Provably reliable Deep learning by design

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@tetraduzione

joint work with Kareem Ahmed, Andreas Grivas, Lorenzo Loconte, Stefano Teso, Kai-Wei Chang, Guy Van den Broeck, Nicola di Mauro, Robert Peharz, Adam Lopez

27th Oct 2023 - **Workshop on Safe and Robust Machine Learning**

april

***a**pril is*
***p**robably a*
***r**ecursive*
***i**dentifier of a*
***l**ab*

april

***a**utonomous &*
***p**rovably*
***r**eliable*
***i**ntelligent*
***l**earners*

deep learning is differentiable lego

just stacking blocks can be unrealiable though...

especially when dealing with hard constraints

part I how to satisfy wanted constraints in NNs by design

part II how the design of NNs implicitly poses unwanted constraints

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part I how to satisfy wanted constraints in NNs by design

Why?

"How can neural nets reason and learn with symbolic constraints reliably and efficiently?"

Why?

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integrate ***hard*** **(logical)** constraints

Why?

"How can neural nets reason and learn with symbolic constraints reliably and efficiently?"

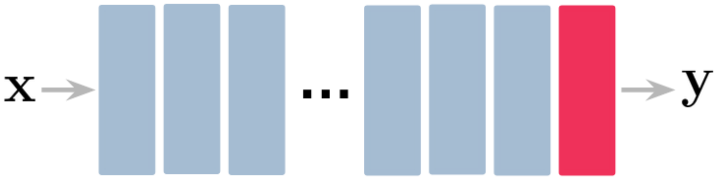
guarantee that predictions ***always satisfy*** constraints

Why?

"How can neural nets reason and learn with symbolic constraints reliably and efficiently?"

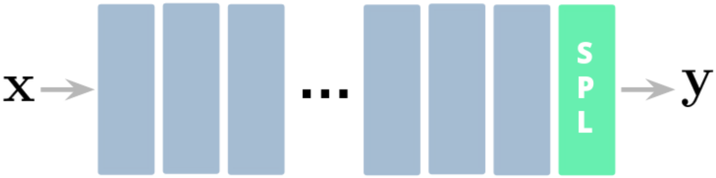
fast and ***exact*** gradients

Why?



make any neural network architecture...

Why?



...guarantee all predictions to conform to constraints

When?

Ground Truth

e.g. predict shortest path in a map

When?

Ground Truth

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

nesy structured output prediction (SOP) tasks

Vlastelica et al., "Differentiation of blackbox combinatorial solvers", ICLR, 2020

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*

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s.t. $\mathbf{y} \models \mathsf{K}$ *// e.g., that form a valid path*

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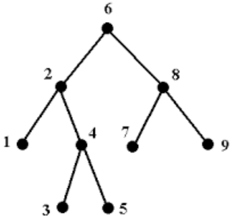
// for a 12×12 grid, 2^{144} states but only 10^{10} valid ones!

nesy structured output prediction (SOP) tasks

Vlastelica et al., "Differentiation of blackbox combinatorial solvers", ICLR, 2020

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

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

hierarchical multi-label classification

Giunchiglia and Lukasiewicz, "Coherent hierarchical multi-label classification networks", NeurIPS, 2020

When?

given $\mathbf{x}$ *// e.g. a user preference over $K - N$ sushi types*

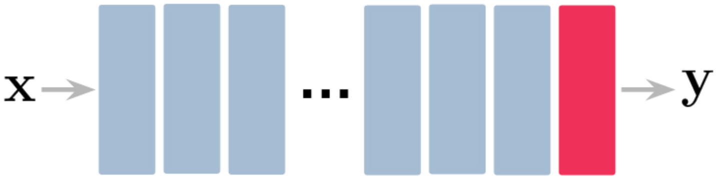
find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_\theta(\mathbf{y} \mid \mathbf{x})$ *// e.g. prefs over N more types*

s.t. $\mathbf{y} \models \mathsf{K}$ *// e.g., output valid rankings*

user preference learning

Choi, Van den Broeck, and Darwiche, "Tractable learning for structured probability spaces: A case study in learning preference distributions", IJCAI, 2015

e.g.,

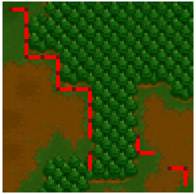


sigmoid linear layers

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

When?

Ground Truth



ResNet-18

neural nets struggle to satisfy validity constraints!

the issues!

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

$\Longrightarrow$ ***a single framework*** *for matching, paths, hierarchies, ...*

II) How to integrate logic and probabilities in a single neural layer

$\Longrightarrow$ ***combining soft and hard constraints***

III) Logical constraints are piecewise constant functions!

$\Longrightarrow$ *differentiable almost everywhere but* ***gradient is zero****!*

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Constraint losses

$$\mathcal{L}(\theta; \mathbf{x}, \mathbf{y}) + \lambda \mathcal{L}_{\mathsf{K}}(\mathbf{x}, \mathbf{y})$$

losses improve consistency during training...

Xu et al., "A Semantic Loss Function for Deep Learning with Symbolic Knowledge", , 2018

Constraint losses

$$\mathcal{L}(\theta; \mathbf{x}, \mathbf{y}) + \lambda \mathcal{L}_{\mathsf{K}}(\mathbf{x}, \mathbf{y})$$

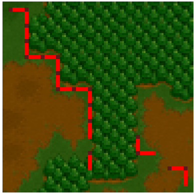
losses improve consistency during training...

e.g., the ***semantic loss***: $\mathcal{L}_{\mathsf{SL}} := -\log \sum_{\mathbf{y} \models \mathsf{K}} \prod_i p(Y_i \mid \mathbf{x})$

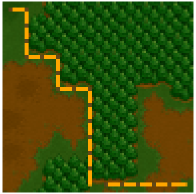
Xu et al., "A Semantic Loss Function for Deep Learning with Symbolic Knowledge", , 2018

Constraint losses

Ground Truth



ResNet-18



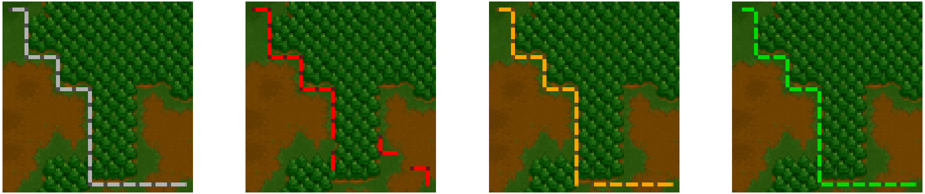
Semantic Loss

...but cannot guarantee consistency at test time!

what?

	Losses			Layers				
Desideratum	DL2 [29]	SL [80]	NeSyEnt [3]	FIL	EBM [43]	MultiplexNet [38]	CCN [33]	SPL *(ours)*
(D1) Probabilistic	✗	✓	✓	✓	✗	✓	✗	✓
(D2) Expressive	✗	✗	✗	✗	✓	✗	✗	✓
(D3) Consistent	✗	✗	✗	✗	✗	✓	✓	✓
(D4) General	✓	✓	✓	✗	✓	✓	✗	✓
(D5) Modular	✓	✓	✓	✓	✓	✓	✓	✓
(D6) Efficient	✓	✓	✓	✓	✗	✗	✓	✓

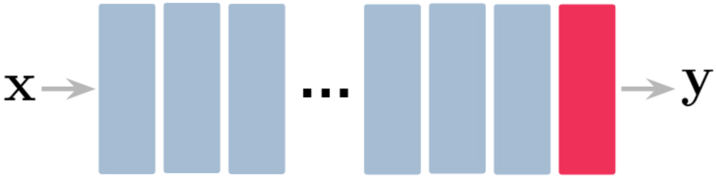
SPL



Ground Truth ResNet-18 Semantic Loss SPL (ours)

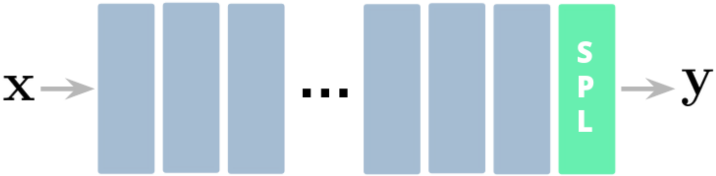
you can predict valid paths 100% of the time!

How?



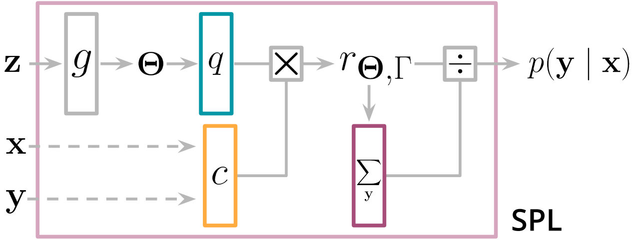
take an unreliable neural network architecture...

How?



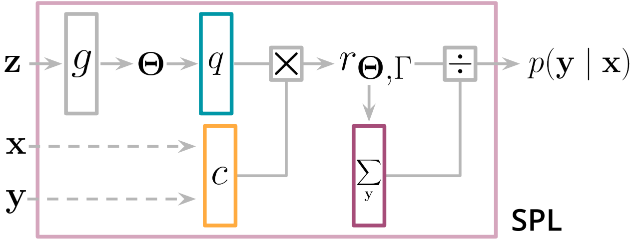
......and replace the last layer with a semantic probabilistic layer

SPL



$\mathbf{z}$
g
$\boldsymbol{\Theta}$
q
$r_{\boldsymbol{\Theta},\Gamma}$
$p(\mathbf{y} \mid \mathbf{x})$
$\mathbf{x}$
$\mathbf{y}$
c
$\sum_{\mathbf{y}}$
SPL

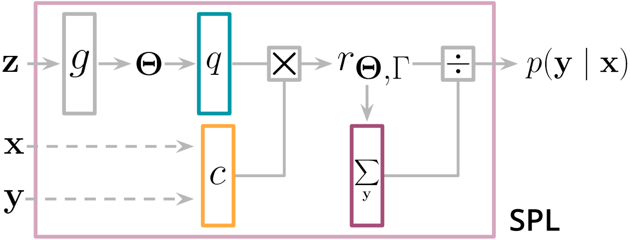
SPL



$$p(\mathbf{y} \mid \mathbf{x}) = q_{\boldsymbol{\Theta}}(\mathbf{y} \mid g(\mathbf{z}))$$

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

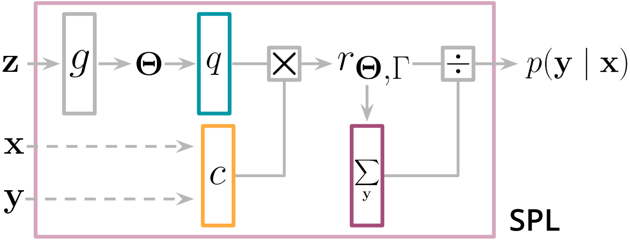
SPL



$$p(\mathbf{y} \mid \mathbf{x}) = q_{\boldsymbol{\Theta}}(\mathbf{y} \mid g(\mathbf{z})) \cdot c_{\mathsf{K}}(\mathbf{x}, \mathbf{y})$$

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

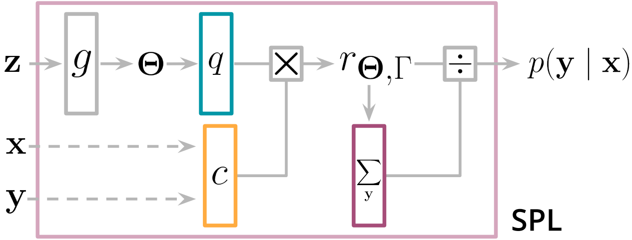
SPL



$$p(\mathbf{y} \mid \mathbf{x}) = q_{\Theta}(\mathbf{y} \mid g(\mathbf{z})) \cdot c_{\mathsf{K}}(\mathbf{x}, \mathbf{y})$$

a product of experts : (

SPL



$$p(\mathbf{y} \mid \mathbf{x}) = q_{\boldsymbol{\Theta}}(\mathbf{y} \mid g(\mathbf{z})) \cdot c_{\mathsf{K}}(\mathbf{x}, \mathbf{y}) / \mathcal{Z}(\mathbf{x})$$

$$\mathcal{Z}(\mathbf{x}) = \sum_{\mathbf{y}} q_{\boldsymbol{\Theta}}(\mathbf{y} \mid \mathbf{x}) \cdot c_{\mathsf{K}}(\mathbf{x}, \mathbf{y})$$

Goal

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

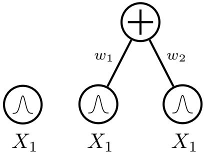
Probabilistic Circuits (PCs)

A grammar for tractable computational graphs

I. *A simple tractable function 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*

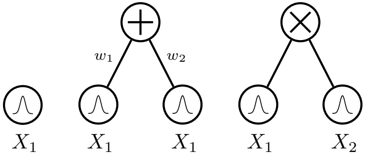
Probabilistic Circuits (PCs)

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*



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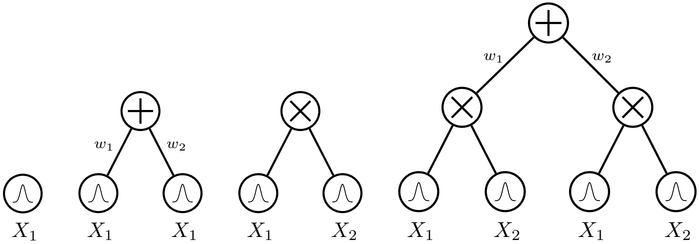
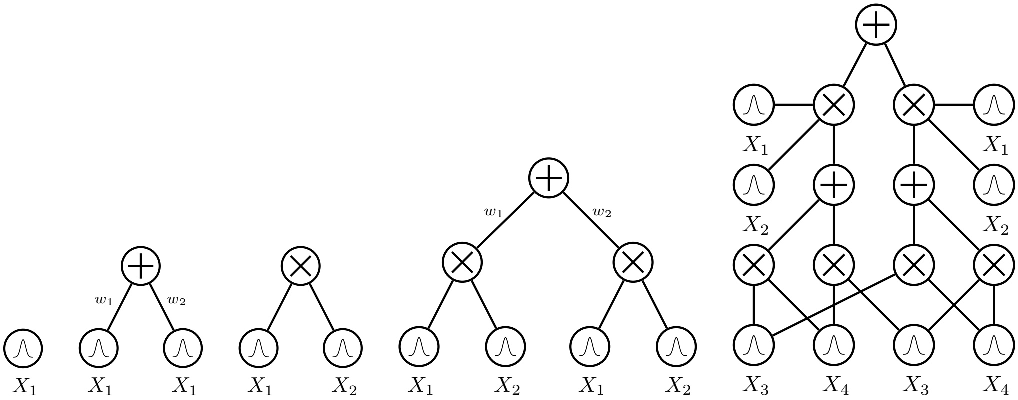


Probabilistic Circuits (PCs)

A grammar for tractable computational graphs



...why PCs?

1. A grammar for tractable models

One formalism to represent many models. *#HMMs #Trees #XGBoost*, ...

2. Expressiveness

Competitive with intractable models, VAEs, Flow...*#hierachical #mixtures #polynomials*

...why PCs?

1. A grammar for tractable models

One formalism to represent many models. *#HMMs #Trees #XGBoost*, ...

2. Expressiveness

Competitive with intractable models, VAEs, Flow...*#hierachical #mixtures #polynomials*

3. Tractability == Structural Properties!!!

Exact computations of reasoning tasks are certified by guaranteeing certain structural properties. *#marginals #expectations #MAP*, *#product* ...

Structural properties

smoothness

decomposability

determinism

compatibility

Vergari *et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021*

Structural properties

property A

property B

property C

property D

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Structural properties

property A

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property C

property D

tractable computation of ***arbitrary integrals***

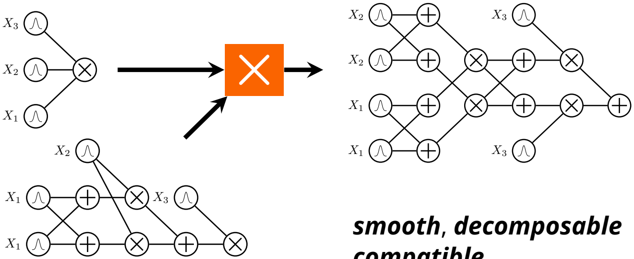
$$p(\mathbf{y}) = \int_{\mathsf{val}(\mathbf{Z})} p(\mathbf{z}, \mathbf{y})\, d\mathbf{Z}, \quad \forall \mathbf{Y} \subseteq \mathbf{X}, \quad \mathbf{Z} = \mathbf{X} \setminus \mathbf{Y}$$

$\implies$ ***sufficient*** *and* ***necessary*** *conditions for a single feedforward evaluation*

$\implies$ *tractable partition function*

__Vergari__ et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021

Tractable products

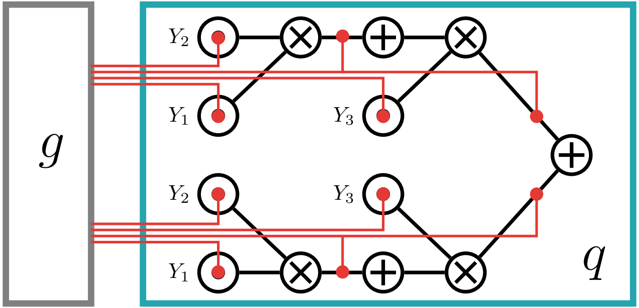


smooth, ***decomposable***
compatible

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

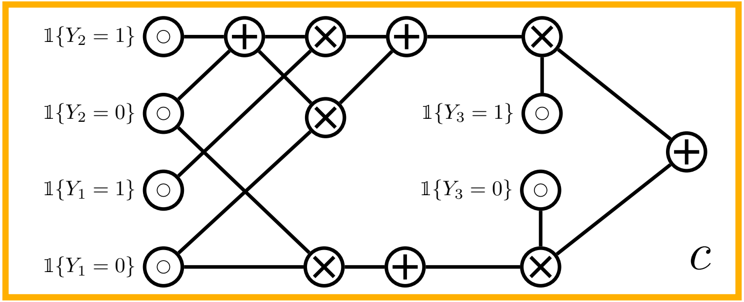
__Vergari__ et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021

SPL



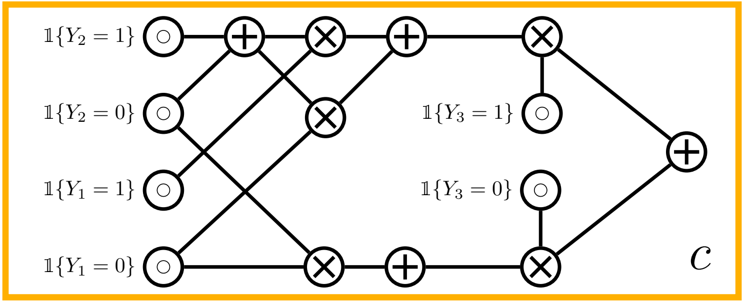
a conditional circuit $\boldsymbol{q}(\mathbf{y}; \boldsymbol{\Theta} = g(\mathbf{z}))$

SPL



and a logical circuit $c(\mathrm{y}, \mathrm{x})$ **encoding** K

SPL



compiling logical formulas into circuits

Knowledge compilation

$$\mathsf{K}: (Y_1 = 1 \implies Y_3 = 1)$$

$$\land \quad (Y_2 = 1 \implies Y_3 = 1)$$

$\mathbb{1}\{Y_1 = 0\}$ $\odot$ $\mathbb{1}\{Y_1 = 1\}$ $\odot$ $\mathbb{1}\{Y_2 = 0\}$ $\odot$

$\mathbb{1}\{Y_2 = 1\}$ $\odot$ $\mathbb{1}\{Y_3 = 0\}$ $\odot$ $\mathbb{1}\{Y_3 = 1\}$ $\odot$

Pipatsrisawat and Darwiche, "New Compilation Languages Based on Structured Decomposability.", AAAI, 2008

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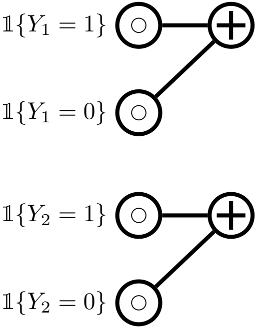

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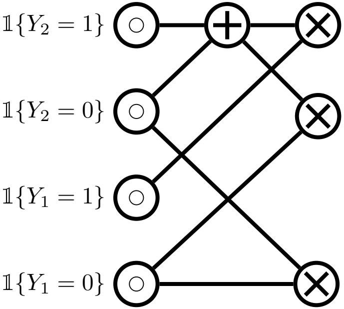

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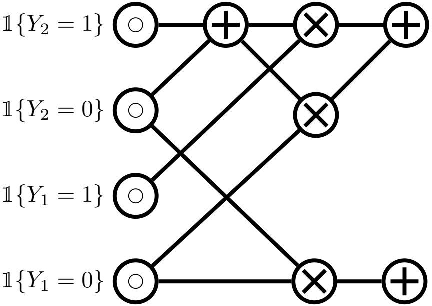

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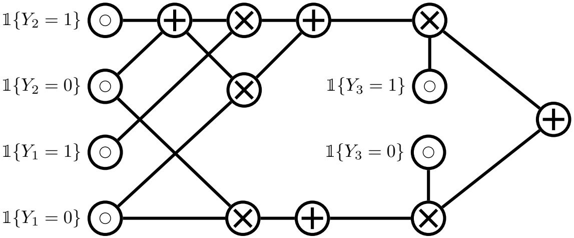

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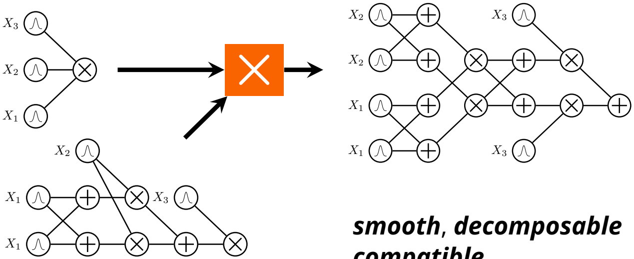
Tractable products



smooth*, *decomposable
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exactly compute $\mathcal{Z}$ in time $O(|\boldsymbol{q}||\boldsymbol{c}|)$

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SPL recipe

$$\mathsf{K} : (Y_1 = 1 \implies Y_3 = 1)$$
$$\land \quad (Y_2 = 1 \implies Y_3 = 1)$$

1) Take a
logical constraint

SPL recipe

$$\mathsf{K}: (Y_1 = 1 \implies Y_3 = 1)$$
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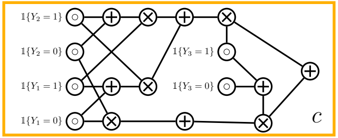
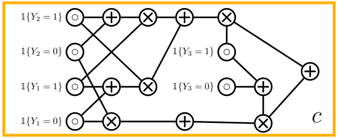


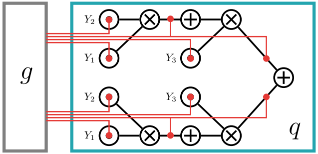
1) Take a logical constraint

2) Compile it into a constraint circuit

SPL recipe

$$\mathsf{K}: (Y_1 = 1 \implies Y_3 = 1) \\ \wedge \quad (Y_2 = 1 \implies Y_3 = 1)$$





1) Take a logical constraint

2) Compile it into a constraint circuit

3) Multiply it by a circuit distribution

SPL recipe

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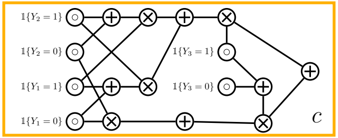
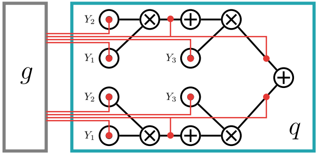




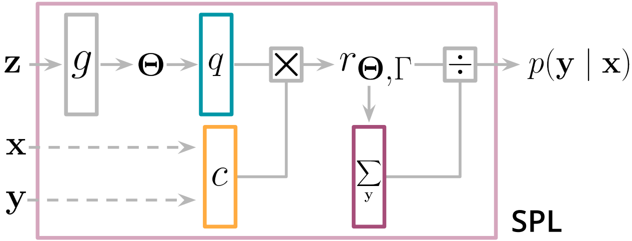
1) Take a logical constraint

2) Compile it into a constraint circuit

3) Multiply it by a circuit distribution

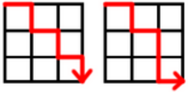
4) train end-to-end by sgd!

Experiments



how good are SPLs?

Experiments

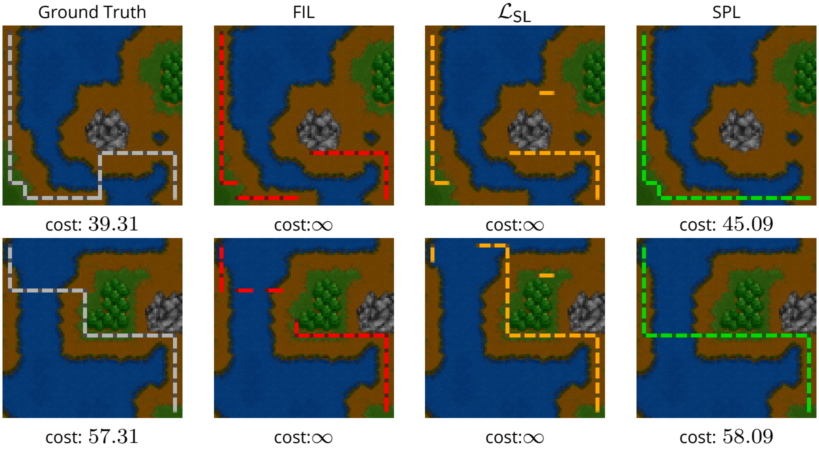


Architecture	Simple Path			Preference Learning		
	Exact	Hamming	Consistent	Exact	Hamming	Consistent
MLP+FIL	5.6	85.9	7.0	1.0	**75.8**	2.7
MLP+$\mathcal{L}_{SL}$	28.5	83.1	75.2	15.0	72.4	69.8
MLP+NeSyEnt	30.1	83.0	91.6	18.2	71.5	96.0
MLP+SPL	**37.6**	**88.5**	**100.0**	**20.8**	72.4	**100.0**

Experiments

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

Experiments



Experiments

Dataset	Exact Match	
	HMCNN	MLP+SPL
CellCycle	3.05 ± 0.11	$\mathbf{3.79 \pm 0.18}$
Derisi	1.39 ± 0.47	$\mathbf{2.28 \pm 0.23}$
Eisen	5.40 ± 0.15	$\mathbf{6.18 \pm 0.33}$
Expr	4.20 ± 0.21	$\mathbf{5.54 \pm 0.36}$
Gasch1	3.48 ± 0.96	$\mathbf{4.65 \pm 0.30}$
Gasch2	3.11 ± 0.08	$\mathbf{3.95 \pm 0.28}$
Seq	5.24 ± 0.27	$\mathbf{7.98 \pm 0.28}$
Spo	$\mathbf{1.97 \pm 0.06}$	1.92 ± 0.11
Diatoms	48.21 ± 0.57	$\mathbf{58.71 \pm 0.68}$
Enron	5.97 ± 0.56	$\mathbf{8.18 \pm 0.68}$
ImCLEF07A	79.75 ± 0.38	$\mathbf{86.08 \pm 0.45}$
ImCLEF07D	76.47 ± 0.35	$\mathbf{81.06 \pm 0.68}$

How to Turn Your Knowledge Graph Embeddings into Generative Models via Probabilistic Circuits

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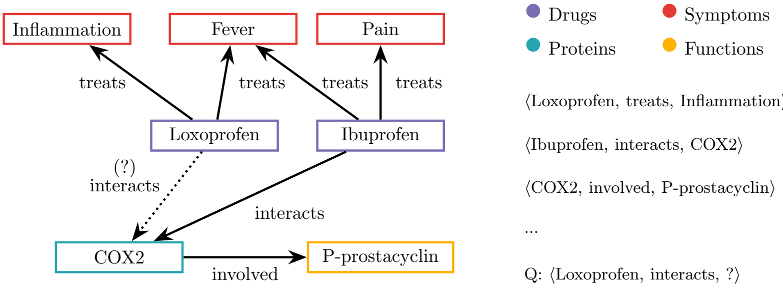
SPL meets knowledge graph embedding models



⟨Loxoprofen, treats, Inflammation⟩

⟨Ibuprofen, interacts, COX2⟩

⟨COX2, involved, P-prostacyclin⟩

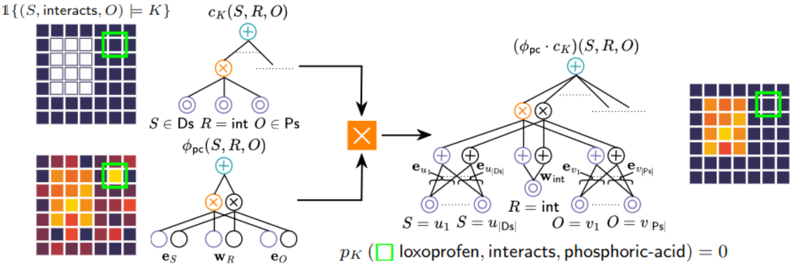
...

Q: ⟨Loxoprofen, interacts, ?⟩

A: ⟨Loxoprofen, interacts, **phosphoric-acid**⟩ !!!

neural link predictors can violate domain constraints

SPL+KGE

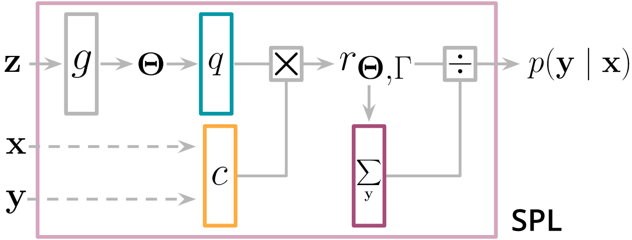


$\mathbb{1}\{(S, \text{interacts}, O) \models K\}$
$c_K(S, R, O)$
$S \in \text{Ds}$ $R = \text{int}$ $O \in \text{Ps}$
$\phi_{\text{pc}}(S, R, O)$
$\mathbf{e}_S$ $\mathbf{w}_R$ $\mathbf{e}_O$
$(\phi_{\text{pc}} \cdot c_K)(S, R, O)$
$\mathbf{e}_{u_1}$ $\mathbf{e}_{u_{|\text{Ds}|}}$ $\mathbf{w}_{\text{int}}$ $\mathbf{e}_{v_1}$ $\mathbf{e}_{v_{|\text{Ps}|}}$
$S = u_1$ $S = u_{|\text{Ds}|}$ $R = \text{int}$ $O = v_1$ $O = v_{|\text{Ps}|}$
p_K (loxoprofen, interacts, phosphoric-acid) $= 0$


MACHINE LEARNERS
COMPLEX REASONING

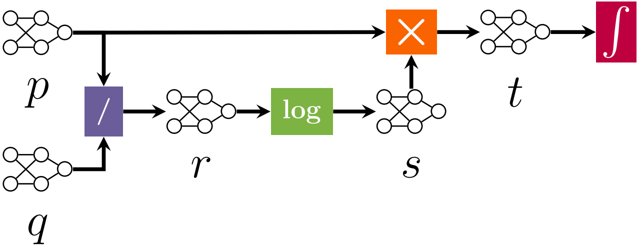

APPROXIMATIONS
imgflip.com

$$p(\mathbf{y} \mid \mathbf{x}) = q_{\boldsymbol{\Theta}}(\mathbf{y} \mid g(\mathbf{z})) \cdot c_{\mathsf{K}}(\mathbf{x}, \mathbf{y}) / \mathcal{Z}(\mathbf{x})$$



efficient and reliable reasoning over constraints

$$\int p(\mathbf{x}) \times \log \left(p(\mathbf{x}) \,/\, q(\mathbf{x}) \right) \, d\mathbf{X}$$



build a LEGO-like query calculus!

Vergari *et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021*

part I how to satisfy wanted constraints in NNs by design

part II how the design of NNs implicitly poses unwanted constraints

Taming the Sigmoid Bottleneck: Provably Argmaxable Sparse Multi-Label Classification

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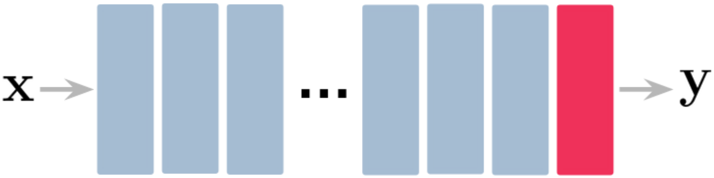


sigmoid linear layers

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

low-rank classifiers

labels (n) $>>$ embedding size (d)

e.g.,

clinically annotated text

$n \approx 9000$
$d \approx 200 - 500$

large-scale biomedical question answering

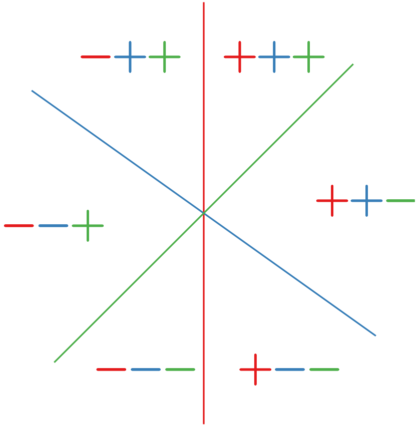
$n \approx 20000$
$d \approx 200 - 500$

OpenImages Dataset
object recognition

$n \approx 9000$
$d \approx 200 - 500$

$n = 3$

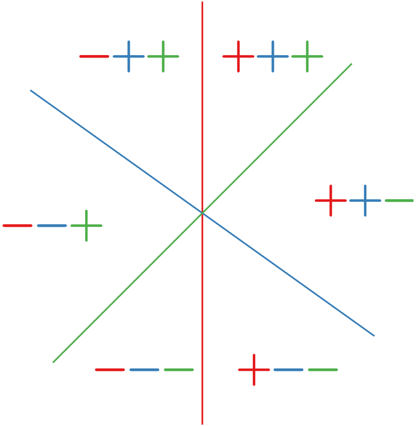
$d = 2$



some label configurations are *unargmaxable*!

$n = 3$

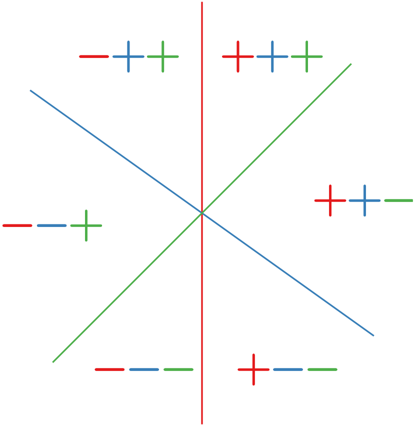
$d = 2$



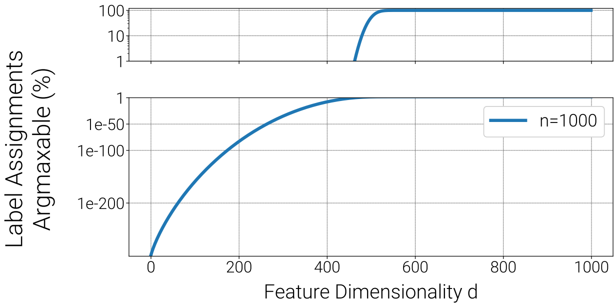
$$\nexists \mathbf{x} : \operatorname*{argmax}_{\mathbf{y}'} p(\mathbf{y}' \mid \mathbf{x}; \mathbf{W}) = \mathbf{y}$$

$n = 3$

$d = 2$



−+− **and** +−+ **are *unargmaxable*!**



exponentially **many configurations are unargmaxable**

but real data is sparse...

K-active labels

clinically annotated text

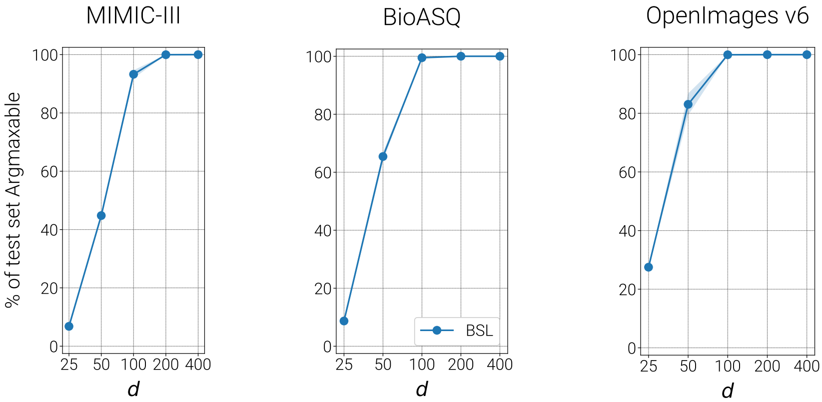
$n \approx 9000$
$K = 80$

large-scale biomedical question answering

$n \approx 20000$
$K = 50$

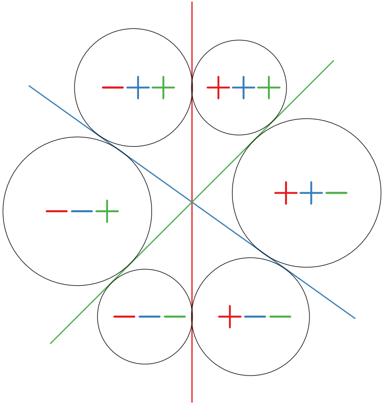
OpenImages Dataset
object recognition

$n \approx 9000$
$K = 50$

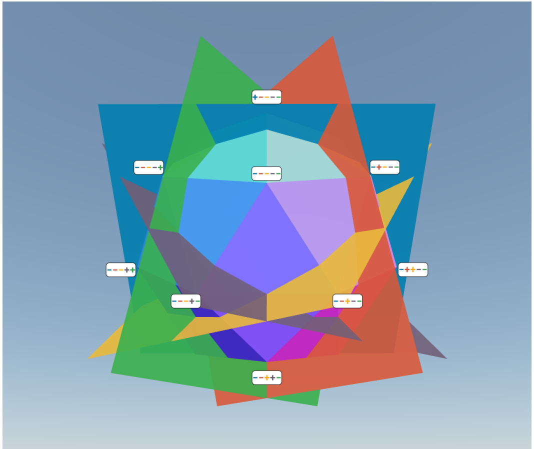


even sparse label configurations are unargmaxable

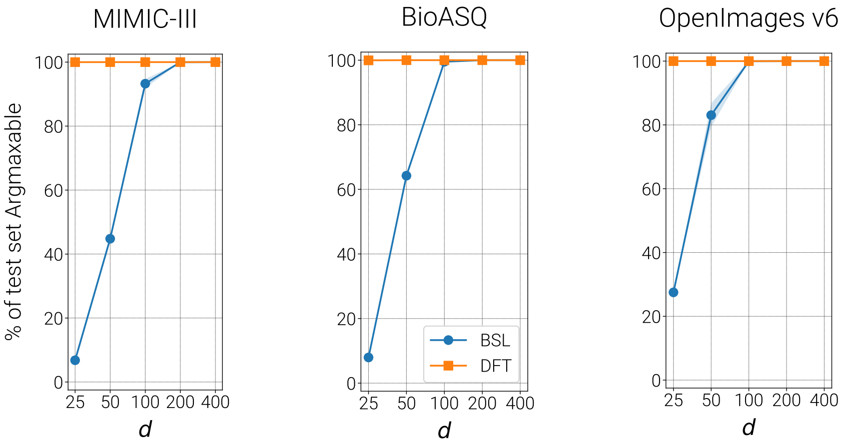
how do we know?



we provide a Chebyshev LP to *verify argmaxability*

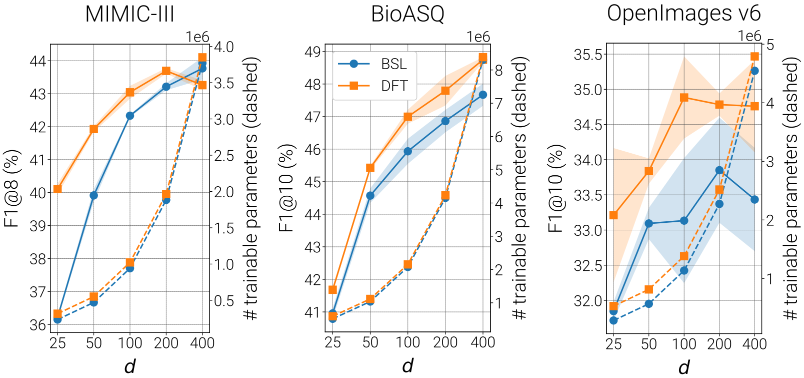


and a new differentiable layer to *guarantee argmaxability*
for K-active label configurations



and a new differentiable layer to guarantee argmaxability

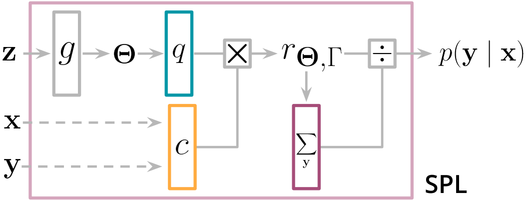
based on the DFT

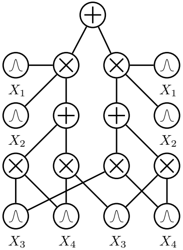


with comparable or better performance

part I how to satisfy wanted constraints in NNs by design

part II how the design of NNs implicitly poses unwanted constraints





Ask me anything!