



logically-consistent deep learning via probabilistic circuits

antonio vergari (he/him)

 @tetraduzione

17th Oct 2024 - **PICS PhD School** - Copenhagen

probabilistic circuits (PCs)

A grammar for tractable computational graphs

1. *A simple tractable function is a circuit*

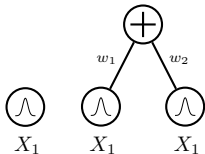
\Rightarrow *e.g., a multivariate Gaussian, or a logical literal*

\bigwedge
 X_1

probabilistic circuits (PCs)

A grammar for tractable computational graphs

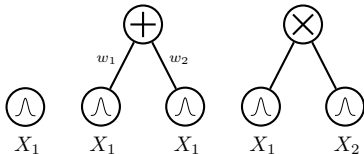
- I. *A simple tractable function is a circuit*
- II. *A weighted combination of circuits is a circuit*



probabilistic circuits (PCs)

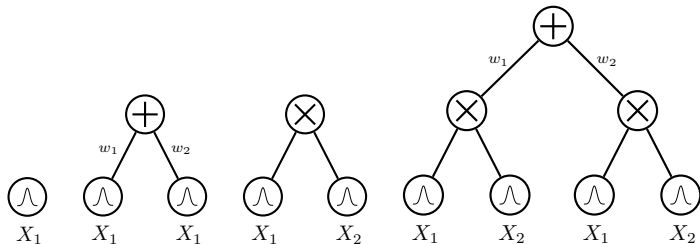
A grammar for tractable computational graphs

- I. A simple tractable function is a circuit
- II. A weighted combination of circuits is a circuit
- III. A product of circuits is a circuit



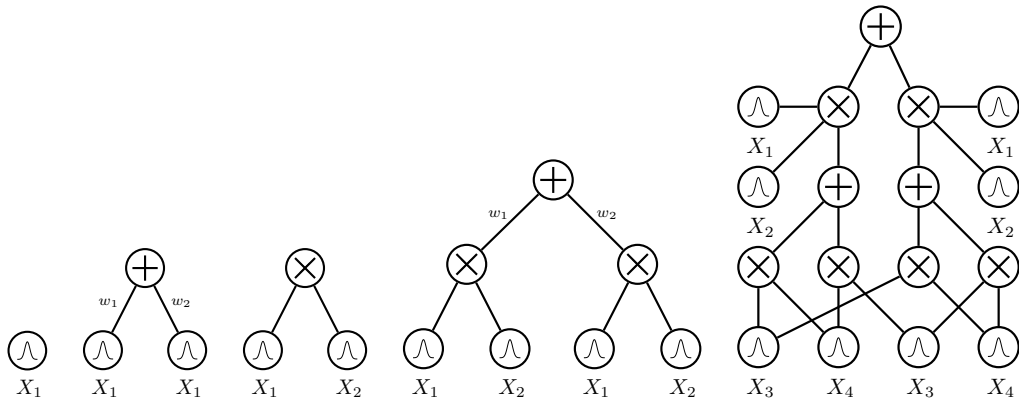
probabilistic circuits (PCs)

A grammar for tractable computational graphs



probabilistic circuits (PCs)

A grammar for tractable computational graphs



structural properties

smoothness

decomposability

compatibility

determinism

structural properties

smoothness

decomposability

compatibility

determinism

structural properties

smoothness

decomposability

compatibility

determinism

structural properties

smoothness

decomposability

compatibility

determinism

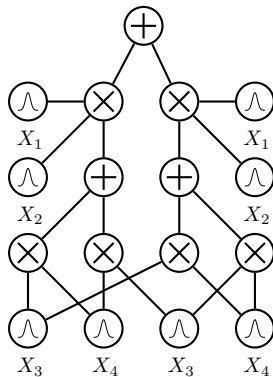
$$\text{determinism} + \text{decomposability} = \text{tractable MAP}$$

Computing maximization with arbitrary evidence \mathbf{e}

\Rightarrow *linear in circuit size!*

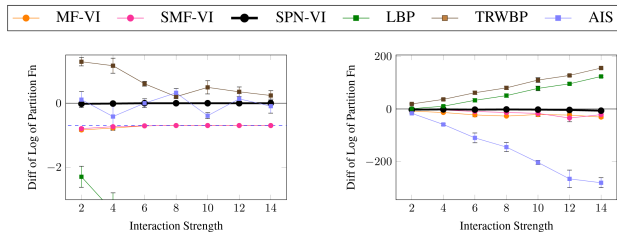
E.g., suppose we want to compute:

$$\max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e})$$



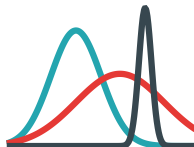
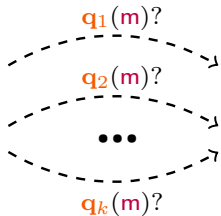
$$\text{determinism} + \text{decomposability} = \text{tractable ELBO}$$

Using deterministic and decomposable PCs as expressive variational family Q for discrete polynomial log-densities, i.e. $\operatorname{argmax}_{q \in Q} \mathbb{E}_{\mathbf{x} \sim q} [\log w(\mathbf{x})] + \mathbb{H}(q)$



Closed-form computation for the entropy \mathbb{H} [Vergari et al. 2021]

Shih and Ermon, "Probabilistic Circuits for Variational Inference in Discrete Graphical Models", *NeurIPS, 2020*



$p_m(\mathbf{X})$

\approx

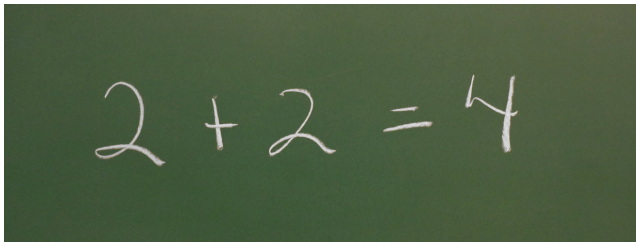
	X^1	X^2	X^3	X^4	X^5
x_8					
x_7					
x_6					
x_5					
x_4					
x_3					
x_2					
x_1					

generative models that can reason probabilistically

...but some events are certain!

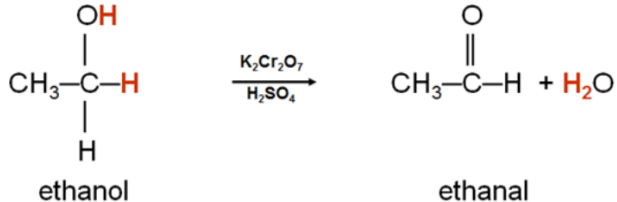
math reasoning

and logical deduction

A photograph of a chalkboard with the equation $2 + 2 = 4$ written in white chalk. The numbers and symbols are written in a simple, slightly cursive hand.

Constraints: carrying out arithmetic tasks, but also ***proving theorems***

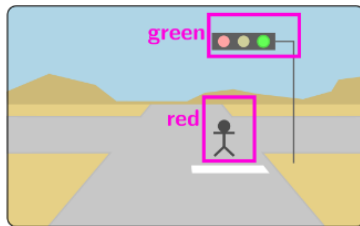
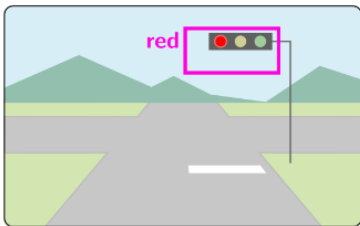
physics laws



Constraints: preserving #atoms, #electrons (RedOx), ...in chemical reactions

AI safety

$$K_1 = (\text{pedestrian} \vee \text{red} \Rightarrow \text{stop})$$



Constraints: traffic rules, scene understanding (objects do not disappear) ...

Marconato et al., "Not all neuro-symbolic concepts are created equal: Analysis and mitigation of reasoning shortcuts", NeurIPS, 2023

***“but how bad
are purely neural models
when dealing with
hard constraints
in the real world?”***

code understanding

Reference

```
def find_length(string, n):  
    current_sum = 0  
    max_sum = 0  
    for i in range(n):  
        current_sum += (1 if string[i] == '0'  
            ↪ else -1)  
        if current_sum < 0:  
            current_sum = 0  
        max_sum = max(current_sum, max_sum)  
    return max_sum if max_sum else 0
```

Transformed

```
def find_length(string, n):  
    current_sum = 0  
    max_sum = 0  
    for i in range(n):  
        current_sum += (1 if string[i] != '0'  
            ↪ else -1)  
        if current_sum < 0:  
            current_sum = 0  
        max_sum = max(current_sum, max_sum)  
    return max_sum if max_sum else 0
```

Model	Prediction
Llama2-7B	YES ✖
Llama2-13B	YES ✖
CodeLlama-7B	YES ✖
CodeLlama-13B	YES ✖
CodeLlama-34B	YES ✖
StarCoder2-3B	YES ✖
StarCoder2-7B	YES ✖
StarCoder2-15B	YES ✖

what about valid molecules?

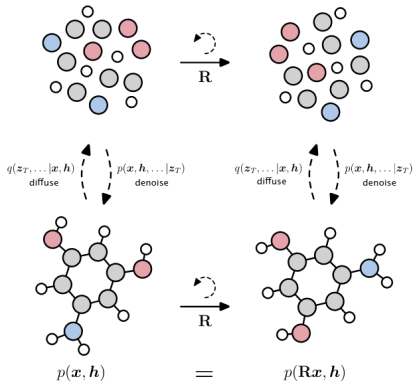
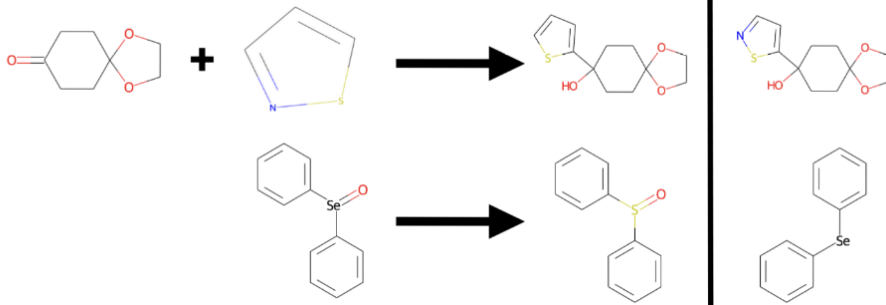


Table 2. Validity and uniqueness over 10000 molecules with standard deviation across 3 runs. Results marked (*) are not directly comparable, as they do not use 3D coordinates to derive bonds.

H: model hydrogens explicitly

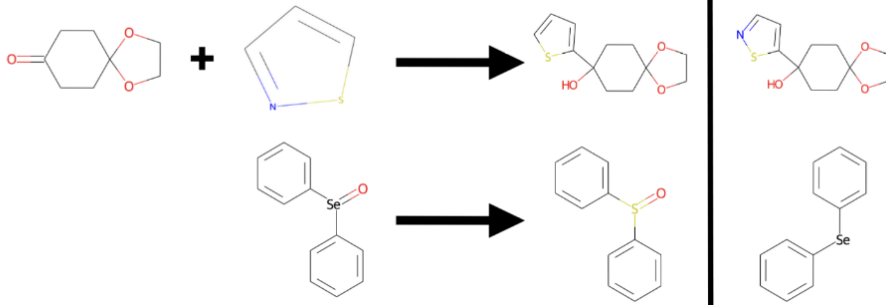
Method	H	Valid (%)	Valid and Unique (%)
Graph VAE (*)		55.7	42.3
GTVAE (*)		74.6	16.8
Set2GraphVAE (*)		59.9 \pm 1.7	56.2 \pm 1.4
EDM (ours)		97.5\pm0.2	94.3\pm0.2
E-NF	✓	40.2	39.4
G-Schnet	✓	85.5	80.3
GDM-aug	✓	90.4	89.5
EDM (ours)	✓	91.9\pm0.5	90.7\pm0.6
Data	✓	97.7	97.7

and valid reactions?



"deep learning is doing alchemy"

and valid reactions?



CHEMALGEBRA: ALGEBRAIC REASONING BY
PREDICTING CHEMICAL REACTIONS

planning

Can Large Language Models Reason and Plan?

Subbarao Kambhampati
School of Computing & Augmented Intelligence
Arizona State University
email: rao@asu.edu

Spoiler: *"To summarize, nothing that I have read, verified, or done gives me any compelling reason to believe that LLMs do reasoning/planning, as normally understood.."*

logical inconsistency

 = LLaMa 2 = LoCo-LLaMa 2

LLMs confabulate and contradict themselves ¹

¹<https://github.com/SuperBruceJia/Awesome-LLM-Self-Consistency>

Logically Consistent Language Models via Neuro-Symbolic Integration

Diego Calanzone*

DISI, University of Trento

`diego.calanzone@studenti.unitn.it`

Stefano Teso



CIMeC & DISI, University of Trento

`stefano.teso@unitn.it`

Antonio Vergari



School of Informatics, University of Edinburgh

`avergari@ed.ac.uk`

Goal

***“How can neural nets
reason and learn with
symbolic constraints
reliably and efficiently?”***

the issues!

I) Logical constraints can be hard to represent in a unified way

⇒ ***a single framework** for implications, negation, paths, hierarchies, ...*

II) How to integrate logic and probabilities in a single architecture

⇒ ***combining soft and hard constraints***

III) Logical constraints are piecewise constant functions!

⇒ *differentiable almost everywhere but **gradient is zero!***

the issues!

I) Logical constraints can be hard to represent in a unified way

⇒ ***a single framework** for implications, negation, paths, hierarchies, ...*

II) How to integrate logic and probabilities in a single architecture

⇒ ***combining soft and hard constraints***

III) Logical constraints are piecewise constant functions!

⇒ *differentiable almost everywhere but **gradient is zero!***

the issues!

I) Logical constraints can be hard to represent in a unified way

⇒ ***a single framework** for implications, negation, paths, hierarchies, ...*

II) How to integrate logic and probabilities in a single architecture

⇒ ***combining soft and hard constraints***

III) Logical constraints are piecewise constant functions!

⇒ *differentiable almost everywhere but **gradient is zero!***

hard vs soft constraints

logic vs probabilities

logic

“If X is a bird, X flies”

$$A(X) \implies B(X)$$

prob logic

“If X is a bird, X might fly”

$$p(A(X) \implies B(X))$$

which logic?

or which kind of constraints to represent?

propositional logic (zeroth-order)

$$(a \wedge b) \vee d \implies c$$

first-order logic (FOL)

$$\forall a \exists b : R(a, b) \vee Q(d) \implies C(x)$$

satisfiability modulo theory (SMT)

which logic?

or which kind of constraints to represent?

propositional logic (zeroth-order)

$$(a \wedge b) \vee d \implies c$$

first-order logic (FOL)

$$\forall a \exists b : R(a, b) \vee Q(d) \implies C(x)$$

satisfiability modulo theory (SMT)

which logical consistency?

factuality



we know that some facts f in a KB are true.

f_1 : "an albatross is a bird"

how to query an LLM?

$$p_{\theta}(z_f = \top) = p_{\theta}(x_t = \ell_{\text{true}} \mid x_1, \dots, x_{t-1} = \text{"Is an albatross a bird?"})$$

which logical consistency?

negation

Negation

$A \oplus \bar{A}$


A: (computer, IsA, airplane)

\bar{A} : (computer, IsNotA, airplane)

Is a computer a airplane? 



No.

Is it true that a computer is not a airplane? 



No.

Logical:  Factual: 



Yes.

Logical:  Factual: 

if we know the following fact

f : "an albatross is a bird"

and what to query the truth value $z_{\tilde{f}}$ of

\tilde{f} : "an albatross is **not** a bird"

because f is the **negation** of \tilde{f} :

$$z_f \oplus z_{\tilde{f}} \iff (z_f \wedge \neg z_{\tilde{f}}) \vee (\neg z_f \wedge z_{\tilde{f}})$$

we expect the answer to be that \tilde{f} is **false**.

which logical consistency?

implication

= LoCo-LLaMa 2
= LLaMa 2


Forward Implication
 $A \rightarrow \neg B$
A: (albatross, isA, bird)
B: (albatross, isA, fish)

Is an albatross a bird?

 Yes.

Is an albatross a fish?

 **Yes.** Logical:  Factual: 

 No. Logical:  Factual: 

if we know the following fact

f_1 : "an albatross is a bird"

and what to query the truth value z_{f_2} of

f_2 : "an albatross is an animal"

because f_1 **implies** f_2 :

$$(z_{f_1} \rightarrow z_{f_2}) \iff (\neg z_{f_1} \vee z_{f_2})$$

we expect the answer to be that f_2 is **true**.

which logical consistency?

reverse implication

Reverse Implication

$\neg B \rightarrow \neg A$ B: (albatross, IsNotA, organism)
A: (albatross, IsNotA, living thing)

Is it true that an albatross is
not an organism?



No.

Is it true that an albatross is
not a living thing?



Yes.

Logical: ✗ Factual: ✗



No.

Logical: ✓ Factual: ✓

we can **reverse an implication**

$$z_{\tilde{f}_2} \rightarrow z_{\tilde{f}_1}$$

where \tilde{f}_2 : "an albatross is **not** an animal"

and we ask if the following is true

\tilde{f}_1 : "an albatross is **not** a bird"

we expect the answer to be that \tilde{f}_1 is **true**.

how

to enforce constraints?

$$\max p_{\theta}(\mathbf{K}_i)$$

maximise the probability of the constraint to hold!

*Xu et al., "A Semantic Loss Function for Deep Learning with Symbolic Knowledge",
Proceedings of the 35th International Conference on Machine Learning (ICML), 2018*

how

to enforce constraints?

$$\min \mathcal{L}(\mathbf{K}_i, p_\theta) = \min -\log \sum_{\mathbf{z} \models \mathbf{K}_i} \prod_{j: \mathbf{z} \models z_{f_j}} p_\theta(z_{f_j}) \prod_{j: \mathbf{z} \models \neg z_{f_j}} (1 - p_\theta(z_{f_j}))$$

minimize the semantic loss

*Xu et al., "A Semantic Loss Function for Deep Learning with Symbolic Knowledge",
Proceedings of the 35th International Conference on Machine Learning (ICML), 2018*

computing the probability of logical formulas

$$p_{\theta}(\mathbf{K}(\mathbf{z})) = \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\mathbb{1}\{\mathbf{z} \models \mathbf{K}\}]$$

computing the probability of \mathbf{K}

WMC

computing the probability of logical formulas

$$\mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\mathbb{1}\{\mathbf{z} \models K\}] = \sum_{\mathbf{z}} p(\mathbf{z}) \mathbb{1}\{\mathbf{z} \models K\} = \sum_{\mathbf{z} \models K} p(\mathbf{z})$$

computing the **weighted model count** (WMC) of K

computing the probability of logical formulas

$$\mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\mathbb{1}\{\mathbf{z} \models \mathbf{K}\}] = \sum_{\mathbf{z} \models \mathbf{K}} \prod_{i: \mathbf{z} \models z_i} p(z_i) \prod_{i: \mathbf{z} \models \neg z_i} (1 - p(z_i))$$

assuming independence of \mathbf{z} (but be careful!)²

²van Krieken et al., “On the Independence Assumption in Neurosymbolic Learning”, 2024
Xu et al., “A Semantic Loss Function for Deep Learning with Symbolic Knowledge”,
Proceedings of the 35th International Conference on Machine Learning (ICML), 2018

computing the probability of logical formulas

$$\mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\mathbb{1}\{\mathbf{z} \models \mathbf{K}\}] = \sum_{\mathbf{z} \models \mathbf{K}} \prod_{i: \mathbf{z} \models z_i} p(z_i) \prod_{i: \mathbf{z} \models \neg z_i} (1 - p(z_i))$$

computing WMC is #P-hard in general : (

more complex constraints

EntailmentBank

$$(z_{f_1} \wedge z_{f_2} \rightarrow z_{f_3}) \wedge z_{f_4} \rightarrow z_{f_5}$$

f_1 : "melting is a kind of phase change"

f_2 : "the ice melts"

f_3 : "the ice undergoes a phase change"

f_4 : "phase changes do not change mass"

f_5 : "the mass of the ice will not change"

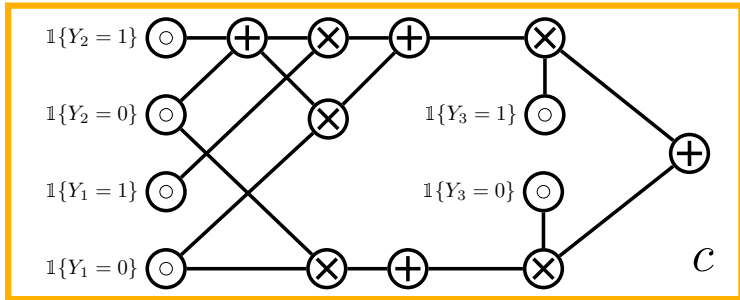
Goal

***Can we encode K
to yield a tractable WMC?***

Goal

***Can we encode K
to yield a tractable WMC?
yes, as a **circuit**!***

semantic loss



compiling logical formulas into circuits

knowledge compilation

$$K : (Y_1 = 1 \implies Y_3 = 1)$$

$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$

$$\mathbb{1}\{Y_1 = 0\} \odot$$

$$\mathbb{1}\{Y_1 = 1\} \odot$$

$$\mathbb{1}\{Y_2 = 0\} \odot$$

$$\mathbb{1}\{Y_2 = 1\} \odot$$

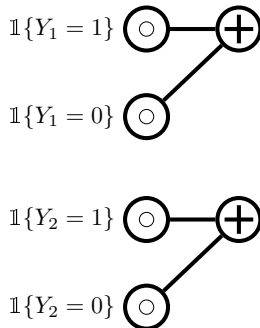
$$\mathbb{1}\{Y_3 = 0\} \odot$$

$$\mathbb{1}\{Y_3 = 1\} \odot$$

knowledge compilation

$$K : (Y_1 = 1 \implies Y_3 = 1)$$

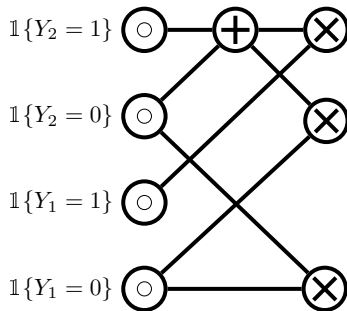
$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$



knowledge compilation

$$K : (Y_1 = 1 \implies Y_3 = 1)$$

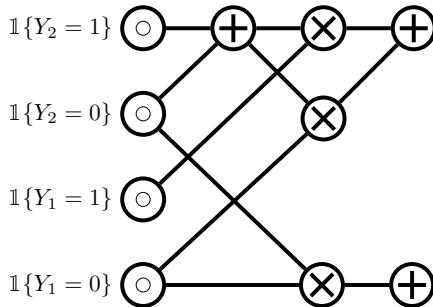
$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$



knowledge compilation

$$K : (Y_1 = 1 \implies Y_3 = 1)$$

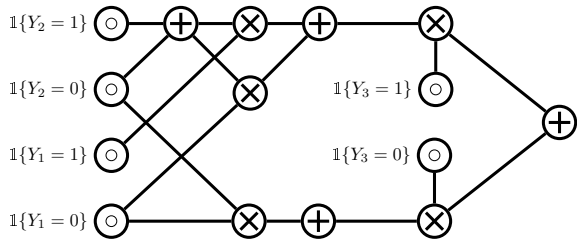
$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$



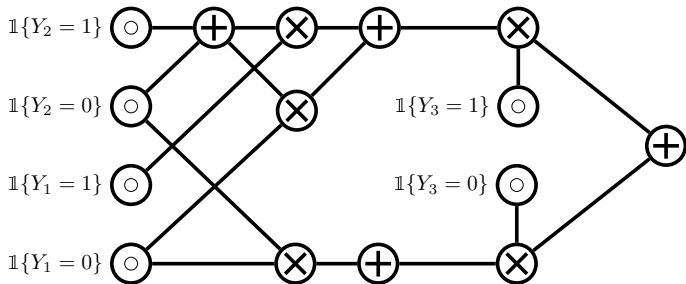
knowledge compilation

$$K : (Y_1 = 1 \implies Y_3 = 1)$$

$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$



tractable WMC



exactly compute **WMC** in time $O(|c|)$

SL recipe

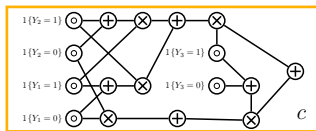
$$K : (Y_1 = 1 \implies Y_3 = 1)$$

$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$

1) Take a
logical constraint

SL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$

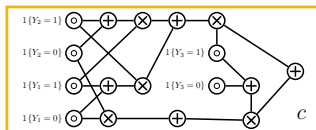


1) Take a
logical constraint

2) Compile it into
a constraint circuit

SL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$



1) Take a
logical constraint

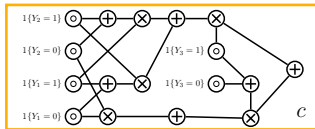
2) Compile it into
a constraint circuit

$$-\log \text{WMC}(K_i, p_\theta)$$

3) minimize the semantic loss

SL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$



$$-\log \text{WMC}(K_i, p_\theta)$$

1) Take a
logical constraint

2) Compile it into
a constraint circuit

3) minimize the semantic loss

4) train end-to-end by sgd!

MODEL	TRAIN	PPL	CONSISTENCY			SELF-CONSISTENCY			AVG
			FAC	IMP	REV	NEG	IMP	REV	
LLAMA-2-7B ZERO SHOT		62.41	0.39	0.52	0.13	0.42	0.30	0.15	0.32
LLAMA-2-7B FEW SHOT		52.30	0.53	0.71	0.34	0.38	0.48	0.47	0.48
LLAMA-2-7B CoT		52.30	0.52	0.64	0.67	0.40	0.64	0.67	0.59
LLAMA-2-70B ZERO SHOT		44.90	0.47	0.69	0.81	0.13	0.31	0.91	0.55
LLAMA-2-7B + XENT	T1+T2	116.85	0.25	0.46	0.01	0.07	0.81	0.01	0.27
LoCo-LLAMA-2-7B (NEG)	T1	62.21	0.44	0.65	0.43	0.96	0.28	0.36	0.52
LoCo-LLAMA-2-7B (F-IMP)	T1	67.15	0.99	0.99	0.07	0.00	0.99	0.07	0.51
LoCo-LLAMA-2-7B (SUPER)	T1	62.23	0.74	0.77	0.77	0.87	0.71	0.77	0.77

greatly improving (self-)consistency

evaluate on unseen constraints

EntailmentBank

$$(z_{f_1} \wedge z_{f_2} \rightarrow z_{f_3}) \wedge z_{f_4} \rightarrow z_{f_5}$$

f_1 : "melting is a kind of phase change"

f_2 : "the ice melts"

f_3 : "the ice undergoes a phase change"

f_4 : "phase changes do not change mass"

f_5 : "the mass of the ice will not change"

MODEL	DEPTH				
	1	2	3	4	5
LLAMA-2-7B	0.87	0.76	0.59	0.61	0.63
LoCo-LLAMA-2-7B (NEG)	0.51	0.51	0.51	0.52	0.52
LoCo-LLAMA-2-7B (F-IMP)	0.98	0.98	0.98	0.98	0.98
LoCo-LLAMA-2-7B (SUPER)	0.69	0.68	0.68	0.68	0.69

finetune on BeliefBank, test on EntailmentBank

nice...

...but!

assuming facts to be independent...

nice...

...but!

assuming facts to be independent...

***no guarantees to satisfy
constraints at test time...***

nice...

...but!

assuming facts to be independent...

***no guarantees to satisfy
constraints at test time...***

WMC

on the independence assumption

$$K : \neg \textcolor{red}{r} \vee \neg \textcolor{green}{g}$$

*a neural net should not output that a traffic light is both **red** and **green***

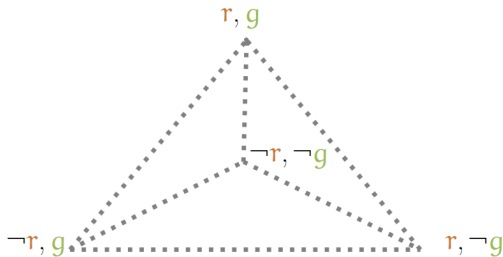


WMC

on the independence assumption

$$K : \neg \mathbf{r} \vee \neg \mathbf{g}$$

a neural net should not output that a traffic light is both **red** and **green**



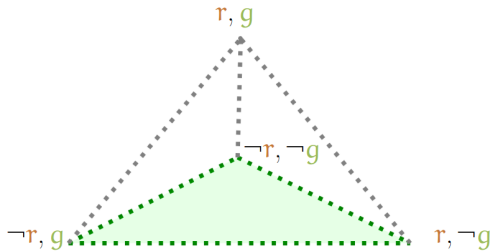
WMC

on the independence assumption

$$K : \neg \mathbf{r} \vee \neg \mathbf{g}$$

a neural net should not output that a traffic light is both **red** and **green**

only some probability assignments should be non-zero (lower triangle)



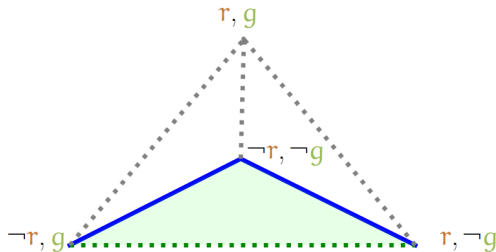
WMC

on the independence assumption

$$K : \neg \mathbf{r} \vee \neg \mathbf{g}$$

a neural net should not output that a traffic light is both **red** and **green**

but assuming $p(\mathbf{r}, \mathbf{g}) = p(\mathbf{r})p(\mathbf{g})$ restricts this even further (only blue lines)



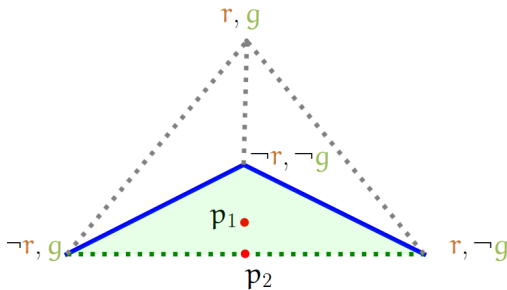
WMC

on the independence assumption

$$K : \neg \mathbf{r} \vee \neg \mathbf{g}$$

a neural net should not output that a traffic light is both **red** and **green**

but assuming $p(\mathbf{r}, \mathbf{g}) = p(\mathbf{r})p(\mathbf{g})$ restricts this even further (only blue lines)



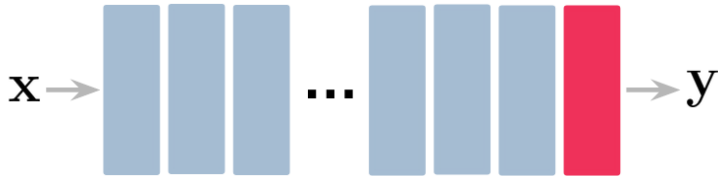
nice...

...but!

assuming facts to be independent...

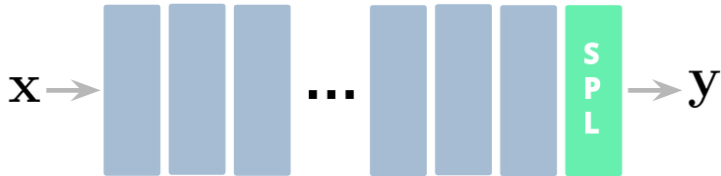
***no **guarantees** to satisfy
constraints at test time...***

how to



make any neural network architecture...

how to



...guarantee all predictions to conform to constraints?

When?



Ground Truth

e.g. predict shortest path in a map

When?



Ground Truth

given x // e.g. a tile map

nesy structured output prediction (SOP) tasks

When?



Ground Truth

given \mathbf{x} // e.g. a tile map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid

nesy structured output prediction (SOP) tasks

When?



Ground Truth

given \mathbf{x} // e.g. a tile map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid
s.t. $\mathbf{y} \models K$ // e.g., that form a valid path

nesy structured output prediction (SOP) tasks

When?



Ground Truth

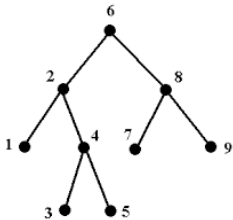
given \mathbf{x} // e.g. a tile map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid
s.t. $\mathbf{y} \models K$ // e.g., that form a valid path

// for a 12×12 grid, 2^{144} states but only 10^{10} valid ones!

nesy structured output prediction (SOP) tasks

When?



given \mathbf{x} // e.g. a feature map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. labels of classes

s.t. $\mathbf{y} \models \mathbf{K}$ // e.g., constraints over superclasses

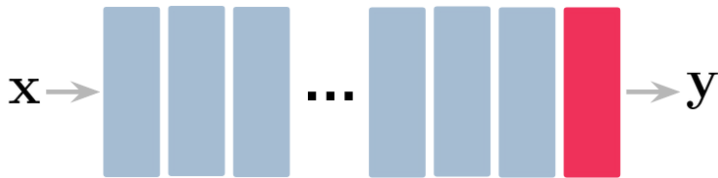
$$\mathbf{K} : (Y_{\text{cat}} \implies Y_{\text{animal}}) \wedge (Y_{\text{dog}} \implies Y_{\text{animal}})$$

hierarchical multi-label classification

How?

***“which neural network
architecture
to use?”***

e.g.,



sigmoid linear layers

$$p(\mathbf{y} \mid \mathbf{x}) = \prod_{i=1}^N p(y_i \mid \mathbf{x})$$

When?



Ground Truth



ResNet-18

neural nets struggle to satisfy validity constraints!

Constraint losses



Ground Truth



ResNet-18



Semantic Loss

...but cannot guarantee consistency at test time!

SPL



Ground Truth



ResNet-18



Semantic Loss



SPL (ours)

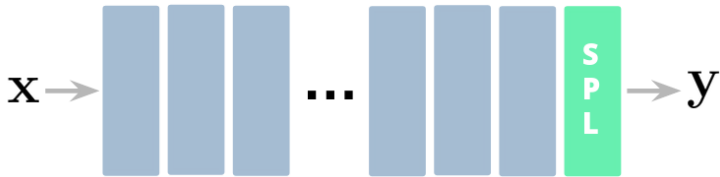
you can predict valid paths 100% of the time!

How?

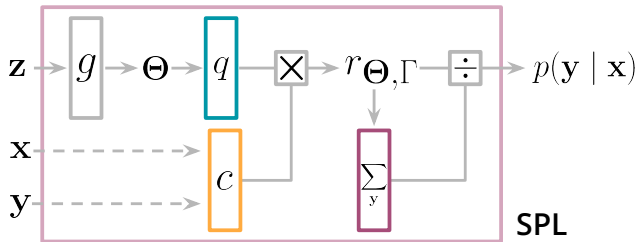


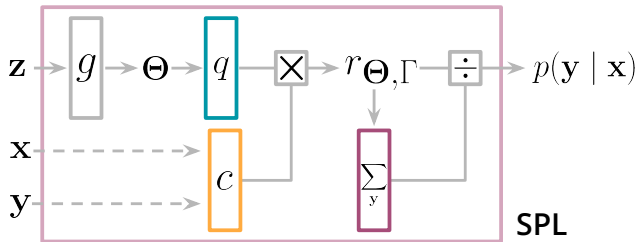
take an unreliable neural network architecture...

How?



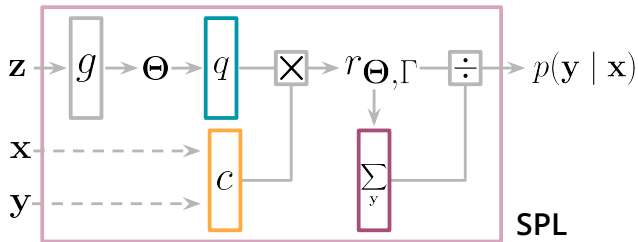
***.....and replace the last layer with
a semantic probabilistic layer***





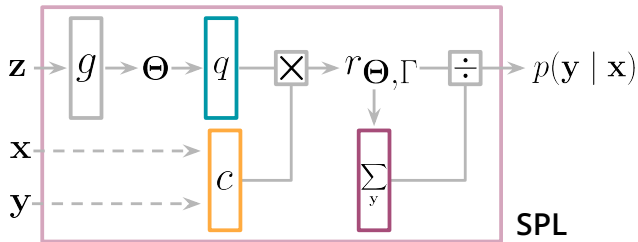
$$p(\mathbf{y} \mid \mathbf{x}) = \mathbf{q}_{\Theta}(\mathbf{y} \mid g(\mathbf{z}))$$

$\mathbf{q}_{\Theta}(\mathbf{y} \mid g(\mathbf{z}))$ is an expressive distribution over labels



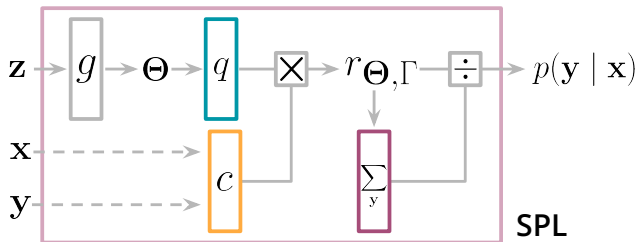
$$p(\mathbf{y} \mid \mathbf{x}) = \mathbf{q}_{\Theta}(\mathbf{y} \mid g(\mathbf{z})) \cdot \mathbf{c}_{\mathbf{K}}(\mathbf{x}, \mathbf{y})$$

$\mathbf{c}_{\mathbf{K}}(\mathbf{x}, \mathbf{y})$ encodes the constraint $\mathbb{1}\{\mathbf{x}, \mathbf{y} \models \mathbf{K}\}$



$$p(y | x) = q_{\Theta}(y | g(z)) \cdot c_K(x, y)$$

a product of experts : (



$$p(\mathbf{y} \mid \mathbf{x}) = \mathbf{q}_{\Theta}(\mathbf{y} \mid g(\mathbf{z})) \cdot \mathbf{c}_{\mathbf{K}}(\mathbf{x}, \mathbf{y}) / \mathbf{Z}(\mathbf{x})$$

$$\mathbf{Z}(\mathbf{x}) = \sum_{\mathbf{y}} \mathbf{q}_{\Theta}(\mathbf{y} \mid \mathbf{x}) \cdot \mathbf{c}_{\mathbf{K}}(\mathbf{x}, \mathbf{y})$$

Goal

*Can we design q and c
to be **expressive models**
yet yielding a tractable product?*

Goal

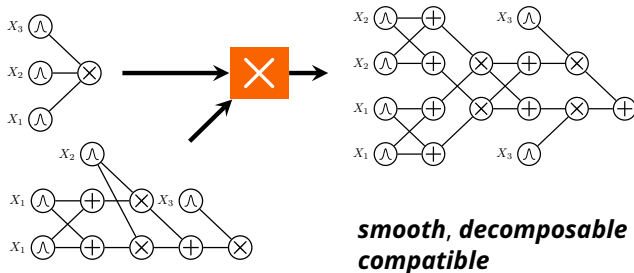
*Can we design q and c
to be **deep computational graphs**
yet yielding a tractable product?*

Goal

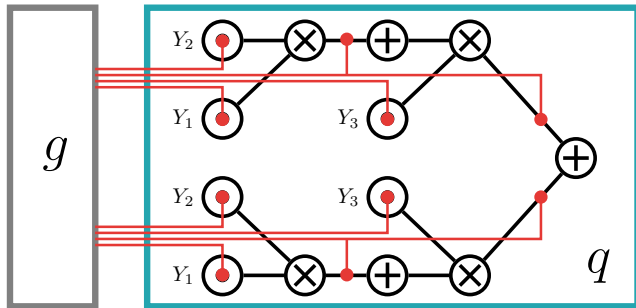
*Can we design q and c
to be **deep computational graphs**
yet yielding a tractable product?*

*yes! as **circuits!***

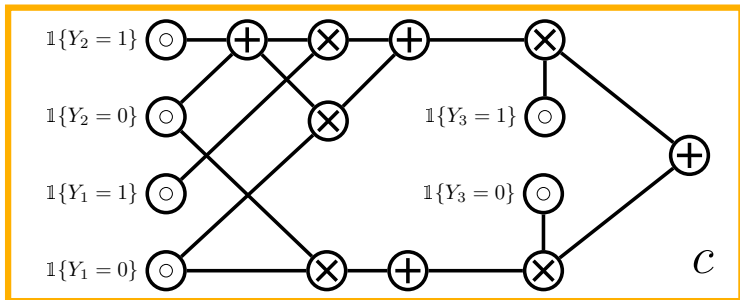
Tractable products



exactly compute \mathcal{Z} in time $O(|q||c|)$

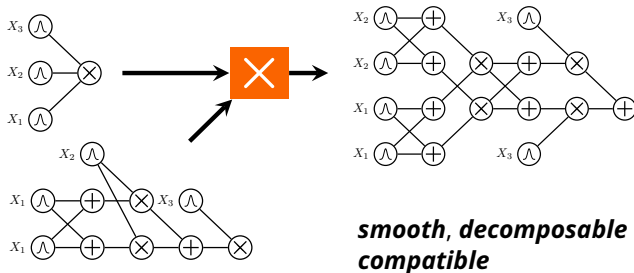


a conditional circuit $q(y; \Theta = g(z))$



and a logical circuit $c(y, x)$ encoding K

Tractable products



exactly compute \mathcal{Z} in time $O(|q||c|)$

SPL recipe

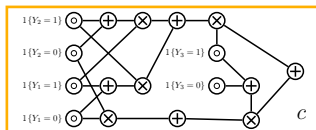
$$K : (Y_1 = 1 \implies Y_3 = 1)$$

$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$

1) Take a
logical constraint

SPL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$

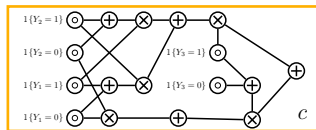


1) Take a
logical constraint

2) Compile it into
a constraint circuit

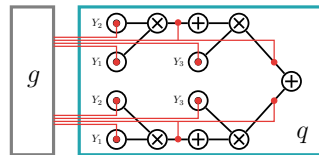
SPL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$



1) Take a
logical constraint

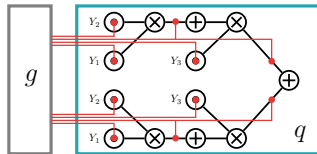
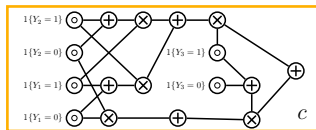
2) Compile it into
a constraint circuit



3) Multiply it
by a circuit distribution

SPL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$



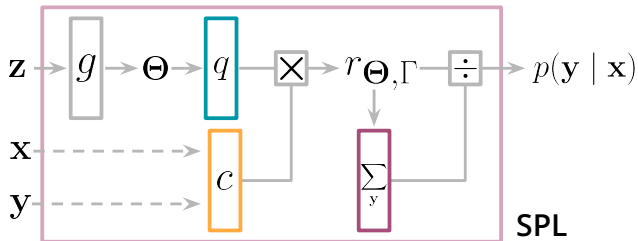
1) Take a
logical constraint

2) Compile it into
a constraint circuit

3) Multiply it
by a circuit distribution

4) train end-to-end by sgd!

Experiments



how good are SPLs?

Experiments



Architecture	Exact	Hamming	Consistent
ResNet-18+FIL	55.0	97.7	56.9
ResNet-18+ \mathcal{L}_{SL}	59.4	97.7	61.2
ResNet-18+SPL	78.2	96.3	100.0

Experiments

Ground Truth



cost: 39.31

FIL



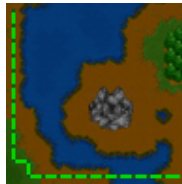
cost: ∞

\mathcal{L}_{SL}



cost: ∞

SPL



cost: 45.09



cost: 57.31



cost: ∞



cost: ∞



cost: 58.09

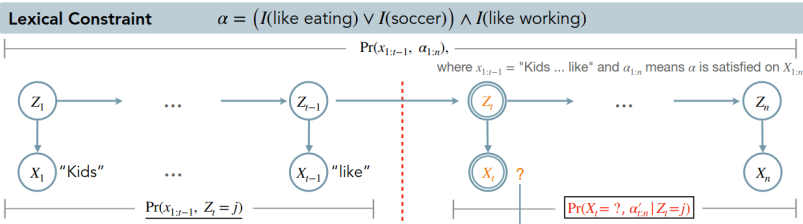
SPLs

(and more circuits)

everywhere

Tractable Control for Autoregressive Language Generation

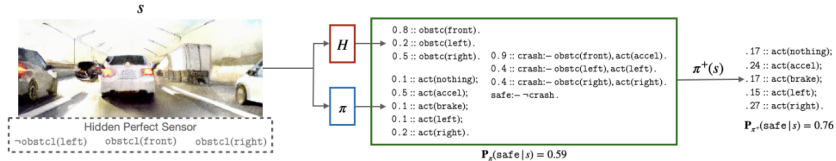
Honghua Zhang^{*1} Meihua Dang^{*1} Nanyun Peng¹ Guy Van den Broeck¹



constrained text generation with LLMs (ICML 2023)

Safe Reinforcement Learning via Probabilistic Logic Shields

Wen-Chi Yang¹, Giuseppe Marra¹, Gavin Rens and Luc De Raedt^{1,2}



reliable reinforcement learning (AAAI 23)

How to Turn Your Knowledge Graph Embeddings into Generative Models

Lorenzo Loconte
University of Edinburgh, UK
l.loconte@sms.ed.ac.uk

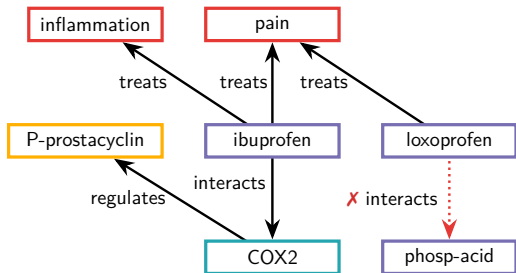
Nicola Di Mauro
University of Bari, Italy
nicola.dimauro@uniba.it

Robert Peharz
TU Graz, Austria
robert.peharz@tugraz.at

Antonio Vergari
University of Edinburgh, UK
avergari@ed.ac.uk

***enforce constraints in knowledge graph embeddings
oral at NeurIPS 2023***

constraints in KGs



- Drugs
- Symptoms
- Proteins
- Functions

K : only drugs and proteins interact

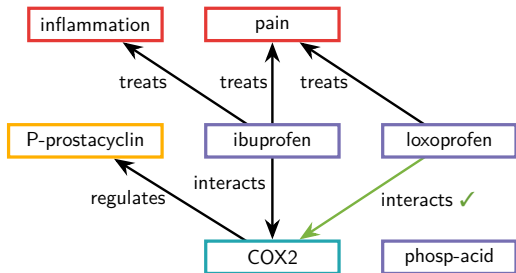
\mathcal{A} : $\langle \text{loxoprofen}, \text{interacts}, \text{phosp-acid} \rangle$



\mathcal{A} : $\langle \text{loxoprofen}, \text{interacts}, \text{COX2} \rangle$



constraints in KGs



- Drugs
- Proteins
- Symptoms
- Functions

K : only drugs and proteins interact

\mathcal{A} : $\langle \text{loxoprofen}, \text{interacts}, \text{phosp-acid} \rangle$

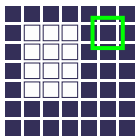


\mathcal{A} : $\langle \text{loxoprofen}, \text{interacts}, \text{COX2} \rangle$

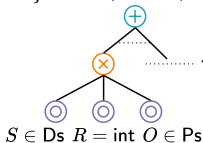


guaranteed satisfaction of constraints

$$\mathbb{1}\{(S, \text{interacts}, O) \models K\}$$

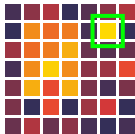


$$c_K(S, R, O)$$

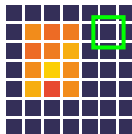
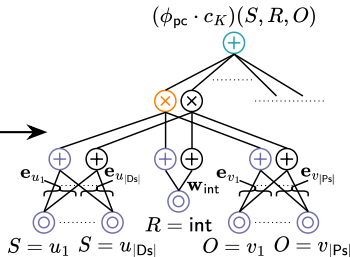
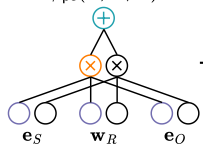


K : only drugs and proteins interact

$$\phi_{\text{pc}}(S, \text{interacts}, O)$$



$$\phi_{\text{pc}}(S, R, O)$$



$$p_K(\text{loxoprofen, interacts, phosp-acid}) = 0$$

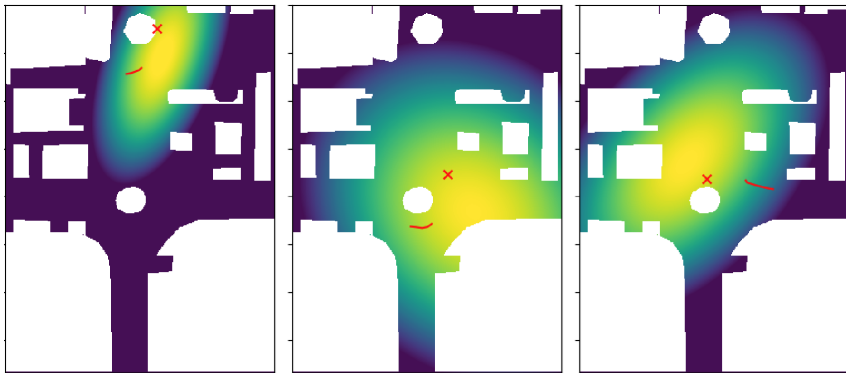
open problems

I constraints over continuous variables

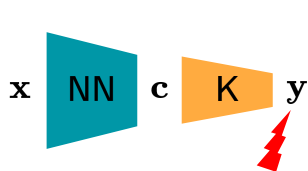
II scaling to H U G E constraints

III learn (partial) constraints

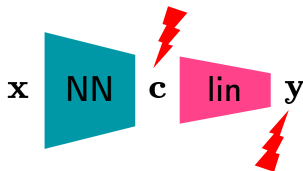
IV revise constraints (continual learning)



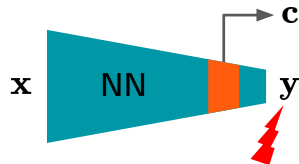
extending it to SMT constraints



SPL & LTN & DPL

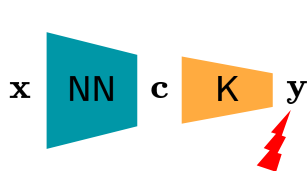


CBMs

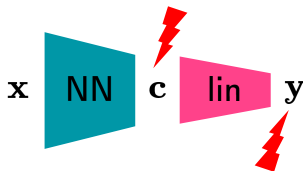


NN + ex-post

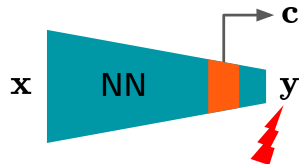
NeSy models are concept bottlenecks



SPL & LTN & DPL



CBMs

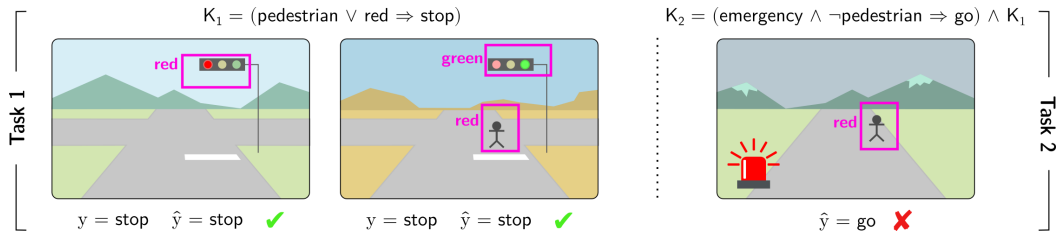


NN + ex-post

NeSy models can suffer from reasoning shortcuts!

Task	Example Data	Knowledge K	Example RS	Impact
MNIST math	$\begin{cases} 2 \cdot \blacksquare + \blacksquare = 6 \\ \blacksquare + \blacksquare = 7 \end{cases}$	Equations must hold.	$\begin{cases} \blacksquare \rightarrow 2 \\ \blacksquare \rightarrow 4 \\ \blacksquare \rightarrow 3 \end{cases}$	$\blacksquare + \blacksquare = 5$

NeSy models can suffer from reasoning shortcuts!



how to **detect** and **mitigate** them

Marconato et al., "Not all neuro-symbolic concepts are created equal: Analysis and mitigation of reasoning shortcuts", NeurIPS, 2023

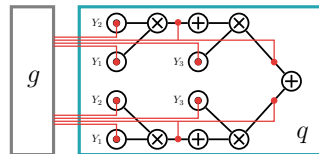
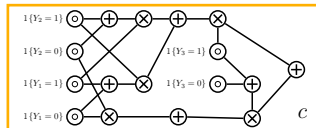
Bortolotti et al., "A Benchmark Suite for Systematically Evaluating Reasoning Shortcuts", NeurIPS Benchmark track, 2024

colorai
connecting
low-rank
representations
in ai

workshop at AAAI-25, Philadelphia

`april-tools.github.io/colorai/`

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$



questions?