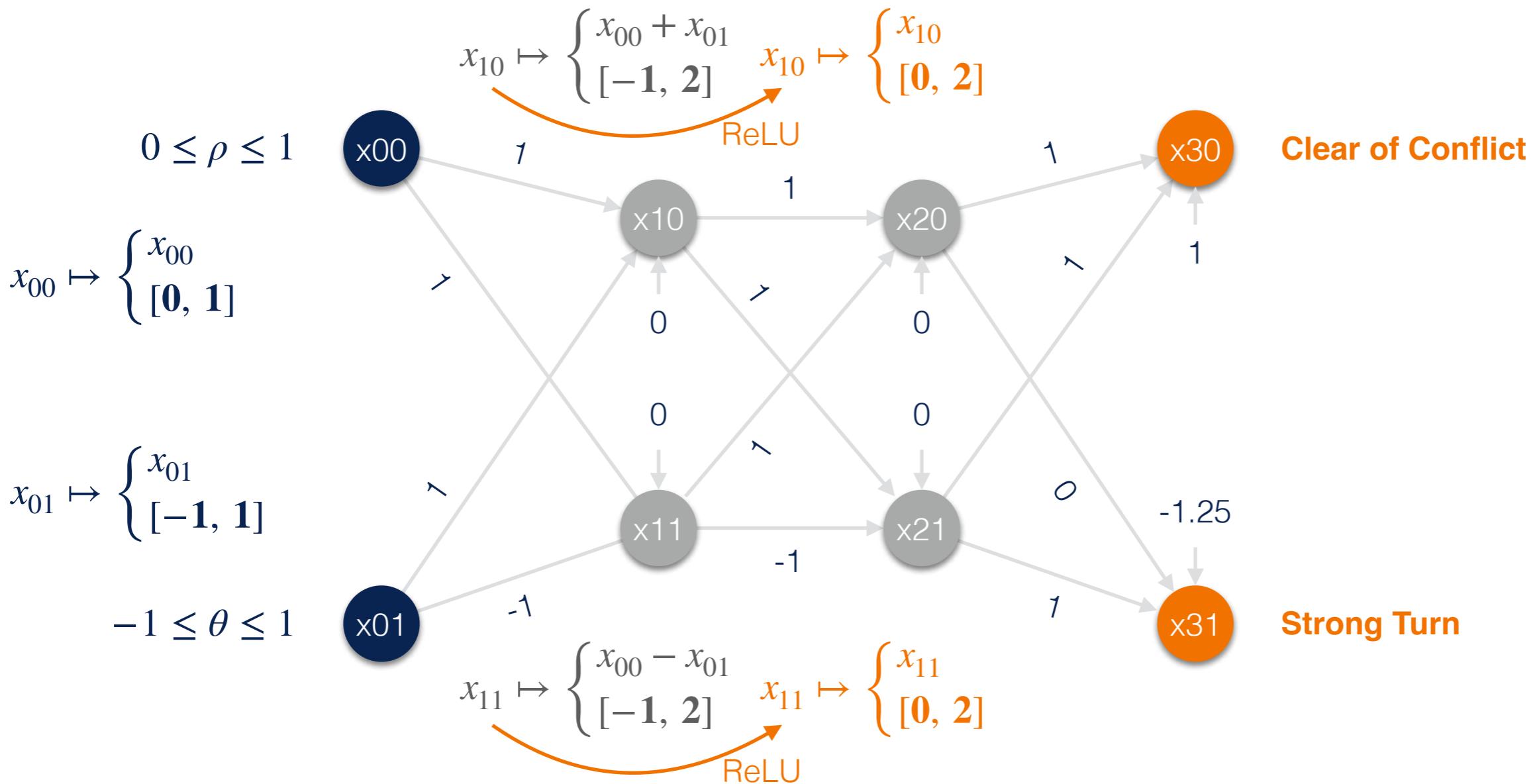
# DeepPoly

[Singh19]



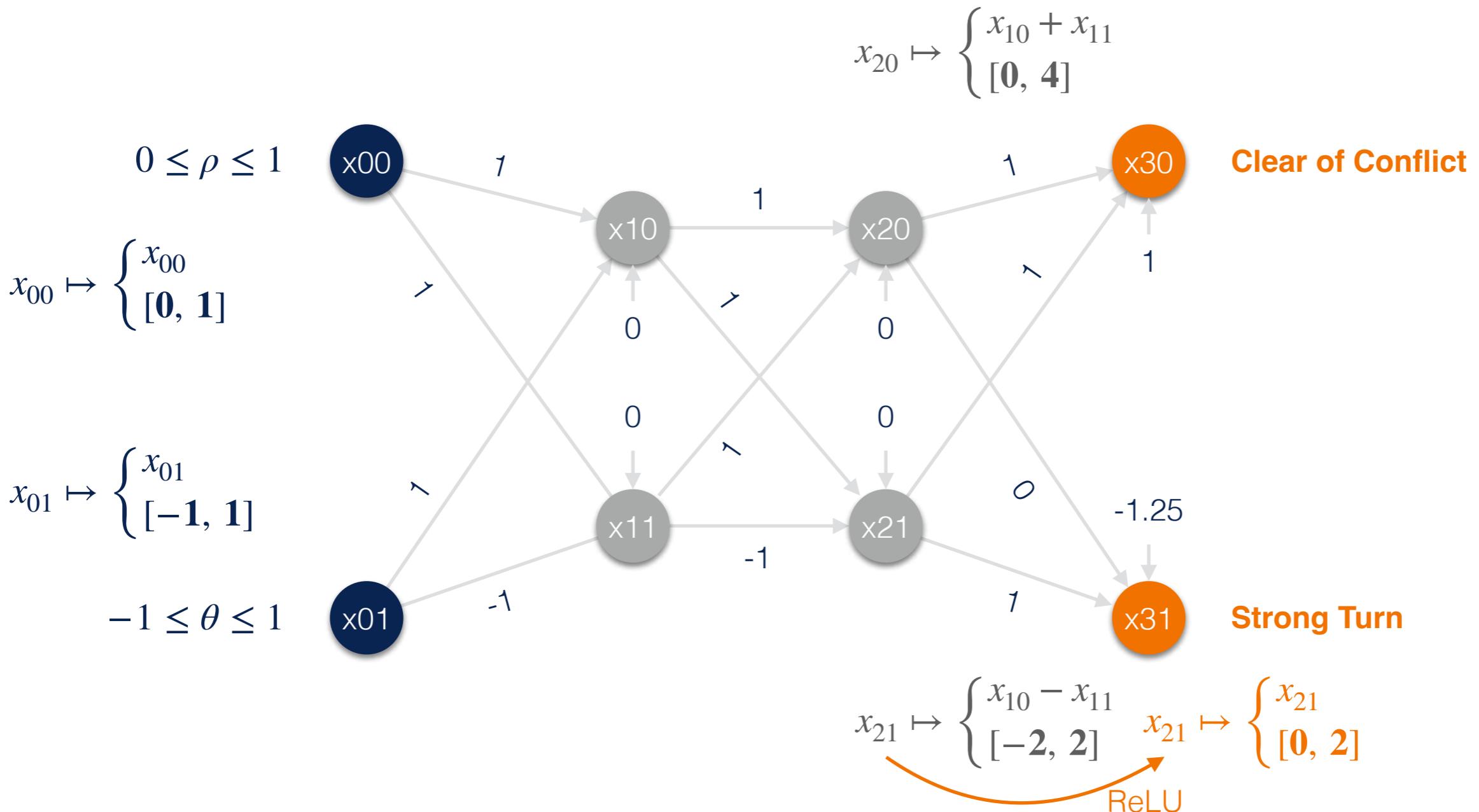
# Interval Abstraction

with Symbolic Constant Propagation [Li19]



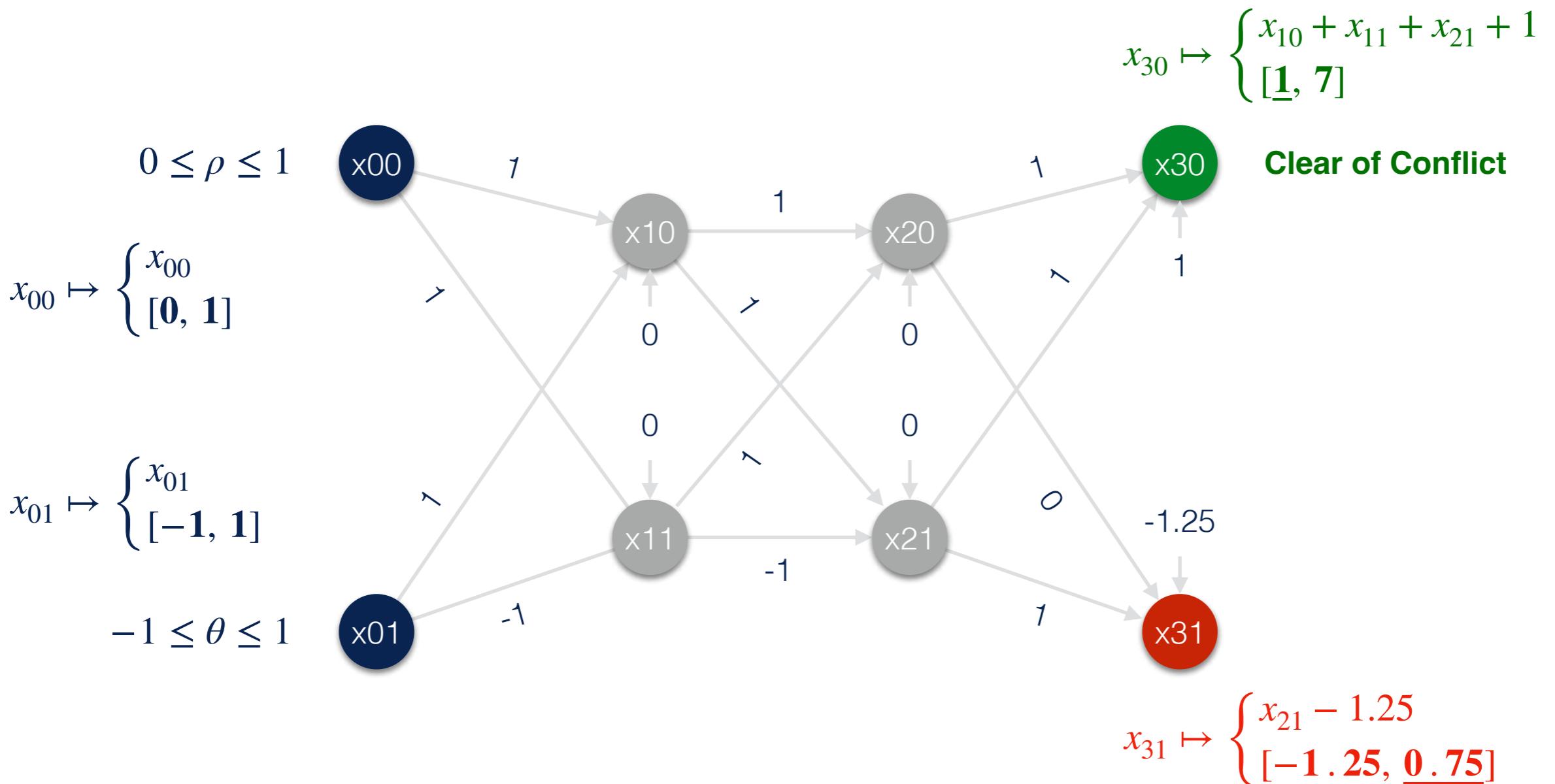
# Interval Abstraction

with Symbolic Constant Propagation [Li19]



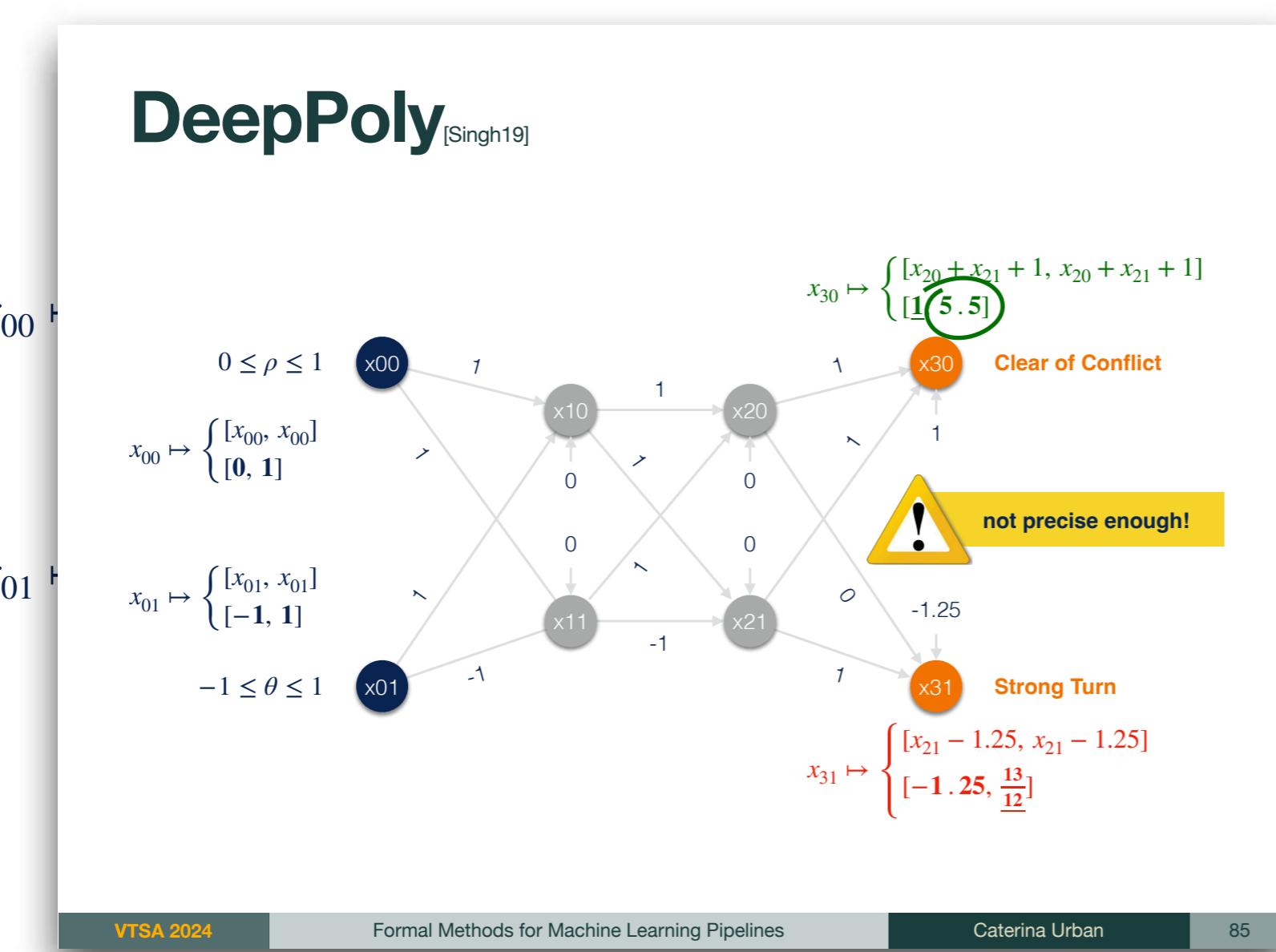
# Interval Abstraction

with **Symbolic Constant Propagation** [Li19]



# Interval Abstraction

with Symbolic Constant Propagation [Li19]



$$x_{30} \mapsto \left\{ \begin{array}{l} x_{10} + x_{11} + x_{21} + 1 \\ [1, 7] \end{array} \right\}$$

**Clear of Conflict**

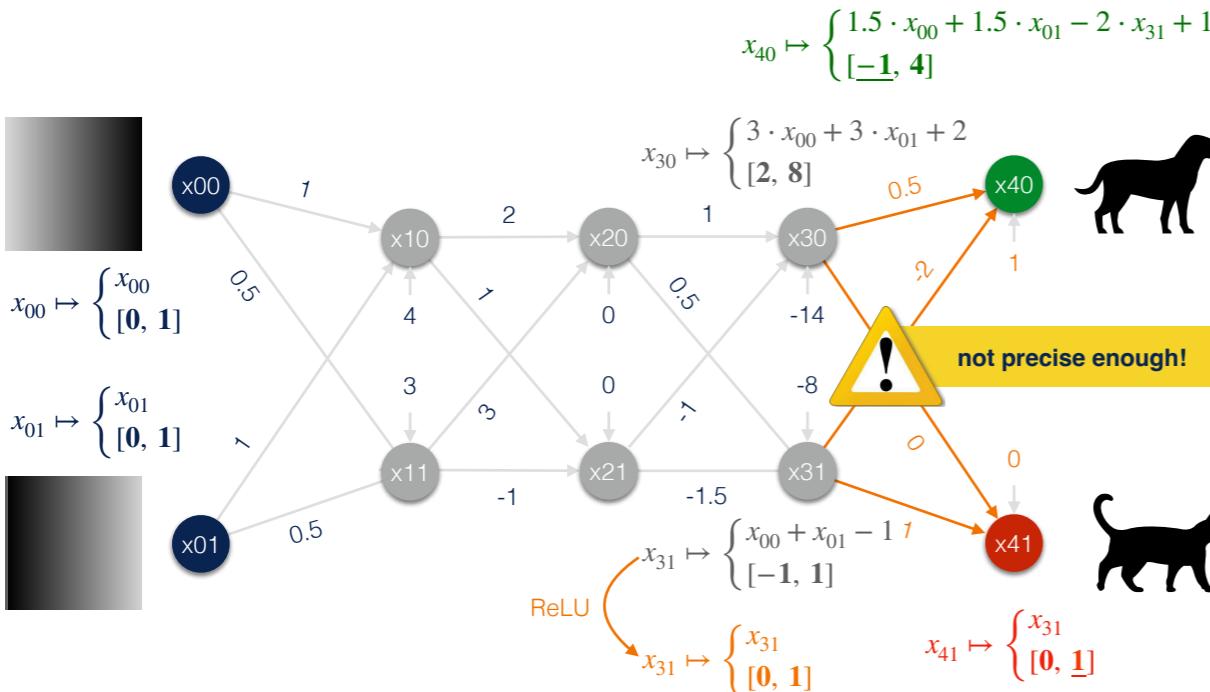
$$x_{31} \mapsto \left\{ \begin{array}{l} x_{21} - 1.25 \\ [-1.25, 0.75] \end{array} \right\}$$

**Strong Turn**

-1.25

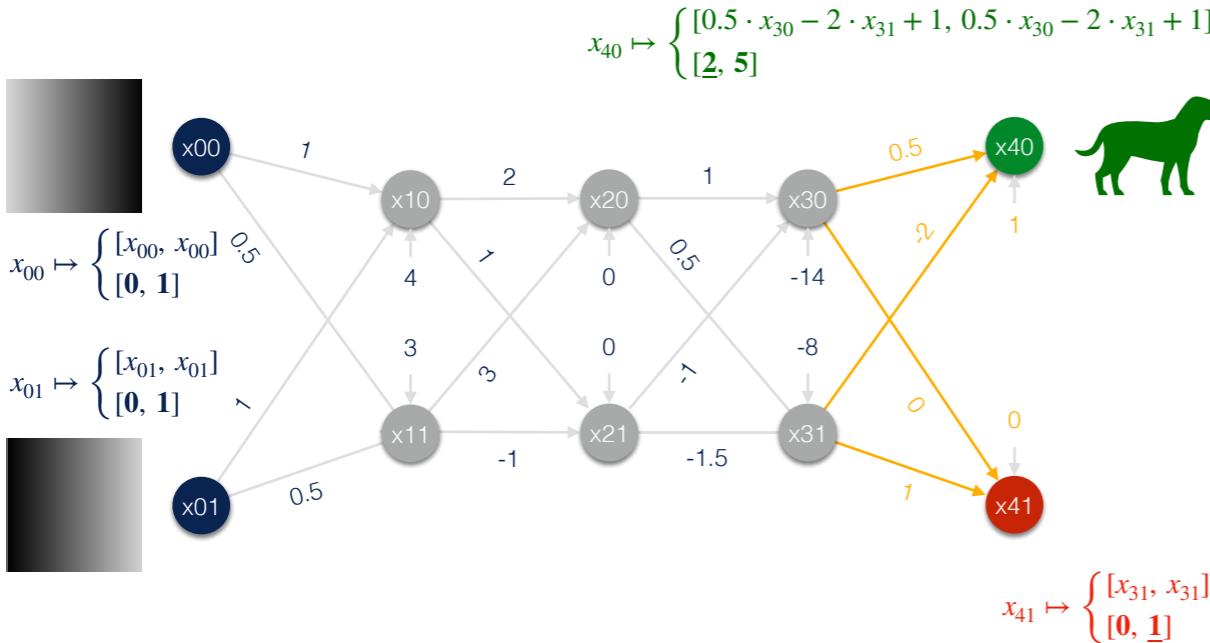
# Interval Abstraction

with Symbolic Constant Propagation [Li19]



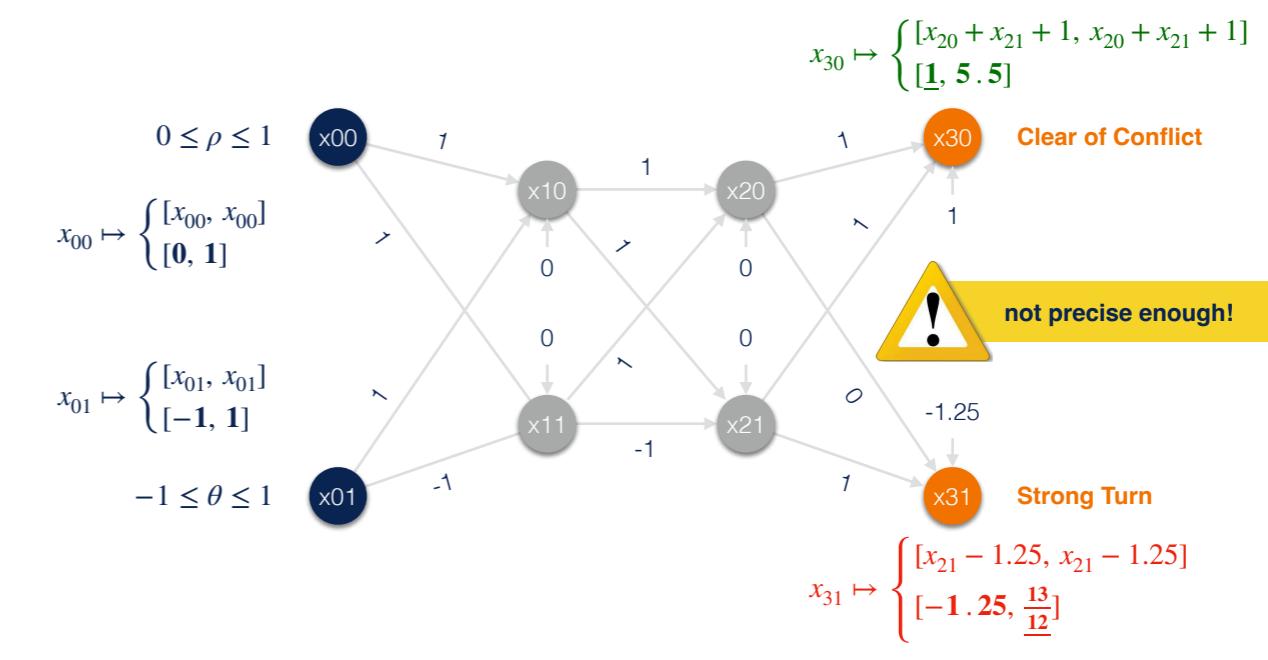
# DeepPoly

[Singh19]



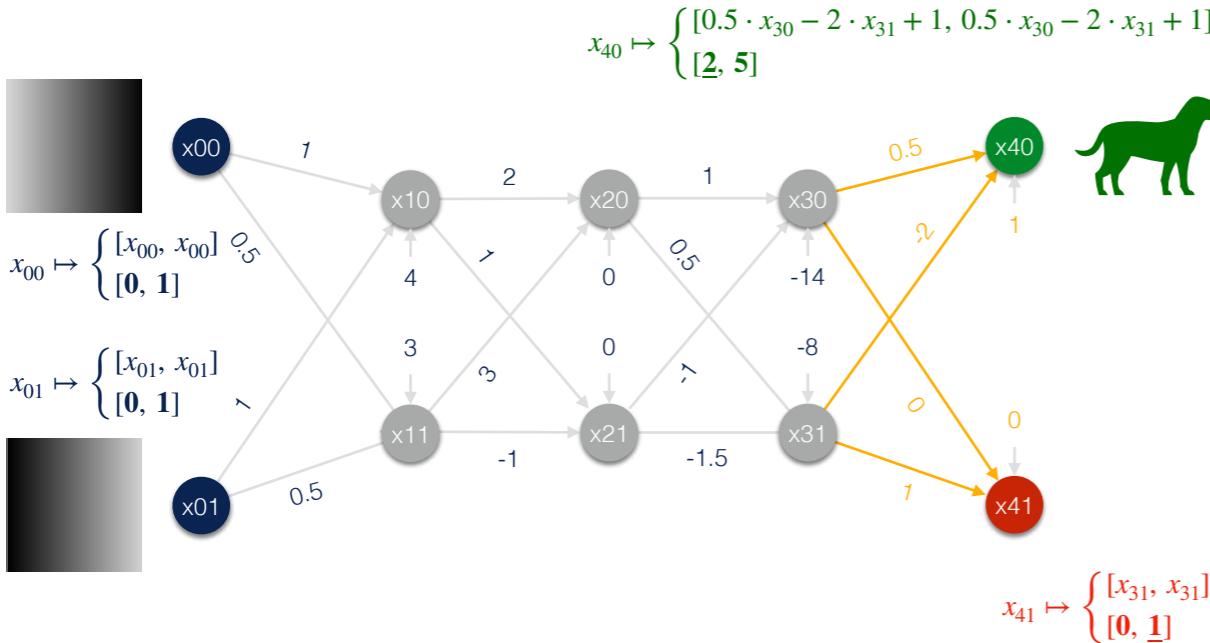
# DeepPoly

[Singh19]



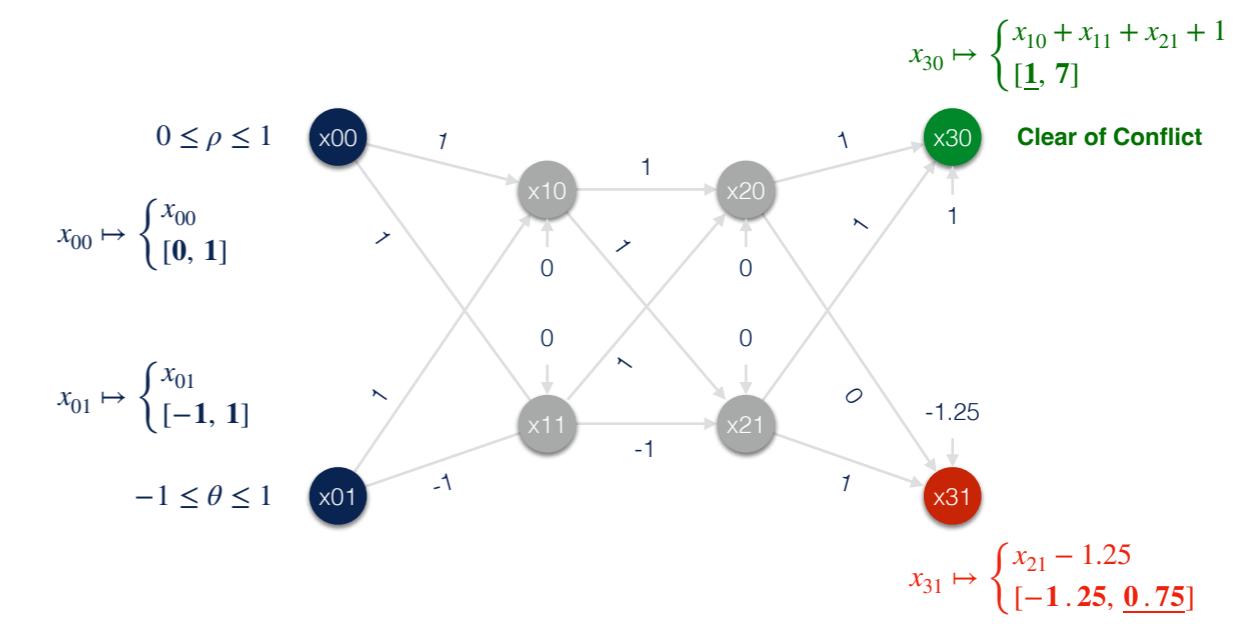
# DeepPoly

[Singh19]



# Interval Abstraction

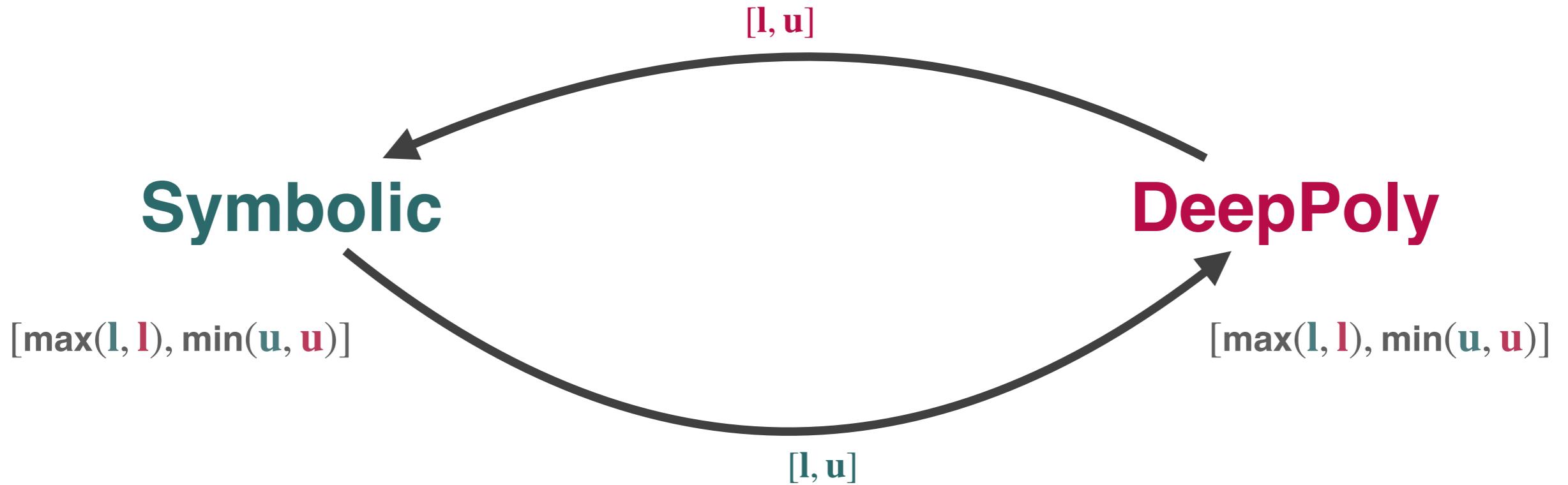
with Symbolic Constant Propagation [Li19]



# Product Domain

[Mazzucato21]

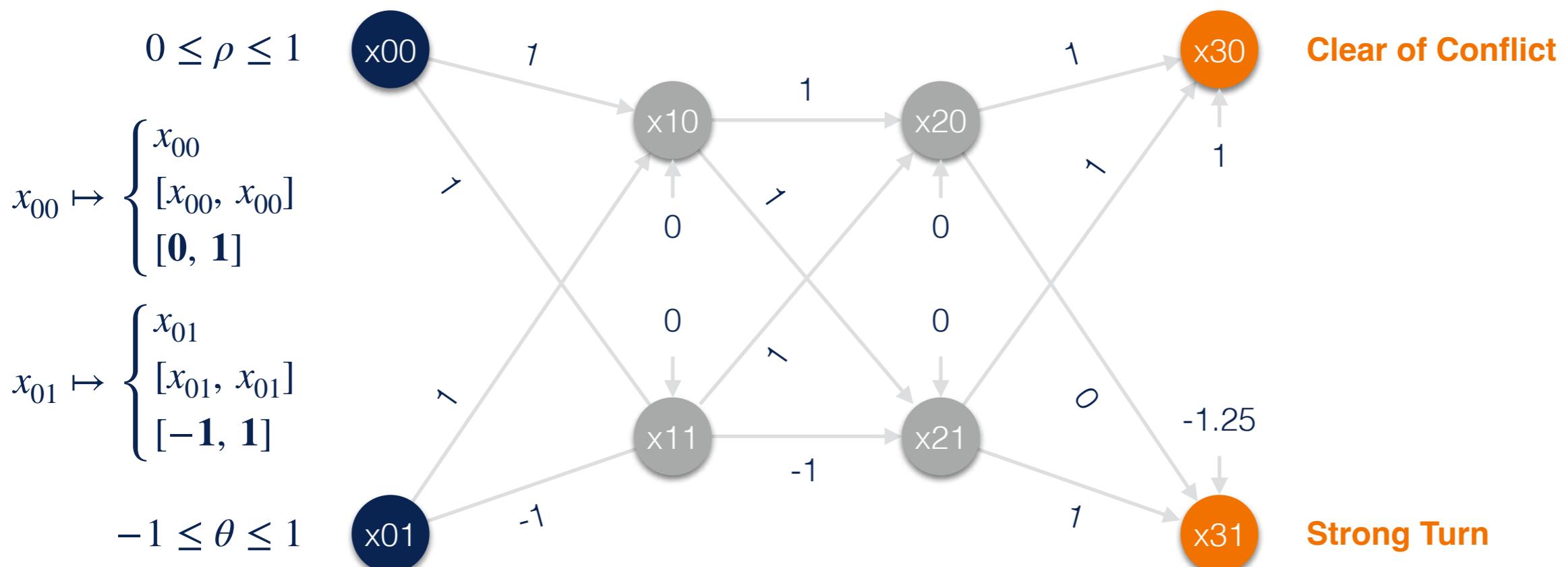
## DeepPoly with Symbolic Constant Propagation



# Product Domain

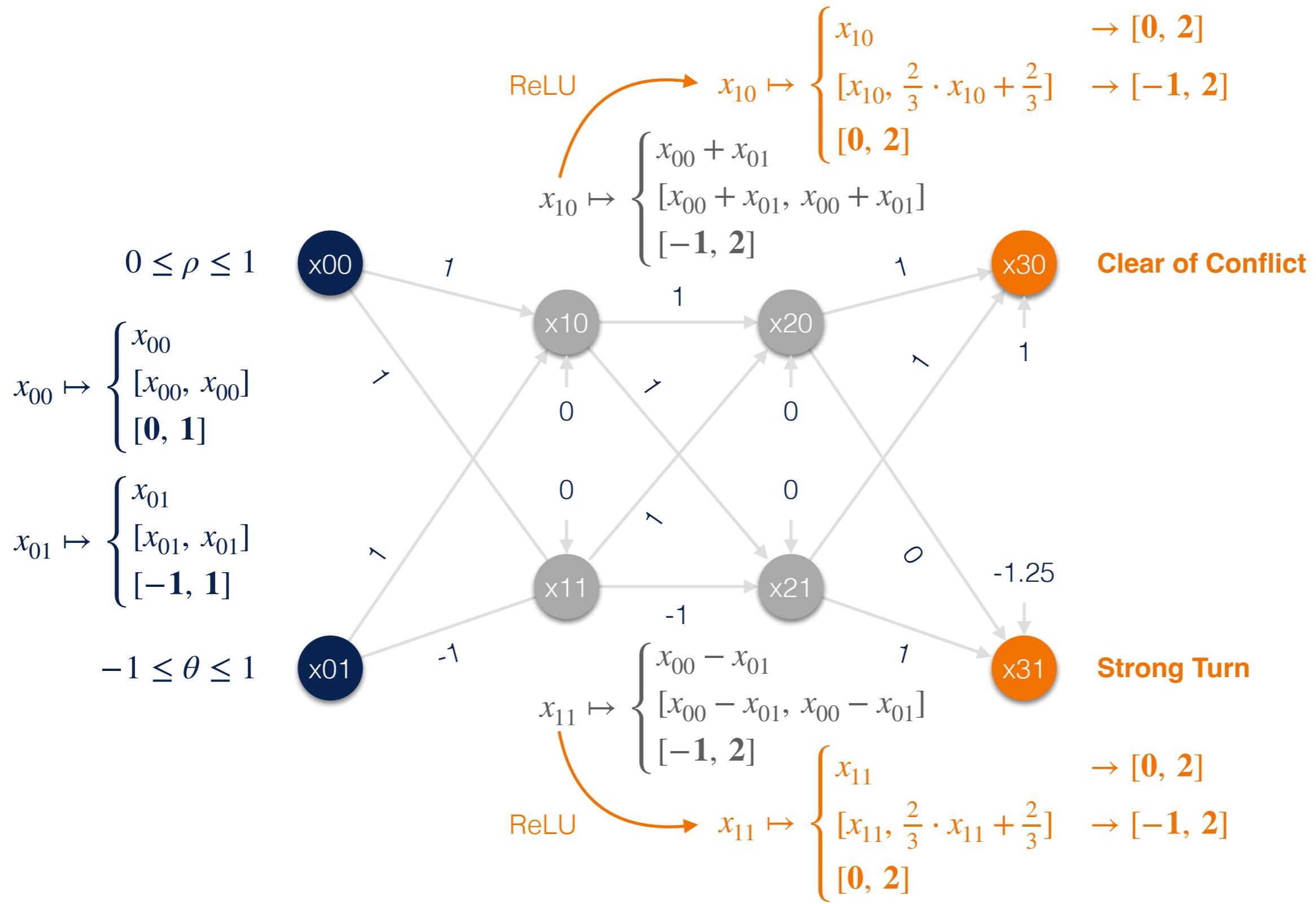
[Mazzucato21]

## DeepPoly with Symbolic Constant Propagation



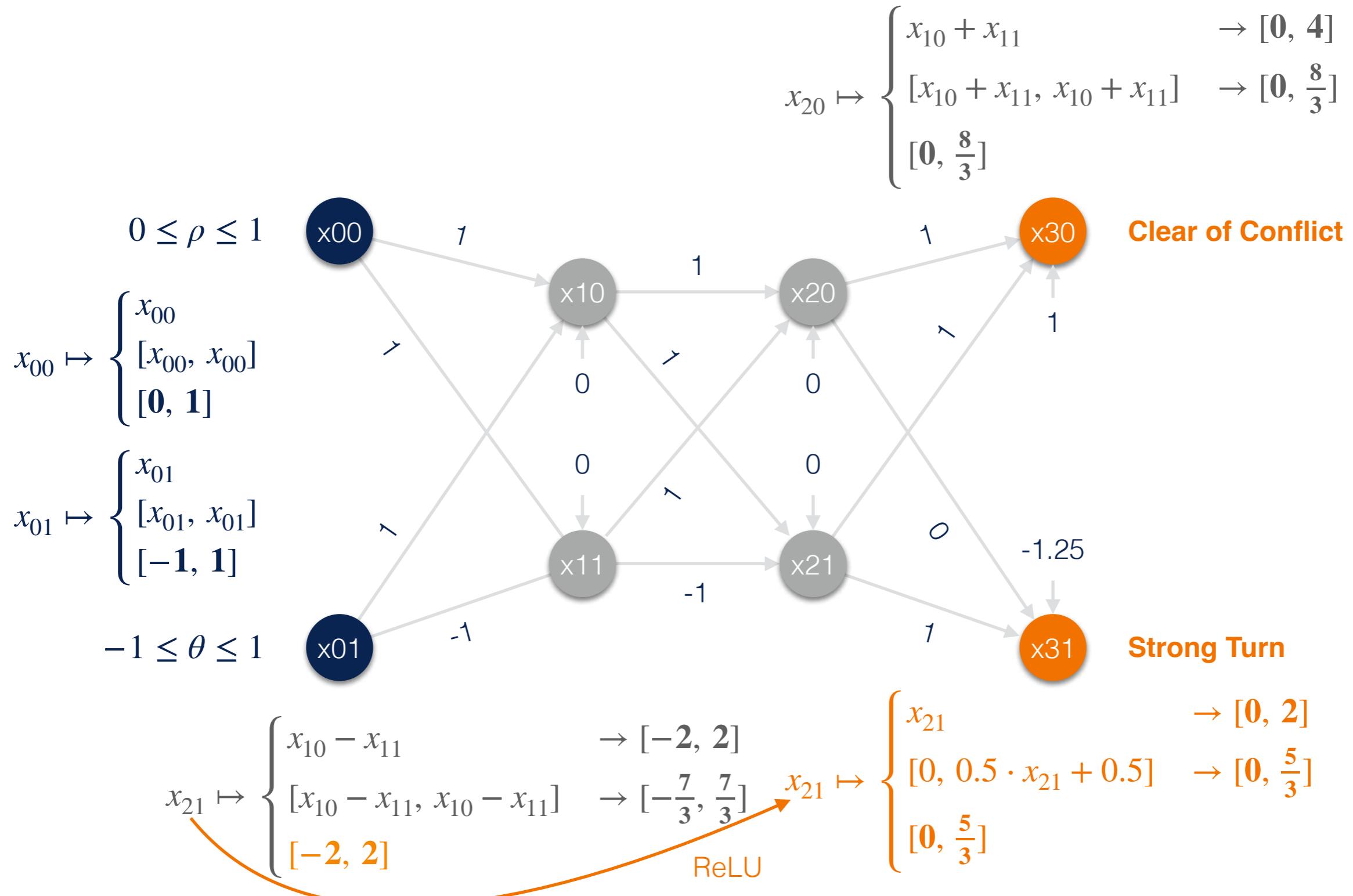
# Product Domain

[Mazzucato21]



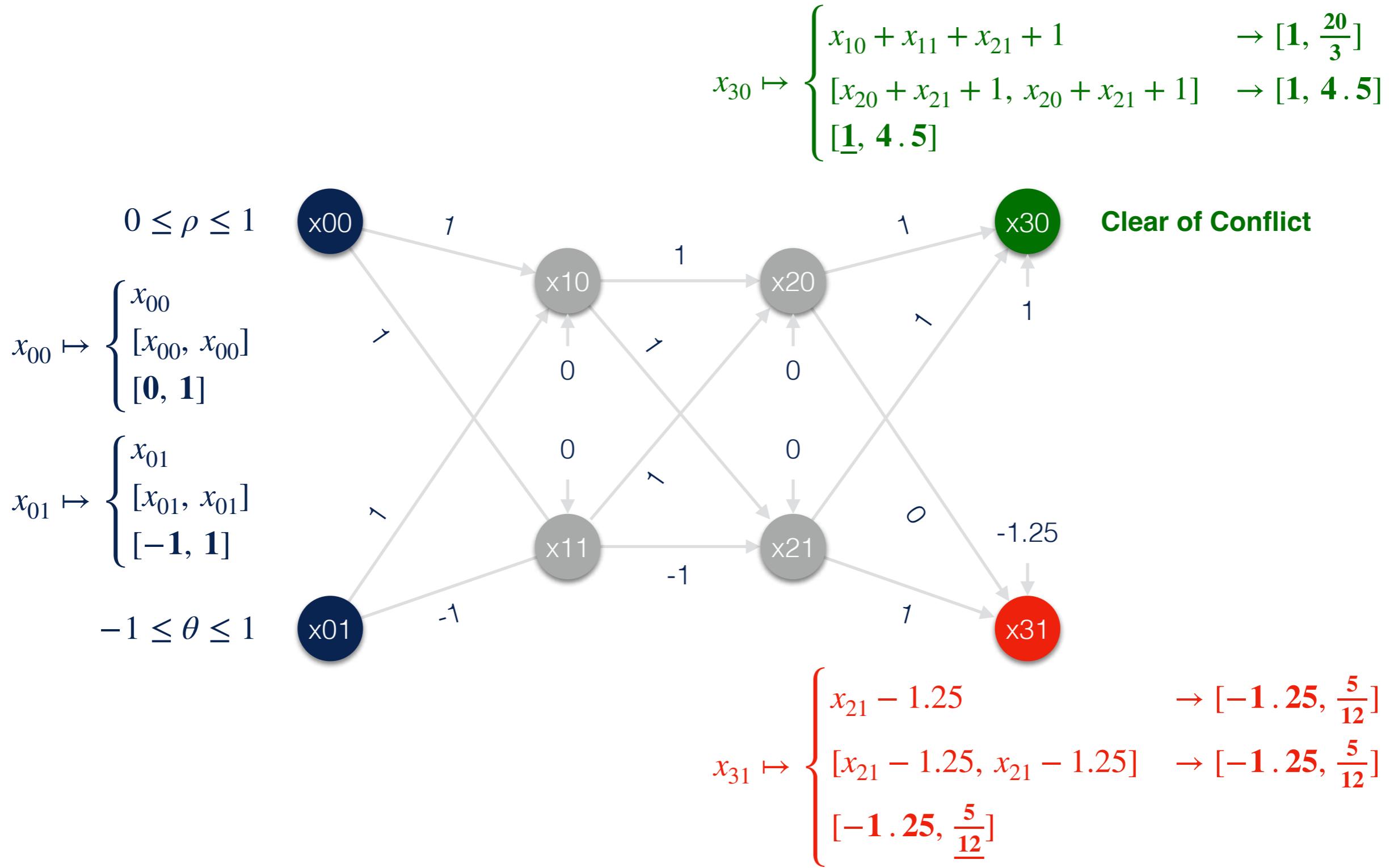
# Product Domain

[Mazzucato21]



# Product Domain

[Mazzucato21]



# Other Complete Methods

# Star Sets



use union of  
efficient representations  
of bounded convex polyhedra

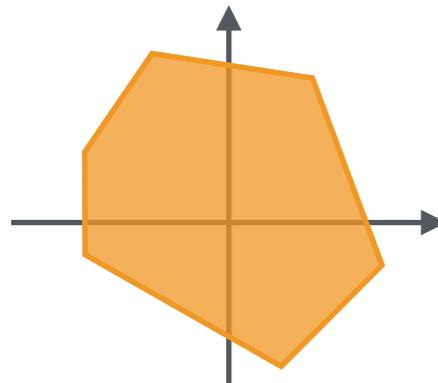
## Exact Static Analysis Method

$$\Theta \stackrel{\text{def}}{=} \langle c, V, P \rangle$$

$c \in \mathcal{R}^n$ : center

$V = \{v_1, \dots, v_m\}$ : basis vectors in  $\mathcal{R}^n$

$P: \mathcal{R}^m \rightarrow \{ \perp, \top \}$ : predicate



$$[\![\Theta]\!] = \{x \mid x = c + \sum_{i=1}^m \alpha_i v_i \text{ such that } P(\alpha_1, \dots, \alpha_m) = \top\}$$

- fast and cheap **affine mapping operations** → neural network layers
- inexpensive **intersections with half-spaces** → ReLU activations

# Star Sets

## Exact Static Analysis Method



Follow-up Work

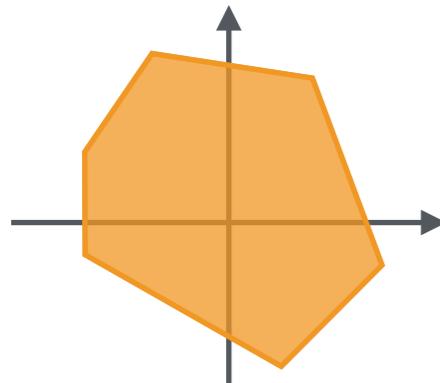
H.-D. Tran et al. -  
Verification of Deep  
Convolutional Neural  
Networks Using  
ImageStars (CAV 2020)

$$\Theta \stackrel{\text{def}}{=} \langle c, V, P \rangle$$

$c \in \mathcal{R}^n$ : center

$V = \{v_1, \dots, v_m\}$ : basis vectors in  $\mathcal{R}^n$

$P: \mathcal{R}^m \rightarrow \{ \perp, \top \}$ : predicate



$$[\![\Theta]\!] = \{x \mid x = c + \sum_{i=1}^m \alpha_i v_i \text{ such that } P(\alpha_1, \dots, \alpha_m) = \top\}$$

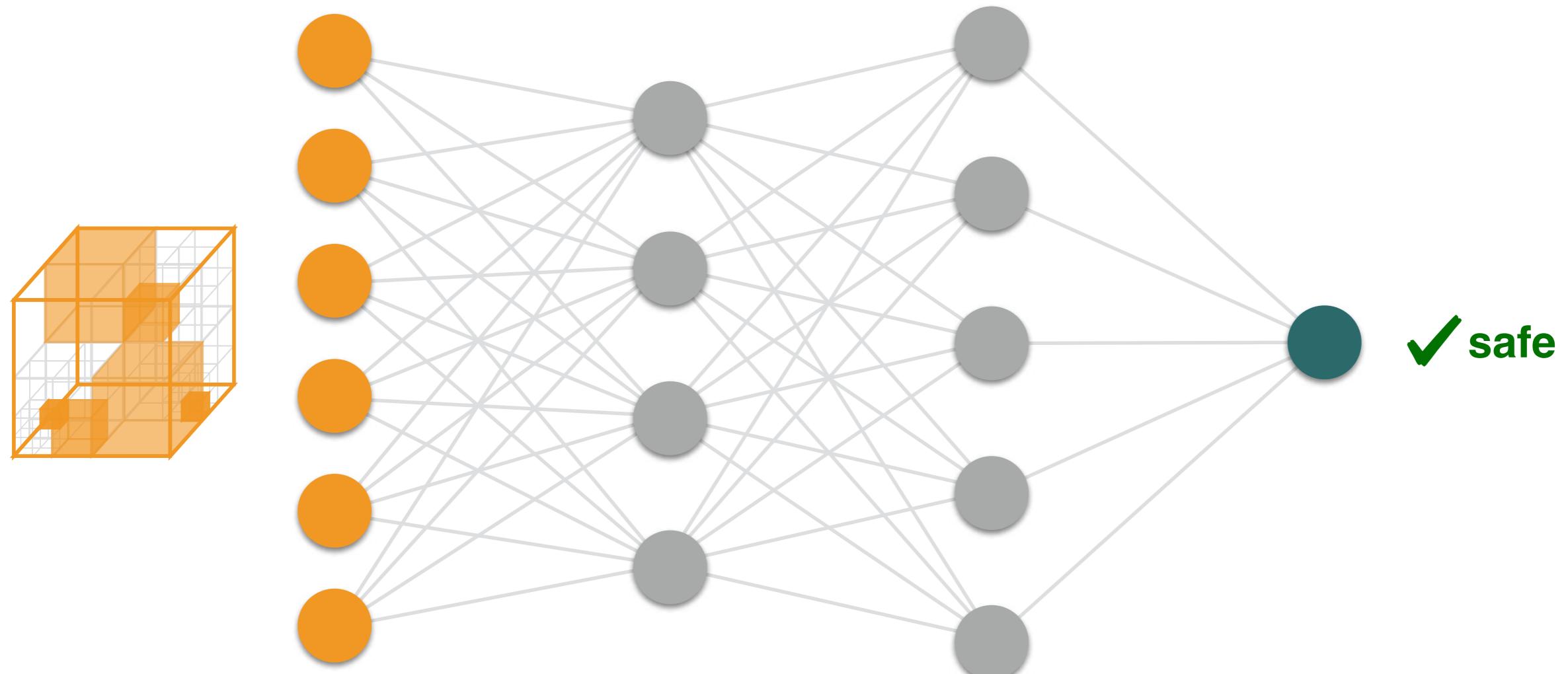
- fast and cheap **affine mapping operations** → neural network layers
- inexpensive **intersections with half-spaces** → ReLU activations

# ReluVal



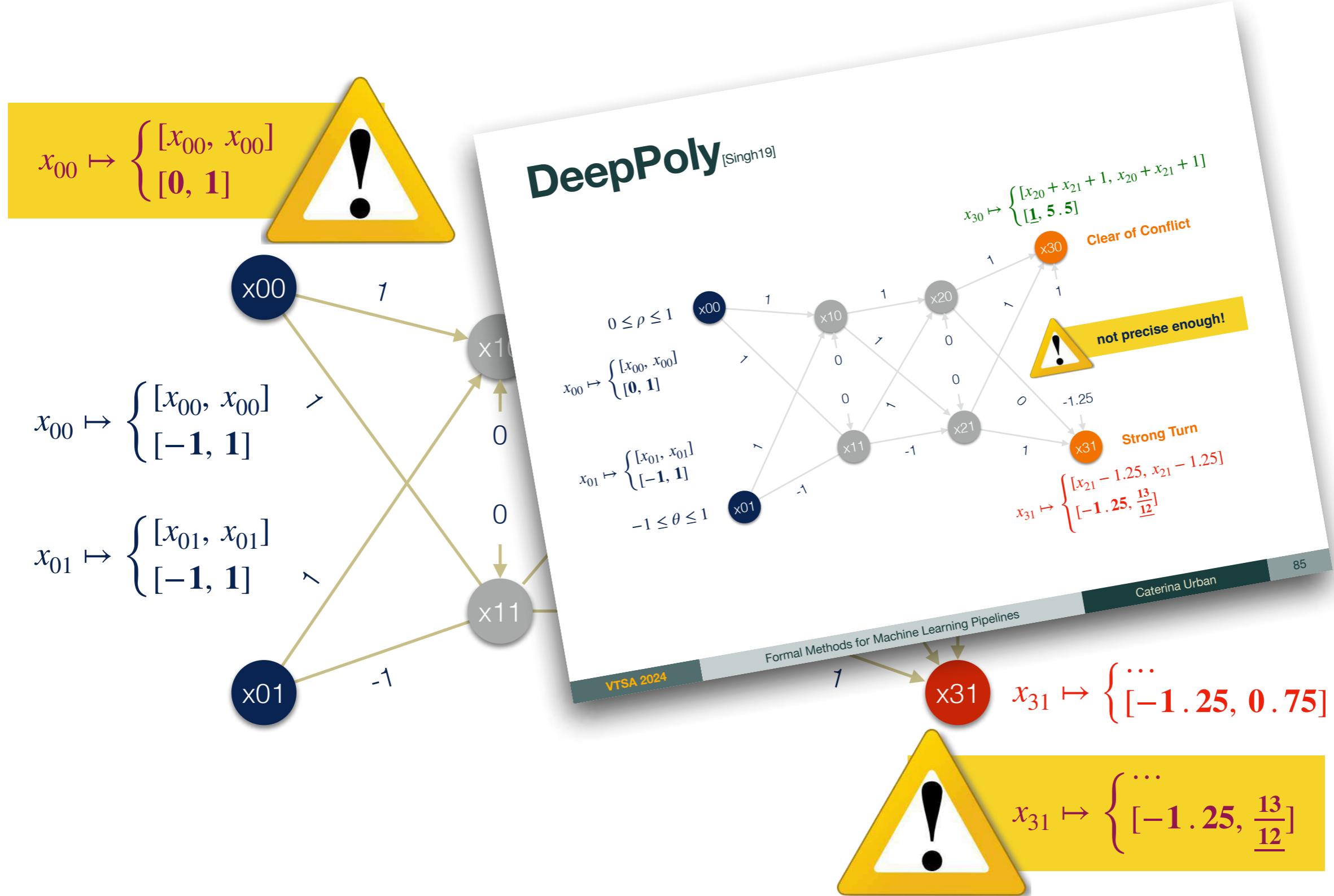
use symbolic propagation  
+ iterative input refinement

## Asymptotically Complete Method



S. Wang et al. - Formal Security Analysis of Neural Networks Using Symbolic Intervals (USENIX Security 2018)

# DeepPoly + Input Refinement





use symbolic propagation +  
convex ReLU approximation +  
iterative input/ReLU refinement

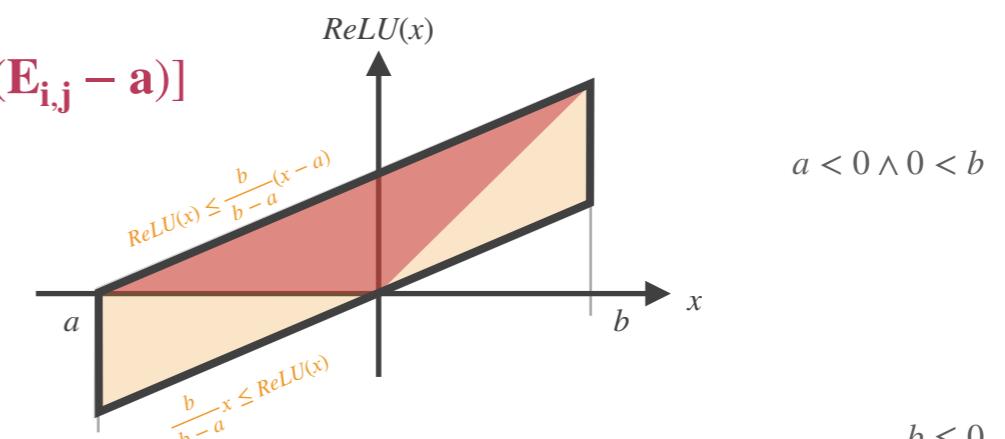
# Neurify

## Asymptotically Complete Method

$$x_{i,j} \mapsto \begin{cases} [\sum_k c_{0,k} \cdot x_{0,k} + c, \sum_k d_{0,k} \cdot x_{0,k} + d] & c_{0,k}, c, d_{0,k}, d \in \mathcal{R} \\ [a, b] & a, b \in \mathcal{R} \end{cases}$$

$$x_{i,j} \mapsto \begin{cases} [\mathbf{E}_{i,j}, \mathbf{E}_{i,j}] \\ [a, b] \end{cases}$$

$$x_{i,j} \mapsto \begin{cases} [\mathbf{0}, \mathbf{0}] \\ [0, 0] \end{cases}$$



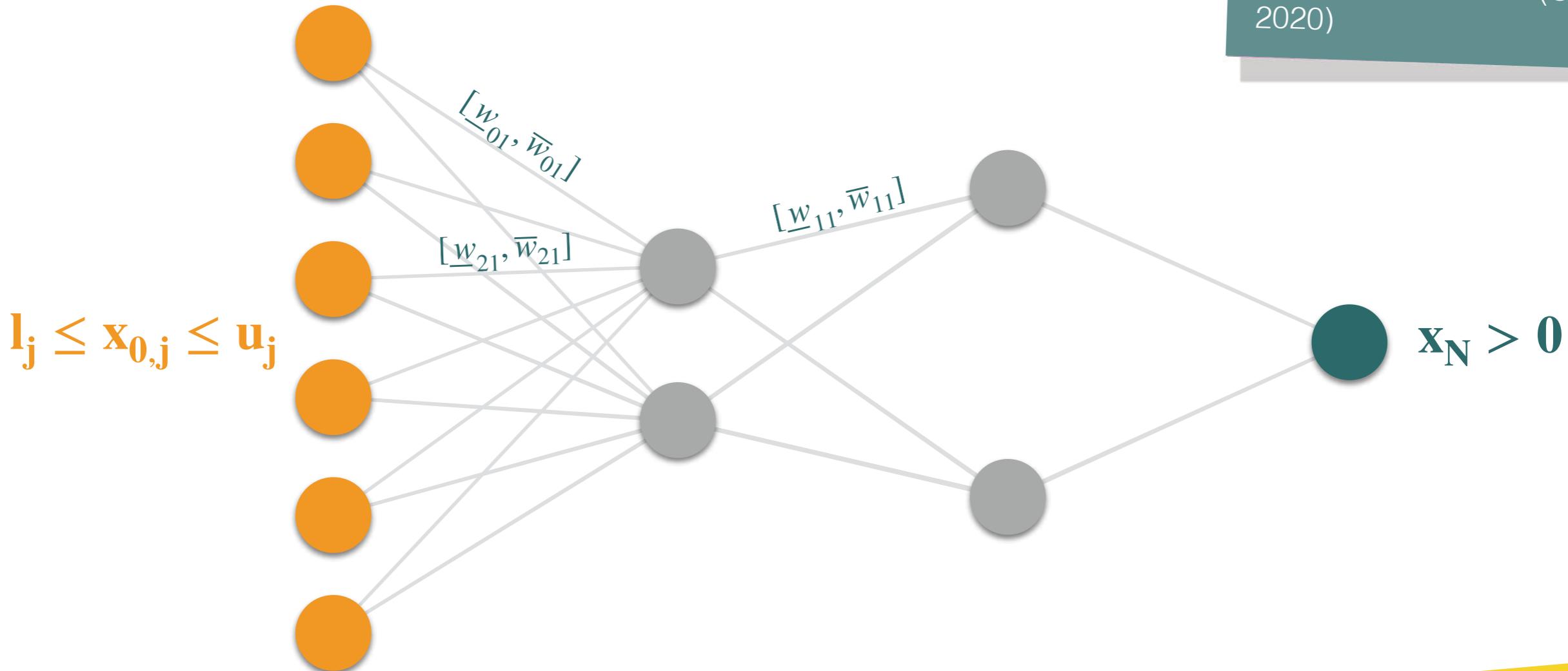
# Further Complete Methods

- **W. Ruan, X. Huang, and M. Kwiatkowska.** *Reachability Analysis of Deep Neural Networks with Provable Guarantees.* In IJCAI, 2018.  
a **global optimization-based approach** for verifying **Lipschitz continuous neural networks**
- **G. Singh, T. Gehr, M. Püschel, and M. Vechev.** *Boosting Robustness Certification of Neural Networks.* In ICLR, 2019.  
an approach combining **abstract interpretation** and **(mixed integer) linear programming**

# Other Incomplete Methods

# Interval Neural Networks

## Abstraction-Based Method



P. Prabhakar and Z. R. Afza - Abstraction based Output Range Analysis for Neural Networks (NeurIPS 2019)

## Related Work

Y. Y. Elboher et al. - An Abstraction-Based Framework for Neural Network Verification (CAV 2020)

# Further Incomplete Methods

- **W. Xiang, H.-D. Tran, and T. T. Johnson.** *Output Reachable Set Estimation and Verification for Multi-Layer Neural Networks.* 2018.  
**an approach combining simulation and linear programming**
- **K. Dvijotham, R. Stanforth, S. Gowal, T. Mann, and P. Kohli.** *A Dual Approach to Scalable Verification of Deep Networks.* In UAI, 2018.  
**an approach based on duality for verifying neural networks**

# Further Incomplete Methods

- **E. Wong and Z. Kolter.** *Provable Defenses Against Adversarial Examples via the Convex Outer Adversarial Polytope.* In ICML, 2018.  
**A. Raghunathan, J. Steinhardt, and P. Liang.** *Certified Defenses against Adversarial Examples.* In ICML, 2018.  
**T.-W. Weng, H. Zhang, H. Chen, Z. Song, C.-J. Hsieh, L. Daniel, D. Boning, and I. Dhillon.** *Towards Fast Computation of Certified Robustness for ReLU Networks.* In ICML, 2018.  
**H. Zhang, T.-W. Weng, P.-Y. Chen, C.-J. Hsieh, and L. Daniel.** *Efficient Neural Network Robustness Certification with General Activation Functions.* In NeurIPS, 2018.  
approaches for finding a **lower bound on robustness** to **adversarial perturbations**

# Further Incomplete Methods

- **A. Boopathy, T.-W. Weng, P.-Y. Chen, S. Liu, and L. Daniel.** *CNN-Cert: An Efficient Framework for Certifying Robustness of Convolutional Neural Networks*. In AAAI, 2019.  
approach focusing on **convolutional neural networks**
- **C.-Y. Ko, Z. Lyu, T.-W. Weng, L. Daniel, N. Wong, and D. Lin.** *POPQORN: Quantifying Robustness of Recurrent Neural Networks*. In ICML, 2019.  
**H. Zhang, M. Shinn, A. Gupta, A. Gurfinkel, N. Le, and N. Narodytska.** *Verification of Recurrent Neural Networks for Cognitive Tasks via Reachability Analysis*. In ECAI, 2020.  
approaches focusing on **recurrent neural networks**
- **D. Gopinath, H. Converse, C. S. Pasareanu, and A. Taly.** *Property Inference for Deep Neural Networks*. In ASE, 2019.  
an approach for **inferring safety properties of neural networks**

# Complete Methods

## Advantages

sound and **complete**

suffer from **false positives**

## Disadvantages

soundness not typically guaranteed  
with respect to **floating-point arithmetic**

**able to scale** to large models

**do not scale** to large models

often **limited** to certain  
model **architectures**

sound often also with respect to  
**floating-point arithmetic**

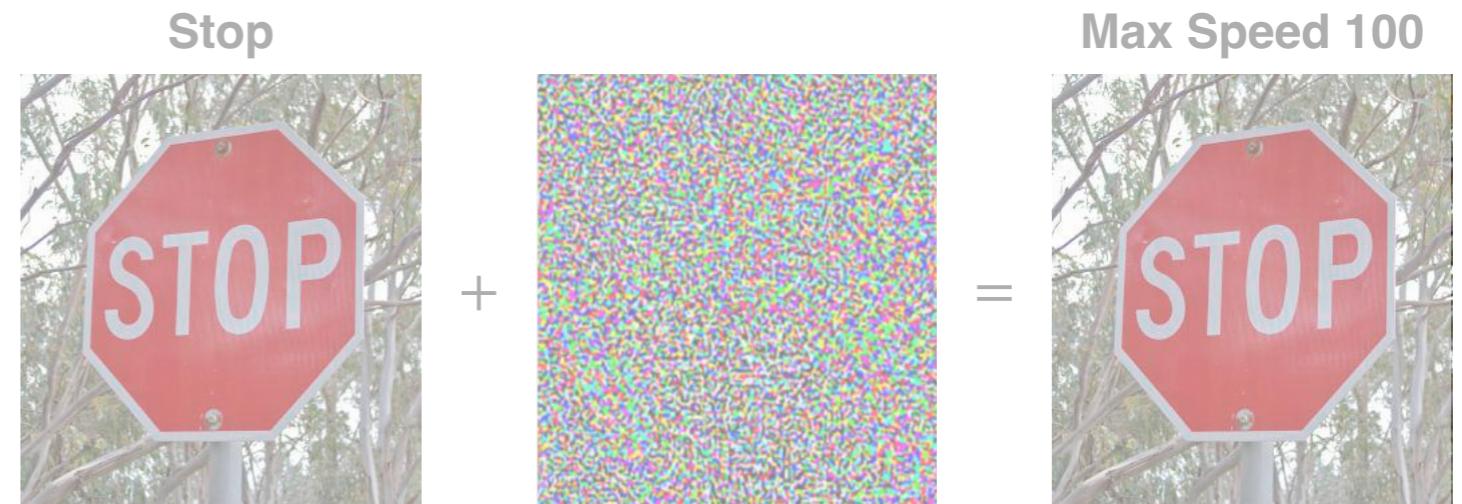
**less limited** to certain  
model **architectures**

## Advantages

# Incomplete Methods

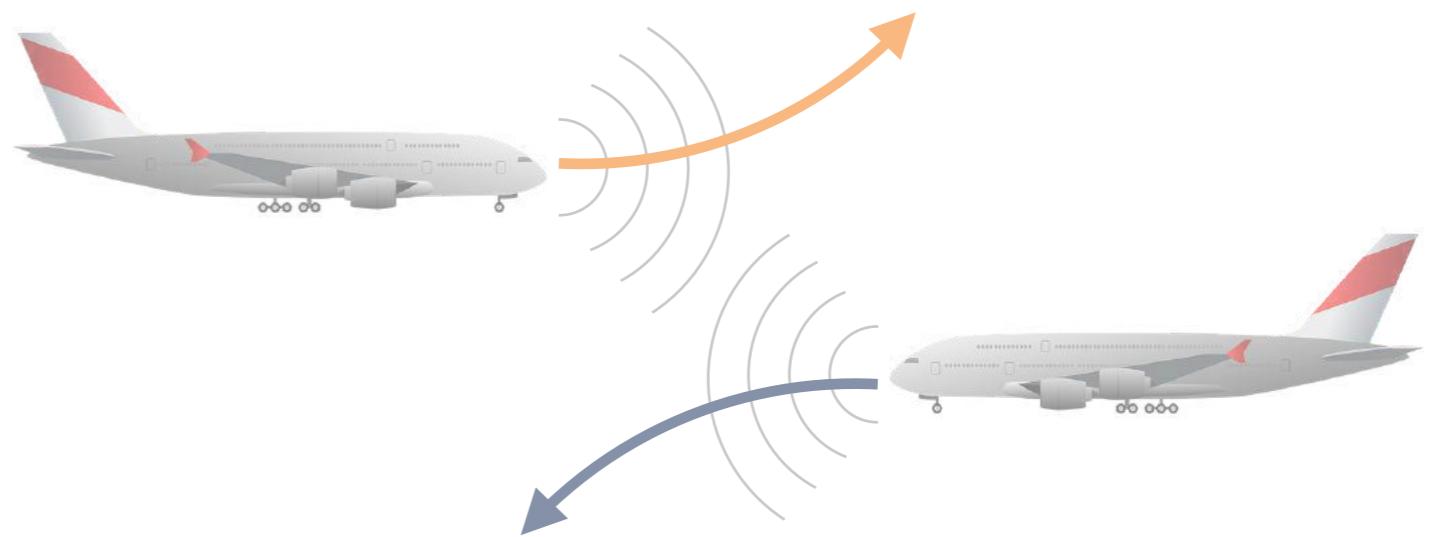
# Stability

Goal G3 in [Kurd03]



# Safety

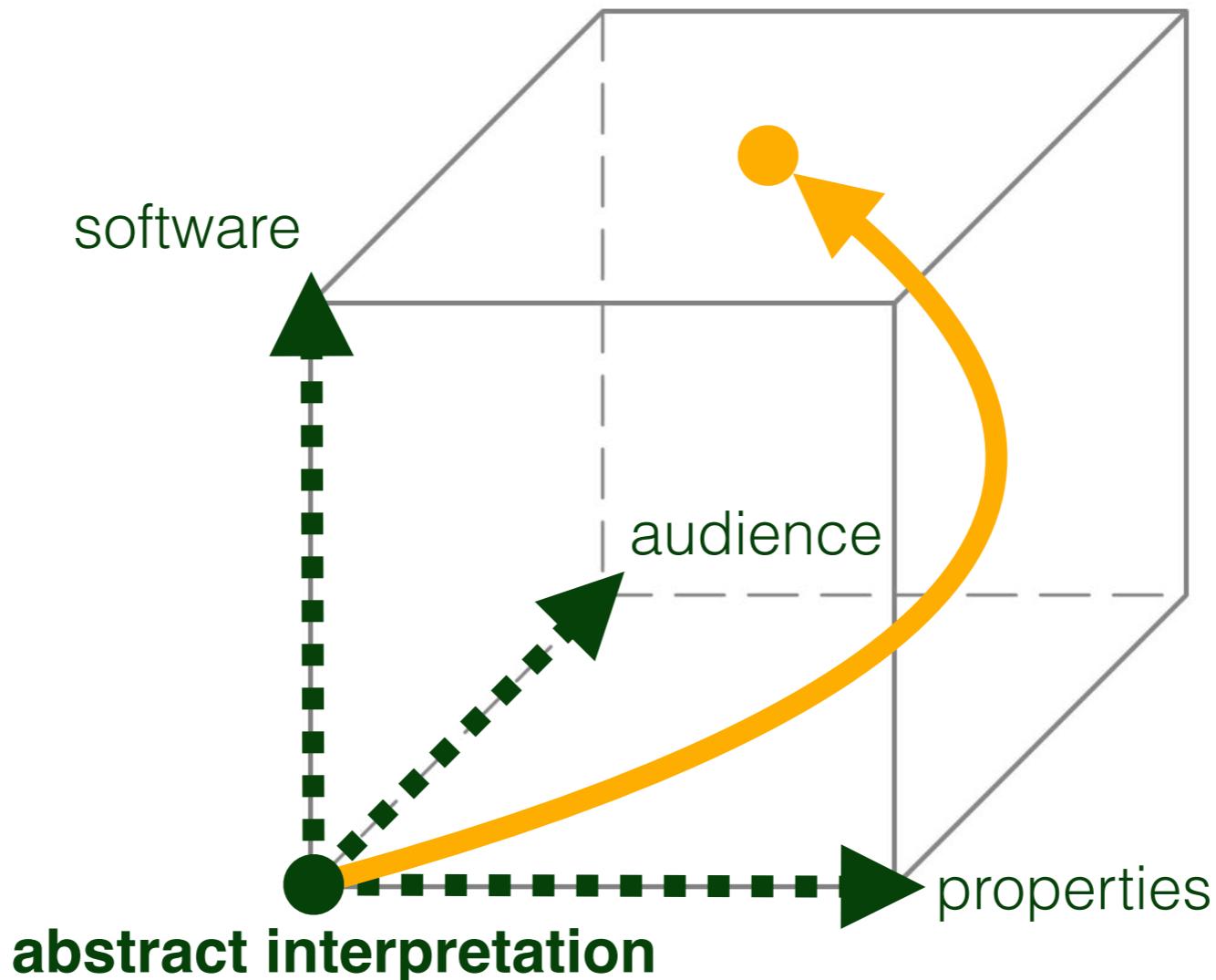
Goal G4 in [Kurd03]



# Fairness



# Fairness Verification



# ML Impacts Our Society

**WIRED**  
*In 2019, predictive algorithms make banks, landlords, and employers*  
**Machine Bias**  
There's software used across the country to predict future criminals. And it's biased against blacks.  
by Julia Angwin, Jeff Larson, Surya Mattu and Lauren Kirchner, ProPublica  
May 23, 2016

**WIRED**  
BUSINESS BUSINESS 03.25.2019 07:00 AM  
**Can AI Be a Fair Judge in Court? Estonia Thinks So**  
Estonia plans to use an artificial intelligence program to handle small-claims cases, part of a push to make government services smarter.

**WIRED**  
BUSINESS BUSINESS OCTOBER 10, 2018 / 5:12 AM / A YEAR AGO  
**Amazon scraps secret AI recruiting tool that showed bias against women**  
Jeffrey Dastin

**DETERMINE WHO GETS APPROVED FOR A HOME**  
MORTGAGE CHECKS ARE BEING MADE AUTOMATICALLY

A large pile of US dollar bills.

A handshake between two people in business suits.

**Translation tutorial:  
21 fairness definitions and their politics**

Arvind Narayanan  
@random\_walker

0:05 / 55:20

Tutorial: 21 fairness definitions and their politics

19,759 views • Mar 1, 2018

196

6

SHARE

SAVE

SUBSCRIBE

Arvind Narayanan  
226 subscribers

Computer scientists and statisticians have devised numerous mathematical criteria to define what it means for a classifier or a model to be fair. The proliferation of these definitions represents an attempt to make technical sense of

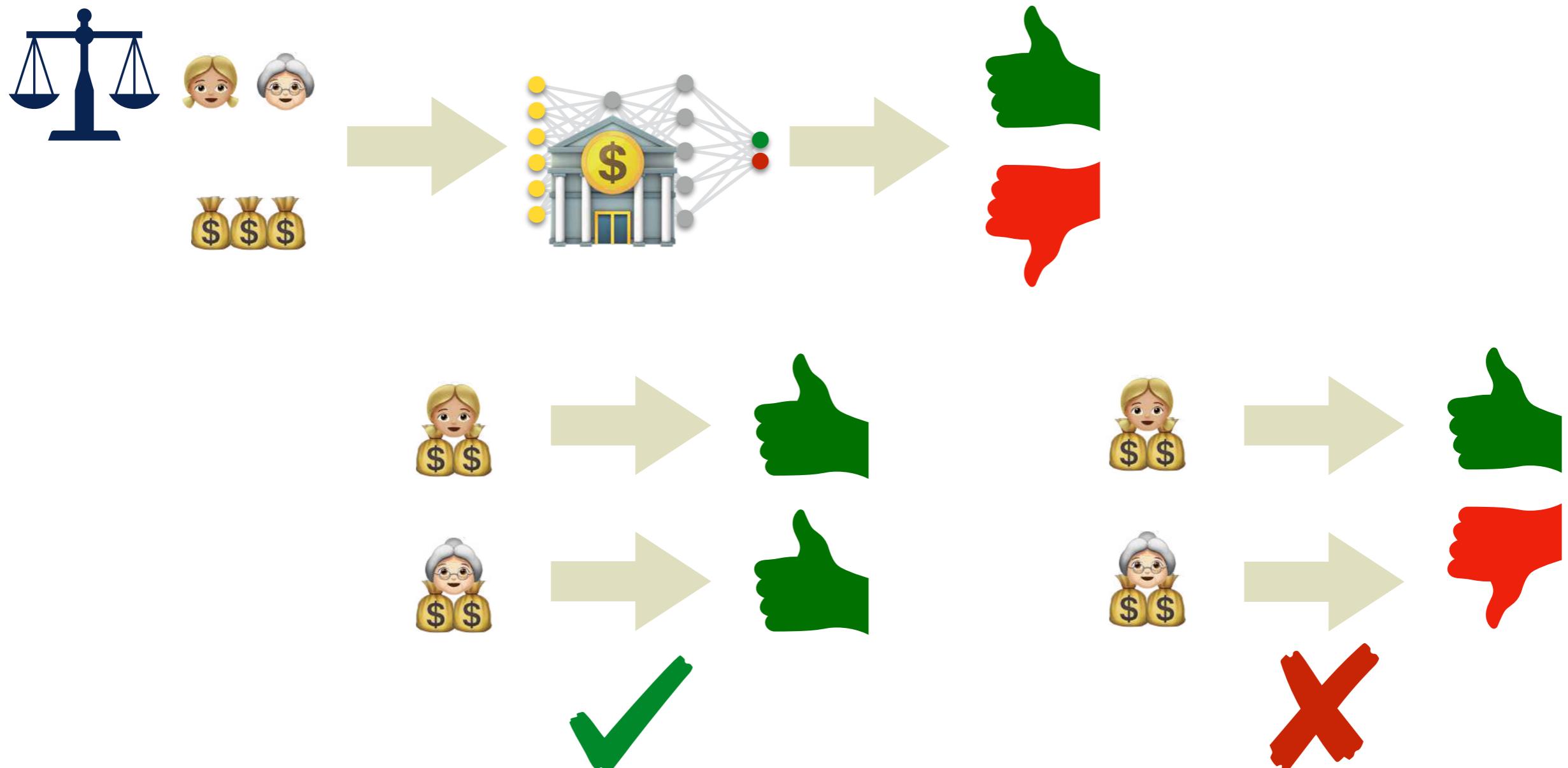
SHOW MORE

The image shows a YouTube video player for a tutorial titled "Translation tutorial: 21 fairness definitions and their politics" by Arvind Narayanan (@random\_walker). The video has 19,759 views and was posted on March 1, 2018. The video duration is 55:20. Below the video player, there is a channel profile for Arvind Narayanan, who has 226 subscribers. A red "SUBSCRIBE" button is visible. The video description below the channel info states: "Computer scientists and statisticians have devised numerous mathematical criteria to define what it means for a classifier or a model to be fair. The proliferation of these definitions represents an attempt to make technical sense of". There is a "SHOW MORE" link at the bottom of this description.

# Dependency Fairness

[Galhotra17]

Prediction is Independent of Sensitive Input Values



# Dependency Fairness

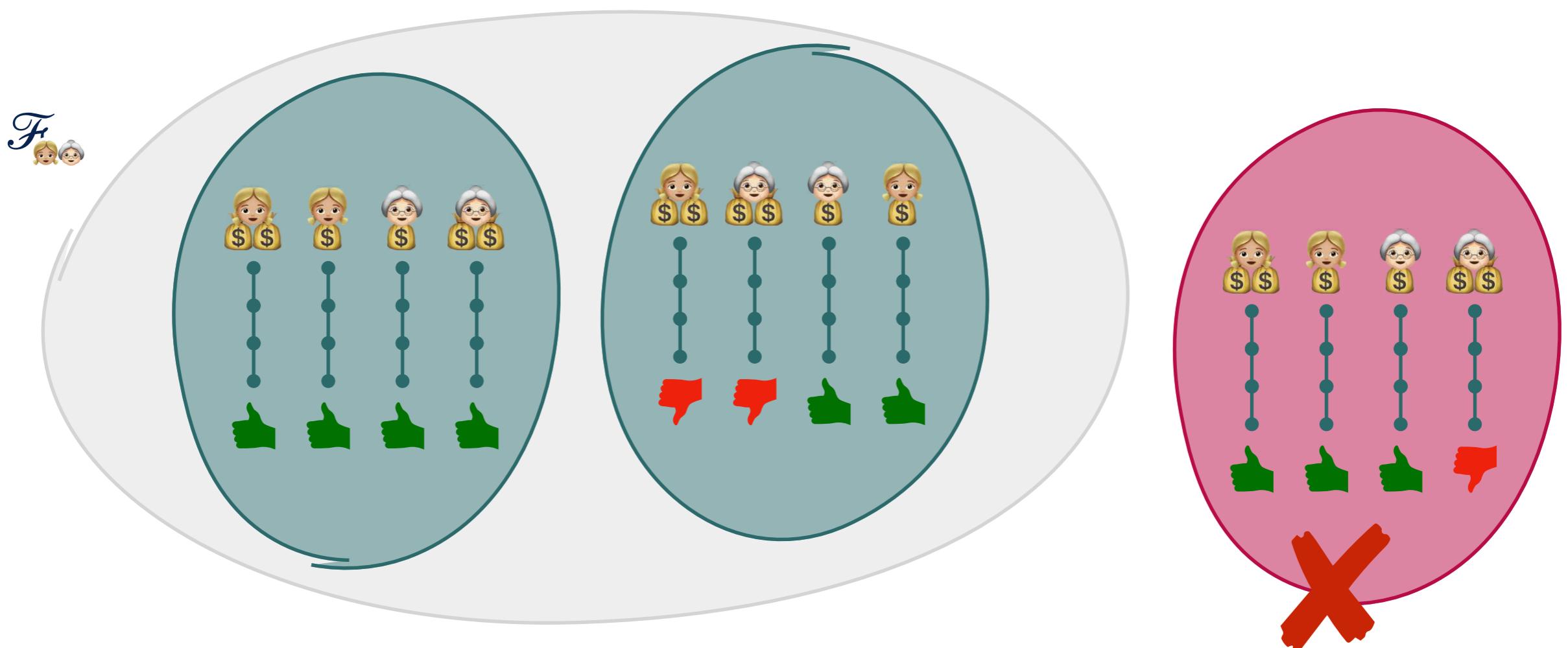
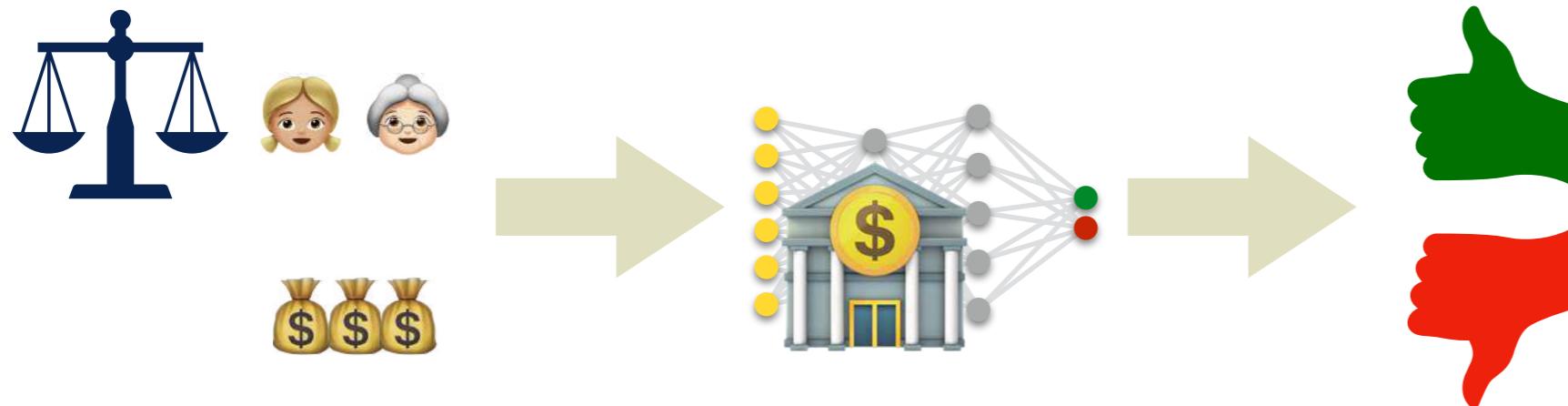
$$\mathcal{F}_i \stackrel{\text{def}}{=} \{[\![M]\!] \mid \text{UNUSED}_i([\![M]\!])\}$$

$\mathcal{F}_i$  is the set of all neural networks M (or, rather, their semantics  $[\![M]\!]$ ) that **do not use** the value of the sensitive input node  $x_{0,i}$  for classification

$$\begin{aligned} \text{UNUSED}_i(T) &\stackrel{\text{def}}{=} \forall t, t' \in T: t_0(x_{0,i}) \neq t'_0(x_{0,i}) \wedge \\ &(\forall 0 \leq j \leq |L_0|: j \neq i \Rightarrow t_0(x_{0,j}) = t'_0(x_{0,j})) \\ &\Rightarrow t_\omega = t'_\omega \end{aligned}$$

Intuitively: inputs differing only on the value of the sensitive input node  $x_{0,i}$  should lead to the same **classification outcome**

# Dependency Fairness



# Dependency Fairness

$$\mathcal{F}_i \stackrel{\text{def}}{=} \{[\![M]\!] \mid \text{UNUSED}_i([\![M]\!])\}$$

$\mathcal{F}_i$  is the set of all neural networks M (or, rather, their semantics  $[\![M]\!]$ ) that **do not use** the value of the sensitive input node  $x_{0,i}$  for classification

$$\begin{aligned} \text{UNUSED}_i(T) &\stackrel{\text{def}}{=} \forall t, t' \in T: t_0(x_{0,i}) \neq t'_0(x_{0,i}) \wedge \\ &(\forall 0 \leq j \leq |L_0|: j \neq i \Rightarrow t_0(x_{0,j}) = t'_0(x_{0,j})) \\ &\Rightarrow t_\omega = t'_\omega \end{aligned}$$

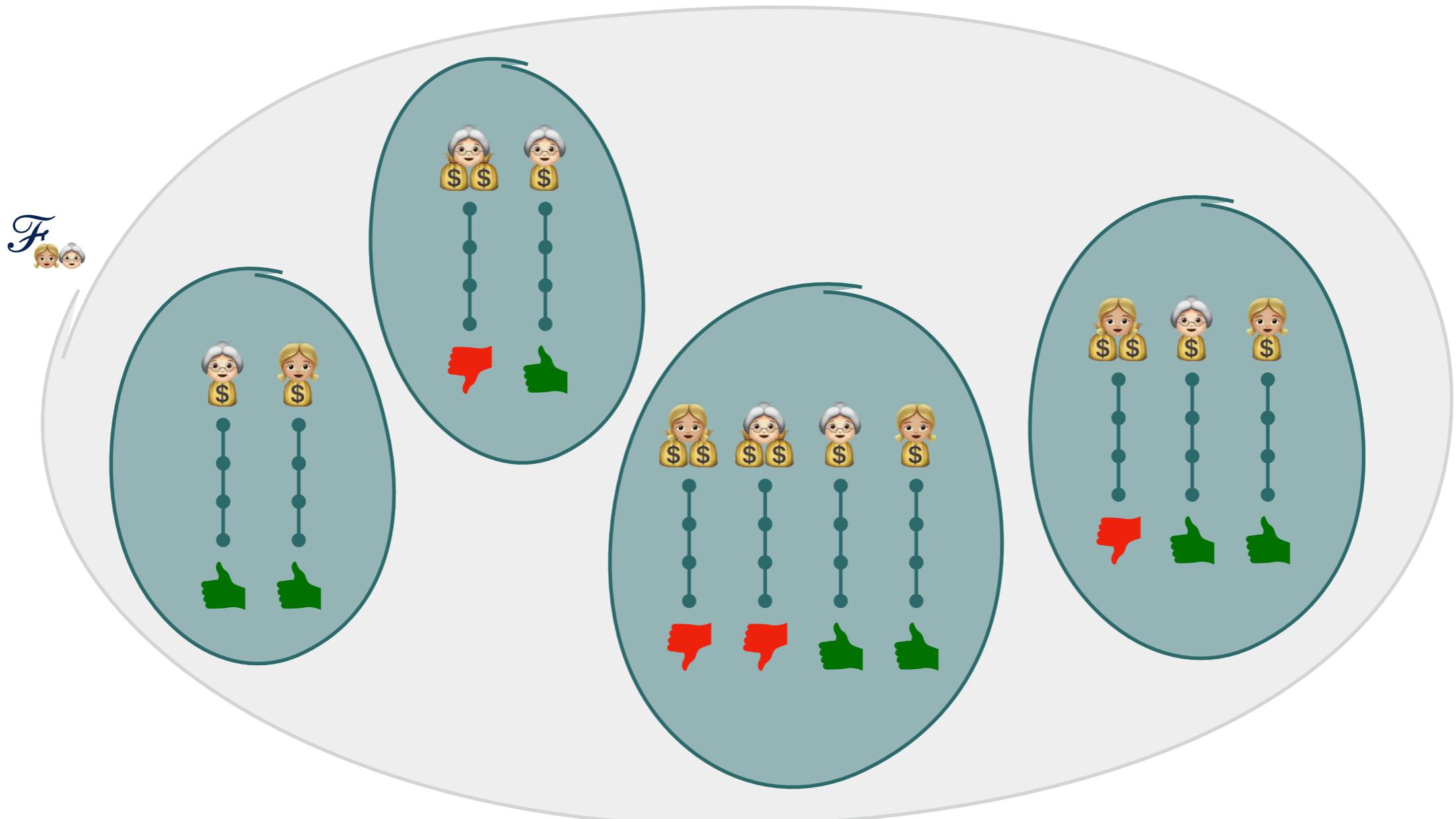
Intuitively: inputs differing only on the value of the sensitive input node  $x_{0,i}$  should lead to the same **classification outcome**

## Theorem

$$M \models \mathcal{F}_i \Leftrightarrow \{[\![M]\!]\} \subseteq \mathcal{F}_i$$

# Dependency Fairness

## Subset-Closed Property (\*)



(\*) ML Models are Deterministic

# Dependency Fairness

$$\mathcal{F}_i \stackrel{\text{def}}{=} \{[\![M]\!] \mid \text{UNUSED}_i([\![M]\!])\}$$

$\mathcal{F}_i$  is the set of all neural networks M (or, rather, their semantics  $[\![M]\!]$ ) that **do not use** the value of the sensitive input node  $x_{0,i}$  for classification

$$\begin{aligned} \text{UNUSED}_i(T) &\stackrel{\text{def}}{=} \forall t, t' \in T: t_0(x_{0,i}) \neq t'_0(x_{0,i}) \wedge \\ &(\forall 0 \leq j \leq |L_0|: j \neq i \Rightarrow t_0(x_{0,j}) = t'_0(x_{0,j})) \\ &\Rightarrow t_\omega = t'_\omega \end{aligned}$$

Intuitively: inputs differing only on the value of the sensitive input node  $x_{0,i}$  should lead to the same **classification outcome**

## Theorem

$$M \models \mathcal{F}_i \Leftrightarrow \{[\![M]\!]\} \subseteq \mathcal{F}_i$$

## Corollary

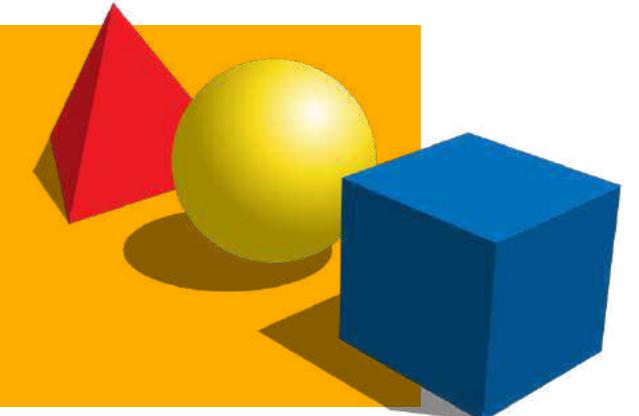
$$M \models \mathcal{F}_i \Leftarrow [\![M]\!] \subseteq [\![M]\!]^\natural \in \mathcal{F}_i$$

# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties



**mathematical models**  
of the program behavior

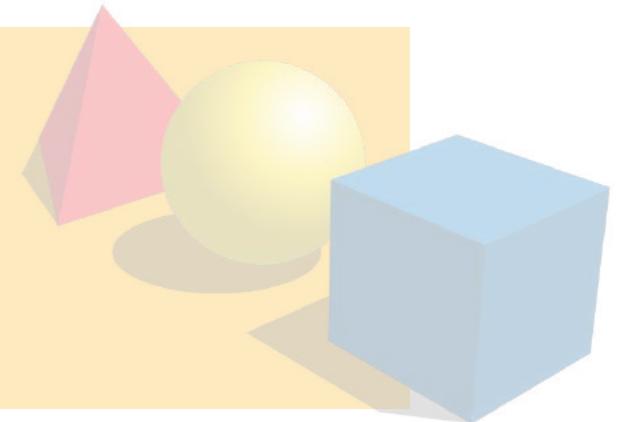


# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties

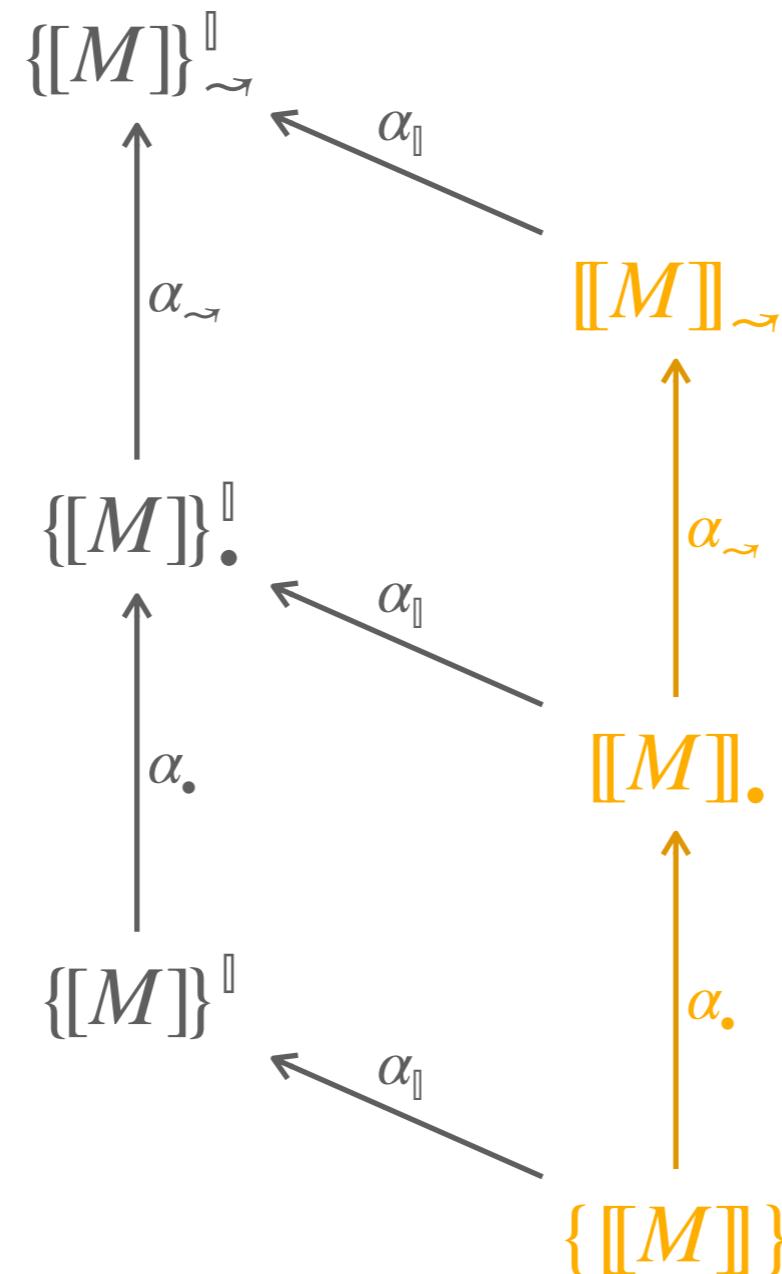


**mathematical models**  
of the program behavior



# Hierarchy of Semantics

parallel semantics

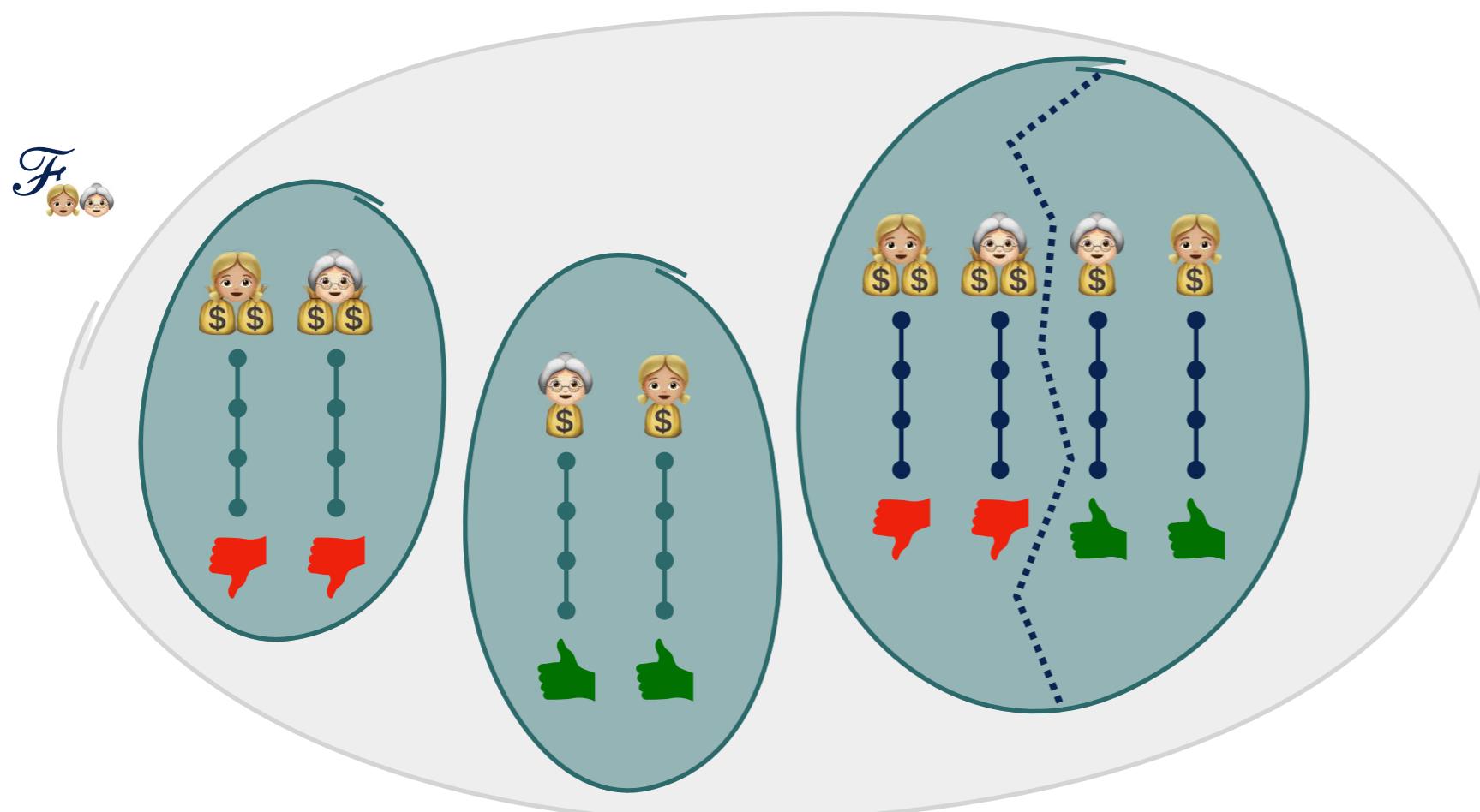
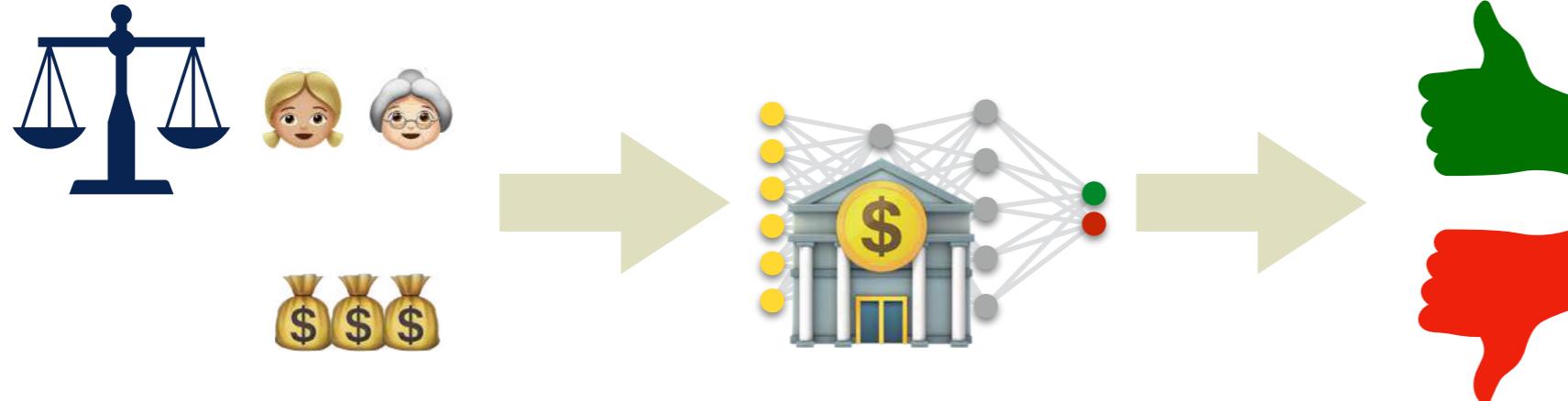


dependency semantics

outcome semantics

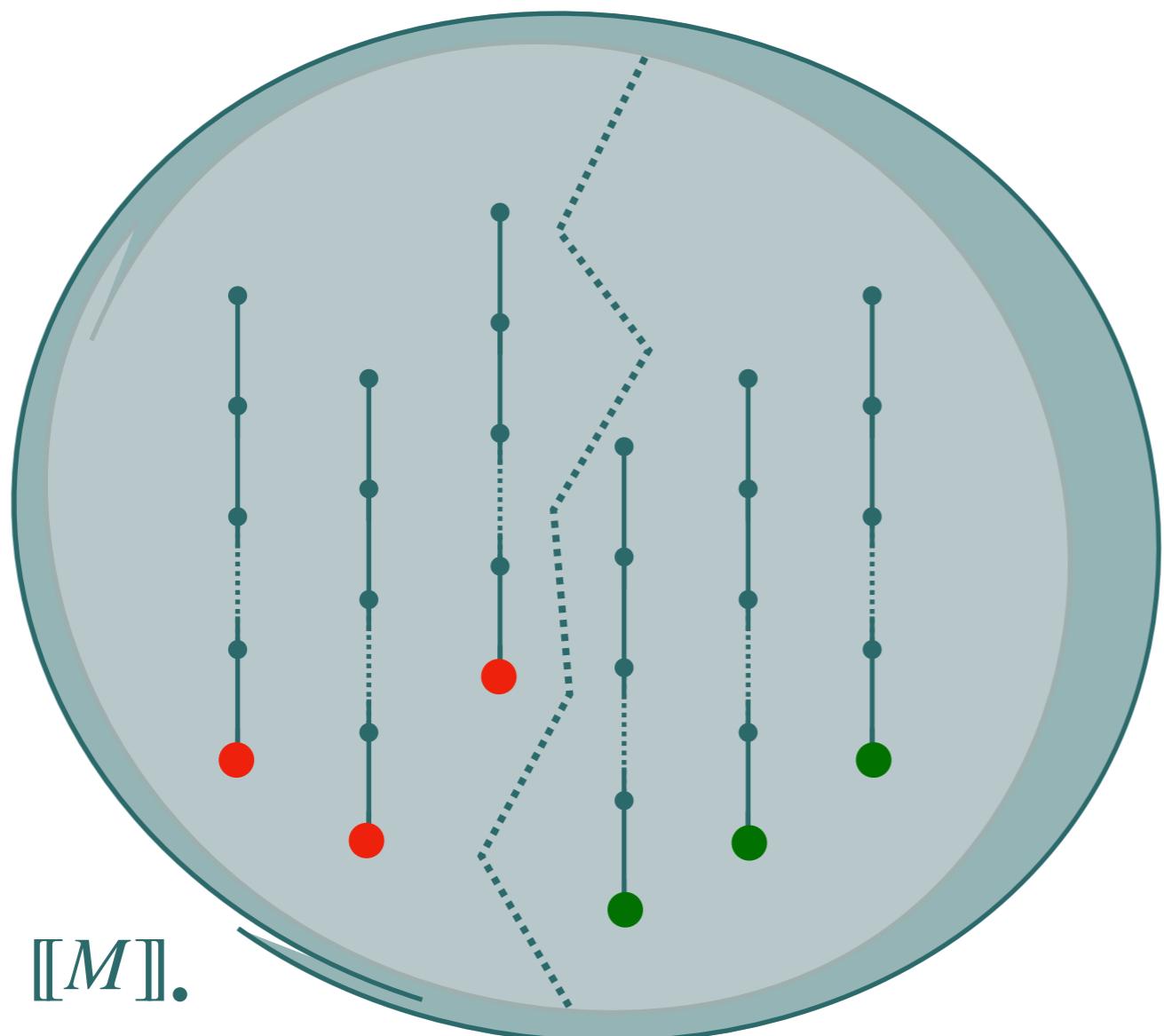
collecting semantics

# Outcome Semantics



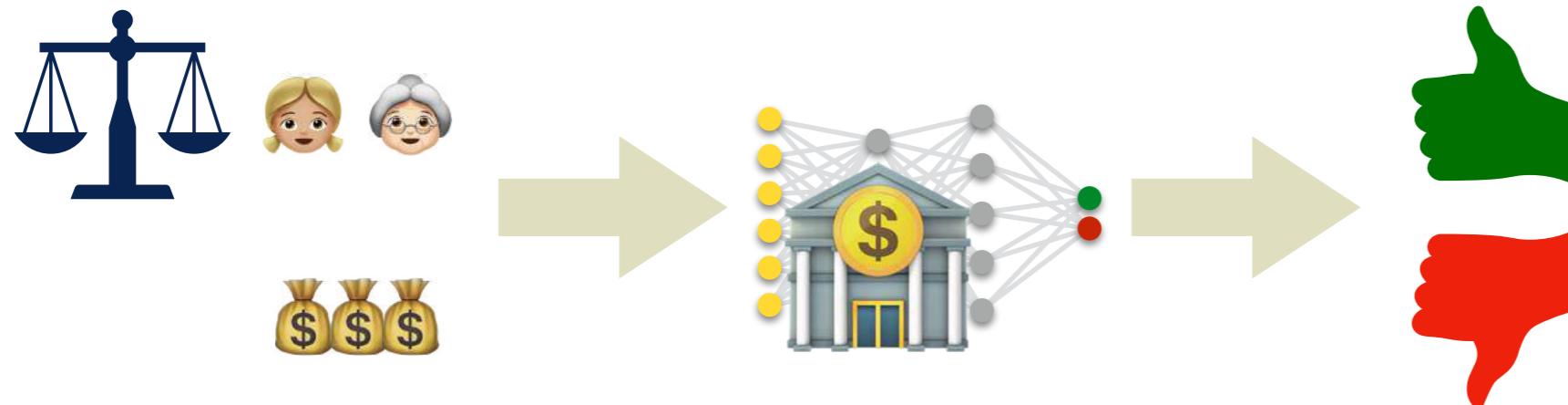
**partitioning** a set of traces that satisfies dependency fairness **with respect to the program outcome** yields sets of traces that also satisfy dependency fairness

# Outcome Semantics

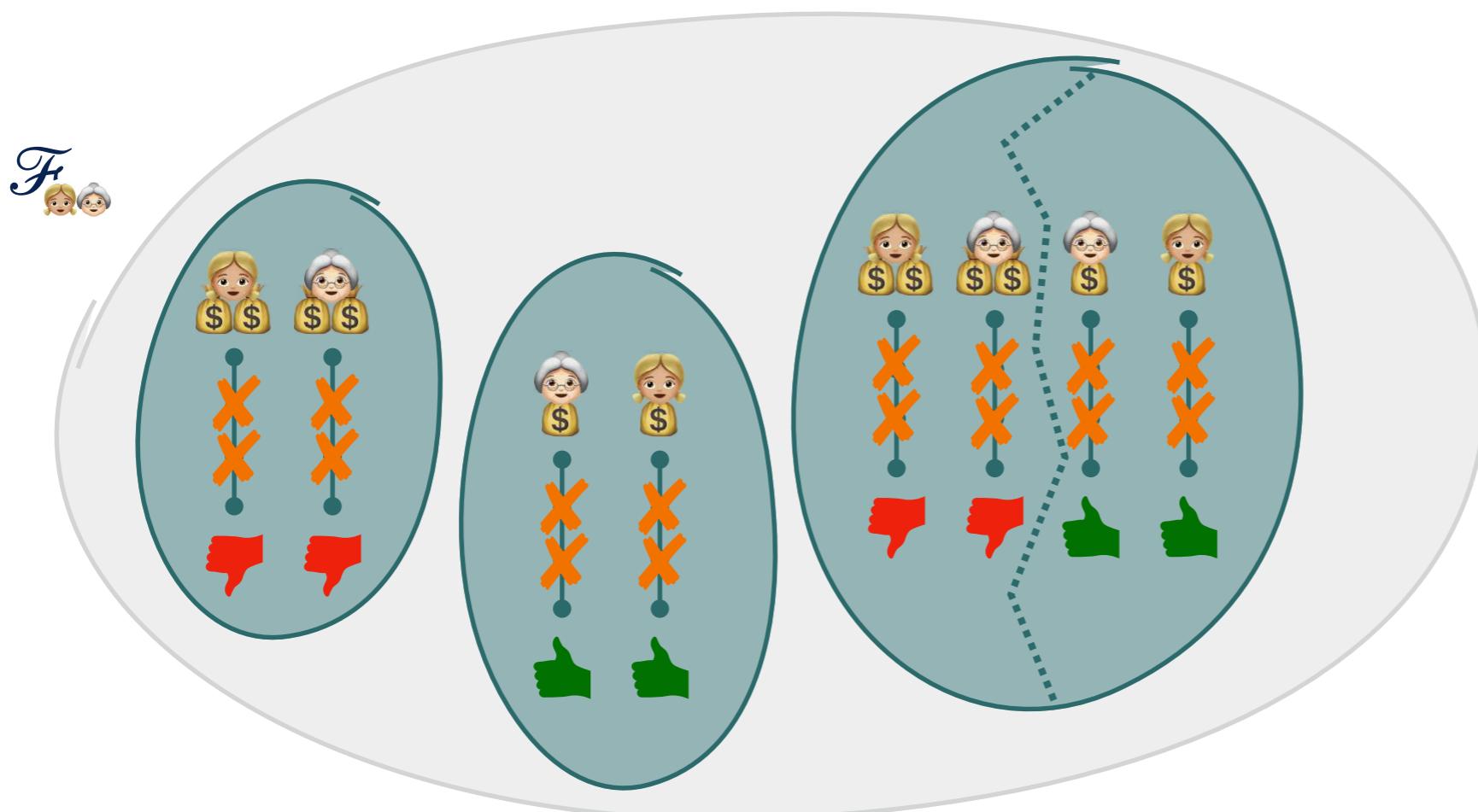


 **partitioning** a set of traces that satisfies dependency fairness **with respect to the program outcome** yields sets of traces that also satisfy dependency fairness

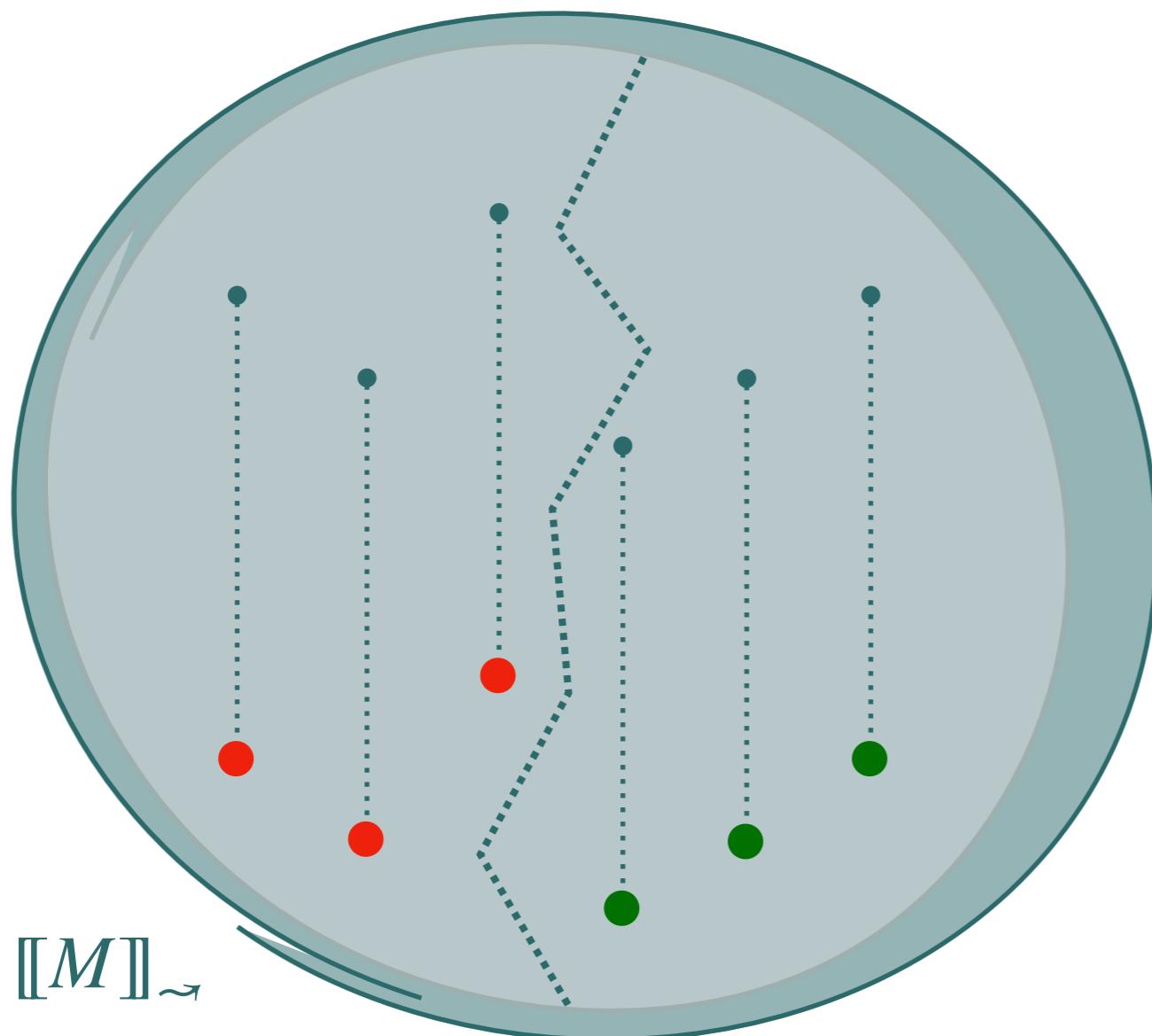
# Dependency Semantics



to reason about dependency fairness **we do not need to consider all intermediate computations** between the initial and final states of a trace (if any)

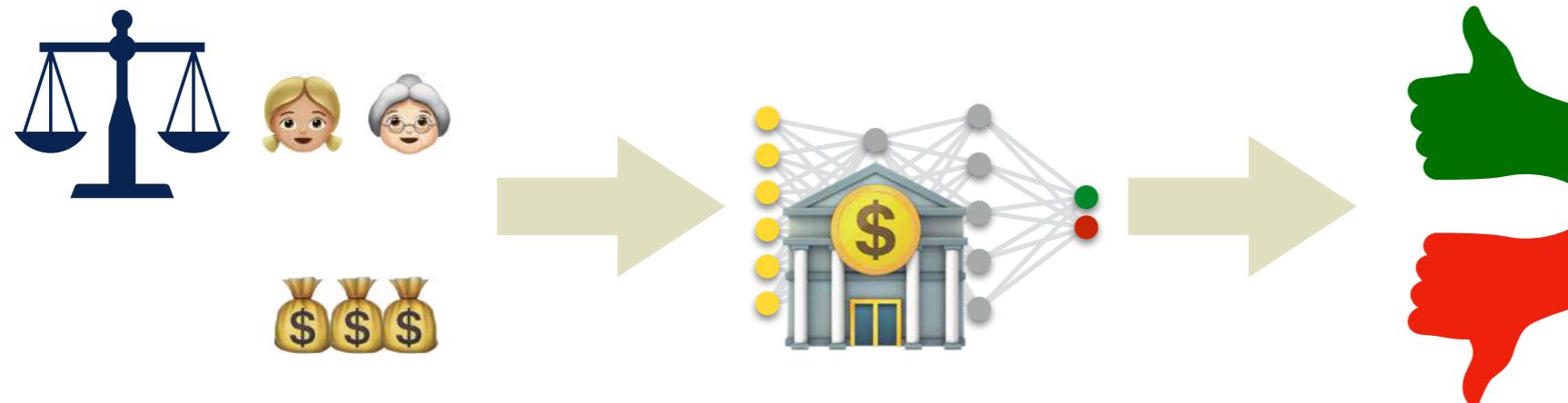


# Dependency Semantics

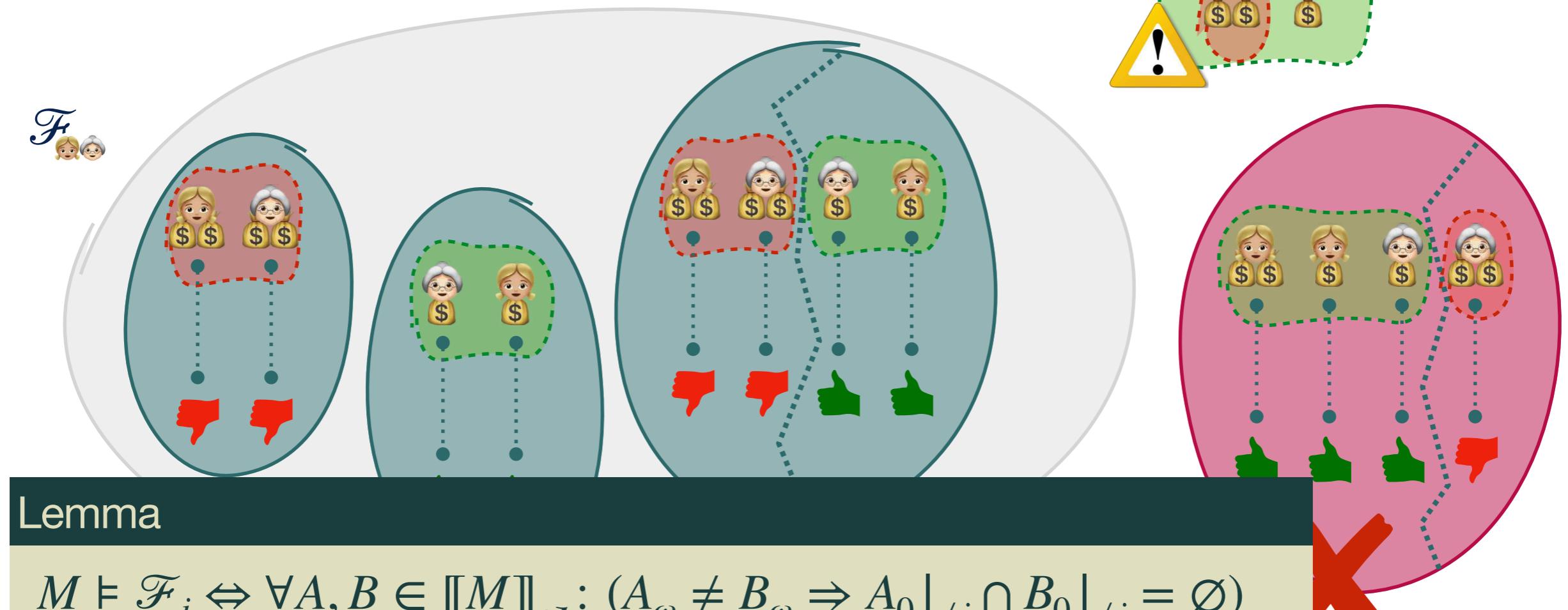


 to reason about dependency fairness **we do not need to consider all intermediate computations** between the initial and final states of a trace (if any)

# Dependency Semantics



💡 partitioning with respect to the outcome classification induces a partition of the space of values of the input nodes used for classification



Lemma

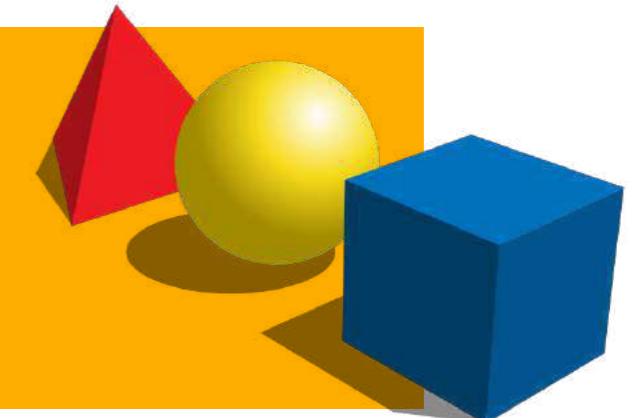
$$M \models \mathcal{F}_i \Leftrightarrow \forall A, B \in \llbracket M \rrbracket_{\sim}: (A_{\omega} \neq B_{\omega} \Rightarrow A_0|_{\neq i} \cap B_0|_{\neq i} = \emptyset)$$

# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties

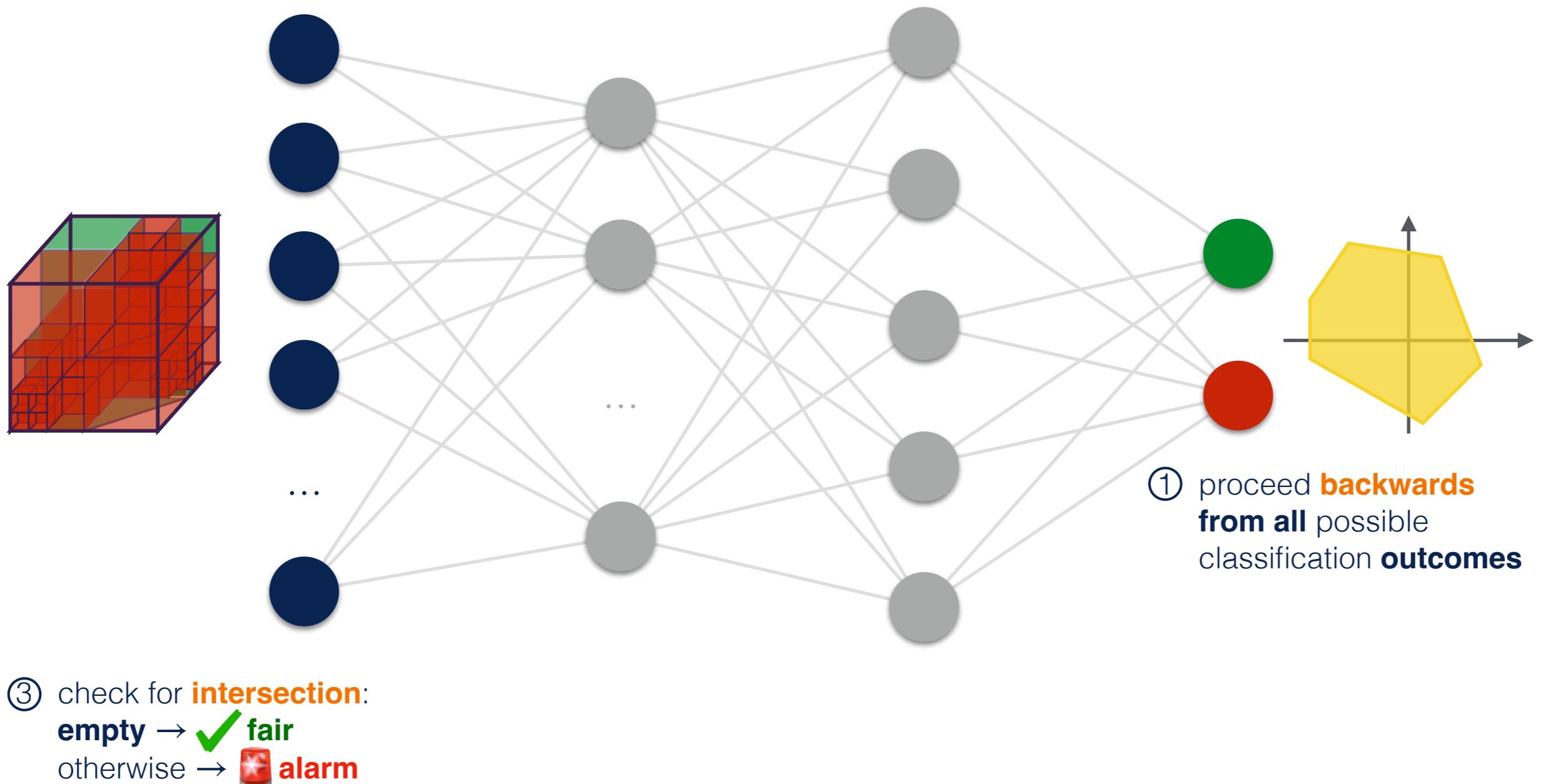


**mathematical models**  
of the program behavior

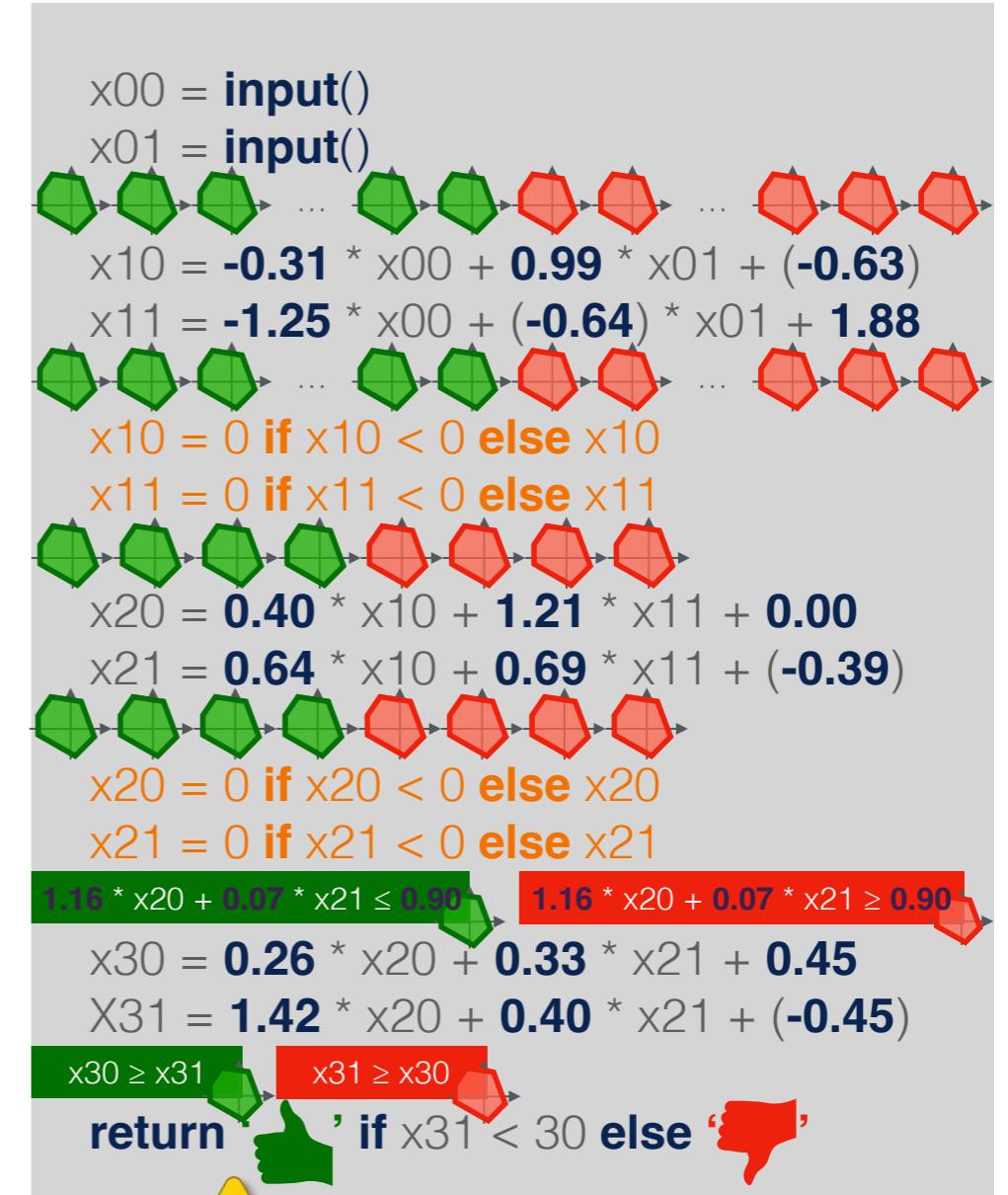
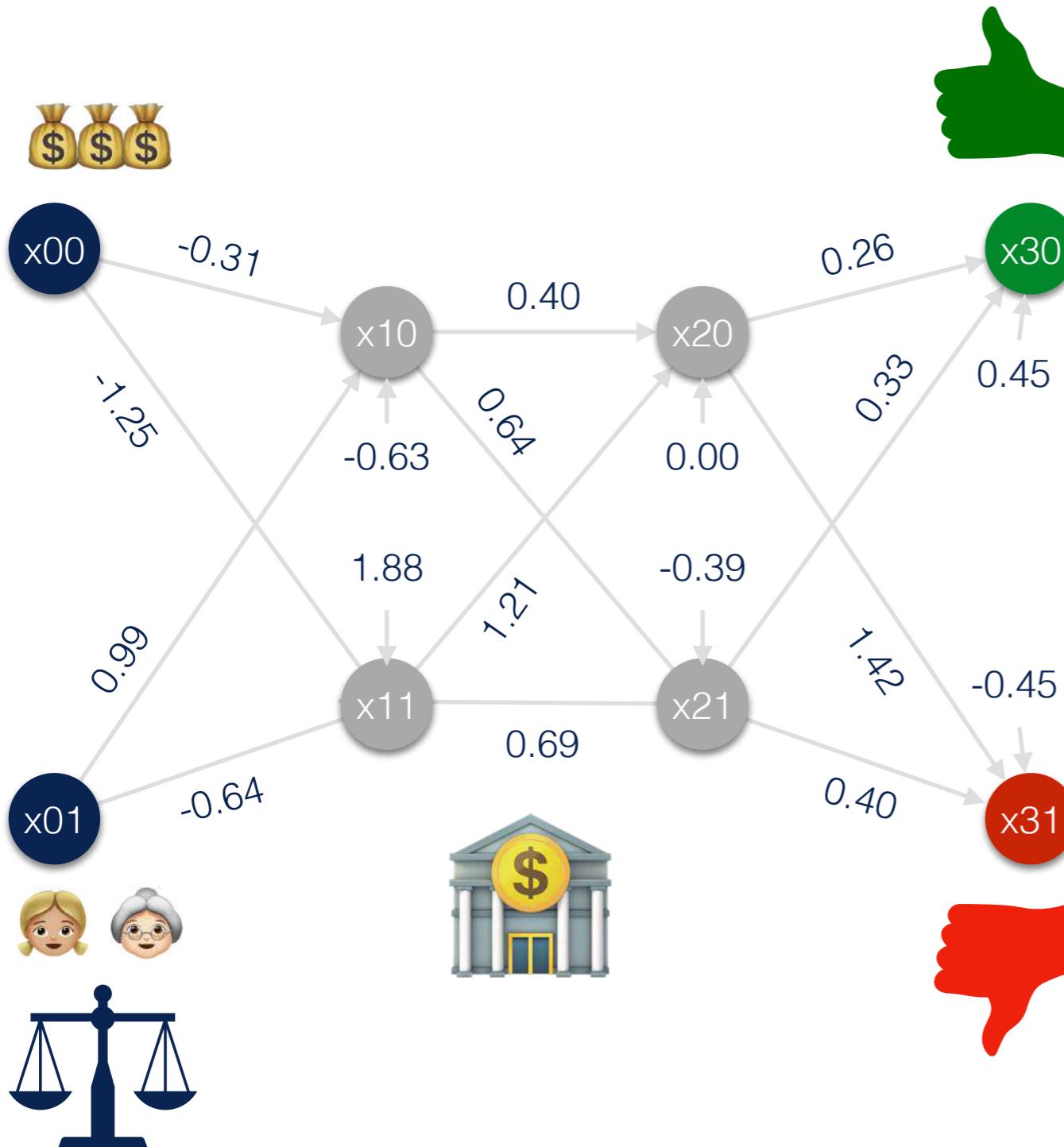


# Naïve Backward Analysis

- ② forget the values of the sensitive input nodes



# Naïve Backward Analysis

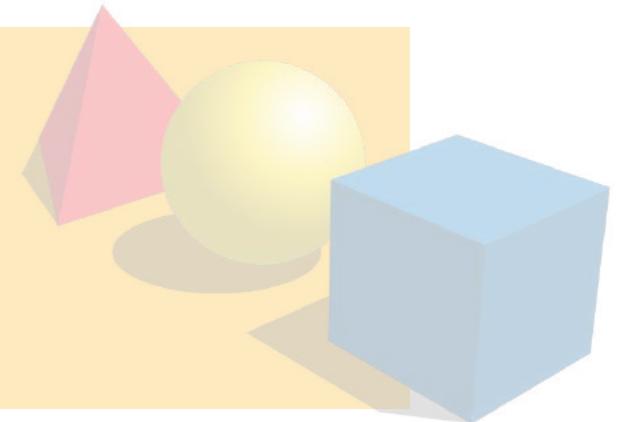


# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties

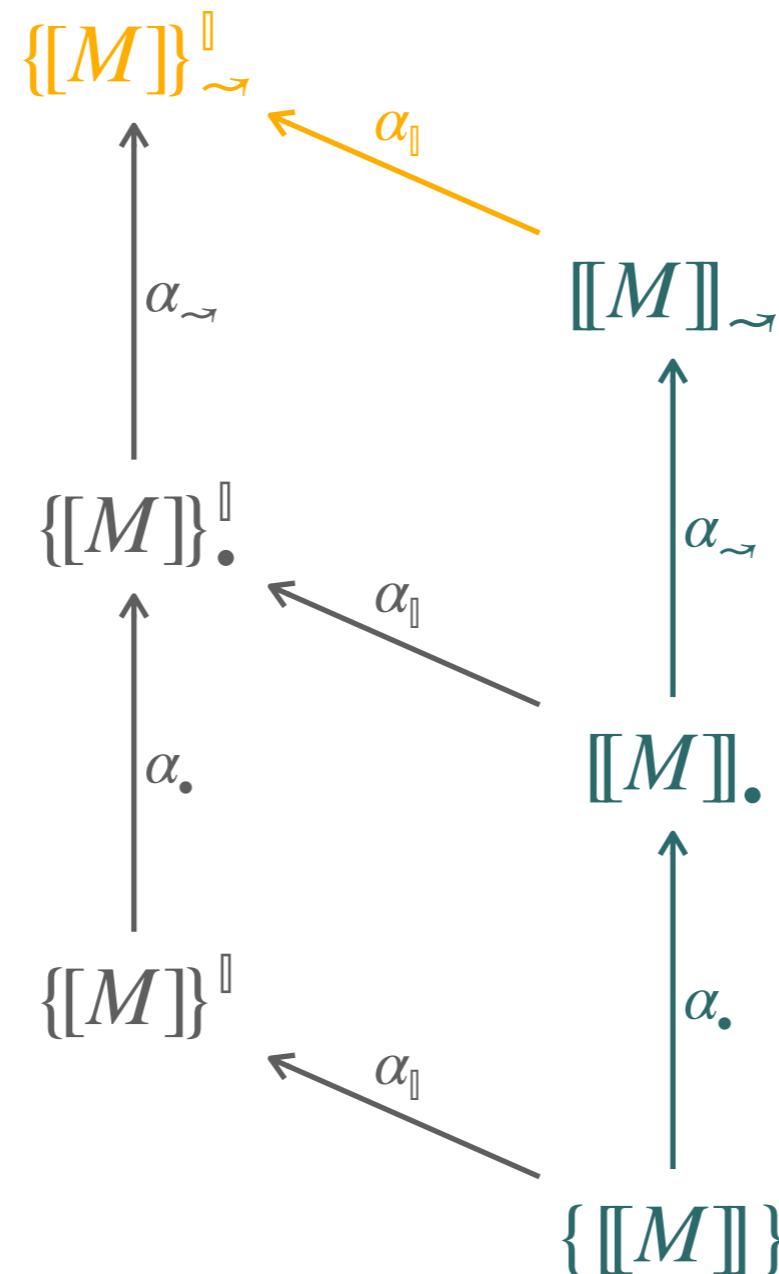


**mathematical models**  
of the program behavior



# Hierarchy of Semantics

parallel semantics

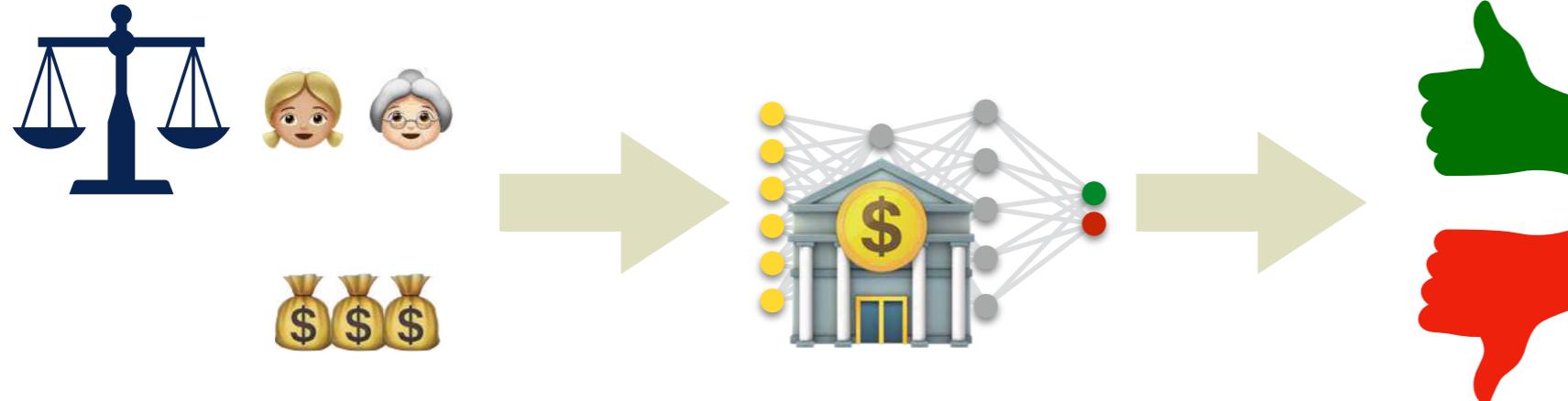


dependency semantics

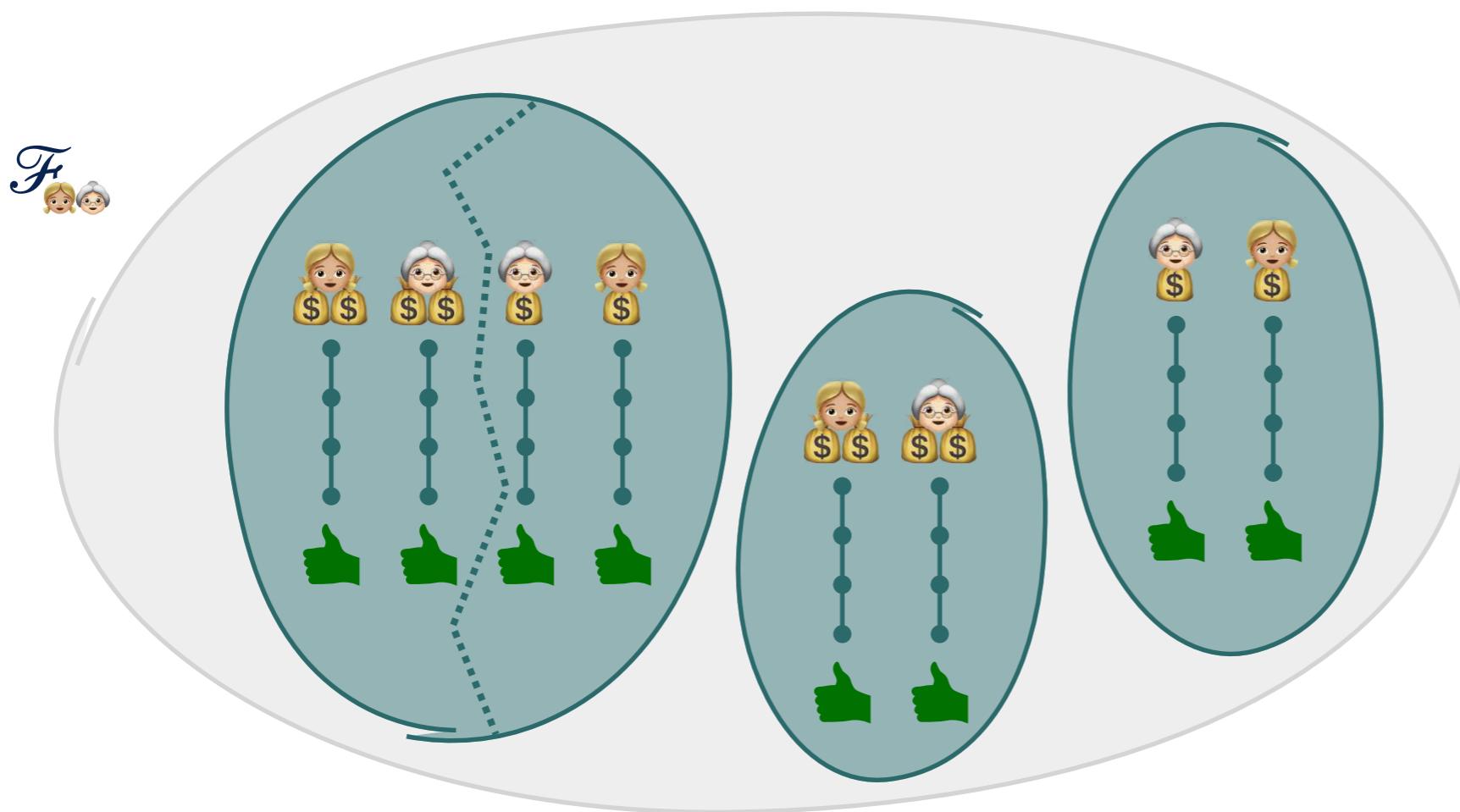
outcome semantics

collecting semantics

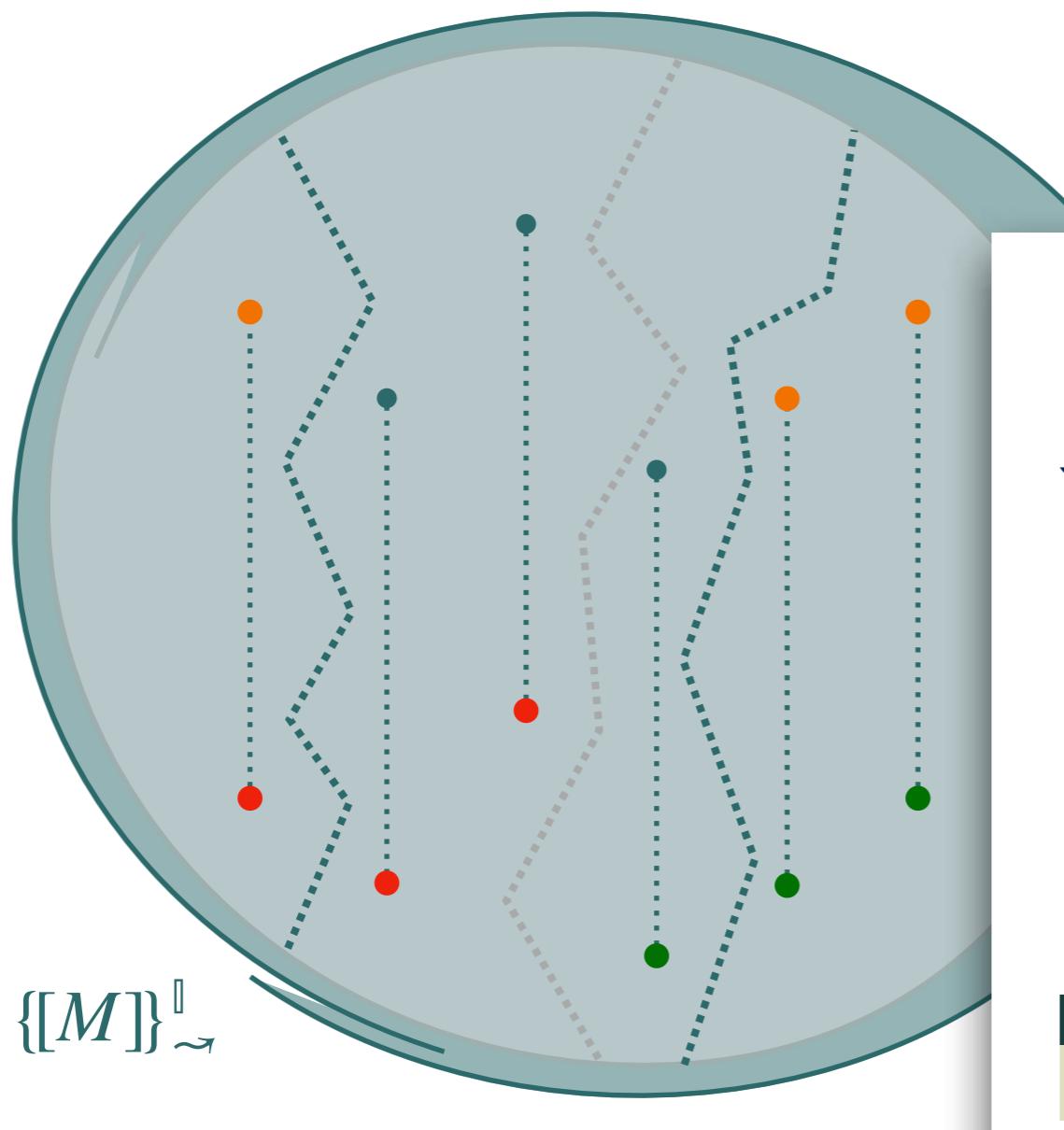
# Parallel Semantics



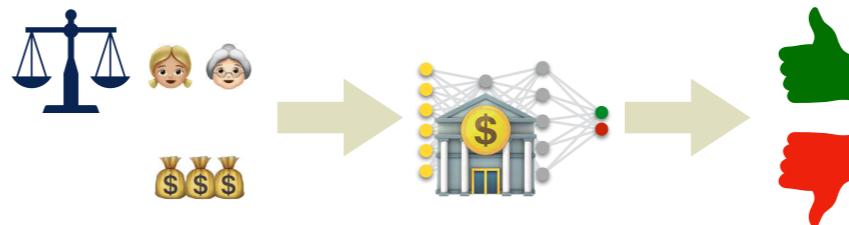
**partitioning** a set of traces that satisfies dependency fairness **with respect to the non-sensitive inputs** yields sets of traces that also satisfy dependency fairness



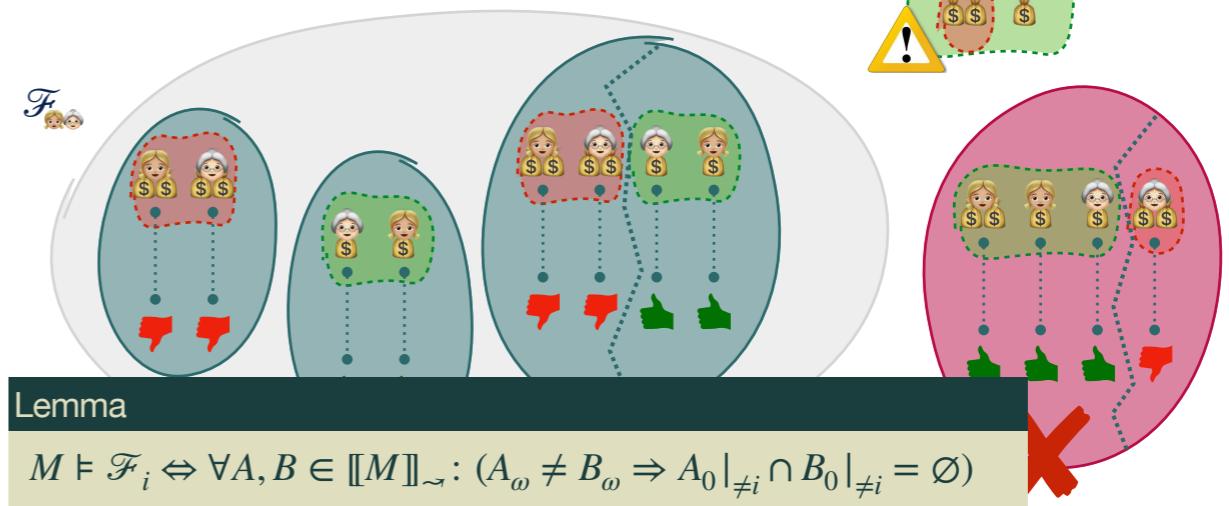
# Parallel Semantics



## Dependency Semantics



partitioning with respect to the outcome classification induces a partition of the space of values of the input nodes used for classification



### Lemma

$$M \models \mathcal{F}_i \Leftrightarrow \forall I \in \mathbb{I}: \forall A, B \in \llbracket M \rrbracket_{\sim}^{\parallel}: (A_{\omega}^I \neq B_{\omega}^I \Rightarrow A_0^I|_{\neq i} \cap B_0^I|_{\neq i} = \emptyset)$$

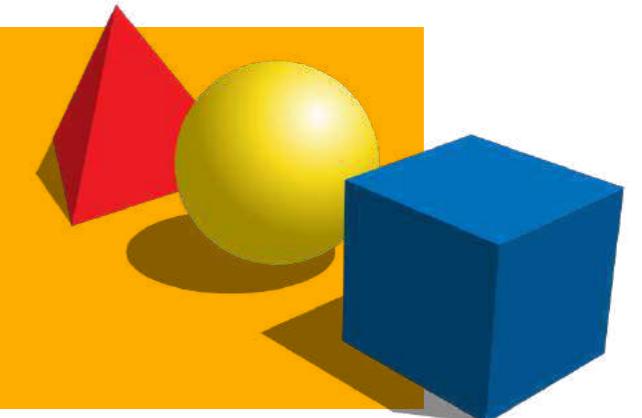
💡 **partitioning** a set of traces that satisfies dependency fairness **with respect to the non-sensitive inputs** yields sets of traces that also satisfy dependency fairness

# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties

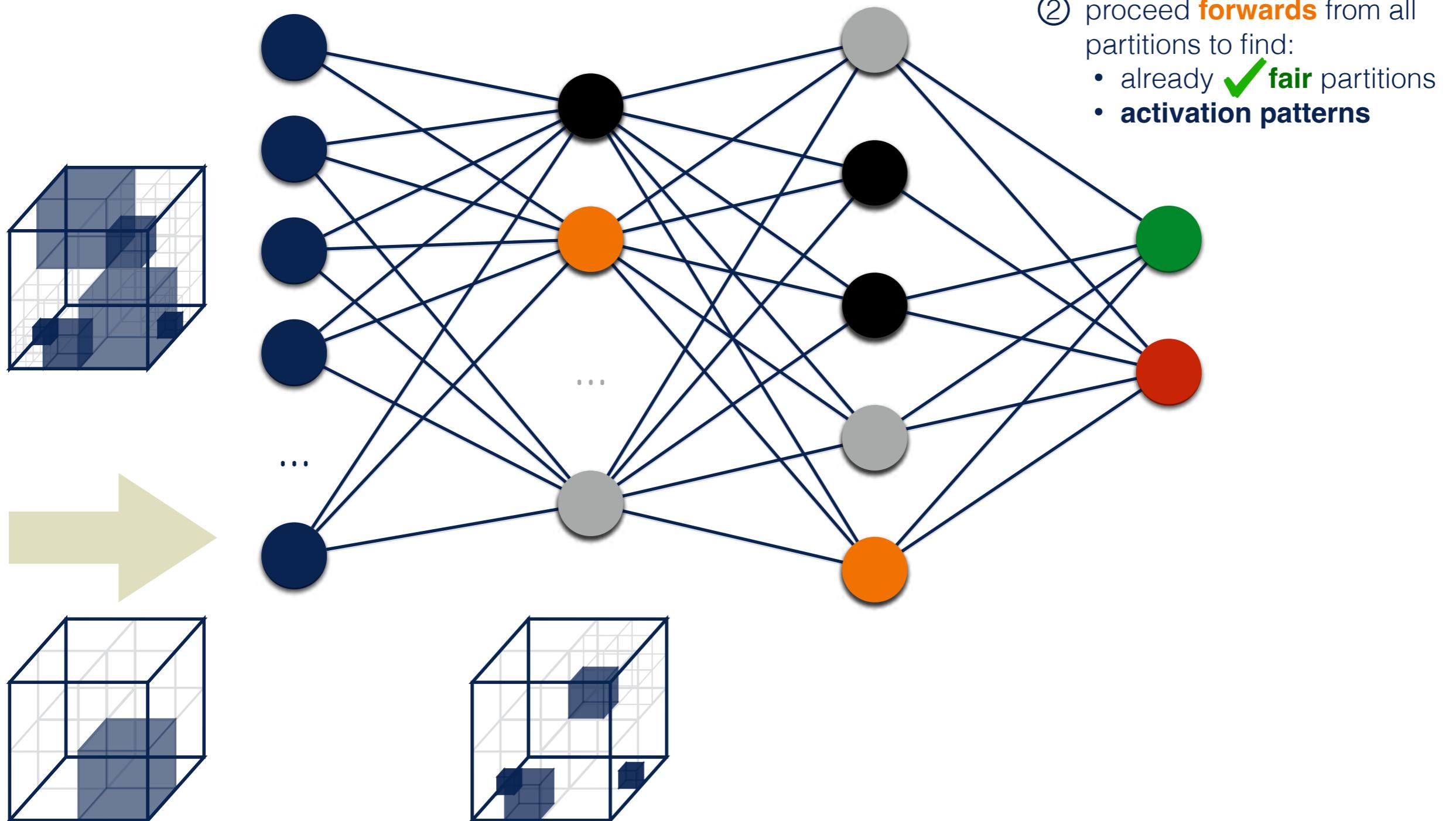


**mathematical models**  
of the program behavior



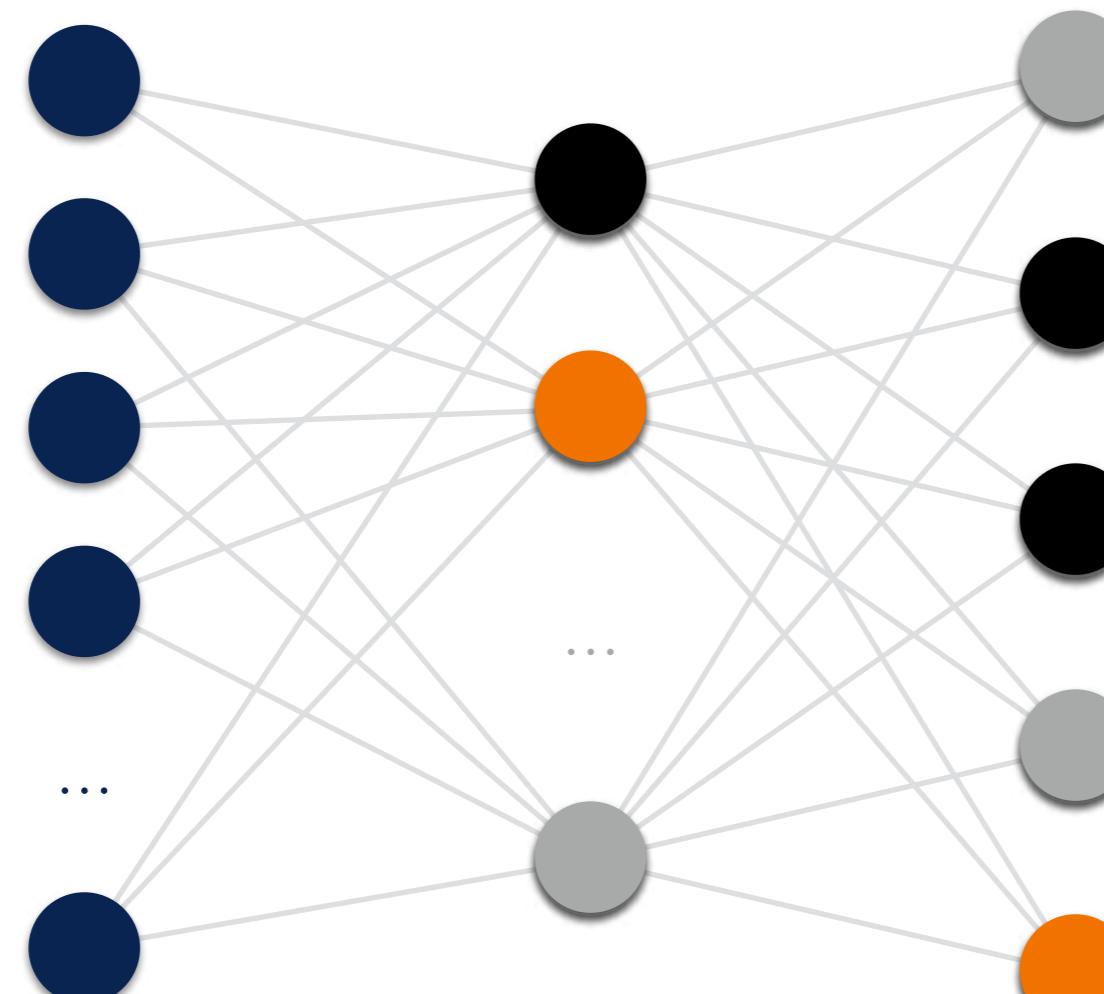
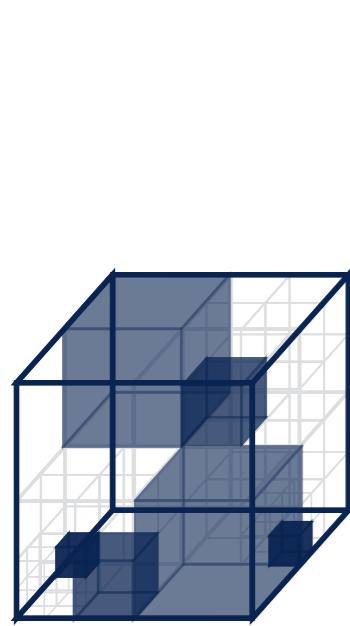
# Forward and Backward Analysis

① **partition** the space of values of the **non-sensitive input** nodes

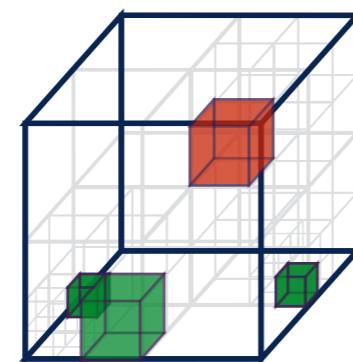
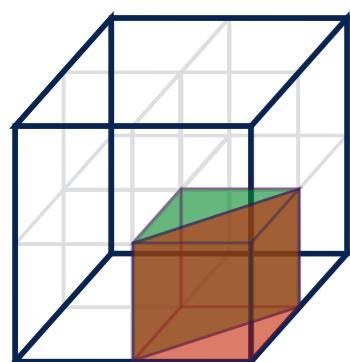
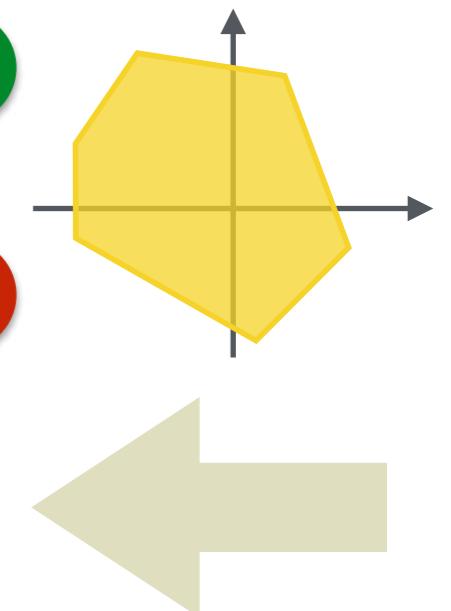


# Forward and Backward Analysis

- ① **partition** the space of values of the **non-sensitive input** nodes



- ② proceed **forwards** from all partitions to find:
- already ✓ **fair** partitions
  - activation patterns**



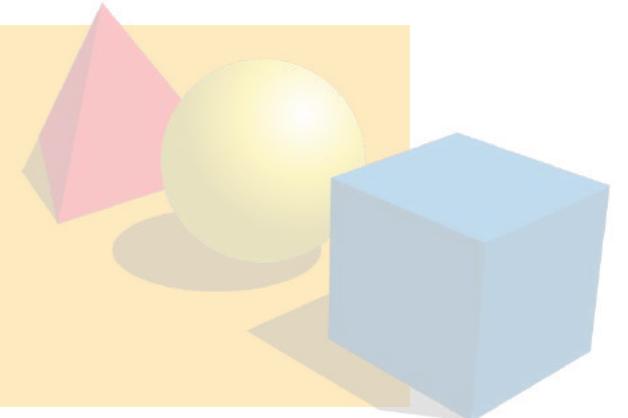
- ③ proceed **backwards** for each activation pattern

# Abstract Interpretation Recipe

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties

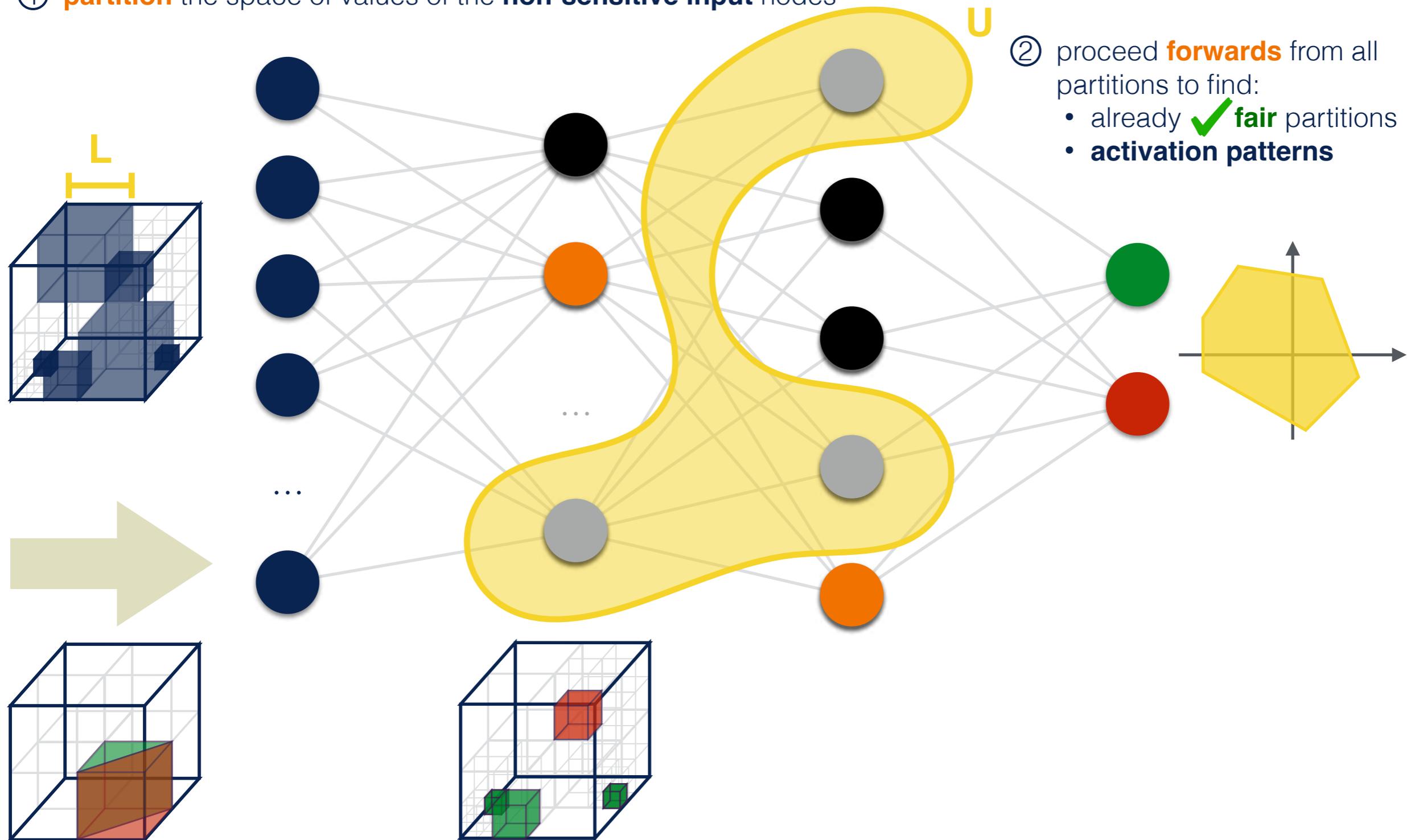


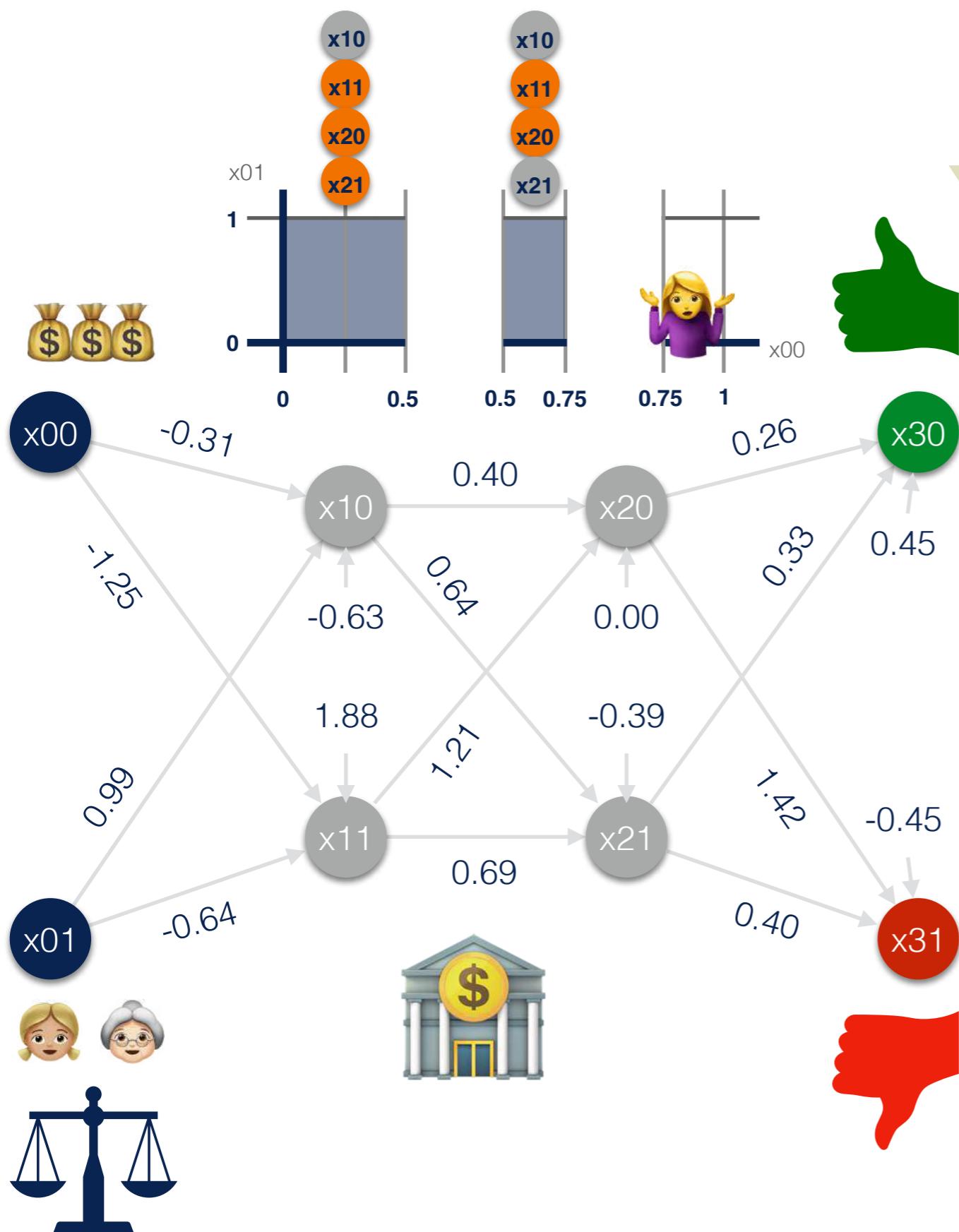
**mathematical models**  
of the program behavior



# Iterative Forward Analysis

① partition the space of values of the **non-sensitive input nodes**





$$L = 0.25$$

$$U = 2$$

$x_{00} = \text{input}()$   
 $x_{01} = \text{input}()$

$$x_{10} = -0.31 * x_{00} + 0.99 * x_{01} + (-0.63)$$

$$x_{11} = -1.25 * x_{00} + (-0.64) * x_{01} + 1.88$$

$$x_{10} = 0 \text{ if } x_{10} < 0 \text{ else } x_{10}$$

$$x_{11} = 0 \text{ if } x_{11} < 0 \text{ else } x_{11}$$

$$x_{20} = 0.40 * x_{10} + 1.21 * x_{11} + 0.00$$

$$x_{21} = 0.64 * x_{10} + 0.69 * x_{11} + (-0.39)$$

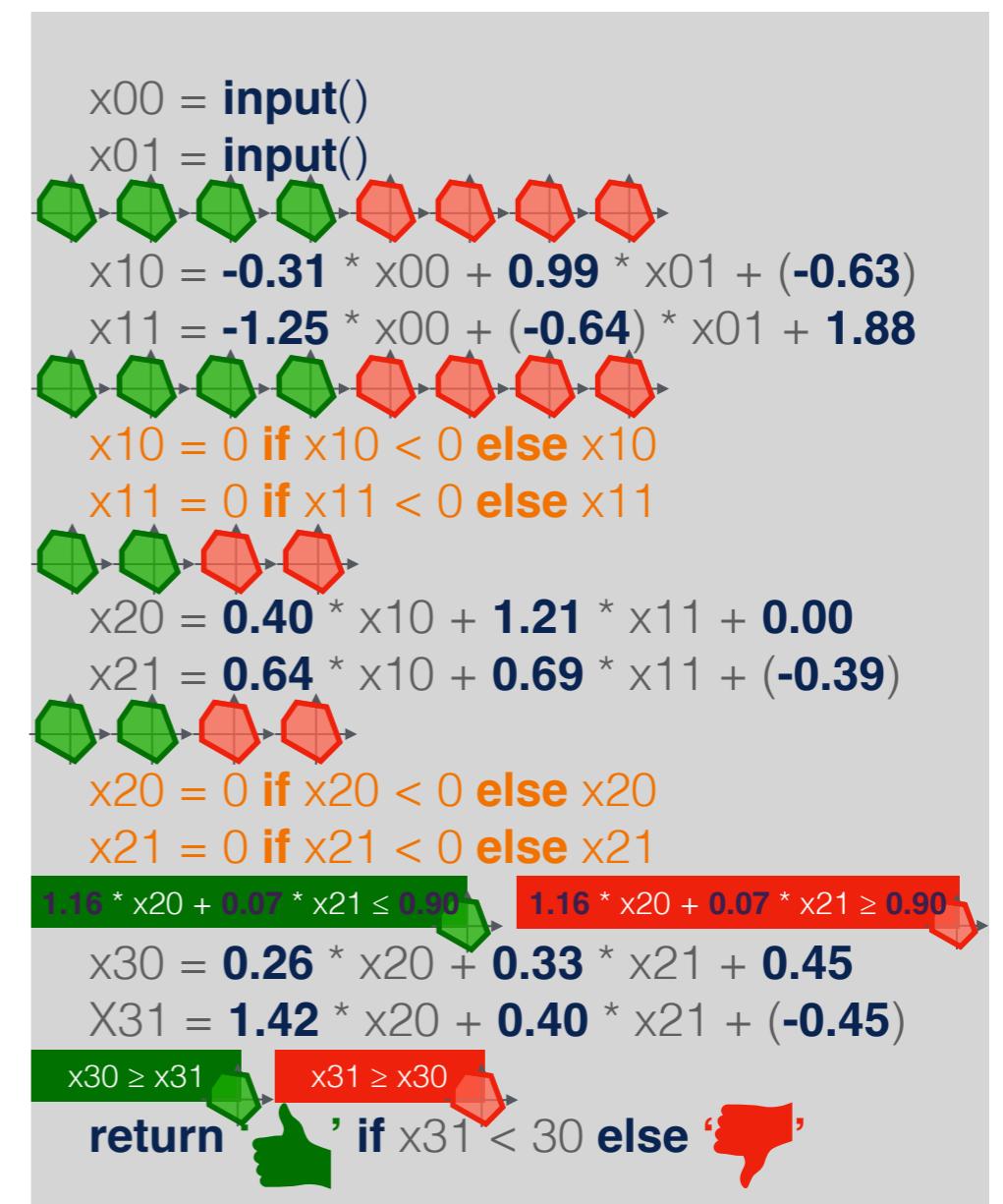
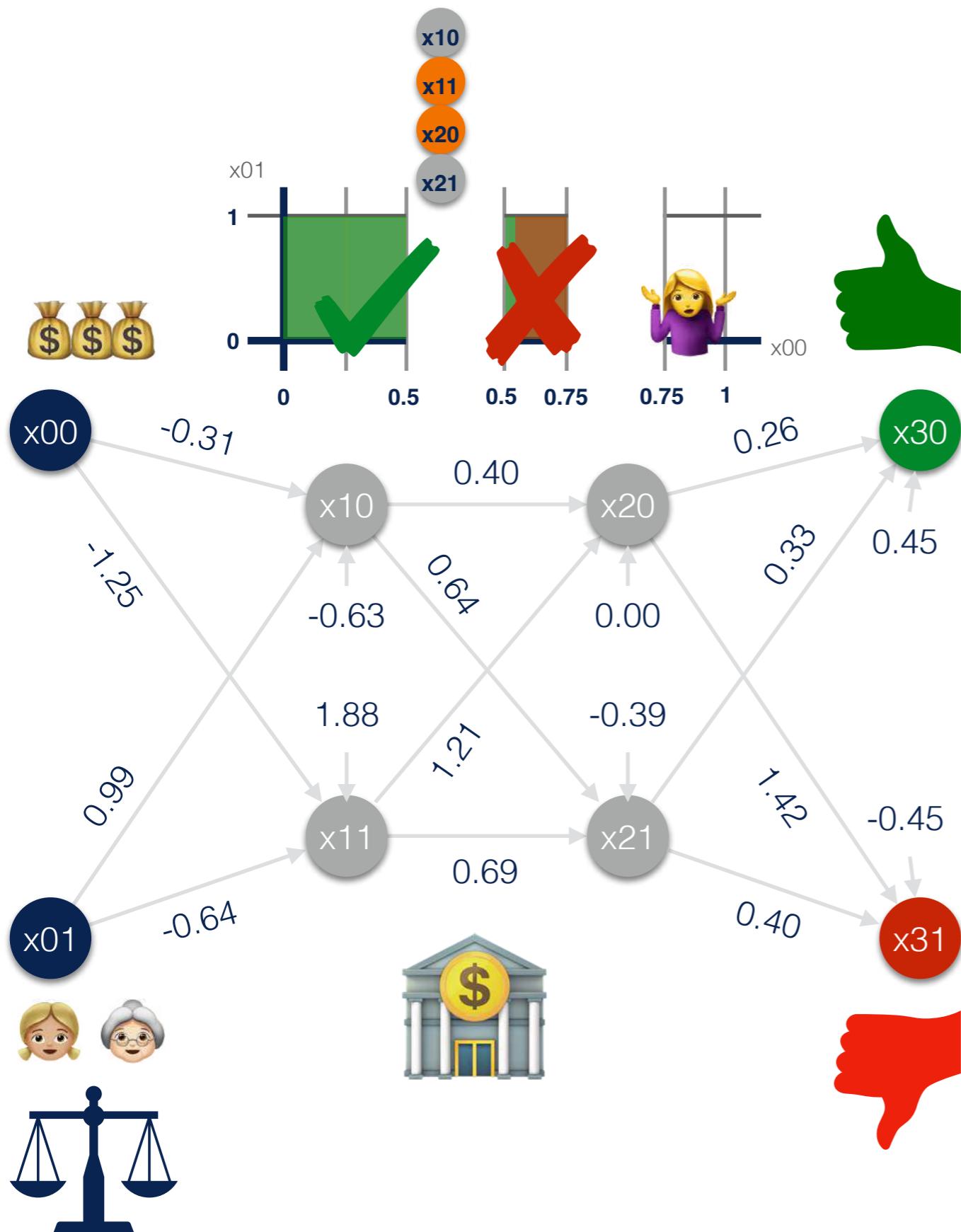
$$x_{20} = 0 \text{ if } x_{20} < 0 \text{ else } x_{20}$$

$$x_{21} = 0 \text{ if } x_{21} < 0 \text{ else } x_{21}$$

$$x_{30} = 0.26 * x_{20} + 0.33 * x_{21} + 0.45$$

$$x_{31} = 1.42 * x_{20} + 0.40 * x_{21} + (-0.45)$$

return ' if  $x_{31} < 30$  else '



# Libra



caterinaurban / Libra

Code Issues Pull requests Actions Projects Security Insights

master ▾ 2 branches 0 tags Go to file Code ▾

caterinaurban README	9f830db on Aug 8	53 commits
src	RQ5 and RQ6 reproducibility	4 months ago
.gitignore	RQ1 reproducibility	4 months ago
LICENSE	Initial prototype	2 years ago
README.md	RQ5 and RQ6 reproducibility	4 months ago
README.pdf	README	4 months ago
icon.png	icon	4 months ago
libra.png	icon	4 months ago
requirements.txt	some documentation	4 months ago
setup.py	some documentation	4 months ago

README.md

## Libra

A yellow icon of a traditional balance scale, symbolizing justice or fairness.

Nowadays, machine-learned software plays an increasingly important role in critical decision-making in our social, economic, and civic lives.

### About

No description or website provided.

#abstract-interpretation

#static-analysis

#machine-learning

#neural-networks #fairness

Readme

MPL-2.0 License

### Releases

No releases published

### Packages

No packages published

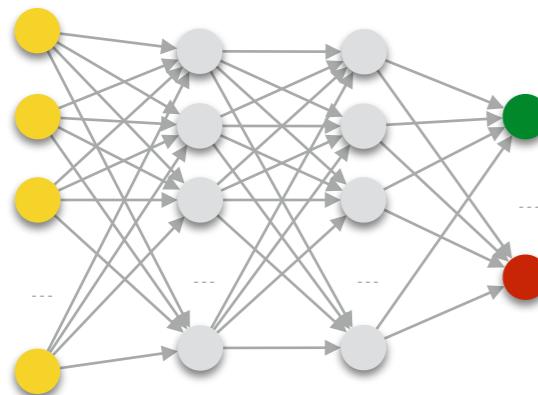
### Languages

Python 98.7%

Shell 1.3%

# Scalability-vs-Precision Tradeoff

## Japanese Credit Screening Dataset

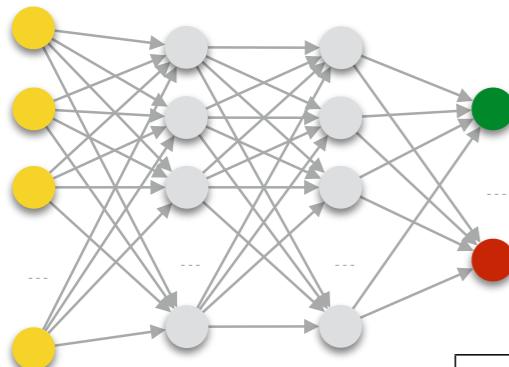


17 inputs  
4 HL \* 5 N  
2 classes  
86% accuracy

L	U	◆ BOXES				▲ SYMBOLIC				★ DEEPPOLY			
		INPUT	C	F	TIME	INPUT	C	F	TIME	INPUT	C	F	TIME
0.5	4	15.28%	37	0 0	8s	58.33%	79	8 20	1m 26s	69.79%	115	10 39	3m 18s
	6	17.01%	39	6 6	51s	69.10%	129	22 61	5m 41s	80.56%	104	23 51	7m 53s
	8	51.39%	90	28 85	12m 2s	82.64%	88	31 67	12m 35s	91.32%	84	27 56	19m 33s
	10	79.86%	89	34 89	34m 15s	93.06%	98	40 83	42m 32s	96.88%	83	29 58	43m 39s
0.25	4	59.09%	1115	20 415	54m 32s	95.94%	884	39 484	54m 31s	98.26%	540	65 293	14m 29s
	6	83.77%	1404	79 944	37m 19s	98.68%	634	66 376	23m 31s	99.70%	322	79 205	13m 25s
	8	96.07%	869	140 761	1h 7m 29s	99.72%	310	67 247	1h 3m 33s	99.98%	247	69 177	22m 52s
	10	99.54%	409	93 403	1h 35m 20s	99.98%	195	52 176	1h 2m 13s	100.00%	111	47 87	34m 56s
0.125	4	97.13%	12449	200 9519	3h 33m 48s	99.99%	1101	60 685	47m 46s	99.99%	768	81 415	19m 1s
	6	99.83%	5919	276 4460	3h 23m	100.00%	988	77 606	26m 47s	100.00%	489	80 298	16m 54s
	8	99.98%	1926	203 1568	2h 14m 25s	100.00%	404	73 309	46m 31s	100.00%	175	57 129	20m 11s
	10	100.00%	428	95 427	1h 39m 31s	100.00%	151	53 141	57m 32s	100.00%	80	39 62	28m 33s
0	4	100.00%	19299	295 15446	6h 13m 24s	100.00%	1397	60 885	40m 5s	100.00%	766	87 425	16m 41s
	6	100.00%	4843	280 3679	2h 24m 7s	100.00%	763	66 446	35m 24s	100.00%	401	81 242	32m 29s
	8	100.00%	1919	208 1567	2h 9m 59s	100.00%	404	73 309	45m 48s	100.00%	193	68 144	24m 16s
	10	100.00%	486	102 475	1h 41m 3s	100.00%	217	55 192	1h 2m 11s	100.00%	121	50 91	30m 53s

# Seeded Bias

## German Credit Dataset ( $L = 0$ )



17 inputs  
4 HL \* 5 N  
2 classes  
71% accuracy

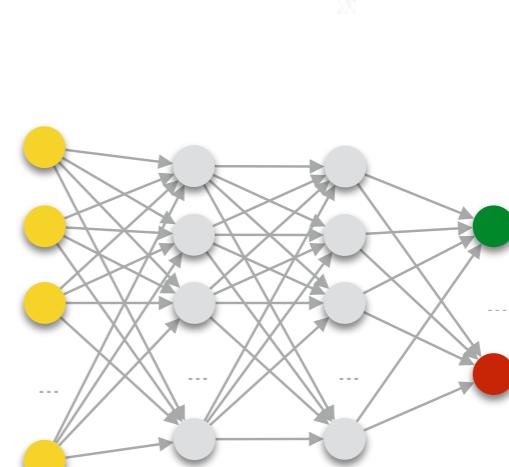
17 inputs  
4 HL \* 5 N  
2 classes  
65% accuracy

CREDIT	DEEPPOLY						BIASED DATA					
	FAIR DATA			TIME			BIASED DATA			TIME		
	U	BIAS	C	F	TIME	U	BIAS	C	F	TIME	TIME	TIME
$\leq 1000$	8	0.33%	170	21	25	3m 40s	8	0.79%	260	42	53	5m 42s
	6	0.17%	211	10	10	4m 5s	4	0.31%	218	9	20	1m 6s
	2	0.09%	176	4	5	14s	12	0.82%	271	53	61	18m 18s
	7	0.15%	212	9	9	1m 31s	4	0.42%	242	21	28	1m 36s
	3	0.23%	217	8	15	32s	10	0.95%	260	42	67	3m 2s
	12	0.30%	213	17	23	5m 45s	2	0.41%	226	20	26	1m 56s
	6	0.20%	193	11	11	52s	3	0.48%	228	19	34	39s
	5	0.16%	193	9	10	10s	1	0.09%	206	5	5	51s
		0.09%			10s		0.09%				39s	
$> 1000$		0.19%			1m 12s		0.45%				1m 46s	
		0.33%			5m 45s		0.95%				18m 18s	
	10	12.08%	321	85	150	10m 30s	11	27.59%	498	234	333	1h 16m 41s
	11	7.43%	329	75	125	22m 33s	7	30.77%	394	70	228	6m 34s
	2	2.21%	217	15	16	39s	7	33.17%	435	185	327	6h 51m 50s
	10	4.29%	239	24	33	4m 4s	6	16.45%	448	162	260	18m 25s
	4	9.73%	268	29	87	4m 0s	13	30.17%	418	141	332	43m 12s
	14	14.96%	403	116	231	1h 9m 45s	5	17.24%	460	91	217	12m 53s
	7	5.83%	313	92	115	4m 17s	8	19.23%	363	79	189	7m 24s
	9	4.61%	264	50	74	5m 38s	2	4.52%	331	45	95	4m 44s
		2.21%			39s		4.52%				4m 44s	
		6.63%			4m 58s		23.41%				15m 39s	
		14.96%			1h 9m 45s		31.17%				6h 51m 50s	

# Bias Queries

## ProPublica COMPAS Dataset ( $L = 0$ )

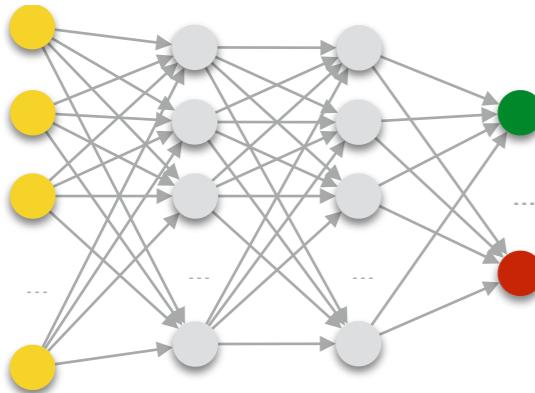
QUERY	DEEPPOLY									
	FAIR DATA					BIASED DATA				
	U	BIAS	C	F	TIME	U	BIAS	C	F	TIME
AGE < 25 RACE BIAS?	10	0.23%	71	18 20	1h 11m 43s	10	0.83%	43	15 33	2h 5m 5s
	10	0.75%	33	14 16	10m 33s	10	6.48%	63	25 34	8m 46s
	10	0.22%	34	17 22	52m 29s	10	1.15%	33	10 14	11m 58s
	10	0.24%	118	28 29	42m 2s	10	0.42%	31	13 30	10m 51s
	10	0.31%	117	49 54	1h 0m 2s	10	0.12%	37	11 16	18m 18s
	10	0.33%	59	18 21	53m 29s	10	2.27%	33	16 24	1h 4m 35s
	10	1.19%	39	17 23	9m 39s	10	3.41%	133	92 102	33m 43s
	10	2.12%	33	17 31	5m 18s	10	0.18%	33	12 17	14m 58s
	MIN	0.22%			5m 18s		0.12%			8m 46s
MEDIAN MAX	MEDIAN	0.32%			47m 16s		0.99%			16m 38s
	MAX	2.12%			1h 11m 43s		6.48%			2h 5m 5s
	MIN									
MALE AGE BIAS?	10	3.86%	242	96 180	2h 30m 23s	10	5.22%	204	65 180	3h 25m 21s
	10	8.84%	100	45 77	19m 47s	10	12.38%	387	152 318	40m 49s
	10	8.14%	204	47 143	28m 12s	10	7.10%	181	63 142	20m 51s
	10	2.70%	563	168 232	1h 49m 9s	10	6.90%	96	23 95	1h 21m 37s
	10	4.65%	545	280 415	1h 33m 36s	10	6.14%	157	62 110	27m 43s
	10	5.77%	217	68 154	1h 35m 25s	10	8.10%	345	61 284	47m 9s
	10	7.76%	252	62 226	23m 10s	10	6.78%	251	141 223	50m 13s
	10	8.70%	267	90 266	53m 26s	10	12.88%	257	124 228	47m 46s
	MIN	2.70%			19m 47s		5.22%			20m 51s
MEDIAN MAX	MEDIAN	6.77%			1h 13m 31s		7.00%			47m 28s
	MAX	8.84%			2h 20m 23s		12.88%			3h 25m 21s
	MIN									
CAUCASIAN PRIORS BIAS?	11	2.18%	106	21 53	2h 32m 44s	11	2.92%	86	26 69	2h 26m 20s
	7	3.66%	105	38 55	18m 26s	11	6.95%	108	33 71	15m 29s
	11	2.73%	100	32 57	39m 5s	14	4.43%	69	12 51	1h 47m 5s
	17	2.19%	101	28 57	16h 19m 14s	7	3.40%	83	21 82	20m 1s
	19	3.17%	86	30 53	52h 10m 2s	13	3.09%	96	24 58	1h 8m 4s
	11	2.45%	94	26 52	2h 18m 42s	14	5.79%	99	45 87	1h 51m 2s
	15	3.94%	87	29 52	2h 39m 18s	17	5.10%	110	73 94	17h 48m 22s
	15	5.36%	90	35 89	3h 41m 16s	14	3.99%	97	38 65	1h 21m 8s
	MIN	2.18%			18m 26s		2.92%			15m 29s
MEDIAN MAX	MEDIAN	2.95%			2h 36m 1s		4.21%			1h 34m 7s
	MAX	5.36%			52h 10m 2s		6.95%			17h 48m 22s



**19 inputs**  
**4 HL \* 5 N**  
**3 classes**  
**55% | 56% accuracy**

# Scalability wrt Model Size

## Adult Census Dataset ( $L = 0.5$ )



**23 inputs**  
**2 HL \* 5 N**  
**2 classes**

**23 inputs**  
**4 HL \* 3 N**  
**2 classes**

**23 inputs**  
**4 HL \* 5 N**  
**2 classes**

**23 inputs**  
**4 HL \* 10 N**  
**2 classes**

**23 inputs**  
**9 HL \* 5 N**  
**2 classes**

M	U	BOXES				SYMBOLIC				DEEPPOLY			
		INPUT	C	F	TIME	INPUT	C	F	TIME	INPUT	C	F	TIME
10 ○ ● ⊕	4	88.26%	1482	77 1136	33m 55s	95.14%	1132	65 686	19m 5s	93.99%	1894	77 992	29m 55s
	6	99.51%	769	51 723	1h 10m 25s	99.93%	578	47 447	39m 8s	99.83%	1620	54 1042	1h 24m 24s
	8	100.00%	152	19 143	3h 47m 23s	100.00%	174	18 146	1h 51m 2s	100.00%	1170	26 824	8h 2m 27s
	10	100.00%	1	1 1	55m 58s	100.00%	1	1 1	56m 8s	100.00%	1	1 1	56m 43s
12 △ ▲ ↖	4	49.83%	719	9 329	13m 43s	72.29%	1177	11 559	24m 9s	60.52%	1498	14 423	10m 32s
	6	72.74%	1197	15 929	2h 6m 49s	98.54%	333	7 195	20m 46s	66.46%	1653	17 594	15m 44s
	8	98.68%	342	9 284	1h 46m 43s	98.78%	323	9 190	1h 27m 18s	70.87%	1764	18 724	2h 19m 11s
	10	99.06%	313	7 260	1h 21m 47s	99.06%	307	5 182	1h 13m 55s	80.76%	1639	18 1007	3h 22m 11s
20 ◊ ♦ ♦	4	38.92%	1044	18 39	2m 6s	51.01%	933	31 92	15m 28s	49.62%	1081	34 79	3m 2s
	6	46.22%	1123	62 255	20m 51s	61.60%	916	67 405	44m 40s	59.20%	1335	90 356	22m 13s
	8	64.24%	1111	96 792	2h 24m 51s	74.27%	1125	78 780	3h 26m 20s	69.69%	1574	127 652	5h 6m 7s
	10	85.90%	1390	71 1339	>13h	89.27%	1435	60 1157	>13h	76.25%	1711	148 839	4h 36m 23s
40 □ ■ ◆	4	0.35%	10	0 0	1m 39s	34.62%	768	1 1	6m 56s	26.39%	648	2 3	10m 11s
	6	0.35%	10	0 0	1m 38s	34.76%	817	4 5	43m 53s	26.74%	592	8 10	1h 23m 11s
	8	0.42%	12	1 2	14m 37s	35.56%	840	21 28	2h 48m 15s	27.74%	686	32 42	2h 43m 2s
	10	0.80%	23	10 13	1h 48m 43s	37.19%	880	50 75	11h 32m 21s	30.56%	699	83 121	>13h
45 ◇ ♪ *	4	1.74%	50	0 0	1m 38s	41.98%	891	14 49	10m 14s	36.60%	805	6 8	2m 47s
	6	2.50%	72	3 22	4m 35s	45.00%	822	32 143	45m 42s	38.06%	847	25 50	5m 7s
	8	9.83%	282	25 234	25m 30s	47.78%	651	46 229	1h 14m 5s	42.53%	975	74 180	25m 1s
	10	18.68%	522	33 488	1h 51m 24s	49.62%	714	51 294	3h 23m 20s	48.68%	1087	110 373	1h 58m 34s

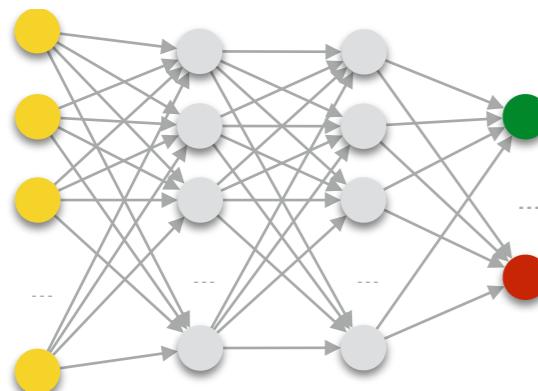
# Scalability wrt Input Space Size

Adult Census Dataset ( $L = 0.25$ ,  $U = 0.1 * |M|$ )

M	QUERY	BOXES				SYMBOLIC				DEEPPOLY			
		INPUT	C	F	TIME	INPUT	C	F	TIME	INPUT	C	F	TIME
80	F 0.009%	99.931% 0.009%	11	0 0	3m 5s	99.961% 0.009%	17	0 0	3m 2s	99.957% 0.009%	10	0 0	2m 36s
	E 0.104%	99.583% 0.104%	61	0 0	3m 6s	99.783% 0.104%	89	0 0	3m 10s	99.753% 0.104%	74	0 0	2m 44s
	D 1.042%	97.917% 1.020%	151	0 0	2m 56s	99.258% 1.034%	297	0 0	3m 41s	98.984% 1.031%	477	0 0	2m 58s
	C 8.333%	83.503% 6.958%	506	2 3	2h 1m	95.482% 7.956%	885	25 34	>13h	93.225% 7.768%	1145	23 33	12h 57m 37s
	B 50%	25.634% 12.817%	5516	7 11	1h 28m 6s	76.563% 38.281%	4917	123 182	>13h	63.906% 31.953%	7139	117 152	>13h
	A 100%	0.052% 0.052%	12	0 0	25m 51s	61.385% 61.385%	5156	73 102	10h 25m 2s	43.698% 43.698%	4757	68 88	>13h
320	F 0.009%	99.931% 0.009%	6	0 0	3m 15s	99.944% 0.009%	9	0 0	3m 35s	99.931% 0.009%	6	0 0	3m 30s
	E 0.104%	99.583% 0.104%	121	0 0	3m 39s	99.627% 0.104%	120	0 0	6m 34s	99.583% 0.104%	31	0 0	4m 22s
	D 1.042%	97.917% 1.020%	151	0 0	6m 18s	98.247% 1.024%	597	0 0	21m 9s	97.917% 1.020%	301	0 0	9m 35s
	C 8.333%	83.333% 6.944%	120	0 0	30m 37s	88.294% 7.358%	755	0 0	1h 36m 35s	83.342% 6.945%	483	0 0	52m 29s
	B 50%	25.000% 12.500%	5744	0 0	2h 24m 36s	46.063% 23.032%	4676	0 0	7h 25m 57s	25.074% 12.537%	5762	4 4	>13h
	A 100%	0.000% 0.000%	0	0 0	2h 54m 25s	24.258% 24.258%	2436	0 0	9h 41m 36s	0.017% 0.017%	4	0 0	5h 3m 33s
1280	F 0.009%	99.931% 0.009%	11	0 0	7m 35s	99.948% 0.009%	10	0 0	24m 42s	99.931% 0.009%	6	0 0	7m 6s
	E 0.104%	99.583% 0.104%	31	0 0	15m 49s	99.674% 0.104%	71	0 0	51m 52s	99.583% 0.104%	31	0 0	15m 14s
	D 1.042%	97.917% 1.020%	151	0 0	1h 49s	98.668% 1.028%	557	0 0	3h 31m 45s	97.917% 1.020%	301	0 0	1h 3m 33s
	C 8.333%	83.333% 6.944%	481	0 0	7h 11m 39s	- -	- -	>13h	83.333% 6.944%	481	0 0	7h 12m 57s	
	B 50%	- -	- -	>13h	- -	- -	>13h	- -	- -	- -	- -	>13h	
	A 100%	- -	- -	>13h	- -	- -	>13h	- -	- -	- -	- -	>13h	

# Scalability-vs-Precision Tradeoff

## Product Domain / Adult Census Dataset



23 inputs  
4 HL \* 5 N  
2 classes

L	U	Intervals	Symbolic	DeepPoly	Neurify	Product
0.5	3	37,9 %	48,8 %	48,9 %	46,5 %	<b>59,2 %</b>
	5	41,0 %	56,1 %	56,3 %	53,1 %	<b>68,2 %</b>
0.25	3	70,6 %	83,6 %	81,8 %	81,4 %	<b>87,0 %</b>
	5	83,1 %	91,7 %	91,6 %	92,3 %	<b>95,5 %</b>
L	U	Intervals	Symbolic	DeepPoly	Neurify	Product
0.5	3	47s	60s	96s	37s	<b>119s</b>
	5	246s	736s	557s	362s	<b>835s</b>
0.25	3	498s	554s	396s	420s	<b>534s</b>
	5	3369s	2674s	2840s	2920s	<b>3716s</b>

+ 10,3%

+ 11,9%

+ 3,4%

+ 3,2%

+ 23-59s

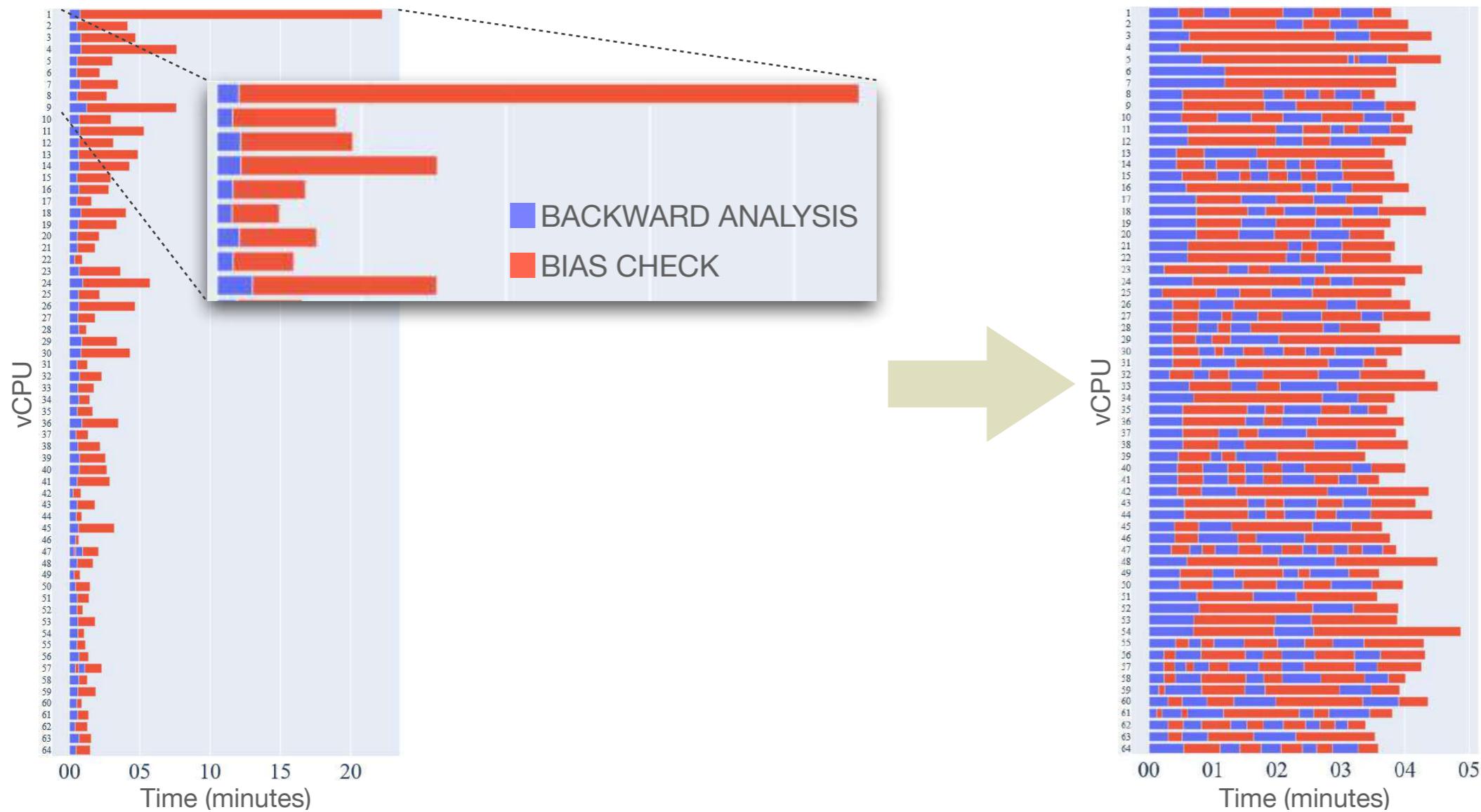
+ 99-278s

- 20s / + 36-138s

+ 796-1042s

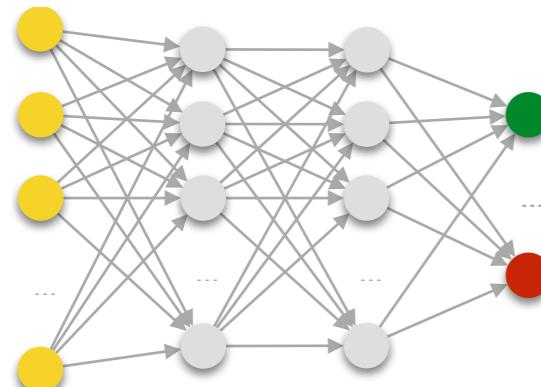
# Forward and Backward Analysis

## Perfect Parallelization



# Scalability-vs-Precision Tradeoff

Perfect Parallelization / Adult Census Dataset



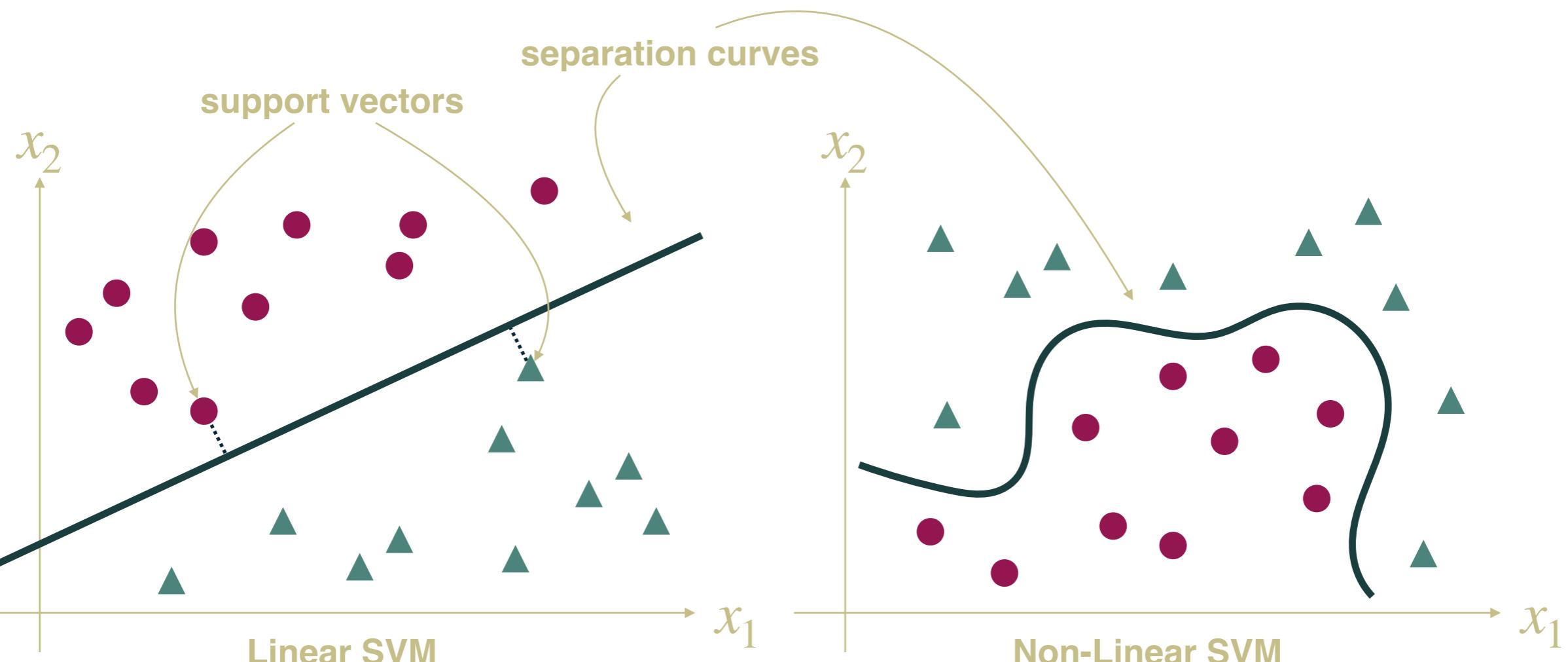
23 inputs  
4 HL \* 5 N  
2 classes

L	U	Intervals	Symbolic	DeepPoly	Neurify	Product					
0.5	3	37,9 %	48,8 %	48,9 %	46,5 %	<b>59,2 %</b>					
	5	41,0 %	56,1 %	56,3 %	53,1 %	<b>68,2 %</b>					
0.25	3	70,6 %	<b>83,6 %</b>	81,8 %	81,4 %	<b>87,0 %</b>					
	5	83,1 %	91,7 %	91,6 %	92,3 %	<b>95,5 %</b>					
L	U	Intervals	Symbolic	DeepPoly	Neurify	Product					
0.5	3	47s	<b>36s</b>	60s	<b>42s</b>	96s	<b>95s</b>	37s	<b>32s</b>	119s	<b>118s</b>
	5	246s	<b>248s</b>	736s	<b>550s</b>	557s	<b>227s</b>	362s	<b>237s</b>	835s	<b>496s</b>
0.25	3	498s	<b>349s</b>	554s	<b>355s</b>	396s	<b>320s</b>	420s	<b>320s</b>	534s	<b>432s</b>
	5	3369s	<b>1603s</b>	2674s	<b>1268s</b>	2840s	<b>1328s</b>	2920s	<b>1554s</b>	3716s	<b>1318s</b>

1.9x - 2.8x FASTER

# Other ML Models

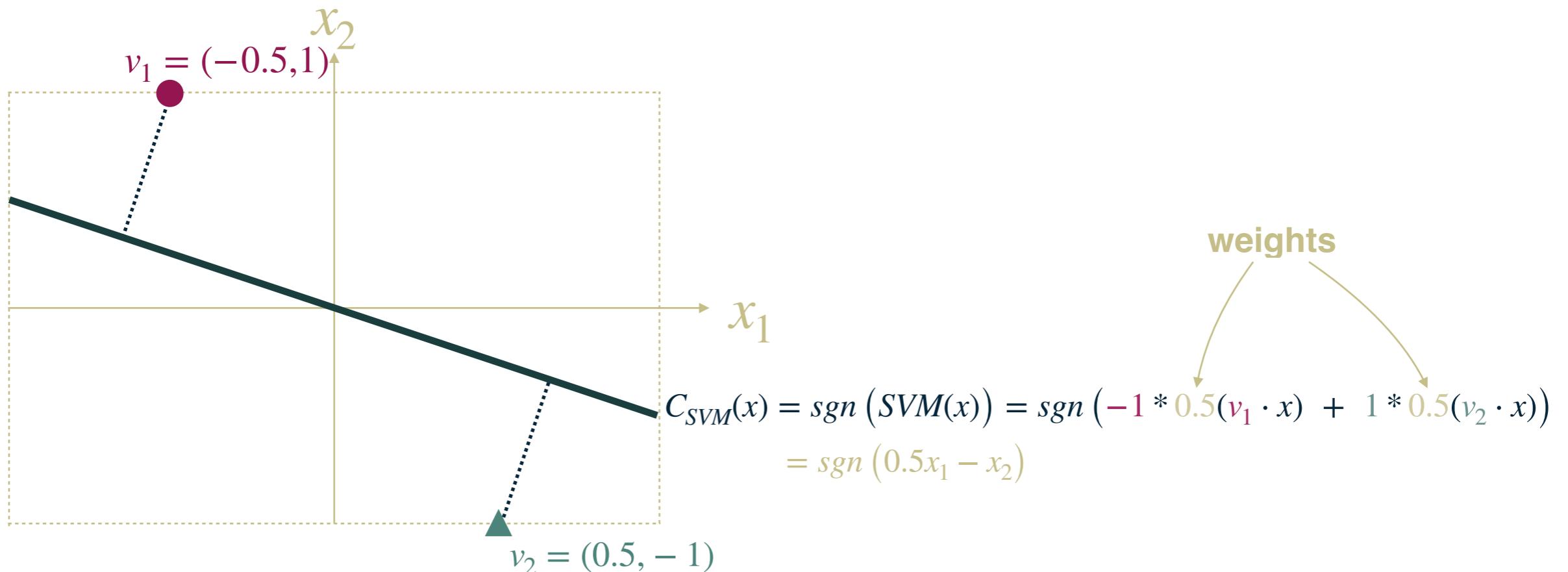
# Support Vector Machines (SVMs)



# Support Vector Machines (SVMs)

## Example

●  $\mapsto -1$   
▲  $\mapsto 1$



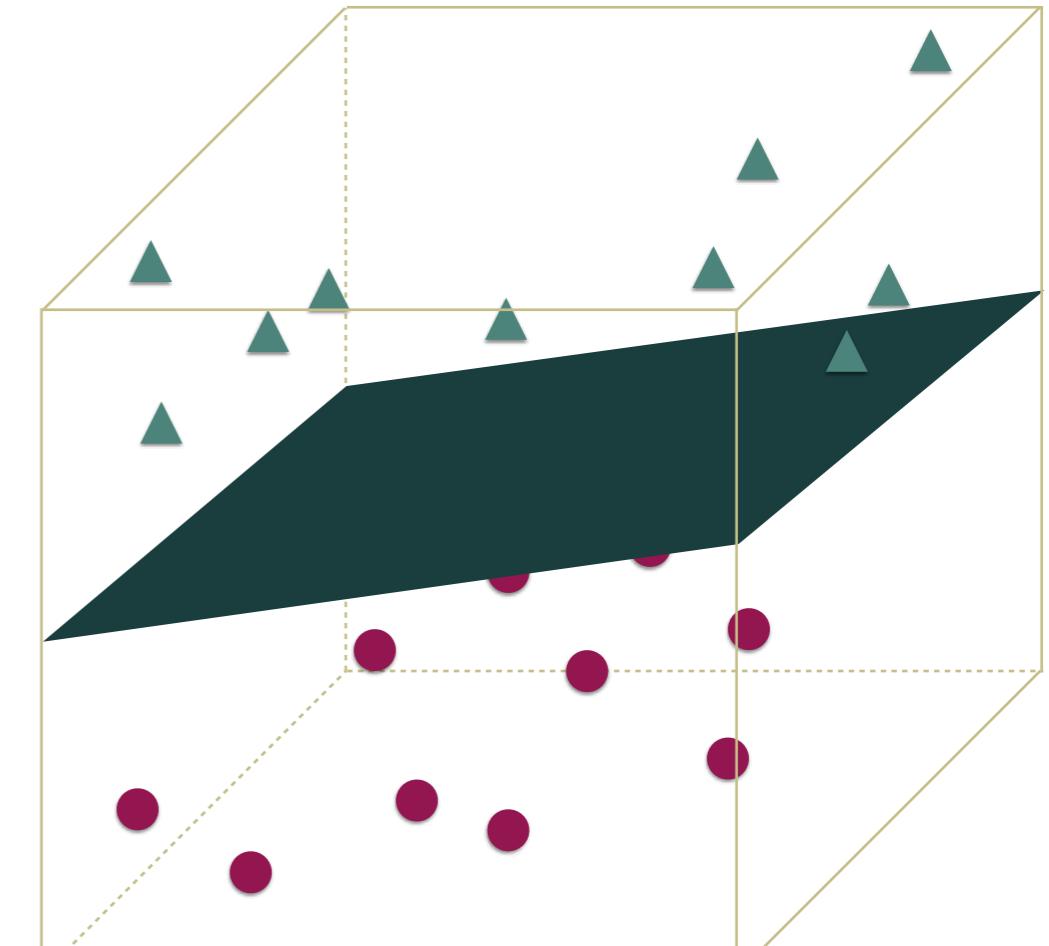
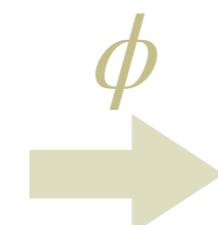
# Non-Linear SVMs

## Kernel Functions

- Polynomial
- Radial Basis Function (RBF)

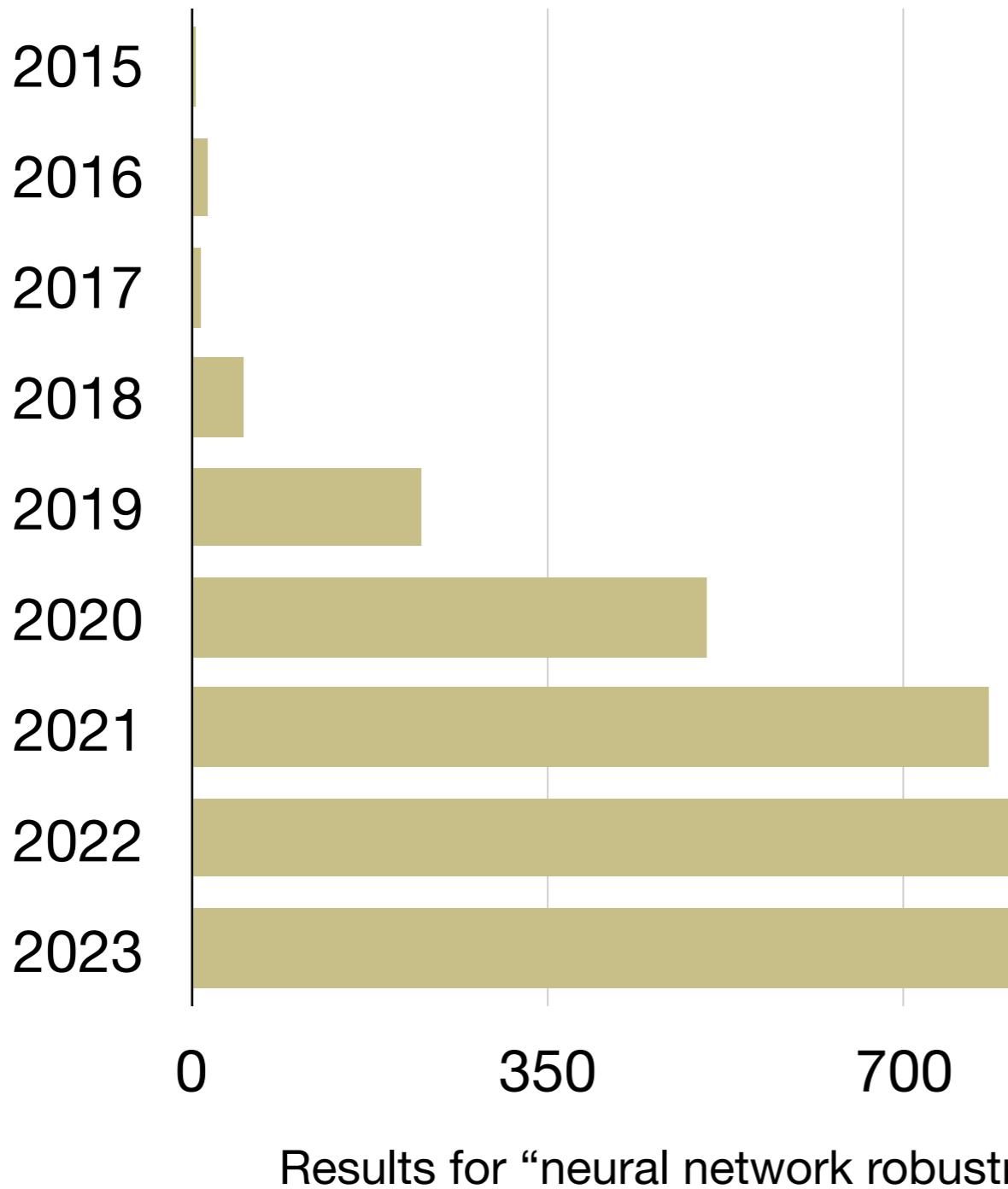


Input Space



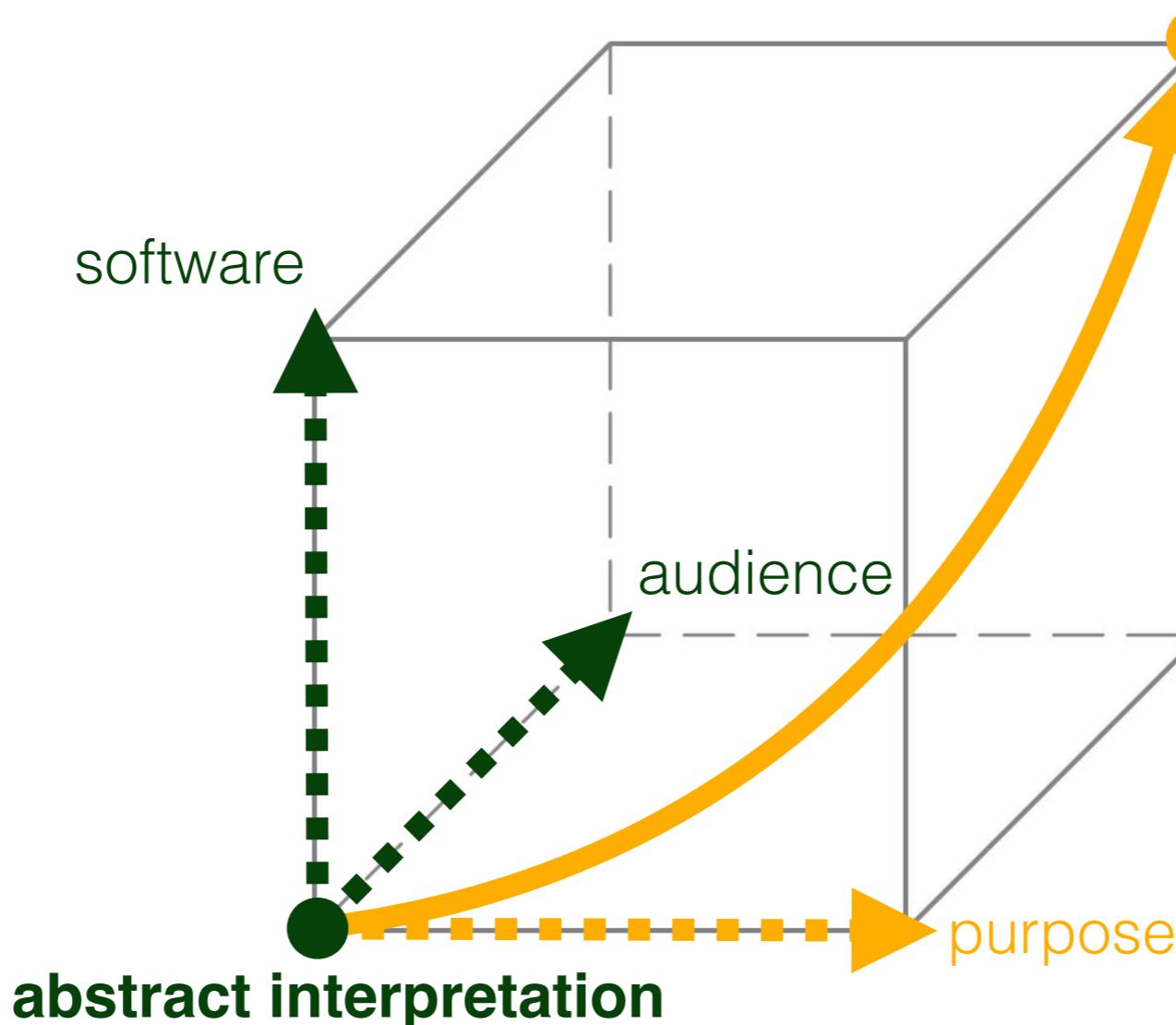
Feature Space

# Formal Methods for ML



# SVM Explainability

# Explainability



# Static Analysis Methods

# Feature Importance Measures

## Contribution of Input Features to Prediction

	Local	Global	Model-Specific		Performance-Based	Effect
			Specific	Agnostic		
Permutation Feature Importance (PFI)		X		X	X	
Partial Dependence (PD) Plots		X		X		X
Individual Conditional Expectation (ICE)		X		X		X
Accumulated Local Effects (ALE) Plots		X		X		X
Local Interpretable Model-Agnostic	X			X		X
SHapley Additive exPlanations (SHAP)	X			X		X
Individual Conditional Importance (ICI)	X			X	X	
Partial Importance (PI) Curves	X			X	X	
Shapley Feature Importance (SFIMP)		X		X	X	
Input Gradients	X			X	X	X
Abstract Feature Importance (AFI)	X	X	X			X

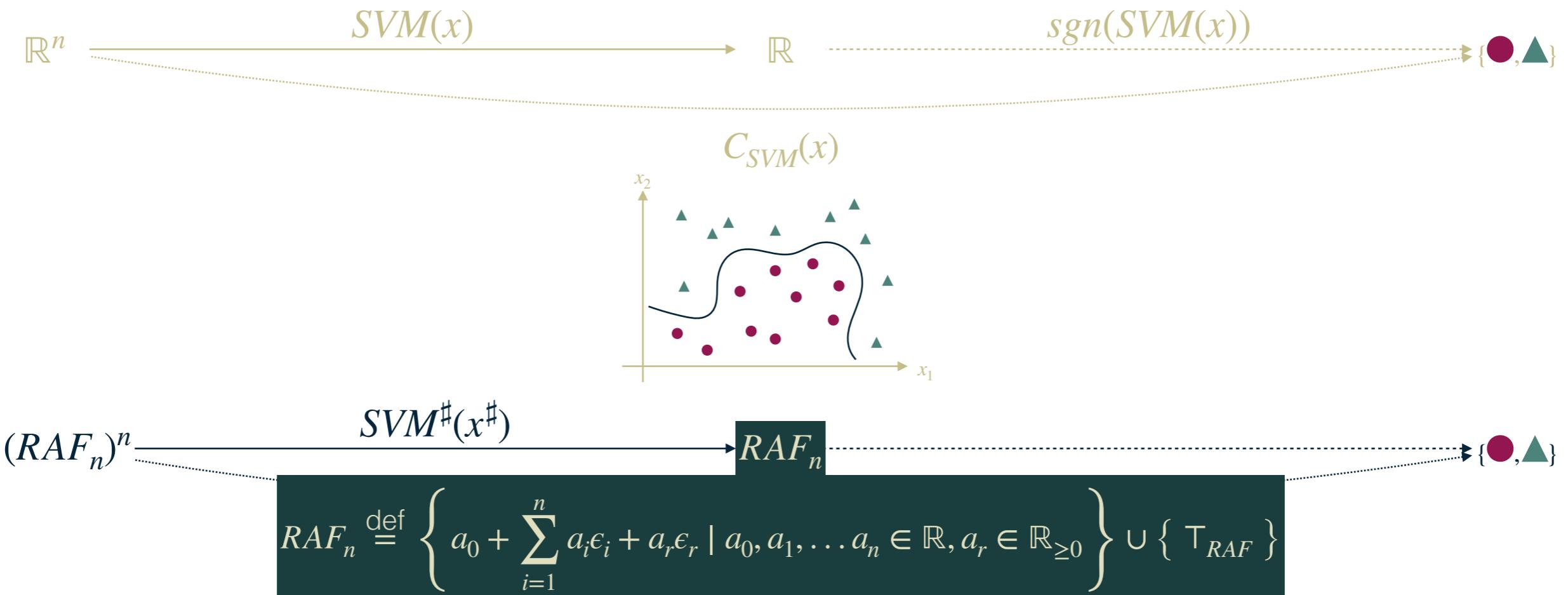
# Abstract Feature Importance [Pal2024]

## Why Another Feature Importance Measure?

Permutation Feature Importance (PFI)	<ul style="list-style-type: none"><li>• result may greatly vary depending on the dataset</li><li>• resource intensive when the number of features is large</li><li>• misleading result when features are correlated</li><li>• quality of the result heavily depends on the model accuracy</li></ul>
Local Interpretable Model-Agnostic Explanations (LIME)	<ul style="list-style-type: none"><li>• requires a large amount of data to find a meaningful optimal neighborhood: may lead to sparse and easily manipulable explanations</li><li>• assumes that the decision boundary is linear at the local level, but there is no theoretically guarantee that this is the case</li></ul>
SHapley Additive exPlanations (SHAP)	<ul style="list-style-type: none"><li>• Shapley values estimations depend on the dataset</li><li>• assumes that features are independent</li><li>• has a very high computational cost, even for small models</li></ul>
Abstract Feature Importance (AFI)	<ul style="list-style-type: none"><li>• yields a formally correct by construction approximation</li><li>• does not depend from a dataset nor the accuracy of the model</li><li>• extremely fast to compute, whatever the number of features</li><li>• supports both linear and non-linear kernel functions</li></ul>

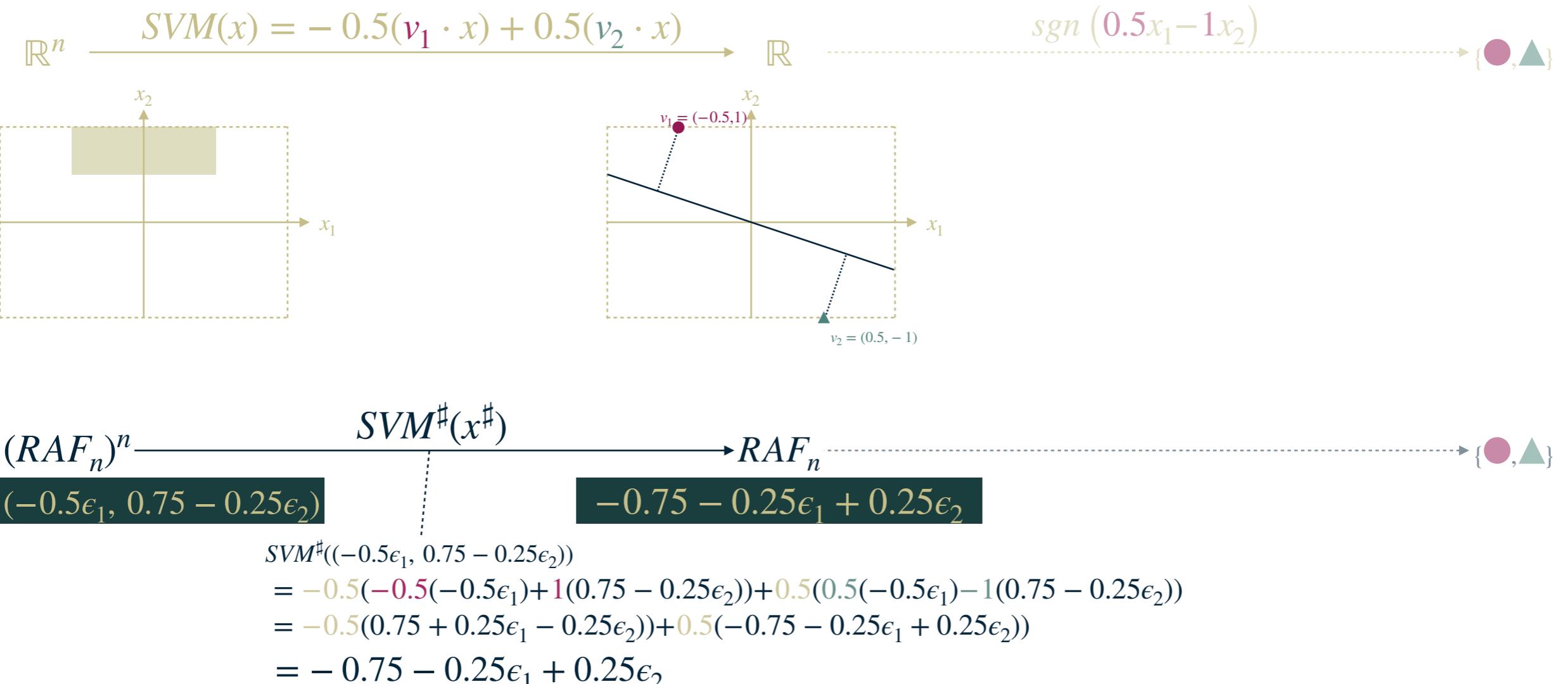
# Abstract Interpretation of SVMs<sup>[R19]</sup>

## Reduced Affine Form (RAF) Abstraction



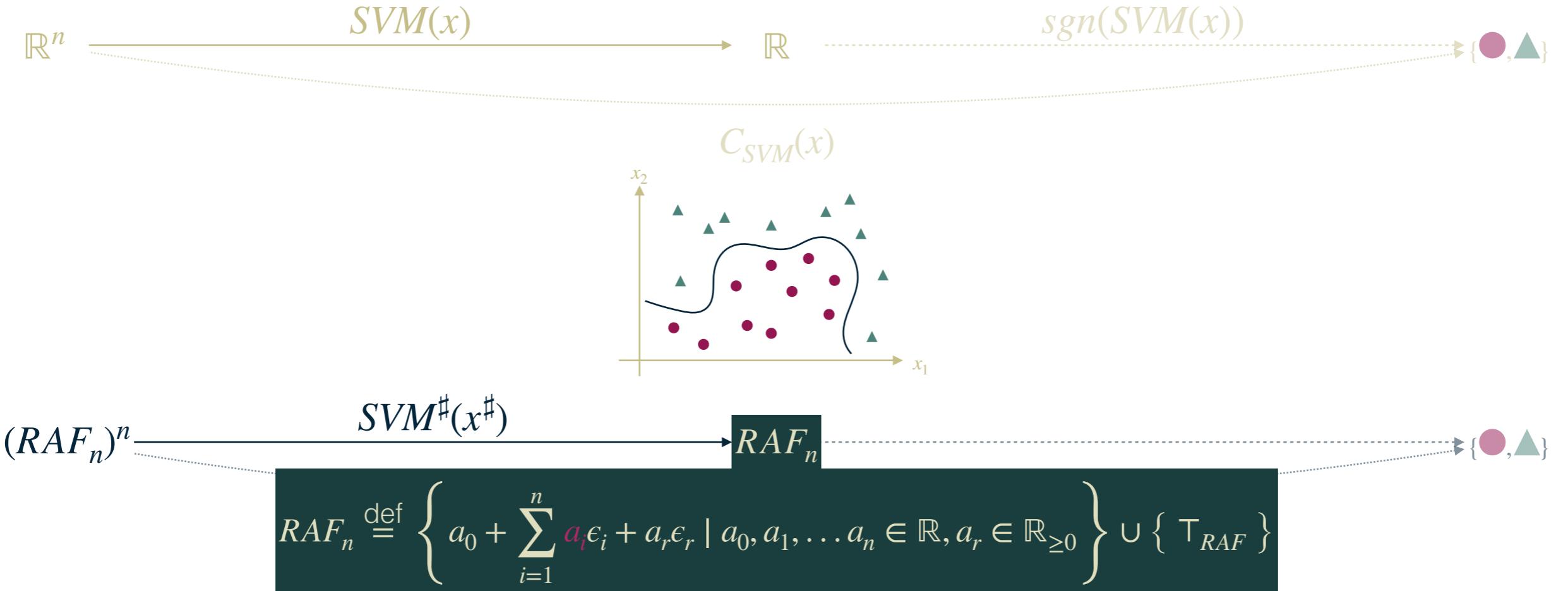
# Abstract Interpretation of SVMs

## Example



# Abstract Feature Importance

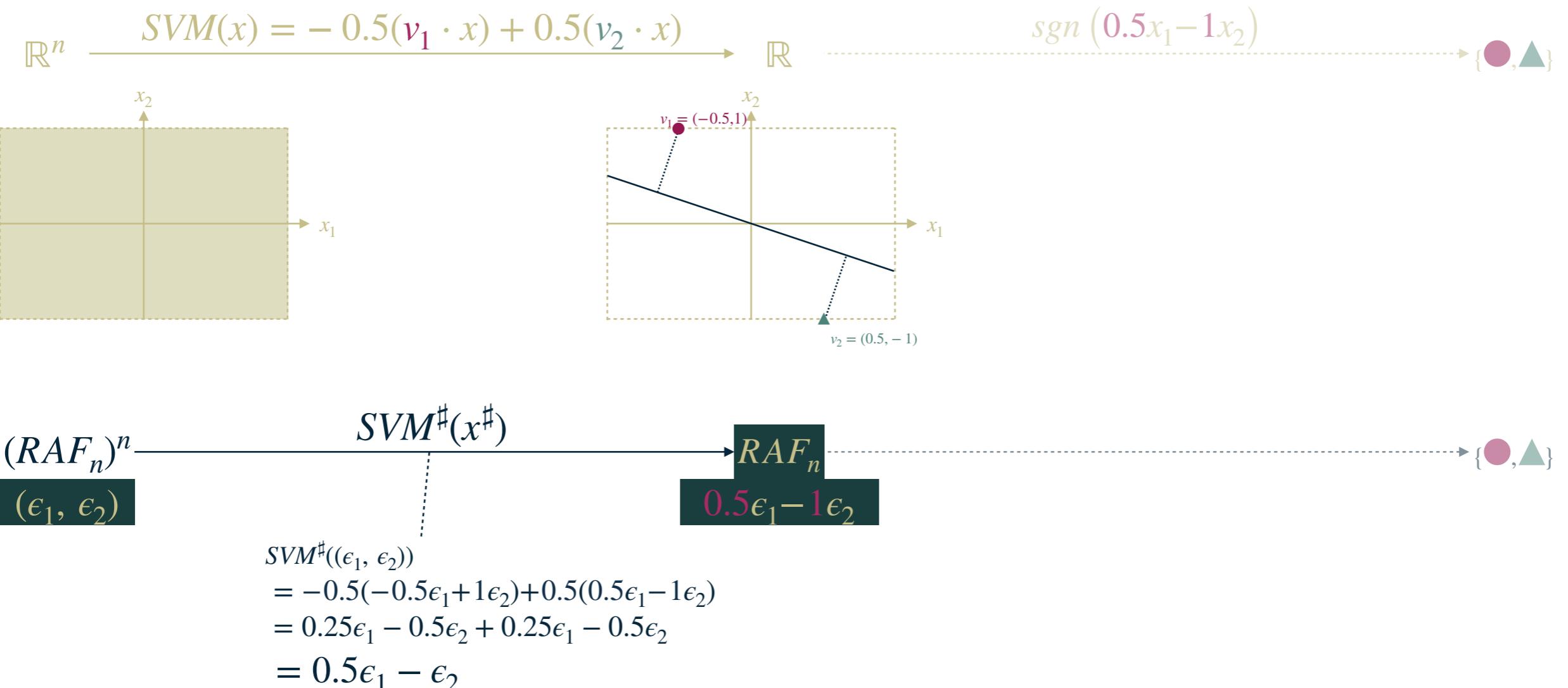
[Pal2024]



# Abstract Feature Importance

[Pal2024]

## Example



# AFI vs PFI

## German Dataset

Grade for each feature												
Linear	Baseline (13.55s)	5	5	5	6	6	7	7	7	7	8	Distance
	AFI (0.01s)	5	5	5	6	6	7	8	7	7	8	1.0
	PFI (4.07s)	5	5	6	7	7	9	6	6	7	7	3.16
RBF	Baseline (17.98s)	5	5	5	6	6	7	7	7	8	8	Distance
	AFI (0.02s)	5	6	5	6	6	8	7	7	8	7	1.73
	PFI (6.23s)	6	7	5	6	7	8	7	6	7	5	4.24
Polynomial	Baseline (15.83s)	5	5	5	6	7	7	7	7	7	8	Distance
	AFI (0.01s)	7	6	7	7	5	7	6	6	5	8	4.47
	PFI (4.15s)	6	7	9	7	6	7	5	6	6	6	5.74

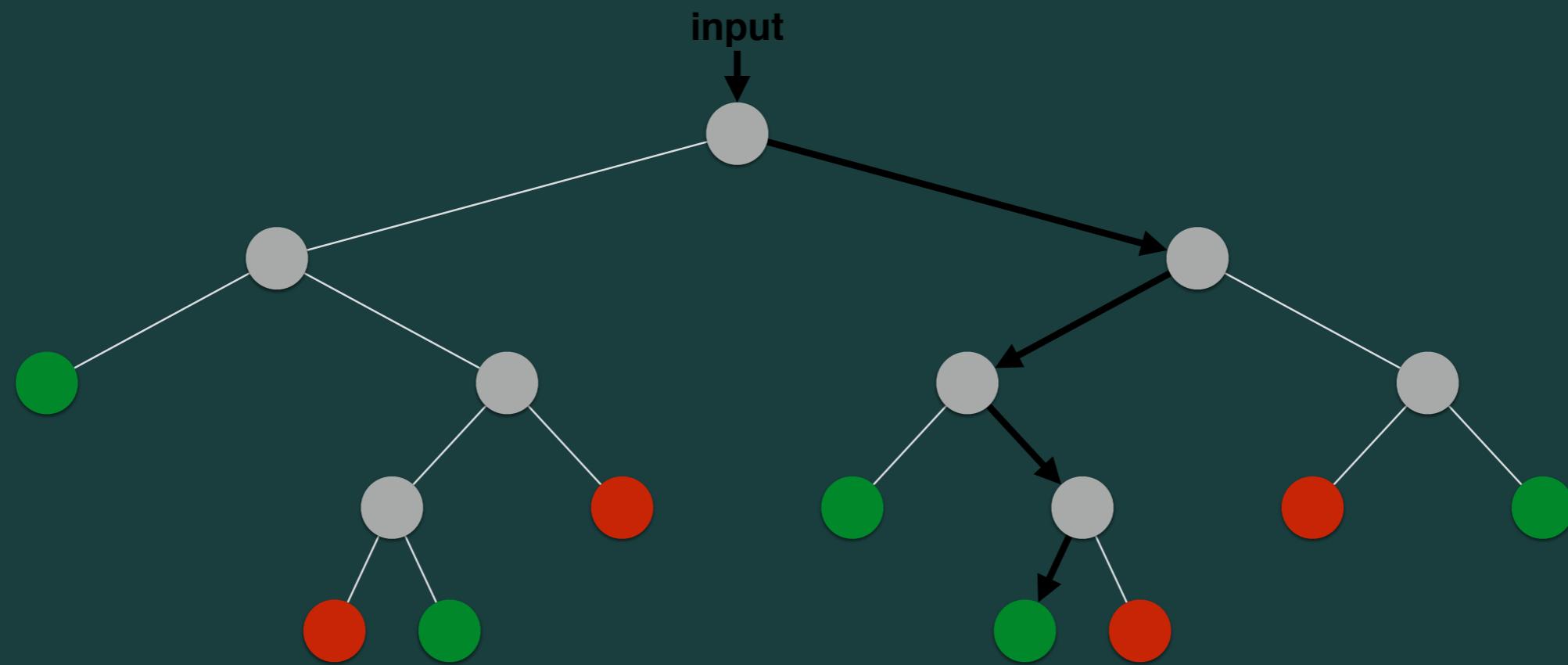
# AFI vs PFI

	Baseline	$N = 2k$ $\epsilon = 0.2$	$N = 10k$ $\epsilon = 0.2$	$N = 2k$ $\epsilon = 0.4$	$N = 10k$ $\epsilon = 0.4$	$N = 2k$ $\epsilon = 0.6$	$N = 5k$ $\epsilon = 0.6$	$N = 10k$ $\epsilon = 0.6$	$N = 2k$ $\epsilon = 0.8$	$N = 5k$ $\epsilon = 0.8$	$N = 10k$ $\epsilon = 0.8$
<b>Adult</b> Linear	AFI (0.27s)	<b>0.0</b>	<b>0.0</b>	<b>1.0</b>	<b>0.0</b>	<b>1.0</b>	<b>1.41</b>	<b>1.0</b>	<b>1.0</b>	<b>1.41</b>	<b>1.0</b>
	PFI (10009s)	2.45	2.45	2.24	2.45	2.24	<b>1.41</b>	2.24	2.24	<b>1.41</b>	2.24
<b>Adult</b> RBF	AFI (0.48s)	<b>1.0</b>	<b>1.41</b>	<b>1.41</b>	<b>1.41</b>	<b>1.73</b>	<b>1.73</b>	<b>1.41</b>	<b>1.41</b>	<b>1.41</b>	<b>1.41</b>
	PFI (25221s)	1.73	2.45	2.45	2.0	2.65	2.65	2.45	2.45	2.45	2.45
<b>Adult</b> Polynomial	AFI (0.44s)	<b>1.0</b>	<b>1.0</b>	<b>0.0</b>	1.41	<b>0.0</b>	<b>0.0</b>	<b>0.0</b>	<b>0.0</b>	<b>0.0</b>	<b>0.0</b>
	PFI (9985s)	<b>1.0</b>	<b>1.0</b>	1.41	<b>1.0</b>	1.41	1.41	1.41	1.41	1.41	1.41
<b>Compas</b> Linear	AFI (0.22s)	<b>1.41</b>	<b>1.41</b>	<b>1.73</b>	<b>1.73</b>	<b>1.41</b>	<b>1.73</b>	<b>1.41</b>	<b>1.41</b>	<b>1.41</b>	<b>1.73</b>
	PFI (1953s)	1.73	1.73	2.0	2.0	2.24	2.0	2.24	2.24	2.24	2.83
<b>Compas</b> RBF	AFI (0.27s)	<b>2.0</b>	<b>2.0</b>	<b>2.65</b>	<b>2.65</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>
	PFI (6827s)	<b>2.0</b>	<b>2.0</b>	<b>2.65</b>	<b>2.65</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>	<b>2.83</b>
<b>Compas</b> Polynomial	AFI (0.22s)	4.24	4.24	4.12	4.12	4.24	4.24	4.24	4.24	4.24	4.24
	PFI (2069s)	<b>2.45</b>	<b>2.45</b>	<b>3.0</b>	<b>3.0</b>	<b>3.74</b>	<b>3.74</b>	<b>3.74</b>	<b>3.74</b>	<b>3.74</b>	<b>3.74</b>
<b>German</b> Linear	AFI (0.01s)	<b>1.0</b>	<b>1.0</b>	<b>1.0</b>	<b>1.0</b>	<b>1.0</b>	<b>1.0</b>	<b>1.0</b>	<b>1.41</b>	<b>1.73</b>	<b>1.41</b>
	PFI (4.07s)	3.16	3.46	3.16	3.16	3.16	3.16	3.16	3.6	3.74	3.0
<b>German</b> RBF	AFI (0.02s)	<b>1.73</b>	<b>1.0</b>	<b>1.73</b>	<b>1.73</b>	<b>2.0</b>	<b>1.41</b>	<b>1.73</b>	<b>1.73</b>	<b>2.0</b>	<b>2.24</b>
	PFI (6.23s)	4.0	3.46	4.24	4.24	4.36	3.61	4.24	4.24	4.36	4.47
<b>German</b> Polynomial	AFI (0.01s)	<b>4.90</b>	<b>4.12</b>	<b>4.47</b>	<b>3.87</b>	<b>3.87</b>	<b>4.24</b>	<b>3.46</b>	<b>3.46</b>	<b>3.46</b>	<b>3.46</b>
	PFI (4.15s)	5.74	5.10	5.74	4.69	4.69	5.0	4.58	4.58	4.58	4.58

# AFI vs LIME

Distance between LIME and ...	Adult			Compas			German		
	Lin.	RBF	Poly	Lin.	RBF	Poly	Lin.	RBF	Poly
AFI ( $\epsilon = 0.1$ )	2.42	2.04	2.98	1.67	1.06	3.05	2.62	2.03	<b>5.31</b>
AFI ( $\epsilon = 0.2$ )	1.68	1.32	2.67	1.63	0.17	2.73	2.21	2.00	5.41
AFI ( $\epsilon = 0.3$ )	1.39	0.51	2.58	<b>1.57</b>	0.14	<b>2.62</b>	1.92	2.05	5.45
AFI (Global)	<b>1.37</b>	<b>0.01</b>	<b>1.01</b>	<b>1.57</b>	<b>0.13</b>	3.16	<b>1.90</b>	<b>1.89</b>	5.53

# Decision Tree Ensembles



- **A. Kantchelian, J. D. Tygar, and A. Joseph.** *Evasion and Hardening of Tree Ensemble Classifiers*. In ICML 2016.  
**H. Chen, H. Zhang, S. Si, Y. Li, D. Boning, and C.-J. Hsieh.** *Robustness Verification of Tree-based Models*. In NeurIPS 2019.  
approaches for finding the **nearest adversarial example**

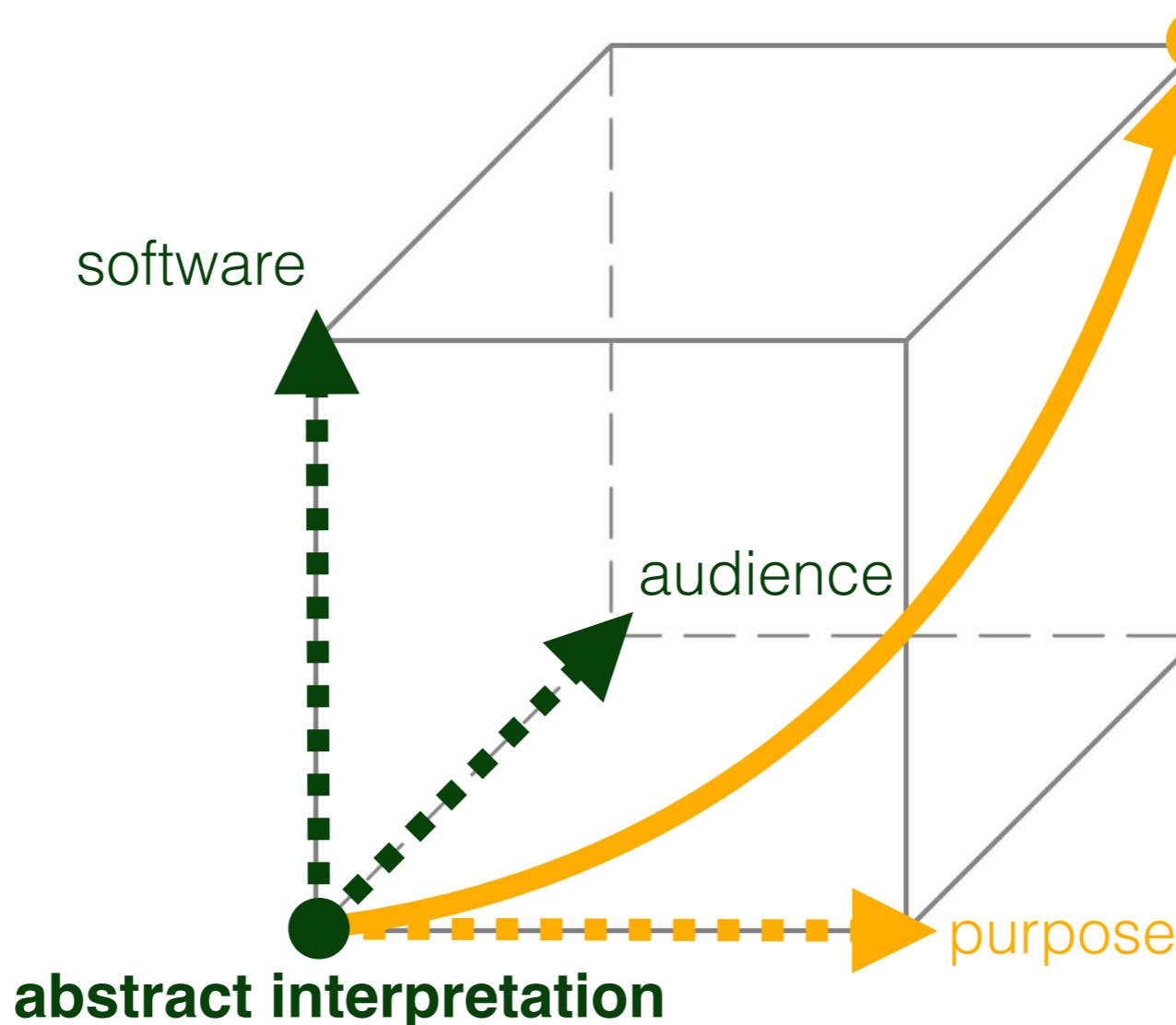
# Decision Tree Ensembles

- **N. Sato, H. Kuruma, Y. Nakagawa, and H. Ogawa.** *Formal Verification of Decision-Tree Ensemble Model and Detection of its Violating-Input-Value Ranges.* 2020.  
**approach for safety verification**
- **G. Einziger, M. Goldstein, Y. Sa'ar, and I. Segall.** *Verifying Robustness of Gradient Boosted Models.* In AAAI 2019.  
**SMT-based approach for local robustness**
- **J. Törnblom and S. Nadjm-Tehrani.** *Formal Verification of Input-Output Mappings of Tree Ensembles.* 2020.  
**F. Ranzato and M. Zanella.** *Abstract Interpretation of Decision Tree Ensemble Classifiers.* In AAAI 2020.  
**S. Calzavara, P. Ferrara, and C. Lucchese.** *Certifying Decision Trees Against Evasion Attacks by Program Analysis.* In ESORICS 2020.  
**abstract interpretation-based approaches for local robustness**

# Formal Methods for Model Training

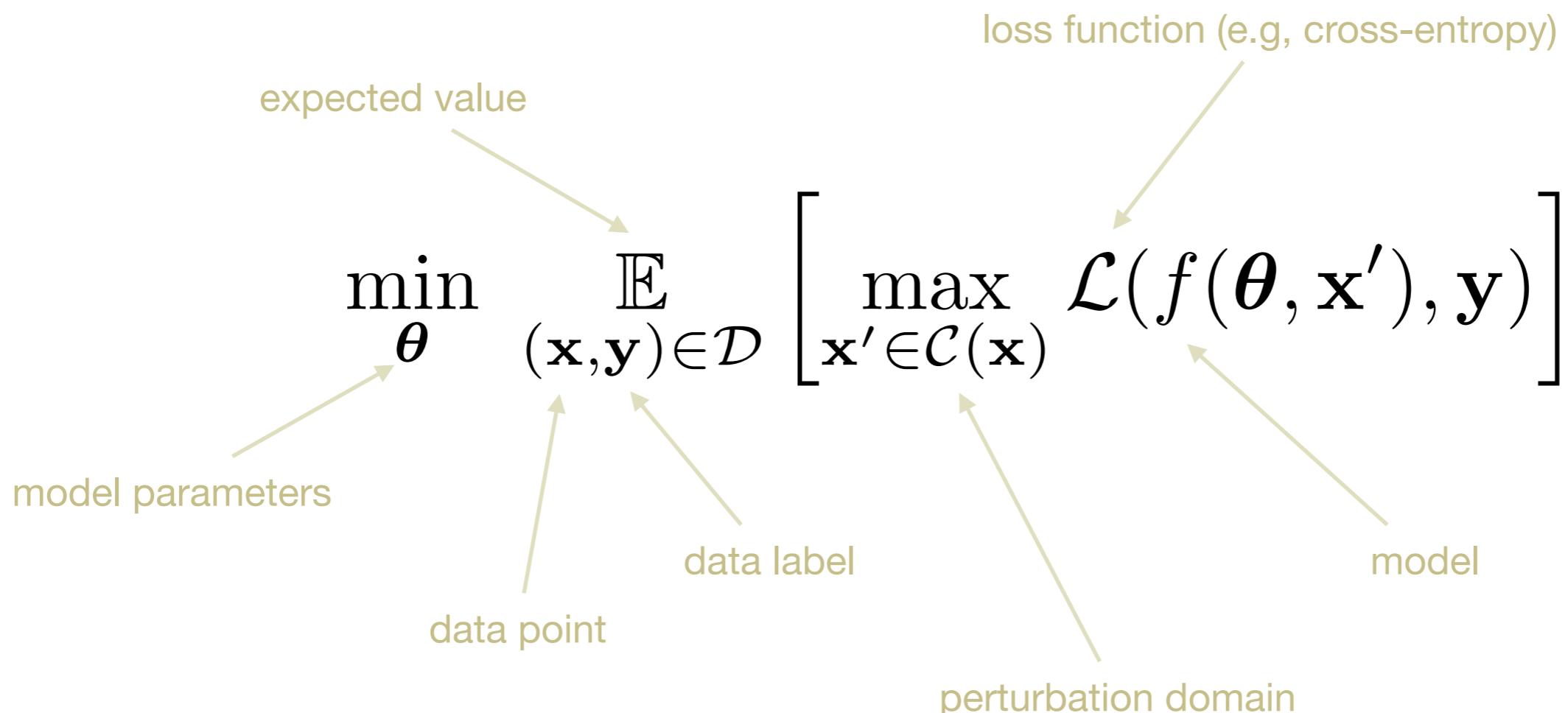


# Formal Methods for Training



# Robust Training

Minimizing the Worst-Case Loss for Each Input

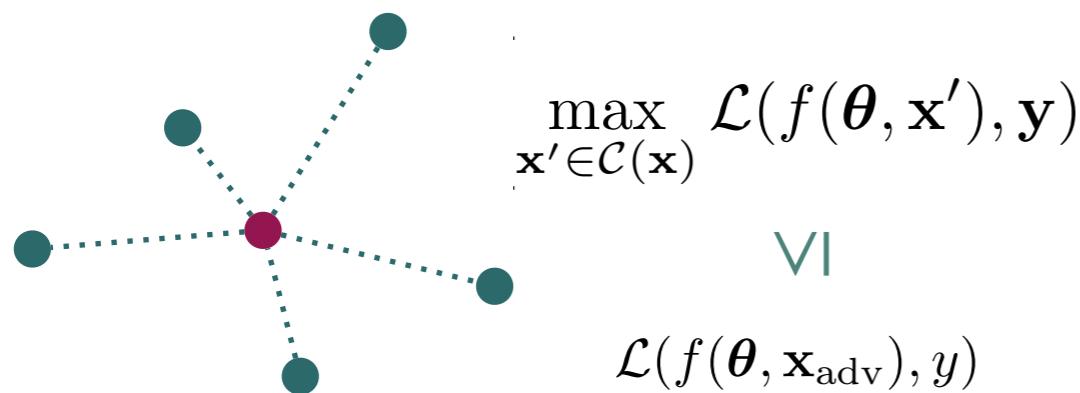


# Robust Training

Minimizing the Worst-Case Loss for Each Input

## Adversarial Training

Minimizing a Lower Bound on the  
Worst-Case Loss for Each Input



generate adversarial inputs  
and use them as training data

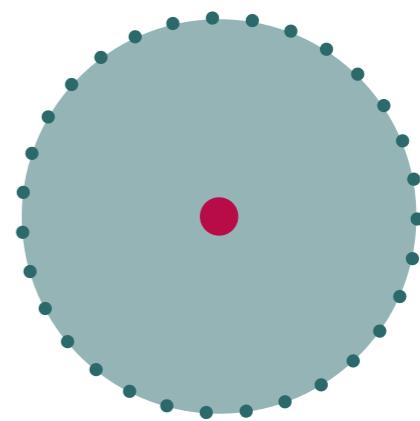
## Certified Training

Minimizing an Upper Bound on the  
Worst-Case Loss for Each Input

$$\max_{\mathbf{x}' \in \mathcal{C}(\mathbf{x})} \mathcal{L}(f(\boldsymbol{\theta}, \mathbf{x}'), \mathbf{y})$$

$\wedge$

$$\mathcal{L}_{\text{ver}}(f(\boldsymbol{\theta}, \mathbf{x}), y)$$



use upper bound as regularizer  
to encourage robustness

# Certified Training

- **M. Andriushchenko, and M. Hein.** *Provably Robust Boosted Decision Stumps and Trees Against Adversarial Attacks.* In NeurIPS 2019.  
approach targeting **decision trees**
- **M. Hein and M. Andriushchenko.** *Formal Guarantees on the Robustness of a Classifier Against Adversarial Manipulation.* In NeurIPS 2017.  
**E. Wong and Z. Kolter.** *Provable Defenses Against Adversarial Examples via the Convex Outer Adversarial Polytope.* In ICML, 2018.  
**A. Raghunathan, J. Steinhardt, and P. Liang.** *Certified Defenses against Adversarial Examples.* In ICML, 2018.  
approaches targeting **neural networks**

# Certified Training

- **M. Mirman, T. Gehr, and M. Vechev.** *Differentiable Abstract Interpretation for Provably Robust Neural Networks* In ICML 2018.  
**abstract interpretation-based approach targeting neural networks**
- **F. Ranzato and M. Zanella.** *Genetic Adversarial Training of Decision Trees.* In GECCO 2021.  
**abstract interpretation-based approach targeting decision trees**

# Certified Training

## Empirical Robustness

Table 7: Comparison of the standard (Acc.), adversarial (Adv. Acc), and certified (Cert. Acc.) accuracy for different certified training methods on the full CIFAR-10 test set. We use MN-BAB (Ferrari et al., 2022) to compute all certified and adversarial accuracies.

$\epsilon_\infty$	Training Method	Source	Acc. [%]	Adv. Acc. [%]	Cert. Acc. [%]
2/255	COLT	Balunovic & Vechev (2020)	78.42	<b>66.17</b>	61.02
	CROWN-IBP	Zhang et al. (2020) <sup>†</sup>	71.27	59.58	58.19
	IBP	Shi et al. (2021)	-	-	-
	SABR	this work	<b>79.52</b>	65.76	<b>62.57</b>
8/255	COLT	Balunovic & Vechev (2020)	51.69	31.81	27.60
	CROWN-IBP	Zhang et al. (2020) <sup>†</sup>	45.41	33.33	33.18
	IBP	Shi et al. (2021)	48.04	35.43	<b>35.30</b>
	SABR	this work	<b>52.00</b>	<b>35.70</b>	35.25

ROBUSTBENCH Leaderboards Paper FAQ Contribute Model Zoo 🚀

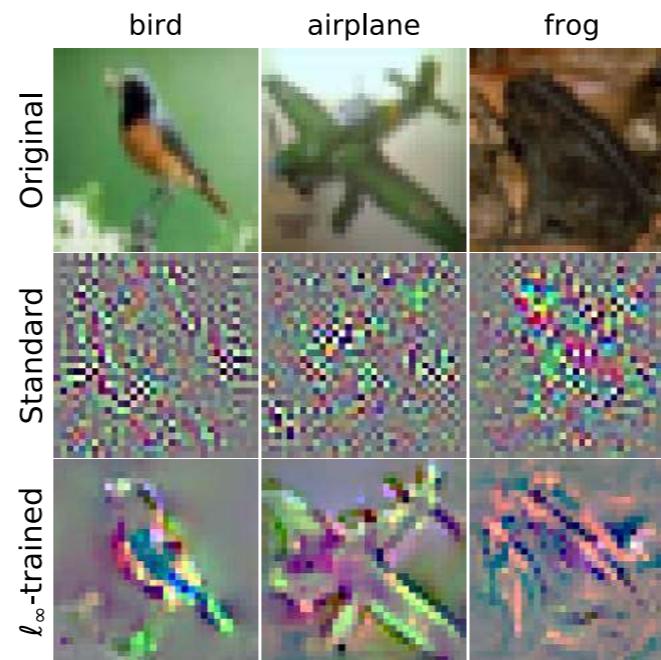
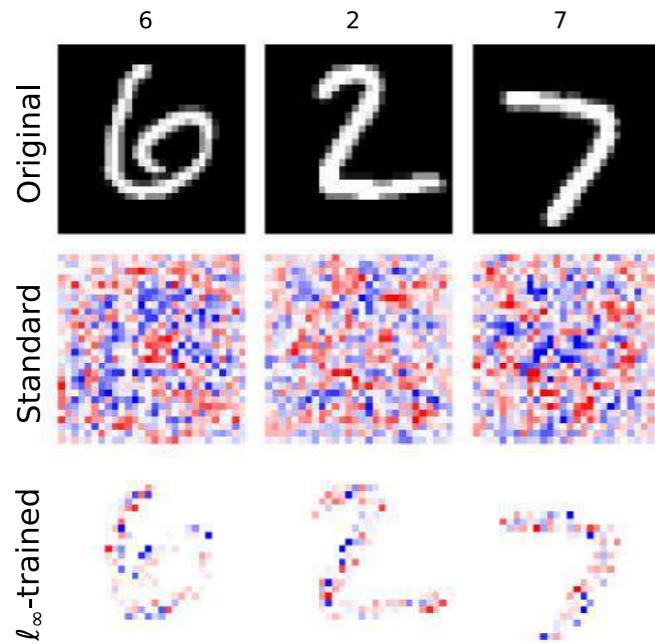
Leaderboard: CIFAR-10,  $\ell_\infty = 8/255$ , untargeted attack

Show 15 entries Search: Papers, architectures, v

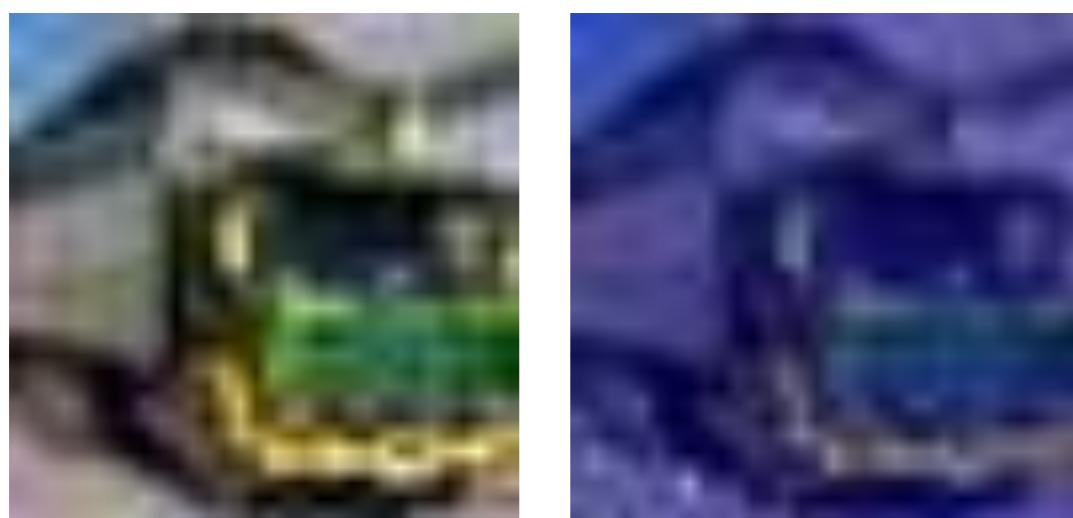
Rank	Method	Standard accuracy	AutoAttack robust accuracy	Best known robust accuracy	AA eval. potentially unreliable	Extradata	Architecture	Venue
1	Robust Principles: Architectural Design Principles for Adversarially Robust CNNs <small>It uses additional 50M synthetic images in training.</small>	93.27%	71.07%	71.07%	X	X	RaWideResNet-70-16	BMVC 2023

# Robust Training

## Perceptually Aligned Gradients



Adversarial Training



Certified Training

Fig. 6. Input Image

Fig. 7. Integrated Gradients

# Robust Training

Minimizing the Worst-Case Loss for Each Input

## Adversarial Training

Minimizing a Lower Bound on the  
Worst-Case Loss for Each Input

## Certified Training

Minimizing an Upper Bound on the  
Worst-Case Loss for Each Input

## Hybrid Training

$$(1 - \alpha) \mathcal{L}(f(\theta, \mathbf{x}_{\text{adv}}), y) + \alpha \mathcal{L}_{\text{ver}}(f(\theta, \mathbf{x}), y)$$

# Hybrid Training

[Ranzato21]

## Random Forests

Dataset	FATT			Natural CART			CART with Hints		
	Accuracy %	Fairness %	Size	Accuracy %	Fairness %	Size	Accuracy %	Fairness %	Size
Adult	80.84	95.21	43	85.32	77.56	270	84.77	87.46	47
Compas	64.11	85.98	75	65.91	22.25	56	65.91	22.25	56
Crime	79.45	75.19	11	77.69	24.31	48	77.44	60.65	8
German	72.00	99.50	2	75.50	57.50	115	73.50	86.00	4
Health	77.87	97.03	84	83.85	79.98	2371	82.25	93.64	100
Average	74.85	<b>90.58</b>	<b>43</b>	<b>77.65</b>	52.32	572	76.77	70.00	<b>43</b>



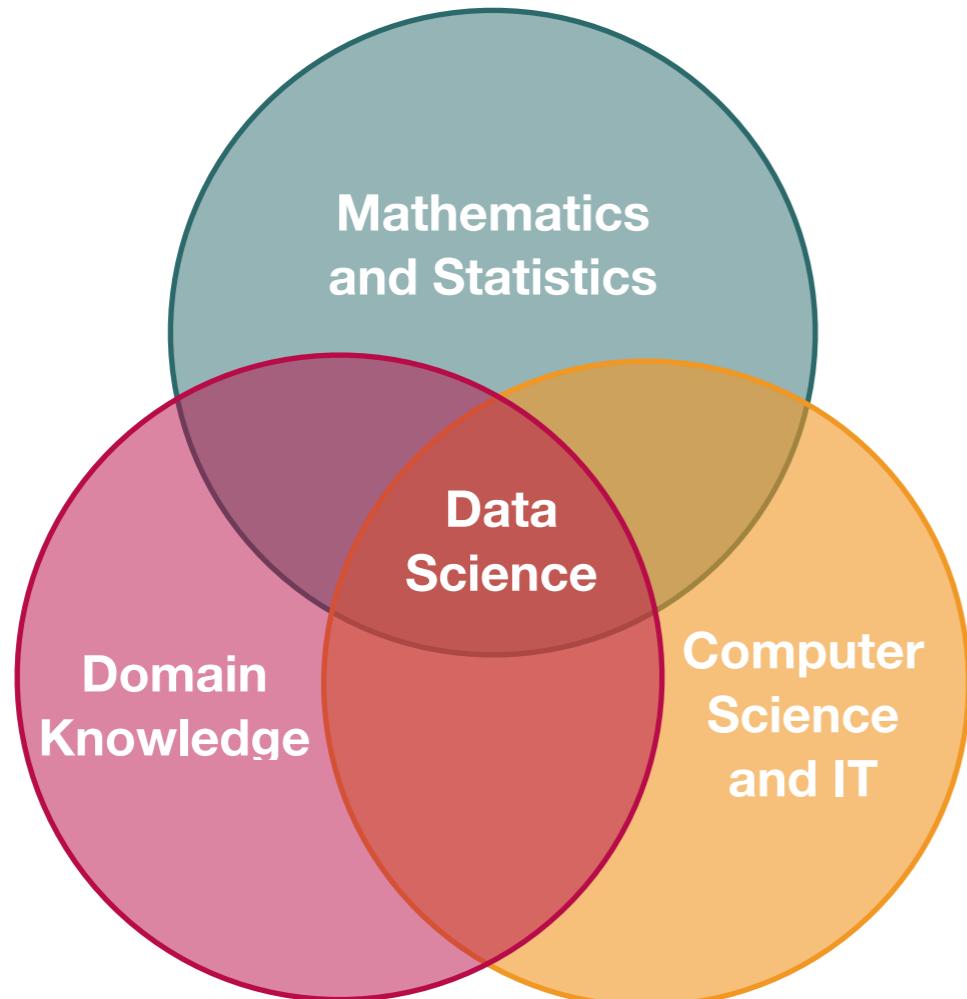
# Hybrid Training

- **Mark Niklas Müller, Franziska Eckert, Marc Fischer, and Martin Vechev.**  
Certified training: Small Boxes Are All You Need. In ICLR, 2023.  
**one of the first instances of hybrid training**
- **Alessandro De Palma, Rudy Bunel, Krishnamurthy Dvijotham, M. Pawan Kumar, Robert Stanforth, Alessio Lomuscio.** Expressive Losses for Verified Robustness via Convex Combinations. In ICLR, 2024.  
**characterization of expressive losses for hybrid training**

# Formal Methods for Data Preparation



# Data Scientists



## Data Scientist: The Sexiest Job of the 21st Century

Andrew McAfee and Erik Brynjolfsson

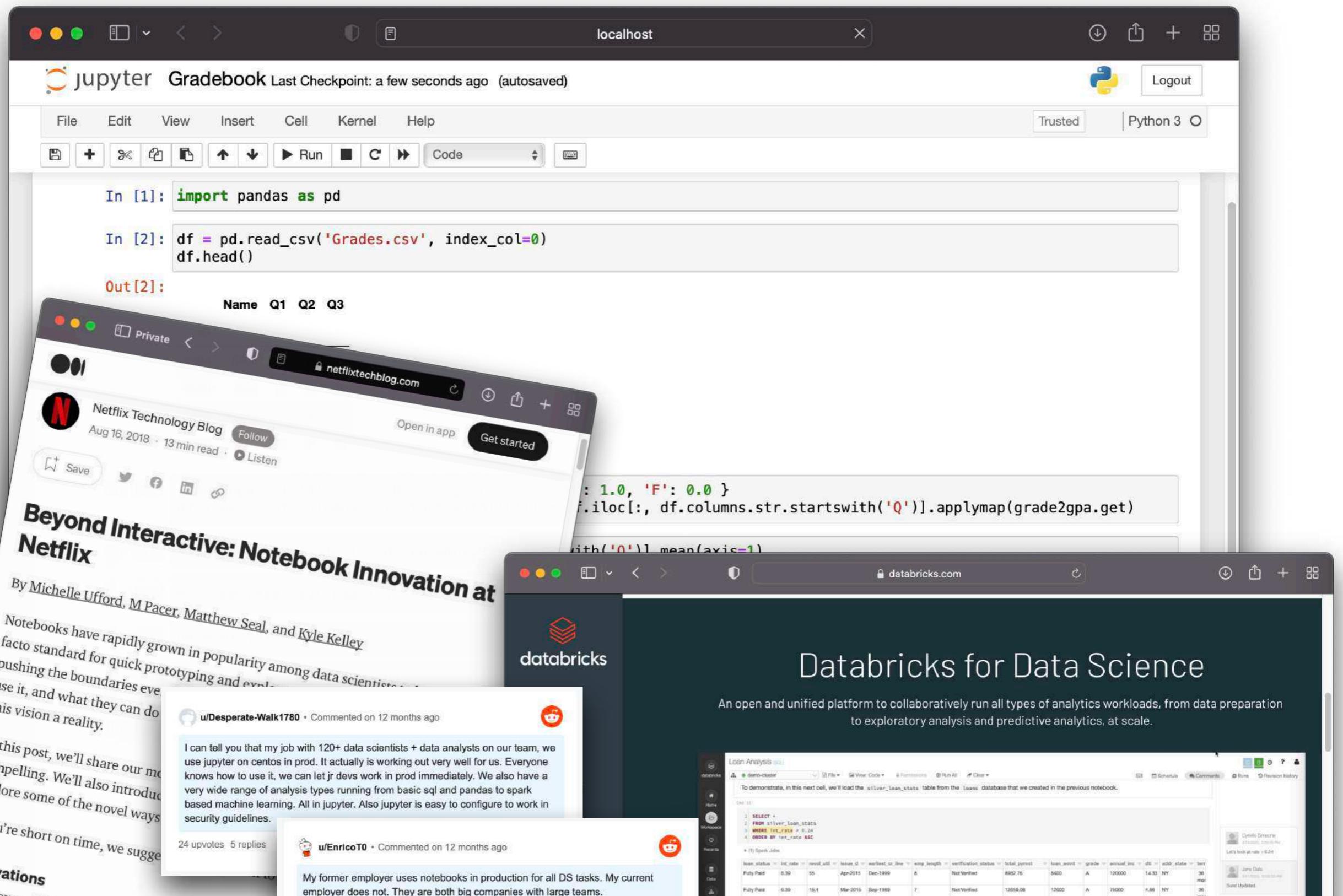


Andrew J Buboltz, silk screen on a page from a high school yearbook, 8.5" x 12", 2011 Tamar Cohen

When Jonathan Goldman arrived for work in June 2006 at [LinkedIn](#), the business networking site, the place still felt like a start-up. The company had just under 8 million accounts, and the number was growing quickly as existing members invited their friends and colleagues to join. But users weren't seeking out connections with the people who were already on the site at the rate executives had expected. Something was apparently missing in the social experience. As one LinkedIn manager put it, "It was like arriving at a conference reception and realizing you don't know

like anyone at a conference reception and realizing you don't know anyone in the social experience. As one LinkedIn manager put it, "It was like arriving at a conference reception and realizing you were the only people who were able to make connections with the people who were there."

# Jupyter Notebooks



# Jupyter Notebooks



UNUSED DATA

```
[1] 1 d = genfromtxt('data.csv')
[2] 1 selector = SelectKBest(k=25)
  2 x = selector.fit_transform(d)
[3] 1 x = genfromtxt('data2.csv')
[4] 1 x_train, x_test, y_train, y_test =
  2 train_test_split(x, ...)
[5] 1 lr = LogisticRegression()
  2 lr.fit(x_train, y_train)
  3 y_pred = lr.predict(x_test)
```

A Jupyter Notebook code cell visualization. On the left, five numbered code cells are shown in a vertical stack. Cell [1] loads data from 'data.csv'. Cell [2] uses a SelectKBest selector and fits it to the data. Cell [3] loads data from 'data2.csv'. Cell [4] splits the data into training and testing sets. Cell [5] creates a LogisticRegression model, fits it to the training data, and makes predictions on the test data. To the right of the cells is a yellow rectangular area containing the text 'UNUSED DATA' in white capital letters. Above this text is a yellow triangle warning sign with a black exclamation mark in the center. A thick orange curved arrow on the far left points from the bottom of cell [1] towards the warning sign, indicating that the data loaded in cell [1] is not used in any subsequent cells.

# Jupyter Notebooks

```
[1] 1 d = genfromtxt('data.csv')
[2] 1 selector = SelectKBest(k=25)
2 x = selector.fit_transform(d)
[3] 1 x = genfromtxt('data2.csv')
[4] 1 x_train, x_test, y_train, y_test =
2 train_test_split(x, ...)
[5] 1 lr = LogisticRegression()
2 lr.fit(x_train, y_train)
3 y_pred = lr.predict(x_test)
```

! DATA LEAK

# Jupyter Notebooks

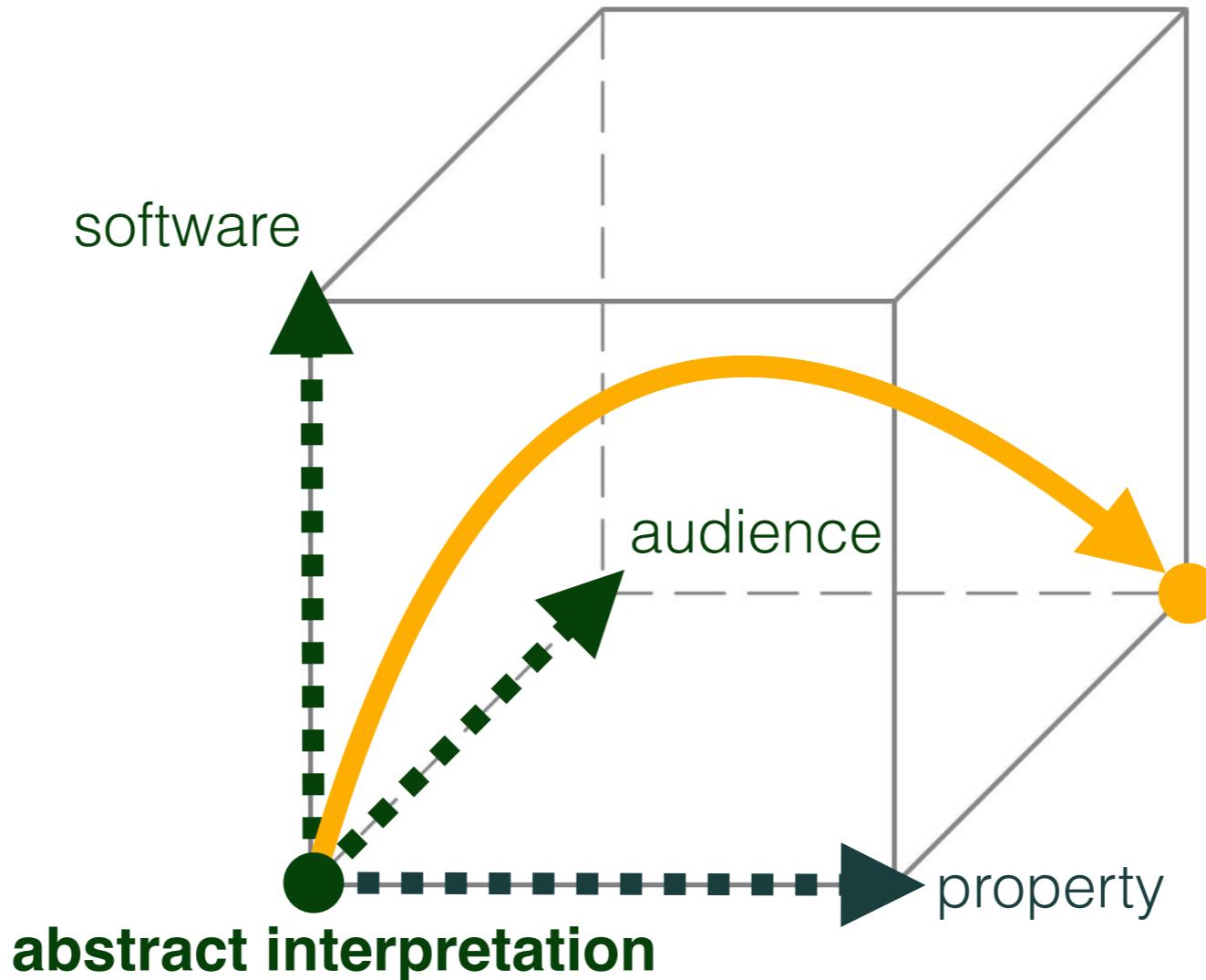
```
[1] 1 d = genfromtxt('data.csv')
[2] 1 selector = SelectKBest(k=25)
2 x = selector.fit_transform(d)
[3] 1 x = genfromtxt('data2.csv')
[4] 1 x_train, x_test, y_train, y_test =
2 train_test_split(x, ...)
[5] 1 lr = LogisticRegression()
2 lr.fit(x_train, y_train)
3 y_pred = lr.predict(x_test)
```

**STALE DATA**



# Anomalously Unused Data

# (Un)used Data Analysis



# The Reinhart-Rogoff Paper

## FAQ: Reinhart, Rogoff, and the Excel Error That Changed History

By Peter Coy  | April 18, 2013

### The Excel Depression

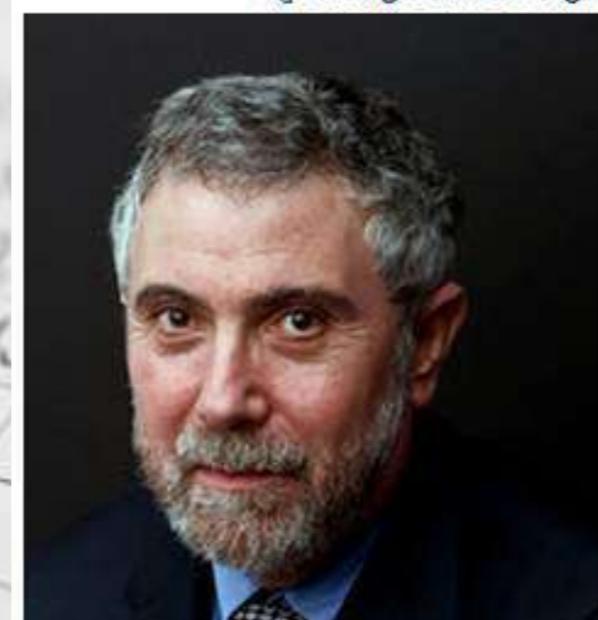
By PAUL KRUGMAN

Published: April 18, 2013 |  470 Comments



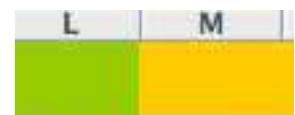
In this age of information, math errors can lead to disaster. NASA's [Mars Orbiter crashed](#) because engineers forgot to convert to metric measurements; JPMorgan Chase's "[London Whale](#)" venture went [bad](#) in part because modelers divided by a sum instead of an average. So, did an Excel coding error destroy the economies of the Western world?

 [Enlarge This Image](#)



The story so far: At the beginning of 2010, two Harvard economists, Carmen Reinhart and Kenneth Rogoff, circulated a paper, "[Growth in a Time of Debt](#)," that purported to identify a critical "threshold," a tipping point, for government indebtedness. Once debt exceeds 90 percent of gross domestic product, they claimed, economic growth drops off sharply.

Ms. Reinhart and Mr. Rogoff had credibility thanks to a



 FACEBOOK

 TWITTER

 GOOGLE+

 SAVE

 EMAIL

 SHARE

 PRINT

 REPRINTS

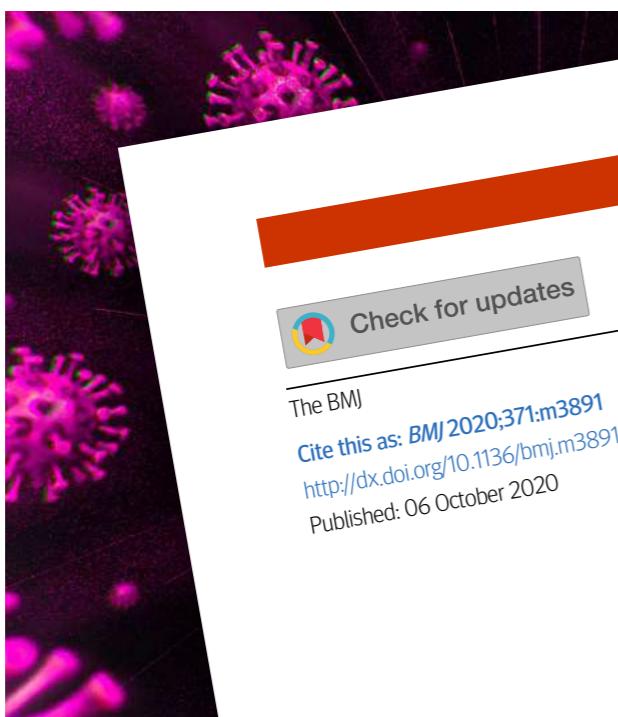
# England Covid-19 Cases Error

SCIENCE \ US & WORLD \ TECH \

## Excel spreadsheet error blamed for UK's 16,000 missing coronavirus cases

*The case went missing after the spreadsheet hit its filesize limit*

By James Vincent | Oct 5, 2020, 9:41am EDT



### Covid-19: Only half of 16 000 patients missed from England's official figures have been contacted

Elisabeth Mahase

Details of nearly 16 000 cases of covid-19 were not transferred to England's NHS Test and Trace service and were missed from official figures because of an error in the process for updating the data.

England's health and social care secretary, Matt Hancock, told the House of Commons on Monday 5 October that after the error was discovered on Friday 2 October "6500 hours of extra contact tracing" had been carried out over the weekend. But as at Monday morning only half (51%) of the people had been reached by contact tracers.

In response, Labour's shadow health secretary, Keir Starmer, said, "Thousands of people are exposed to covid, and we must make sure that they can get tested and traced."

data and furthermore have issued guidance on validation and risk management for these products if they are to be used in such a safety critical manner."

The error came as the Labour Party's leader, Keir Starmer, said that the prime minister had "lost control" of covid-19, with no clear strategy for beating it. Speaking to the Observer, Starmer set out his five point plan for covid-19, which starts with publishing the criteria for local restrictions, as the German government did. Secondly, he said public health messaging should be improved by adding a feature to the NHS covid-19 app so people can search their postcode and find out their local restrictions.

Starmer has also said he would fix the contact tracing system by investing in NHS and university facilities to expand testing and at the same time bring in high

NEWS

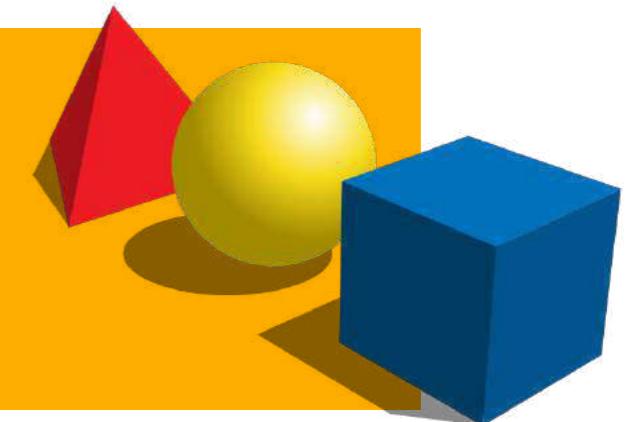
BMJ: first published as 10.1136/bmj.m3891 on 6 October 2020. DOI: <http://dx.doi.org/10.1136/bmj.m3891>

# Data Usage Static Analysis [CU18]

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties



**mathematical models**  
of the program behavior



# Data (Non-)Usage

$$\mathcal{N}_J \stackrel{\text{def}}{=} \{\llbracket P \rrbracket \mid \text{UNUSED}_J(\llbracket P \rrbracket)\}$$

$\mathcal{N}_J$  is the set of all programs  $P$  (or, rather, their semantics  $\llbracket P \rrbracket$ ) that **do not use** the value of the input variables in  $J$

$$\begin{aligned} \text{UNUSED}_J(\llbracket P \rrbracket) &\stackrel{\text{def}}{=} \forall t \in \llbracket P \rrbracket, V \in \mathcal{R}^{|J|}: t_0(J) \neq V \Rightarrow \exists t' \in \llbracket P \rrbracket : \\ &(\forall i: i \notin J \Rightarrow t_0(i) = t'_0(i)) \\ &\wedge t'_0(J) = V \\ &\wedge t_\omega = t'_\omega \end{aligned}$$

Intuitively: **any possible program outcome** is possible from **any value of the input variable  $i$**

## Theorem

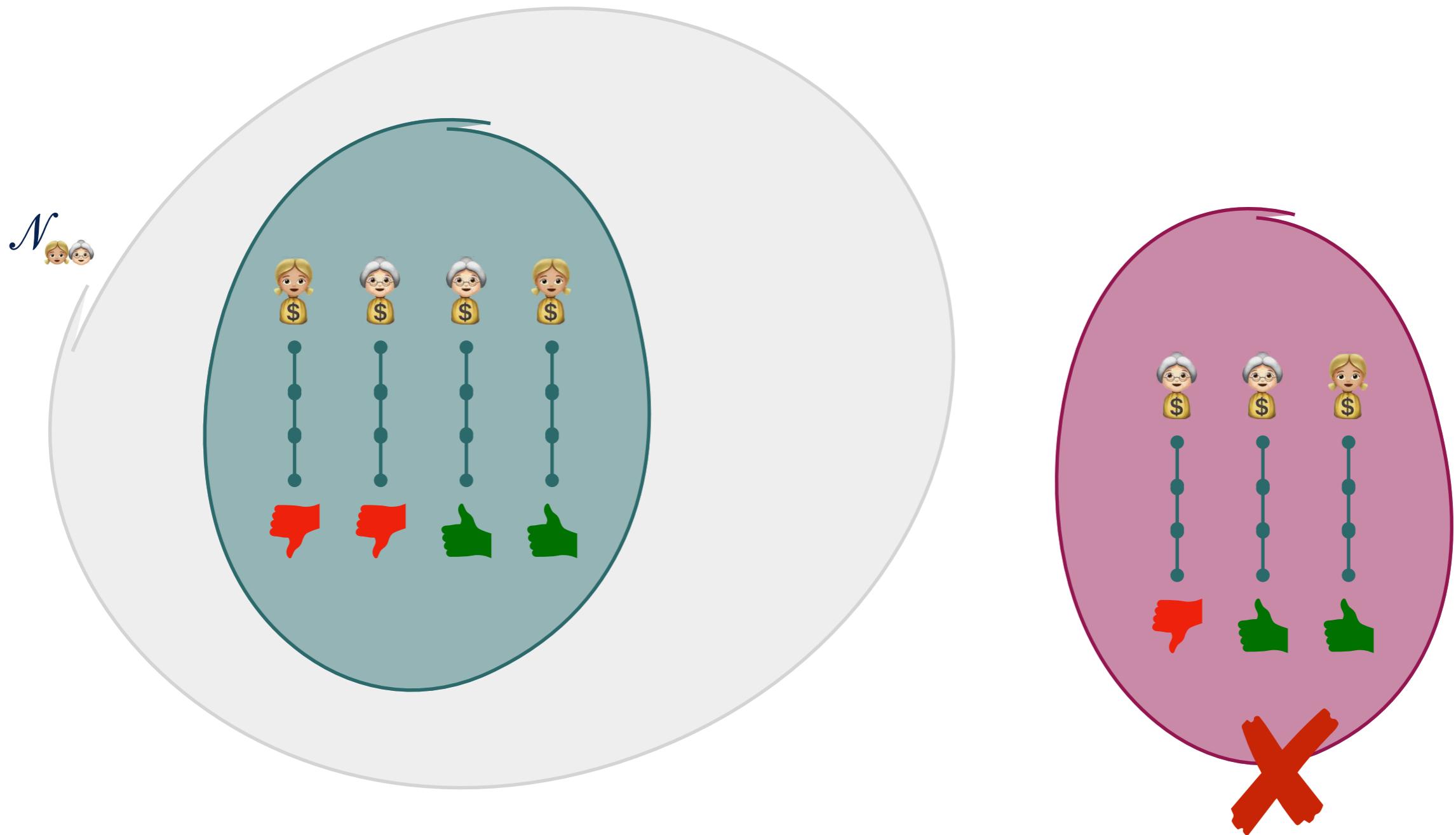
$$P \models \mathcal{N}_J \Leftrightarrow \{\llbracket P \rrbracket\} \subseteq \mathcal{N}_J$$

## Corollary

$$P \models \mathcal{N}_J \Leftrightarrow \{\llbracket P \rrbracket^\natural\} \subseteq \llbracket P \rrbracket^\natural \in \mathcal{N}_J$$

# Data (Non-) Usage

Not a Subset-Closed Property



# Data Usage Static Analysis [CU18]

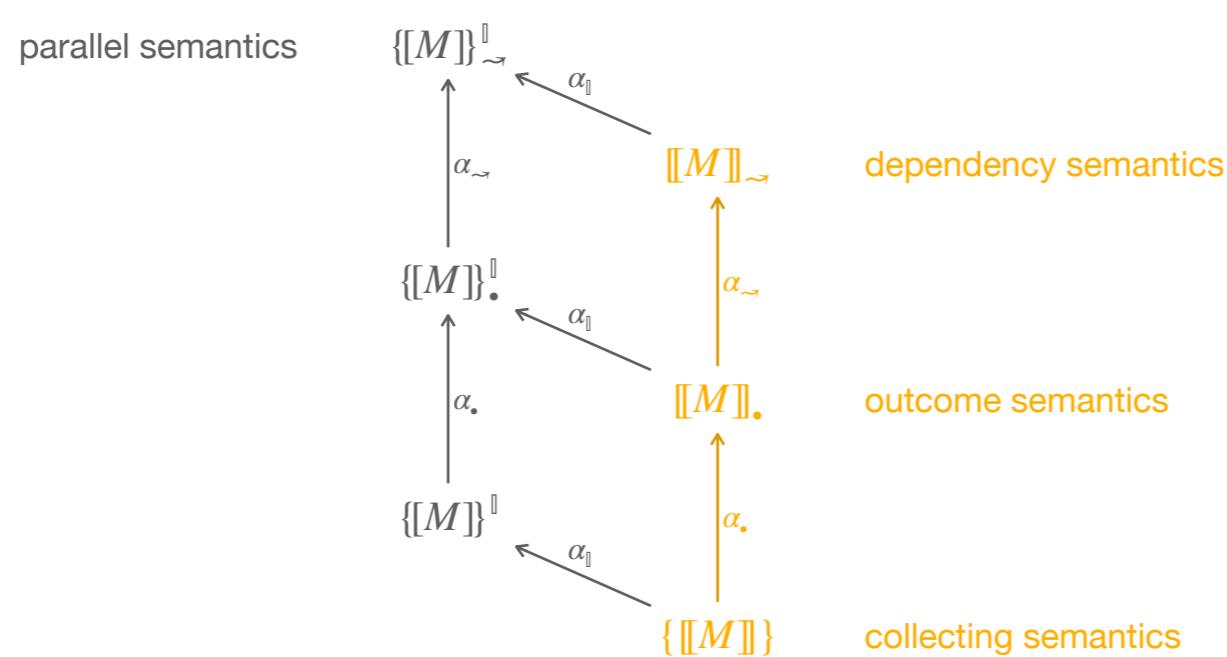
practical tools

task

algo  
to

ma

of the program behavior



EJCP 2024

Formal Methods for Machine Learning Pipelines

Caterina Urban

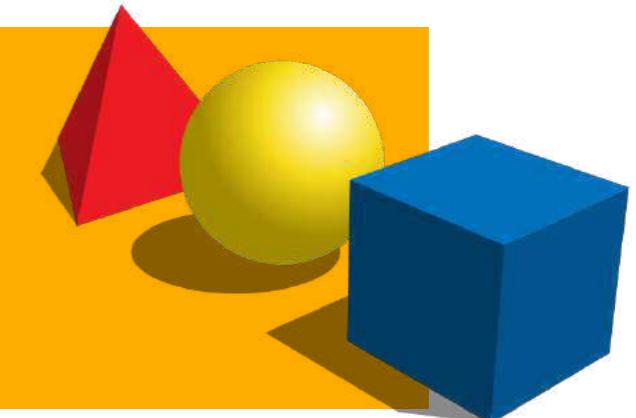
115

# Data Usage Static Analysis [CU18]

**practical tools**  
targeting specific programs



**algorithmic approaches**  
to decide program properties



**mathematical models**  
of the program behavior



# Data (Non-)Usage Abstractions

Over-Approximation of the Used Input Data

⇒ Under-Approximation of the Unused Input Data

$$P \models \mathcal{N}_{J \setminus \underline{J}} \Leftarrow \llbracket P \rrbracket \subseteq \llbracket P \rrbracket_A^\natural \subseteq \mathcal{N}_{J \setminus \underline{J}}$$

# Example

```
english = bool(input())
math = bool(input())
science = bool(input())
bonus = bool(input())

passing = True
if not english:
    english = False
if not math:
    passing = False or bonus
if not science:
    science = False or bonus

print(passing)
```

INPUT VARIABLES

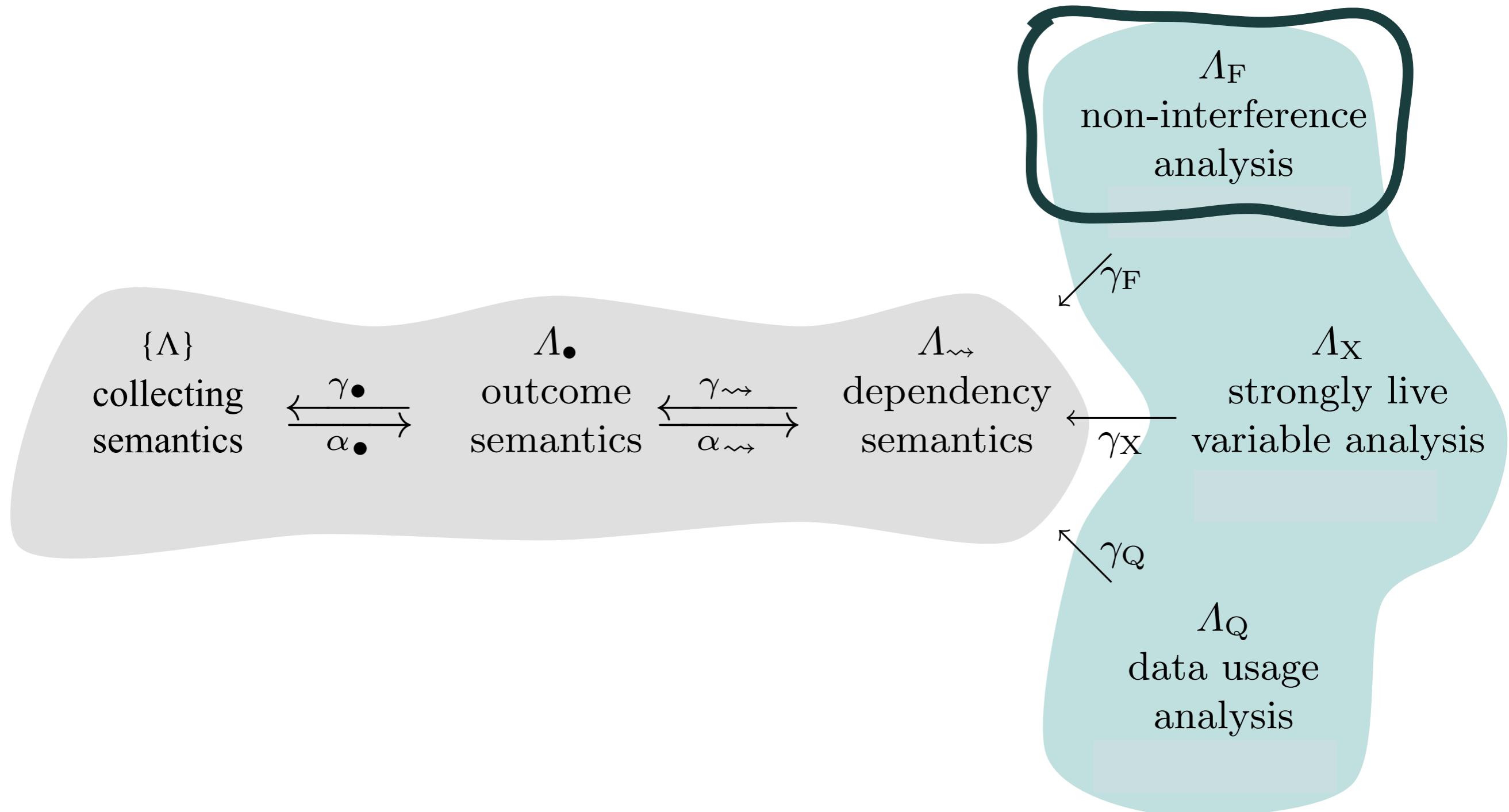
ERROR: english SHOULD BE passing

ERROR: math SHOULD BE science

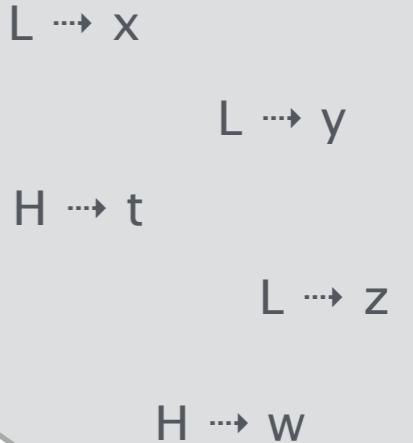
OUTPUT VARIABLES



the input variables english and science are unused



# Secure Information Flow



**probabilistic non-interference** coincides with input data (non-)usage when the set J of unused input variables contains *all* input variables:

- input variables are **high-security variables**
- output variables are **low-security variables**

explicit usage flows

implicit usage flows

$$\Theta_F[\text{skip}](S) \stackrel{\text{def}}{=} S$$

$$\Theta_F[x = e](S) \stackrel{\text{def}}{=} \{L \rightsquigarrow y \in S \mid y \neq x\} \cup \{L \rightsquigarrow x \mid \mathcal{V}_F[e]S\}$$

$$\Theta_F[\text{if } e: s_1 \text{ else: } s_2](S) \stackrel{\text{def}}{=} \begin{cases} \Theta_F[s_1](S) \sqcup_F \Theta_F[s_2](S) & \text{if } \mathcal{V}_F[e]S \\ \{L \rightsquigarrow x \in S \mid x \notin W(s_1) \cup W(s_2)\} & \text{otherwise} \end{cases}$$

$$\Theta_F[\text{while } e: s](S) \stackrel{\text{def}}{=} \text{lfp}_S^{\sqsubseteq_F} \Theta_F[\text{if } e: s \text{ else: skip}]$$

$$\Theta_F[s_1 \ s_2](S) \stackrel{\text{def}}{=} \Theta_F[s_2] \circ \Theta_F[s_1](S)$$

$$\mathcal{L} \stackrel{\text{def}}{=} \{L, H\} : \text{set of security levels}$$

$$L \rightsquigarrow x : \text{dependency constraint}$$

$$F \stackrel{\text{def}}{=} \{L \rightsquigarrow x \mid x \in X\}$$

$$\langle P(F), \sqsubseteq_F, \sqcup_F \rangle : \text{abstract domain}$$

$$S_1 \sqsubseteq_F S_2 \stackrel{\text{def}}{=} S_1 \supseteq S_2$$

$$S_1 \sqcup_F S_2 \stackrel{\text{def}}{=} S_1 \cap S_2$$

$e ::= v \mid x \mid \text{not } e \mid e \text{ and } e \mid e \text{ or } e$   
 $s ::= \text{skip} \mid x = e \mid \text{if } e: s \text{ else: } s \mid \text{while } e: s \mid s\ s$

(expressions)  
 (statements)

$\mathcal{V}_F[x]S \Leftrightarrow L \rightsquigarrow x \in S$

S guarantees a unique value for  $x$  independently of values of input variables

set of variables modified by  $s_i$

Hypercollecting Semantics and Its Application to Static Analysis of Information Flow

Mounir Assaf  
Stevens Institute of Technology,  
Hoboken, US  
first.last@stevens.edu

Éric Totel  
CIDRE, CentraleSupélec,  
Rennes, FR  
first.last@centralesupelec.fr

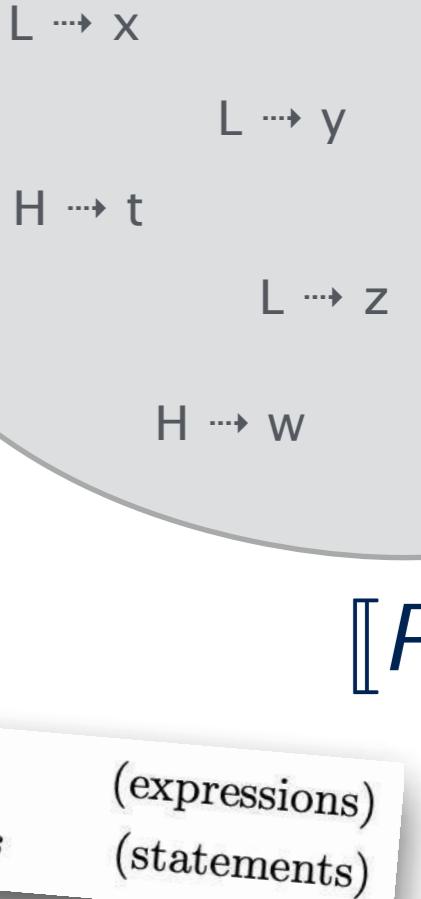
David A. Naumann  
Stevens Institute of Technology,  
Hoboken, US  
first.last@stevens.edu

Julien Signoles  
Software Reliability and Security Lab,  
CEA LIST, Saclay, FR  
first.last@cea.fr

Frédéric Tronel  
CIDRE, CentraleSupélec,  
Rennes, FR  
first.last@centralesupelec.fr

program is correct if all its traces satisfy the predicate. By c with such trace properties, extensional definitions of depen involve more than one trace. To express that the final va depend only on the initial value of a variab interference in the security trac with

# Secure Information Flow



**probabilistic non-interference coincides with input data (non-)usage when the set  $J$  of unused input variables contains *all* input variables:**

- **input variables are high-security variables**
- **output variables are low-security variables**

$$\Theta_F[\text{skip}](S) \stackrel{\text{def}}{=} S$$

$$\Theta_F[x = e](S) \stackrel{\text{def}}{=} \{L \rightsquigarrow y \in S \mid y \neq x\} \cup \{L \rightsquigarrow x \mid \mathcal{V}_F[e]S\}$$

$$\Theta_F[\text{if } e: s_1 \text{ else: } s_2](S) \stackrel{\text{def}}{=} \begin{cases} \Theta_F[s_1](S) \sqcup_F \Theta_F[s_2](S) & \text{if } \mathcal{V}_F[e]S \\ \{L \rightsquigarrow x \in S \mid x \notin W(s_1) \cup W(s_2)\} & \text{otherwise} \end{cases}$$

$$\Theta_F[\text{while } e: s](S) \stackrel{\text{def}}{=} \text{lfp}_S^{\sqsubseteq_F} \Theta_F[\text{if } e: s \text{ else: skip}]$$

$$\Theta_F[s_1 \ s_2](S) \stackrel{\text{def}}{=} \Theta_F[s_2] \circ \Theta_F[s_1](S)$$

$$e ::= v \mid x \mid \text{not } e \mid e \text{ and } e \mid e \text{ or } e$$

$$s ::= \text{skip} \mid x = e \mid \text{if } e: s \text{ else: } s \mid \text{while } e: s \mid s \ s$$

(expressions)  
(statements)

```

passing = True
if not english:
    english = False
if not math:
    passing = False or bonus
if not math:
    passing = False or bonus
  
```

$\leftarrow \dots \dots \dots \quad L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$   
 $\leftarrow \dots \dots \dots \quad L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$   
 $\leftarrow \dots \dots \dots \quad L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$   
 $\leftarrow \dots \dots \dots \quad H \rightarrow \text{english, math, science, bonus, passing}$   
 $\leftarrow \dots \dots \dots \quad H \rightarrow \text{english, math, science, bonus, passing}$

# Secure Information Flow

$L \rightarrow x$   
 $L \rightarrow y$   
 $H \rightarrow t$   
 $L \rightarrow z$   
 $H \rightarrow w$

$\llbracket P \rrbracket_F$

**probabilistic non-interference coincides with input data (non-)usage when the set  $J$  of unused input variables contains *all* input variables:**

- **input variables are high-security variables**
- **output variables are low-security variables**
- **and the program is terminating**

$$\Theta_F[\text{skip}](S) \stackrel{\text{def}}{=} S$$

$$\Theta_F[x = e](S) \stackrel{\text{def}}{=} \{L \rightsquigarrow y \in S \mid y \neq x\} \cup \{L \rightsquigarrow x \mid \mathcal{V}_F[e]S\}$$

$$\Theta_F[\text{if } e: s_1 \text{ else: } s_2](S) \stackrel{\text{def}}{=} \begin{cases} \Theta_F[s_1](S) \sqcup_F \Theta_F[s_2](S) & \text{if } \mathcal{V}_F[e]S \\ \{L \rightsquigarrow x \in S \mid x \notin W(s_1) \cup W(s_2)\} & \text{otherwise} \end{cases}$$

$$\Theta_F[\text{while } e: s](S) \stackrel{\text{def}}{=} \text{lfp}_S^{\sqsubseteq_F} \Theta_F[\text{if } e: s \text{ else: skip}]$$

$$\Theta_F[s_1 \ s_2](S) \stackrel{\text{def}}{=} \Theta_F[s_2] \circ \Theta_F[s_1](S)$$

$e ::= v \mid x \mid \text{not } e \mid e \text{ and } e \mid e \text{ or } e$

$s ::= \text{skip} \mid x = e \mid \text{if } e: s \text{ else: } s \mid \text{while } e: s \mid s \ s$

(expressions)  
(statements)

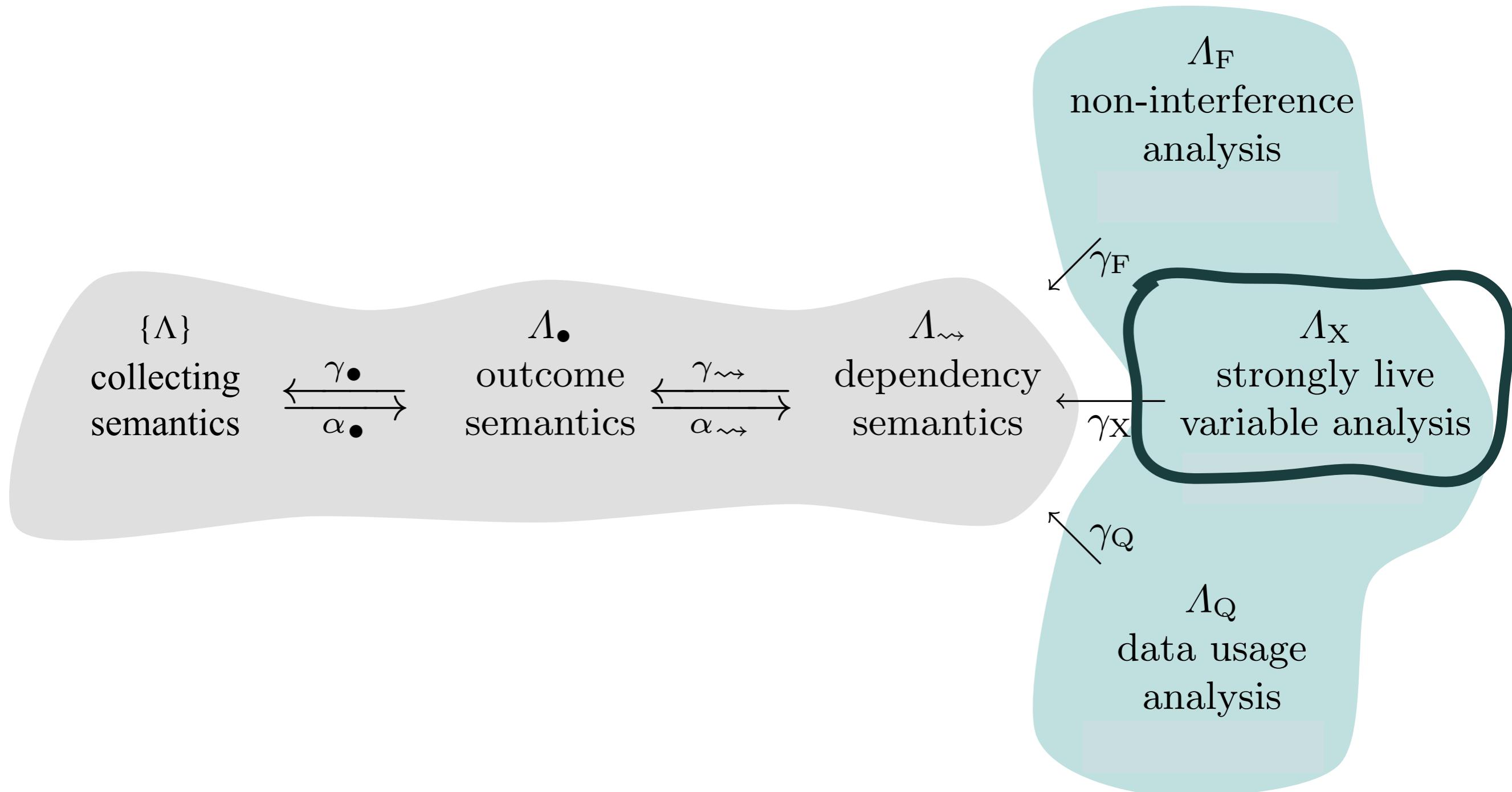
```

passing = True
while not english:
    english = False
  
```

$\xleftarrow{\dots} L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$   
 $\xleftarrow{\dots} L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$   
 $\xleftarrow{\dots} L \rightarrow \text{passing}, H \rightarrow \text{english, math, science, bonus}$

## Theorem

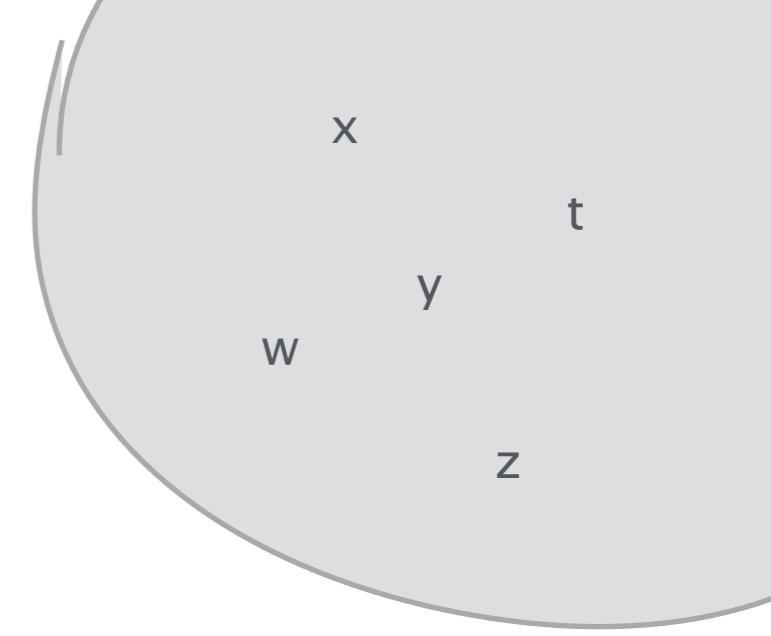
$$P \models \mathcal{N}_J^+ \Leftarrow \llbracket P \rrbracket \subseteq \llbracket P \rrbracket_F^\natural \subseteq \mathcal{N}_J^+$$



# Strong-Liveness

a variable is **strongly live** if

- it is used in an assignment to another strongly live variable
- it is used in a statement other than an assignment



$\llbracket P \rrbracket_X$

$$\Theta_X[\text{skip}](S) \stackrel{\text{def}}{=} S$$

$$\Theta_X[x = e](S) \stackrel{\text{def}}{=} \begin{cases} (S \setminus \{x\}) \cup \text{VARS}(e) & x \in S \\ S & \text{otherwise} \end{cases}$$

$$\Theta_X[\text{if } b: s_1 \text{ else: } s_2](S) \stackrel{\text{def}}{=} \text{VARS}(b) \cup \Theta_X[s_1](S) \cup \Theta_X[s_2](S)$$

$$\Theta_X[\text{while } b: s](S) \stackrel{\text{def}}{=} \text{VARS}(b) \cup \Theta_X[s](S)$$

$$\Theta_X[s_1 \ s_2](S) \stackrel{\text{def}}{=} \Theta_X[s_1] \circ \Theta_X[s_2](S)$$

$e ::= v \mid x \mid \text{not } e \mid e \text{ and } e \mid e \text{ or } e$

$s ::= \text{skip} \mid x = e \mid \text{if } e: s \text{ else: } s \mid \text{while } e: s \mid s \ s$

(expressions)  
(statements)

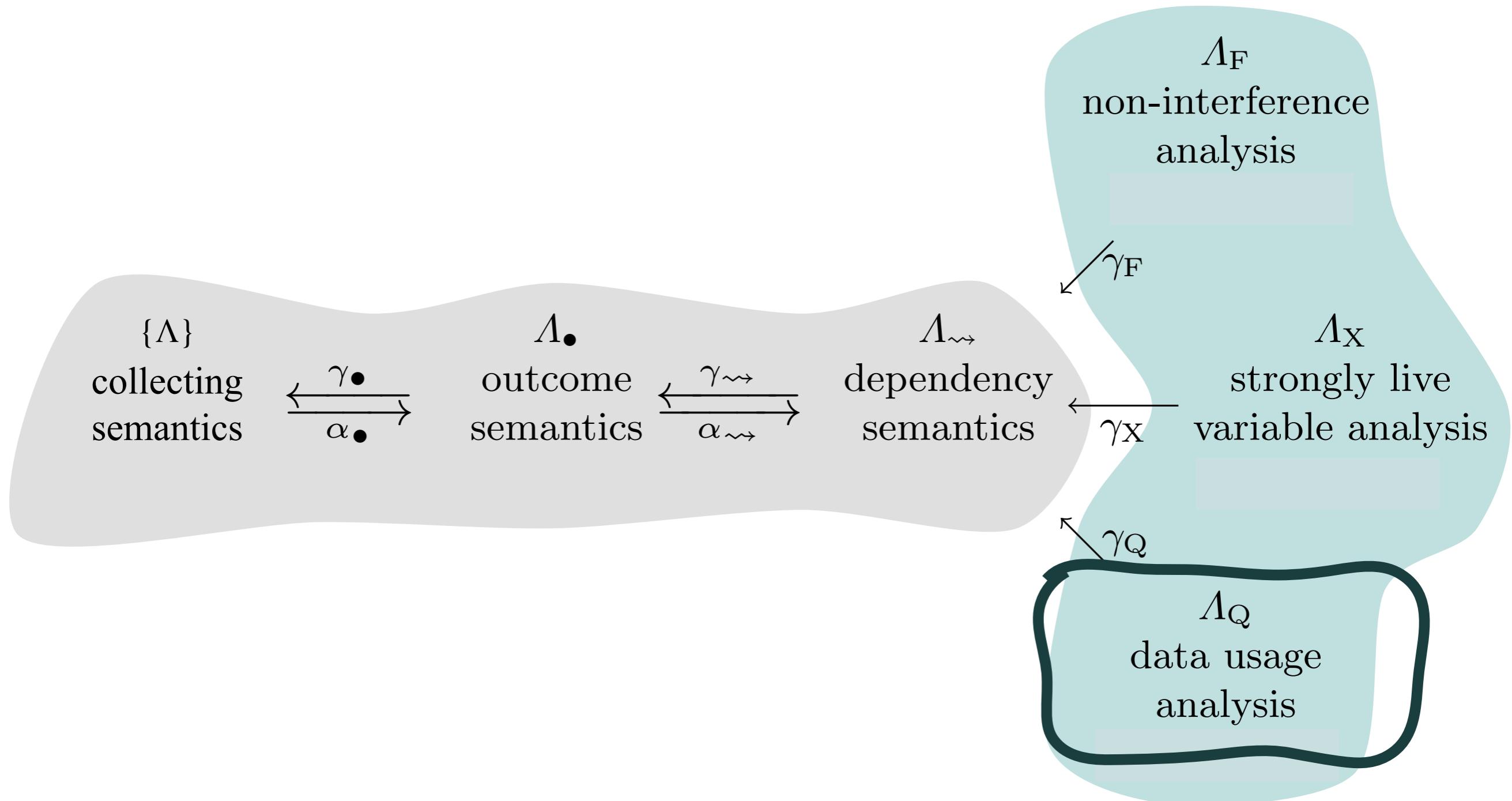
## Theorem

$$P \models \mathcal{N}_J \Leftarrow \llbracket P \rrbracket \subseteq \llbracket P \rrbracket_X^\natural \subseteq \mathcal{N}_J$$

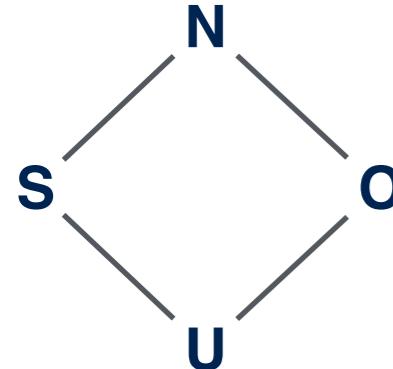
```

passing = True
if not english:
    english = False
if not math:
    passing = False or bonus
if not math:
    passing = False or bonus
  
```

-----	{ bonus, math, english }
-----	{ bonus, math, english }
-----	{ bonus, math }
-----	{ bonus, math }
-----	{ bonus, math }
-----	{ bonus, math }
-----	{ bonus }
-----	{ passing }



# Syntactic (Non-)Usage



- **U**: used in the current scope (or an inner scope)
- **S**: used in an outer scope
- **O**: used in an outer scope and overridden in the current scope
- **N**: not used

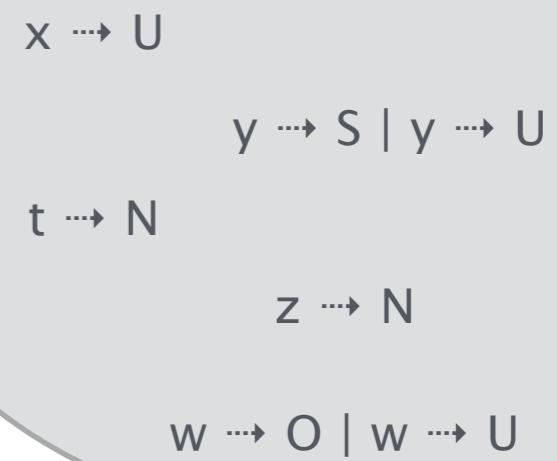
passing = **True**

**if not** english:

english = **False**

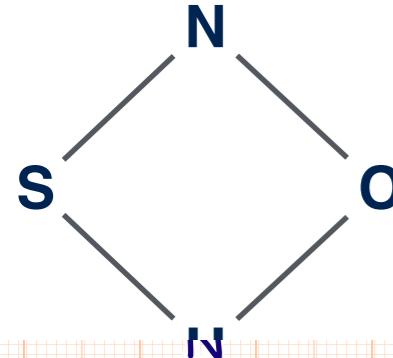
●	math, bonus, passing → S   math, bonus, passing → U
●	math, bonus, passing → U
<b>if not</b> math:	math → S, bonus → U, passing → O   ...
●	math, bonus, passing → S   math, bonus, passing → U
●	math, bonus, passing → U
<b>if not</b> math:	bonus → U, passing → O   passing → U
●	passing → S   passing → U
●	passing → U

$$\begin{aligned} \Theta_Q[\text{skip}](q) &\stackrel{\text{def}}{=} q \\ \Theta_Q[x = e](q) &\stackrel{\text{def}}{=} \text{ASSIGN}[x = e](q) \\ \Theta_Q[\text{if } b: s_1 \text{ else: } s_2](q) &\stackrel{\text{def}}{=} \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_1] \circ \text{PUSH}(q) \\ &\quad \sqcup_Q \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_2] \circ \text{PUSH}(q) \\ \Theta_Q[\text{while } b: s](q) &\stackrel{\text{def}}{=} \text{lfp}_t^{\sqsubseteq_Q} \Theta_Q[\text{if } b: s \text{ else: skip}] \\ \Theta_Q[s_1 \ s_2](q) &\stackrel{\text{def}}{=} \Theta_Q[s_1] \circ \Theta_Q[s_2](q) \end{aligned}$$



$\llbracket P \rrbracket_Q$

# Syntactic (Non-)Usage



- **U**: used in the current scope (or an inner scope)
- **S**: used in an outer scope
- **O**: used in an outer scope and overridden in the current scope
- **N**: not used

●  
passing = **True**

●  
if not english:  
●  
**english = False**

●  
if not math:  
●  
passing = **False or bonus**

●  
if not math:  
●  
passing = **False or bonus**

●  
passing

VTSA 2024

Formal Methods for Machine Learning Pipelines

Caterina Urban

228

the input variables **english**  
and **science** are definitely not used  
by the program

math, bonus  $\rightarrow$  U, passing  $\rightarrow$  O

math, bonus, passing  $\rightarrow$  U

math, bonus, passing  $\rightarrow$  S | math, bonus, passing  $\rightarrow$  U

math, bonus, passing  $\rightarrow$  S | math, bonus, passing  $\rightarrow$  U

math, bonus, passing  $\rightarrow$  U

$\Theta_Q[\text{skip}](q) \stackrel{\text{def}}{=} q$

$\Theta_Q[x = e](q) \stackrel{\text{def}}{=} \text{ASSIGN}[x = e](q)$

$\Theta_Q[\text{if } b: s_1 \text{ else: } s_2](q) \stackrel{\text{def}}{=} \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_1] \circ \text{PUSH}(q)$

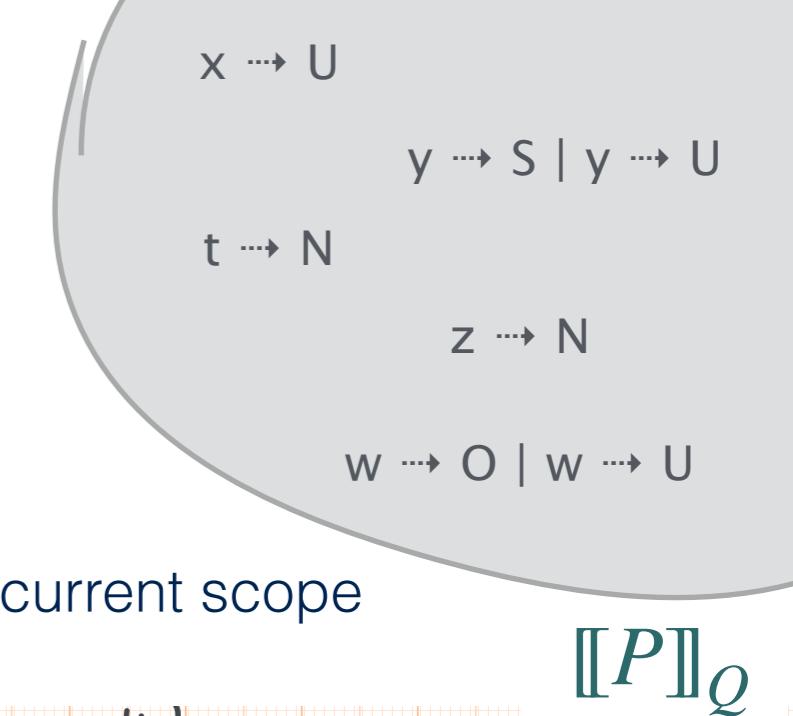
$\sqcup_Q \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_2] \circ \text{PUSH}(q)$

$\Theta_Q[\text{while } b: s](q) \stackrel{\text{def}}{=} \text{lfp}_t^{\sqsubseteq_Q} \Theta_Q[\text{if } b: s \text{ else: skip}]$

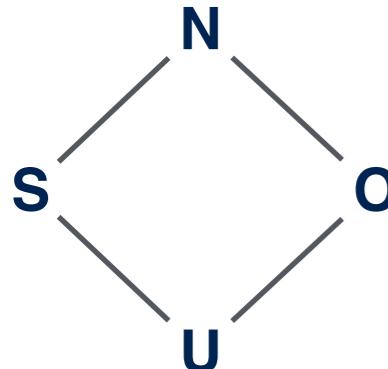
$\Theta_Q[s_1 \ s_2](q) \stackrel{\text{def}}{=} \Theta_Q[s_1] \circ \Theta_Q[s_2](q)$

passing

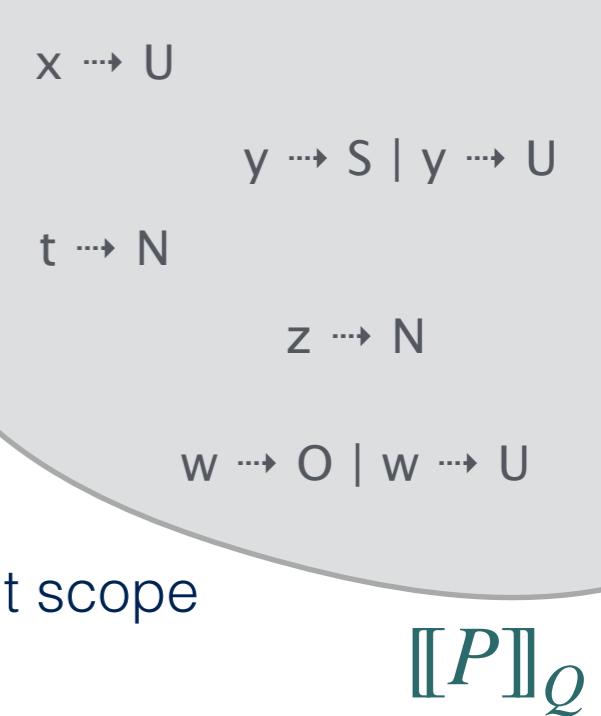
passing  $\rightarrow$  U



# Syntactic (Non-)Usage



- **U**: used in the current scope (or an inner scope)
- **S**: used in an outer scope
- **O**: used in an outer scope and overridden in the current scope
- **N**: not used



$$\Theta_Q[\text{skip}](q) \stackrel{\text{def}}{=} q$$

$$\Theta_Q[x = e](q) \stackrel{\text{def}}{=} \text{ASSIGN}[x = e](q)$$

$$\Theta_Q[\text{if } b: s_1 \text{ else: } s_2](q) \stackrel{\text{def}}{=} \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_1] \circ \text{PUSH}(q)$$

$$\sqcup_Q \text{POP} \circ \text{FILTER}[b] \circ \Theta_Q[s_2] \circ \text{PUSH}(q)$$

$$\Theta_Q[\text{while } b: s](q) \stackrel{\text{def}}{=} \text{lfp}_t^{\sqsubseteq_Q} \Theta_Q[\text{if } b: s \text{ else: skip}]$$

$$\Theta_Q[s_1 \ s_2](q) \stackrel{\text{def}}{=} \Theta_Q[s_1] \circ \Theta_Q[s_2](q)$$

$e ::= v \mid x \mid \text{not } e \mid e \text{ and } e \mid e \text{ or } e$   
 $s ::= \text{skip} \mid x = e \mid \text{if } e: s \text{ else: } s \mid \text{while } e: s \mid s \ s$ 

(expressions)  
(statements)

```

passing = True
while not english:
  english = False
  
```

←..... passing  $\rightarrow O$   
 ←..... passing  $\rightarrow U$   
 ←..... passing  $\rightarrow U$

## Theorem

$$P \models \mathcal{N}_J^+ \Leftarrow \llbracket P \rrbracket \subseteq \llbracket P \rrbracket_Q^\natural \subseteq \mathcal{N}_J^+$$

# Data Usage Static Analysis [CU18]

**practical tools**  
targeting specific programs



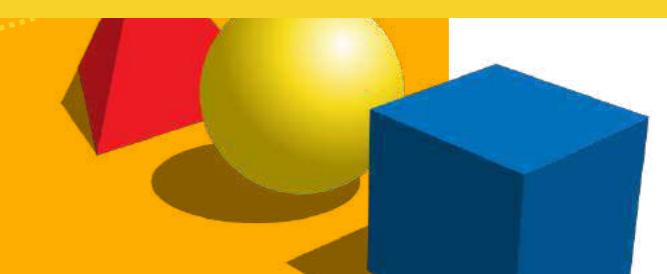
**algorithmic approaches**  
to decide program properties

**strongly-live variable analysis**

**mathematical models**  
of the program behavior

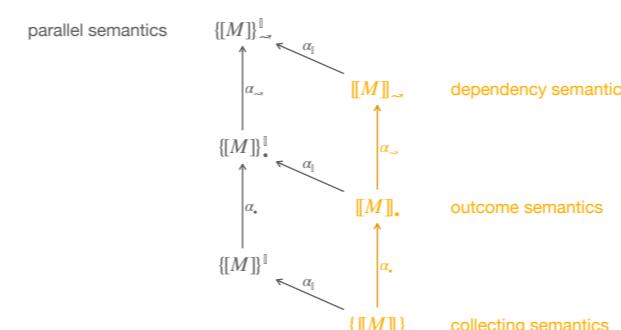


**secure information flow**



**syntactic non-usage**

Hierarchy of Semantics



github.com

caterinaurban / Lyra

Type ⌘ to search

Code Issues Pull requests Actions Projects Wiki Security Insights Settings

Lyra Public

Unpin Unwatch 4 Fork 9 Star 25

master 1 branch 0 tags Go to file Add file Code

caterinaurban update for Python 3.9 e37b228 on Nov 7 1,144 commits

File	Description	Time
docs	documentation	5 years ago
src	update for Python 3.9	last month
.gitignore	[wip] adding .DS_Store mac file	9 months ago
.travis.yml	added fulara unittests to travis	5 years ago
LICENSE	Initial commit	6 years ago
README.md	Merge pull request #78 from caterinaurban/build-status	5 years ago
icon.png	various	6 years ago
lyra.png	logo	6 years ago
requirements.txt	list creation	5 years ago
setup.py	main file	6 years ago

Readme MPL-2.0 license Activity 25 stars 4 watching 9 forks

No description or website provided.

python data-science static-analysis abstract-interpretation

Readme MPL-2.0 license Activity 25 stars 4 watching 9 forks

25 stars 4 watching 9 forks

Initial commit

Merge pull request #78 from caterinaurban/build-status

various

logo

list creation

main file

README.md

Lyra - Static Analyzer for Data Science Applications

Contributors 9

Deployment 188

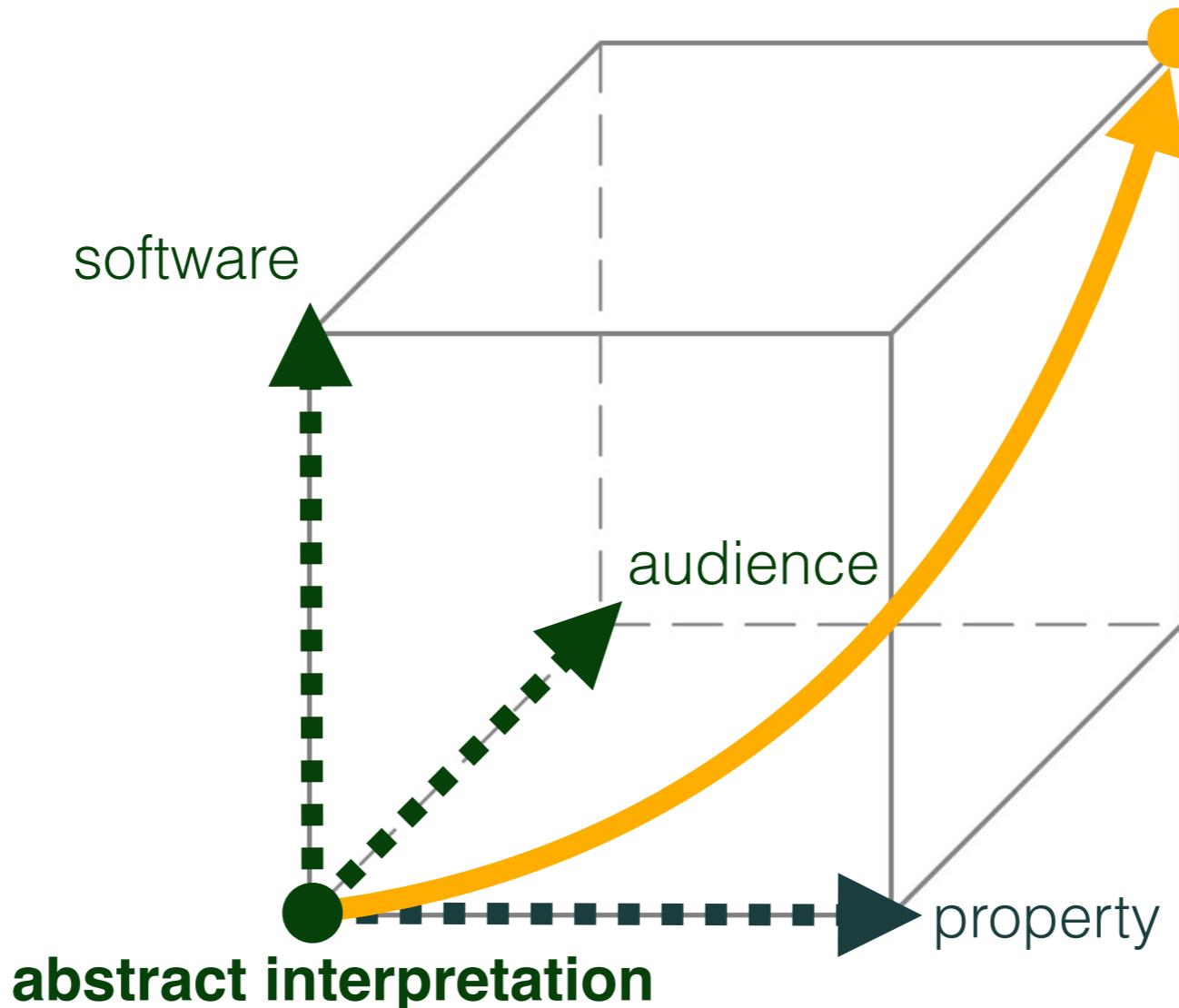
VTSA 2024 Formal Methods for Machine Learning Pipelines Caterina Urban 231



# Data Leakage



# Data Leakage Analysis



## A case study of algorithm-assisted decision making in child maltreatment hotline screening decisions

Alexandra Chouldechova

Heinz College  
Carnegie Mellon University  
Pittsburgh, PA, 15213, USA

Emily Putnam-Hornstein

Suzanne Dworak-Peck School of Social Work  
University of Southern California  
Los Angeles, CA, 90089, USA

Diana Benavides-Prado

Oleksandr Fialko  
Rhema Vaithianathan

Centre for Social Data Analytics  
Auckland University of Technology  
Auckland, New Zealand

Editors: Sorelle A. Friedler and Christo Wilson

### Abstract

Every year there are more than 3.6 million referrals made to child protection agencies across the US. The practice of screening calls is left to each jurisdiction to follow local practices and policies, potentially leading to large variation in the way which referrals are treated across the country. Whilst increasing access to linked administrative data is available, it is often for welfare workers to make systematic use of historical information about all children and adults on a single reference. Risk prediction models that use collected administrative data can help workers to better identify cases likely to result in adverse outcomes; however, the use of predictive analysis in the area of child welfare is contentious. It is a possibility that some communities, such as those in poverty or from particular racial and ethnic groups, are advantaged by the reliance on administrative data. On the other hand, these analytics tools can augment or replace human judgments, which themselves are biased and imperfect. In this paper we describe our work on developing, validating, and deploying a risk assessment tool for child maltreatment auditing, and deploying a risk

ACHOULD@CMU.EDU

EHORNSTE@USC.EDU

<https://www.aisnakeoil.com/p/the-bait-and-switch-behind-ai-risk>

## Family separation in Allegheny county

In 2016, Allegheny county in Pennsylvania adopted the Allegheny Family Screening Tool (AFST) to predict which children are at risk of maltreatment. AFST is used to decide which families should be investigated by social workers. In these investigations, social workers can forcibly remove children from their families and place them in foster care, **even if there are no allegations of abuse**—only poverty-based neglect.

Two years later, it was **discovered** that AFST suffered from data leakage, leading to exaggerated claims about its performance. In addition, the tool was **systematically biased** against Black families. When questioned, the creators trotted out the familiar defense that the **final decision is always made by a human decision-maker**.

and linked administrative data is available, it is difficult for child welfare workers to make systematic use of historical information about all the children and adults on a single reference. R. Vaithianathan.

A STAT INVESTIGATION

## Epic's sepsis algorithm is going off the rails in the real world. The use of these variables may explain why

By Casey Ross  Sept. 27, 2021



<https://www.aisnakeoil.com/p/the-bait-and-switch-behind-ai-risk>

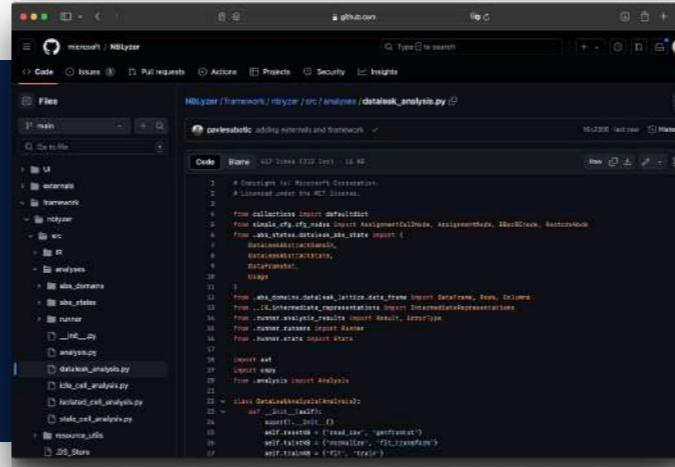
### Epic's sepsis prediction debacle

Epic is a large healthcare software company. It stores health data for over 300 million patients. In 2017, Epic released a sepsis prediction model. Over the next few years, it was deployed in hundreds of hospitals across the U.S. However, a [2021 study](#) from researchers at the University of Michigan found that Epic's model vastly underperformed compared to the developer's claims.

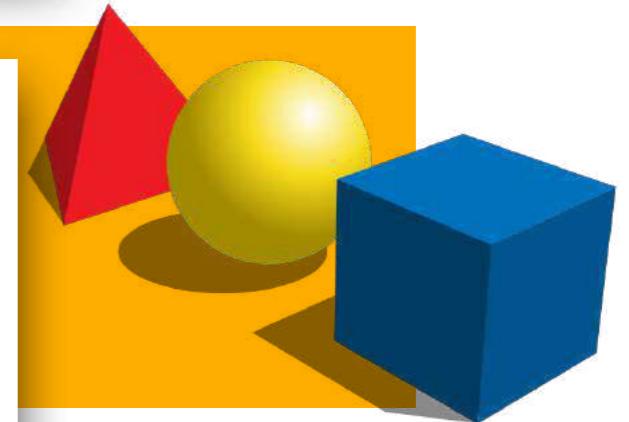
The tool's inputs included information about whether a patient was given antibiotics. But if a patient is given antibiotics, they have [already been diagnosed with sepsis](#)—making the tool's prediction useless. These cases were still counted as successes when the developer evaluated the tool, leading to exaggerated claims about how well it performed. This is an example of [data leakage](#), a common error in building AI tools.

# Data Leakage Analysis [Subotic24]

practical tools  
targeting specific programs



algorithmic approaches  
to decide program properties



mathematical models  
of the program behavior

As artificial intelligence (AI) continues its unprecedented impact on society, ensuring machine learning (ML) models are accurate is crucial. To this end, ML models must be trained on independent training and testing datasets. This can be challenging, especially when training datasets are large. This can lead to overfitting, followed by a significant drop in performance when models are deployed in the real world. This can be dangerous, notably when models are used for risk prediction in high-stakes applications.

In this paper, we propose an abstract interpretation-based static analysis to identify signs of data leakage. We implemented it in the NBLyzer framework and we demonstrate its performance and precision on 2111 Jupyter notebooks from the Kaggle competition platform.

## 1 Introduction

As artificial intelligence (AI) continues its unprecedented impact on society, ensuring machine learning (ML) models are accurate is crucial. To this end, ML models must be trained on independent training and testing datasets. This can be challenging, especially when training datasets are large. This can lead to overfitting, followed by a significant drop in performance when models are deployed in the real world. This can be dangerous, notably when models are used for risk prediction in high-stakes applications.

In this paper, we propose an abstract interpretation-based static analysis to identify signs of data leakage. We implemented it in the NBLyzer framework and we demonstrate its performance and precision on 2111 Jupyter notebooks from the Kaggle competition platform.

Example 1 (Motivating Example). Consider the following excerpt of a data science notebook (based on 569.ipynb from our benchmarks, and written in the small language that we introduce in Section 3.3):

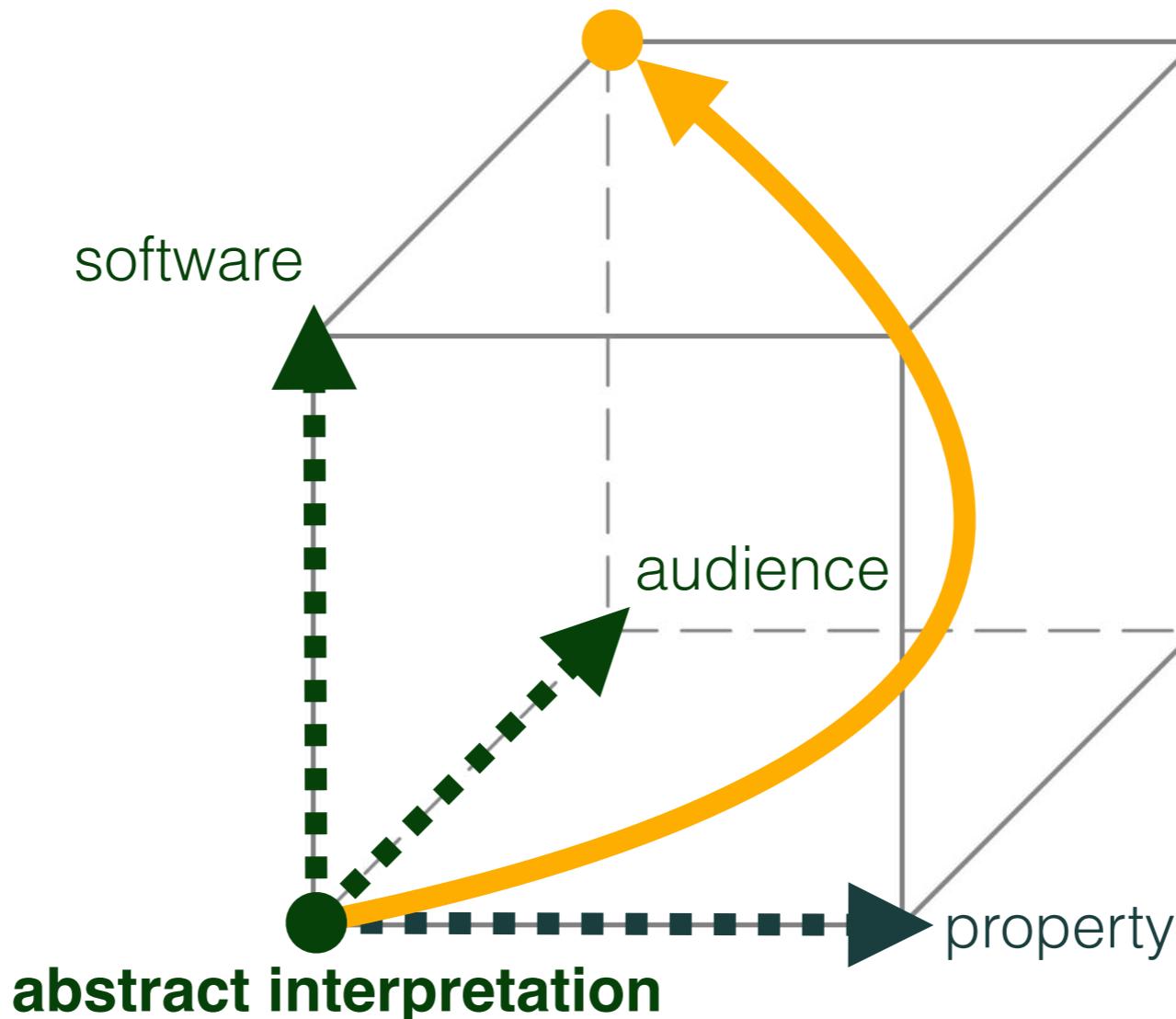
```
1 data = read("data.csv")
2 X_norm = normalize(X)
3 X_train = X_norm.select([(0.025 * R_norm) + 1, ..., R_norm]) []
4 X_test = X_norm.select([0, ..., (0.025 * R_norm)]) []
5 train(X,train)
6 test(X,test)
```



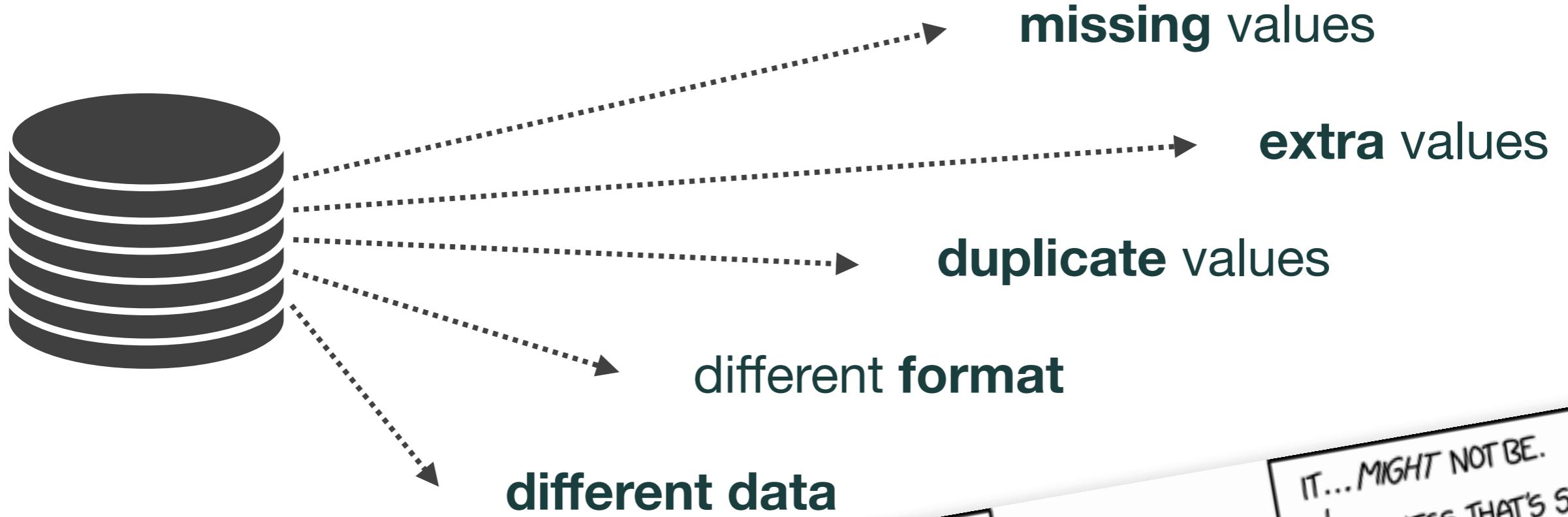
# Unexpected Data



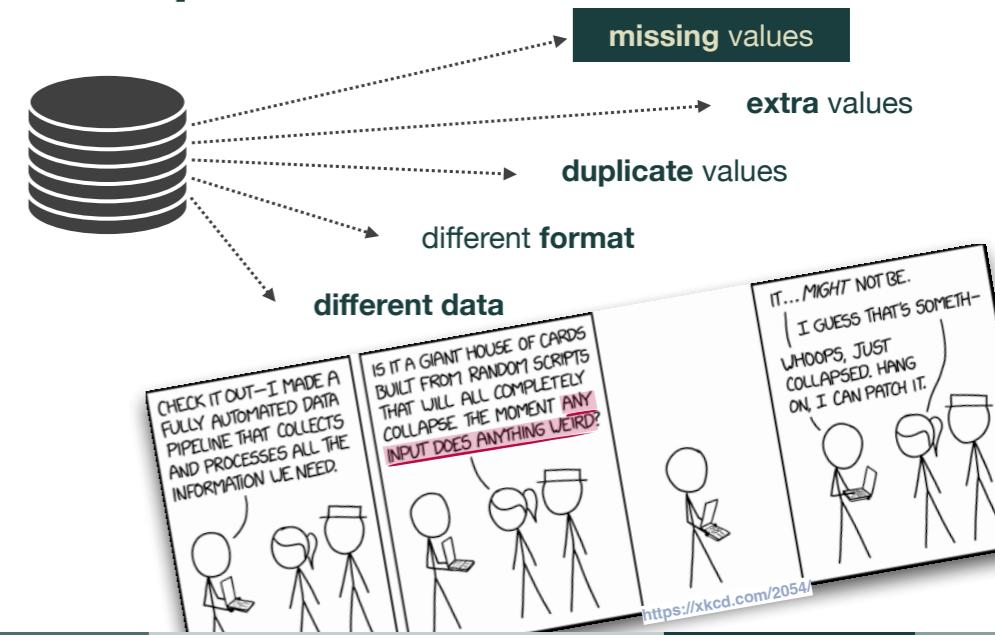
# (Un)expected Data Analysis



# Unexpected Data



# Unexpected Data



jupyter Gradebook Last Checkpoint: a few seconds ago (autosaved)

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv')`  
df.head()

Out [2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B	B
3956	Carol	F	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv')`

In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
res.head()

Out [7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	2.0
3956	carol@uni.eu	2.0
9578	david@uni.eu	1.0

jupyter Gradebook Last Checkpoint: a minute ago (unsaved)

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv', index_col=0)`  
df.head()

Out [2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B	B
3956	Carol	Nan	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv', index_col=0)`

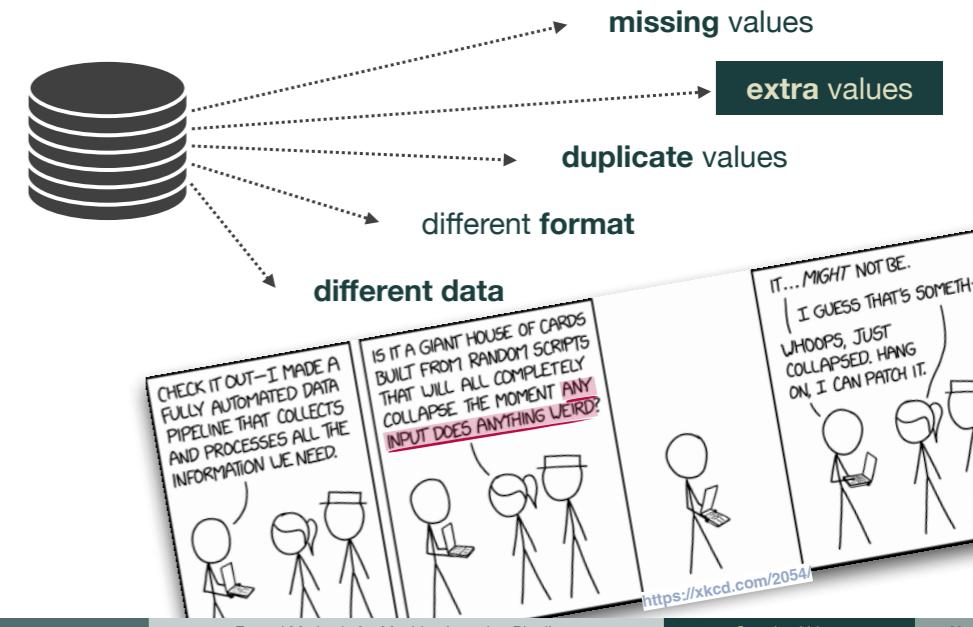
In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
res.head()

Out [7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	2.0
3956	carol@uni.eu	3.0
9578	david@uni.eu	1.0

# Unexpected Data



jupyter Gradebook Last Checkpoint: a few seconds ago (autosaved)

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv')`  
`df.head()`

Out[2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B	B
3956	Carol	F	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa.get)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv')`

In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
`res.head()`

Out[7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	2.0
3956	carol@uni.eu	2.0
9578	david@uni.eu	1.0

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv', index_col=0)`  
`df.head()`

Out[2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B	B
3956	Carol	F	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa.get)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv', index_col=0)`

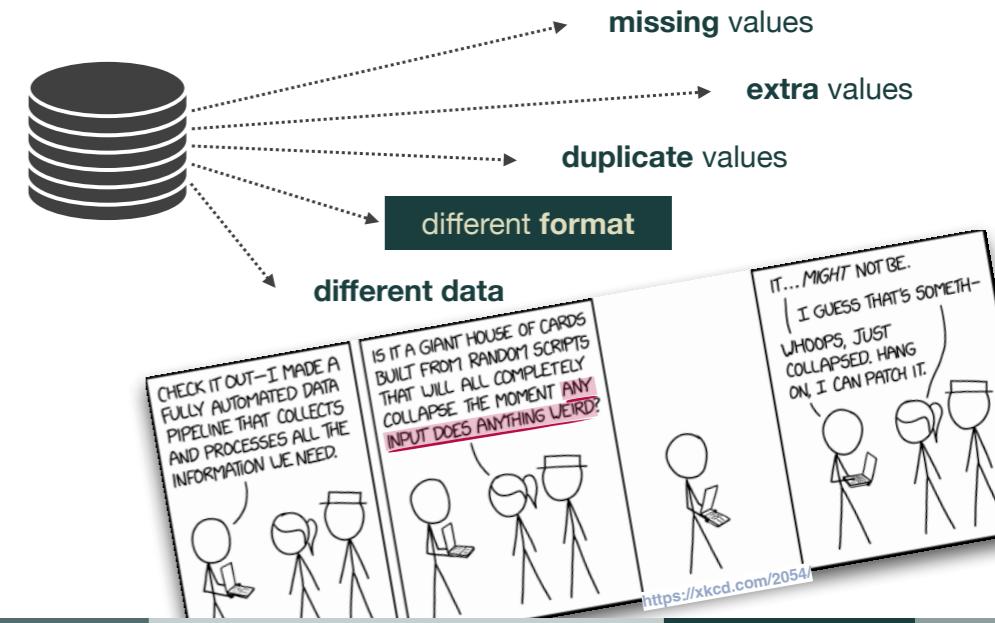
In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
`res.head()`

Out[7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	3.0
3956	carol@uni.eu	3.0
9578	david@uni.eu	1.0

# Unexpected Data



jupyter Gradebook Last Checkpoint: a few seconds ago (autosaved)

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv')`  
`df.head()`

Out [2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B	B
3956	Carol	F	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv')`

In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
`res.head()`

Out [7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	2.0
3956	carol@uni.eu	2.0
9578	david@uni.eu	1.0

In [1]: `import pandas as pd`

In [2]: `df = pd.read_csv('Grades.csv', index_col=0)`  
`df.head()`

Out [2]:

ID	Name	Q1	Q2	Q3
2394	Alice	A	A	A
4583	Bob	F	B+	B
3956	Carol	F	A	C
9578	David	D	F	C

In [3]: `grade2gpa = { 'A': 4.0, 'B': 3.0, 'C': 2.0, 'D': 1.0, 'F': 0.0 }`  
`df.iloc[:, df.columns.str.startswith('Q')] = df.iloc[:, df.columns.str.startswith('Q')].applymap(grade2gpa)`

In [4]: `df['Mean'] = df.iloc[:, df.columns.str.startswith('Q')].mean(axis=1)`

In [5]: `es = pd.read_csv('Emails.csv', index_col=0)`

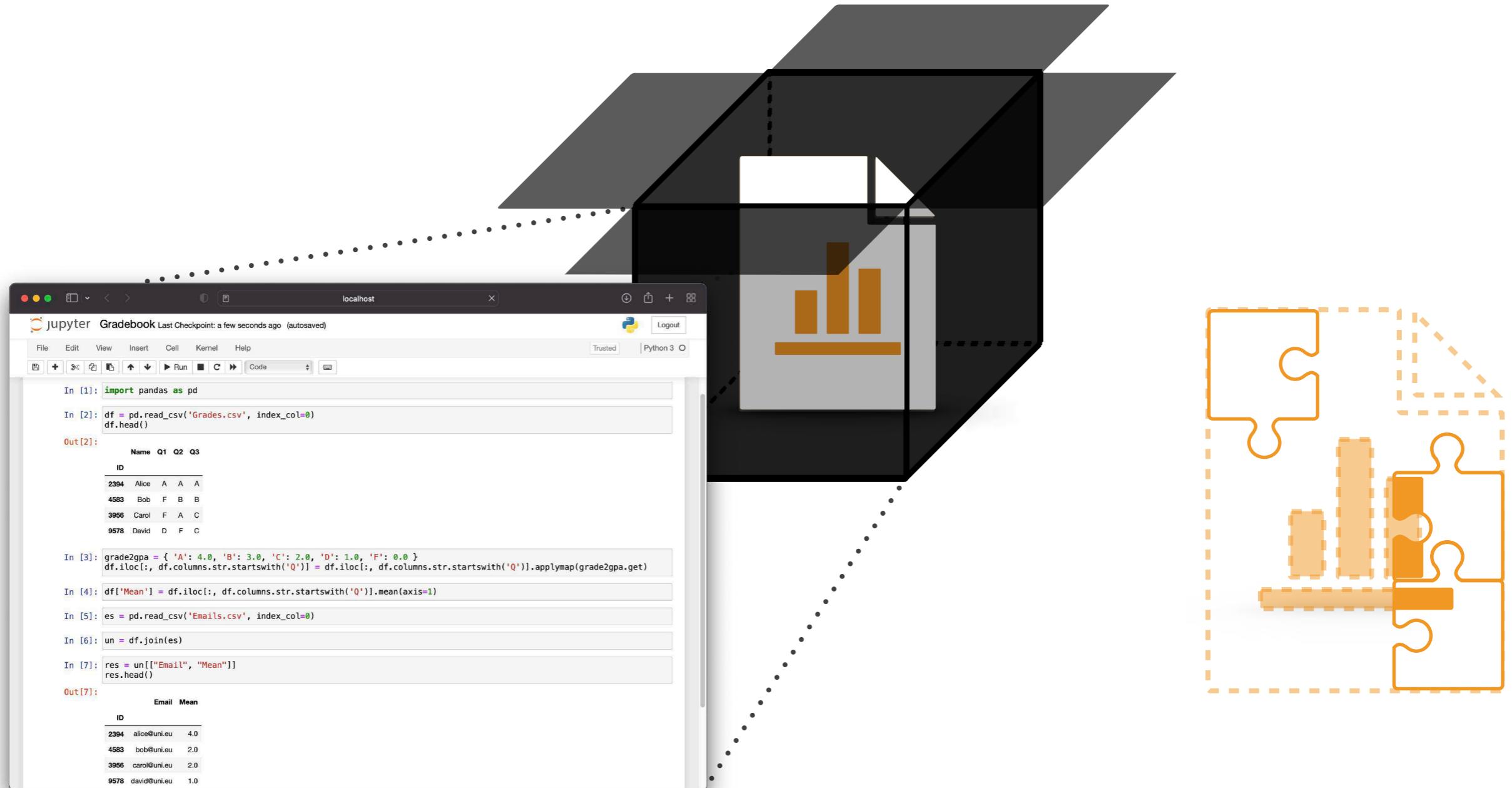
In [6]: `un = df.join(es)`

In [7]: `res = un[['Email', 'Mean']]`  
`res.head()`

Out [7]:

ID	Email	Mean
2394	alice@uni.eu	4.0
4583	bob@uni.eu	1.5
3956	carol@uni.eu	2.0
9578	david@uni.eu	1.0

# Data Expectations Analysis



# Data

## 1st Challenge: Multi-Dimensional Data Structures



# Data Expectations Analysis

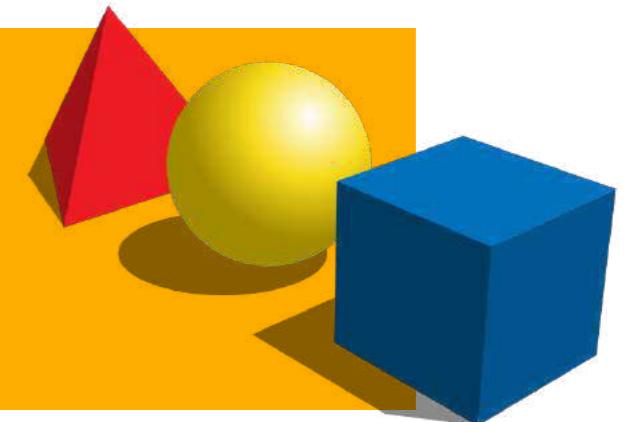
**practical tools**

targeting specific programs



**algorithmic approaches**

to decide program properties



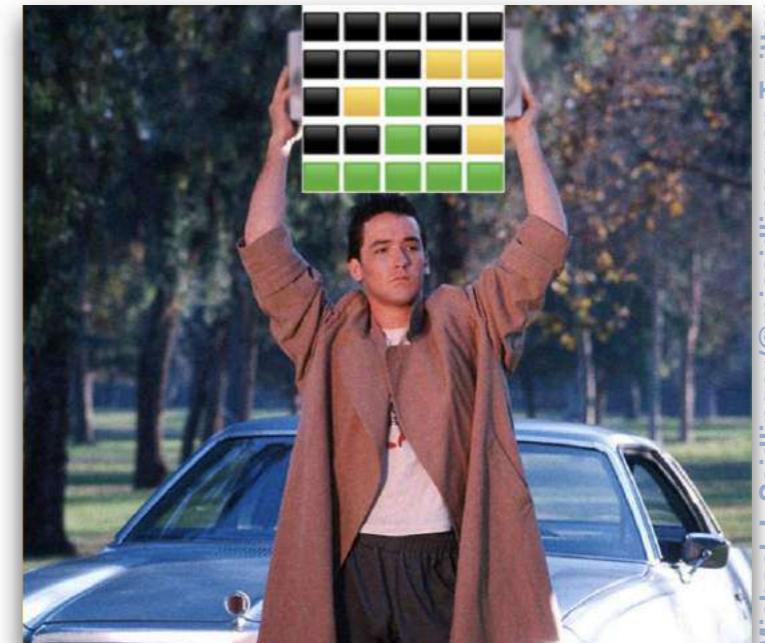
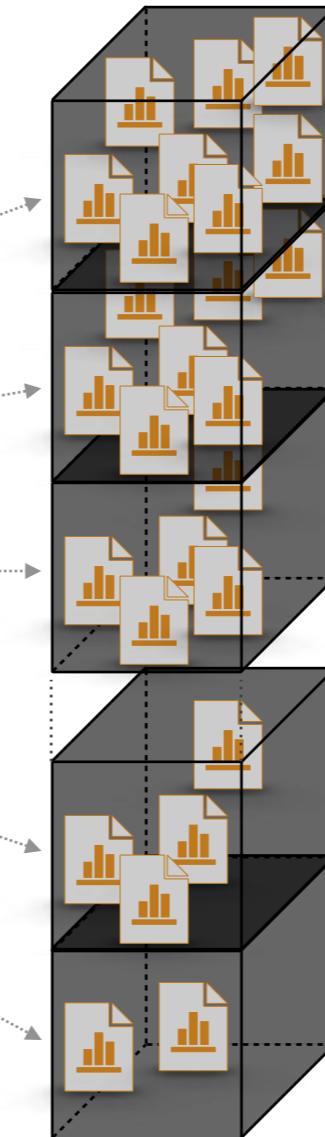
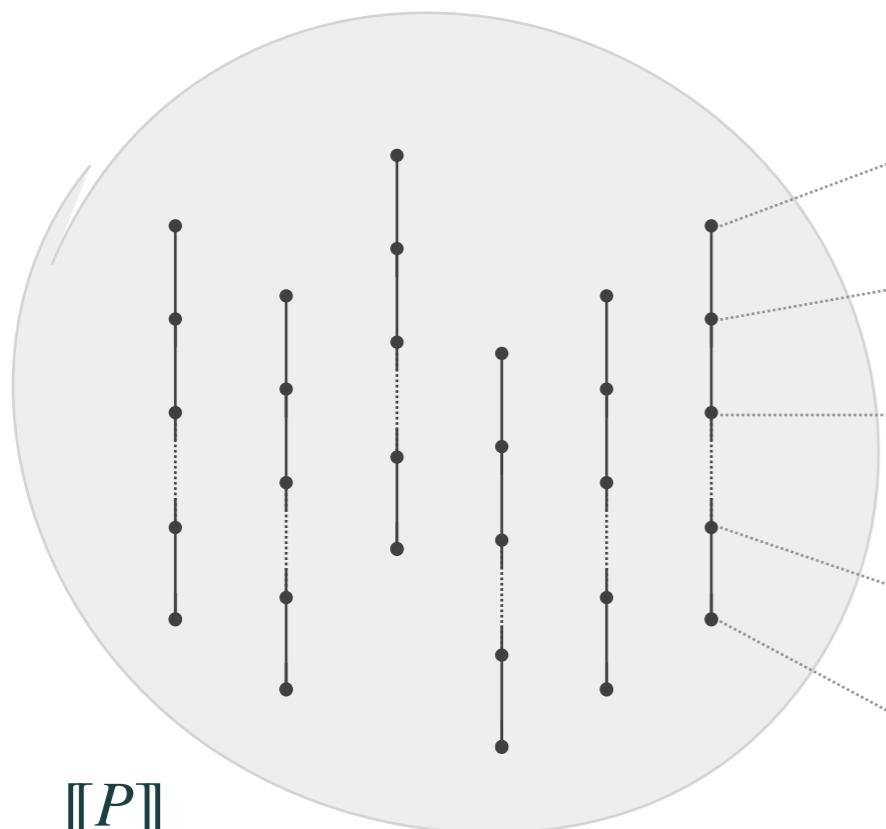
**mathematical models**

of the program behavior



# Concrete Semantics

## 2nd Challenge: Indirect Reasoning

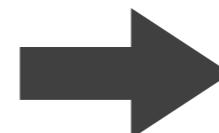


Michael J. Seidlinger/@mjseidlinger on Twitter

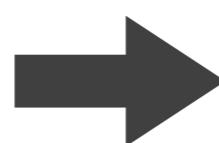
# Abstract Semantics

## 3rd Challenge: Complex Library Calls

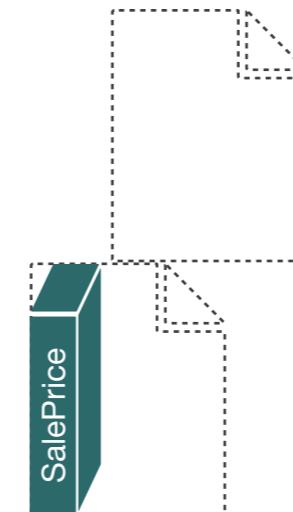
```
import pandas as pd  
df = pd.read_csv("HousePrices.csv")
```



```
ex = df[df.SalePrice >= 1000000]
```



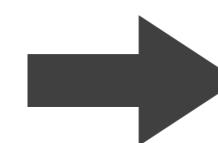
```
ex['Profit'] = ex['SalePrice'] - ex['BuyPrice']
```



ex = df



```
:  
dL = pd.read_csv("L.csv")  
dP = dL.pivot(index=c, columns=y, values=1)  
dR = pd.read_csv("R.csv")  
dG = dP.loc[:, 0:35].groupby(dR[r])
```



$$\begin{aligned} dR[r] &\in dG \\ dP \cap dR &\end{aligned}$$

# Practical Static Analysis

## Necessary vs Sufficient Data Expectations

### Automatic Inference of Necessary Preconditions

Patrick Cousot<sup>1</sup>, Radhia Cousot<sup>2</sup>, Manuel Fähndrich<sup>3</sup>, and Francesco Logozzo<sup>3</sup>

<sup>1</sup> NYU, ENS, CNRS, INRIA

[pcousot@cims.nyu.edu](mailto:pcousot@cims.nyu.edu)

<sup>2</sup> CNRS, ENS, INRIA

[rcousot@ens.fr](mailto:rcousot@ens.fr)

<sup>3</sup> Microsoft Research

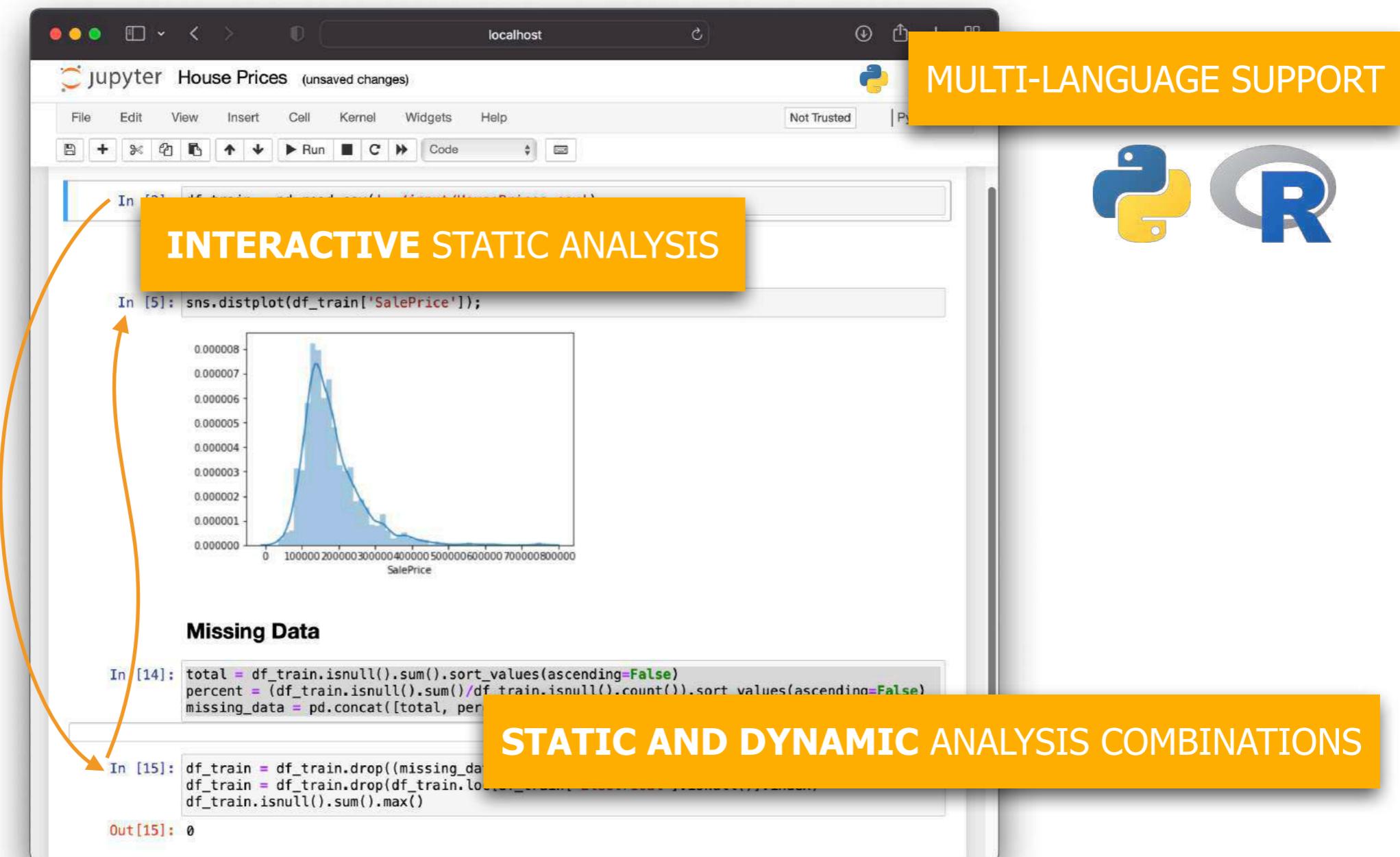
[{maf,logozzo}@microsoft.com](mailto:{maf,logozzo}@microsoft.com)

**Abstract.** We consider the problem of *automatic* precondition inference. We argue that the common notion of *sufficient* precondition inference (*i.e.*, under which precondition is the program correct?) imposes too large a burden on callers, and hence it is unfit for automatic program analysis. Therefore, we define the problem of *necessary* precondition inference (*i.e.*, under which precondition, if violated, will the program *always* be incorrect?). We designed and implemented several new abstract interpretation-based analyses to infer atomic, disjunctive, universally and existentially quantified necessary preconditions.

We experimentally validated the analyses on large scale industrial

# Implementation

## Wish List



# Data Expectations Analysis

**practical tools**

targeting specific program

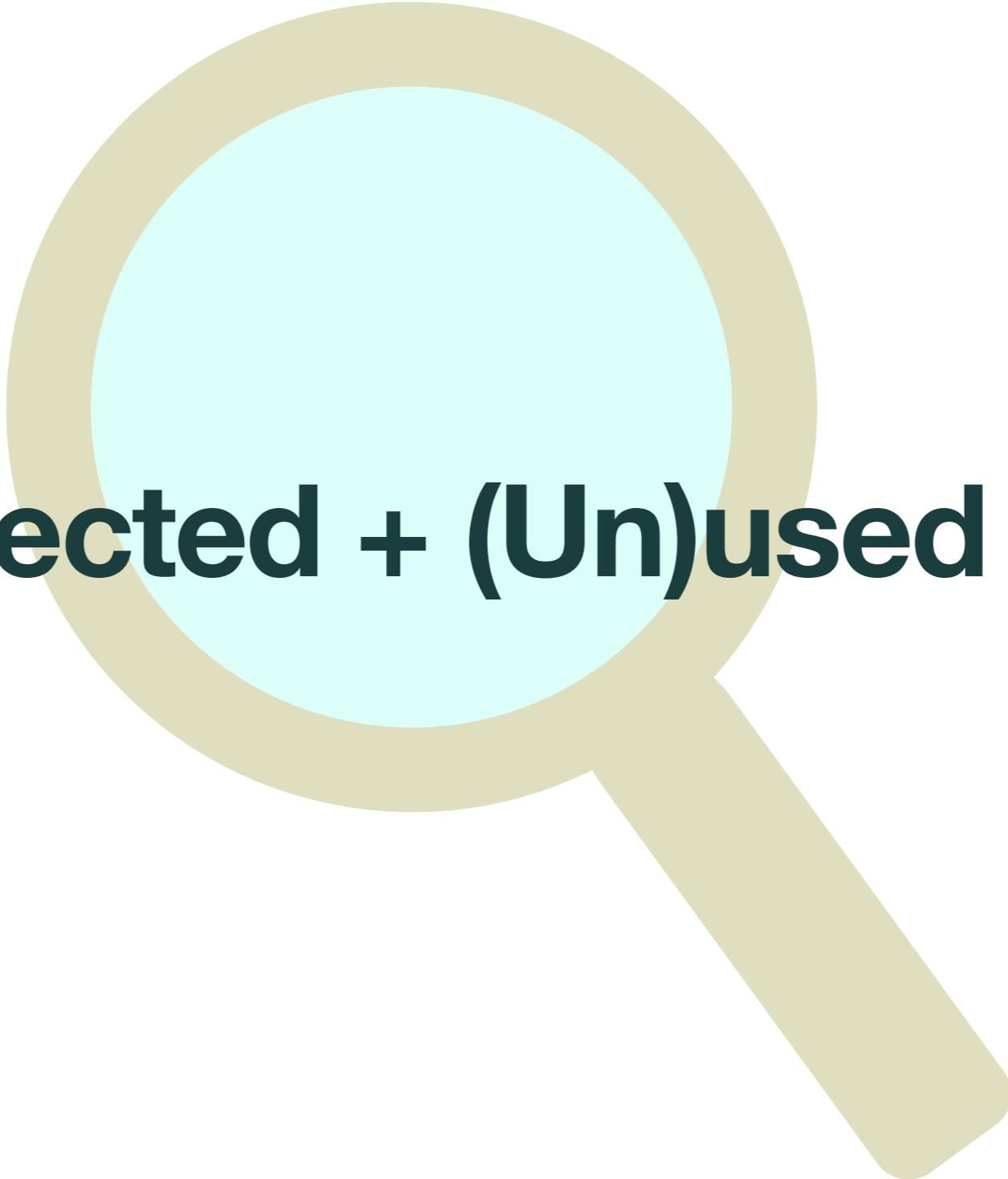
**algorithmic approach**

to decide program

**mathematical models**

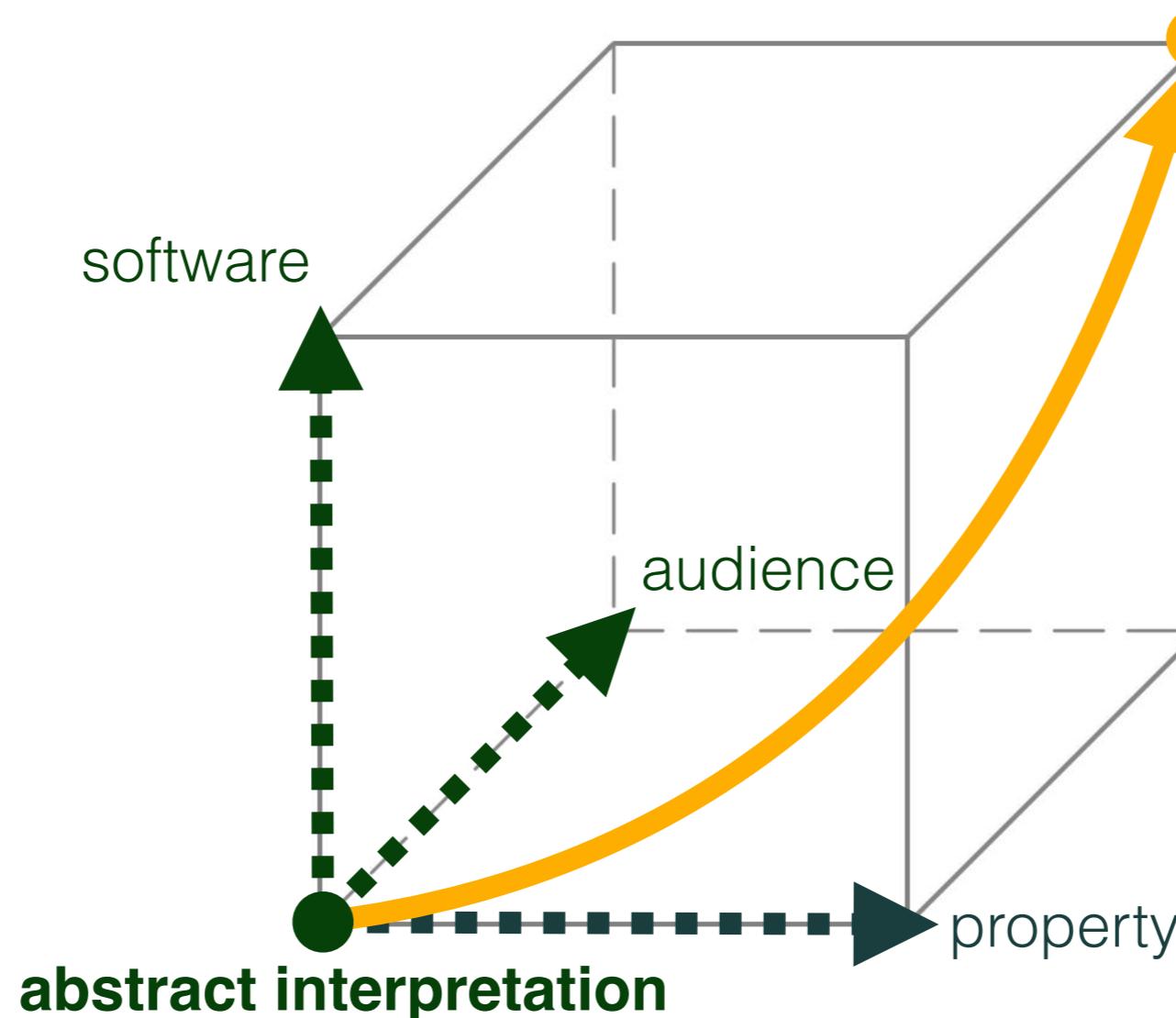
of the program behav





**(Un)expected + (Un)used Data**

# (Un)expected + (Un)used Analysis

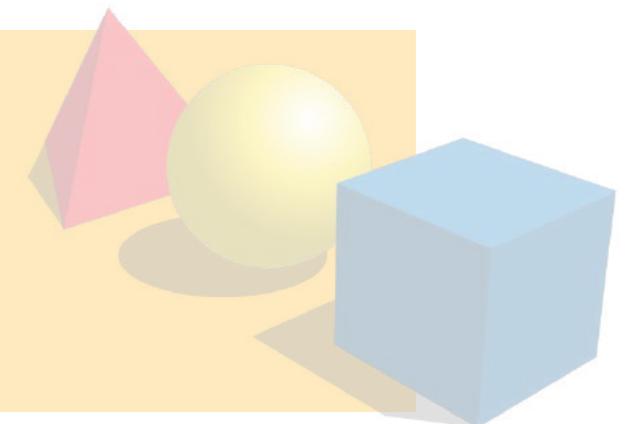


# Expectations + Usage Analysis

**practical tools**  
targeting specific programs

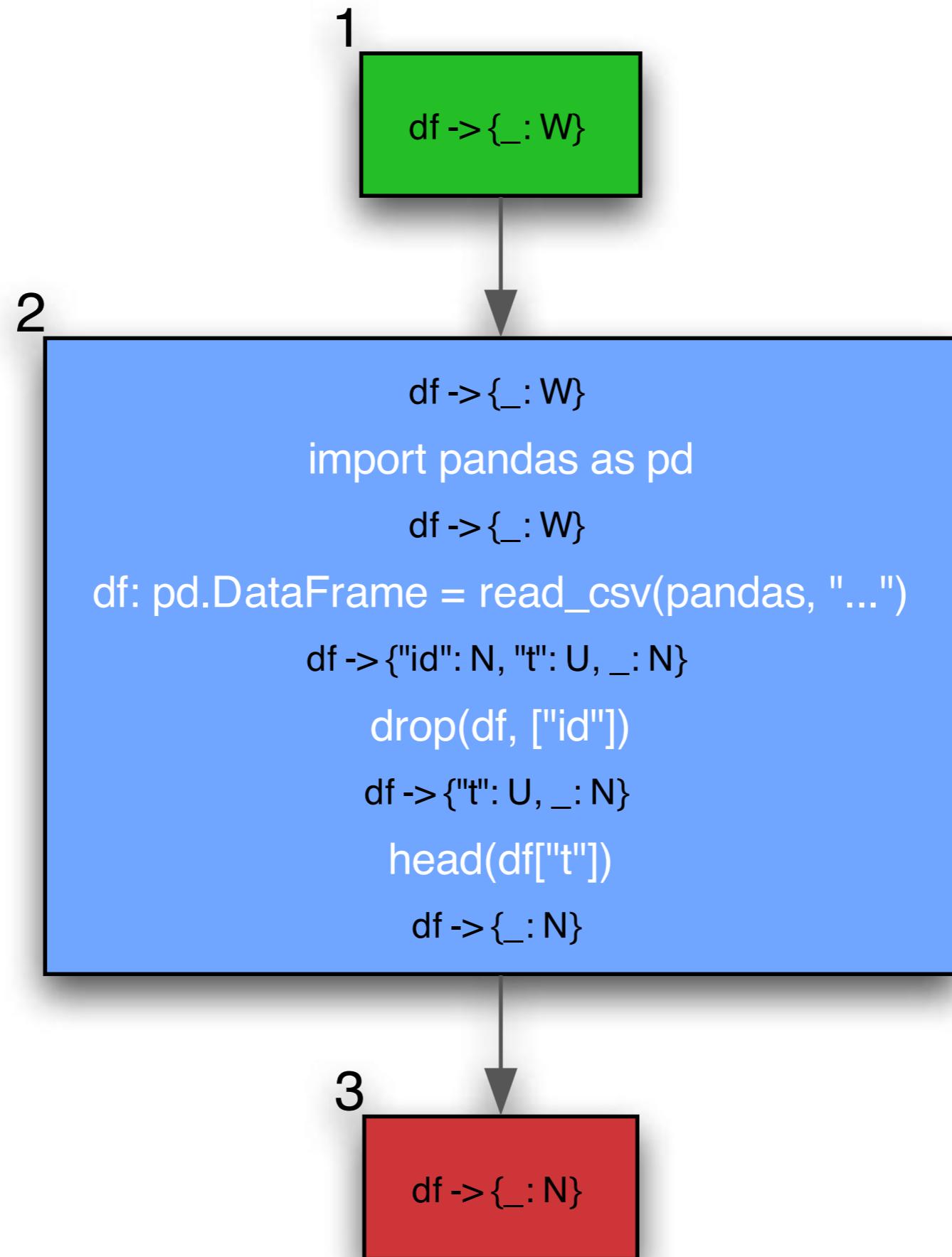


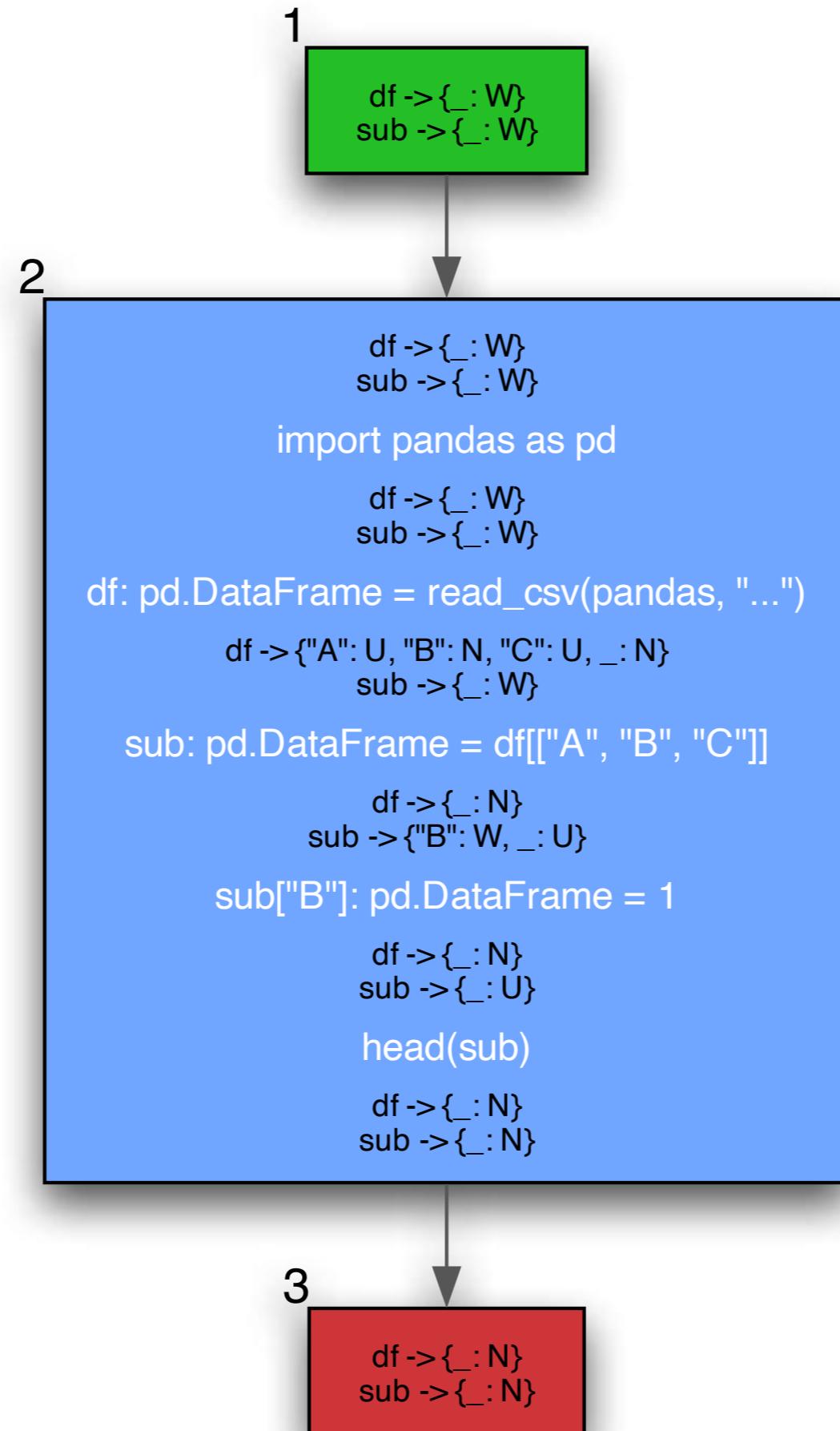
**algorithmic approaches**  
to decide program properties



**mathematical models**  
of the program behavior







# Bibliography

- [Kurd03] **Zeshan Kurd, Tim Kelly.** Establishing Safety Criteria for Artificial Neural Networks. In KES, 2003.
- [Li19] **Jianlin Li, Jiangchao Liu, Pengfei Yang, Liqian Chen, Xiaowei Huang, and Lijun Zhang.** Analyzing Deep Neural Networks with Symbolic Propagation: Towards Higher Precision and Faster Verification. In SAS, 2019.
- [Singh19] **Gagandeep Singh, Timon Gehr, Markus Püschel, and Martin T. Vechev.** An Abstract Domain for Certifying Neural Networks. In POPL, 2019.
- [Munakata23] **Satoshi Munakata, CU, Haruki Yokoyama, Koji Yamamoto, Kazuki Munakata.** Verifying Attention Robustness of Deep Neural Networks against Semantic Perturbations. In NFM, 2023.
- [Mohapatra20] Jeet Mohapatra, Tsui-Wei Weng, Pin-Yu Chen, Sijia Liu, Luca Daniel. Towards Verifying Robustness of Neural Networks Against A Family of Semantic Perturbations. In CVPR, 2020.

# Bibliography

[Mazzucato21] **Denis Mazzucato and CU.** Reduced Products of Abstract Domains for Fairness Certification of Neural Networks. In SAS, 2021.

[Julian16] **Kyle D. Julian, Jessica Lopez, Jeffrey S. Brush, Michael P. Owen, Mykel J. Kochenderfer.** Policy Compression for Aircraft Collision Avoidance Systems. In DASC, 2016.

[Katz17] **Guy Katz, Clark W. Barrett, David L. Dill, Kyle Julian, Mykel J. Kochenderfer.** Reluplex: An Efficient SMT Solver for Verifying Deep Neural Networks. In CAV, 2017.

[Galhotra17] **Sainyam Galhotra, Yuriy Brun, and Alexandra Meliou.** Fairness Testing: Testing Software for Discrimination. In FSE, 2017.

[Urban20] **CU, Maria Christakis, Valentin Wüstholtz, and Fuyuan Zhang.** Perfectly Parallel Fairness Certification of Neural Networks. In OOPSLA, 2020.

# Bibliography

[Urban21] **CU and Antoine Miné.** A Review of Formal Methods applied to Machine Learning. <https://arxiv.org/abs/2104.02466>, 2021.

[Pal24] **Abhinandan Pal, Francesco Ranzato, CU, Marco Zanella.** Abstract Interpretation-Based Feature Importance for Support Vector Machines. In VMCAI, 2024.

[R19] **Francesco Ranzato and Marco Zanella.** Robustness Verification of Support Vector Machines. In SAS, 2019.

[Ranzato21] **Francesco Ranzato, CU, and Marco Zanella.** *Fairness-Aware Training of Decision Trees by Abstract Interpretation.* In CIKM 2021.

[CU18] **CU and Peter Müller.** An Abstract Interpretation Framework for Data Usage. In ESOP 2018.

[Subotic24] **Filip Drobnjaković, Pavle Subotić, CU.** An Abstract Interpretation-Based Data Leakage Static Analysis. In TASE 2024.