Towards a New Synthesis of Reasoning and Learning

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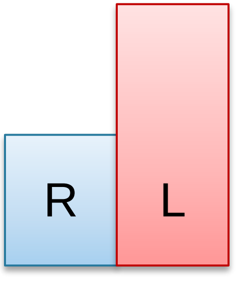
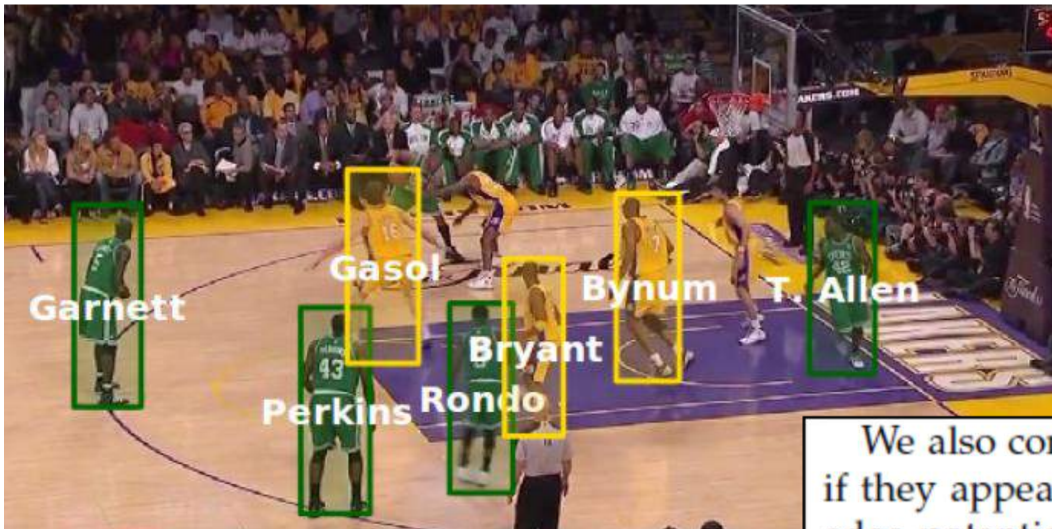
Outline: Reasoning ∩ Learning

1. Deep Learning with Symbolic Knowledge
2. Efficient Reasoning During Learning
3. Probabilistic and Logistic Circuits
4. High-Level Probabilistic Reasoning

Deep Learning with Symbolic Knowledge



Motivation: Vision



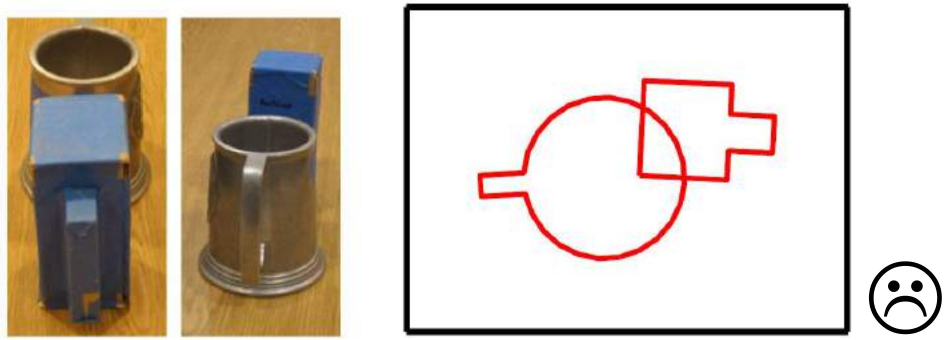
We also connect all pairs of identity nodes $y_{t,i}$ and $y_{t,j}$ if they appear in the same time t. We then introduce an edge potential that enforces mutual exclusion:

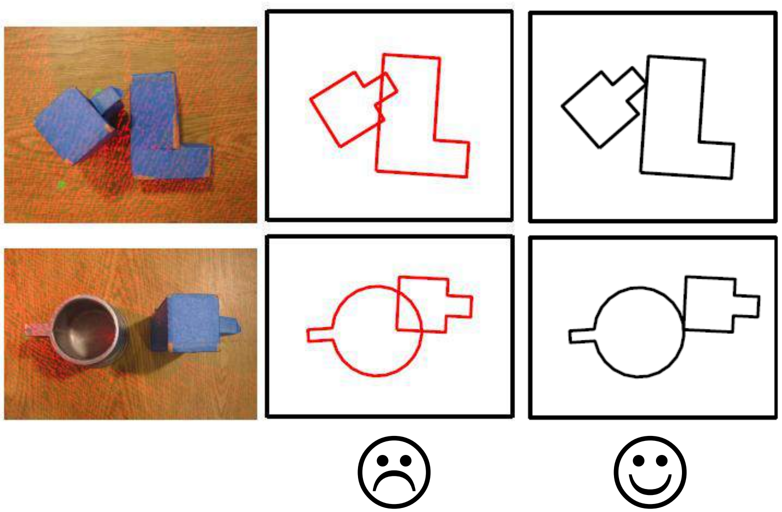
$$\psi_{\text{mutex}}(y_{t,i}, y_{t,j}) = \begin{cases} 1 & \text{if } y_{t,i} \neq y_{t,j} \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

This potential specifies the constraint that a player can be appear only *once* in a frame. For example, if the i-th detection $y_{t,i}$ has been assign to Bryant, $y_{t,j}$ cannot have the same identity because Bryant is impossible to appear twice in a frame.

[Lu, W. L., Ting, J. A., Little, J. J., & Murphy, K. P. (2013). Learning to track and identify players from broadcast sports videos.]

Motivation: Robotics





The method developed in this paper can be used in a broad variety of semantic mapping and object manipulation tasks, providing an efficient and effective way to incorporate collision constraints into a recursive state estimator, obtaining optimal or near-optimal solutions.

[Wong, L. L., Kaelbling, L. P., & Lozano-Perez, T., Collision-free state estimation. ICRA 2012]

Motivation: Language

- Non-local dependencies:

  "At least one verb in each sentence"

- Sentence compression

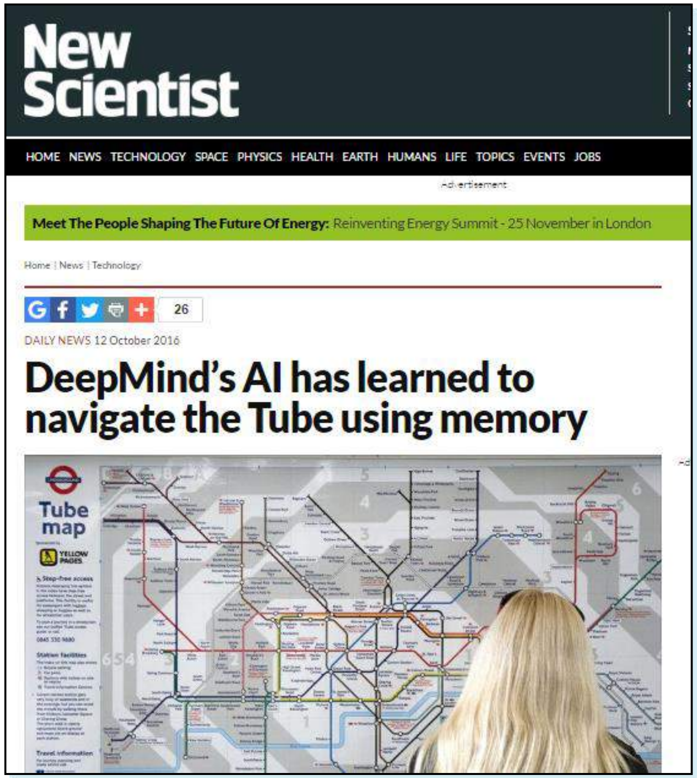
  "If a modifier is kept, its subject is also kept"

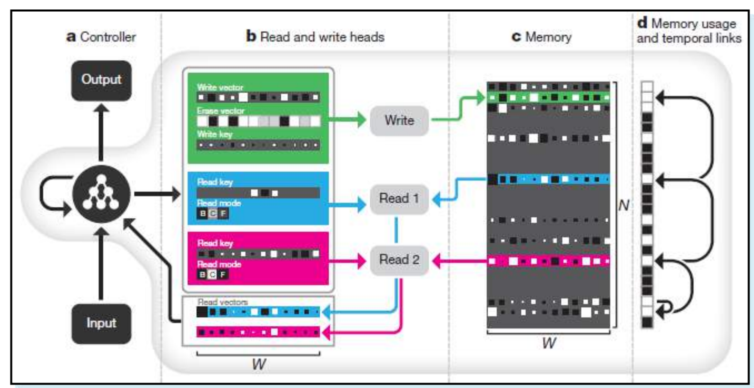
… and many more!

Citations	
Start	The citation must start with author or editor.
AppearsOnce	Each field must be a consecutive list of words, and can appear at most once in a citation.
Punctuation	State transitions must occur on punctuation marks.
BookJournal	The words *proc*, *journal*, *proceedings*, *ACM* are *JOURNAL* or *BOOKTITLE*.
...	...
TechReport	The words *tech*, *technical* are *TECH_REPORT*.
Title	Quotations can appear only in titles.
Location	The words *CA*, *Australia*, *NY* are *LOCATION*.

[Chang, M., Ratinov, L., & Roth, D. (2008). Constraints as prior knowledge],
[Ganchev, K., Gillenwater, J., & Taskar, B. (2010). Posterior regularization for structured latent variable models]

Motivation: Deep Learning

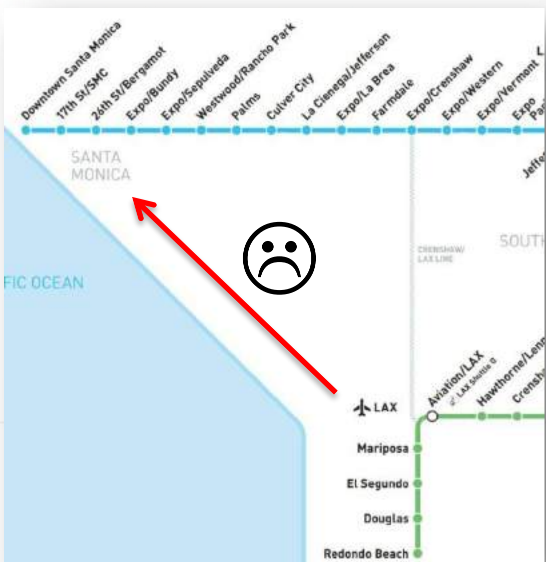




[Graves, A., Wayne, G., Reynolds, M., Harley, T., Danihelka, I., Grabska-Barwińska, A., et al.. (2016). Hybrid computing using a neural network with dynamic external memory. *Nature*, *538*(7626), 471-476.]

Motivation: Deep Learning

DeepMind's latest technique uses external memory to **solve tasks that require logic and reasoning — a step toward more human-like AI.**



… but …

optimal planner recalculating a shortest path to the end node. To ensure that the network always moved to a valid node, the output distribution was renormalized over the set of possible triples outgoing from the current node. The performance

it also received input triples during the answer phase, indicating the actions chosen on the previous time-step. This makes the problem a 'structured prediction'

[Graves, A., Wayne, G., Reynolds, M., Harley, T., Danihelka, I., Grabska-Barwińska, A., et al.. (2016). Hybrid computing using a neural network with dynamic external memory. *Nature*, *538*(7626), 471-476.]

Learning with Symbolic Knowledge

L	K	P	A	Students
0	0	1	0	6
0	0	1	1	54
0	1	1	1	10
1	0	0	0	5
1	0	1	0	1
1	0	1	1	0
1	1	0	0	17
1	1	1	0	4
1	1	1	1	3

Data + **Constraints**
(Background Knowledge)
(Physics)

$$P \vee L$$
$$A \Rightarrow P$$
$$K \Rightarrow (P \vee L)$$

1. Must take at least one of Probability (**P**) or Logic (**L**).
2. Probability (**P**) is a prerequisite for AI (**A**).
3. The prerequisites for KR (**K**) is either AI (**A**) or Logic (**L**).

Learning with Symbolic Knowledge

L	K	P	A	Students
0	0	1	0	6
0	0	1	1	54
0	1	1	1	10
1	0	0	0	5
1	0	1	0	1
1	0	1	1	0
1	1	0	0	17
1	1	1	0	4
1	1	1	1	3

Data + **Constraints**
(Background Knowledge)
(Physics)

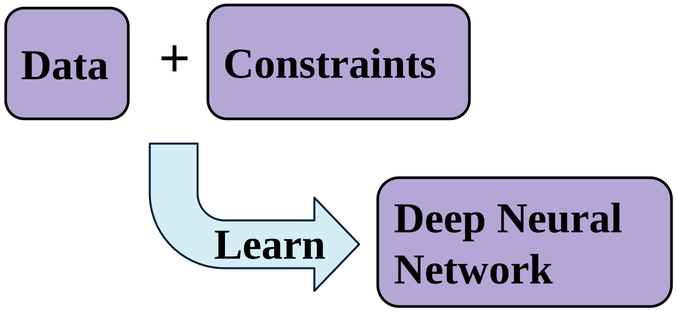
$$P \vee L$$
$$A \Rightarrow P$$
$$K \Rightarrow (P \vee L)$$

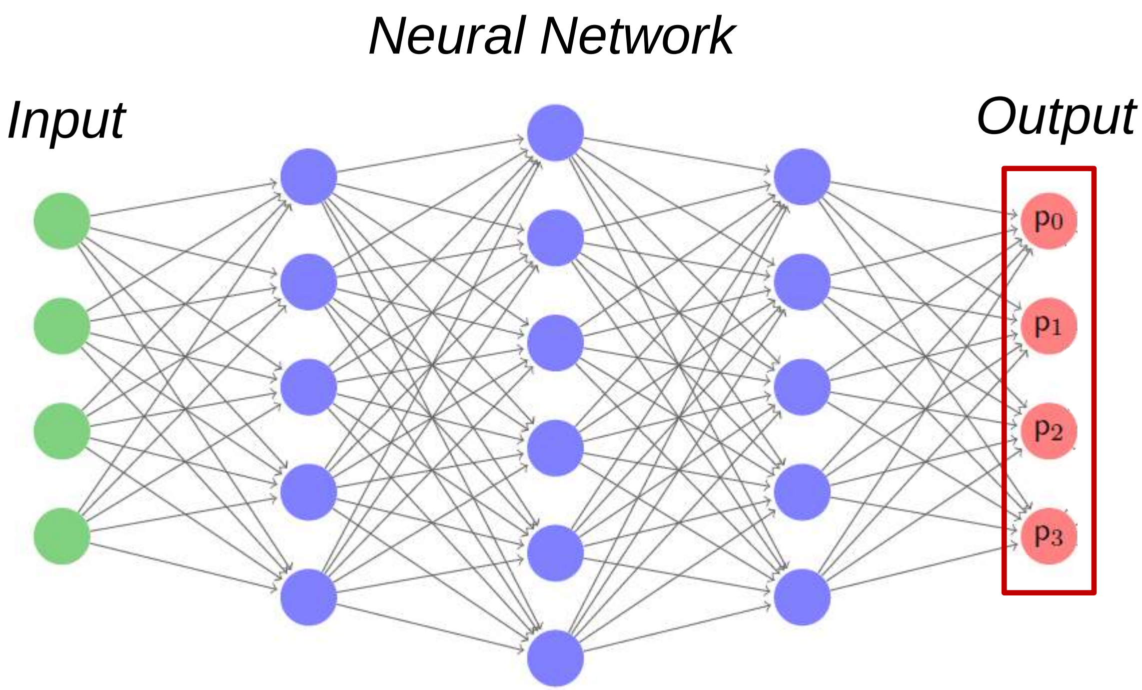
Learn

ML Model

Today's machine learning tools don't take knowledge as input! ☹

Deep Learning with Symbolic Knowledge





Output is probability vector **p**, not Boolean logic!

Semantic Loss

<u>Q</u>: How close is output ***p*** *to satisfying constraint α?*

*<u>Answer</u>: Semantic loss function L(α,**p**)*

- Axioms, for example:
  - If **p** is Boolean then L(**p**,**p**) = 0
  - If α implies β then L(α,**p**) ≥ L(β,**p**) (*α more strict*)

- Implied Properties:
  - If α is equivalent to β then L(α,**p**) = L(β,**p**)
  - If **p** is Boolean and satisfies α then L(α,**p**) = 0

SEMANTIC Loss!

Semantic Loss: Definition

Theorem: Axioms imply unique semantic loss:

$$L^s(\alpha, \mathsf{p}) \propto -\log \sum_{\mathbf{x} \models \alpha} \prod_{i:\mathbf{x} \models X_i} \mathsf{p}_i \prod_{i:\mathbf{x} \models \neg X_i} (1 - \mathsf{p}_i)$$

Probability of getting state **x** after flipping coins with probabilities **p**

Probability of satisfying α after flipping coins with probabilities **p**

Simple Example: Exactly-One

- Data must have some label

  We agree this must be one of the 10 digits:

- Exactly-one constraint

  → For 3 classes: $\begin{cases} x_1 \lor x_2 \lor x_3 \\ \neg x_1 \lor \neg x_2 \\ \neg x_2 \lor \neg x_3 \\ \neg x_1 \lor \neg x_3 \end{cases}$

- Semantic loss:

$$\mathrm{L}^{\mathrm{s}}(\text{exactly-one}, \mathrm{p}) \propto -\log \sum_{i=1}^{n} \mathrm{p}_i \underbrace{\prod_{j=1, j \neq i}^{n} (1 - \mathrm{p}_j)}$$

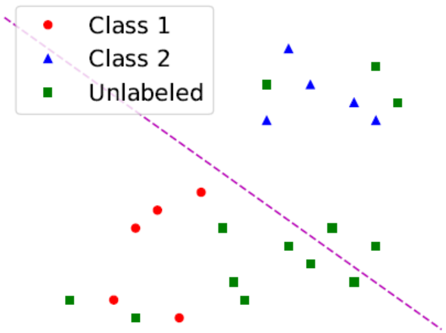
Only $x_i = 1$ after flipping coins

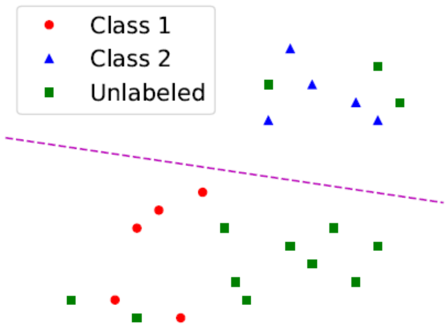
Exactly one true x after flipping coins

Semi-Supervised Learning

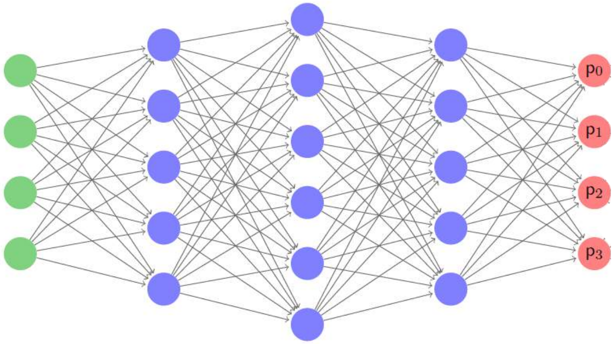
- Intuition: Unlabeled data must have some label

  Cf. entropy minimization, manifold learning





- Minimize exactly-one semantic loss on unlabeled data



Train with

$$existing\ loss + w \cdot semantic\ loss$$

Experimental Evaluation

Accuracy % with # of used labels	100	1000	ALL
AtlasRBF (Pitelis et al., 2014)	91.9 (±0.95)	96.32 (±0.12)	98.69
Deep Generative (Kingma et al., 2014)	96.67(±0.14)	97.60 (±0.02)	99.04
Virtual Adversarial (Miyato et al., 2016)	97.67	98.64	99.36
Ladder Net (Rasmus et al., 2015)	**98.94** (±0.37)	**99.16** (±0.08)	99.43 (±0.02)
Baseline: MLP, Gaussian Noise	78.46 (±1.94)	94.26 (±0.31)	99.34 (±0.08)
Baseline: Self-Training	72.55 (±4.21)	87.43 (±3.07)	
Baseline: MLP with Entropy Regularizer	96.27 (±0.64)	98.32 (±0.34)	99.37 (±0.12)
MLP with Semantic Loss	98.38 (±0.51)	98.78 (±0.17)	99.36 (±0.02)

Competitive with state of the art in semi-supervised deep learning

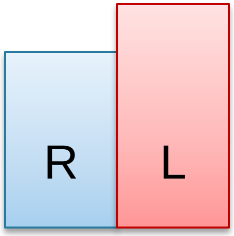
Accuracy % with # of used labels	100	500	1000	ALL
Ladder Net (Rasmus et al., 2015)	81.46 (±0.64)	85.18 (±0.27)	86.48 (±0.15)	90.46
Baseline: MLP, Gaussian Noise	69.45 (±2.03)	78.12 (±1.41)	80.94 (±0.84)	89.87
MLP with Semantic Loss	**86.74** (±0.71)	**89.49** (±0.24)	**89.67** (±0.09)	89.81

Outperforms SoA!

Same conclusion on CIFAR10

Accuracy % with # of used labels	4000	ALL
CNN Baseline in Ladder Net	76.67 (± 0.61)	90.73
Ladder Net (Rasmus et al., 2015)	79.60 (±0.47)	
Baseline: CNN, Whitening, Cropping	77.13	90.96
CNN with Semantic Loss	**81.79**	90.92

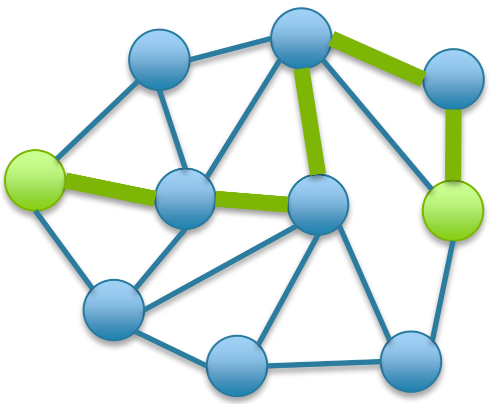
Efficient Reasoning
During Learning



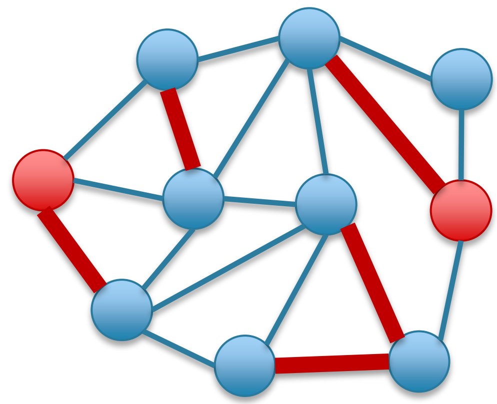
But what about *real* constraints?

- Path constraint

cf. Nature paper



vs.



- Example: 4x4 grids

  2^{24} = 184 paths + 16,777,032 non-paths

- Easily encoded as logical constraints ☺

[Nishino et al., Choi et al.]

How to Compute Semantic Loss?

- In general: #P-hard ☹

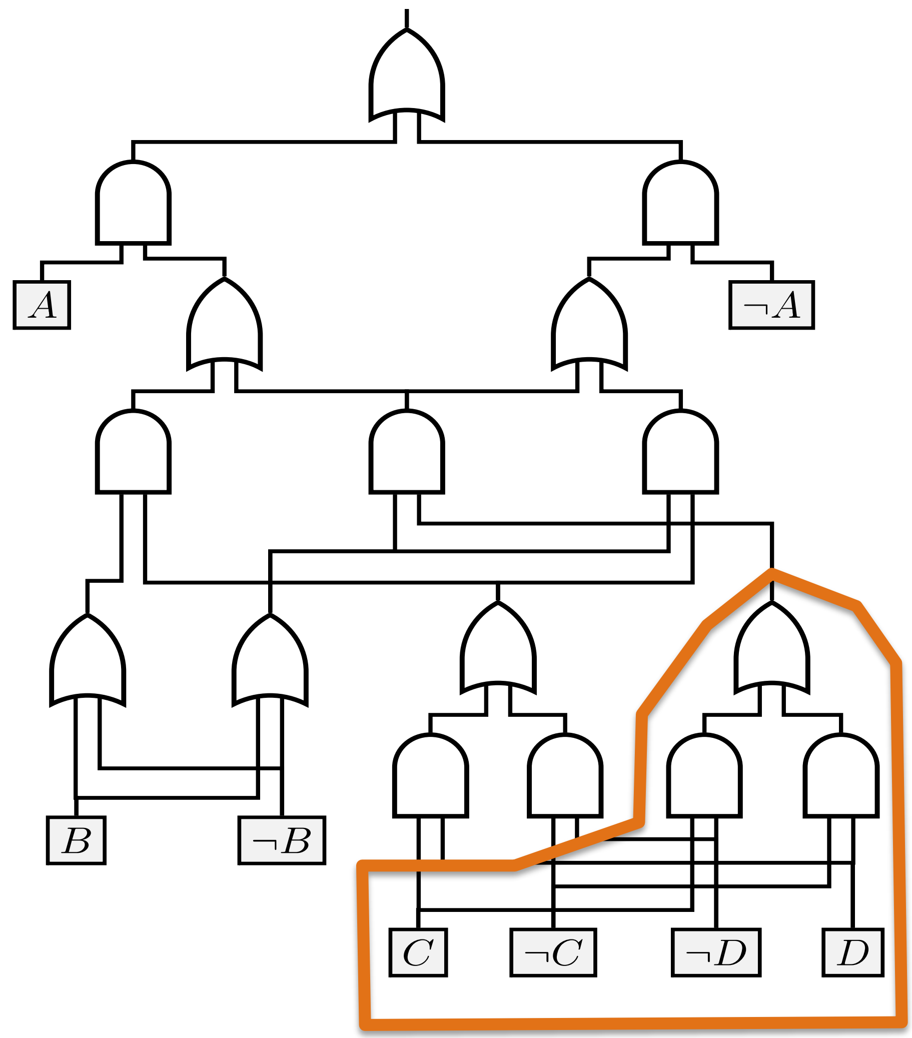
$$L^s(\alpha, \mathsf{p}) \propto -\log \sum_{\mathbf{x} \models \alpha} \prod_{i:\mathbf{x} \models X_i} \mathsf{p}_i \prod_{i:\mathbf{x} \models \neg X_i} (1 - \mathsf{p}_i)$$

Reasoning Tool: Logical Circuits

Representation of logical sentences:

$(C \wedge \neg D) \vee (\neg C \wedge D)$

C XOR D

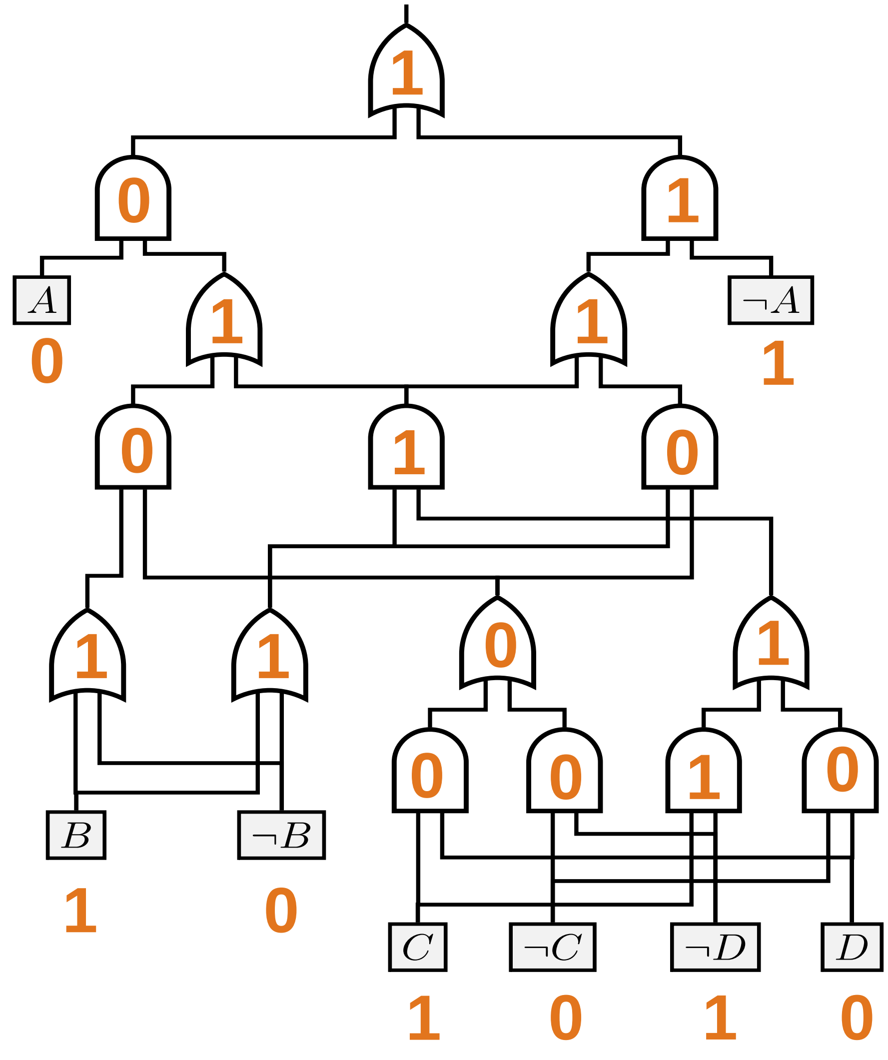


Reasoning Tool: Logical Circuits

Representation of logical sentences:

Input:

A	B	C	D
0	1	1	0

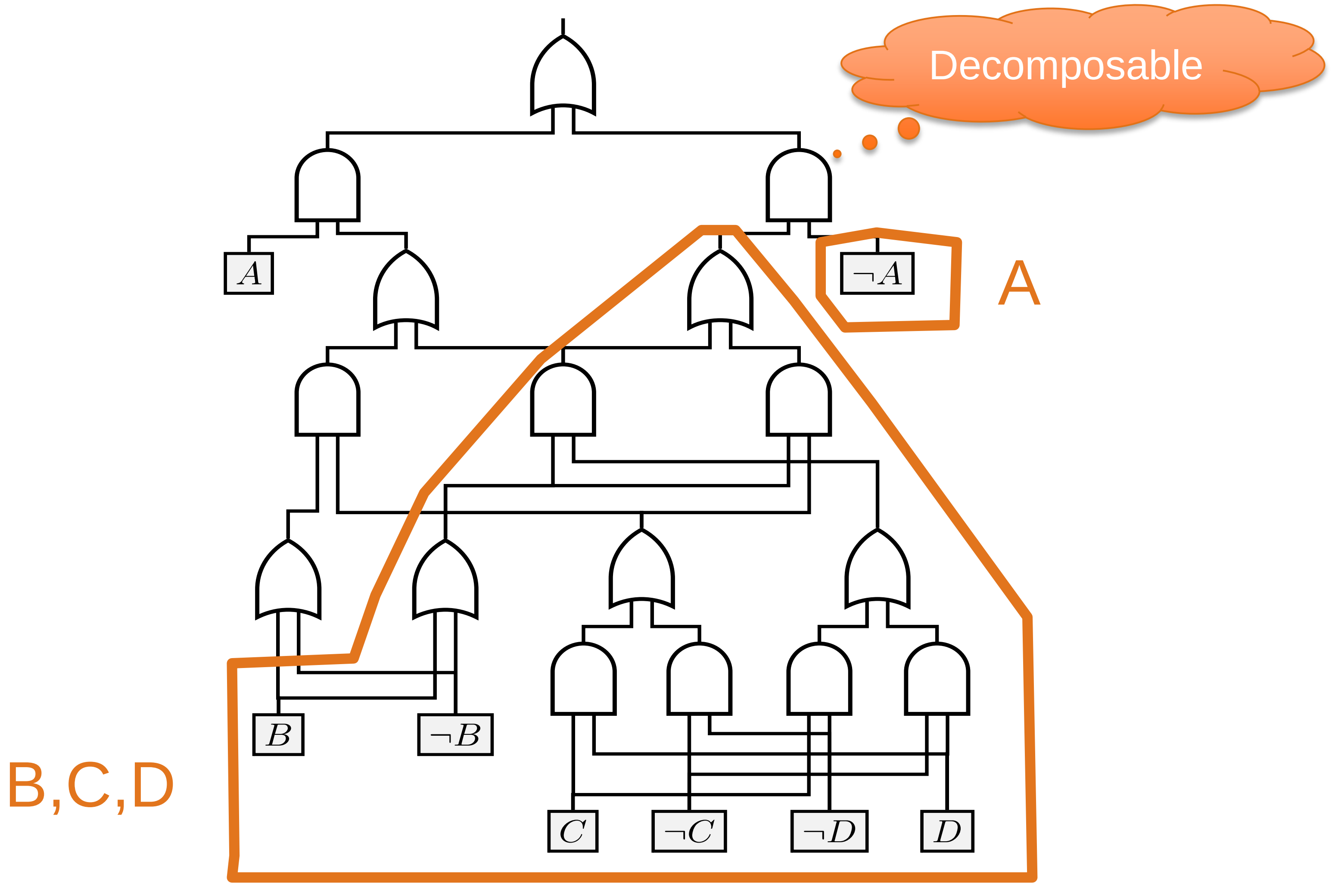


Bottom-up Evaluation

Tractable for Logical Inference

- Is there a solution? (SAT)
  - SAT($\alpha \lor \beta$) iff SAT(α) or SAT(β) (*always*)
  - SAT($\alpha \land \beta$) iff ***???***

Decomposable Circuits

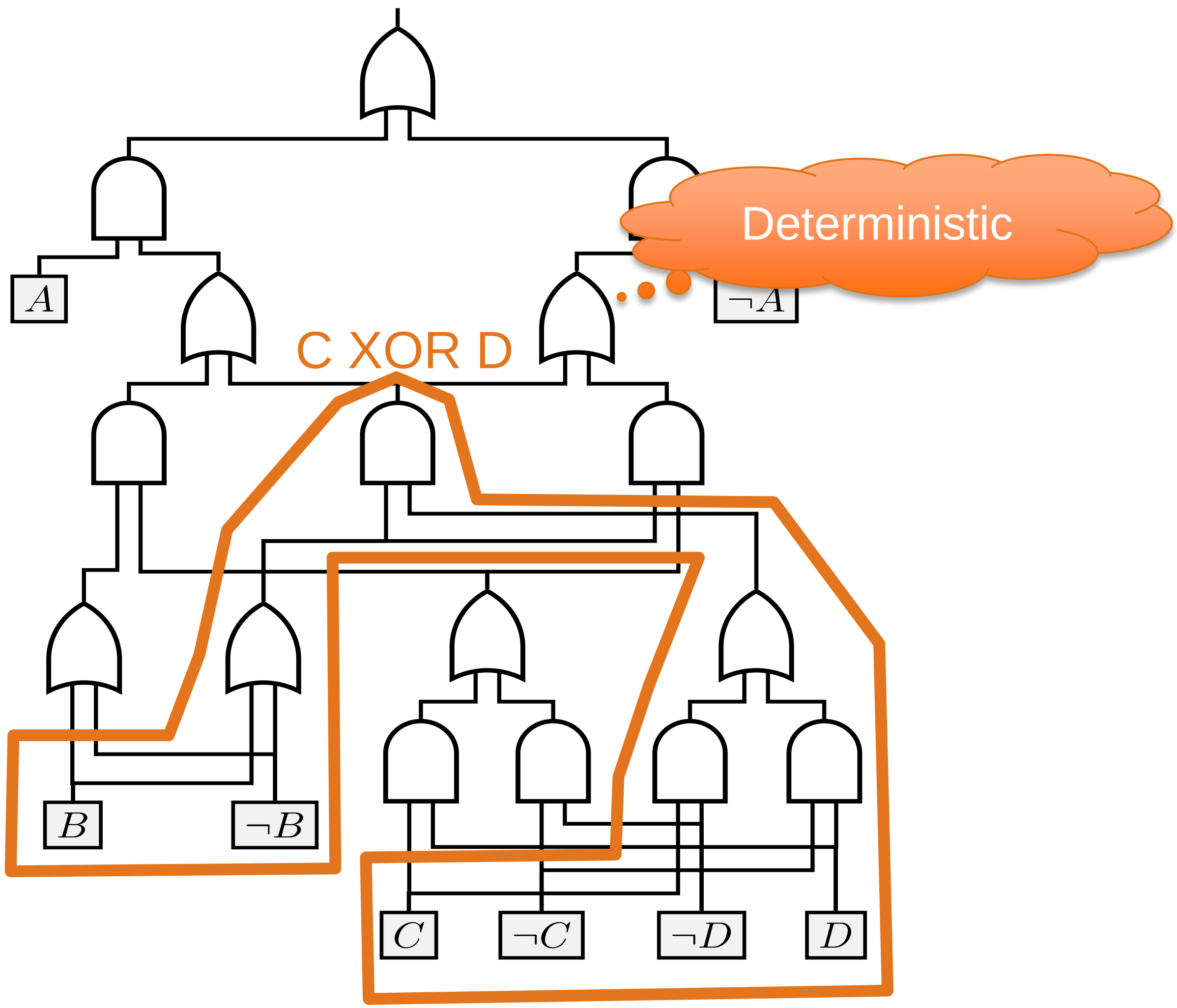


Tractable for Logical Inference

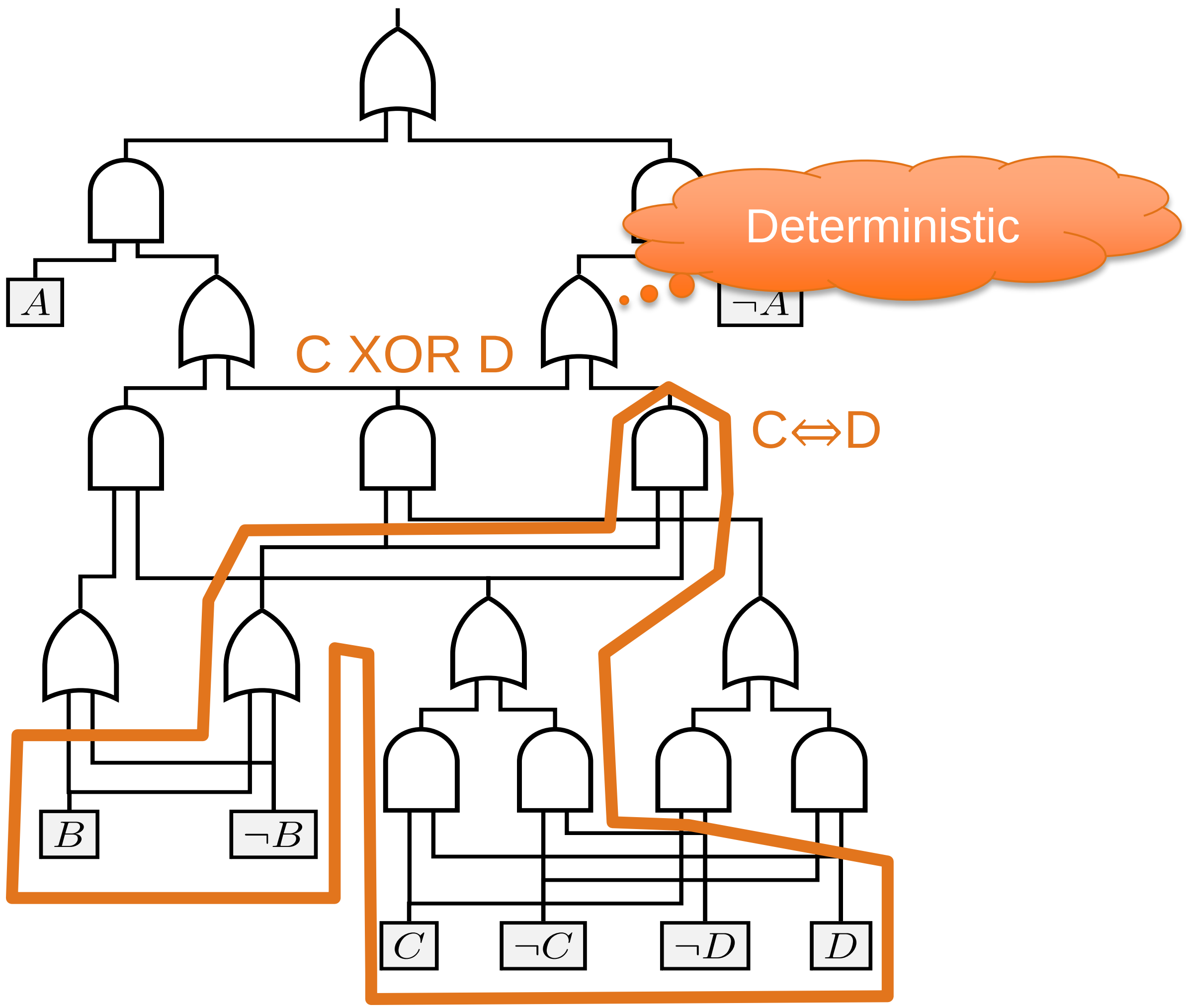
- Is there a solution? (SAT) ✓
  - SAT($\alpha \vee \beta$) iff SAT(α) or SAT(β) (*always*)
  - SAT($\alpha \wedge \beta$) iff SAT(α) and SAT(β) (*decomposable*)
- How many solutions are there? (#SAT)

- Complexity linear in circuit size ☺

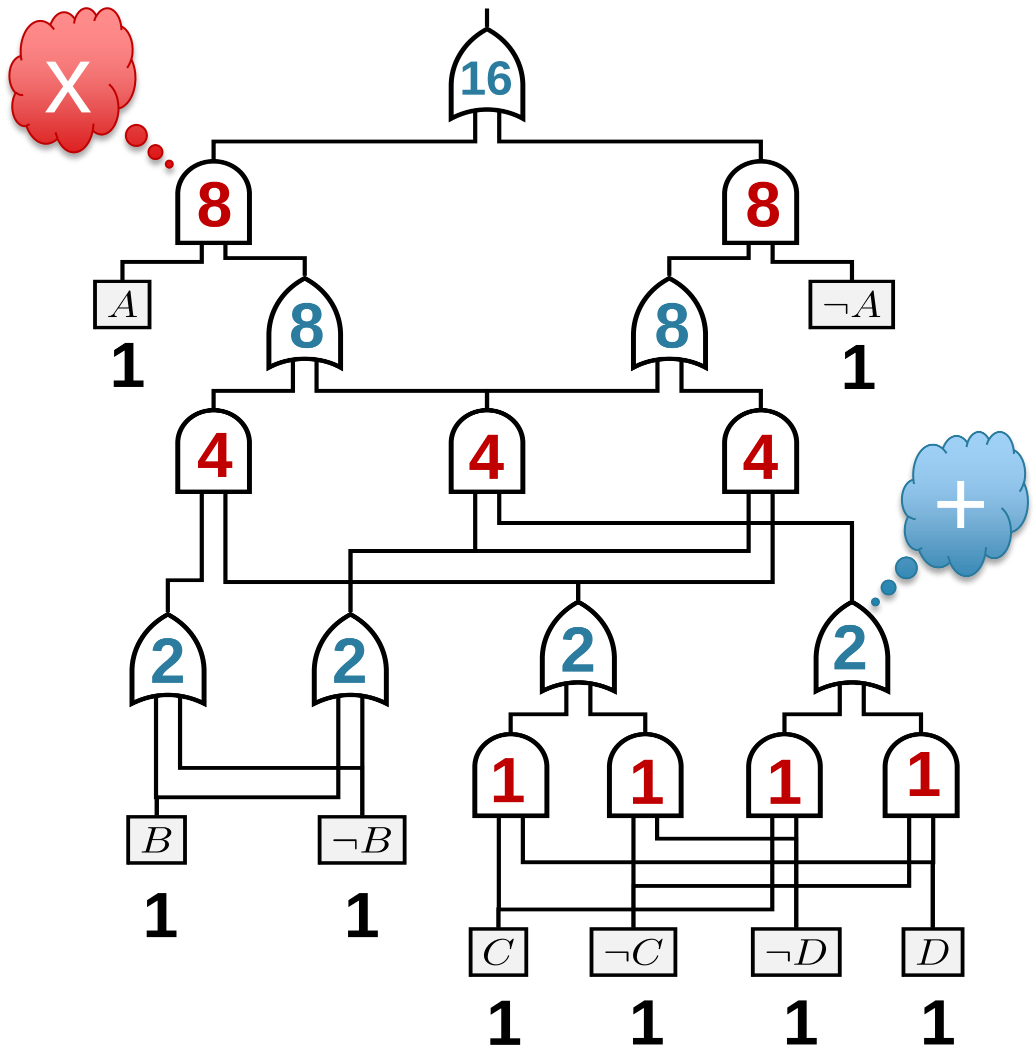
Deterministic Circuits



Deterministic Circuits



How many solutions are there? (#SAT)



Tractable for Logical Inference

- Is there a solution? (SAT) ✓
- How many solutions are there? (#SAT) ✓

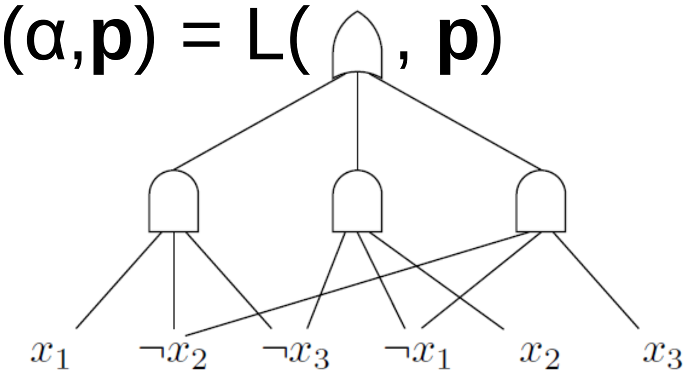
- Complexity linear in circuit size ☺

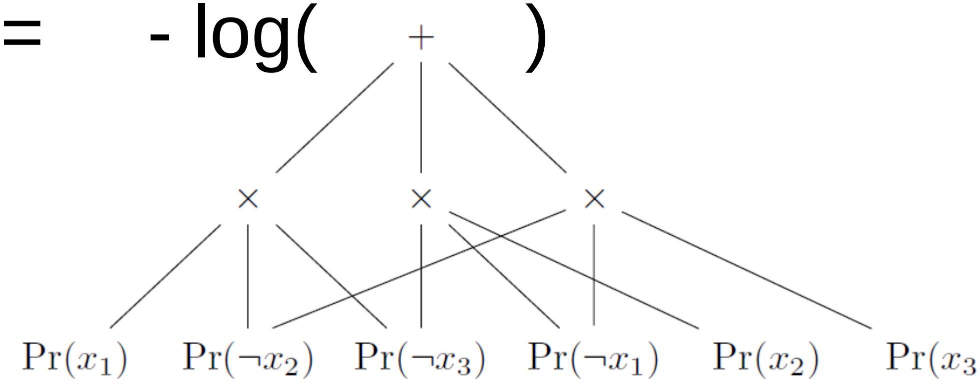
- Compilation into circuit by
  - ↓ exhaustive SAT solver
  - ↑ conjoin/disjoin/negate

[Darwiche and Marquis, JAIR 2002]

How to Compute Semantic Loss?

- In general: #P-hard ☹
- With a logical circuit for α: Linear ☺
- Example: exactly-one constraint:

L(α,**p**) = L(

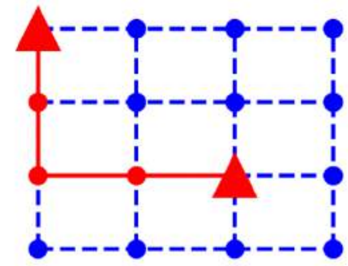
, **p**) = - log(

)

- *Why?* Decomposability and determinism!

Predict Shortest Paths

Add semantic loss
for path constraint



Test accuracy %	Coherent	Incoherent	Constraint
5-layer MLP	5.62	**85.91**	6.99
Semantic loss	**28.51**	83.14	**69.89**

Is prediction the shortest path?
This is the real task!

Are individual edge predictions correct?

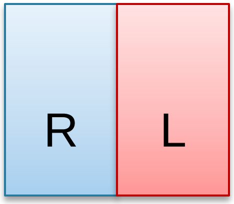
Is output a path?

(same conclusion for predicting sushi preferences, see paper)

Conclusions 1

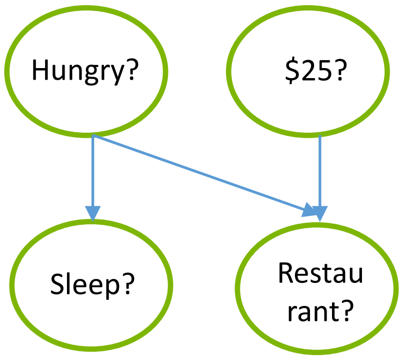
- Knowledge is (hidden) everywhere in ML
- Semantic loss makes logic differentiable
- Performs well semi-supervised
- Requires hard reasoning in general
  - Reasoning can be encapsulated in a circuit
  - No overhead during learning
- Performs well on structured prediction
- A little bit of reasoning goes a long way!

Probabilistic and Logistic Circuits



A False Dilemma?

Classical AI Methods



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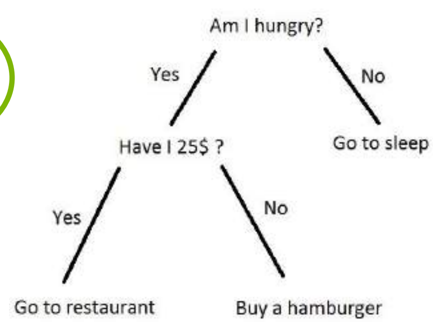
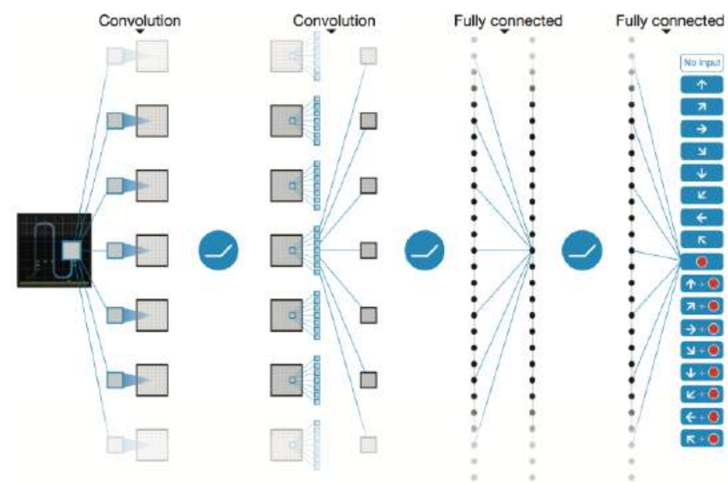


Clear Modeling Assumption
Well-understood

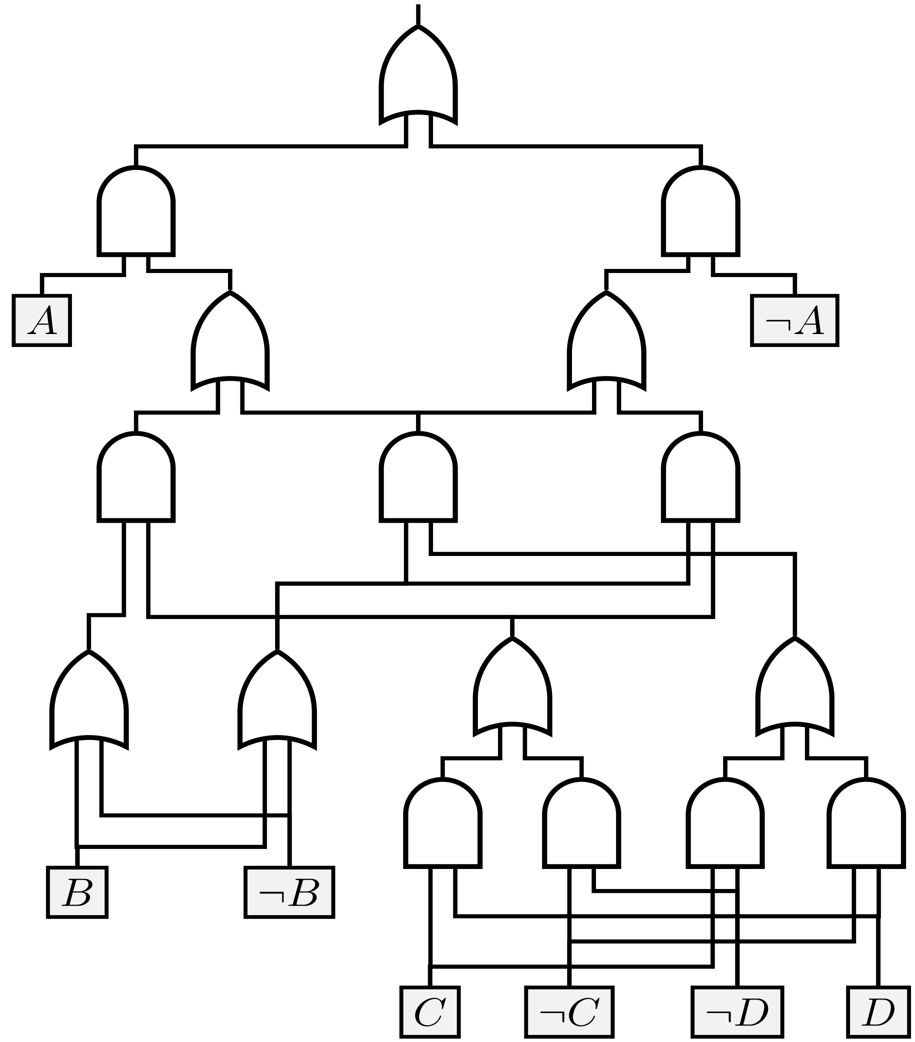
Neural Networks



“Black Box”
Empirical performance

Inspiration: Probabilistic Circuits

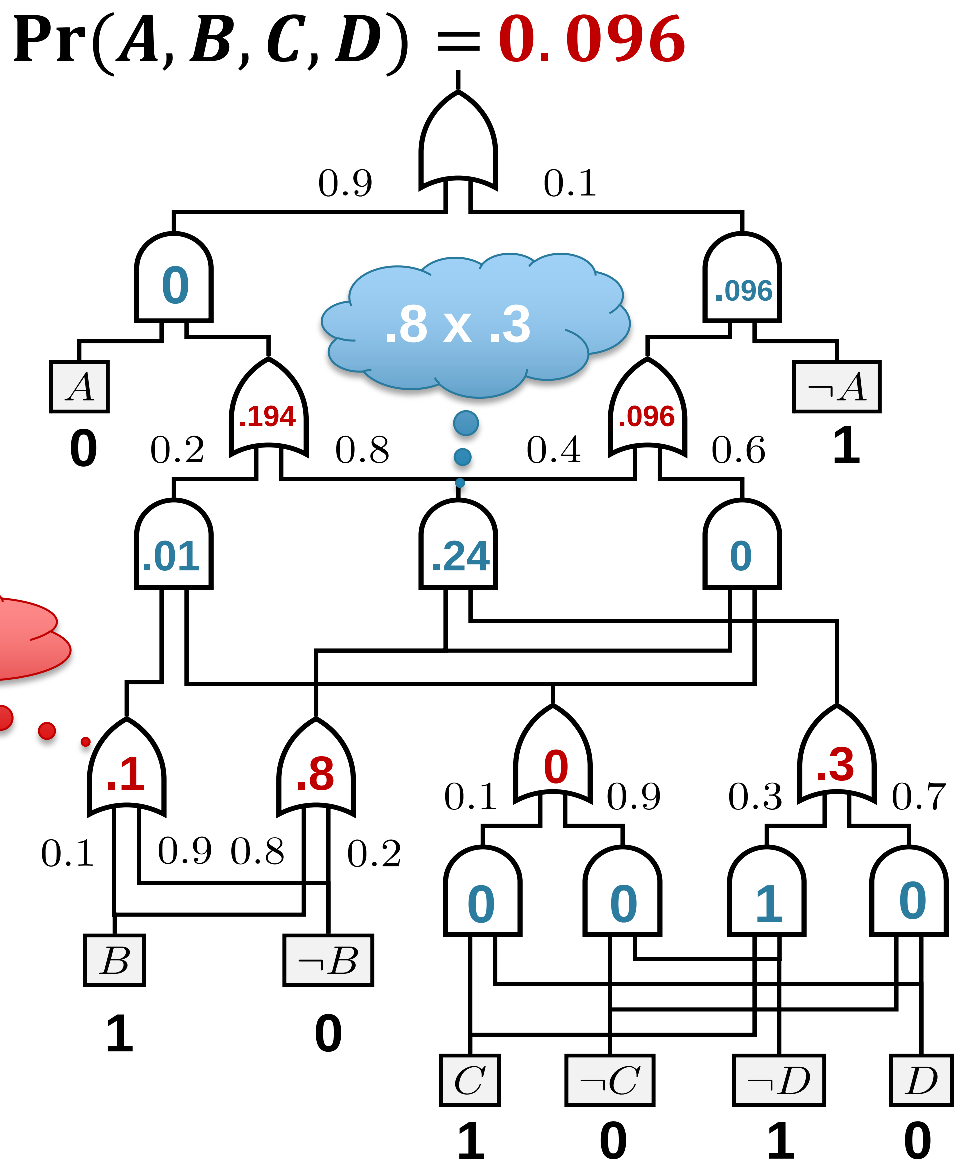
Can we turn **logic circuits** into a **statistical model?**



Probabilistic Circuits

Probability on edges

Bottom-up evaluation



Input:

A	B	C	D	$\Pr(A, B, C, D)$
0	1	1	0	?

Properties, Properties, Properties!

- Read conditional independencies from structure
- Interpretable parameters (XAI)
  (conditional probabilities of logical sentences)
- Closed-form parameter learning
- Efficient reasoning
  - **MAP inference**: most-likely assignment to x given y
    (otherwise NP-hard)
  - Computing **conditional probabilities** Pr(x|y)
    (otherwise #P-hard)
  - Algorithms linear in circuit size ☺

Side Note: Discrete Density Estimation

Datasets	|Var|	LearnPSDD Ensemble	Best-to-Date
NLTCS	16	$-5.99^{\dagger}$	-6.00
MSNBC	17	$-6.04^{\dagger}$	$-6.04^{\dagger}$
KDD	64	$-2.11^{\dagger}$	-2.12
Plants	69	-13.02	$-11.99^{\dagger}$
Audio	100	-39.94	$-39.49^{\dagger}$
Jester	100	-51.29	$-41.11^{\dagger}$
Netflix	100	$-55.71^{\dagger}$	-55.84
Accidents	111	-30.16	$-24.87^{\dagger}$
Retail	135	$-10.72^{\dagger}$	-10.78
Pumsb-Star	163	-26.12	$-22.40^{\dagger}$
DNA	180	-88.01	$-80.03^{\dagger}$
Kosarek	190	$-10.52^{\dagger}$	-10.54
MSWeb	294	-9.89	$-9.22^{\dagger}$
Book	500	-34.97	$-30.18^{\dagger}$
EachMovie	500	-58.01	$-51.14^{\dagger}$
WebKB	839	-161.09	$-150.10^{\dagger}$
Reuters-52	889	-89.61	$-80.66^{\dagger}$
20NewsGrp.	910	-155.97	$-150.88^{\dagger}$
BBC	1058	-253.19	$-233.26^{\dagger}$
AD	1556	-31.78	$-14.36^{\dagger}$

LearnPSDD
state of the art
on 6 datasets!

Q: “Help! I need to learn a discrete probability distribution…”

A: Learn probabilistic circuits!

Strongly outperforms

- Bayesian network learners
- Markov network learners

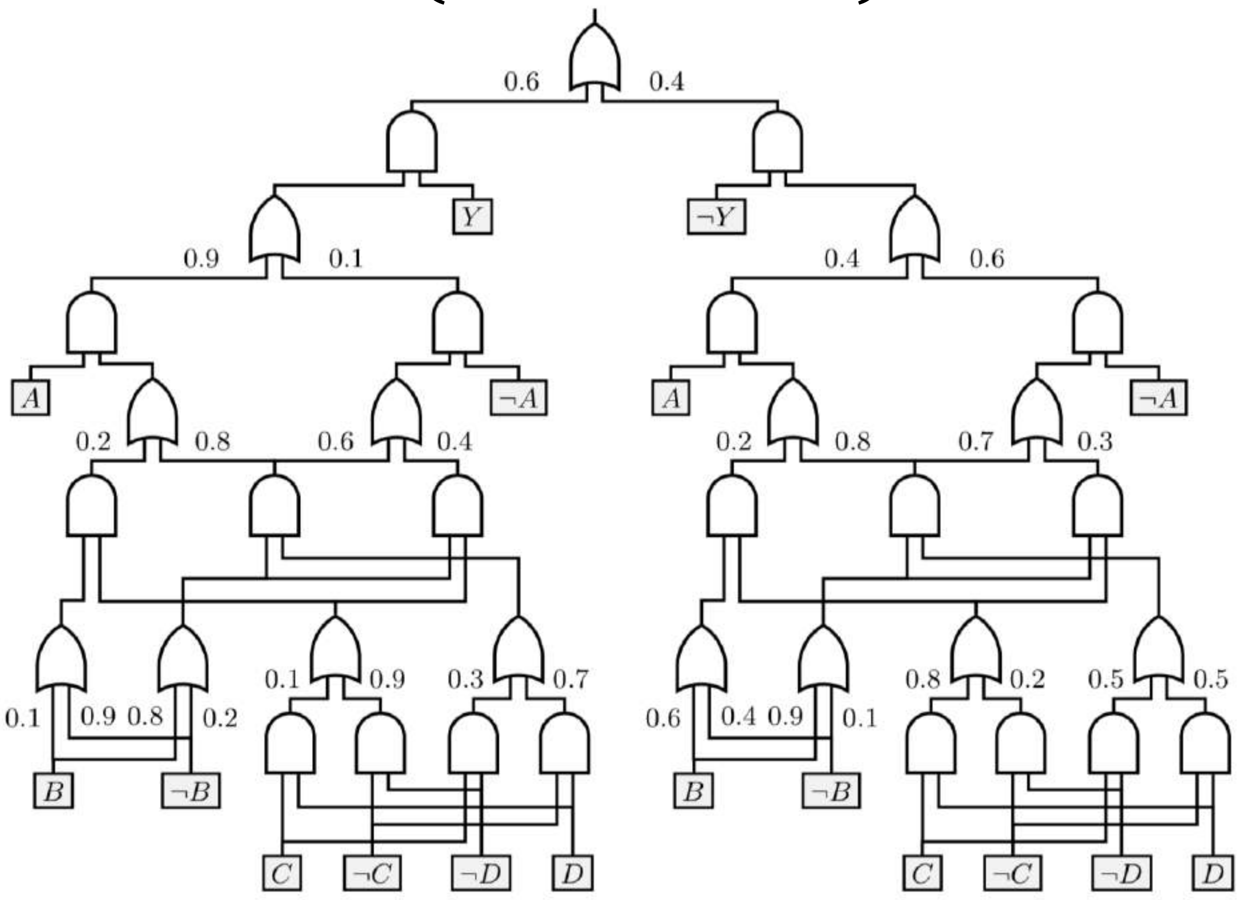
Competitive with SPN learners

(State of the art for approximate inference in discrete factor graphs)

But what if I only want to classify Y?

$$\Pr(Y|A, B, C, D)$$

~~$\Pr(Y, A, B, C, D)$~~



Logistic Circuits

$$\Pr(Y = 1 \mid A, B, C, D) = \frac{1}{1 + exp(-1.9)} = 0.869$$

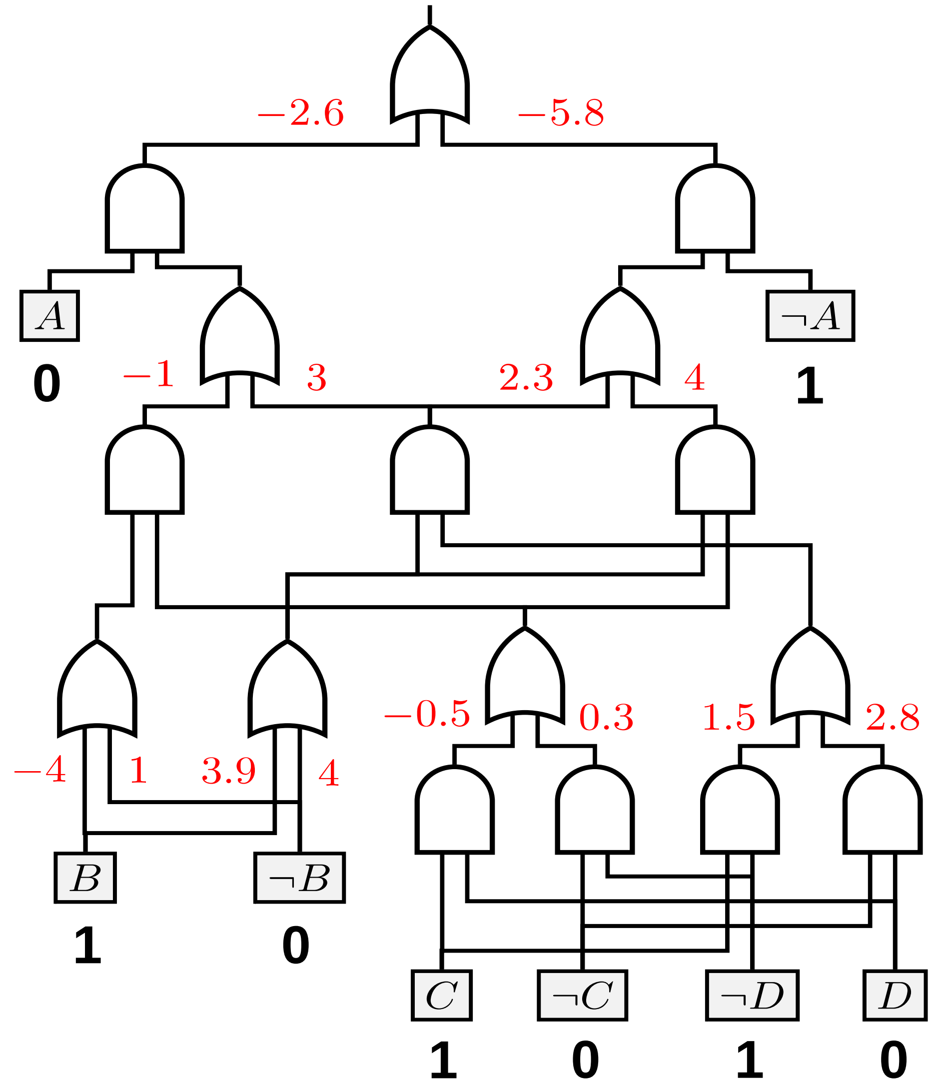
Weights on edges

Logistic function on output weight

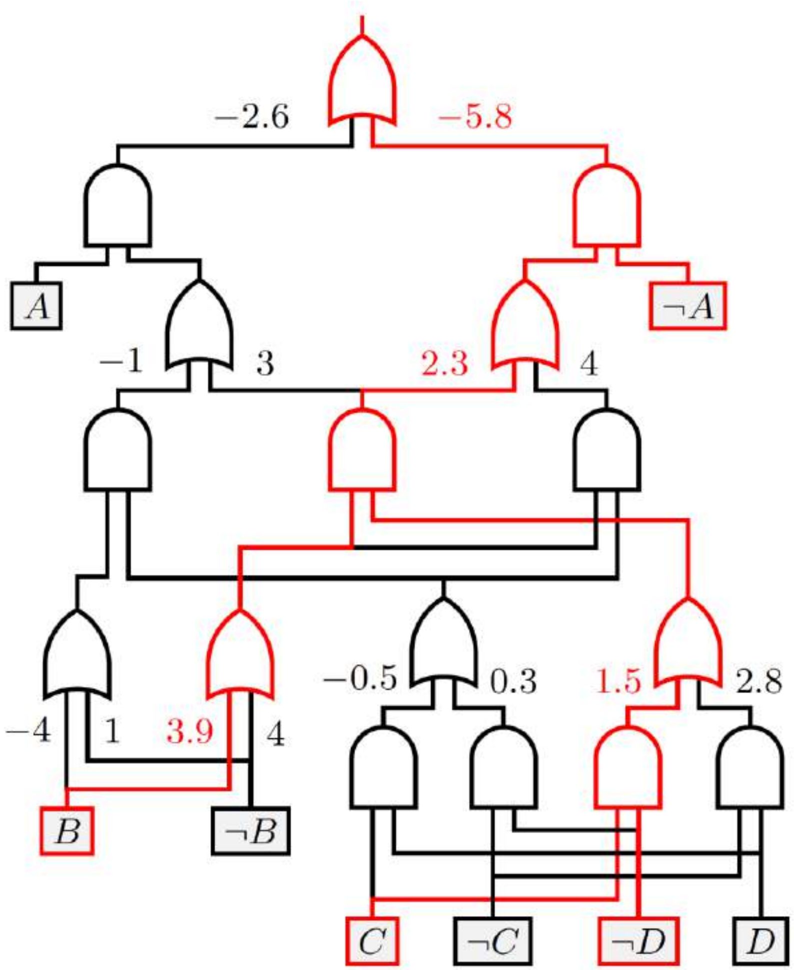
Bottom-up evaluation

Input:

A	B	C	D	$\Pr(Y \mid A, B, C, D)$
0	1	1	0	?



Alternative Semantics

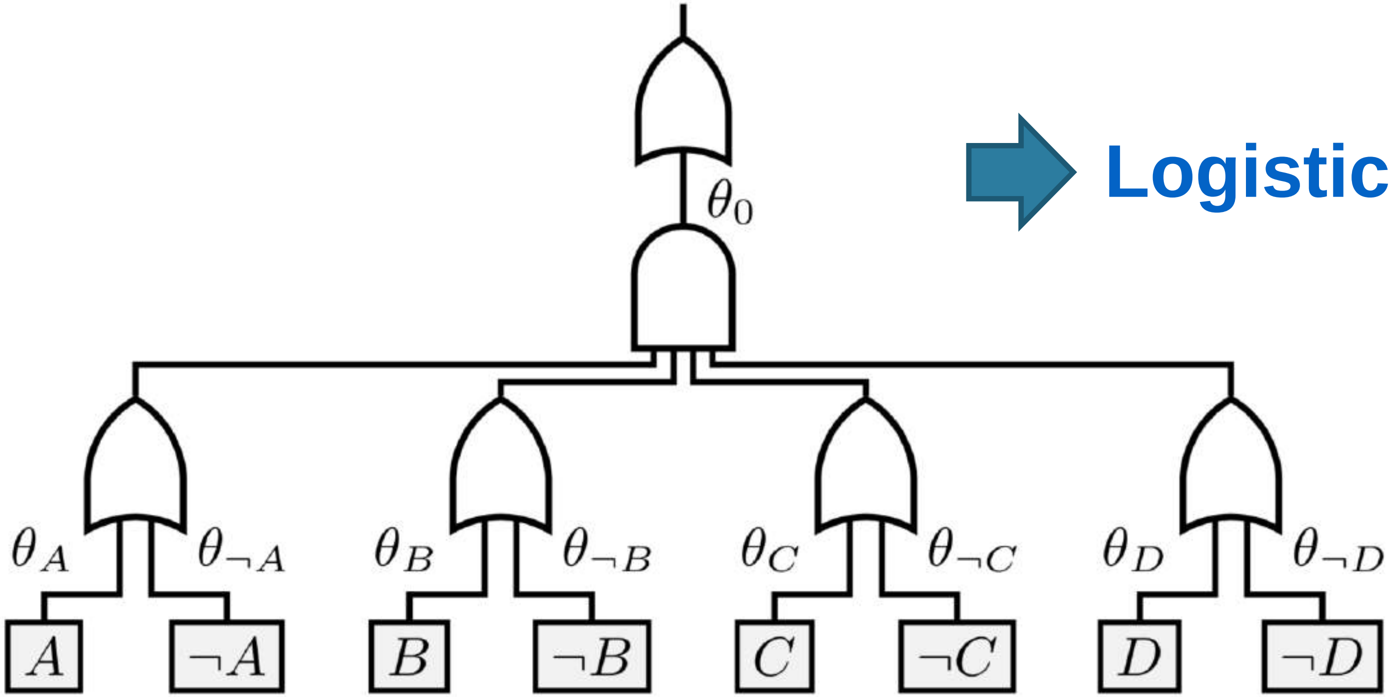


Represents $\Pr(Y \mid A, B, C, D)$

- Take all ‘hot’ wires
- Sum their weights
- Push through logistic function

A	B	C	D	$g_r(ABCD)$	$\Pr(Y=1 \mid ABCD)$
1	0	1	1	-3.1	4.31%
0	1	1	0	1.9	86.99%
1	1	1	0	5.8	99.70%

Special Case: Logistic Regression



Logistic Regression

$$\Pr(Y = 1 | A, B, C, D) = \frac{1}{1 + \exp(-A * \theta_A - \neg A * \theta_{\neg A} - B * \theta_B - \cdots)}$$

Is this a coincidence?

What about more general circuits?

Parameter Learning

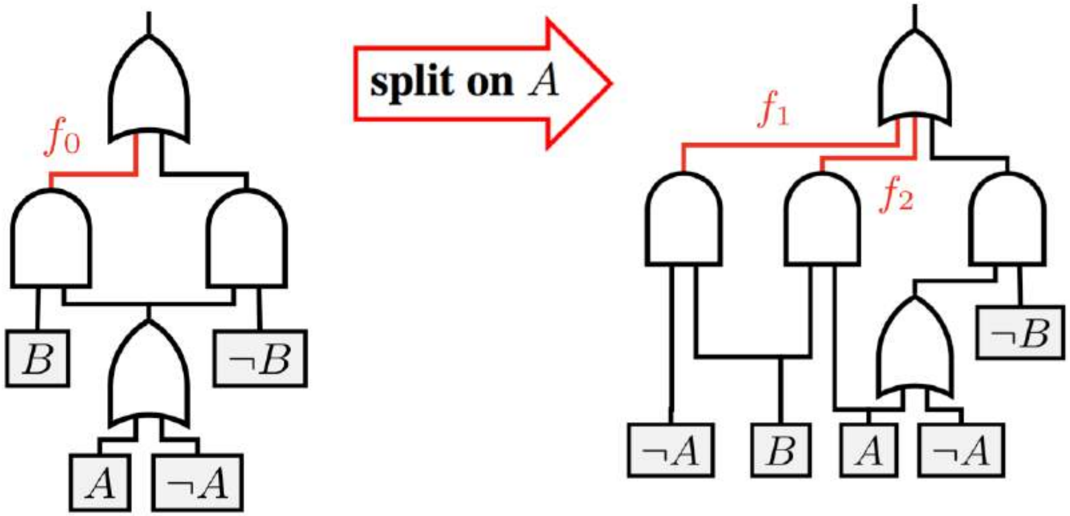
Reduce to logistic regression:

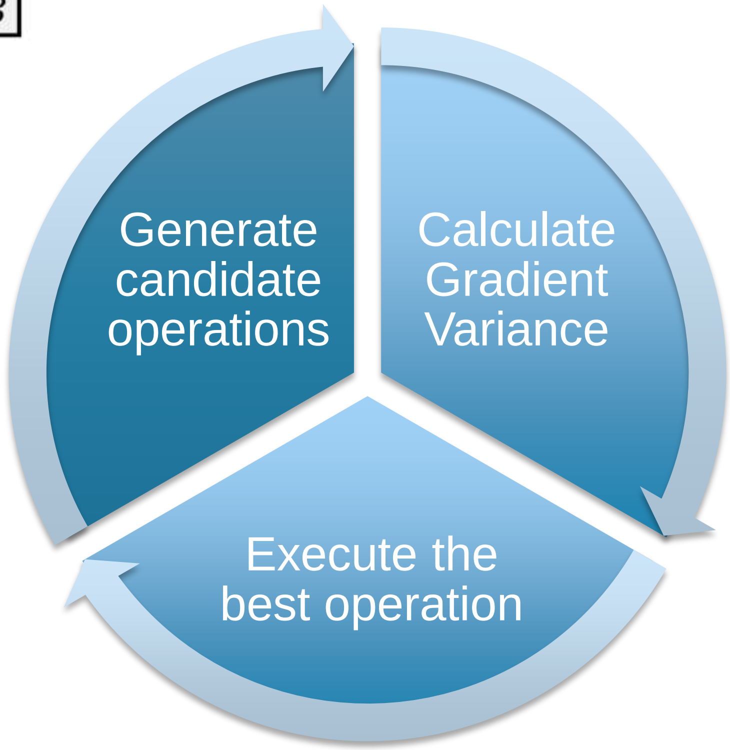
$$\Pr(Y = 1 \mid \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{x} \cdot \boldsymbol{\theta})}$$

Features associated with each wire
"Global Circuit Flow" features

Learning parameters θ is convex optimization!

Logistic Circuit Structure Learning





Comparable Accuracy with Neural Nets

Accuracy % on Dataset	Mnist	Fashion
Baseline: Logistic Regression	85.3	79.3
Baseline: Kernel Logistic Regression	97.7	88.3
Random Forest	97.3	81.6
3-layer MLP	97.5	84.8
RAT-SPN (Peharz et al. 2018)	98.1	89.5
SVM with RBF Kernel	98.5	87.8
5-Layer MLP	99.3	89.8
Logistic Circuit (binary)	97.4	87.6
Logistic Circuit (real-valued)	99.4	91.3
CNN with 3 conv layers	99.1	90.7
Resnet (He et al. 2016)	99.5	93.6

Significantly Smaller in Size

Number of Parameters	Mnist	Fashion
Baseline: Logistic Regression	<1K	<1K
Baseline: Kernel Logistic Regression	1,521 K	3,930K
Logistic Circuit (real-valued)	182K	467K
Logistic Circuit (binary)	268K	614K
3-layer MLP	1,411K	1,411K
RAT-SPN (Peharz et al. 2018)	8,500K	650K
CNN with 3 conv layers	2,196K	2,196K
5-layer MLP	2,411K	2,411K
Resnet (He et al. 2016)	4,838K	4,838K

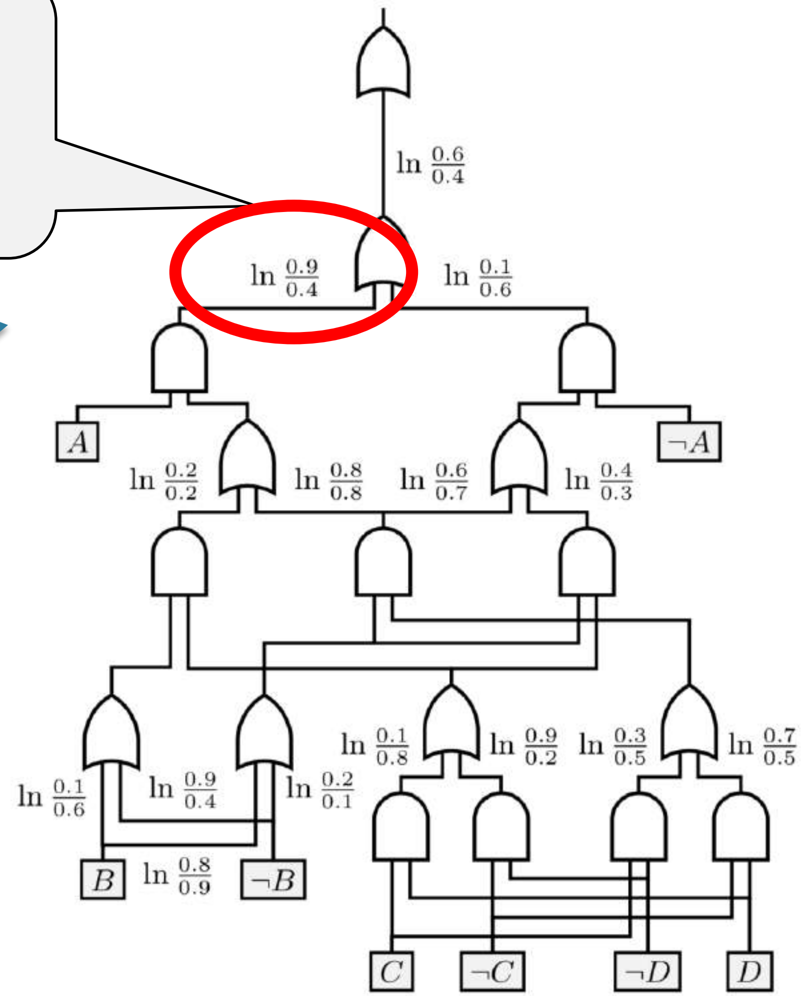
Better Data Efficiency

Accuracy % with % of Training Data	MNIST			Fashion		
	100%	10%	2%	100%	10%	2%
5-layer MLP	99.3	**98.2**	94.3	89.8	86.5	80.9
CNN with 3 Conv Layers	99.1	98.1	95.3	90.7	87.6	83.8
Logistic Circuit (Binary)	97.4	96.9	94.1	87.6	86.7	83.2
Logistic Circuit (Real-Valued)	**99.4**	97.6	**96.1**	**91.3**	**87.8**	**86.0**

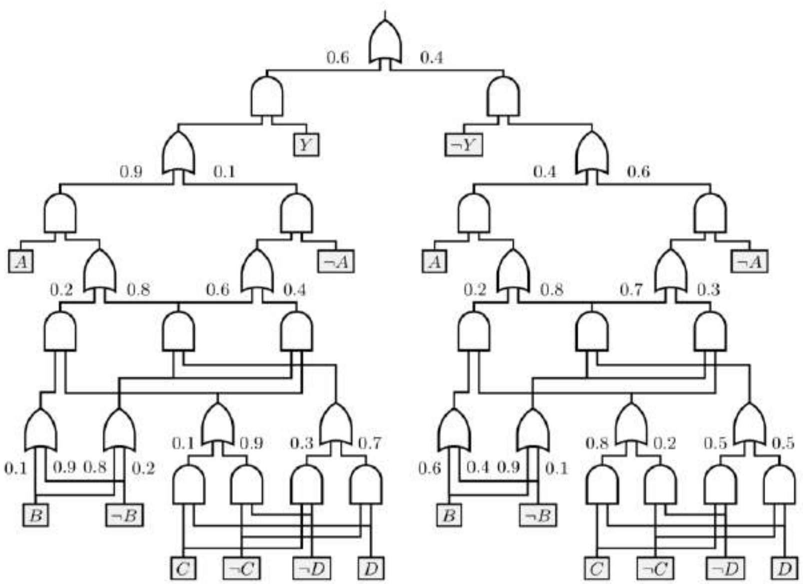
Logistic vs. Probabilistic Circuits

$\Pr(Y \mid A, B, C, D)$

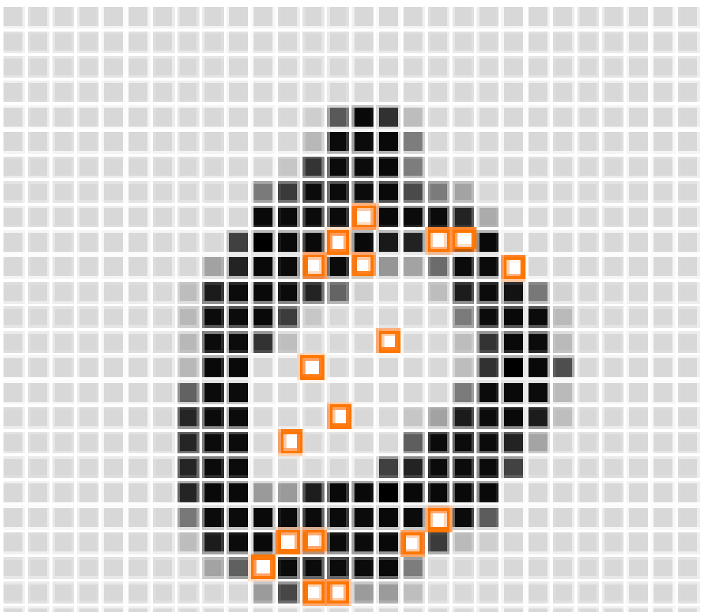
Probabilities become log-odds

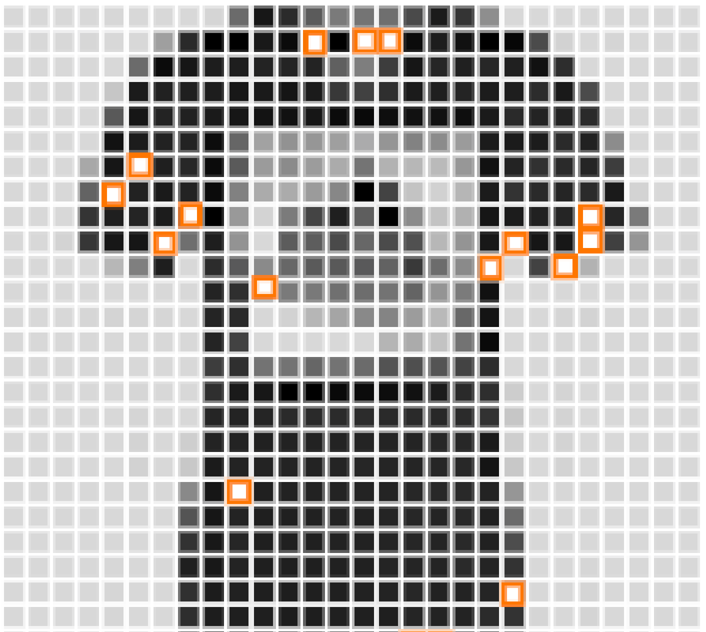


$\Pr(Y, A, B, C, D)$

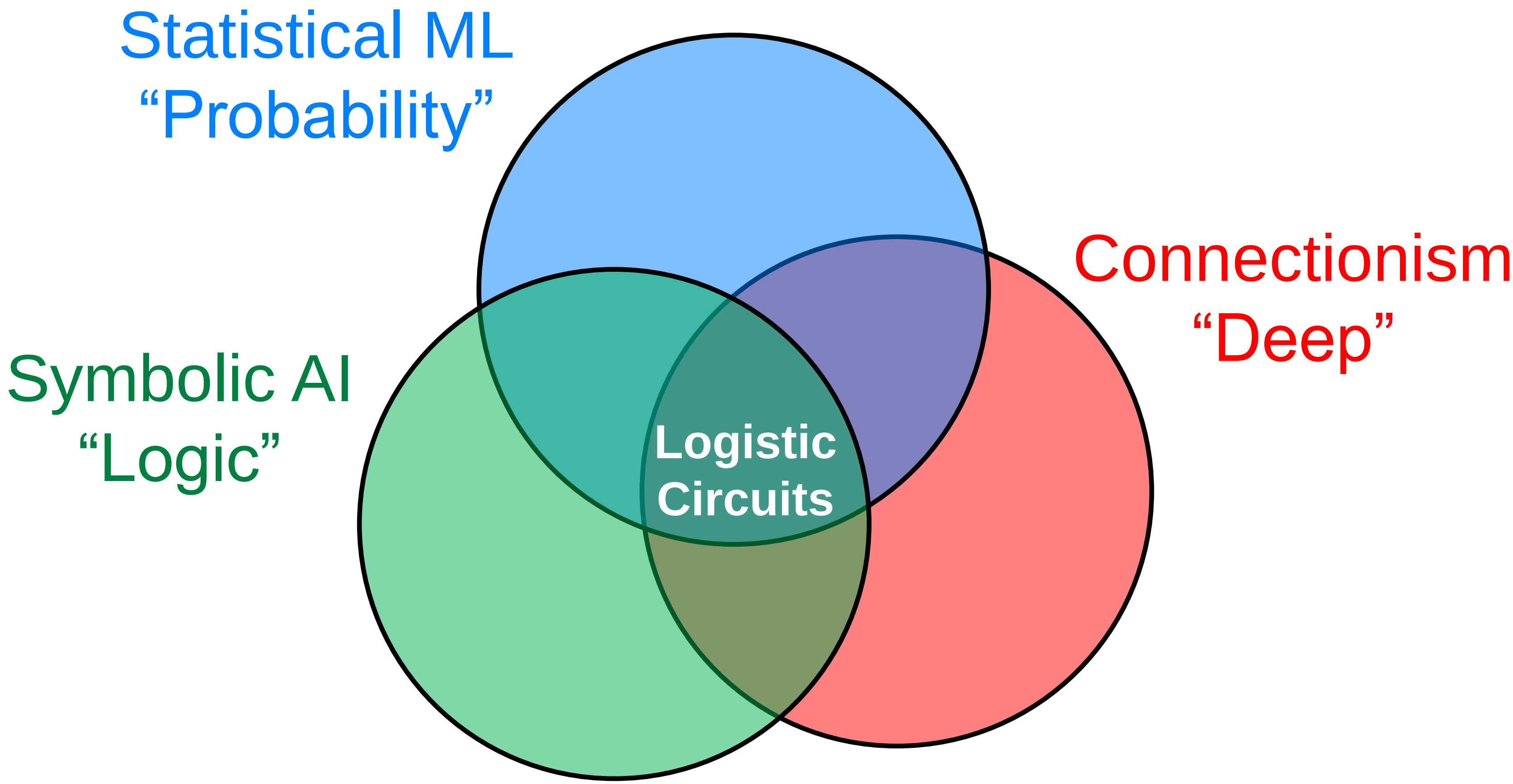


Interpretable?

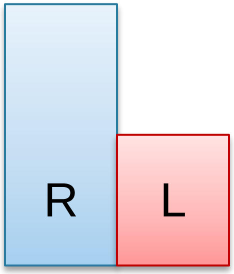




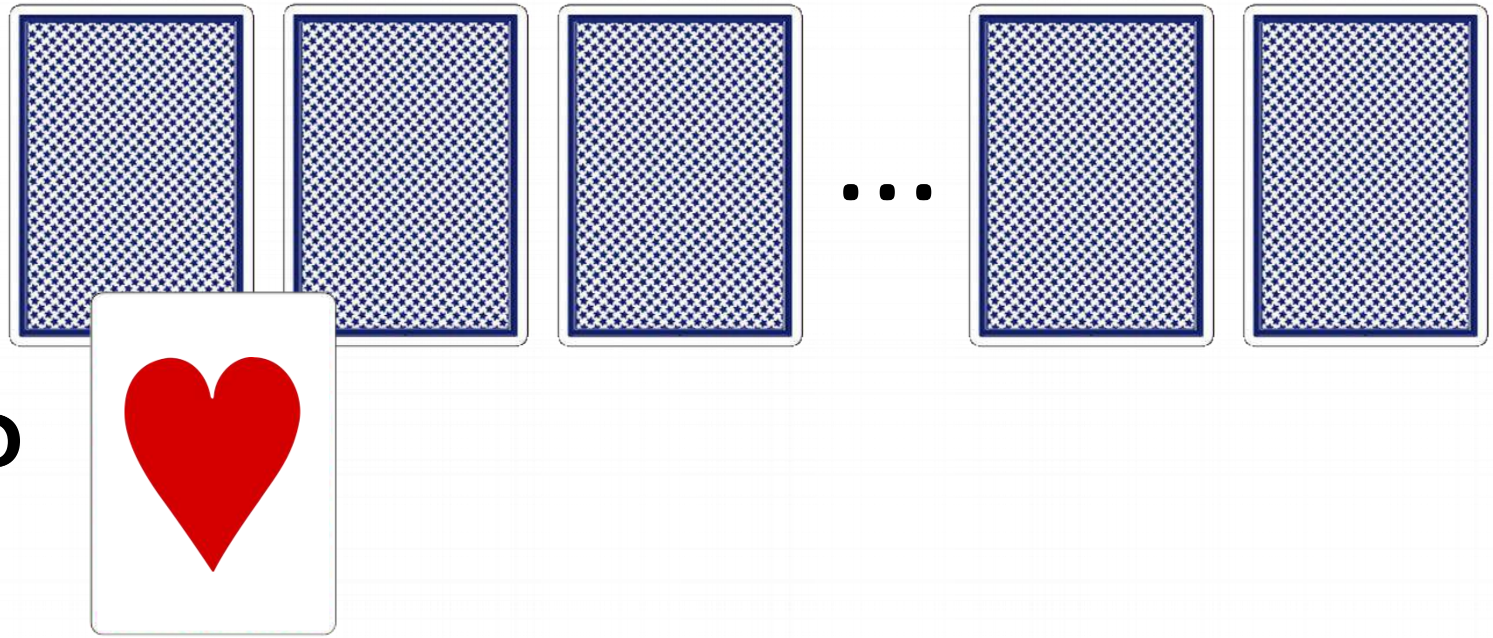
Conclusions 2



High-Level Probabilistic Inference



Simple Reasoning Problem



?

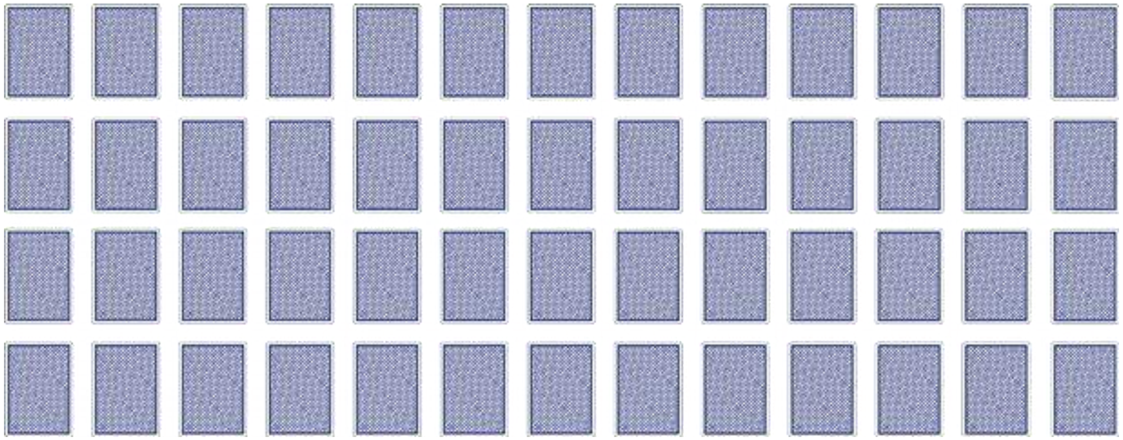
Probability that Card1 is Hearts? 1/4

[Van den Broeck; AAAI-KRR'15]

Automated Reasoning

Let us automate this:

1. Probabilistic graphical model (e.g., factor graph)



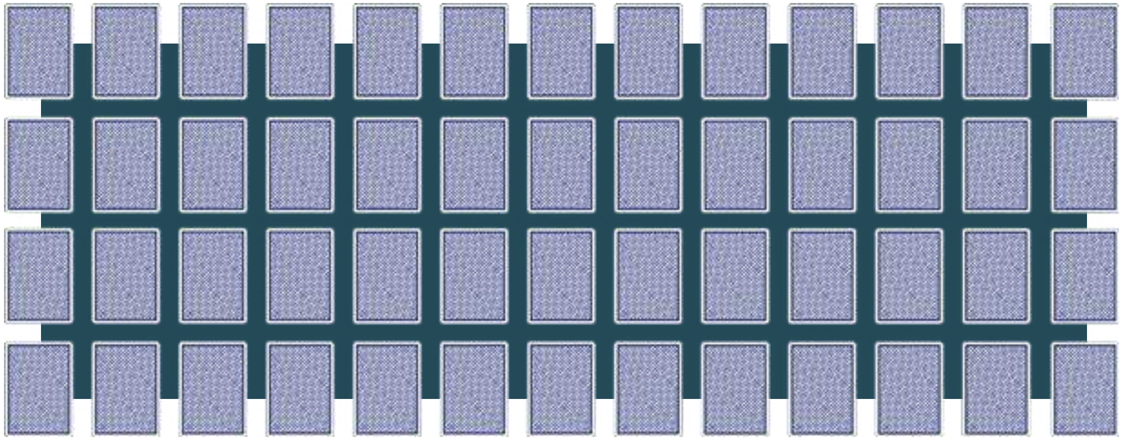
2. Probabilistic inference algorithm
   (e.g., variable elimination or junction tree)

[Van den Broeck; AAAI-KRR'15]

Automated Reasoning

Let us automate this:

1. Probabilistic graphical model (e.g., factor graph)
   is fully connected!

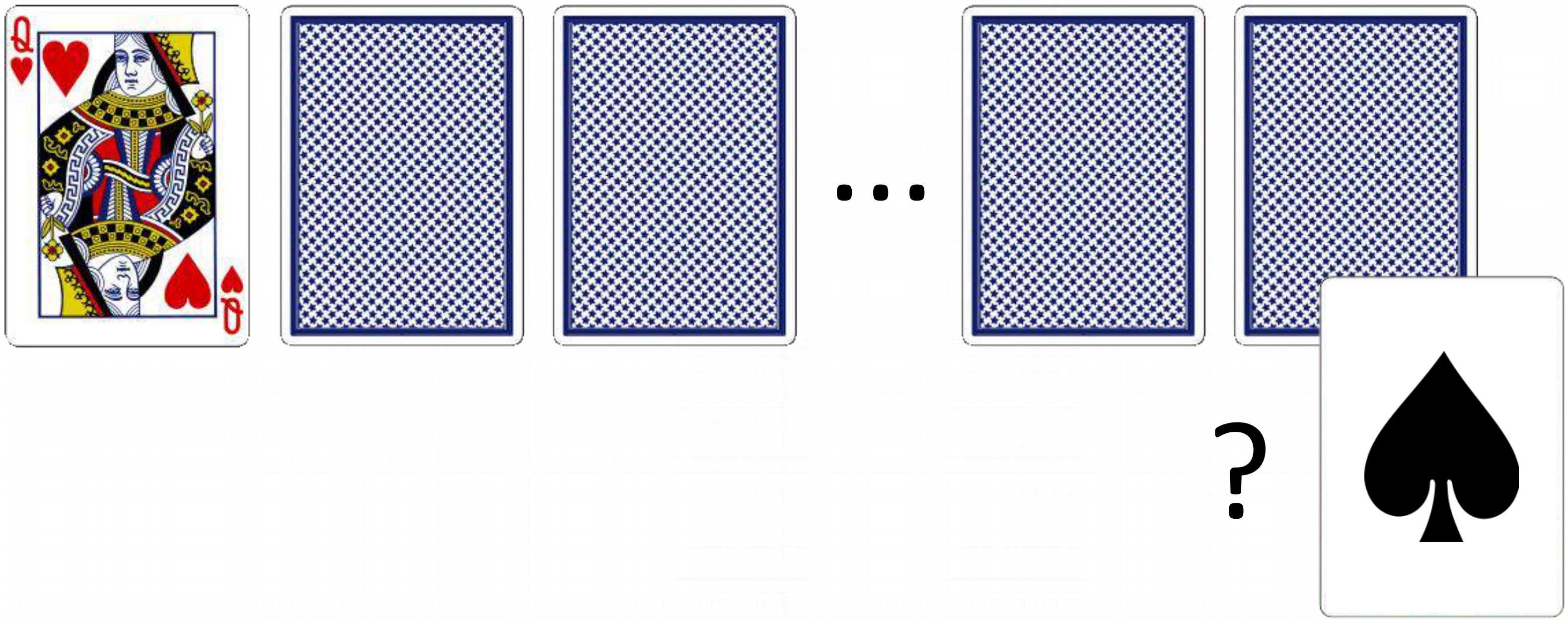


(artist's impression)

2. Probabilistic inference algorithm
   (e.g., variable elimination or junction tree)
   builds a table with $\mathbf{52}^{52}$ rows

[Van den Broeck; AAAI-KRR'15]

What's Going On Here?

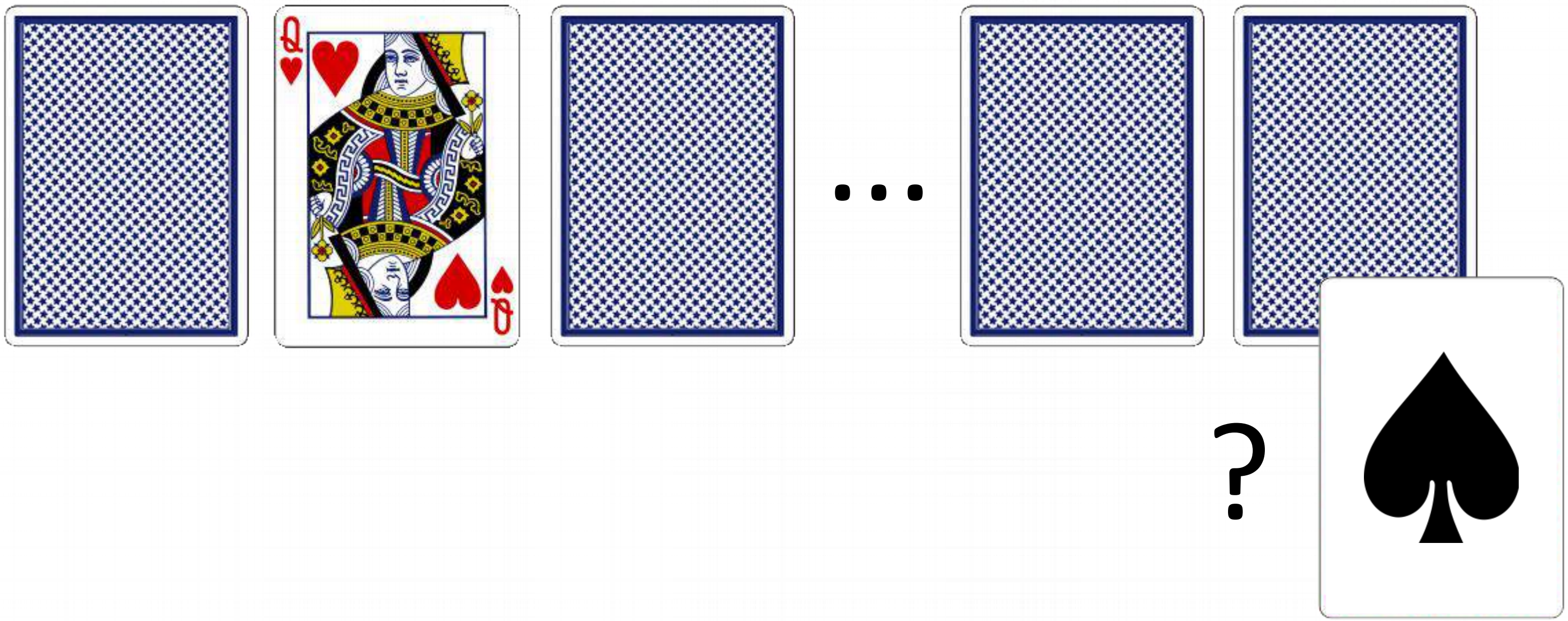


Probability that Card52 is Spades given that Card1 is QH?

13/51

[Van den Broeck; AAAI-KRR’15]

What's Going On Here?

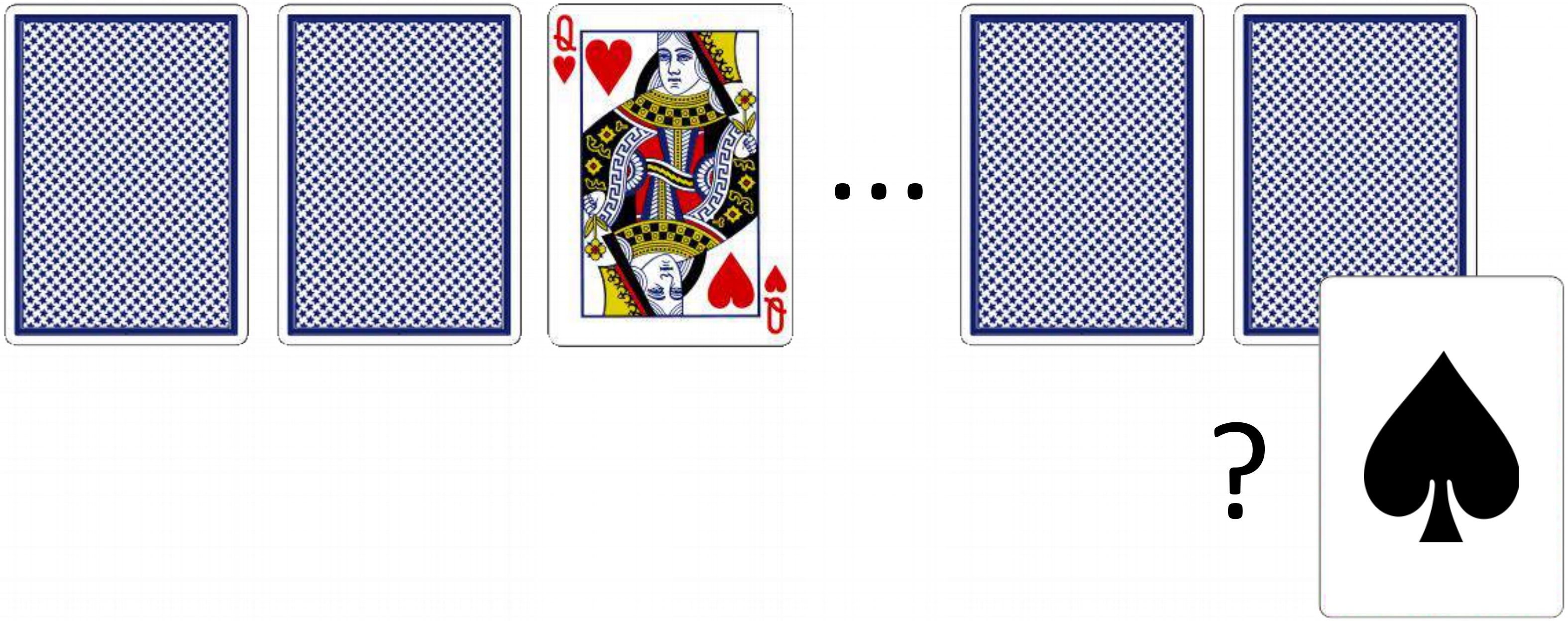


Probability that Card52 is Spades given that Card2 is QH?

13/51

[Van den Broeck; AAAI-KRR'15]

What's Going On Here?

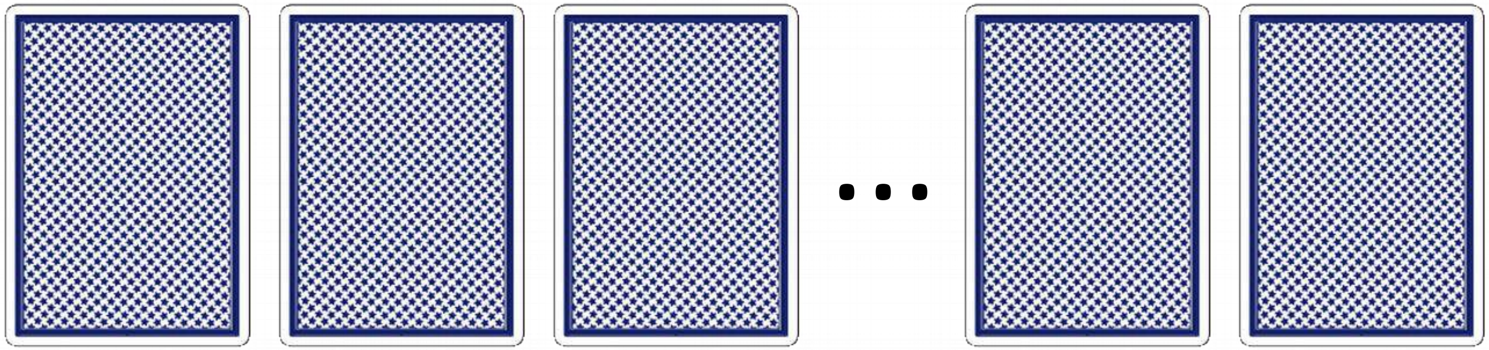


Probability that Card52 is Spades given that Card3 is QH?

13/51

[Van den Broeck; AAAI-KRR'15]

Tractable Reasoning



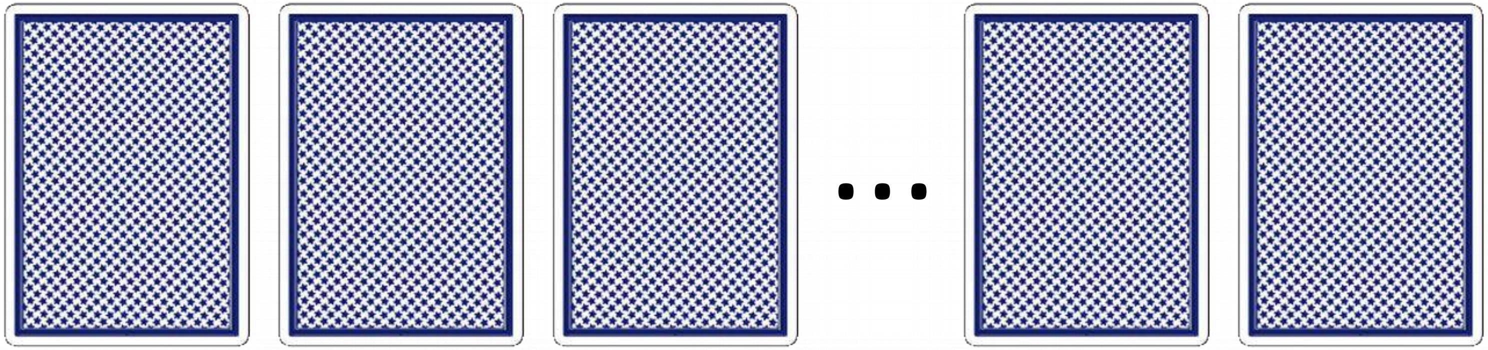
What's going on here?

Which property makes reasoning tractable?

- High-level (first-order) reasoning
- Symmetry
- Exchangeability

⇒ Lifted Inference

[Niepert and Van den Broeck, AAAI' 14], [Van den Broeck, AAAI-KRR'15]



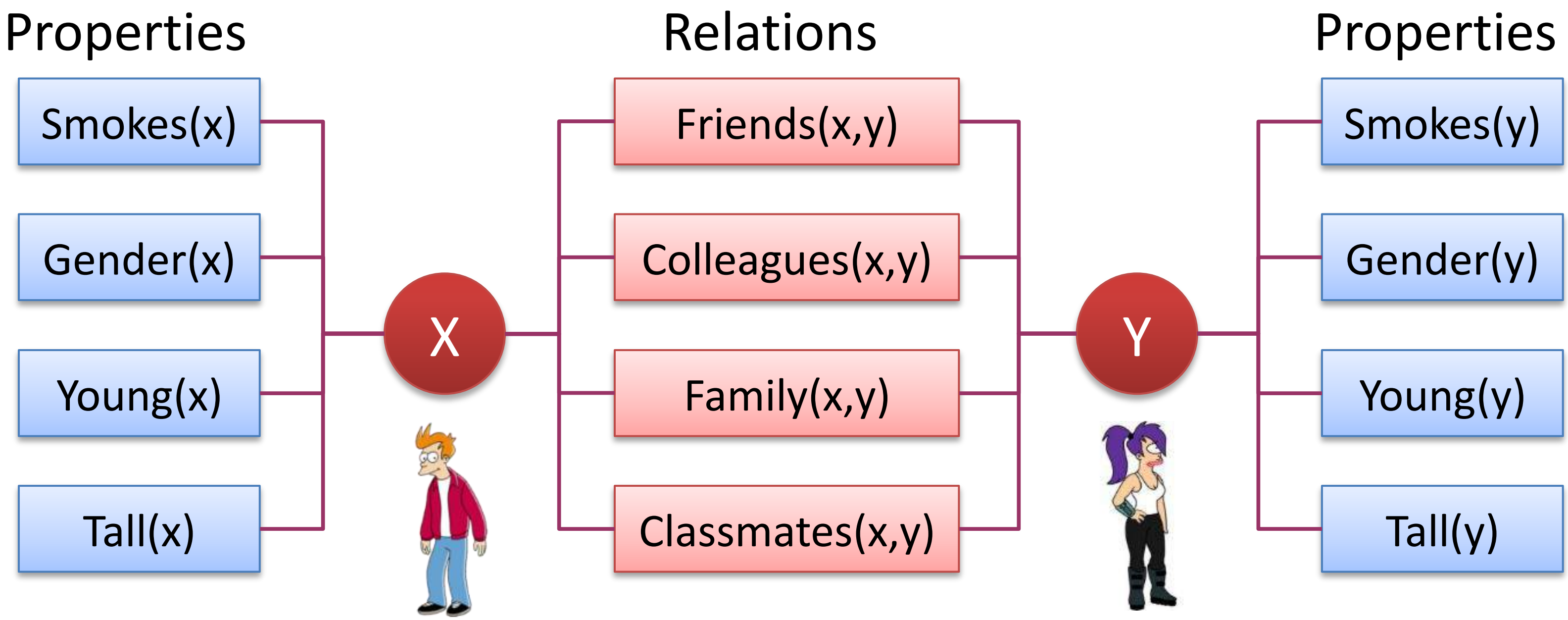
Model distribution at first-order level:

Δ = $\forall p, \exists c, Card(p,c)$
$\forall c, \exists p, Card(p,c)$
$\forall p, \forall c, \forall c', Card(p,c) \wedge Card(p,c') \Rightarrow c = c'$

Can we now be efficient
in the size of our domain?

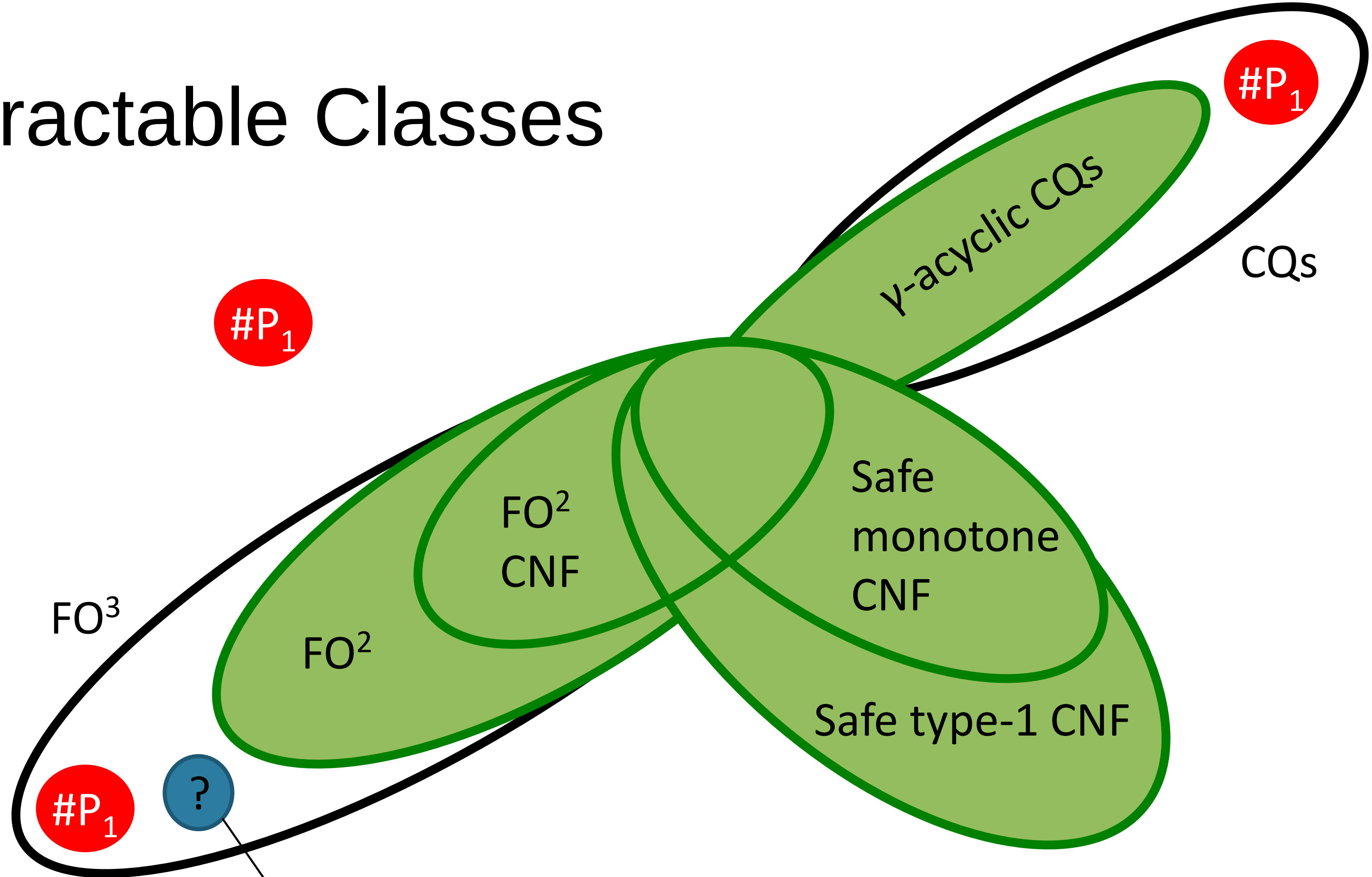
[Van den Broeck 2015]

FO^2 is liftable!



"Smokers are more likely to be friends with other smokers."
"Colleagues of the same age are more likely to be friends."
"People are either family or friends, but never both."
"If X is family of Y, then Y is also family of X."
"Universities in the Bay Area are more likely to be rivals."

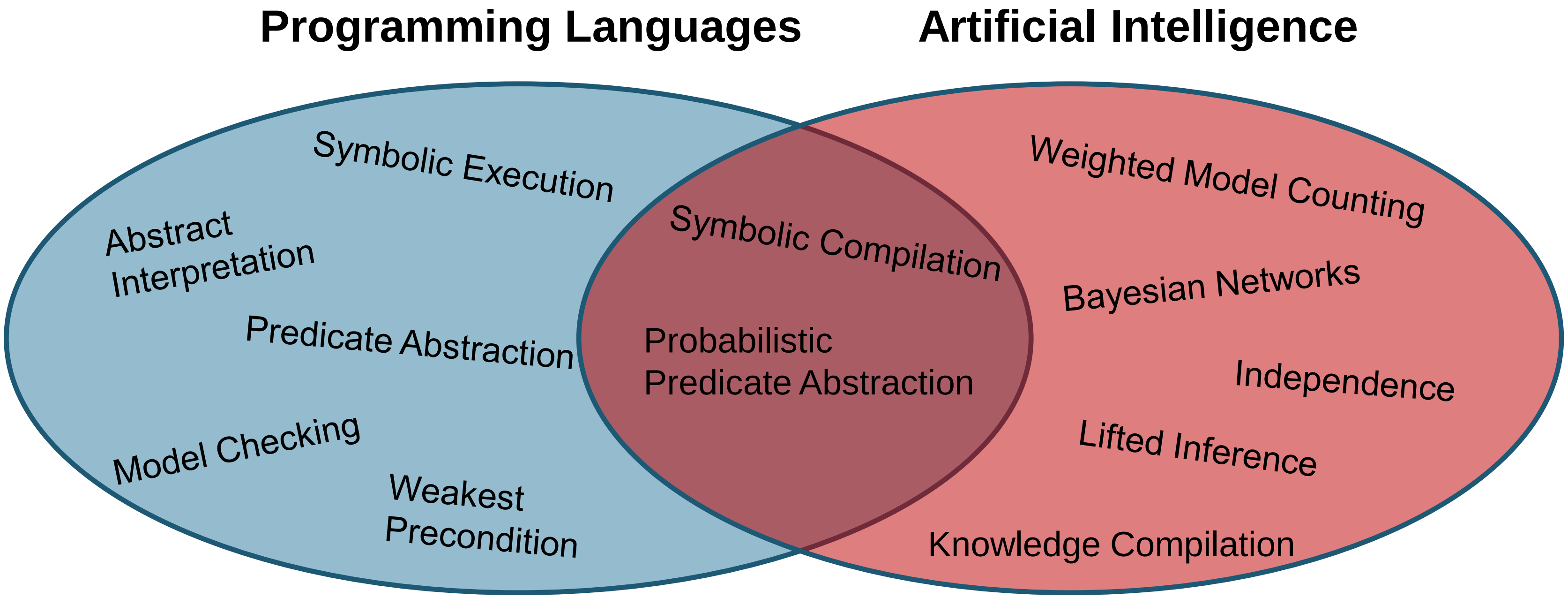
Tractable Classes



Δ = ∀x,y,z, Friends(x,y) ∧ Friends(y,z) ⇒ Friends(x,z)

[VdB; NIPS'11], [VdB et al.; KR'14], [Gribkoff, VdB, Suciu; UAI'15], [Beame, VdB, Gribkoff, Suciu; PODS'15], etc.

Probabilistic Programming



Similar picture for *probabilistic databases*
probabilistic SMT, probabilistic datalog,
probabilistic logic programming, …

Conclusions 3

- Challenge is even greater at first-order level
- Existing reasoning algorithms cannot cut it!

- Integration of first-order logic and probability is long-standing goal of AI
- First-order probabilistic reasoning is **frontier** and **integration** of
  AI, KR, ML, DBs, theory, PL, etc.

Final Conclusions

- Knowledge is everywhere in learning
- Some concepts not easily learned from data
- Make knowledge first-class citizen in ML

- Logical circuits turned statistical models
- Strong properties produce strong learners
- There is no dilemma between understanding and accuracy?

- A wealth of high-level reasoning approaches are still absent from ML discussion

Acknowledgements

Thanks to my students and collaborators!

Thanks for your attention!

Questions?