

AI can learn from data. But can it learn to reason?

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Oregon State University - Feb 3 2023

Outline

1. The paradox of learning to reason from data

~~deep learning~~

2. Architectures for Learning and Reasoning

logical reasoning + deep learning

a. Constrained language generation

b. Constrained structured prediction

c. Secret sauce: tractable circuits

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Can Language Models Perform Logical Reasoning?

Language Models achieve high performance on various “reasoning” benchmarks in NLP.

<p>Kristin and her son Justin went to visit her mother Carol on a nice Sunday afternoon. They went out for a movie together and had a good time.</p> 	<p>Q: How is Carol related to Justin ?</p> <p>A: Carol is the grandmother of Justin</p> 
--	---

Reasoning Example
from the CLUTRR
dataset

It is unclear whether they solve the tasks following the rules of logical deduction.

Language Models:

input → ? → *Carol is the grandmother of Justin.*

Logical Reasoning:

input → *Justin is Kristin's son; Carol is Kristin's mother;* → *Carol is Justin's mother's mother; if X is Y's mother's mother then X is Y's grandmother* → *Carol is the grandmother of Justin.*

SimpleLogic

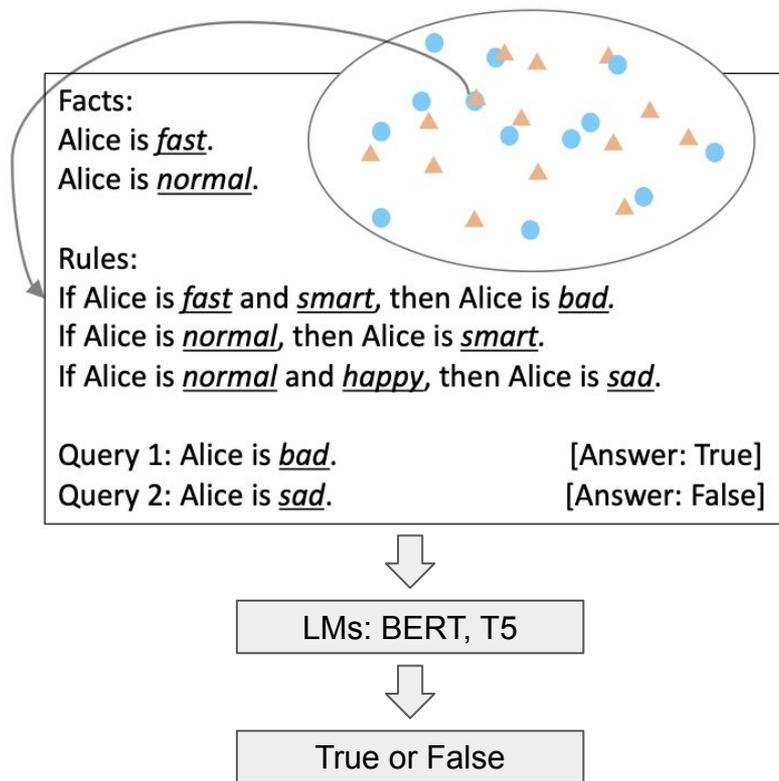
Generate textual train and test examples of the form:

Rules: If witty, then diplomatic. If careless and condemned and attractive, then blushing. If dishonest and inquisitive and average, then shy. If average, then stormy. If popular, then blushing. If talented, then hurt. If popular and attractive, then thoughtless. If blushing and shy and stormy, then inquisitive. If adorable, then popular. If cooperative and wrong and stormy, then thoughtless. If popular, then sensible. If cooperative, then wrong. If shy and cooperative, then witty. If polite and shy and thoughtless, then talented. If polite, then condemned. If polite and wrong, then inquisitive. If dishonest and inquisitive, then talented. If blushing and dishonest, then careless. If inquisitive and dishonest, then troubled. If blushing and stormy, then shy. If diplomatic and talented, then careless. If wrong and beautiful, then popular. If ugly and shy and beautiful, then stormy. If shy and inquisitive and attractive, then diplomatic. If witty and beautiful and frightened, then adorable. If diplomatic and cooperative, then sensible. If thoughtless and inquisitive, then diplomatic. If careless and dishonest and troubled, then cooperative. If hurt and witty and troubled, then dishonest. If scared and diplomatic and troubled, then average. If ugly and wrong and careless, then average. If dishonest and scared, then polite. If talented, then dishonest. If condemned, then wrong. If wrong and troubled and blushing, then scared. If attractive and condemned, then frightened. If hurt and condemned and shy, then witty. If cooperative, then attractive. If careless, then polite. If adorable and wrong and careless, then diplomatic. Facts: Alice sensible Alice condemned Alice thoughtless Alice polite Alice scared Alice average
Query: Alice is shy ?

Problem Setting: SimpleLogic

The easiest of reasoning problems:

1. **Propositional logic** fragment
 - a. bounded vocabulary & number of rules
 - b. bounded reasoning depth (≤ 6)
 - c. finite space ($\approx 10^{360}$)
2. **No language variance**: templated language
3. **Self-contained**
No prior knowledge
4. **Purely symbolic** predicates
No shortcuts from word meaning
5. **Tractable** logic (definite clauses)
Can always be solved efficiently

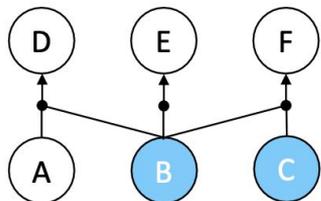


Training a BERT model on SimpleLogic

(1) Randomly sample facts & rules.

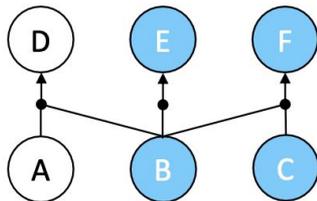
Facts: B, C

Rules: $A, B \rightarrow D$. $B \rightarrow E$. $B, C \rightarrow F$.



Rule-Priority

(2) Compute the correct labels for all predicates given the facts and rules.



Label-Priority



(1) Randomly assign labels to predicates.

True: B, C, E, F.

False: A, D.

(2) Set B, C (randomly chosen among B, C, E, F) as facts and sample rules (randomly) consistent with the label assignments.

Test accuracy for different reasoning depths

Test	0	1	2	3	4	5	6
RP	99.9	99.8	99.7	99.3	98.3	97.5	95.5

Test	0	1	2	3	4	5	6
LP	100.0	100.0	99.9	99.9	99.7	99.7	99.0

Has BERT learned to reason from data?

1. Easiest of reasoning problems (no variance, self-contained, purely symbolic, tractable)
2. RP/LP data covers the whole problem space
3. The learned model has almost 100% test accuracy
4. There exist BERT parameters that compute the ground-truth reasoning function:

Theorem 1: *For a BERT model with n layers and 12 attention heads, by construction, there exists a set of parameters such that the model can correctly solve any reasoning problem in SimpleLogic that requires at most $n - 2$ steps of reasoning.*

**Surely, under these conditions,
BERT has learned the ground-truth reasoning function!**



The Paradox of Learning to Reason from Data

Train	Test	0	1	2	3	4	5	6
RP	RP	99.9	99.8	99.7	99.3	98.3	97.5	95.5
	LP	99.8	99.8	99.3	96.0	90.4	75.0	57.3
LP	RP	97.3	66.9	53.0	54.2	59.5	65.6	69.2
	LP	100.0	100.0	99.9	99.9	99.7	99.7	99.0

The BERT model trained on one distribution fails to generalize to the other distribution within the same problem space.



1. If BERT **has learned** to reason, it should not exhibit such generalization failure.
2. If BERT **has not learned** to reason, it is baffling how it achieves near-perfect in-distribution test accuracy.

Why? Statistical Features

Monotonicity of entailment:

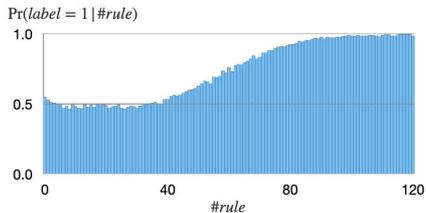
Any rules can be freely added to the hypothesis of any proven fact.



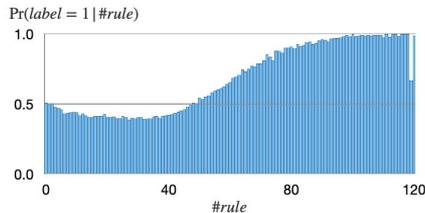
The more rules given, the more likely a predicate will be proved.



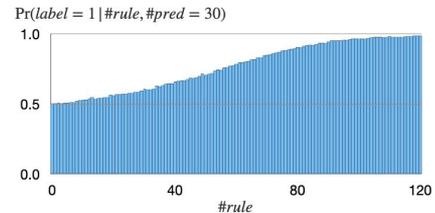
$\Pr(\text{label} = \text{True} \mid \text{Rule \#} = x)$ should increase (roughly) monotonically with x



(a) Statistics for examples generated by Rule-Priority (RP).



(b) Statistics for examples generated by Label-Priority (LP).



(c) Statistics for examples generated by uniform sampling;

BERT leverages statistical features to make predictions

RP_b downsamples from RP such that $\Pr(\text{label} = \text{True} \mid \text{rule\#} = x) = 0.5$ for all x

Train	Test	0	1	2	3	4	5	6
	RP	99.9	99.8	99.7	99.3	98.3	97.5	95.5
RP	RP_b	99.0	99.3	98.5	97.5	96.7	93.5	88.3

1. Accuracy drop from RP to RP_b indicates that **the model is using rule# as a statistical feature to make predictions.**
2. Potentially countless statistical features
3. Such features are **inherent to the reasoning problem**, cannot make data “clean”

First Conclusion

Experiments unveil the fundamental difference between

1. learning to reason, and
2. learning to achieve high performance on benchmarks using statistical features.

Be careful deploying AI in applications where this difference matters.

Is more data going to solve this problem?

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~~deep learning~~

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logical reasoning + deep learning

a. Constrained language generation

b. Constrained structured prediction

c. Secret sauce: tractable circuits

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Is ChatGPT all you need?

 generate a sentence using the following keywords: fish watch kid swim tank

 A kid watches a fish swim in the tank.

 generate a sentence using the following keywords: cook top pan stove vegetable

 The cook used a pan on the stove top to prepare the vegetable.

Large language models are *not* all you need

fine-grained control (e.g., generation given lexical constraints) is challenging ...



using the keywords "fish" "watch" "kid" "swim" "tank", generate a sentence with seven words:



Kid watches fish swim in tank. 

Large language models are *not* all you need

fine-grained control (e.g., generation given lexical constraints) is challenging ...

H

generate a sentence using the following keywords and the keywords should appear in the order as listed: pan vegetable cook stove top



"She placed a pan of chopped vegetables on the stove top to cook"



Large language models are *not* all you need

fine-grained control (e.g., generation given lexical constraints) is challenging ...



generate a sentence with "pan" as the third word and "vegetable" as the fifth word.



The chef used the pan to gently sauté the diced vegetable for their delicious stir-fry dish.



Key Challenge: intractable conditioning

Given lexical constraint α :

“pan” “vegetable” “cook” “stove” “top” appears in the generated sentence

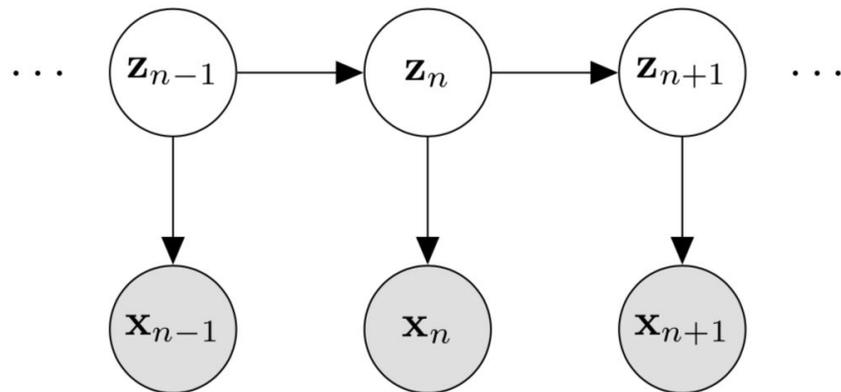
Goal: generate from the conditional distribution $\Pr(\text{sentence} \mid \alpha)$

Computing $\Pr(\text{sentence} \mid \alpha)$ is *intractable* for auto-regressive large language models (LLMs); in particular, computing $\Pr(\text{next-token} \mid \alpha, \text{prefix})$ is *intractable*.

Solution: language models that allow efficient conditioning

Tractable Probabilistic
Models

Step 1: distill a TPM that *approximates* the distribution of an LLM.



A simple *Hidden Markov Model* architecture will suffice!

- 50k emission tokens x
- 4096 hidden states z
- trained as a *Probabilistic Circuit* in Juice.jl from LLM samples
- scaled up using *Latent Variable Distillation* [ICLR 2023]

Step 2: compute $\Pr(\text{next-token} \mid \text{prefix}, \alpha)$ via TPM

Dynamic programming algorithm in PyTorch that takes logical constraints α .

Can be quite complex: all inflections, all positions in seq, ...

Step 3: control auto-regressive generation with the LLM.

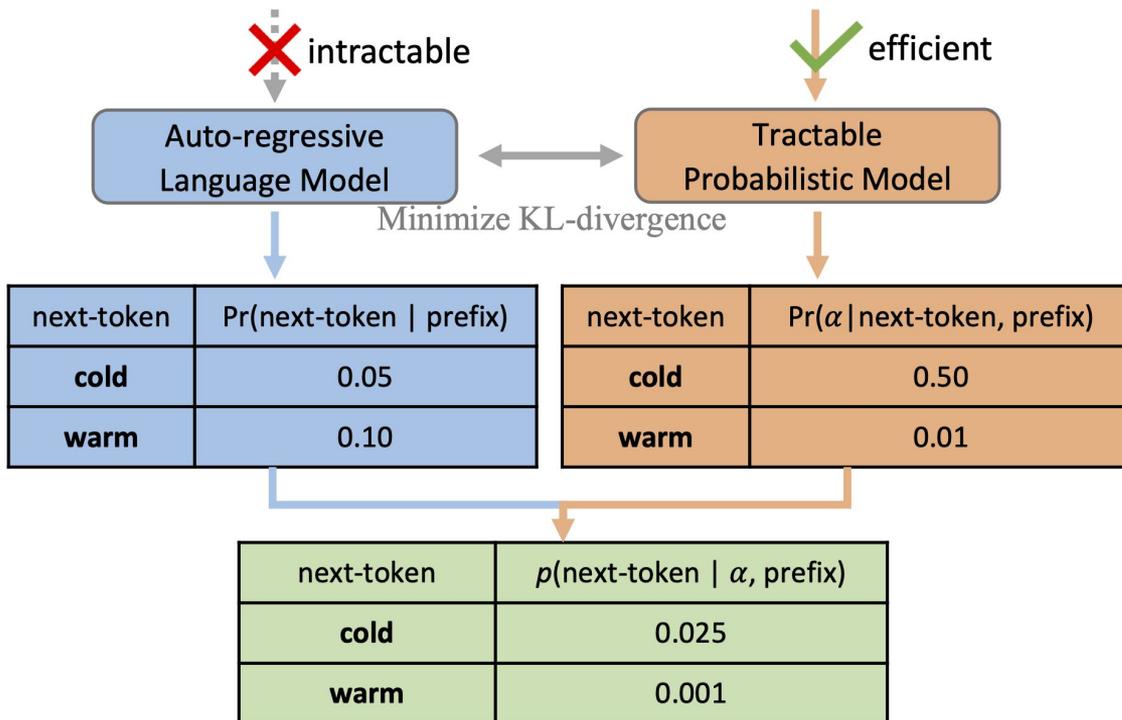
Assume independence between fluency β and constraint α

$$\begin{aligned} & \Pr_{\text{TPM}}(x_{t+1} \mid x_{1:t}, \alpha, \beta) \\ & \propto \Pr_{\text{TPM}}(\alpha \mid x_{1:t+1}, \beta) \cdot \Pr_{\text{TPM}}(x_{t+1} \mid x_{1:t}, \beta) \\ & \propto \Pr_{\text{TPM}}(\alpha \mid x_{1:t+1}) \cdot \Pr_{\text{LM}}(x_{t+1} \mid x_{1:t}) \\ & \quad \downarrow \text{sleight of hand} \end{aligned}$$

Controlling Language Generation via TPM

Lexical Constraint α : the sentence contains keyword “**winter**”

Probabilistic Query: $\Pr(\text{next-token} \mid \alpha, \text{prefix} = \text{“the weather is”})$



CommonGen: a challenging constrained generation task

Method	<i>Generation Quality</i>				<i>Constraint Satisfaction</i>			
	ROUGE-L		BLEU-4		Coverage		Success Rate	
	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>
<i>Unsupervised</i>								
InsNet (Lu et al., 2022a)	-	-	18.7	-	100.0		100.0	-
NeuroLogic (Lu et al., 2021)	-	41.9	-	24.7	-	96.7	-	-
A*esque (Lu et al., 2022b)	-	44.3	-	28.6	-	97.1	-	-
NADO (Meng et al., 2022)	-	-	26.2	-	96.1	-	-	-
Ours	44.6	44.1	29.9	29.4	100.0	100.0	100.0	100.0
<i>Supervised</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>
NeuroLogic (Lu et al., 2021)	-	42.8	-	26.7	-	97.7	-	93.9 [†]
A*esque (Lu et al., 2022b)	-	43.6	-	28.2	-	97.8	-	97.9 [†]
NADO (Meng et al., 2022)	44.4 [†]	-	30.8	-	97.1	-	88.8 [†]	-
Ours	46.0	45.6	34.1	32.9	100.0	100.0	100.0	100.0

State-of-the-art performance on the CommonGen dataset, beating baselines from various families of constrained generation techniques with a large margin. All baselines use GPT2-large as the base model.

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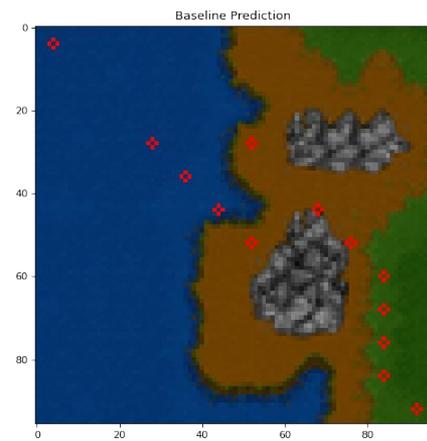
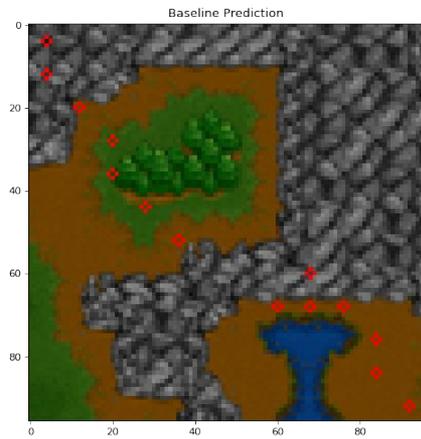
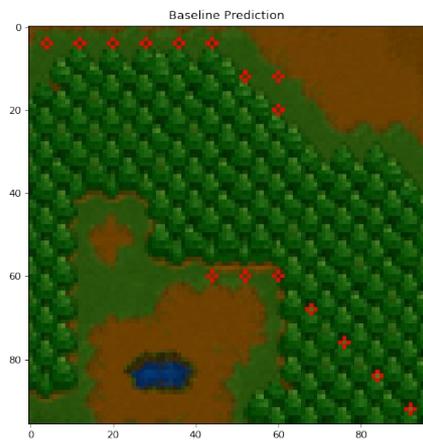
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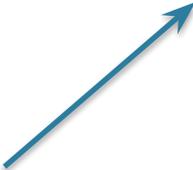
a. Constrained language generation

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ARCHITECTURE	EXACT MATCH	HAMMING SCORE	CONSISTENCY
RESNET-18+FIL	55.0	97.7	56.9



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

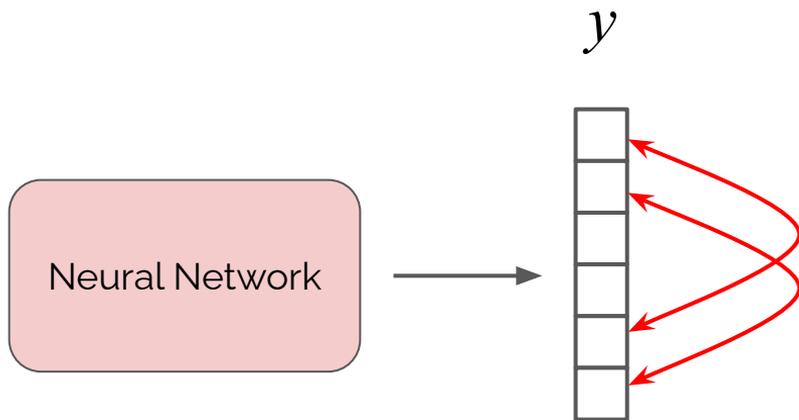


*Are individual
edge predictions
correct?*

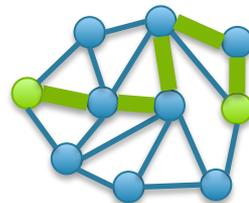


*Is output
a path?*

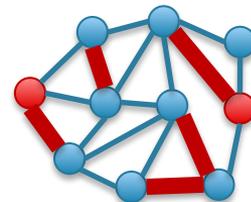
Declarative Knowledge of the Output



How is the output structured?
Are all possible outputs valid?



vs.



How are the outputs related to each other?

Learning this from data is inefficient
Much easier to express this declaratively

pylon

PyTorch Code

```
for i in range(train_iters):  
    ...  
    py = model(x)  
    ...  
    loss = CrossEntropy(py, ...)
```

1

Specify knowledge as a predicate

```
def check(y):  
    ...  
    return isValid
```

pylon

PyTorch Code

```
for i in range(train_iters):  
    ...  
    py = model(x)  
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    loss = CrossEntropy(py, ...)  
    loss += constraint_loss(check)(py)
```

1

Specify knowledge as a predicate

```
def check(y):  
    ...  
    return isValid
```

2

Add as loss to training

```
loss += constraint_loss(check)
```

pylon

PyTorch Code

```
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1 Specify knowledge as a predicate

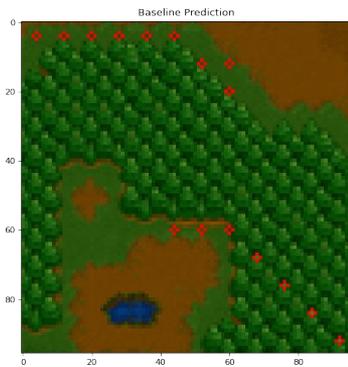
```
def check(y):  
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2 Add as loss to training

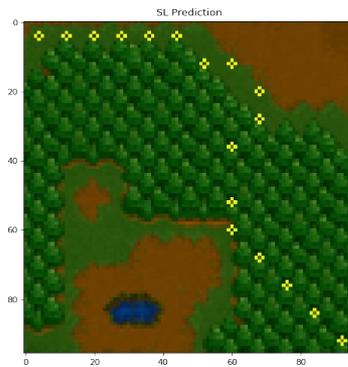
```
loss += constraint_loss(check)
```

3 pylon derives the gradients
(solves a combinatorial problem)

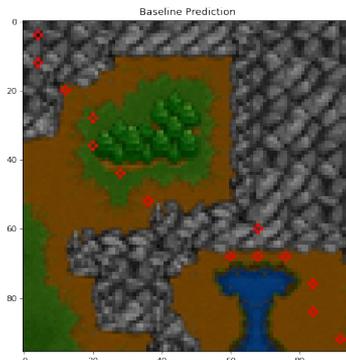
without constraint



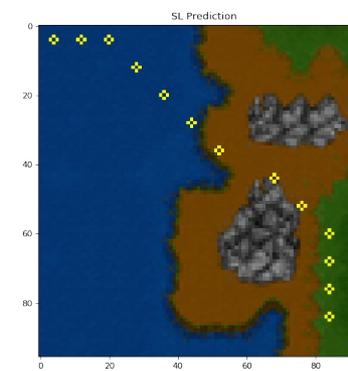
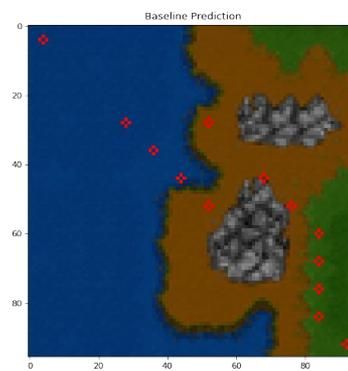
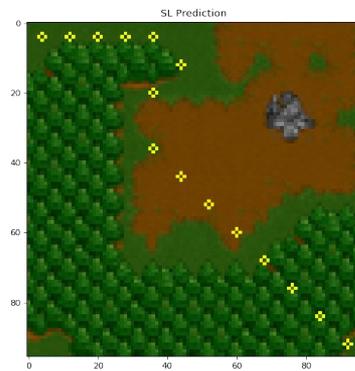
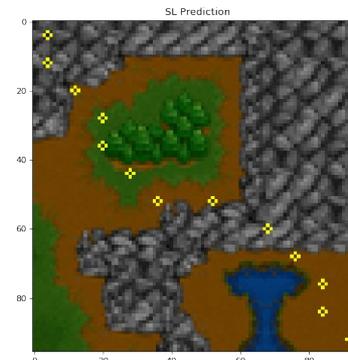
with constraint

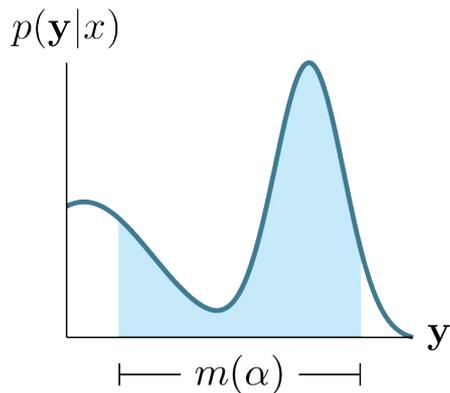


without constraint

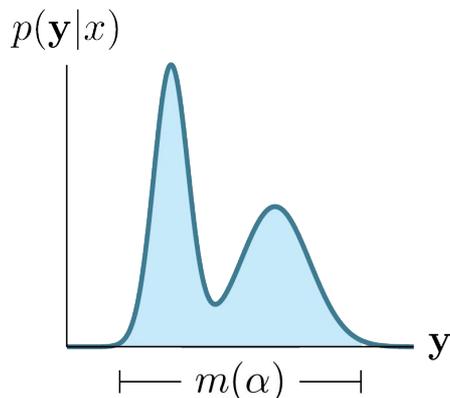


with constraint





a) A network uncertain over both valid & invalid predictions



c) A network allocating most of its mass to models of constraint

$$L^S(\alpha, \mathbf{p}) \propto -\log \underbrace{\sum_{\mathbf{x} \models \alpha} \prod_{i: \mathbf{x} \models X_i} p_i \prod_{i: \mathbf{x} \models \neg X_i} (1 - p_i)}_{\text{Probability of satisfying constraint } \alpha \text{ after sampling from neural net output layer } \mathbf{p}}$$



Semantic Loss

Probability of satisfying constraint α after sampling from neural net output layer \mathbf{p}

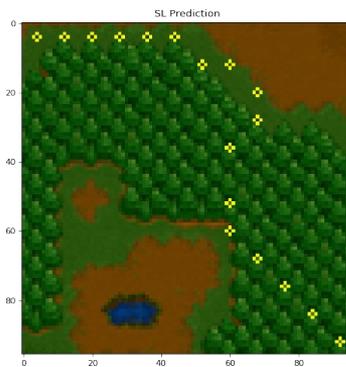
In general: #P-hard 😞

Do this probabilistic-logical reasoning during learning in a computation graph

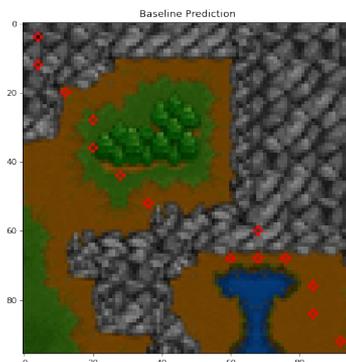
without constraint



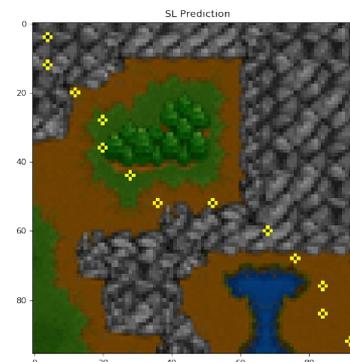
with constraint



without constraint



with constraint



ARCHITECTURE

EXACT MATCH

HAMMING SCORE

CONSISTENCY

RESNET-18+FIL

55.0

97.7

56.9

RESNET-18+ \mathcal{L}_{SL}

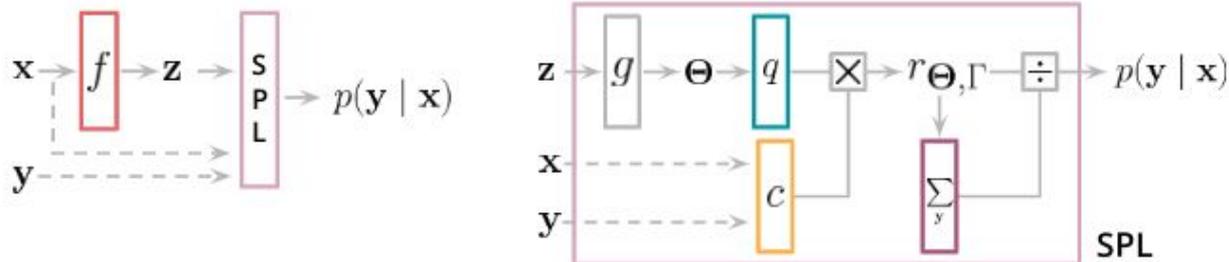
59.4

97.7

61.2

Semantic Probabilistic Layers

- How to give a 100% guarantee that Boolean constraints will be satisfied?
- Bake the constraint into the neural network as a special layer



- Secret sauce is tractable circuits – computation graphs for reasoning



GROUND TRUTH



RESNET-18



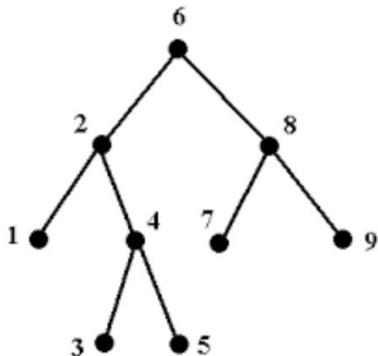
SEMANTIC LOSS



SPL (ours)

ARCHITECTURE	EXACT MATCH	HAMMING SCORE	CONSISTENCY
RESNET-18+FIL	55.0	97.7	56.9
RESNET-18+ \mathcal{L}_{SL}	59.4	97.7	61.2
RESNET-18+SPL	75.1	97.6	100.0
OVERPARAM. SDD	78.2	96.3	100.0

Hierarchical Multi-Label Classification

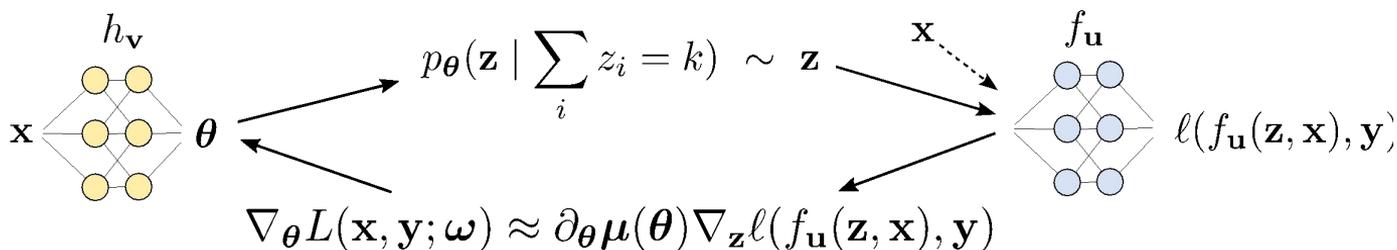


“if the image is classified as a dog, it must also be classified as an animal”

“if the image is classified as an animal, it must be classified as either cat or dog”

DATASET	EXACT MATCH	
	HMCNN	MLP+SPL
CELLCYCLE	3.05 ± 0.11	3.79 ± 0.18
DERISI	1.39 ± 0.47	2.28 ± 0.23
EISEN	5.40 ± 0.15	6.18 ± 0.33
EXPR	4.20 ± 0.21	5.54 ± 0.36
GASCH1	3.48 ± 0.96	4.65 ± 0.30
GASCH2	3.11 ± 0.08	3.95 ± 0.28
SEQ	5.24 ± 0.27	7.98 ± 0.28
SPO	1.97 ± 0.06	1.92 ± 0.11
DIATOMS	48.21 ± 0.57	58.71 ± 0.68
ENRON	5.97 ± 0.56	8.18 ± 0.68
IMCLEF07A	79.75 ± 0.38	86.08 ± 0.45
IMCLEF07D	76.47 ± 0.35	81.06 ± 0.68

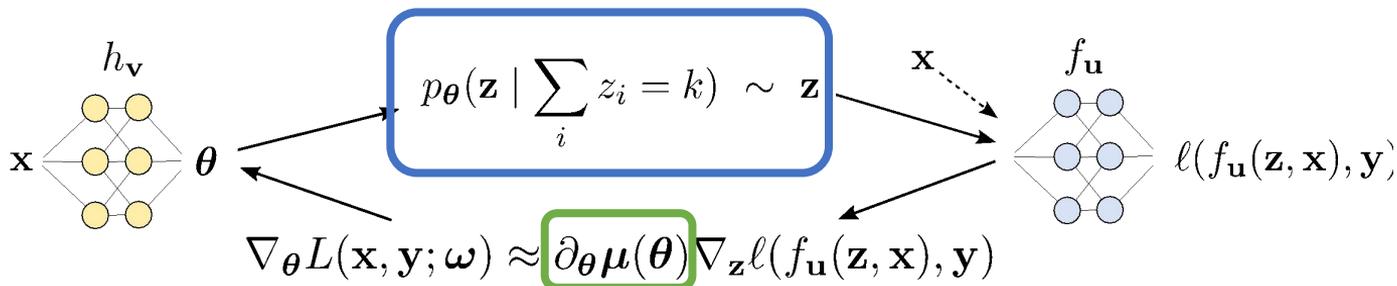
SIMPLE: Gradient Estimator for k -Subset Sampling



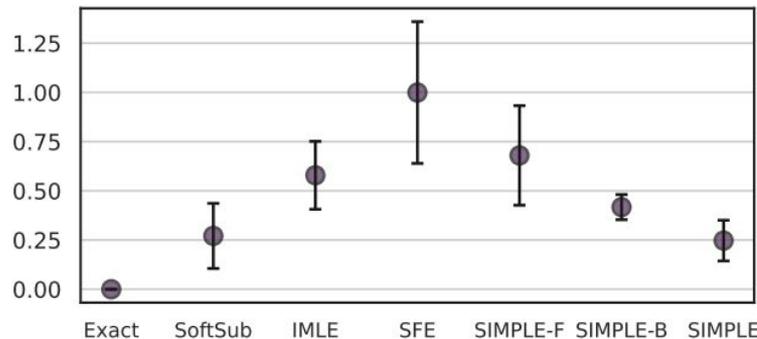
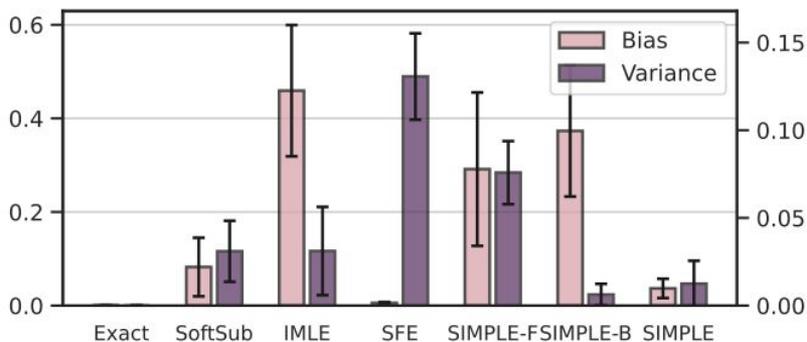
Example.
Learning to Explain (L2X)

Taste Score	Key Words ($k = 10$)
0.7	a lite bodied beer with a pleasant taste. was like a reddish color. a little like wood and caramel with a hop finish. has a sort of fruity flavor like grapes or cherry that is sort of buried in there. mouth feel was lite, sort of bubbly. not hard to down, though a bit harder then one would expect given the taste.

SIMPLE: Gradient Estimator for k -Subset Sampling



We achieve **lower bias and variance** by **exact, discrete samples** and **exact derivative of conditional marginals**.



Experiment: Learn to Explain (L2X)

Taste Score	Key Words ($k = 10$)
0.7	a lite bodied beer with a pleasant taste . was like a reddish color. a little like wood and caramel with a hop finish. has a sort of fruity flavor like grapes or cherry that is sort of buried in there. mouth feel was lite , sort of bubbly . not hard to down, though a bit harder then one would expect given the taste.

Results for three aspects with $k = 10$

Method	Appearance		Palate		Taste	
	Test MSE	Precision	Test MSE	Precision	Test MSE	Precision
SIMPLE (Ours)	2.35 ± 0.28	66.81 ± 7.56	2.68 ± 0.06	44.78 ± 2.75	2.11 ± 0.02	42.31 ± 0.61
L2X ($t = 0.1$)	10.70 ± 4.82	30.02 ± 15.82	6.70 ± 0.63	50.39 ± 13.58	6.92 ± 1.61	32.23 ± 4.92
SoftSub ($t = 0.5$)	2.48 ± 0.10	52.86 ± 7.08	2.94 ± 0.08	39.17 ± 3.17	2.18 ± 0.10	41.98 ± 1.42
I-MLE ($\tau = 30$)	2.51 ± 0.05	65.47 ± 4.95	2.96 ± 0.04	40.73 ± 3.15	2.38 ± 0.04	41.38 ± 1.55

Results for aspect Aroma, for k in {5, 10, 15}

Method	$k = 5$		$k = 10$		$k = 15$	
	Test MSE	Precision	Test MSE	Precision	Test MSE	Precision
SIMPLE (Ours)	2.27 ± 0.05	57.30 ± 3.04	2.23 ± 0.03	47.17 ± 2.11	3.20 ± 0.04	53.18 ± 1.09
L2X ($t = 0.1$)	5.75 ± 0.30	33.63 ± 6.91	6.68 ± 1.08	26.65 ± 9.39	7.71 ± 0.64	23.49 ± 10.93
SoftSub ($t = 0.5$)	2.57 ± 0.12	54.06 ± 6.29	2.67 ± 0.14	44.44 ± 2.27	2.52 ± 0.07	37.78 ± 1.71
I-MLE ($\tau = 30$)	2.62 ± 0.05	54.76 ± 2.50	2.71 ± 0.10	47.98 ± 2.26	2.91 ± 0.18	39.56 ± 2.07

Outline

1. The paradox of learning to reason from data

~~deep learning~~

2. **Architectures for Learning and Reasoning**

logical reasoning + deep learning

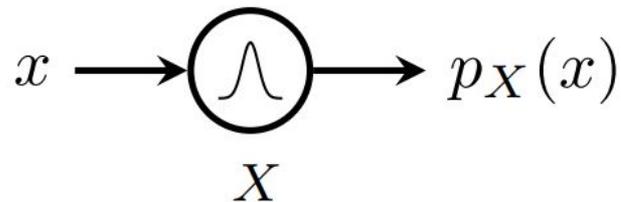
a. Constrained language generation

b. Constrained structured prediction

c. **Secret sauce: tractable circuits**

Probabilistic circuits

computational graphs that recursively define distributions



Simple distributions are tractable “black boxes” for:

- EVI: output $p(\mathbf{x})$ (density or mass)
- MAR: output 1 (normalized) or Z (unnormalized)
- MAP: output the mode

Probabilistic circuits

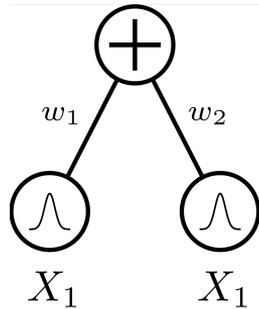
computational graphs that recursively define distributions



$\neg X$



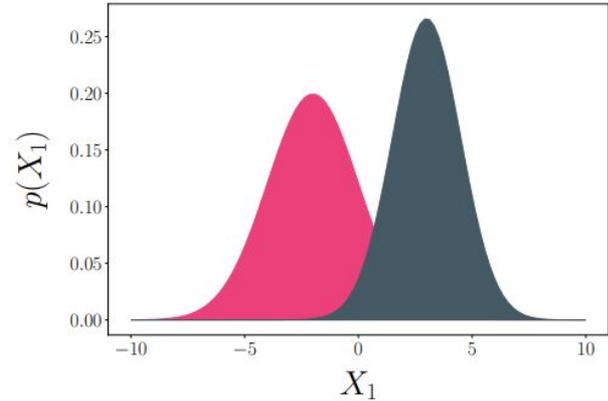
X_1



$$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$$

\Rightarrow

mixtures



$$p(X) = p(Z = \mathbf{1}) \cdot p_1(X|Z = \mathbf{1}) \\ + p(Z = \mathbf{2}) \cdot p_2(X|Z = \mathbf{2})$$

Probabilistic circuits

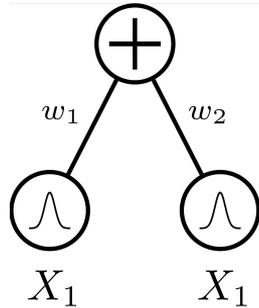
computational graphs that recursively define distributions



$\neg X$



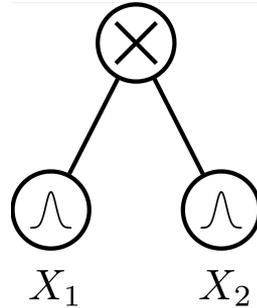
X_1



$$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$$

\Rightarrow

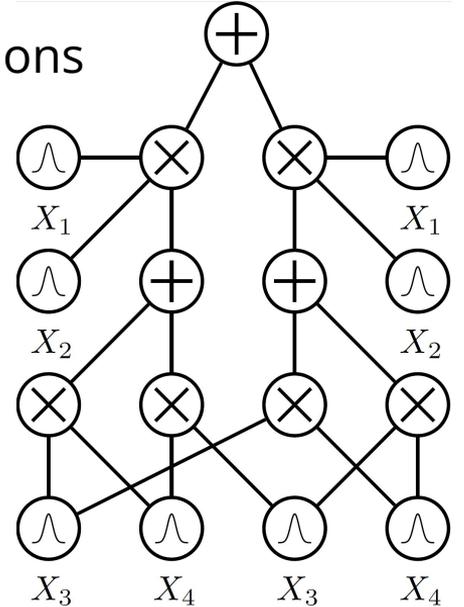
mixtures



$$p(X_1, X_2) = p(X_1) \cdot p(X_2)$$

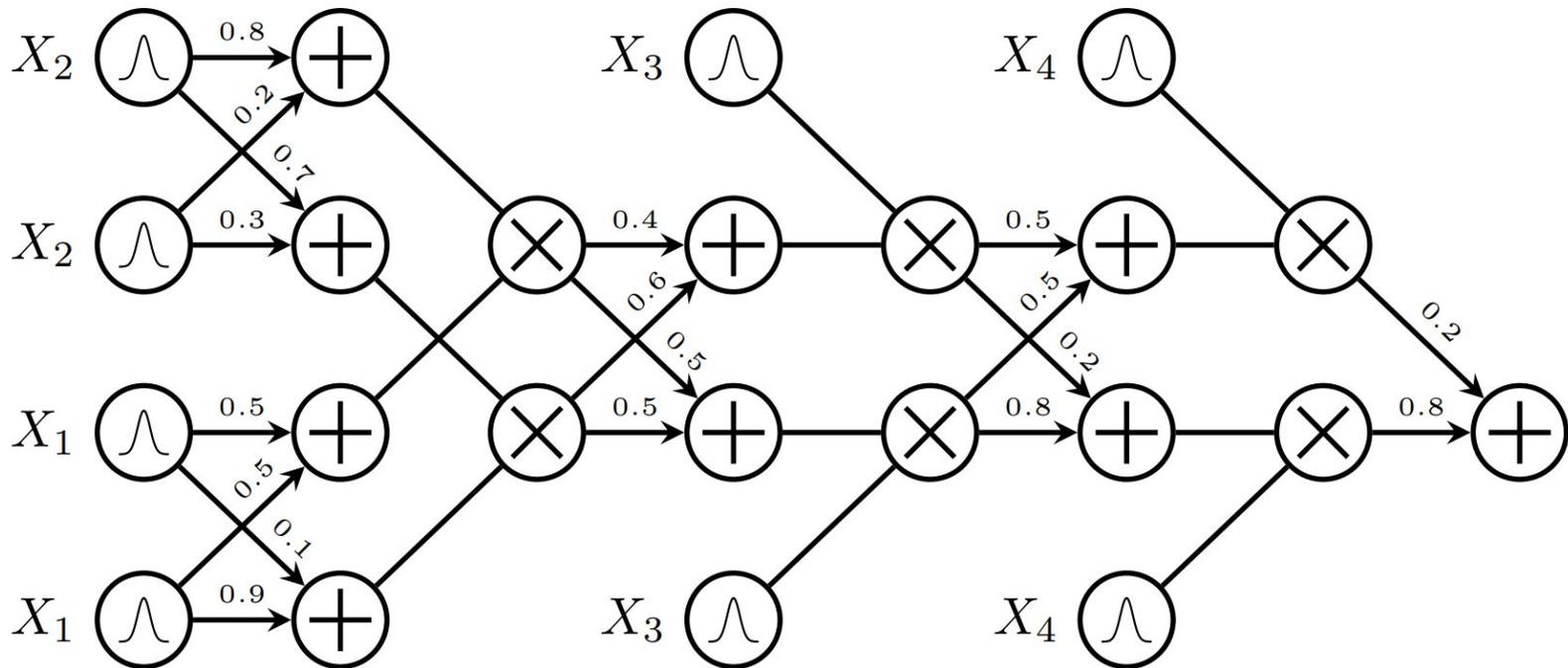
\Rightarrow

factorizations



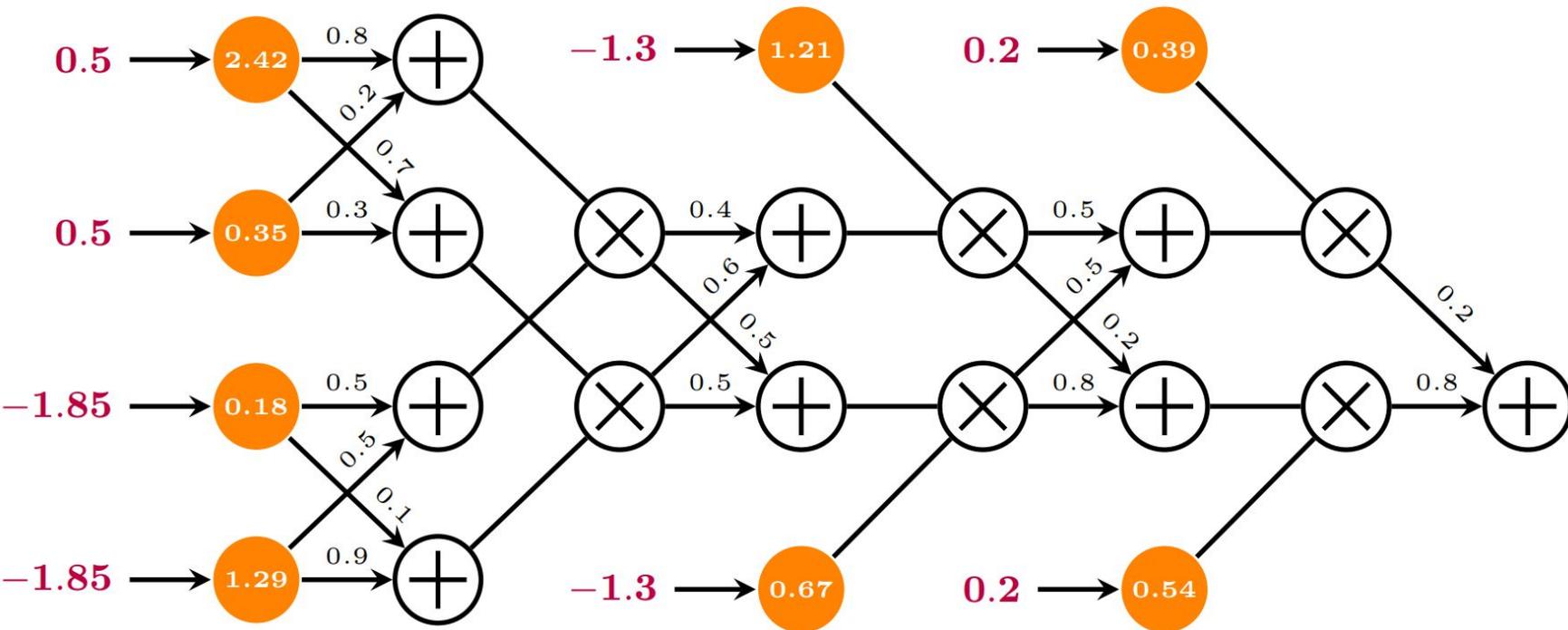
Likelihood

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



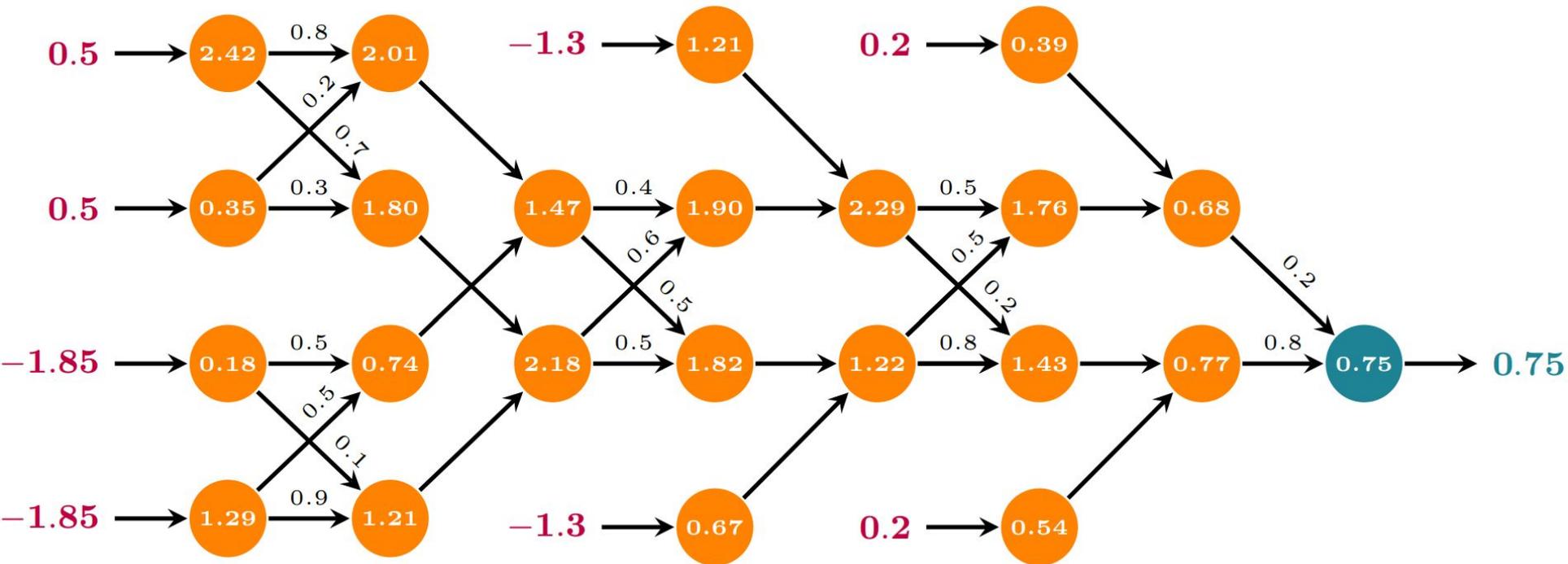
Likelihood

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Likelihood

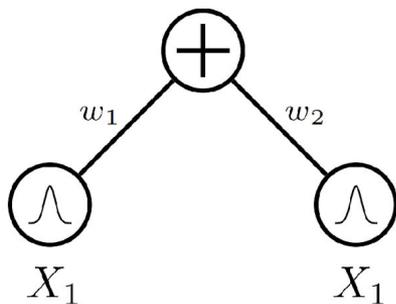
$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



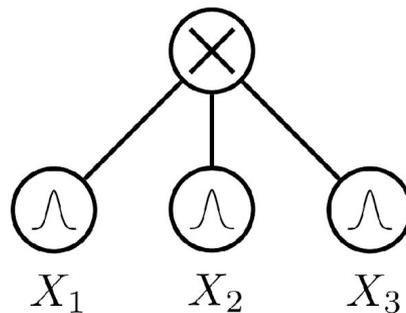
Tractable marginals

A sum node is *smooth* if its children depend on the same set of variables.

A product node is *decomposable* if its children depend on disjoint sets of variables.



smooth circuit



decomposable circuit

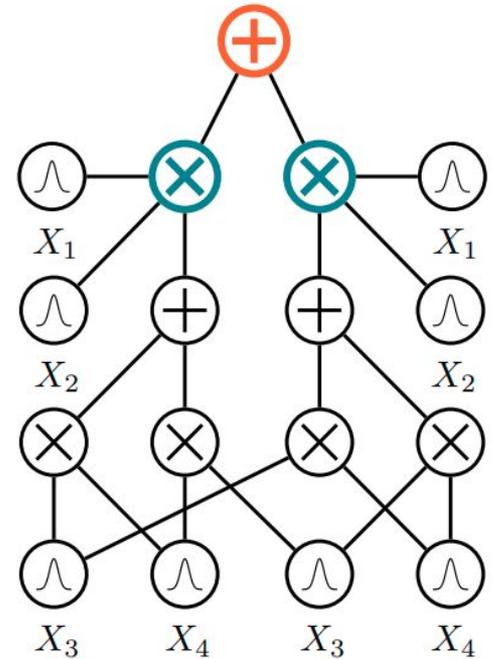
Smoothness + decomposability = tractable MAR

If $p(\mathbf{x}) = \sum_i w_i p_i(\mathbf{x})$, (**smoothness**):

$$\int p(\mathbf{x}) d\mathbf{x} = \int \sum_i w_i p_i(\mathbf{x}) d\mathbf{x} =$$

$$= \sum_i w_i \int p_i(\mathbf{x}) d\mathbf{x}$$

\Rightarrow integrals are "pushed down" to children

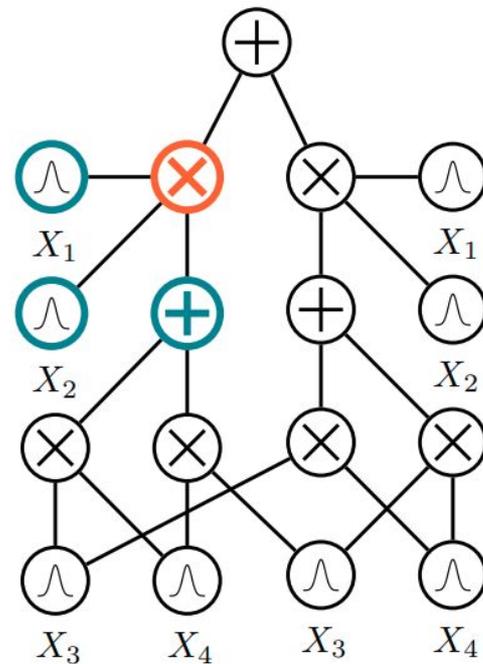


Smoothness + decomposability = tractable MAR

If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (**decomposability**):

$$\begin{aligned} & \int \int \int p(\mathbf{x}, \mathbf{y}, \mathbf{z}) dx dy dz = \\ &= \int \int \int p(\mathbf{x})p(\mathbf{y})p(\mathbf{z}) dx dy dz = \\ &= \int p(\mathbf{x}) dx \int p(\mathbf{y}) dy \int p(\mathbf{z}) dz \end{aligned}$$

\Rightarrow integrals decompose into easier ones



Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

\Rightarrow linear in circuit size!

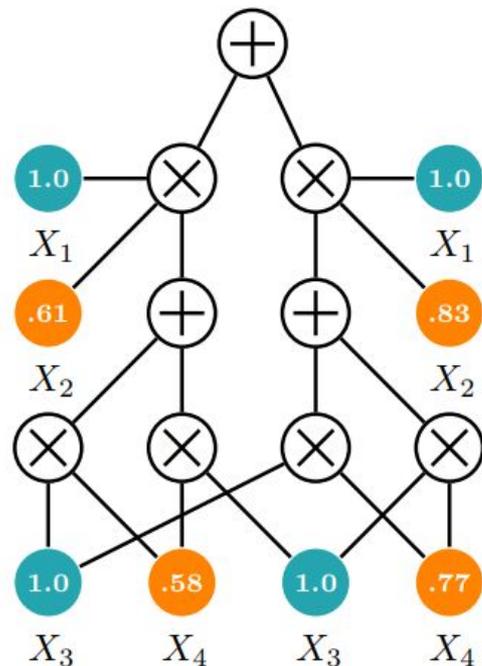
E.g. to compute $p(x_2, x_4)$:

leaves over X_1 and X_3 output $Z_i = \int p(x_i) dx_i$

\Rightarrow for normalized leaf distributions: 1.0

leaves over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)



Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

\Rightarrow linear in circuit size!

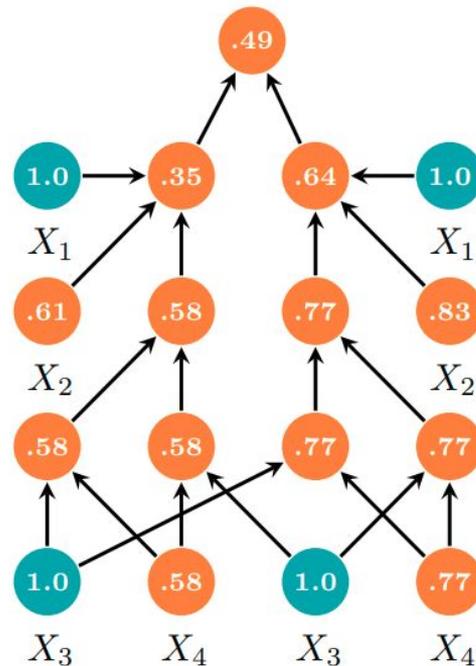
E.g. to compute $p(x_2, x_4)$:

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\Rightarrow for normalized leaf distributions: 1.0

leaves over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)



Learn more about probabilistic circuits?



Tutorial (3h)

Probabilistic Circuits

*Inference
Representations
Learning
Theory*

Antonio Vergari
University of California, Los Angeles

Robert Peharz
TU Eindhoven

YooJung Choi
University of California, Los Angeles

Guy Van den Broeck
University of California, Los Angeles

September 14th, 2020 - Ghent, Belgium - ECML-PKDD 2020

<https://youtu.be/2RAG5-L9R70>

Overview Paper (80p)

Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Models*

YooJung Choi
Antonio Vergari
Guy Van den Broeck
*Computer Science Department
University of California
Los Angeles, CA, USA*

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1	Introduction	3
2	Probabilistic Inference: Models, Queries, and Tractability	4
2.1	Probabilistic Models	5
2.2	Probabilistic Queries	6
2.3	Tractable Probabilistic Inference	8
2.4	Properties of Tractable Probabilistic Models	9

<http://starai.cs.ucla.edu/papers/ProbCirc20.pdf>

Outline

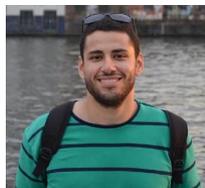
1. The paradox of learning to reason from data
deep learning
2. Architectures for Learning and Reasoning
logical (and probabilistic) reasoning + deep learning
 - a. Constrained language generation
 - b. Constrained structured prediction
 - c. Secret sauce: tractable circuits

Thanks

This was the work of many wonderful students/postdocs/collaborators!



Honghua



Kareem



Zhe



Meihua



Anji

References: <http://starai.cs.ucla.edu/publications/>