UCLA Computer Science

STAR AI RESEARCH LAB UCLA

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

Guy Van den Broeck

nCSI Workshop @ NeurIPS 2022 - Dec 8 2022

Outline

1. The paradox of learning to reason from data

   ~~deep learning~~

2. Learning with symbolic knowledge

   logical reasoning + *deep learning*

Outline

1. **The paradox of learning to reason from data**

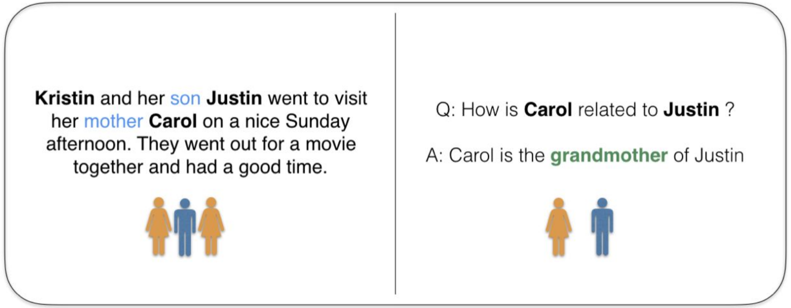
   ~~deep learning~~

2. Learning with symbolic knowledge

   logical reasoning + deep learning

Can Language Models Perform Logical Reasoning?

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



Reasoning Example from the CLUTRR dataset

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

<u>Language Models</u>:
input → ? → Carol is the grandmother of Justin.

<u>Logical Reasoning</u>:
input → Justin in 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.

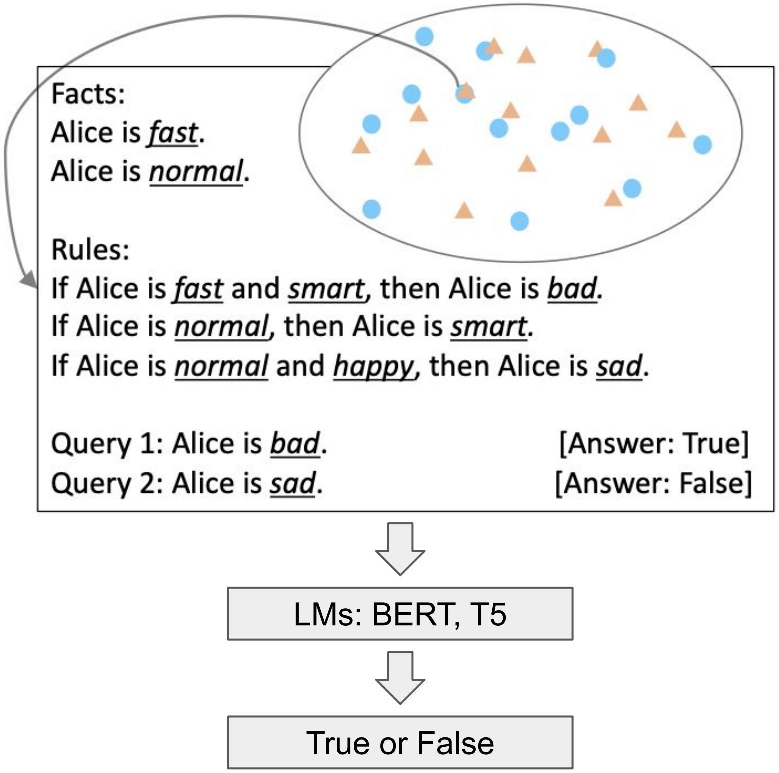
Problem Setting: SimpleLogic

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 ?

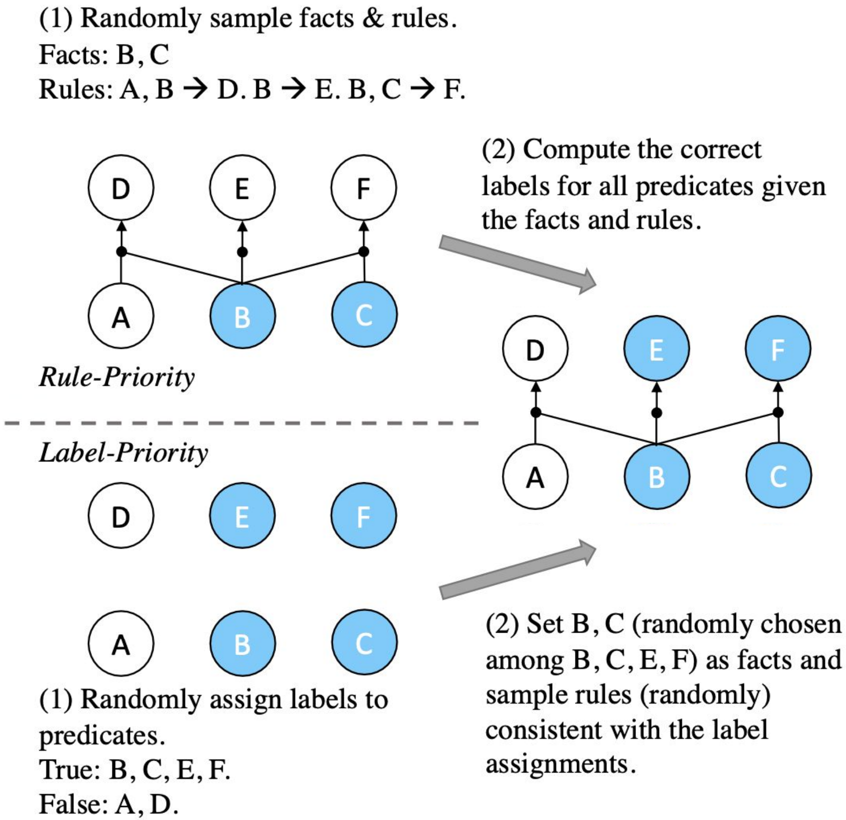
Problem Setting: SimpleLogic

The easiest of reasoning problems:

1. **Propositional logic** fragment
   a. bounded vocabulary & number of rules
   b. bounded reasoning depth (≤ 6)
   c. finite space (≈ 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



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

Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang and Guy Van den Broeck. On the Paradox of Learning to Reason from Data, 2022

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!

Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang and Guy Van den Broeck. On the Paradox of Learning to Reason from Data, 2022

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.

Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang and Guy Van den Broeck. On the Paradox of Learning to Reason from Data, 2022

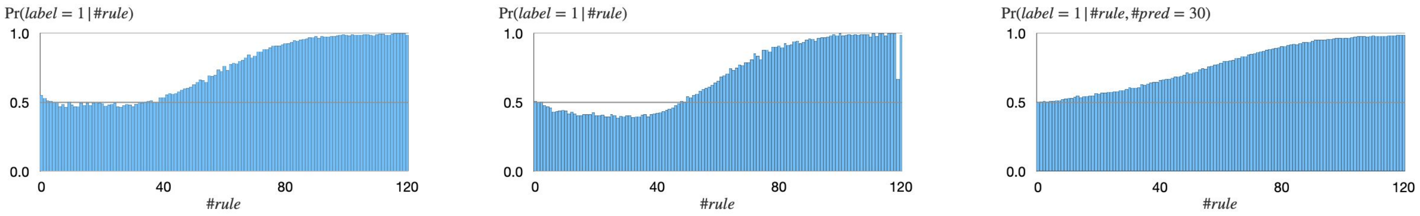
Why? Statistical Features

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(label = True | 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(label = True | rule# = x) = 0.5 for all x

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
	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. Though removing one statistical feature from training data can help with model generalization, there are potentially countless statistical features and it is computationally infeasible to jointly remove them.

Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang and Guy Van den Broeck. On the Paradox of Learning to Reason from Data, 2022

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.

Honghua Zhang, Liunian Harold Li, Tao Meng, Kai-Wei Chang and Guy Van den Broeck. On the Paradox of Learning to Reason from Data, 2022

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1. The paradox of learning to reason from data

   ~~deep learning~~

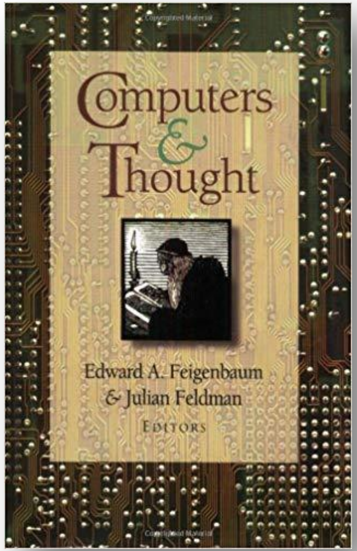
2. **Learning with symbolic knowledge**

   logical reasoning + deep learning

The AI Dilemma of 2022

Deep learning
approaches the problem of designing intelligent machines by postulating a large number of very simple information processing elements, arranged in a [.] network, and certain processes for facilitating or inhibiting their activity.

Knowledge representation and reasoning
take a much more macroscopic approach [.].
They believe that intelligent performance by a machine is an end difficult enough to achieve without "starting from scratch", and so they build into their systems as much complexity of information processing as they are able to understand and communicate to a computer.

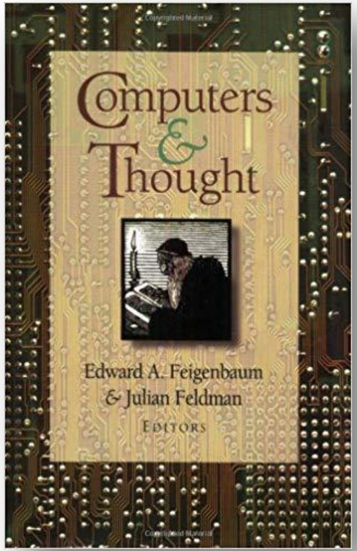


Edward Feigenbaum and Julian Feldman

The AI Dilemma of ~~2022~~ **1963**

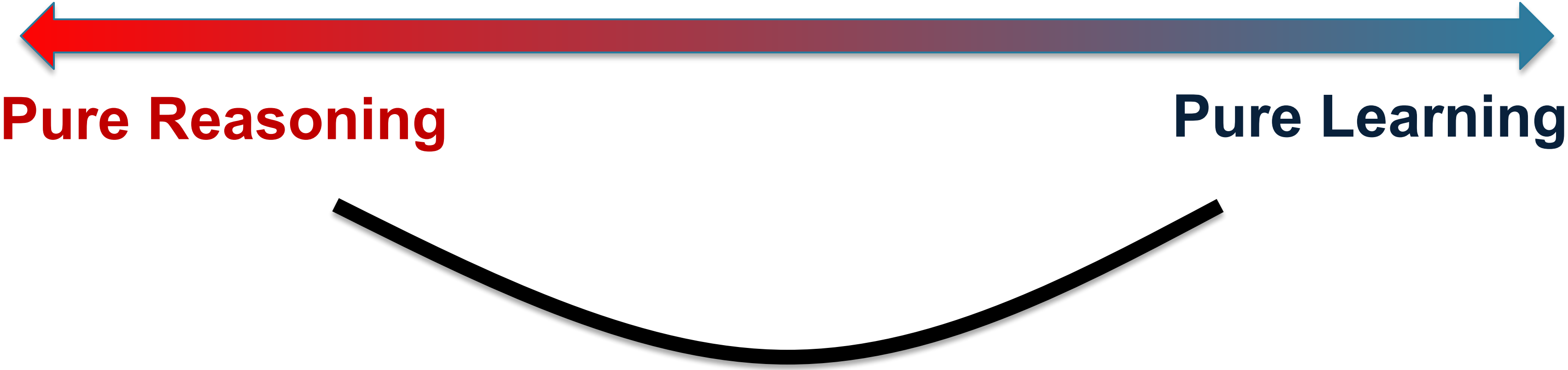
Neural cybernetics
approaches the problem of designing intelligent machines by postulating a large number of very simple information processing elements, arranged in a [.] network, and certain processes for facilitating or inhibiting their activity.

Cognitive model builders
take a much more macroscopic approach [.].
They believe that intelligent performance by a machine is an end difficult enough to achieve without "starting from scratch" , and so they build into their systems as much complexity of information processing as they are able to understand and communicate to a computer.



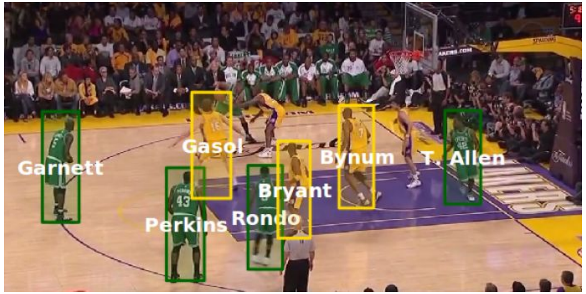
Edward Feigenbaum and Julian Feldman

The AI Dilemma

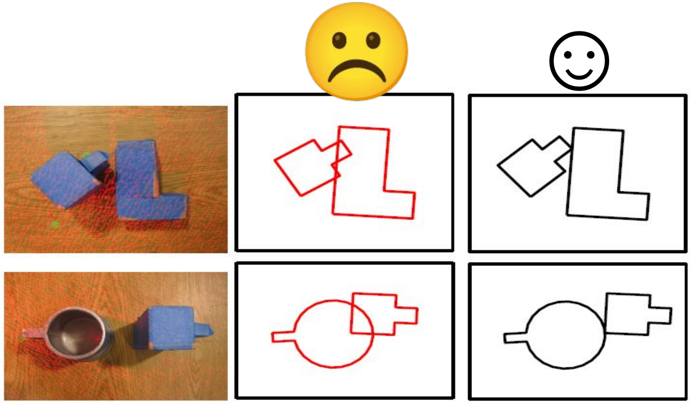


Integrate reasoning into modern deep learning algorithms

Knowledge in Vision, Robotics, NLP, Activity Recognition



People appear at most
once in a frame



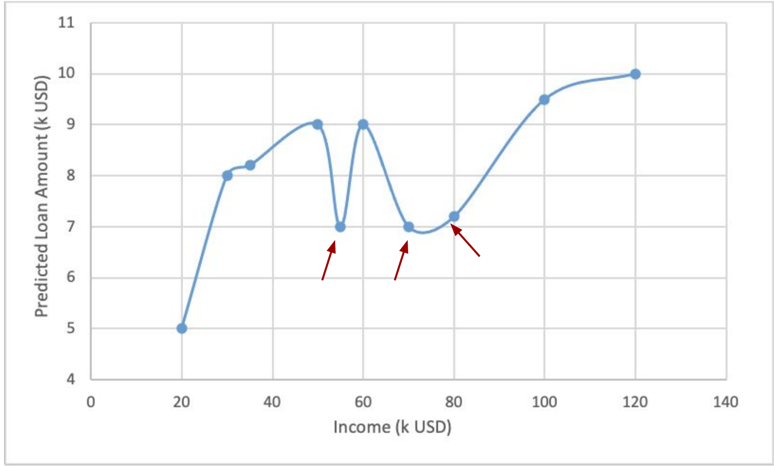
Rigid objects don't overlap

At least one verb
in each sentence.
If X and Y are married,
then they are people.

Cut the orange before
squeezing the orange

[Lu, W. L., Ting, J. A., Little, J. J., & Murphy, K. P. (2013). Learning to track and identify players from broadcast sports videos.], [Wong, L. L., Kaelbling, L. P., & Lozano-Perez, T., Collision-free state estimation. ICRA 2012], [Chang, M., Ratinov, L., & Roth, D. (2008). Constraints as prior knowledge], [Ganchev, K., Gillenwater, J., & Taskar, B. (2010). Posterior regularization for structured latent variable models]… and many many more!

Predict Loan Amount



Neural Network Model: Increasing income can decrease the approved loan amount

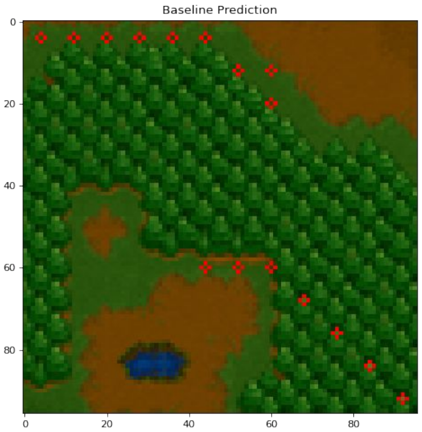
Monotonicity (Prior Knowledge):
Increasing income should increase the approved loan amount

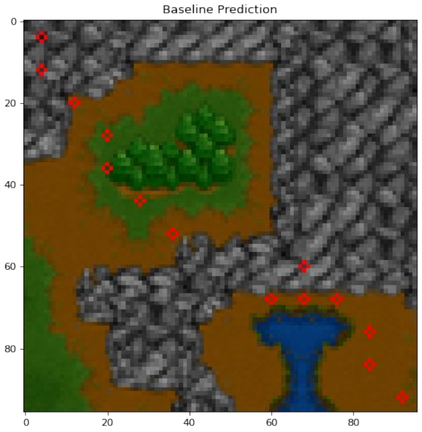
Aishwarya Sivaraman, Golnoosh Farnadi, Todd Millstein and Guy Van den Broeck. Counterexample-Guided Learning of Monotonic Neural Networks, *NeurIPS*, 2020.

Warcraft Shortest Path

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

[Differentiation of Blackbox Combinatorial Solvers, Marin Vlastelica, Anselm Paulus, Vít Musil, Georg Martius, Michal Rolínek, 2019]


Baseline Prediction
0
20
40
60
80
0
20
40
60
80


Baseline Prediction
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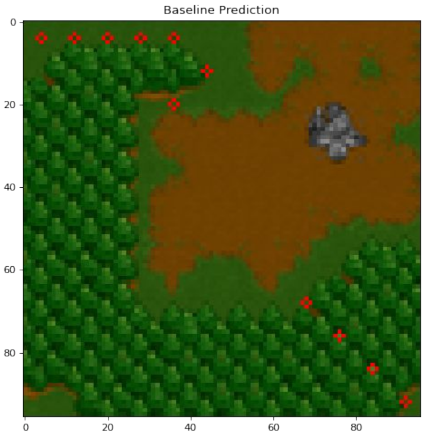
40
60
80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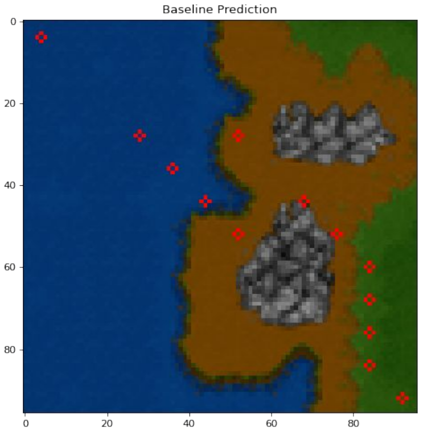

Baseline Prediction
0
20
40
60
80
0
20
40
60
80

Knowledge vs. Data

- Where did the world knowledge go?
  - Python scripts
    - Decode/encode/search cleverly
    - Fix inconsistent beliefs
  - Rule-based decision systems
  - Dataset design
  - “a big hack” (with author’s permission)
- In some sense we went backwards

  Less principled, scientific, and intellectually satisfying ways of incorporating knowledge

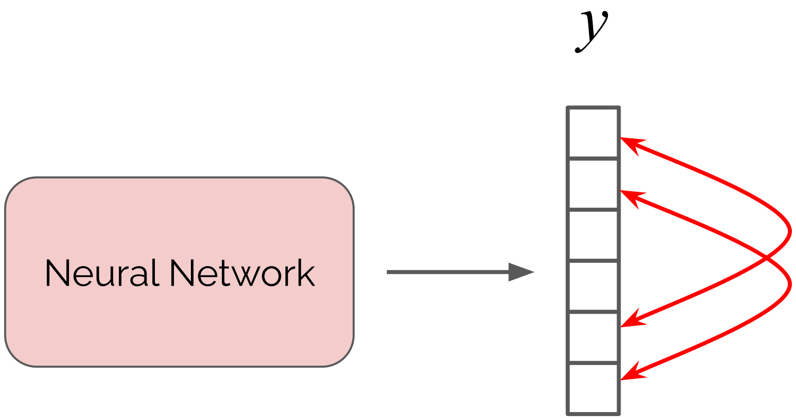
pylon

A PyTorch Framework for Learning with Constraints

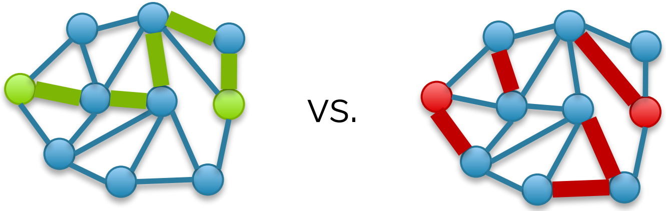
Kareem Ahmed Tao Li Thy Ton Quan Guo,
Kai-Wei Chang Parisa Kordjamshidi Vivek Srikumar
Guy Van den Broeck Sameer Singh

http://pylon-lib.github.io

Declarative Knowledge of the Output



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



How are the outputs related to each other?

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

pylon

Library that extends PyTorch to allow injection of declarative knowledge

- **Easy to Express Knowledge:** users write arbitrary constraints on the output
- **Integrates with PyTorch:** minimal change to existing code
- **Efficient Training:** compiles into loss that can be efficiently optimized
    - Exact semantic loss (see later)
    - Monte-carlo estimate of loss
    - T-norm approximation
    - *your solver?*

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)
    ...
    loss = CrossEntropy(py,...)

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

1 Specify knowledge as a predicate

```
def check(y):
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```

2 Add as loss to training

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

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PyTorch Code

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```

1 Specify knowledge as a predicate

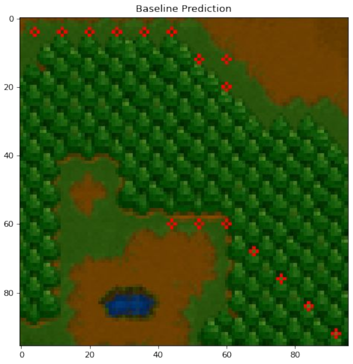
```
def check(y):
    ...
    return isValid
```

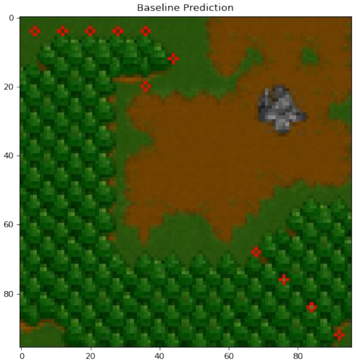
2 Add as loss to training

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

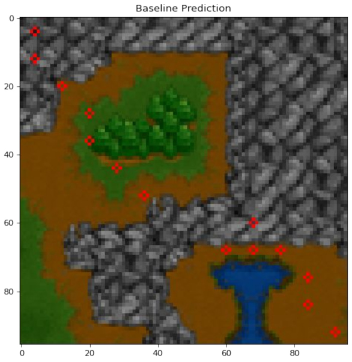
3 pylon derives the gradients
(solves a combinatorial problem)

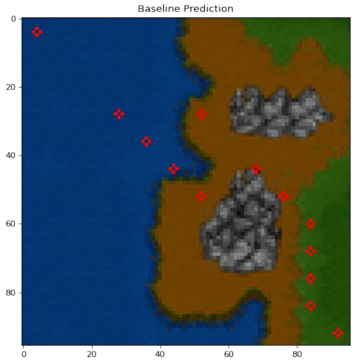
without constraint





without constraint





Warcraft min-cost simple-path prediction results

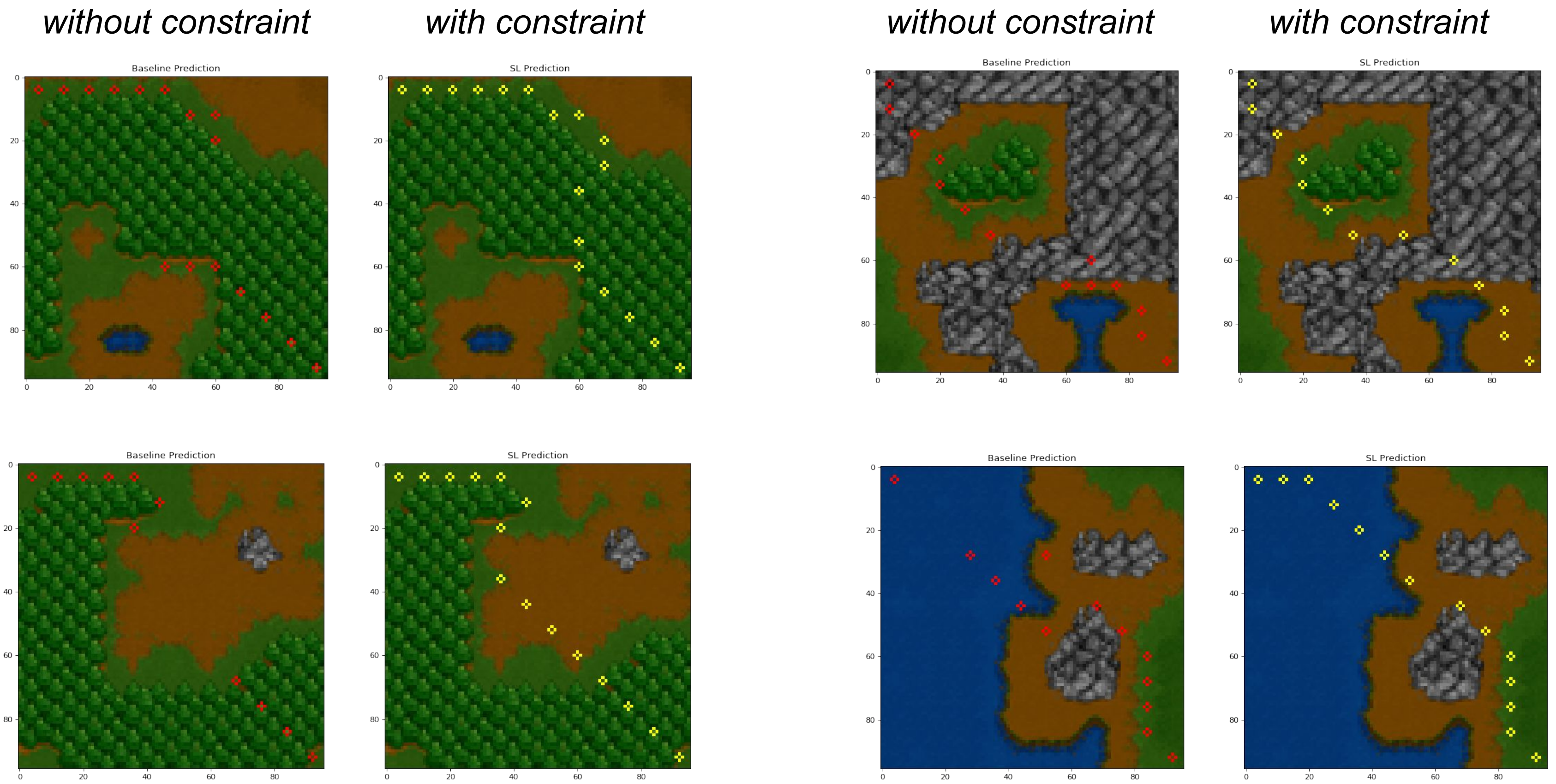
Test accuracy %	Coherent	Incoherent	Constraint
ResNet-18	44.8	**97.7**	56.9

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

Are individual edge predictions correct?

Is output a path?

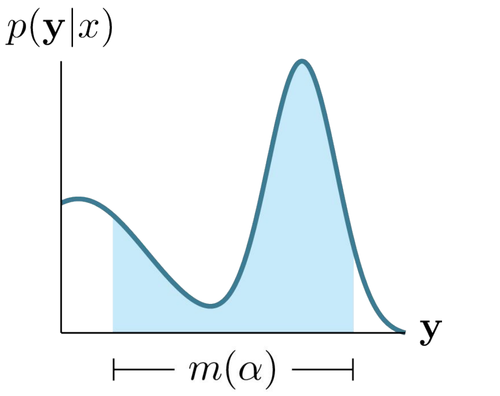
Kareem Ahmed, Eric Wang, Kai-Wei Chang and Guy Van den Broeck. Neuro-Symbolic Entropy Regularization, 2021.


without constraint
with constraint
without constraint
with constraint
Baseline Prediction
SL Prediction
Baseline Prediction
SL Prediction
Baseline Prediction
SL Prediction
Baseline Prediction
SL Prediction

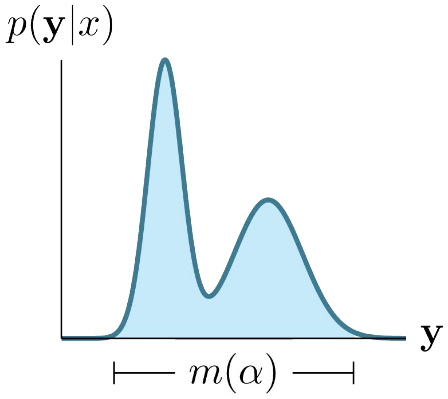
Warcraft min-cost simple-path prediction results

Test accuracy %	Coherent	Incoherent	Constraint
ResNet-18	44.8	**97.7**	56.9
+ Semantic loss	**50.9**	**97.7**	**67.4**

Kareem Ahmed, Eric Wang, Kai-Wei Chang and Guy Van den Broeck. Neuro-Symbolic Entropy Regularization, 2021.



a) A network uncertain over both valid & invalid predictions



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

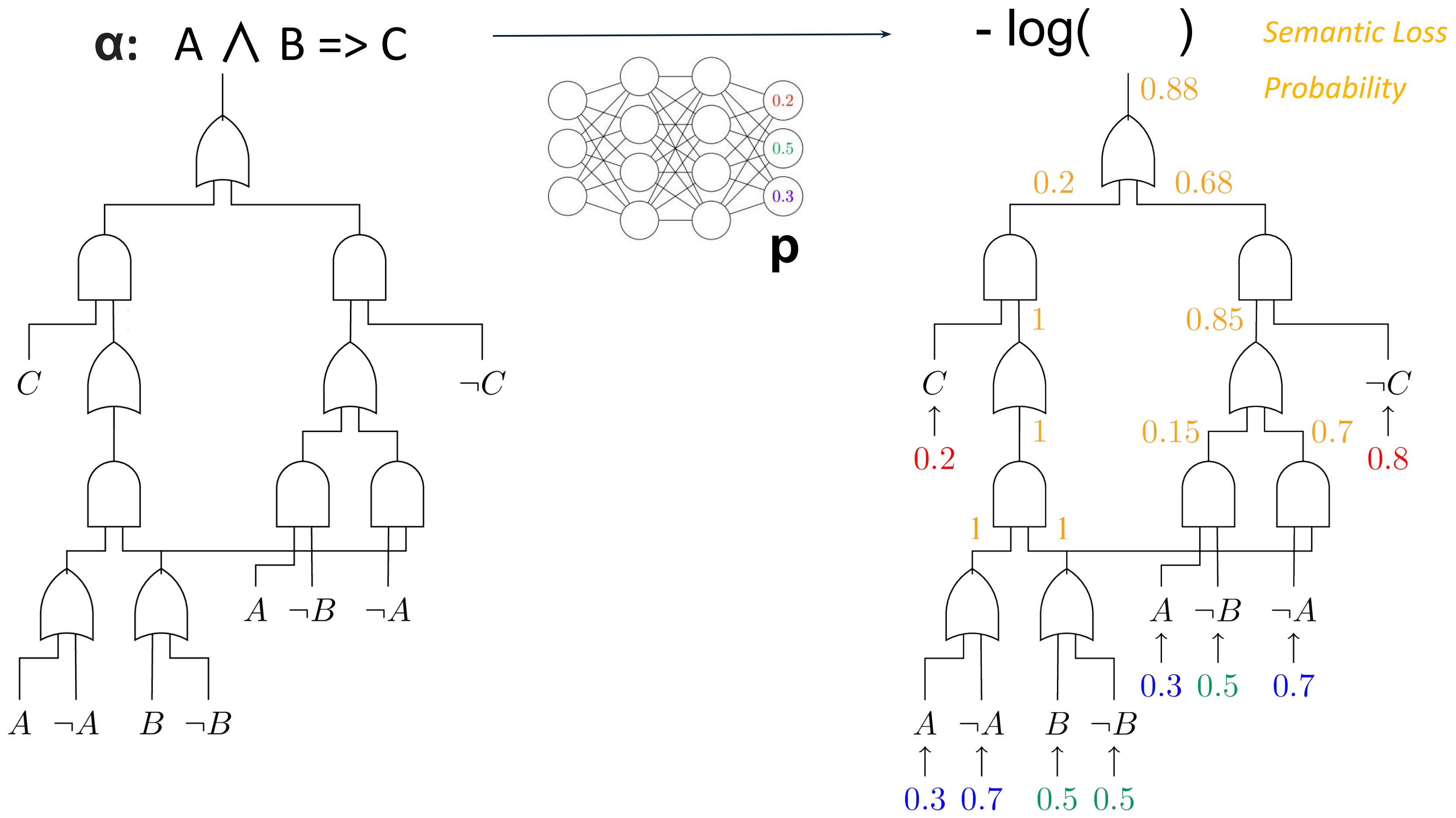
Neuro-Symbolic Learning

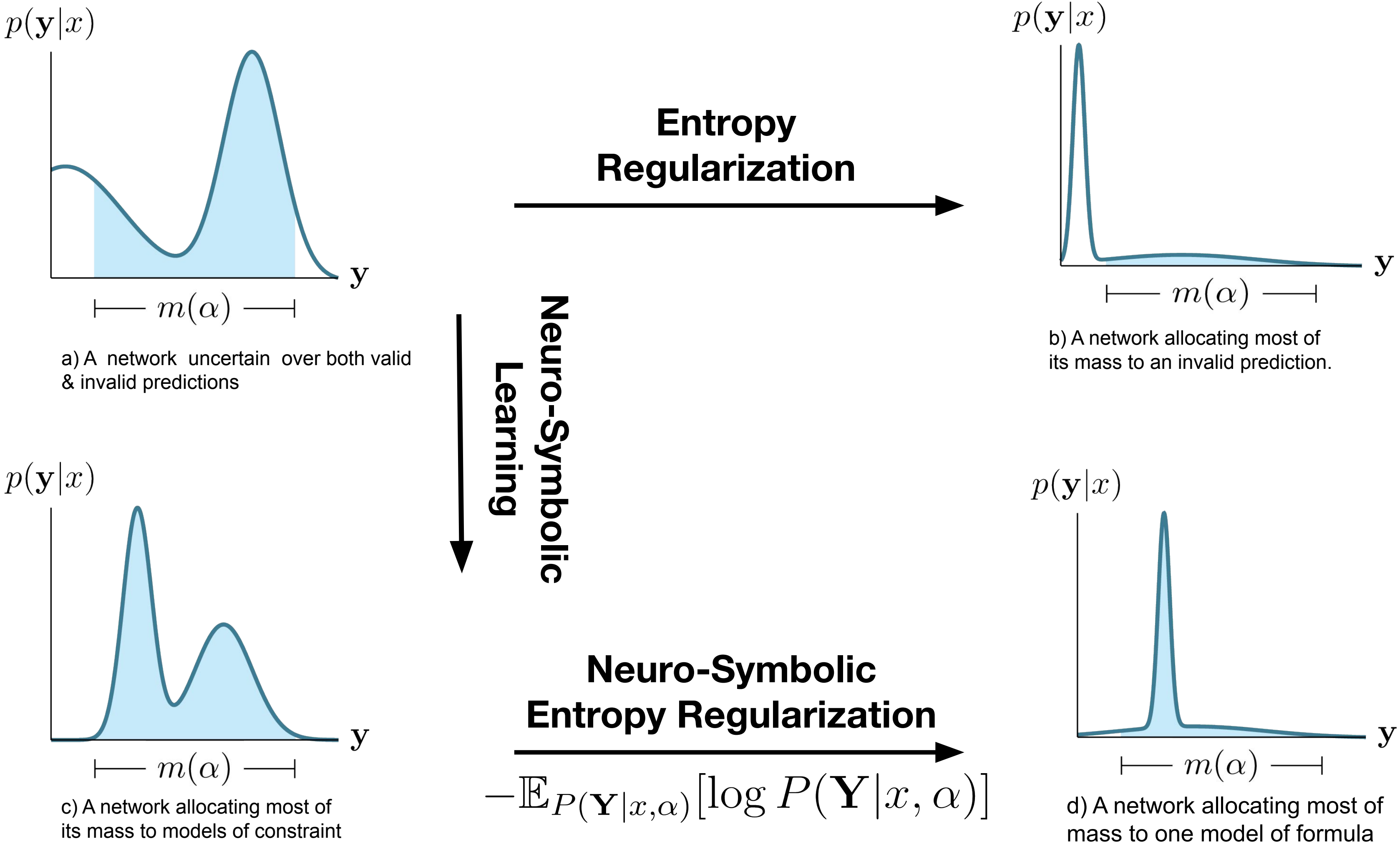
$$\mathrm{L}^{s}(\alpha, \mathsf{p}) \propto -\log \sum_{\mathbf{x} \models \alpha} \prod_{i:\mathbf{x} \models X_i} \mathsf{p}_i \prod_{i:\mathbf{x} \models \neg X_i} (1 - \mathsf{p}_i)$$

Probability of satisfying constraint α after sampling from neural net output layer **p**

In general: #P-hard ☹

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


α: A ∧ B => C
- log( )
Semantic Loss
Probability
p
0.2
0.5
0.3
0.88
0.68
1
0.85
0.15
0.7
0.8
C
¬C
A
¬A
B
¬B



$p(\mathbf{y}|x)$
$\mathbf{y}$
$m(\alpha)$
a) A network uncertain over both valid & invalid predictions
Entropy Regularization
b) A network allocating most of its mass to an invalid prediction.
Neuro-Symbolic Learning
c) A network allocating most of its mass to models of constraint
Neuro-Symbolic Entropy Regularization
$-\mathbb{E}_{P(\mathbf{Y}|x,\alpha)}[\log P(\mathbf{Y}|x,\alpha)]$
d) A network allocating most of mass to one model of formula

Warcraft min-cost simple-path prediction results

Test accuracy %	Coherent	Incoherent	Constraint
ResNet-18	44.8	97.7	56.9
Semantic loss	50.9	97.7	67.4
+ Full Entropy	51.5	97.6	67.7
+ NeSy Entropy	**55.0**	**97.9**	**69.8**

Kareem Ahmed, Eric Wang, Kai-Wei Chang and Guy Van den Broeck. Neuro-Symbolic Entropy Regularization, 2021.

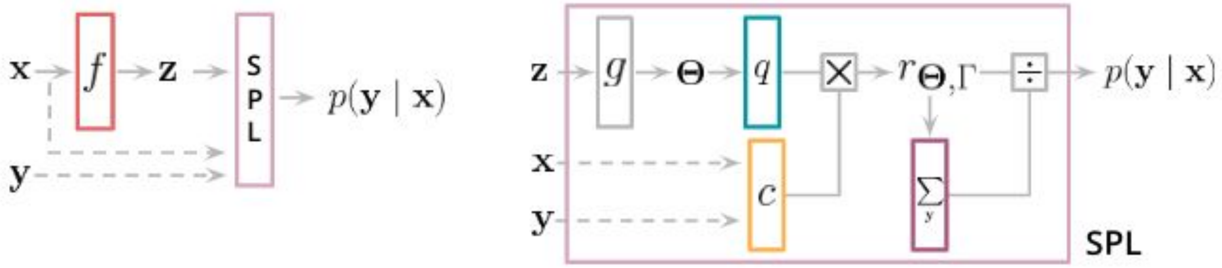
Joint entity-relation extraction in natural language processing

#		3	5	10	15	25	50	75
ACE05	Baseline	4.92 ± 1.12	7.24 ± 1.75	13.66 ± 0.18	15.07 ± 1.79	21.65 ± 3.41	28.96 ± 0.98	33.02 ± 1.17
	Self-training	7.72 ± 1.21	12.83 ± 2.97	16.22 ± 3.08	17.55 ± 1.41	27.00 ± 3.66	32.90 ± 1.71	37.15 ± 1.42
	Product t-norm	8.89 ± 5.09	14.52 ± 2.13	19.22 ± 5.81	21.80 ± 7.67	30.15 ± 1.01	34.12 ± 2.75	37.35 ± 2.53
	Semantic Loss	12.00 ± 3.81	14.92 ± 3.14	22.23 ± 3.64	27.35 ± 3.10	30.78 ± 0.68	36.76 ± 1.40	38.49 ± 1.74
	+ Full Entropy	**14.80** ± 3.70	15.78 ± 1.90	23.34 ± 4.07	28.09 ± 1.46	31.13 ± 2.26	36.05 ± 1.00	39.39 ± 1.21
	+ NeSy Entropy	14.72 ± 1.57	**18.38** ± 2.50	**26.41** ± 0.49	**31.17** ± 1.68	**35.85** ± 0.75	**37.62** ± 2.17	**41.28** ± 0.46
SciERC	Baseline	2.71 ± 1.10	2.94 ± 1.00	3.49 ± 1.80	3.56 ± 1.10	8.83 ± 1.00	12.32 ± 3.00	12.49 ± 2.60
	Self-training	3.56 ± 1.40	3.04 ± 0.90	4.14 ± 2.60	3.73 ± 1.10	9.44 ± 3.80	14.82 ± 1.20	13.79 ± 3.90
	Product t-norm	**6.50** ± 2.00	8.86 ± 1.20	10.92 ± 1.60	13.38 ± 0.70	13.83 ± 2.90	19.20 ± 1.70	19.54 ± 1.70
	Semantic Loss	6.47 ± 1.02	**9.31** ± 0.76	11.50 ± 1.53	12.97 ± 2.86	14.07 ± 2.33	20.47 ± 2.50	23.72 ± 0.38
	+ Full Entropy	6.26 ± 1.21	8.49 ± 0.85	11.12 ± 1.22	14.10 ± 2.79	17.25 ± 2.75	**22.42** ± 0.43	24.37 ± 1.62
	+ NeSy Entropy	6.19 ± 2.40	8.11 ± 3.66	**13.17** ± 1.08	**15.47** ± 2.19	**17.45** ± 1.52	22.14 ± 1.46	**25.11** ± 1.03

Kareem Ahmed, Eric Wang, Kai-Wei Chang and Guy Van den Broeck. Neuro-Symbolic Entropy Regularization, 2022.

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 again tractable circuits – computation graphs for reasoning

Kareem Ahmed, Stefano Teso, Kai-Wei Chang, Guy Van den Broeck and Antonio Vergari. Semantic Probabilistic Layers for Neuro-Symbolic Learning, 2022.

Warcraft Shortest Path

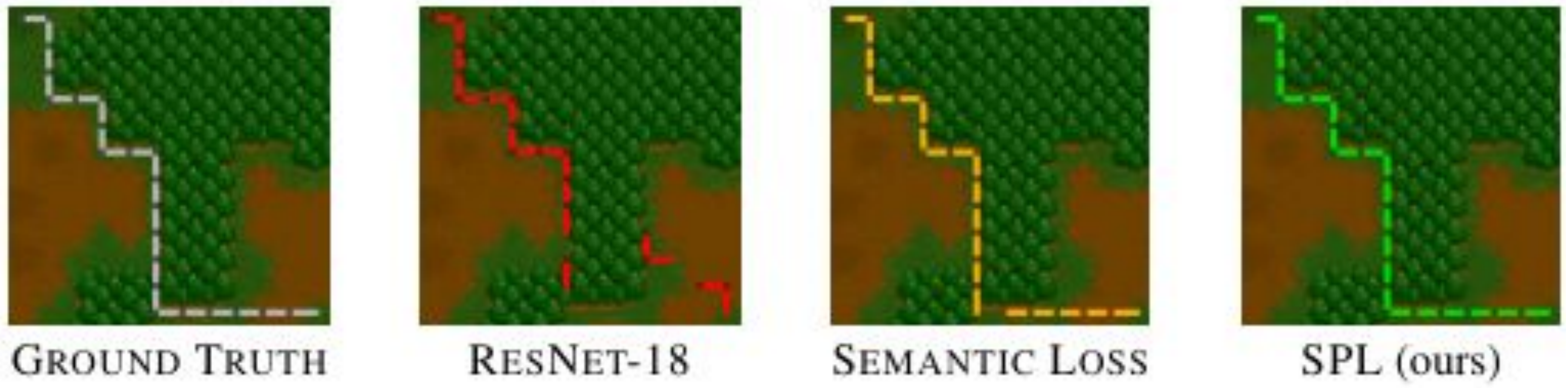
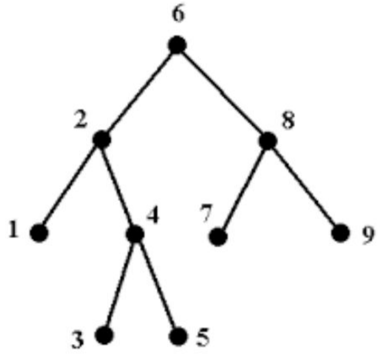


Table 3: Warcraft shortest path prediction results

ARCHITECTURE	EXACT MATCH	HAMMING SCORE	CONSISTENCY
RESNET-18+FIL	55.0	**97.7**	56.9
RESNET-18+$\mathcal{L}_{\text{SL}}$	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	$\mathbf{3.79 \pm 0.18}$
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	$\mathbf{81.06 \pm 0.68}$

Outline

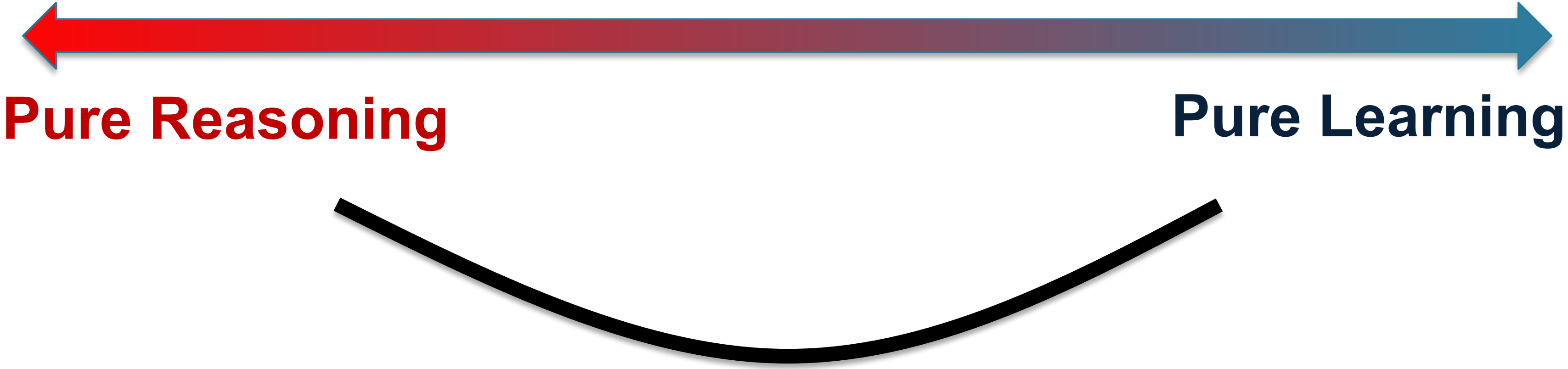
1. The paradox of learning to reason from data

   ~~deep learning~~

2. Learning with symbolic knowledge

   logical (and probabilistic) reasoning + deep learning

The AI Dilemma

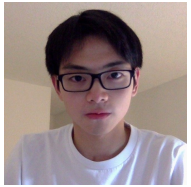


Integrate reasoning into modern deep learning algorithms

- Knowledge is (hidden) everywhere in ML
- A little bit of reasoning goes a long way!

Thanks

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



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