Probabilistic and Logistic Circuits:

A New Synthesis of Logic and Machine Learning

Guy Van den Broeck

UCLA

RelationalAI ArrowCon

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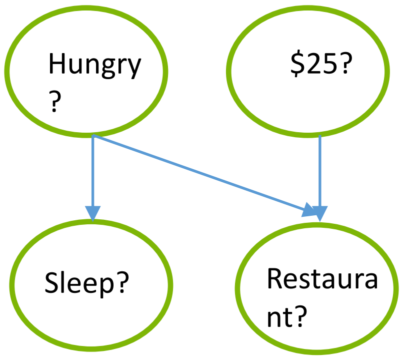
STAR AI
RESEARCH LAB
UCLA

Which method to choose?

Classical AI Methods:



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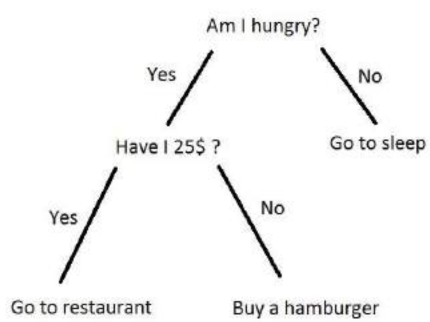
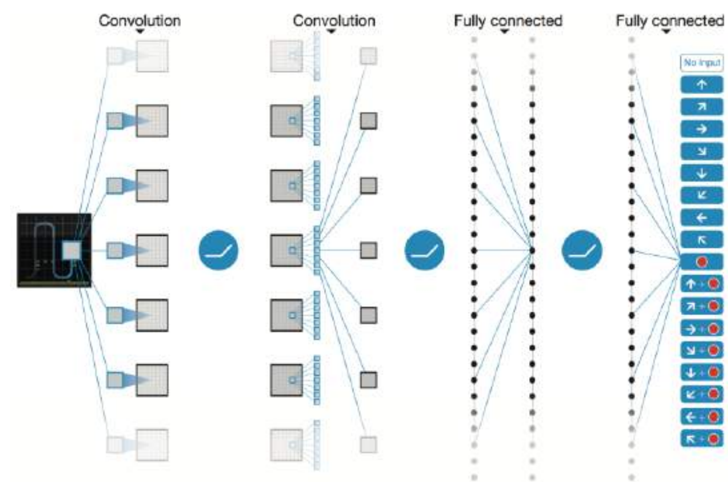


Clear Modeling Assumption
Well-understood

Neural Networks:



“Black Box”
Good performance
on Image Classification

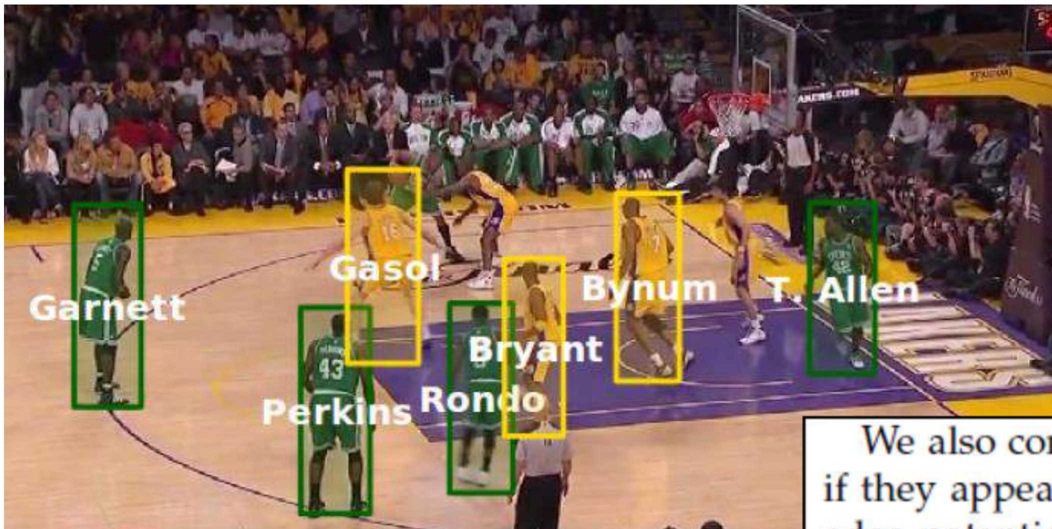
Outline

- Adding knowledge to deep learning
- Probabilistic circuits
- Logistic circuits for image classification

Outline

- **Adding knowledge to deep learning**
- Probabilistic circuits
- Logistic circuits for image classification

Motivation: Video



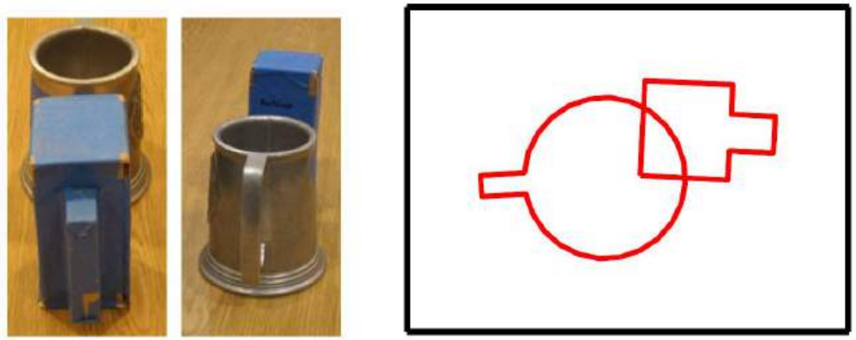
We also connect all pairs of identity nodes $y_{t,i}$ and $y_{t,j}$ if they appear in the same time t. We then introduce an edge potential that enforces mutual exclusion:

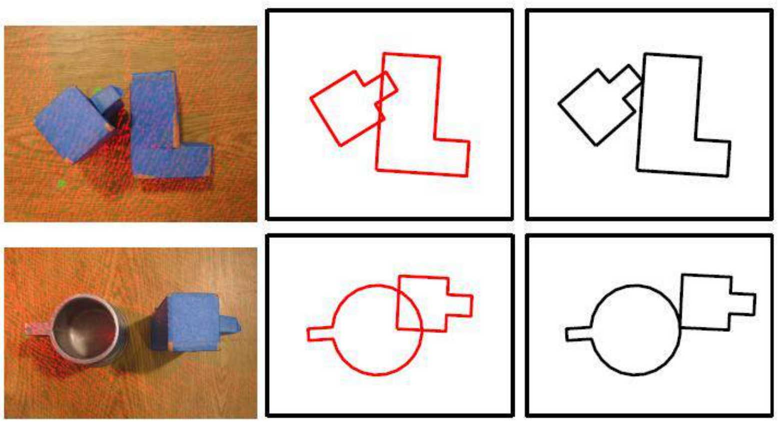
$$\psi_{\text{mutex}}(y_{t,i}, y_{t,j}) = \begin{cases} 1 & \text{if } y_{t,i} \neq y_{t,j} \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

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

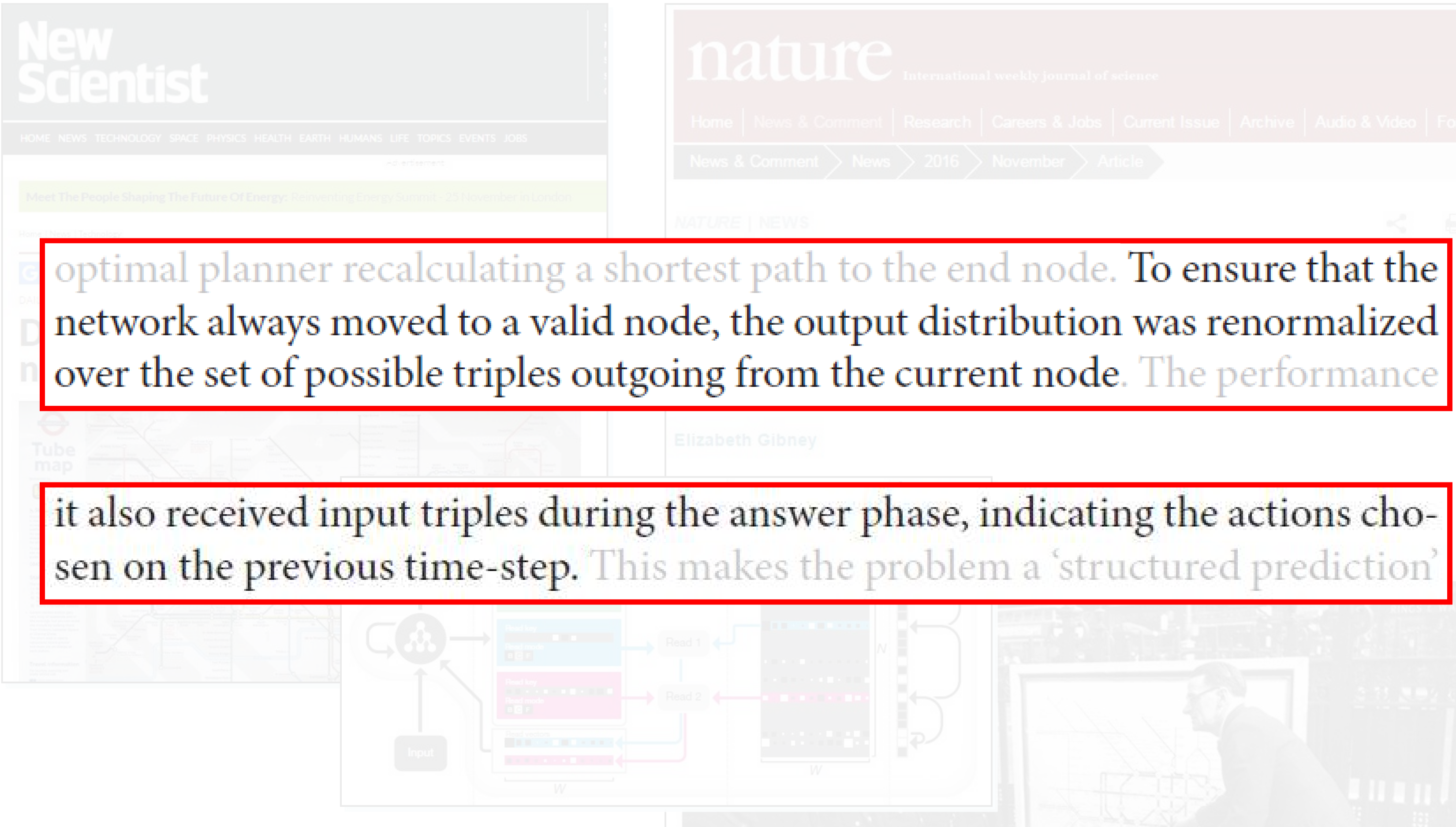
- Information extraction
- Semantic role labeling

… 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],…, [Chang, M. W., Ratinov, L., & Roth, D. (2012). Structured learning with constrained conditional models.], [https://en.wikipedia.org/wiki/Constrained_conditional_model]

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.]

Running Example

Courses:

- Logic (L)
- Knowledge Representation (K)
- Probability (P)
- Artificial Intelligence (A)

Constraints

- Must take at least one of Probability or Logic.
- Probability is a prerequisite for AI.
- The prerequisites for KR is either AI or Logic.

Data

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

Structured Space

unstructured

L	K	P	A
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

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

7 out of 16 instantiations are impossible

structured

L	K	P	A
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

Boolean Constraints

unstructured

L	K	P	A
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

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

7 out of 16 instantiations are impossible

structured

L	K	P	A
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

Learning in Structured Spaces

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)

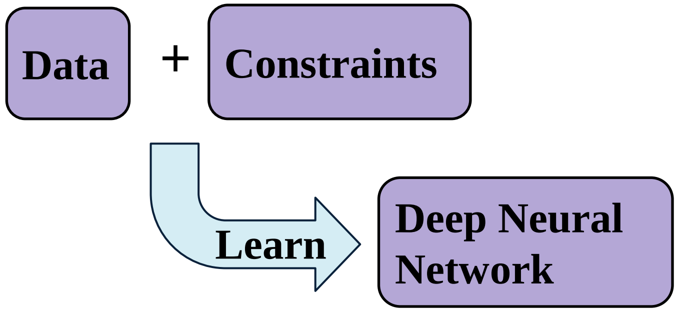
$$P \vee L$$
$$A \Rightarrow P$$
$$K \Rightarrow (P \vee L)$$

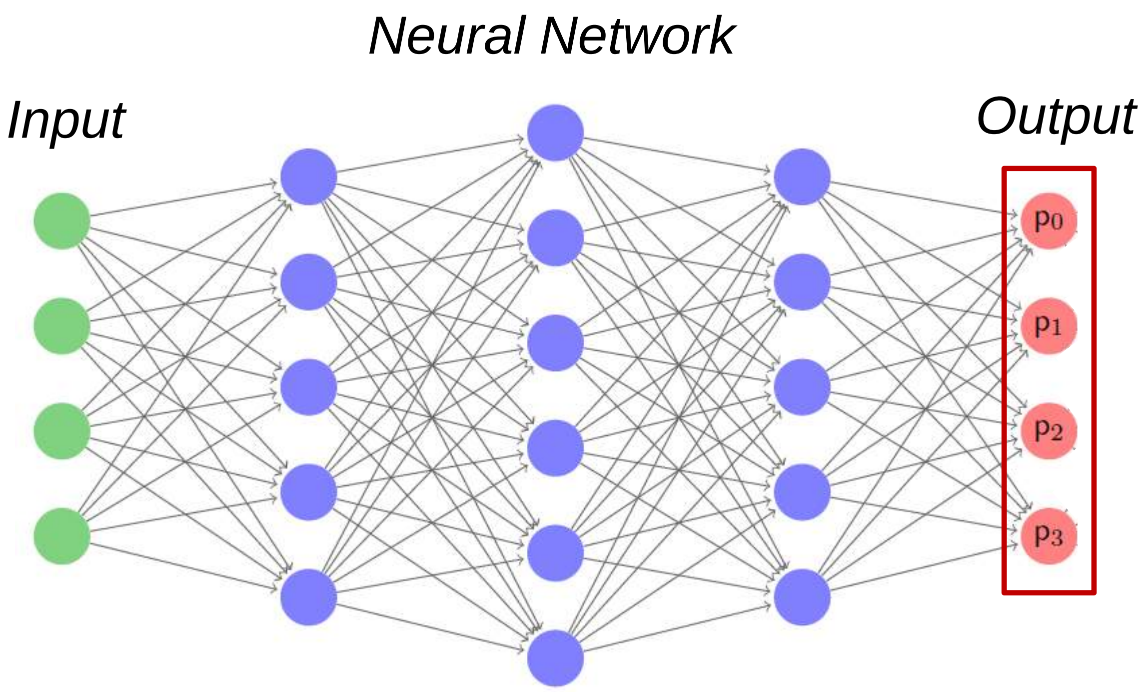
Learn

ML Model

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

Deep Learning with Logical Knowledge





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

Semantic Loss

Q: How close is output **p** *to satisfying constraint?*

Answer: Semantic loss function $L(\alpha,\mathbf{p})$

- Axioms, for example:
  - If **p** is Boolean then $L(\mathbf{p},\mathbf{p}) = 0$
  - If α implies β then $L(\alpha,\mathbf{p}) \geq L(\beta,\mathbf{p})$ (*α more strict*)
- Properties:
  - If α is equivalent to β then $L(\alpha,\mathbf{p}) = L(\beta,\mathbf{p})$
  - If **p** is Boolean and satisfies α then $L(\alpha,\mathbf{p}) = 0$

SEMANTIC
Loss!

Semantic Loss: Definition

Theorem: Axioms imply unique semantic loss:

$$\mathrm{L}^{\mathrm{s}}(\alpha, \mathsf{p}) \propto -\log \underbrace{\sum_{\mathbf{x} \models \alpha} \underbrace{\prod_{i : \mathbf{x} \models X_i} \mathsf{p}_i \prod_{i : \mathbf{x} \models \neg X_i} (1 - \mathsf{p}_i)}_{\text{Probability of getting } \mathbf{x} \text{ after flipping coins with prob. } \mathbf{p}}}_{\text{Probability of satisfying } \alpha \text{ after flipping coins with prob. } \mathbf{p}}$$

Example: Exactly-One

- Data must have some label

  We agree this must be one of the 10 digits:

- Exactly-one constraint

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

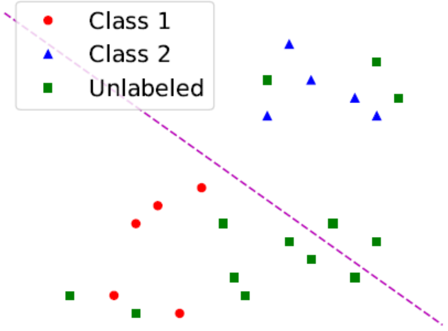
- Semantic loss:

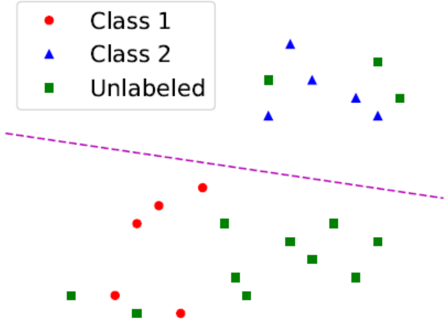
$$\mathrm{L}^{\mathrm{s}}(\text{exactly-one}, \mathrm{p}) \propto -\log \underbrace{\sum_{i=1}^{n} \mathrm{p}_i \underbrace{\prod_{j=1, j \neq i}^{n} (1 - \mathrm{p}_j)}_{\text{Only } x_i = 1 \text{ after flipping coins}}}_{\text{Exactly one true } x \text{ after flipping coins}}$$

Semi-Supervised Learning

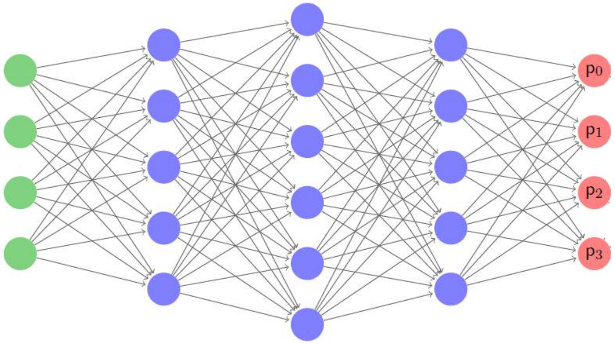
- Intuition: Unlabeled data must have some label

  Cf. entropy constraints, manifold learning





- Minimize exactly-one semantic loss on unlabeled data



Train with

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

MNIST Experiment

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)	
MLP with Semantic Loss	98.38 (±0.51)	98.78 (±0.17)	99.36 (±0.02)

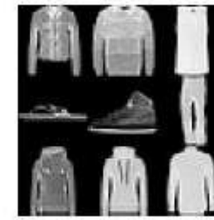
Competitive with state of the art
in semi-supervised deep learning

FASHION Experiment

(a) Confidently Correct

(b) Unconfidently Correct

(c) Unconfidently Incorrect



(d) Confidently Incorrect

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 Ladder Nets!

Same conclusion on CIFAR10

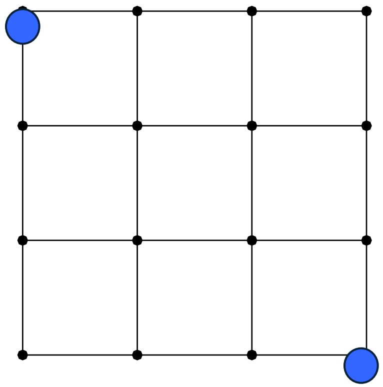
Accuracy % with # of used labels	4000	ALL
CNN Baseline in Ladder Net	76.67 (± 0.61)	90.73
Ladder Net (Rasmus et al., 2015)	79.60 (±0.47)	
Baseline: CNN, Whitening, Cropping	77.13	90.96
CNN with Semantic Loss	**81.79**	90.92

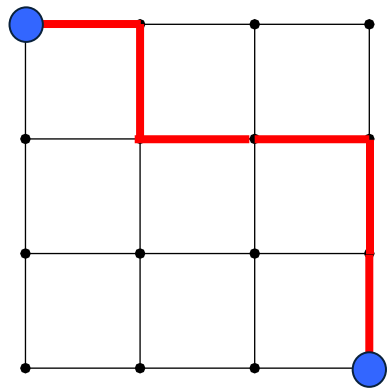
What about real constraints? Paths

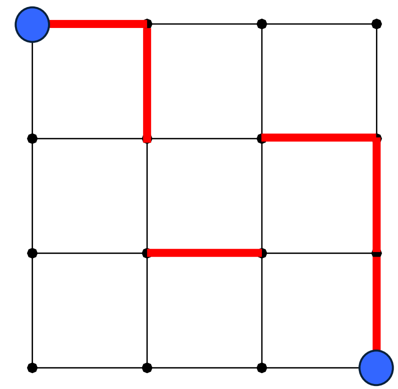
cf. Nature paper


nature

Google's AI reasons its way around the London Underground







Good variable assignment (represents route)

184

Bad variable assignment (does not represent route)

16,777,032

Unstructured probability space: 184+16,777,032 = 2^{24}

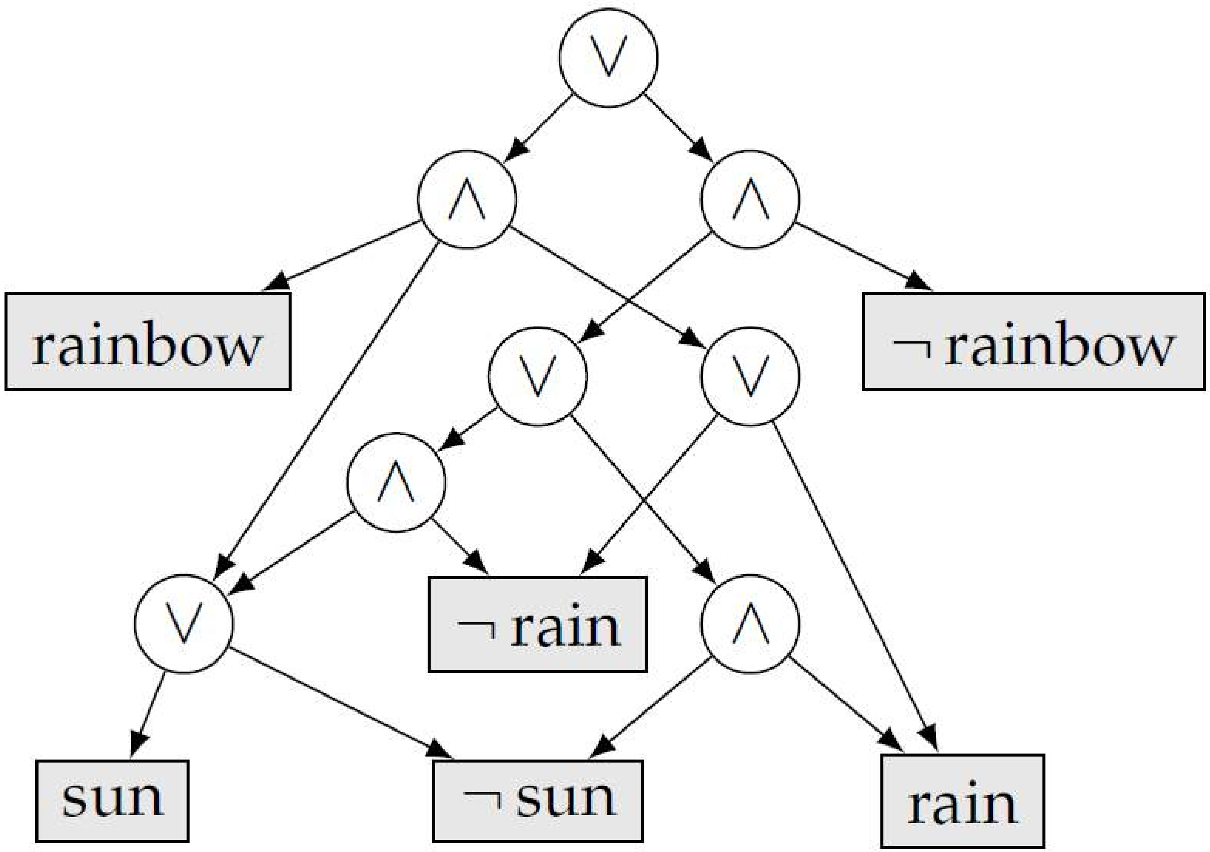
Space easily encoded in logical constraints ☺ [Nishino et al.]

How to Compute Semantic Loss?

- In general: #P-hard ☹

Negation Normal Form Circuits

$\Delta = (\text{sun} \land \text{rain} \Rightarrow \text{rainbow})$



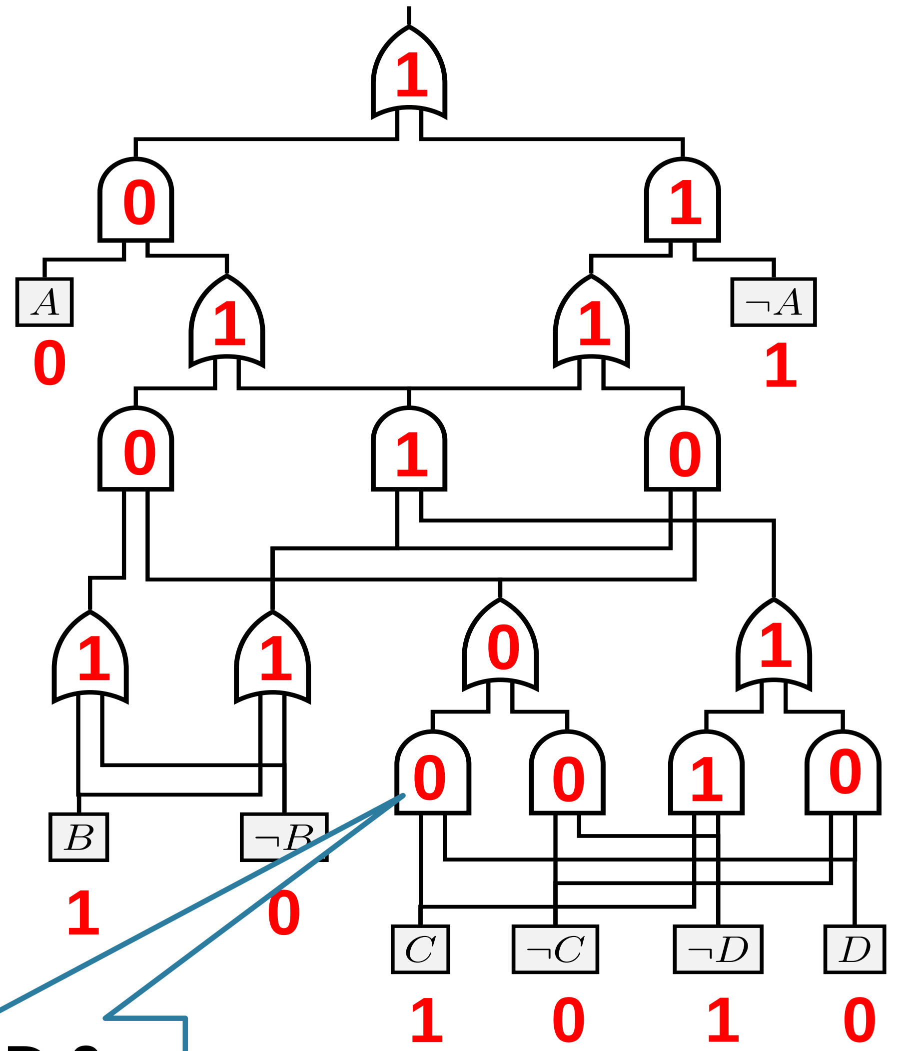
[Darwiche 2002]

Logical Circuits

Input:

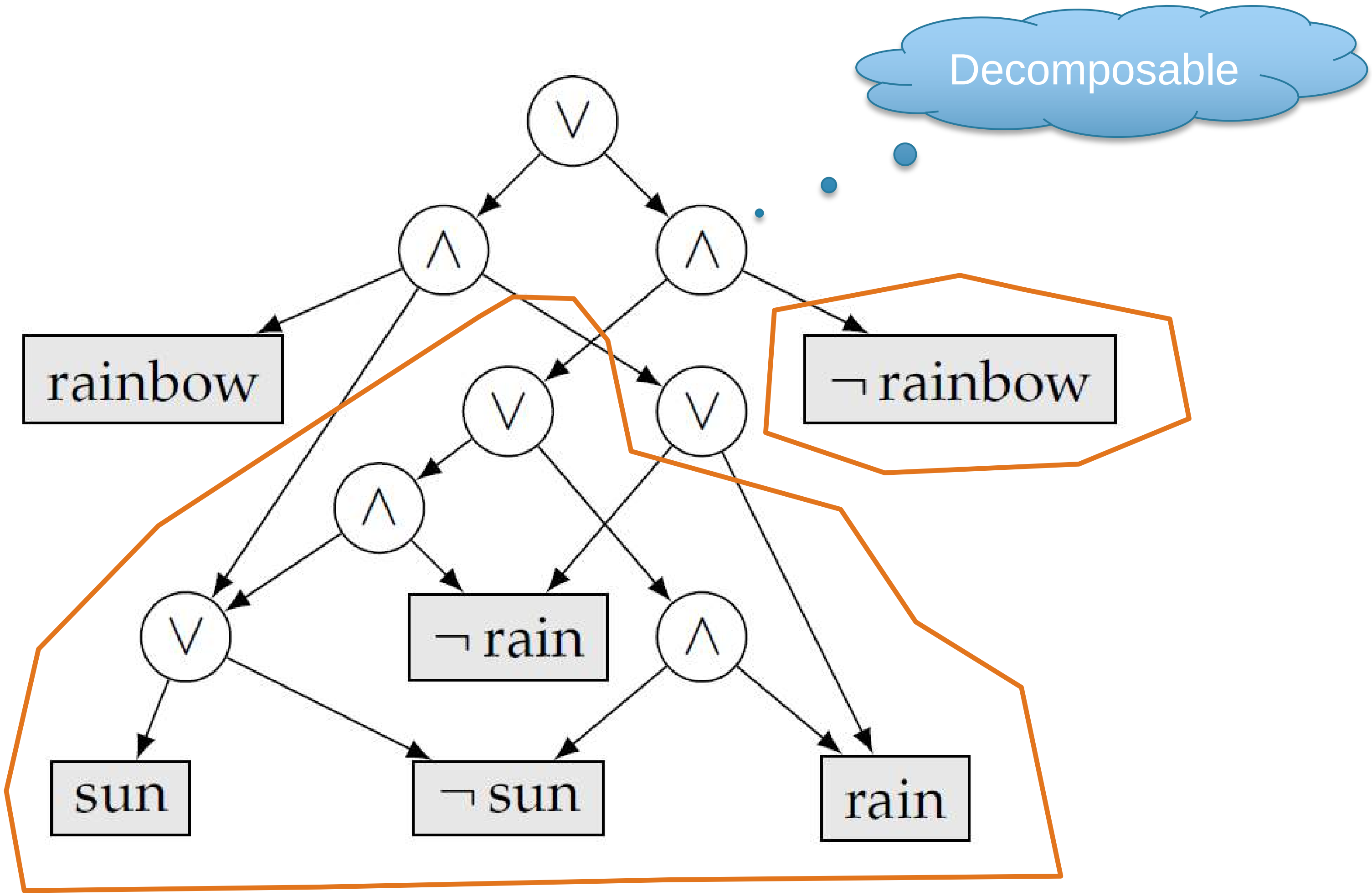
A	B	C	D
0	1	1	0

Bottom-up Evaluation



0 = 1 AND 0

Decomposable Circuits



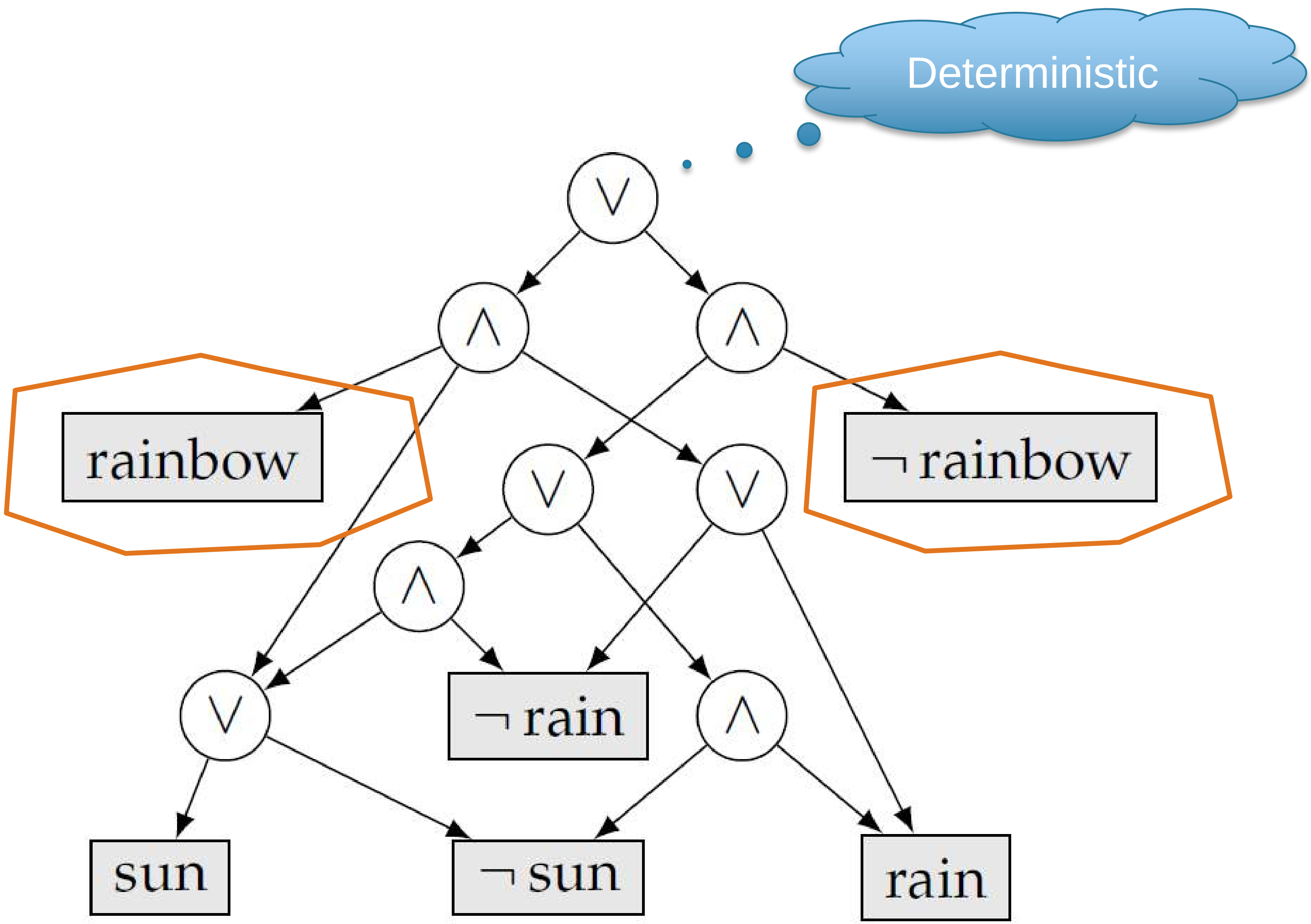
[Darwiche 2002]

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)

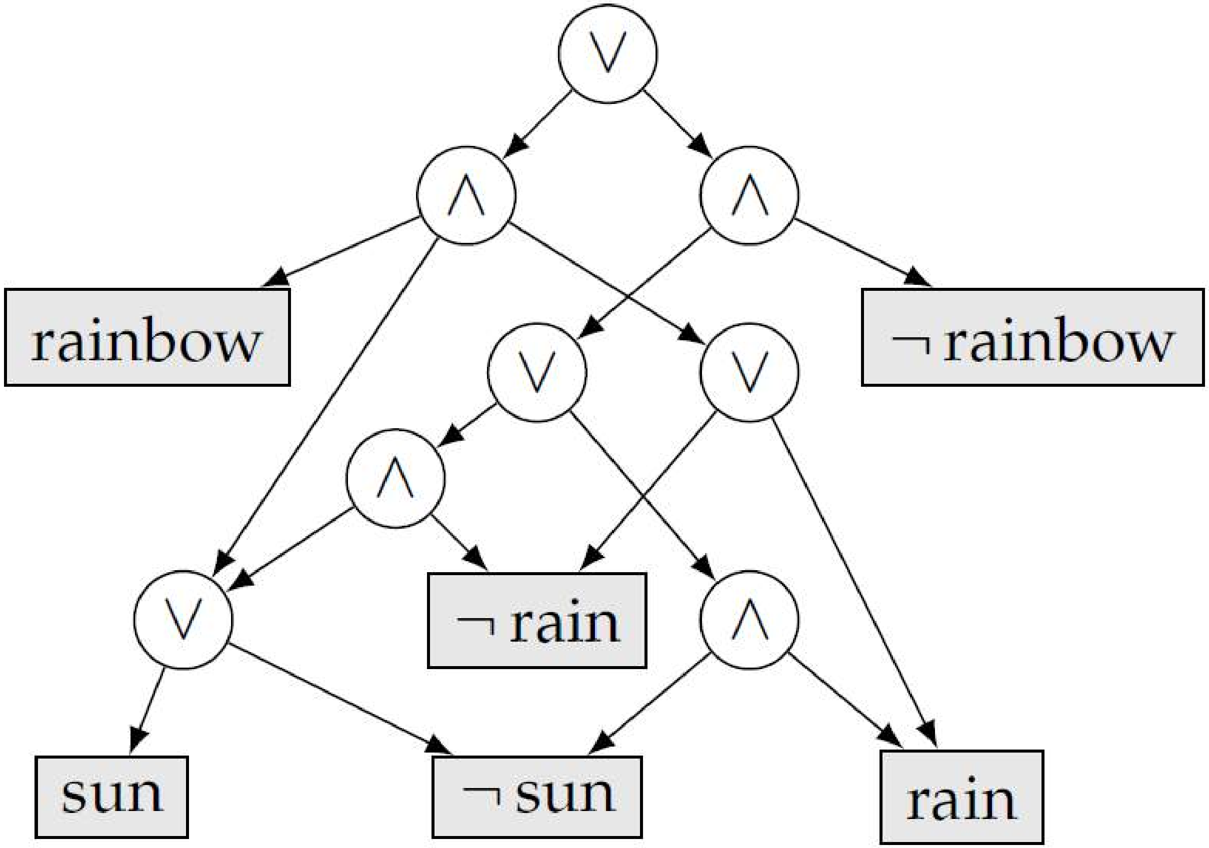
- Complexity linear in circuit size ☺

Deterministic Circuits

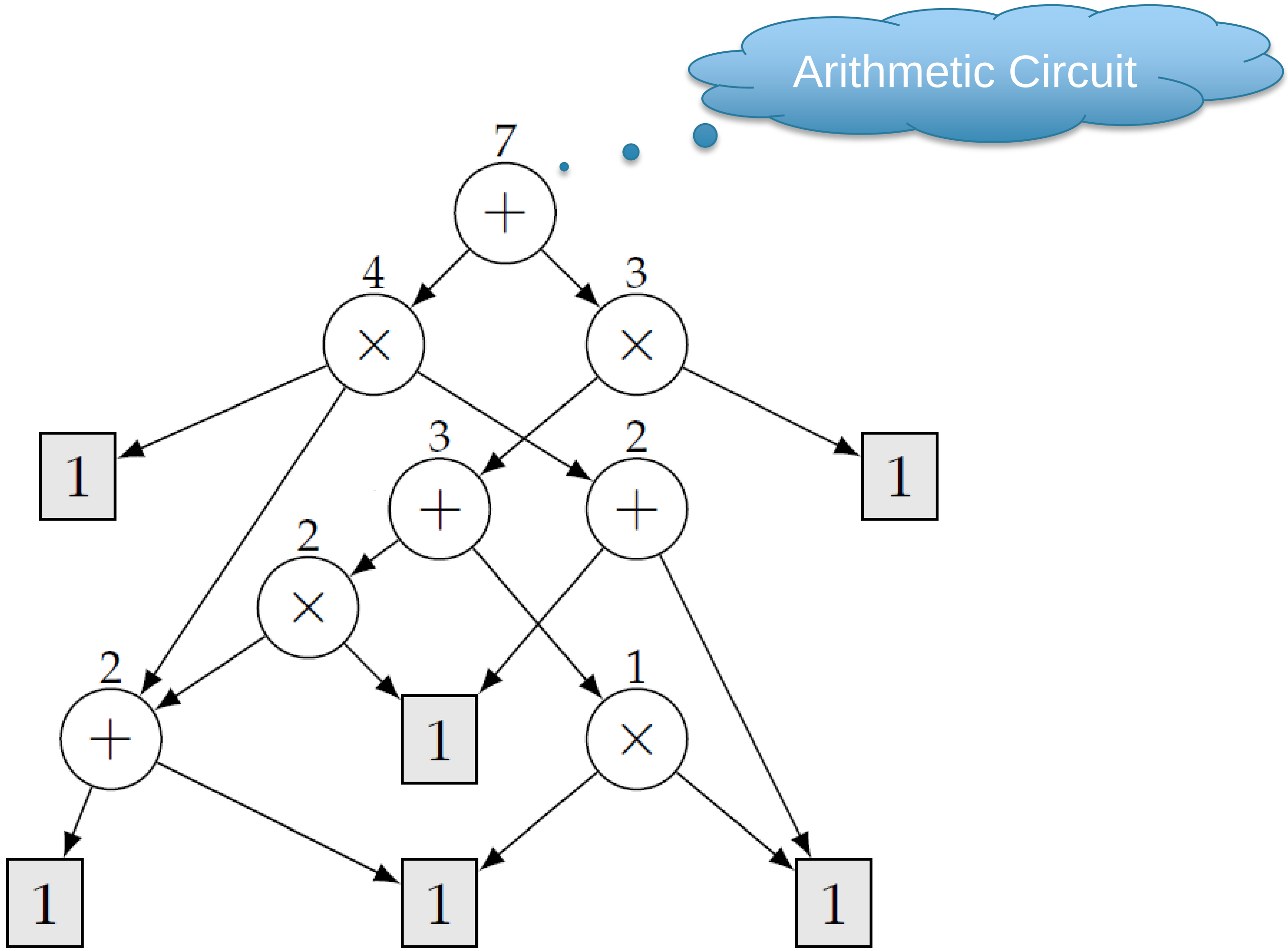


[Darwiche 2002]

How many solutions are there? (#SAT)



How many solutions are there? (#SAT)

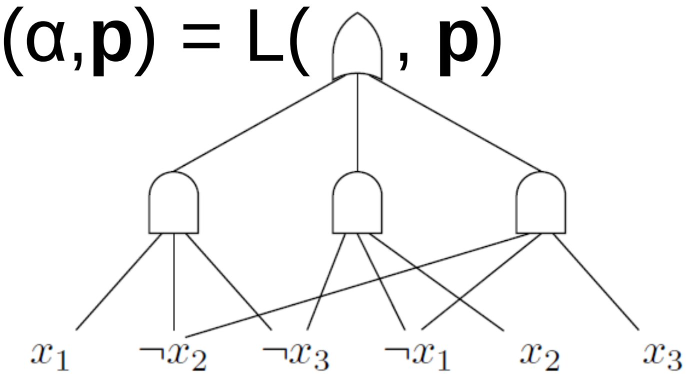


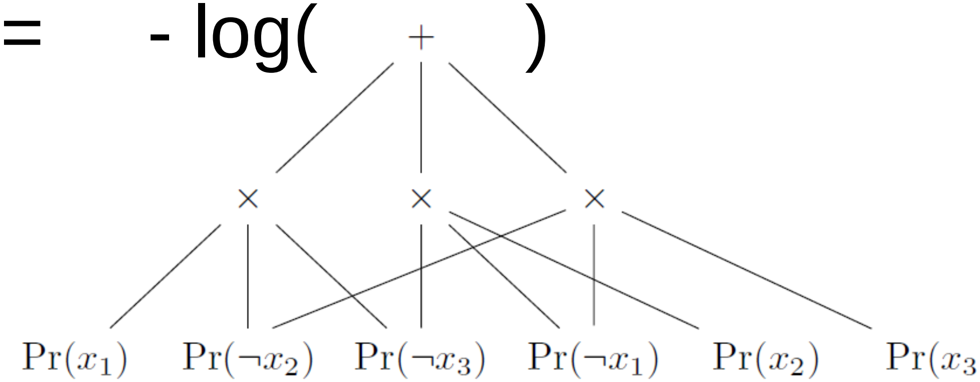
Tractable for Logical Inference

- Is there a solution? (SAT) ✓
- How many solutions are there? (#SAT) ✓
- Stricter languages (e.g., BDD, SDD):
  - Equivalence checking ✓
  - Conjoin/disjoint/negate circuits ✓
- Complexity linear in circuit size ☺
- Compilation into circuit language by either
  - ↓ exhaustive SAT solver
  - ↑ conjoin/disjoin/negate

How to Compute Semantic Loss?

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

$L(\alpha,\mathbf{p}) = L($ 

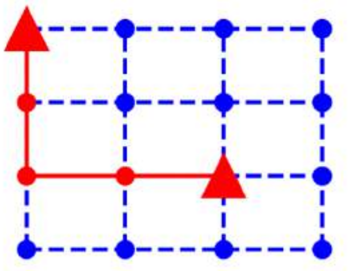
$, \mathbf{p}) = -\log($ 

$)$

- *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?

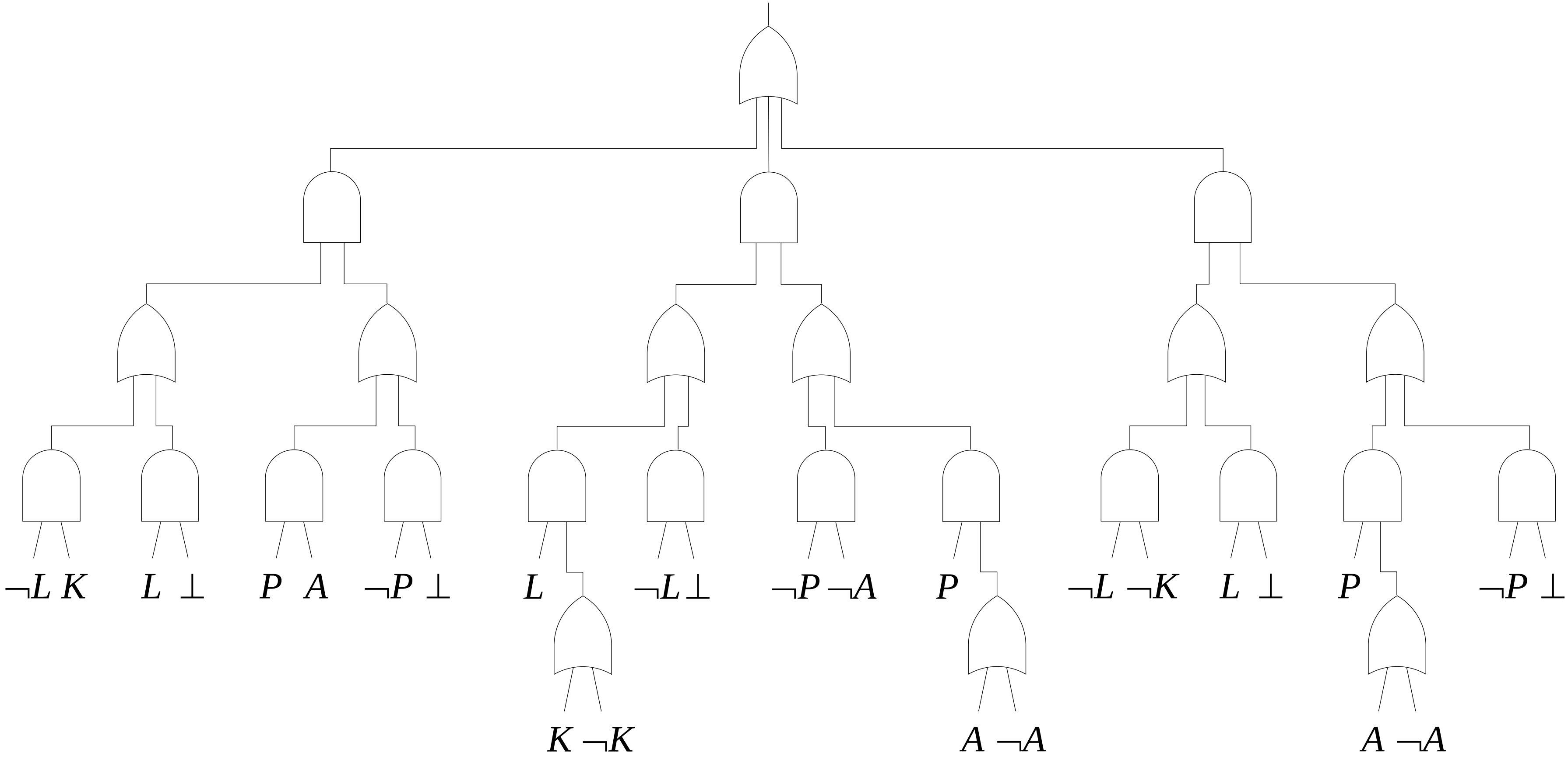
(same conclusion for predicting sushi preferences, see paper)

Outline

- Adding knowledge to deep learning
- **Probabilistic circuits**
- Logistic circuits for image classification

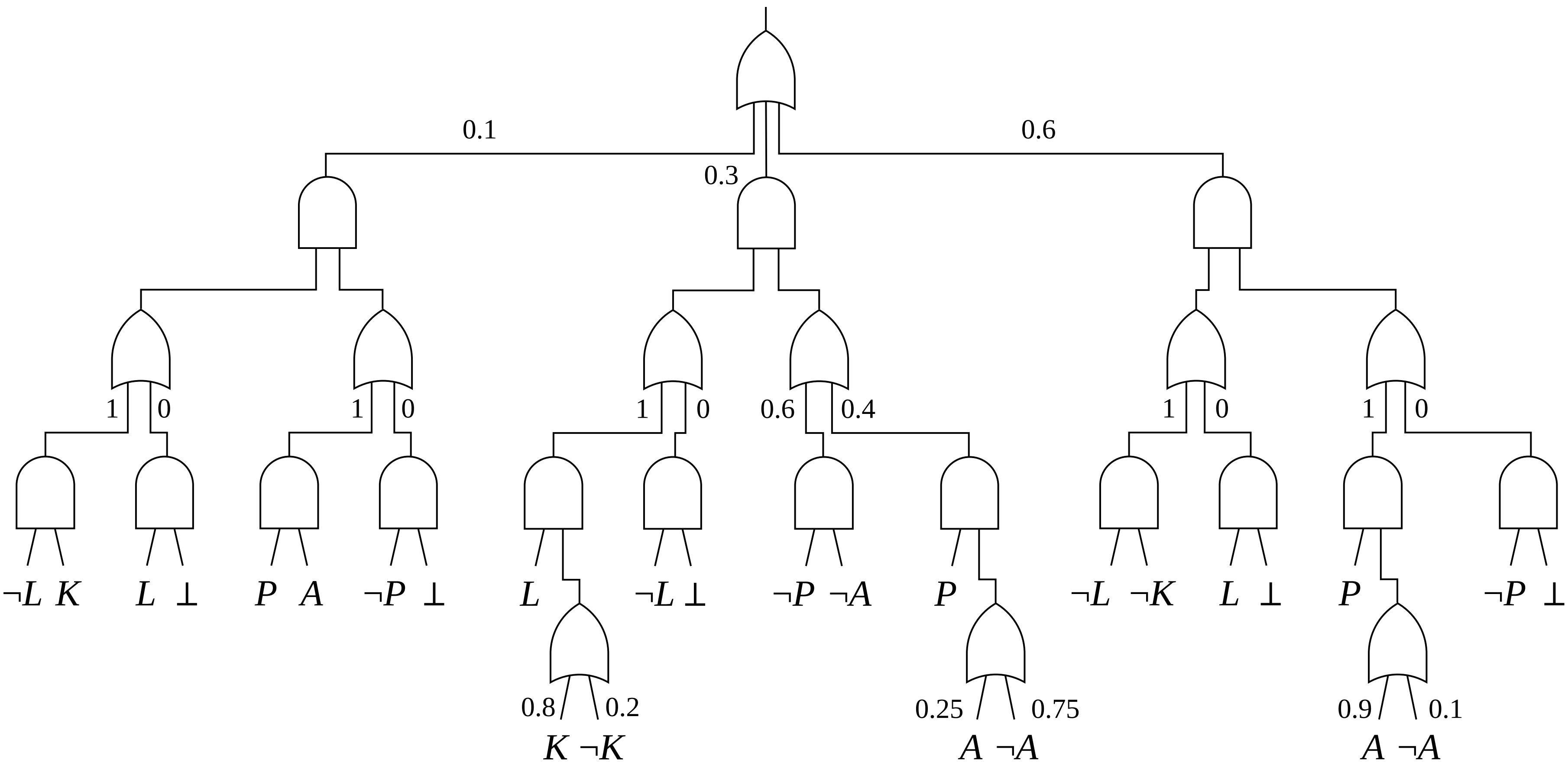
Logical Circuits

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



Can we represent a **distribution** over the solutions to the constraint?

Probabilistic Circuits



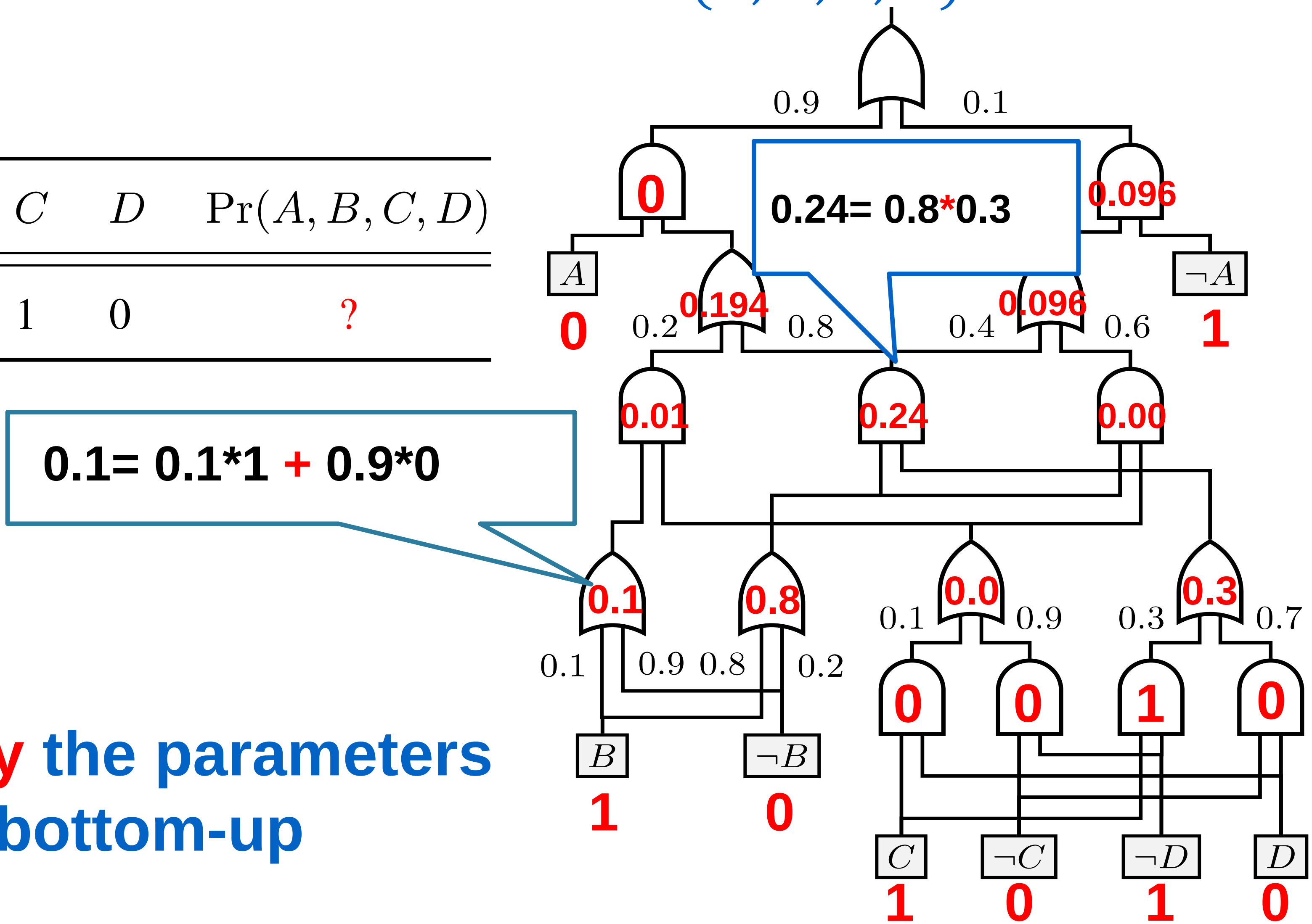
Syntax: assign a normalized probability to each OR gate input

Bottom-Up Evaluation of PSDDs

$\mathbf{Pr}(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \boldsymbol{D}) = \mathbf{0.096}$

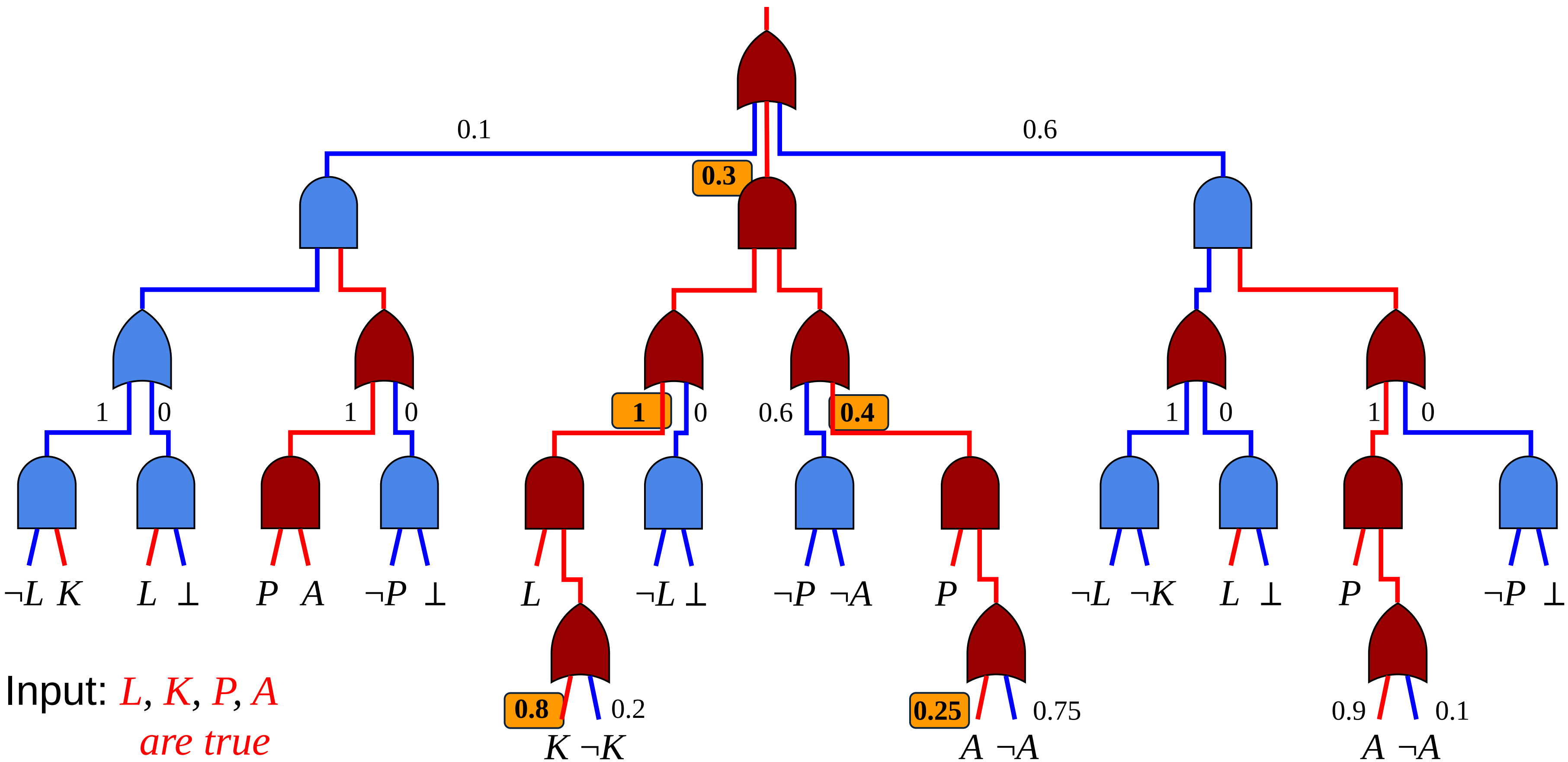
Input:

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



Multiply the parameters bottom-up

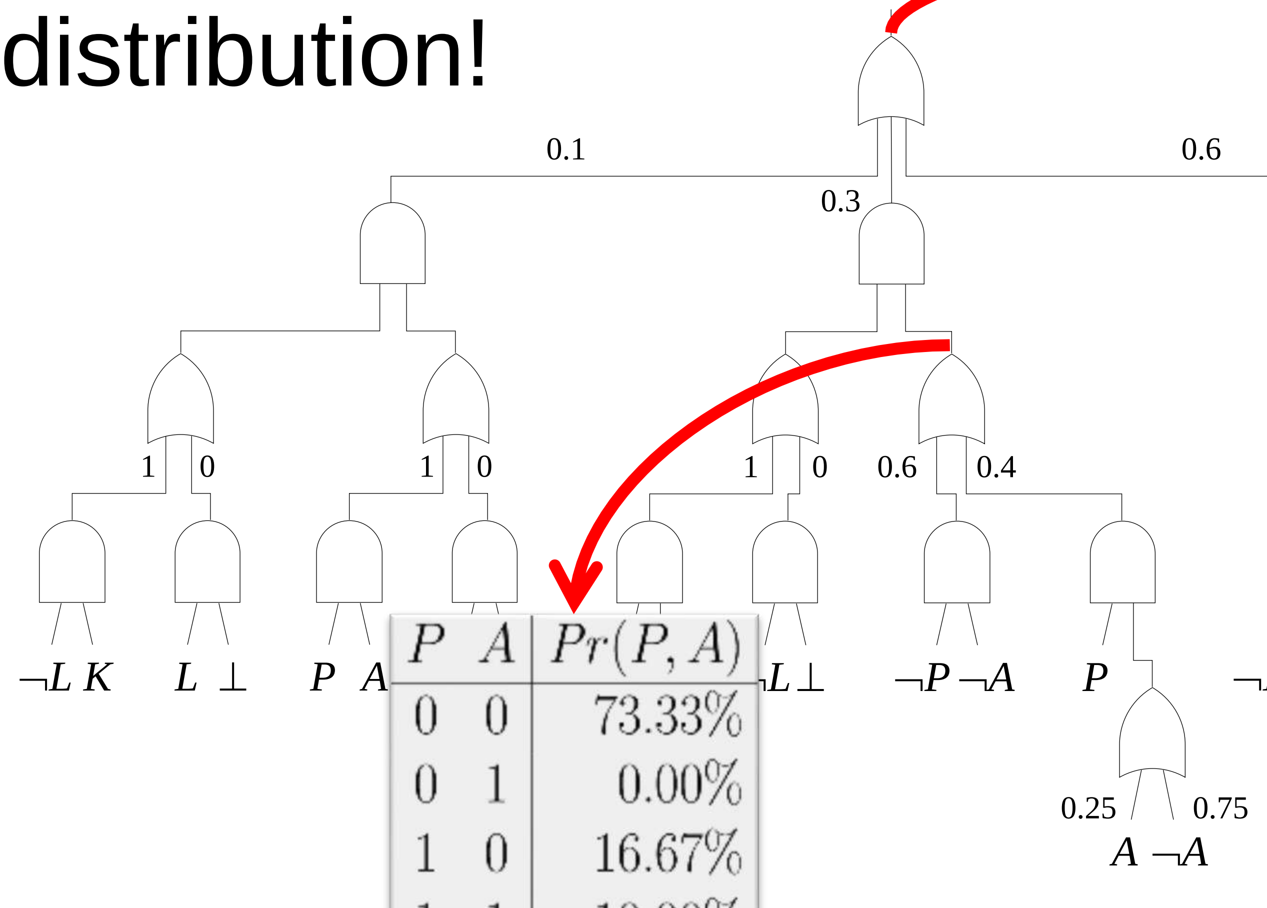
Alternative View of PSDDs



Input: *L*, *K*, *P*, *A*
are true

$$\Pr(L,K,P,A) = 0.3 \times 1 \times 0.8 \times 0.4 \times 0.25 = \mathbf{0.024}$$

Each node represents a normalized distribution!



P	A	$Pr(P, A)$
0	0	73.33%
0	1	0.00%
1	0	16.67%
1	1	10.00%

L	K	P	A	$Pr(L, K, P, A)$
0	0	0	0	0.00%
0	0	0	1	0.00%
0	0	1	0	6.00%
0	0	1	1	54.00%
0	1	0	0	0.00%
0	1	0	1	0.00%
0	1	1	0	0.00%
0	1	1	1	10.00%
1	0	0	0	4.40%
1	0	0	1	0.00%
1	0	1	0	1.00%
1	0	1	1	0.60%
1	1	0	0	17.6%
1	1	0	1	0.00%
1	1	1	0	4.00%
1	1	1	1	2.40%

Can read probabilistic independences off the circuit structure!

Can interpret every parameter as a conditional probability! (XAI)

Tractable for Probabilistic Inference

- **MAP inference**:
  Find most-likely assignment to x given y
  (otherwise NP-hard)
- Computing **conditional probabilities** Pr(x|y)
  (otherwise #P-hard)
- **Sample** from Pr(x|y)

- Algorithms linear in circuit size ☺
  (pass up, pass down, similar to backprop)

Parameter Learning Algorithms

- Closed form
  max likelihood
  from complete data

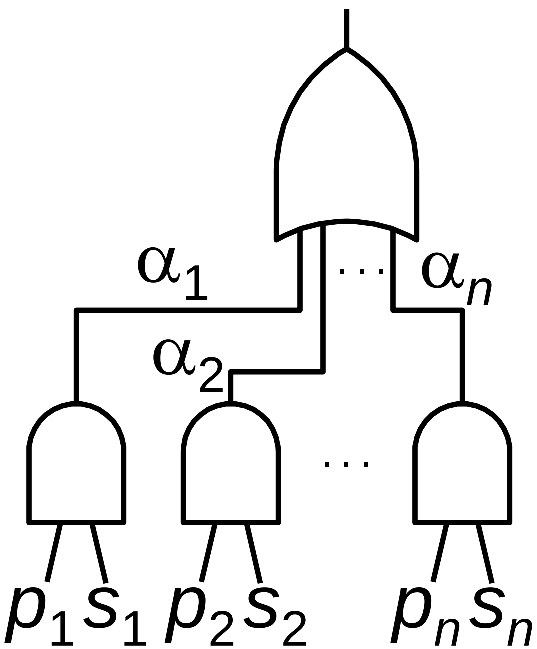
L	K	P	A	Students
0	0	1	0	6
0	0	1	1	54
0	1	1	1	10
1	0	0	0	5
1	0	1	0	1
1	0	1	1	0
1	1	0	0	17
1	1	1	0	4
1	1	1	1	3

- One pass over data to estimate Pr(x|y)

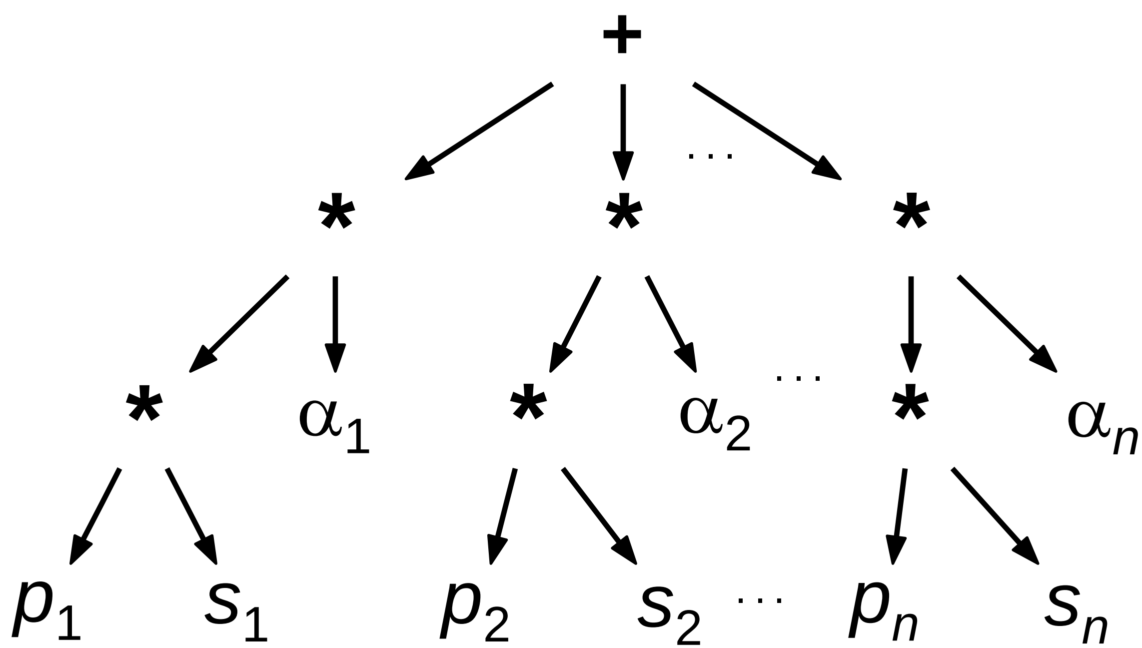
Not a lot to say: very easy! ☺

PSDDs

…are Sum-Product Networks …are Arithmetic Circuits



PSDD



AC

Learn Mixtures of PSDD Structures

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	$-14.36^{\dagger}$

State of the art on 6 datasets!

Q: "Help! I need to learn a discrete probability distribution…"
A: Learn mixture of PSDDs!

Strongly outperforms
- Bayesian network learners
- Markov network learners

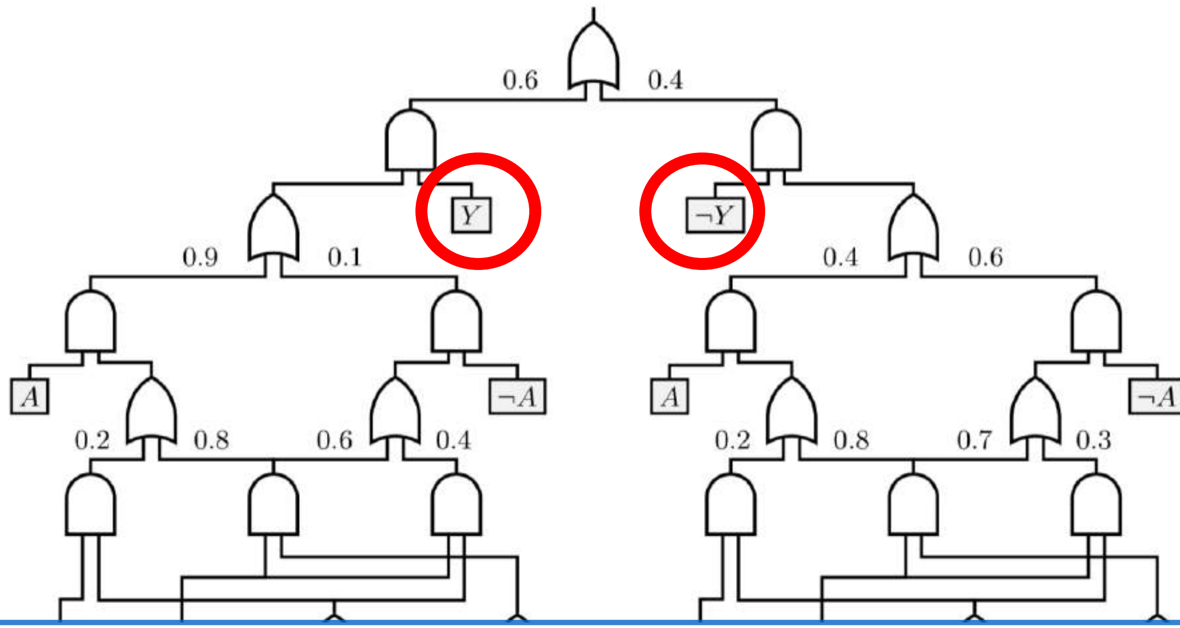
Competitive with
- SPN learners
- Cutset network learners

Outline

- Adding knowledge to deep learning
- Probabilistic circuits
- **Logistic circuits for image classification**

What if I only want to classify Y?

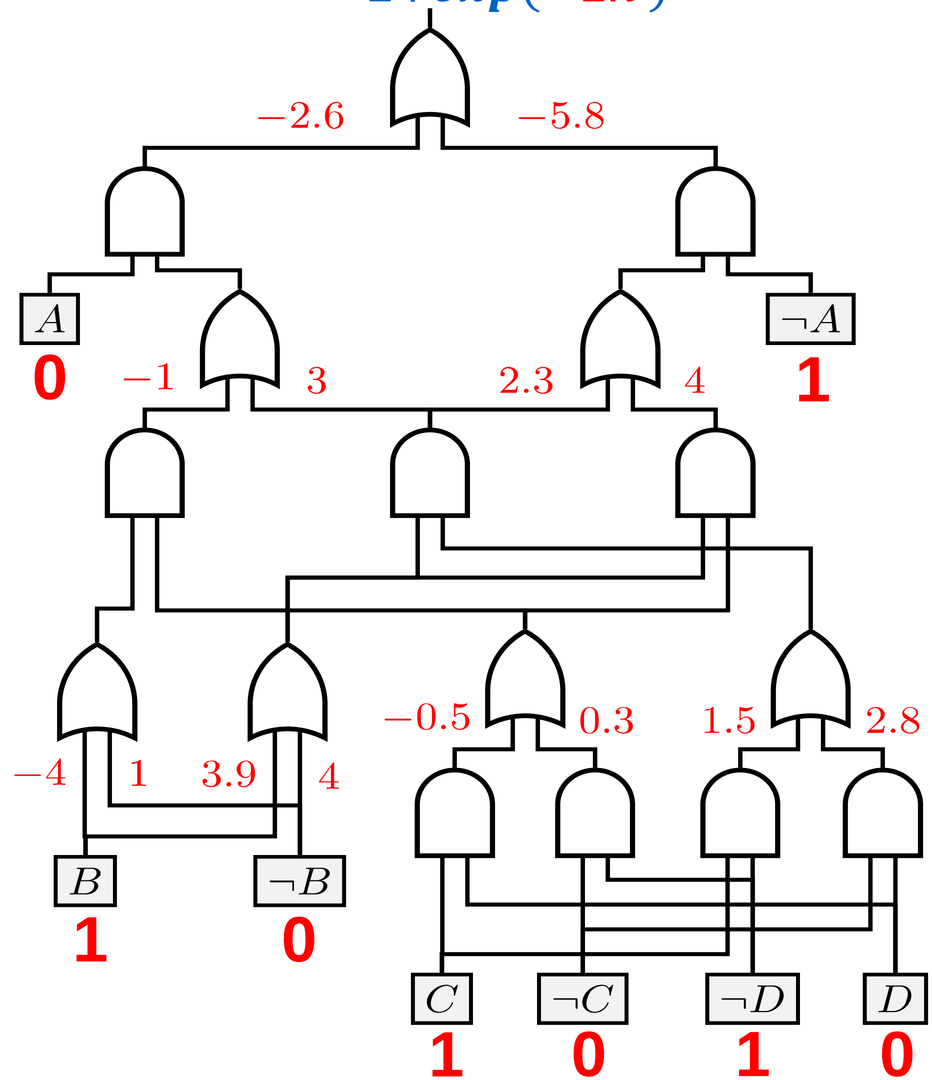
$\Pr(Y, A, B, C, D)$



What if we only want to learn a classifier $\Pr(Y|X)$

Logistic Circuits: Evaluation

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



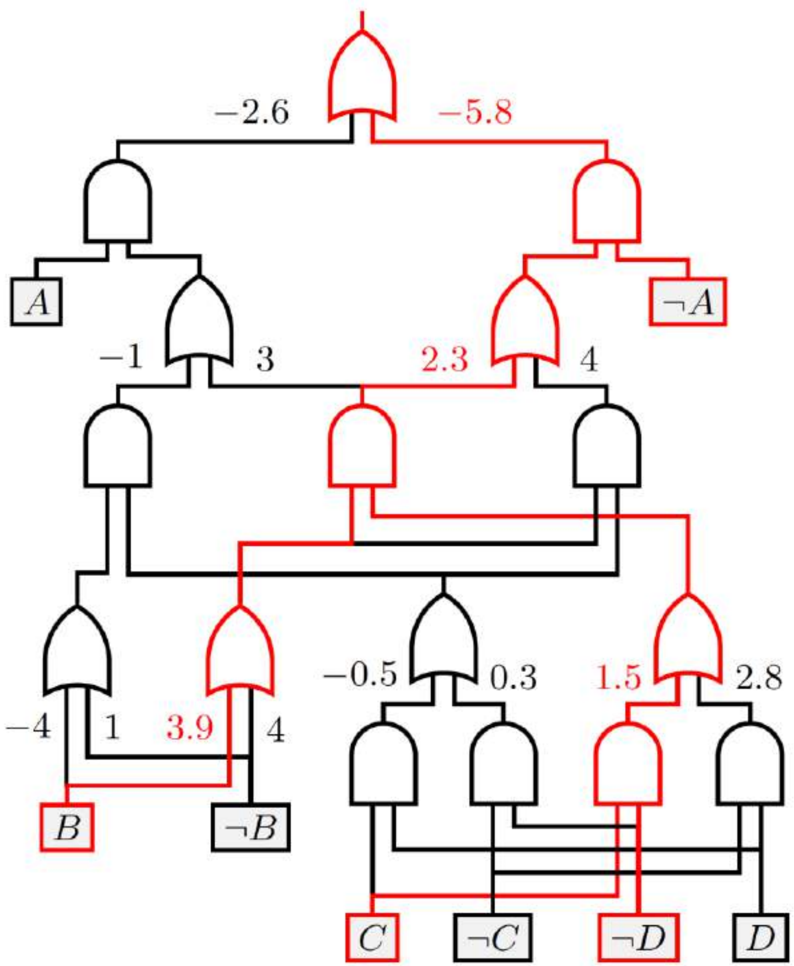
Input:

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

Aggregate the parameters bottom-up

Logistic function on final output

Alternative View on Logistic Circuits

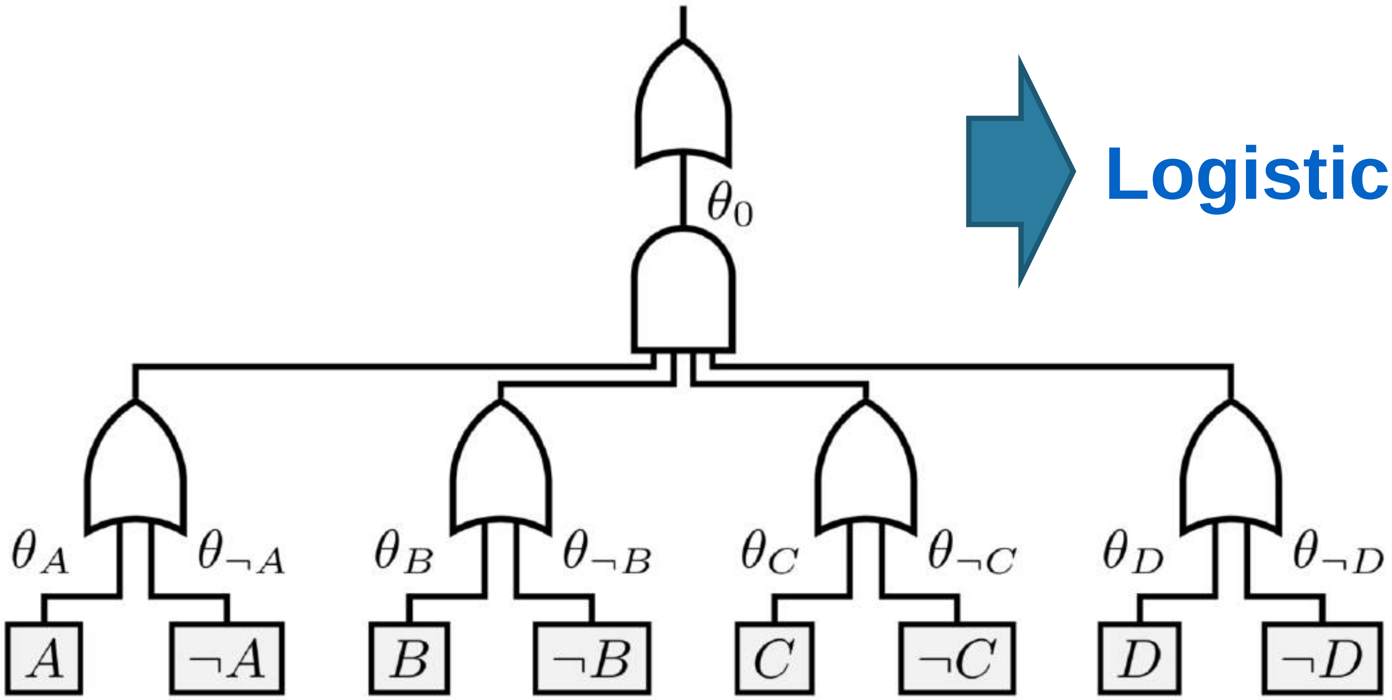


Represents $\Pr(Y \mid A, B, C, D)$

- 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

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

What about other logistic circuits in more general forms?

Parameter Learning

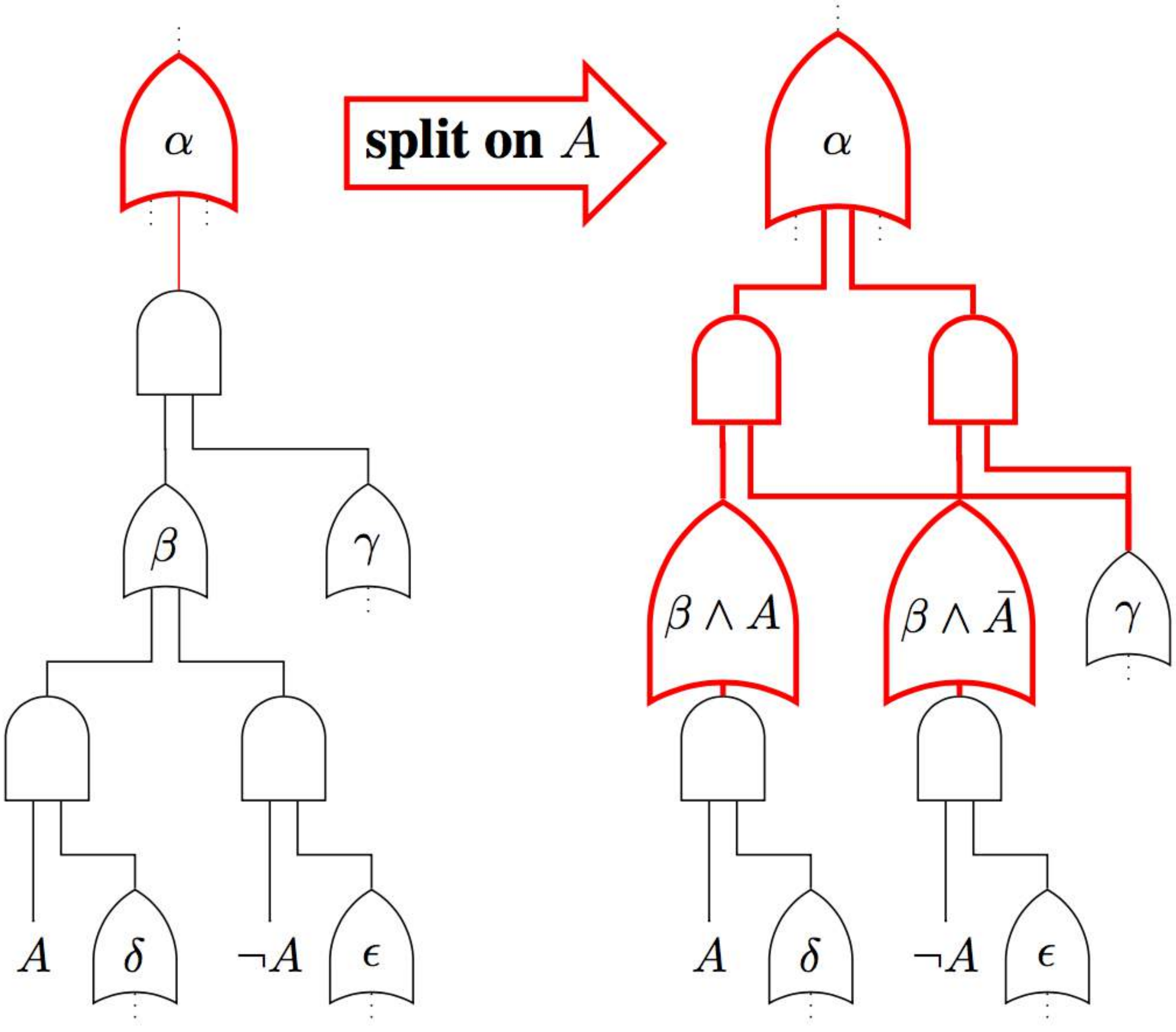
Reduce to logistic regression:

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

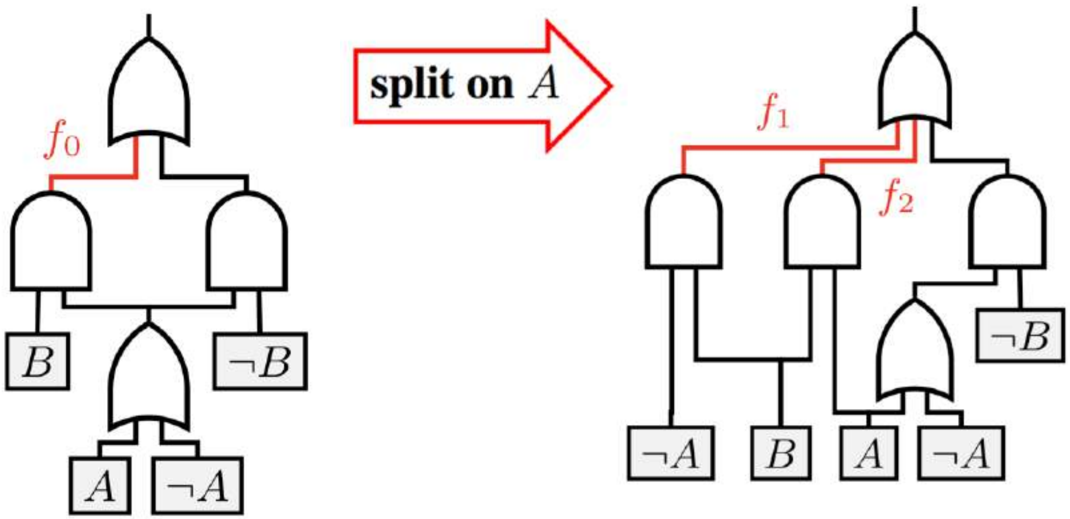
Features associated with each wire
"Global Circuit Flow" features

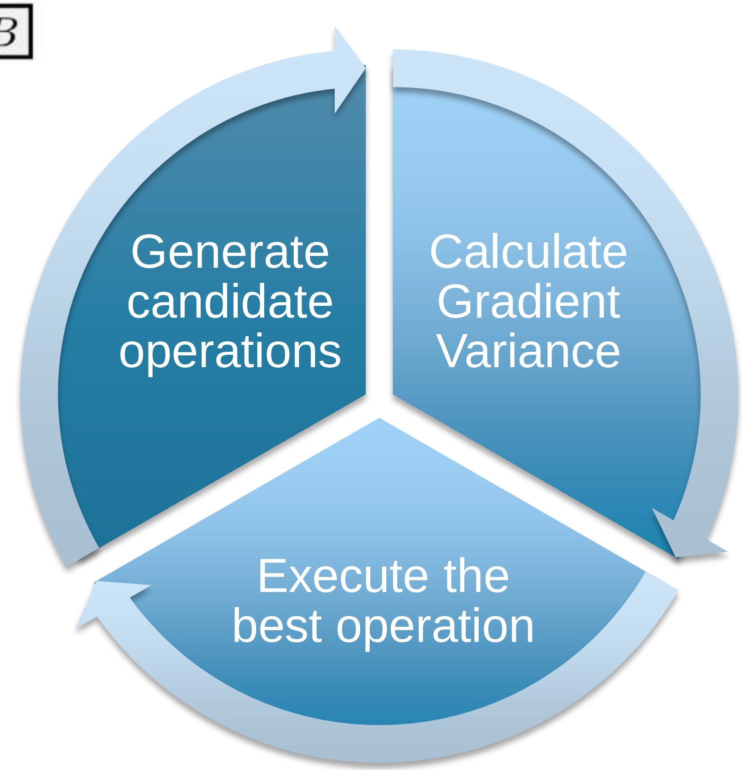
Learning parameters θ is convex optimization!

Structure Learning Primitive



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

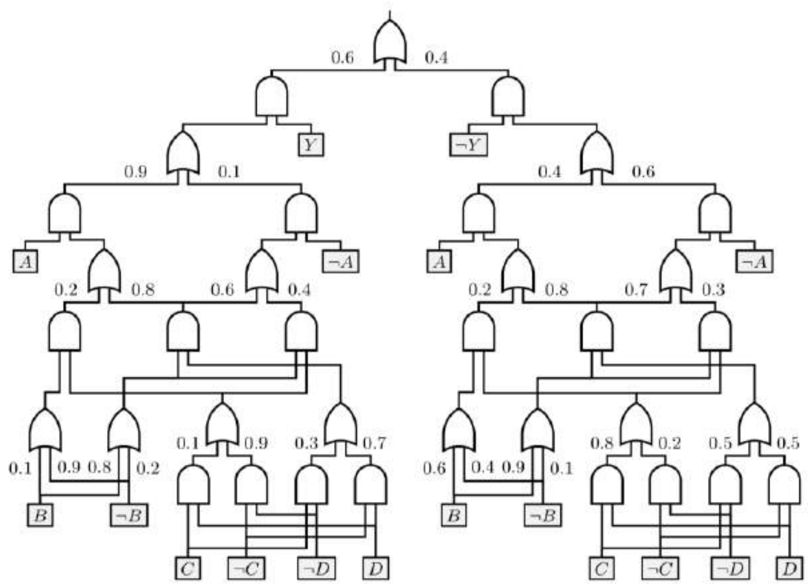
Better Data Efficiency

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**

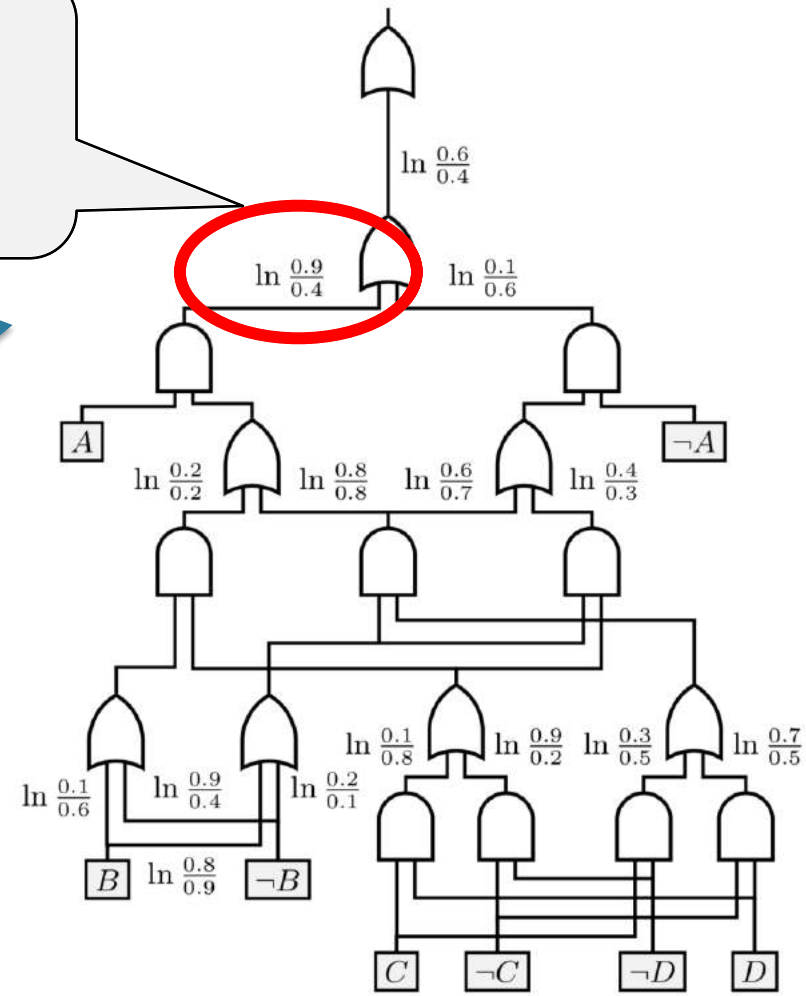
Logistic vs. Probabilistic Circuits

Probabilities become log-odds

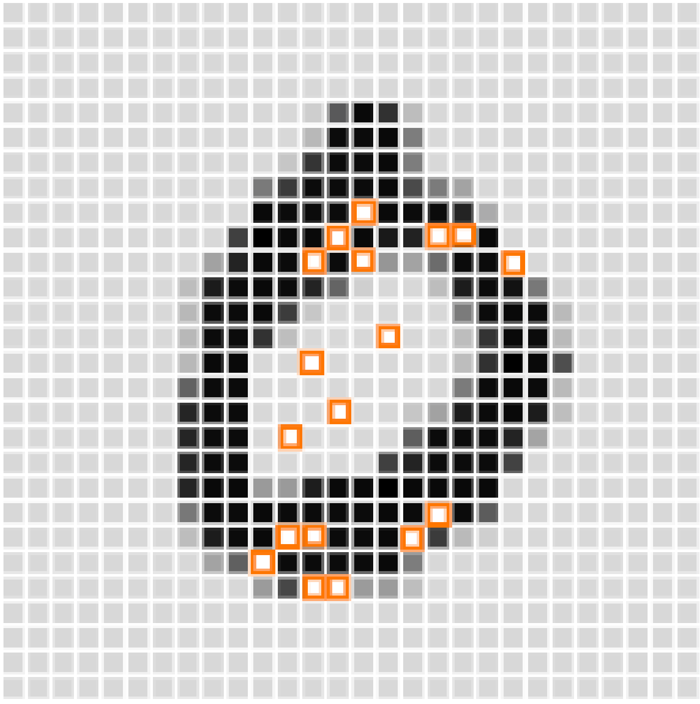
$\Pr(Y, A, B, C, D)$

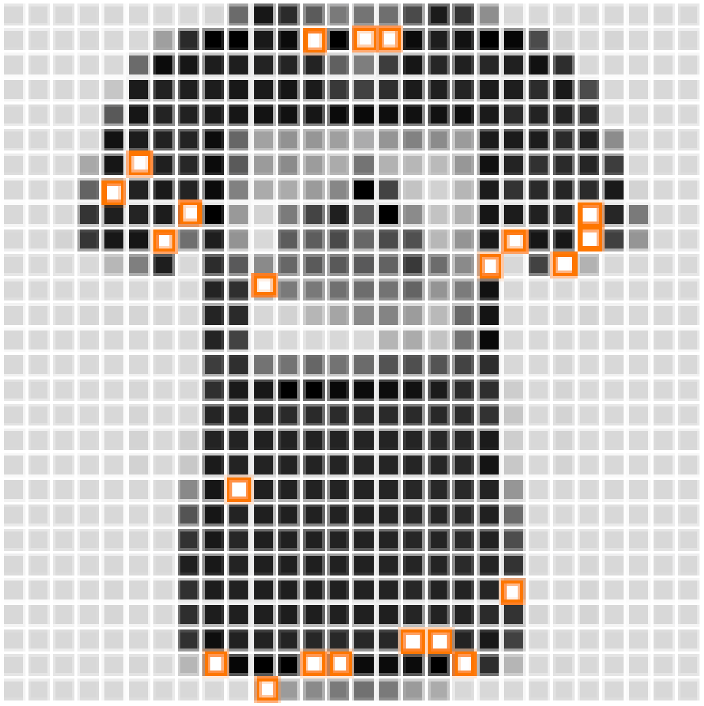


$\Pr(\, Y \mid A, B, C, D \,)$



Interpretable?





Logistic Circuits: Conclusions

- Synthesis of symbolic AI and statistical learning
- Discriminative counterparts of probabilistic circuits
- Convex parameter learning
- Simple heuristic for structure learning
- Good performance
- Easy to interpret

Conclusions