End-to-End Differentiable Proving

Tim Rocktäschel

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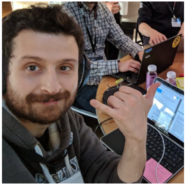
Logic and Learning Workshop at The Alan Turing Institute

January 12, 2018

Joint Work With

Sebastian Riedel
University College London



Pasquale Minervini
University College London

Thomas Demeester
Ghent University

Sameer Singh
University of California, Irvine

What vegetable is on the plate?
Neural Net: broccoli
Ground Truth: broccoli

What color are the shoes on the person's feet ?
Neural Net: brown
Ground Truth: brown

How many school busses are there?
Neural Net: 2
Ground Truth: 2

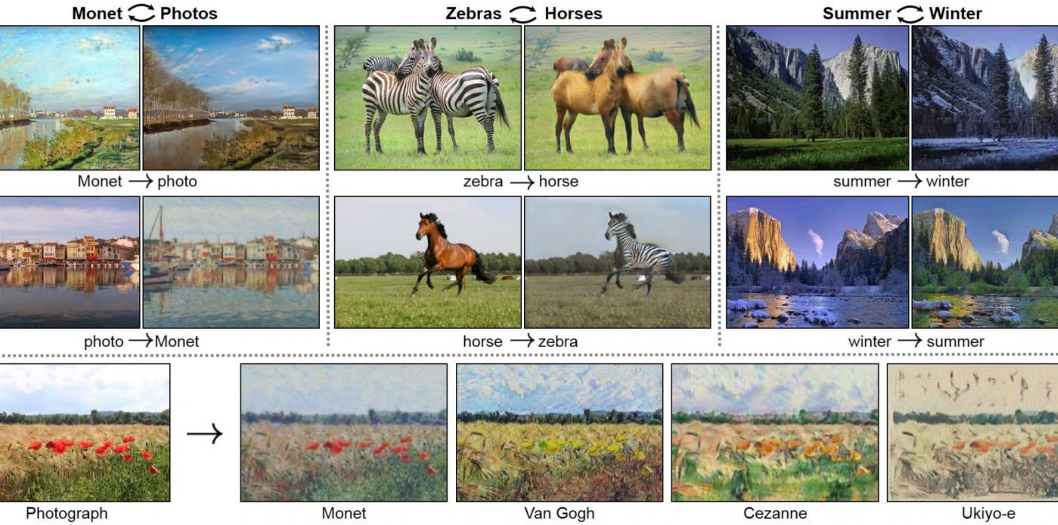
What sport is this?
Neural Net: baseball
Ground Truth: baseball

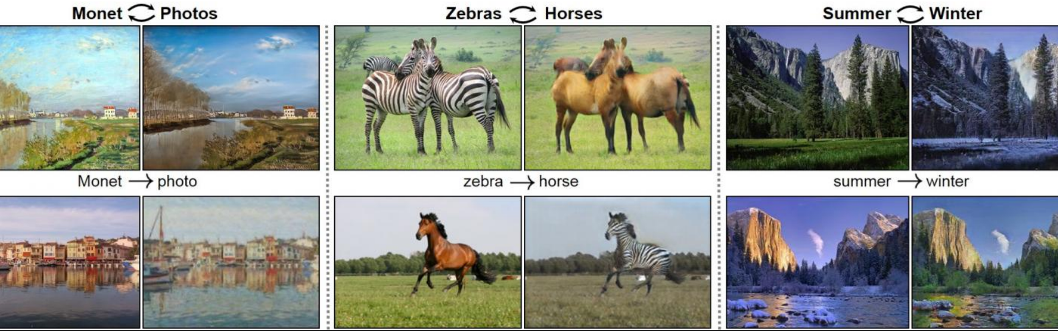
What is on top of the refrigerator?
Neural Net: magnets
Ground Truth: cereal

What uniform is she wearing?
Neural Net: shorts
Ground Truth: girl scout

What is the table number?
Neural Net: 4
Ground Truth:40

What are people sitting under in the back?
Neural Net: bench
Ground Truth: tent


Monet ⇄ Photos
Zebras ⇄ Horses
Summer ⇄ Winter
Monet → photo
zebra → horse
summer → winter
photo → Monet
horse → zebra
winter → summer
Photograph
Monet
Van Gogh
Cezanne
Ukiyo-e



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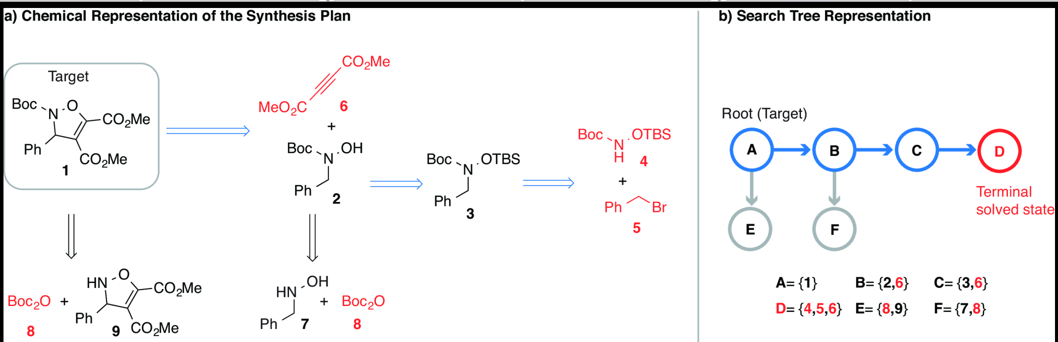
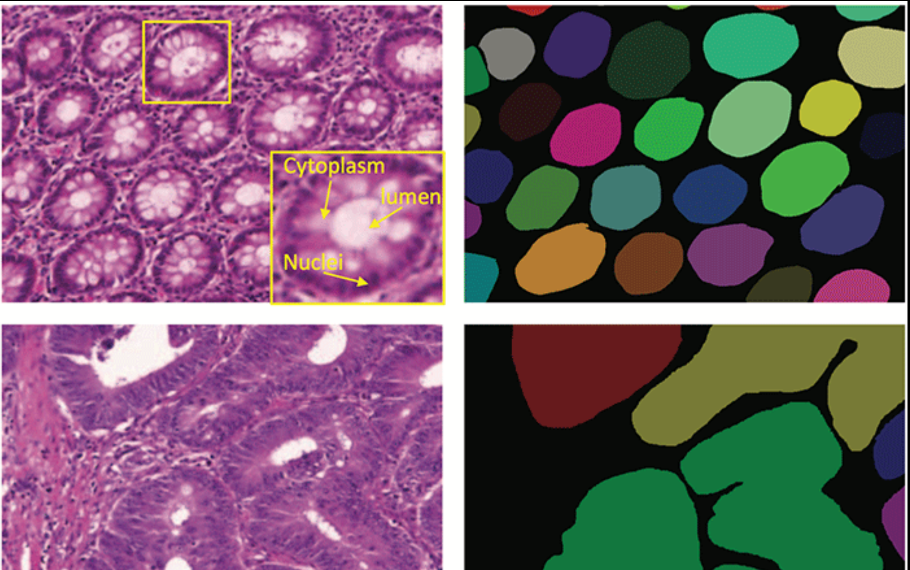
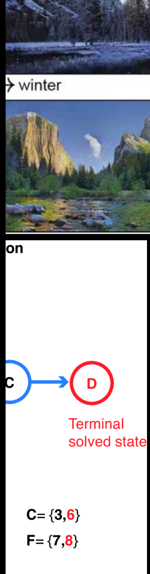
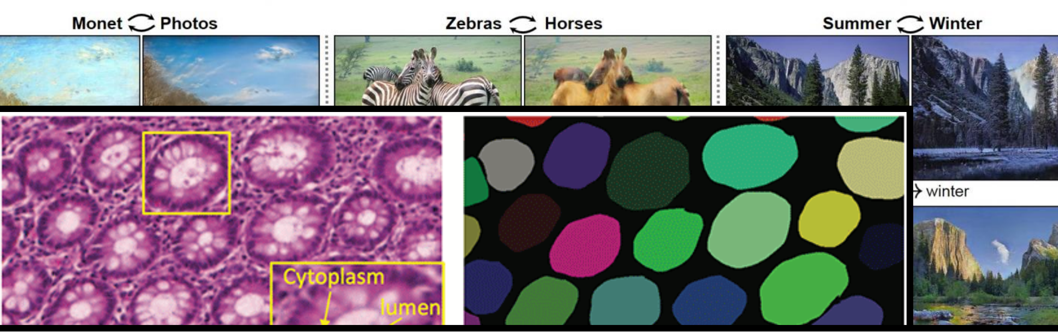


a) Chemical Representation of the Synthesis Plan
Target
Boc
N
O
CO_2Me
Ph
CO_2Me
1
CO_2Me
MeO_2C
6
+
Boc
N
OH
Ph
2
Boc
N
OTBS
Ph
3
Boc
N
H
OTBS
4
+
Ph
Br
5
Boc_2O
8
+
HN
O
CO_2Me
Ph
9
CO_2Me
HN
OH
Ph
7
+
Boc_2O
8
b) Search Tree Representation
Root (Target)
A
B
C
D
E
F
Terminal solved state
A= {1}
B= {2,6}
C= {3,6}
D= {4,5,6}
E= {8,9}
F= {7,8}


Monet Photos
Zebras Horses
Summer Winter


Cytoplasm
lumen
Nuclei


winter
on
C
D
Terminal
solved state
C= {3,6}
F= {7,8}



Translate from **GERMAN** (detected)

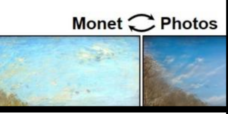
Translate into **ENGLISH**

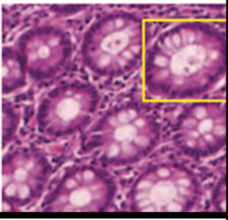
Die Polizei in den USA darf sich wieder schwere Ausrüstung und Waffen beim Militär besorgen. Das hat US-Präsident Donald Trump entschieden und so eine Anordnung seines Vorgängers Barack Obama aufgehoben, nach der es dem Verteidigungsministerium verboten war, die Polizei mit Granatwerfern, gepanzerten Fahrzeugen, Bajonetten, großkalibrigen Waffen und Munition auszurüsten.

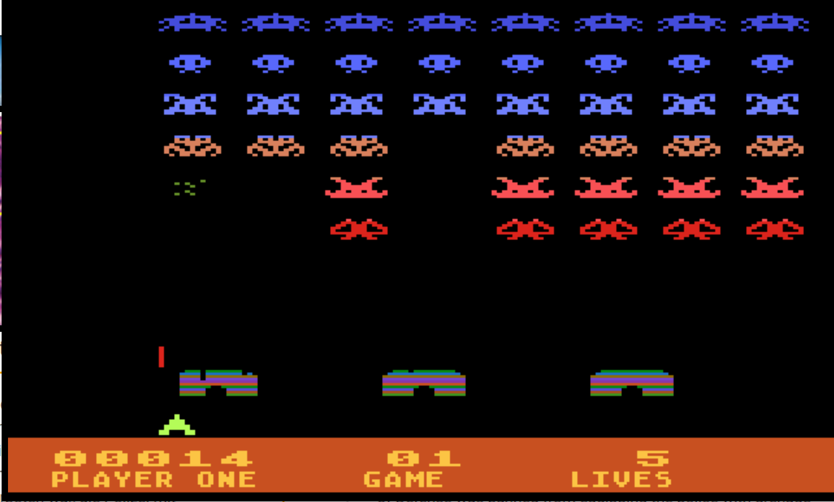
Mit der Maßnahme soll sichergestellt werden, dass die Polizei die lebensrettende Ausrüstung bekomme, die sie brauche, um ihren Job zu machen, sagte US-Justizminister Jeff Sessions.

The police in the USA are allowed to get heavy equipment and weapons from the military again. This was decided by US President Donald Trump, who overturned an order from his predecessor Barack Obama, according to which the Department of Defense was banned from equipping the police with grenade launchers, armoured vehicles, bayonets, large-calibre weapons and ammunition.

The measure is designed to ensure that the police get the life-saving equipment they need to do their job, US Attorney General Jeff Sessions said.







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XKCD, 17th May 2017

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Explanations

- Rules
- (Partial) Programs
- Natural Language

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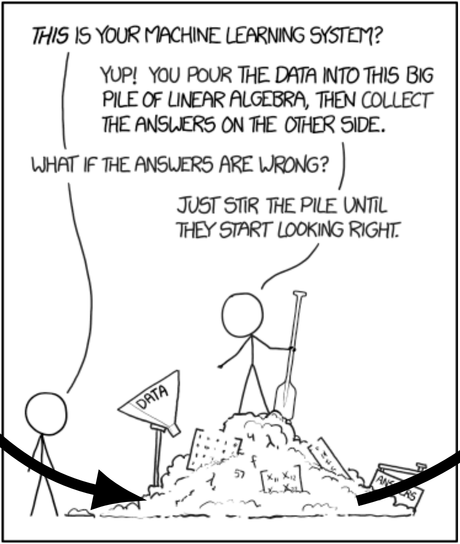

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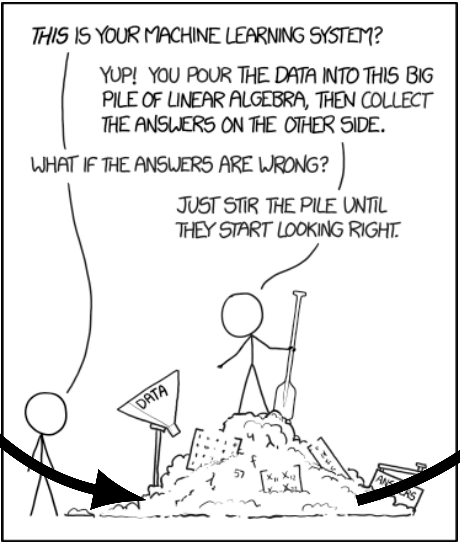

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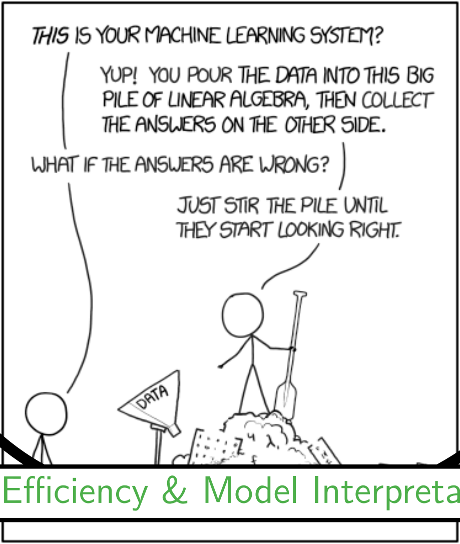

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Data Efficiency & Model Interpretability

Lecture Notes

PROLOG AND NATURAL-LANGUAGE ANALYSIS

Fernando C.N. Pereira
and
Stuart M. Shieber

CSLI CENTER FOR THE STUDY OF LANGUAGE AND INFORMATION

```
goal problem.

rule 1
  if not turn_over and
    battery_bad
  then problem is battery cf 100.

rule 2
  if lights_weak
  then battery_bad cf 50.

rule 3
  if radio_weak
  then battery_bad cf 50.

rule 4
 if turn_over and
    smell_gas
  then problem is flooded cf 80.

rule 5
  if turn_over and
    gas_gauge is empty
  then problem is out_of_gas cf 90.

rule 6
  if turn_over and
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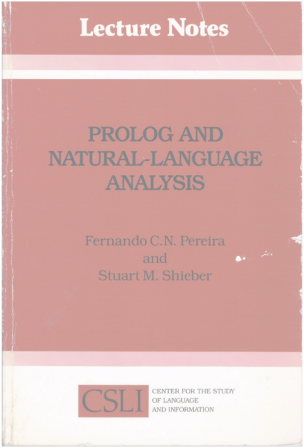

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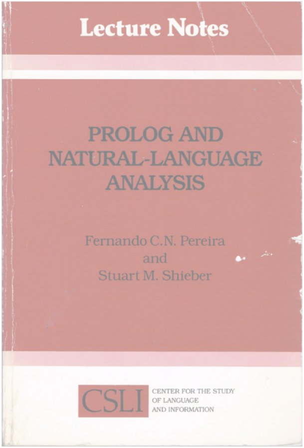

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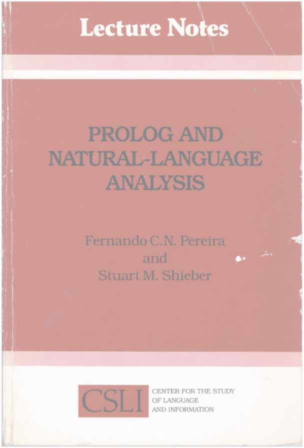

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- Rules manually defined
- No generalization

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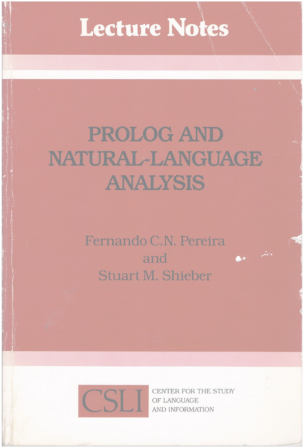

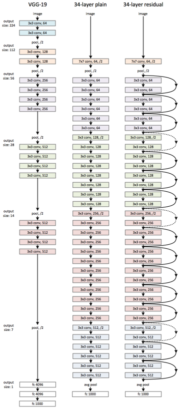

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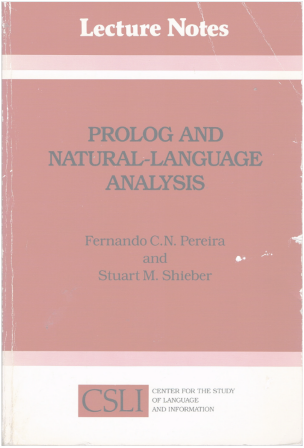

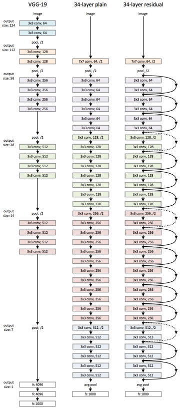

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Neural Networks

- Trained end-to-end
- Strong generalization

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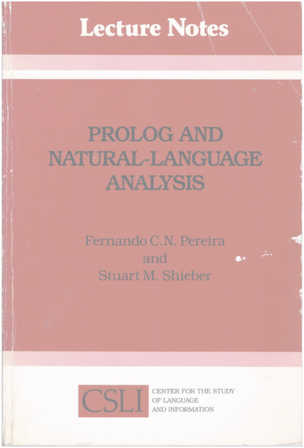

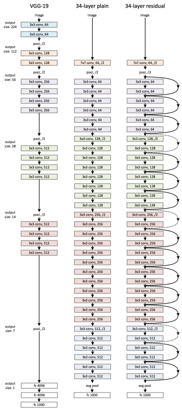

Expert Systems

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- Interpretable
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Neural Networks

- Need a lot of training data
- Not interpretable
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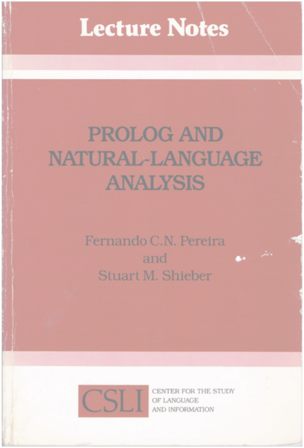

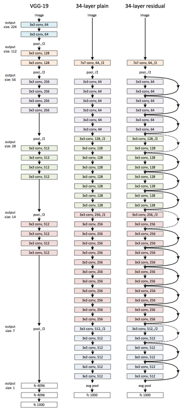

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For overviews see Besold et al. (2017) and d'Avila Garcez et al. (2012)

Outline

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4. Outlook & Summary

Notation

- **Constant**: HOMER, BART, LISA etc. (lowercase)

Notation

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- **Fact**: ground rule (no free variables) with empty body, e.g.,
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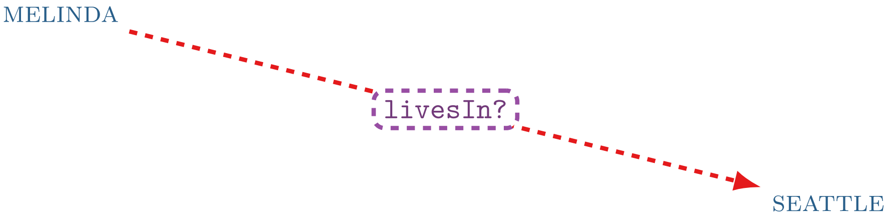

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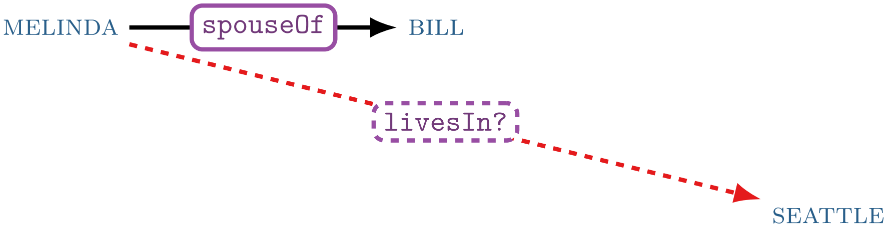

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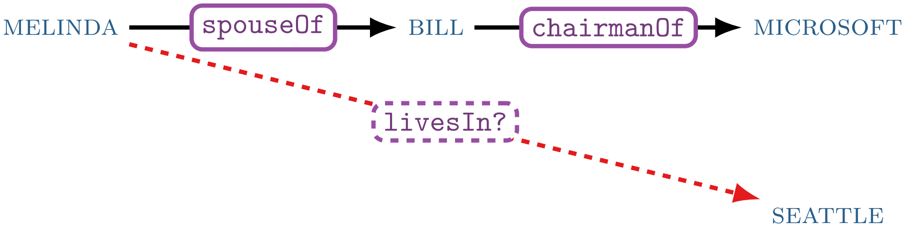

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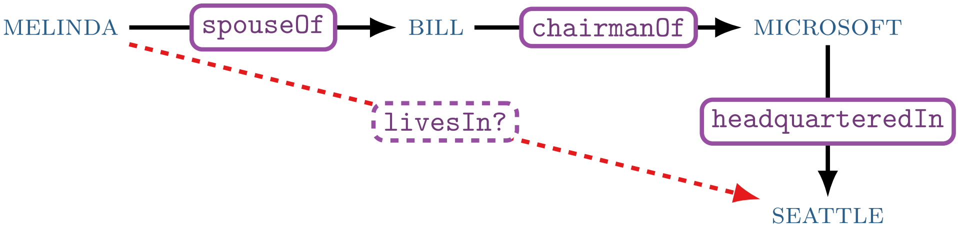

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- Fairly easy to debug and trivial to incorporate domain knowledge:
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$$\texttt{livesIn}(\text{MELINDA}, \text{SEATTLE})? = f_{\boldsymbol{\theta}}(\boldsymbol{v}_{\texttt{livesIn}}, \boldsymbol{v}_{\text{MELINDA}}, \boldsymbol{v}_{\text{SEATTLE}})$$

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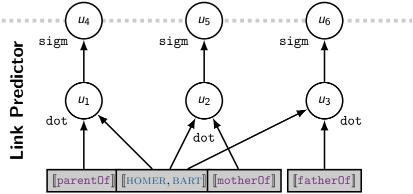
- Obtain gradients $\nabla_{\boldsymbol{v}_s}\mathfrak{L}$, $\nabla_{\boldsymbol{v}_i}\mathfrak{L}$, $\nabla_{\boldsymbol{v}_j}\mathfrak{L}$ by backprop

Regularization by Propositional Logic



Rocktäschel et al. (2015), NAACL

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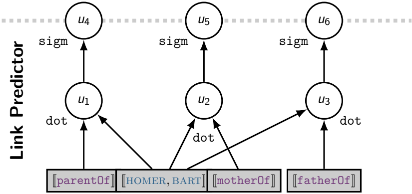

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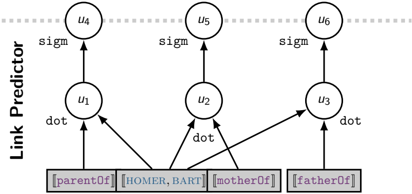

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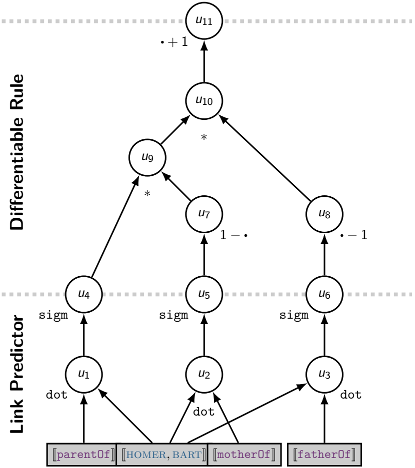

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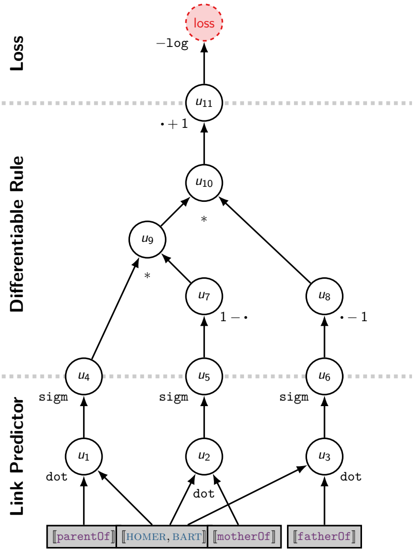


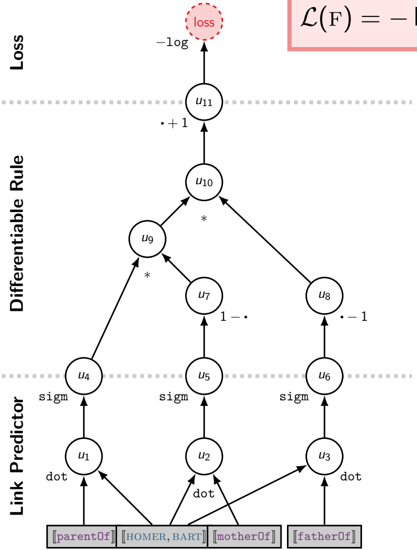
$$\mathtt{fatherOf}(\mathrm{X},\mathrm{Y}) \text{ :– } \mathtt{parentOf}(\mathrm{X},\mathrm{Y}), \neg\,\mathtt{motherOf}(\mathrm{X},\mathrm{Y})$$

$$p(F) = [\![F]\!] = \begin{cases} f_\theta(s,i,j) & \text{if } F = s(i,j) \\ 1 - [\![A]\!] & \text{if } F = \neg A \\ [\![A]\!]\,[\![B]\!] & \text{if } F = A \wedge B \\ [\![A]\!] + [\![B]\!] - [\![A]\!]\,[\![B]\!] & \text{if } F = A \vee B \\ [\![B]\!]\,([\![A]\!] - 1) + 1 & \text{if } F = A \text{ :– } B \end{cases}$$

$$\mathcal{L}\Big([\![\mathtt{fatherOf}(\mathrm{HOMER},\mathrm{BART}) \text{ :– } \mathtt{parentOf}(\mathrm{HOMER},\mathrm{BART}) \wedge \neg\,\mathtt{motherOf}(\mathrm{HOMER},\mathrm{BART})]\!]\Big)$$

Rocktäschel et al. (2015), NAACL

Regularization by Propositional Logic



$$\boxed{\mathcal{L}(\mathrm{F}) = -\log\left(\llbracket \forall \mathrm{X}, \mathrm{Y} : \mathrm{F}(\mathrm{X}, \mathrm{Y}) \rrbracket\right) = -\sum_{(e_i, e_j) \in \mathcal{C}^2} \log \llbracket \mathrm{F}(e_i, e_j) \rrbracket}$$

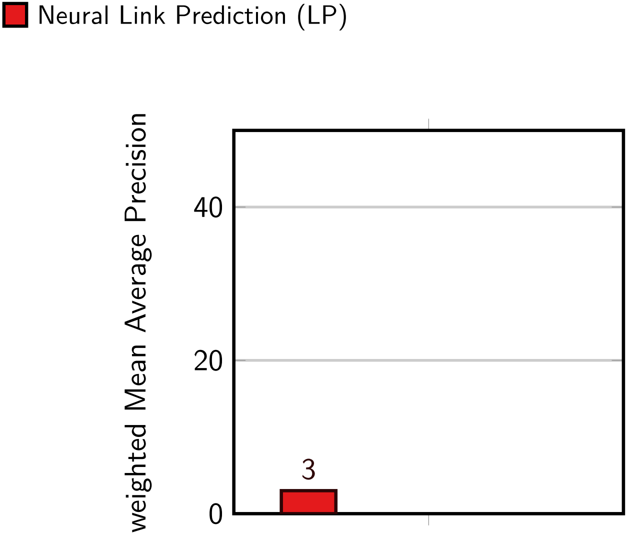
$$\texttt{fatherOf}(\mathrm{X}, \mathrm{Y}) :\!- \texttt{parentOf}(\mathrm{X}, \mathrm{Y}), \neg\, \texttt{motherOf}(\mathrm{X}, \mathrm{Y})$$

$$p(F) = \llbracket F \rrbracket = \begin{cases} f_\theta(s, i, j) & \text{if } F = s(i, j) \\ 1 - \llbracket A \rrbracket & \text{if } F = \neg A \\ \llbracket A \rrbracket \llbracket B \rrbracket & \text{if } F = A \wedge B \\ \llbracket A \rrbracket + \llbracket B \rrbracket - \llbracket A \rrbracket \llbracket B \rrbracket & \text{if } F = A \vee B \\ \llbracket B \rrbracket (\llbracket A \rrbracket - 1) + 1 & \text{if } F = A :\!- B \end{cases}$$

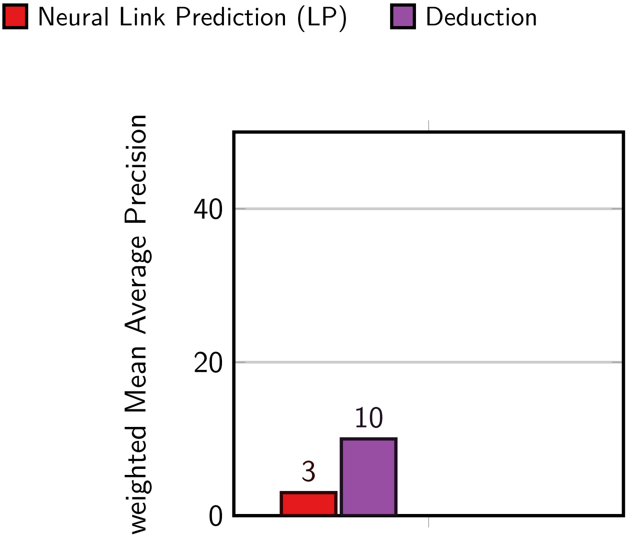
$$\mathcal{L}\Big(\llbracket \texttt{fatherOf}(\mathrm{HOMER}, \mathrm{BART}) :\!- \texttt{parentOf}(\mathrm{HOMER}, \mathrm{BART}) \wedge \neg\, \texttt{motherOf}(\mathrm{HOMER}, \mathrm{BART}) \rrbracket\Big)$$

Rocktäschel et al. (2015), NAACL

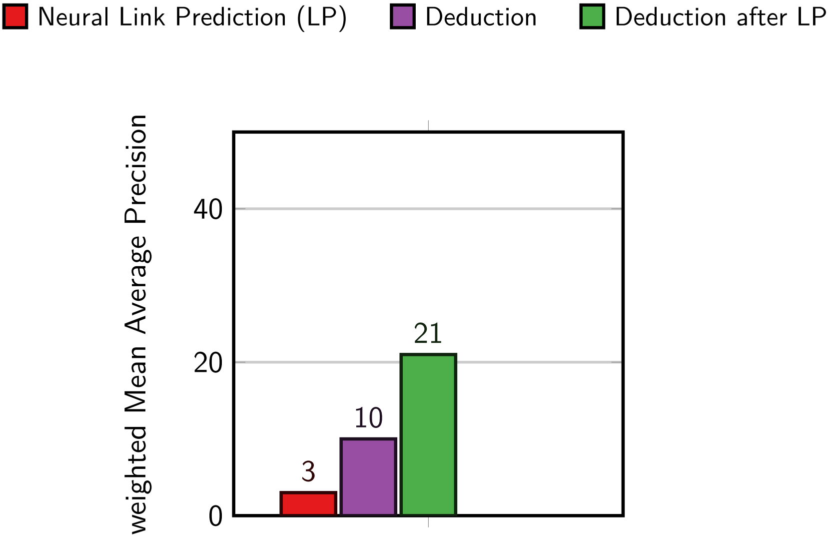
Zero-shot Learning Results



Zero-shot Learning Results



Zero-shot Learning Results



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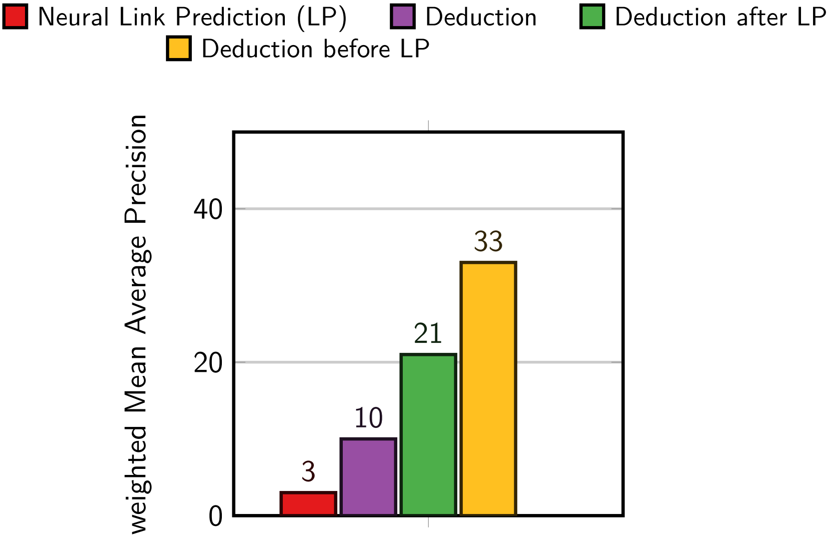
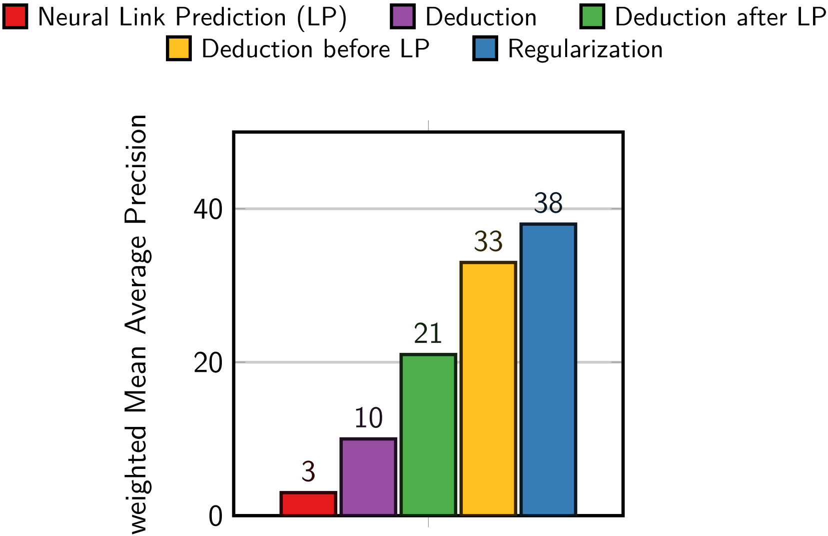
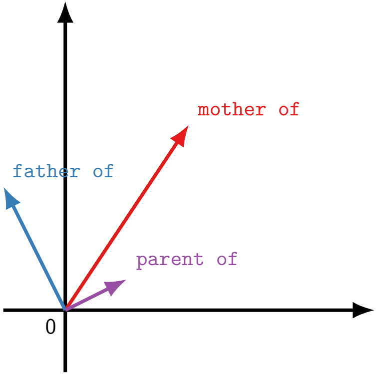


Zero-shot Learning Results



Lifted Regularization by Implications

Every father is a parent
Every mother is a parent



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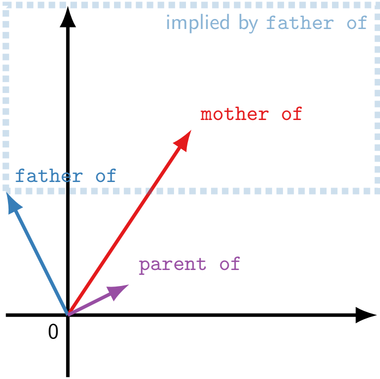

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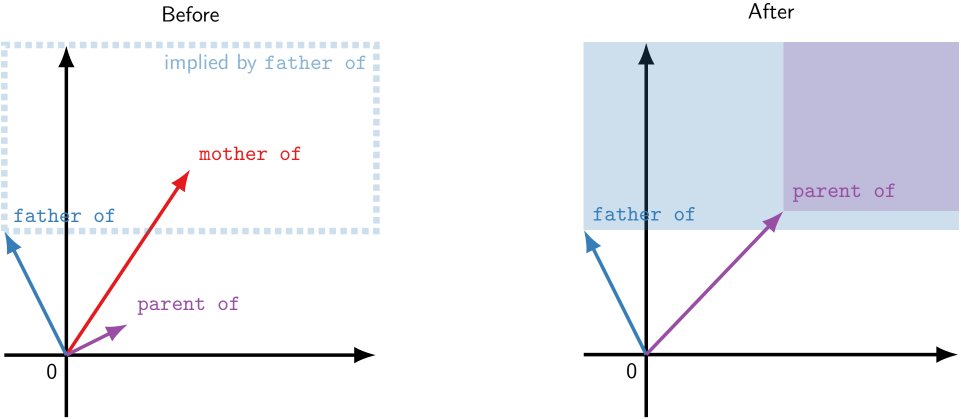

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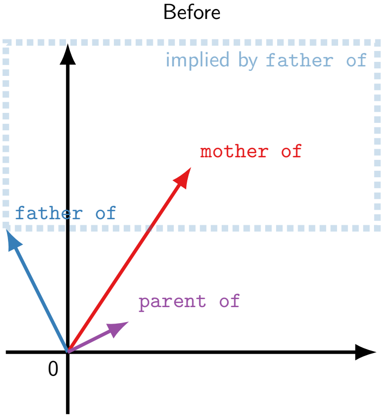
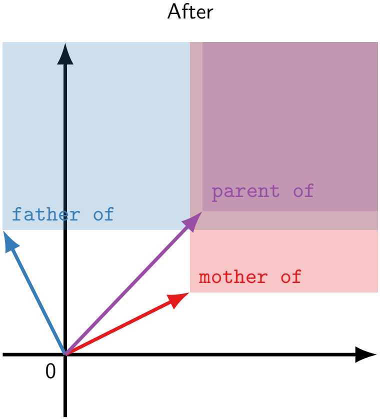
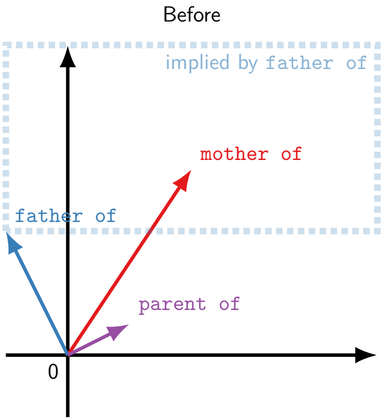
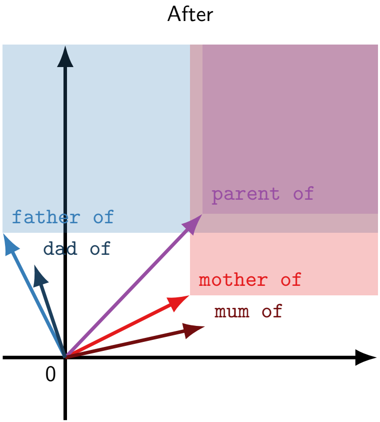




Lifted Regularization by Implications

Every father is a parent Generalises to similar relations (*e.g.* dad)
Every mother is a parent Generalises to similar relations (*e.g.* mum)



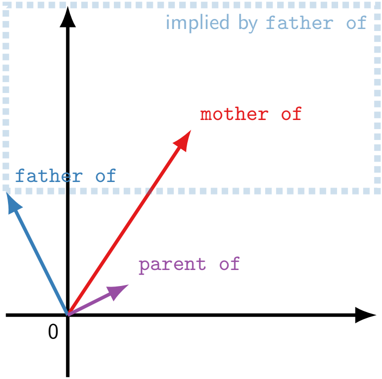


Demeester et al. (2016), EMNLP

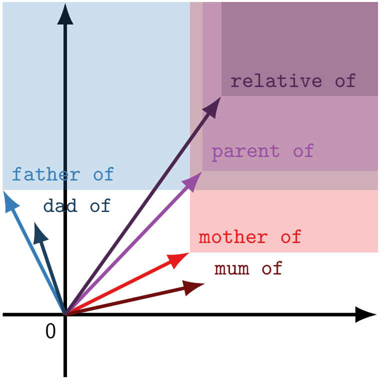
Lifted Regularization by Implications

Every father is a parent	Generalises to similar relations (*e.g.* dad)
Every mother is a parent	Generalises to similar relations (*e.g.* mum)
Every parent is a relative	**No training facts needed!**

Before



After

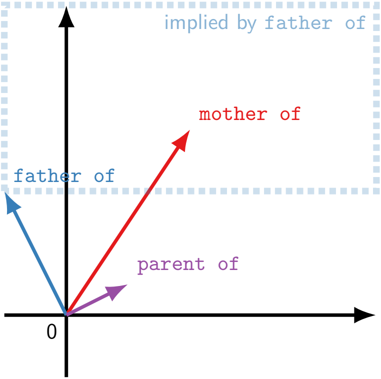


Lifted Regularization by Implications

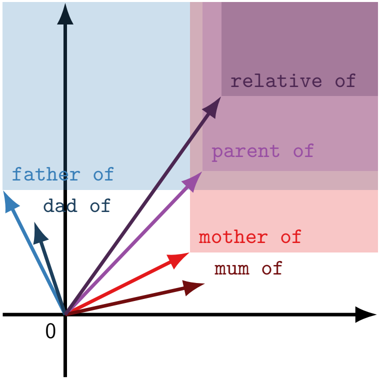
Every father is a parent
Every mother is a parent
Every parent is a relative

$$\forall \mathrm{X}, \mathrm{Y} \;:\; \mathtt{h}(\mathrm{X}, \mathrm{Y}) \coloneq \mathtt{b}(\mathrm{X}, \mathrm{Y})$$
$$\forall (e_i, e_j) \in \mathcal{C}^2 : [\![\mathtt{h}]\!]^\top [\![e_i, e_j]\!] \geq [\![\mathtt{b}]\!]^\top [\![e_i, e_j]\!]$$
$$[\![\mathtt{h}]\!] \geq [\![\mathtt{b}]\!], \quad \forall (e_i, e_j) \in \mathcal{C}^2 : [\![e_i, e_j]\!] \in \mathbb{R}_+^k$$

Before

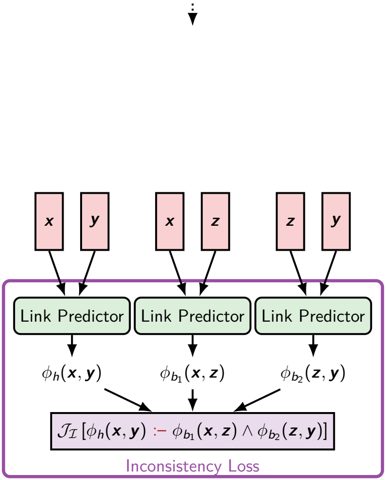


After



Adversarial Regularization

Clause $\mathcal{A}$: $h(\mathrm{X}, \mathrm{Y}) \coloneq b_1(\mathrm{X}, \mathrm{Z}) \wedge b_2(\mathrm{Z}, \mathrm{Y})$

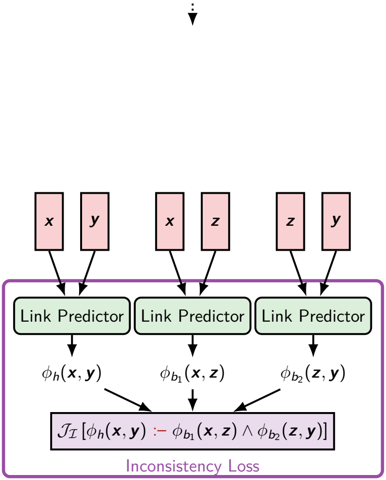


- Regularization by propositional rules needs grounding – does not scale to large domains!

Minervini et al. (2017), UAI

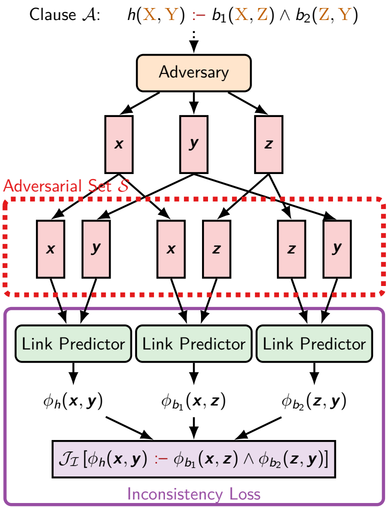
Adversarial Regularization

Clause $\mathcal{A}$: $h(\mathrm{X}, \mathrm{Y}) :- b_1(\mathrm{X}, \mathrm{Z}) \wedge b_2(\mathrm{Z}, \mathrm{Y})$



- Regularization by propositional rules needs grounding – does not scale to large domains!
- Lifted regularization only supports direct implications

Adversarial Regularization



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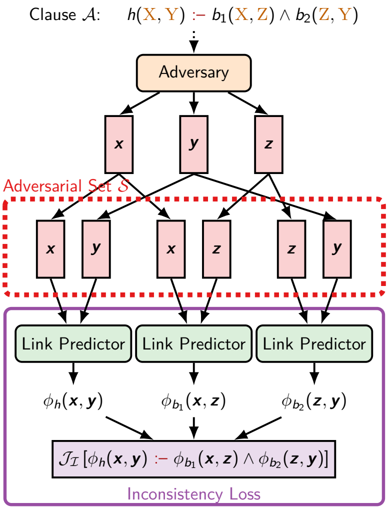
- Lifted regularization only supports direct implications
- Idea: let grounding be generated by an adversary and optimize minimax game...

Minervini et al. (2017), UAI

Adversarial Regularization



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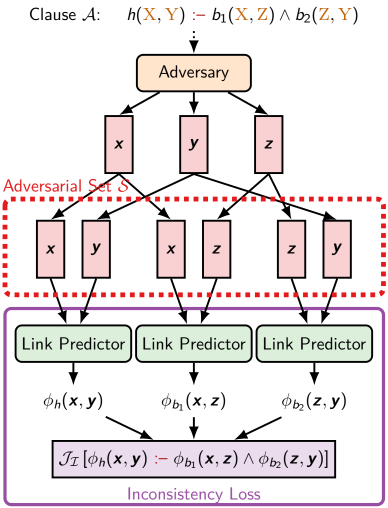
- Adversary finds maximally violating grounding for a given rule

Adversarial Regularization



- Regularization by propositional rules needs grounding – does not scale to large domains!
- Lifted regularization only supports direct implications
- Idea: let grounding be generated by an adversary and optimize minimax game...
- Adversary finds maximally violating grounding for a given rule
- Neural link predictor attempts to minimize rule violation for given generated groundings

Minervini et al. (2017), UAI

End-to-End Differentiable Prover

- Neural network for proving queries to a knowledge base

End-to-End Differentiable Prover

- Neural network for proving queries to a knowledge base
- Proof success differentiable w.r.t. vector representations of symbols

End-to-End Differentiable Prover

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- **Learn vector representations of symbols** end-to-end from proof success

Rocktäschel and Riedel (2017), NIPS

End-to-End Differentiable Prover

- Neural network for proving queries to a knowledge base
- Proof success differentiable w.r.t. vector representations of symbols
- **Learn vector representations of symbols** end-to-end from proof success
- **Make use of provided rules** in soft proofs

End-to-End Differentiable Prover

- Neural network for proving queries to a knowledge base
- Proof success differentiable w.r.t. vector representations of symbols
- **Learn vector representations of symbols** end-to-end from proof success
- **Make use of provided rules** in soft proofs
- **Induce interpretable rules** end-to-end from proof success

Rocktäschel and Riedel (2017), NIPS

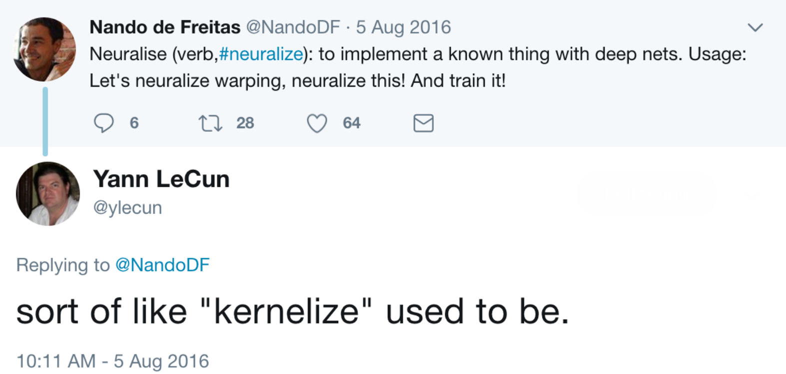
Approach


Nando de Freitas @NandoDF · 5 Aug 2016

Neuralise (verb,#neuralize): to implement a known thing with deep nets. Usage: Let's neuralize warping, neuralize this! And train it!

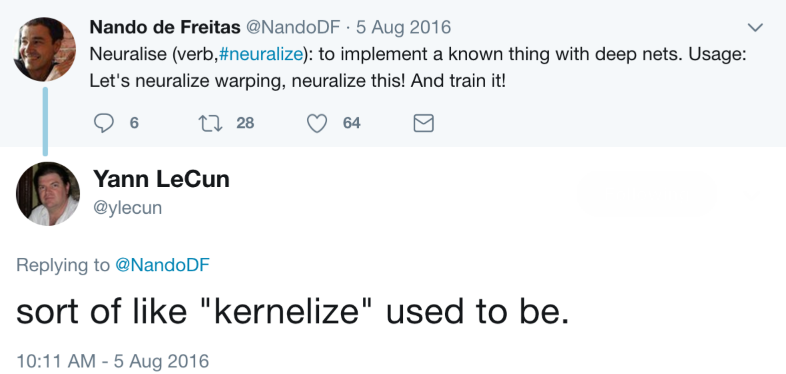
6 28 64

Approach



Nando de Freitas @NandoDF · 5 Aug 2016
Neuralise (verb,#neuralize): to implement a known thing with deep nets. Usage: Let's neuralize warping, neuralize this! And train it!
6
28
64
Yann LeCun
@ylecun
Replying to @NandoDF
sort of like "kernelize" used to be.
10:11 AM - 5 Aug 2016

Approach



Let's **neuralize** Prolog's Backward Chaining using a Radial Basis Function **kernel** for unifying vector representations of symbols!

Prolog's Backward Chaining

Example Knowledge Base:

1. `fatherOf`(ABE, HOMER).
2. `parentOf`(HOMER, BART).
3. `grandfatherOf`(X, Y) :–
   `fatherOf`(X, Z),
   `parentOf`(Z, Y).

Prolog's Backward Chaining

Example Knowledge Base:

1. $\texttt{fatherOf}(\textsc{abe}, \textsc{homer})$.
2. $\texttt{parentOf}(\textsc{homer}, \textsc{bart})$.
3. $\texttt{grandfatherOf}(X, Y)$:–
   $\texttt{fatherOf}(X, Z)$,
   $\texttt{parentOf}(Z, Y)$.

Intuition:

- Backward chaining translates a query into subqueries via rules, *e.g.*,
  $\texttt{grandfatherOf}(\textsc{abe}, \textsc{bart}) \xrightarrow{3.} \texttt{fatherOf}(\textsc{abe}, Z), \texttt{parentOf}(Z, \textsc{bart})$

Prolog's Backward Chaining

Example Knowledge Base:

1. $\texttt{fatherOf}(\text{ABE}, \text{HOMER})$.
2. $\texttt{parentOf}(\text{HOMER}, \text{BART})$.
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Intuition:

- Backward chaining translates a query into subqueries via rules, *e.g.*,
  $\texttt{grandfatherOf}(\text{ABE}, \text{BART}) \xrightarrow{\boxed{3.}} \texttt{fatherOf}(\text{ABE}, Z), \texttt{parentOf}(Z, \text{BART})$
- It attempts this for all rules in the knowledge base and thus specifies a depth-first search

Unification

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
2. parentOf(HOMER, BART).
3. grandfatherOf(X, Y) :–
   fatherOf(X, Z),
   parentOf(Z, Y).

Query

grandfatherOf ABE BART

Unification

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
2. parentOf(HOMER, BART).
3. grandfatherOf(X, Y) :–
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Query

grandfatherOf	ABE	BART

1.

fatherOf	ABE	HOMER

Unification

Example Knowledge Base:

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2. parentOf(HOMER, BART).
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Query

grandfatherOf	ABE	BART
$\stackrel{?}{=}$	$\stackrel{?}{=}$	$\stackrel{?}{=}$
fatherOf	ABE	HOMER

1.

Unification

Example Knowledge Base:

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2. parentOf(HOMER, BART).
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Query

	grandfatherOf	ABE	BART
	$\stackrel{?}{=}$	$\stackrel{?}{=}$	$\stackrel{?}{=}$
1.	fatherOf	ABE	HOMER
	FAIL	SUCCESS	FAIL

Unification

Example Knowledge Base:

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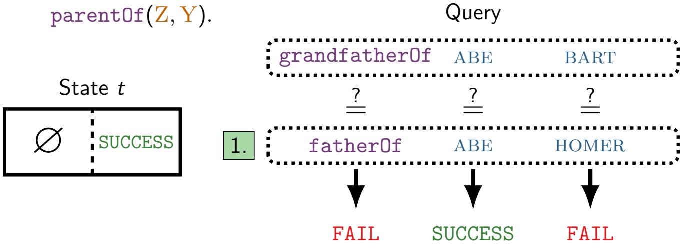

Unification

Example Knowledge Base:

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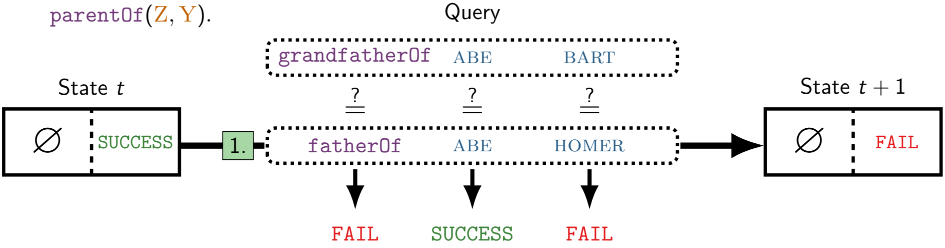

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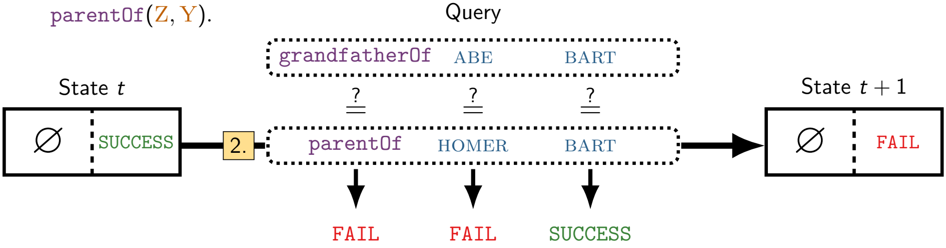

Unification

Example Knowledge Base:

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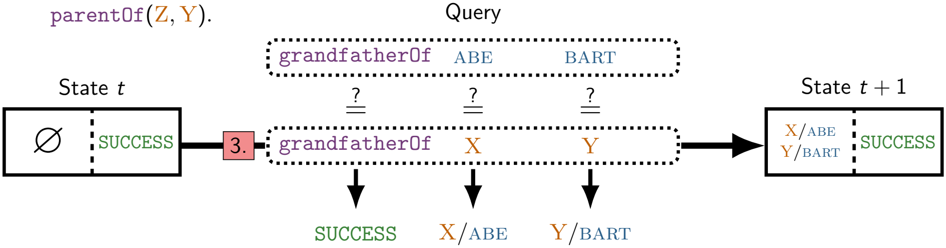

Unification Failure

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
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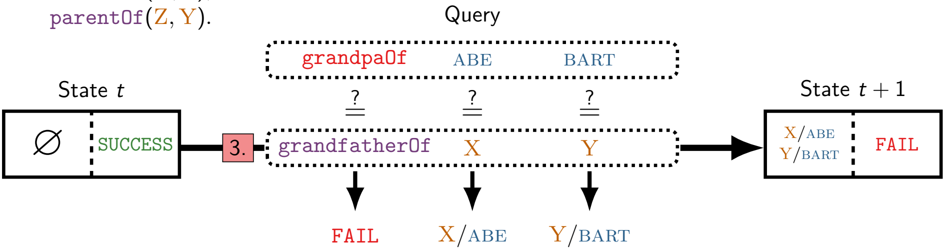

Neural Unification

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
2. parentOf(HOMER, BART).
3. grandfatherOf(X, Y) :–
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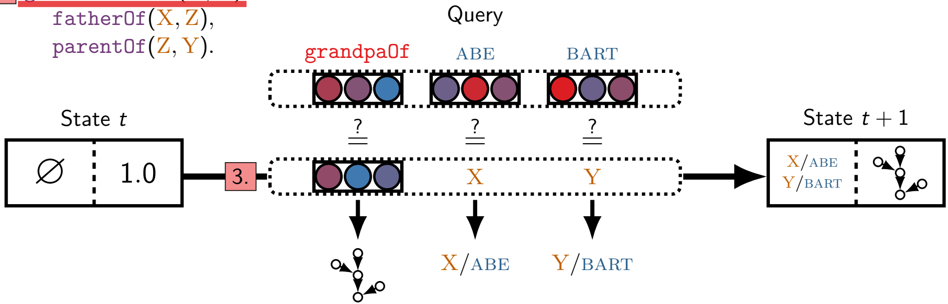

Neural Unification

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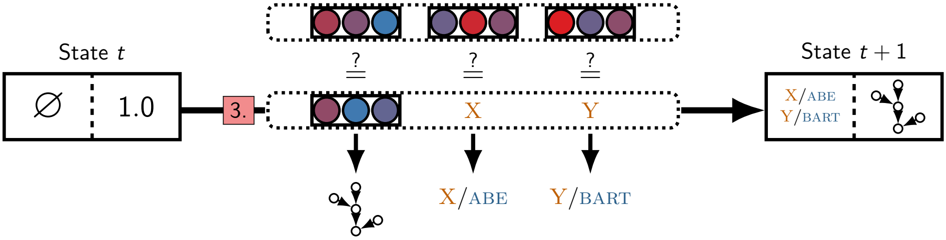

$$\min\left(1.0, \exp\left(\frac{-\|\mathbf{v}_{\texttt{grandpaOf}} - \mathbf{v}_{\texttt{grandfatherOf}}\|_2}{2\mu^2}\right)\right)$$

Differentiable Prover

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
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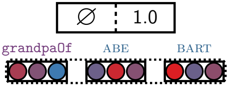

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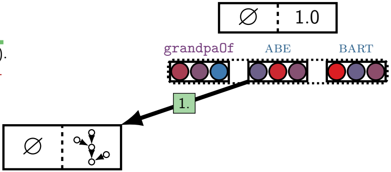

Differentiable Prover

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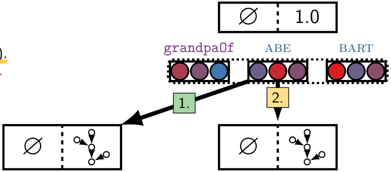

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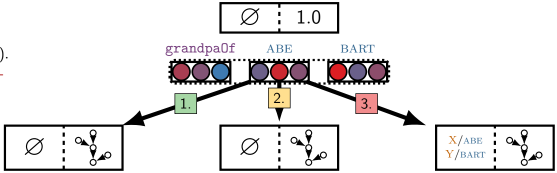

3.1 fatherOf(X, Z)
3.2 parentOf(Z, Y)

Differentiable Prover

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
2. parentOf(HOMER, BART).
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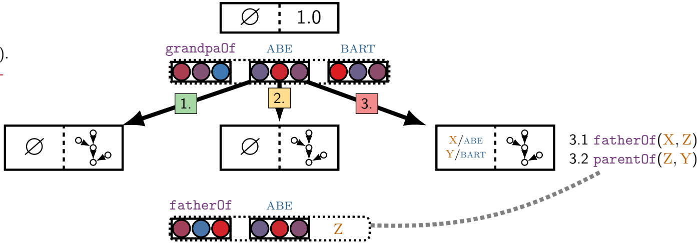

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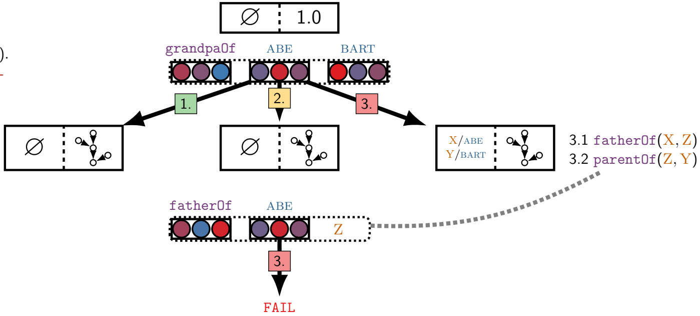

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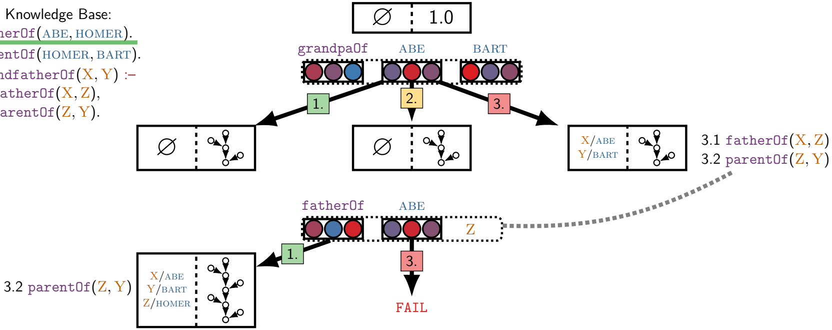

Differentiable Prover

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
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3. grandfatherOf(X, Y) :–
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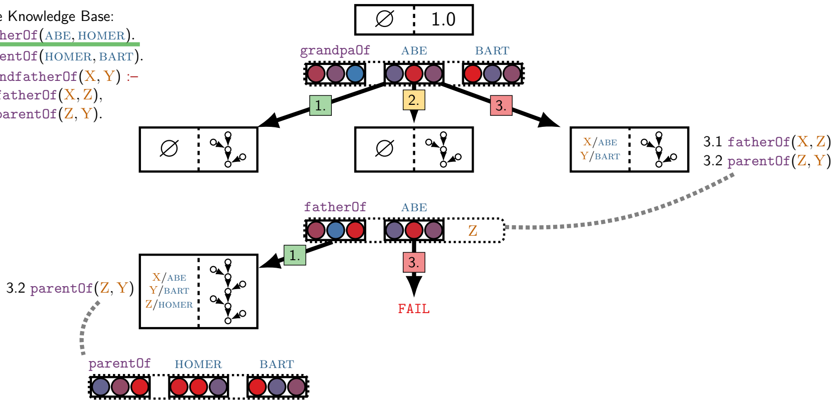

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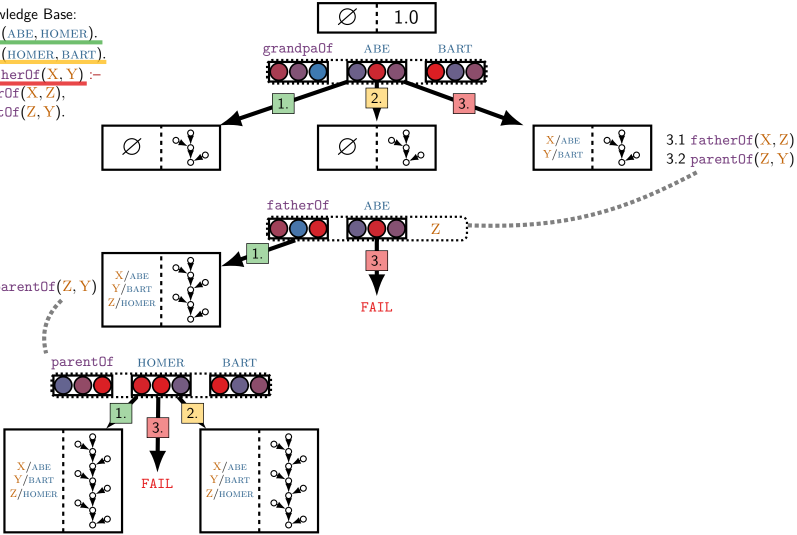

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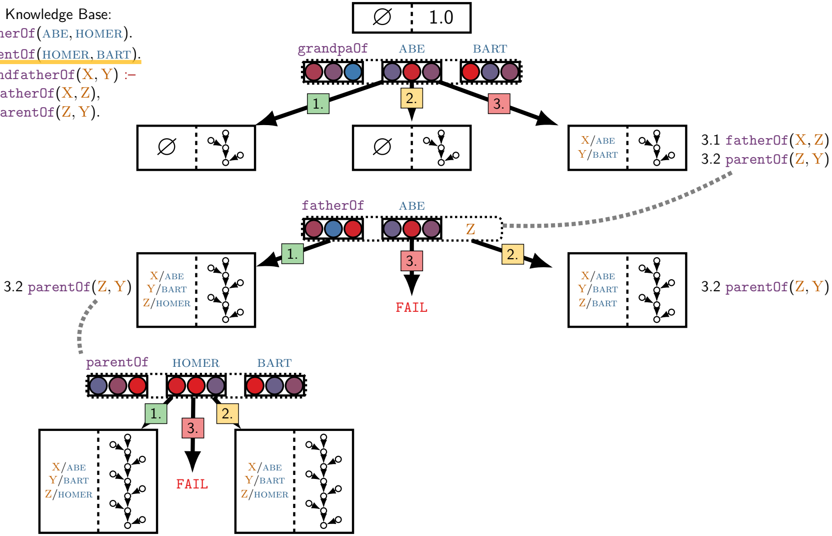

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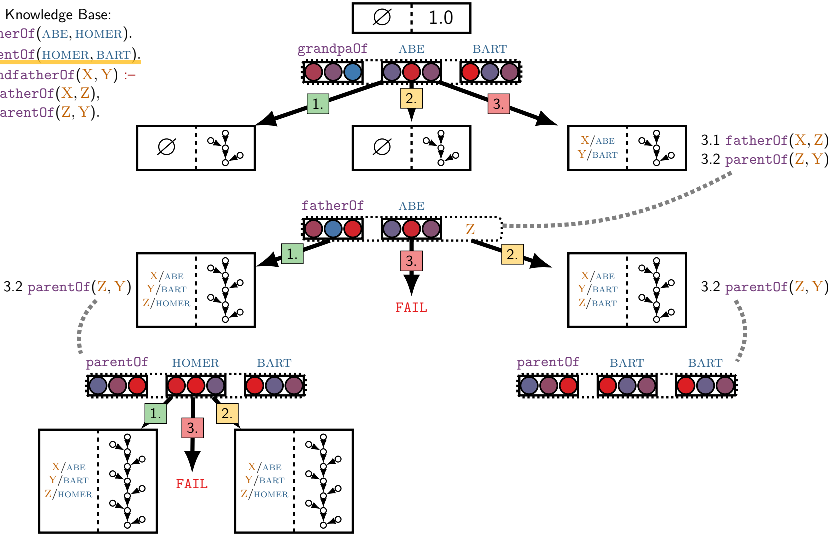

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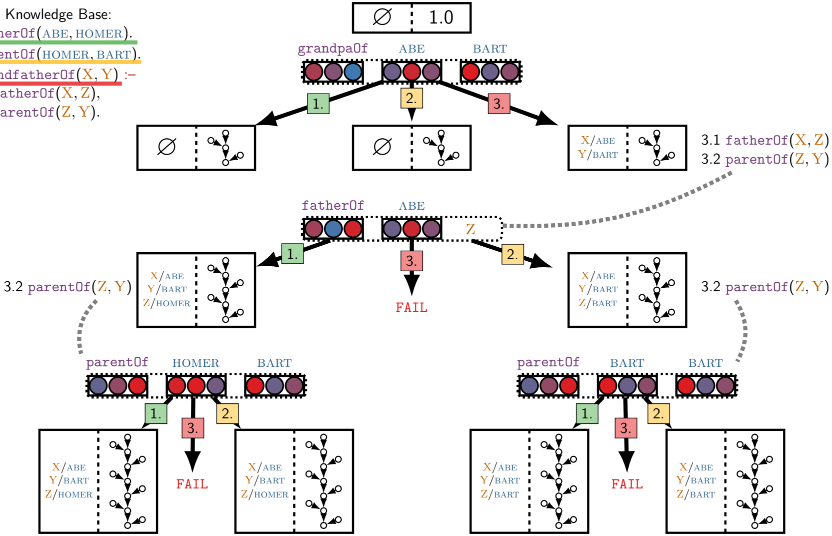

Neural Program Induction

Example Knowledge Base:

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3. grandfatherOf(X, Y) :–
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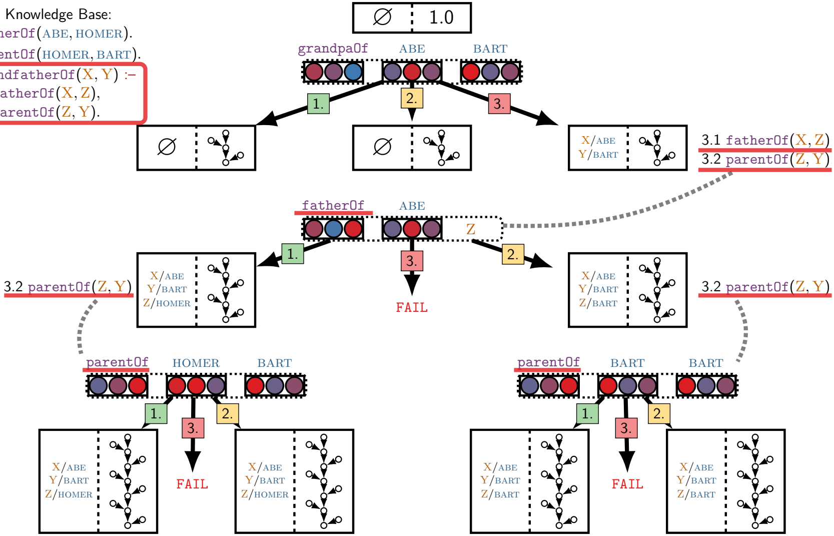
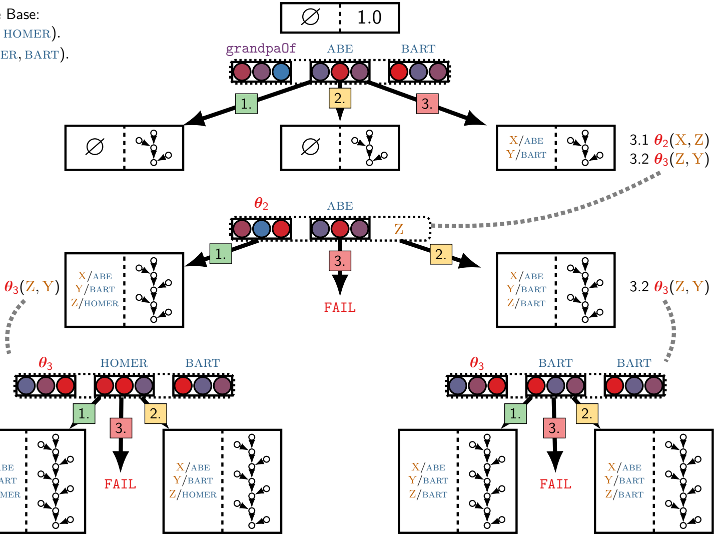


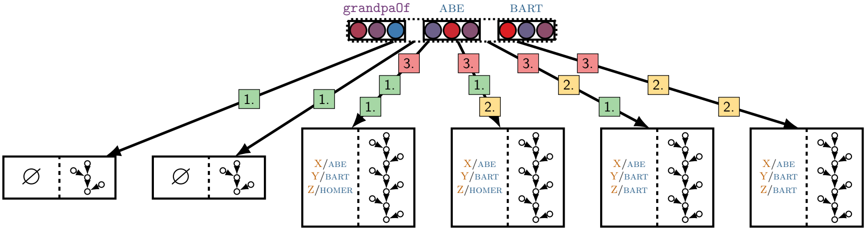
Neural Program Induction

Example Knowledge Base:

1. fatherOf(ABE, HOMER).
2. parentOf(HOMER, BART).
3. $\theta_1(X, Y)$:–
   $\theta_2(X, Z)$,
   $\theta_3(Z, Y)$.



Training Objective



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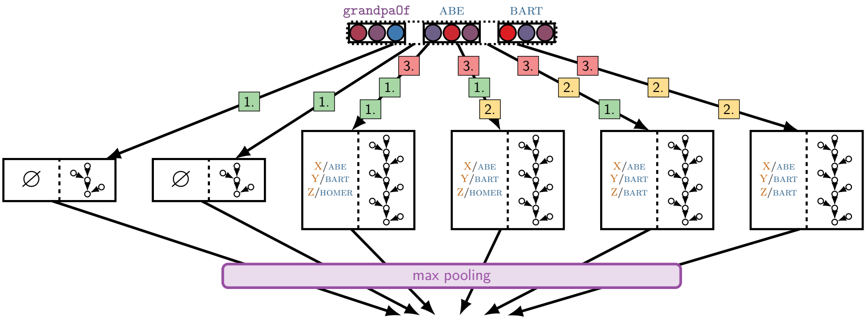
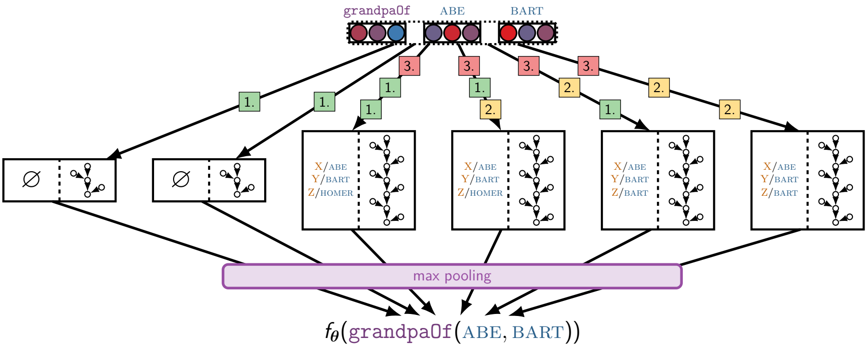


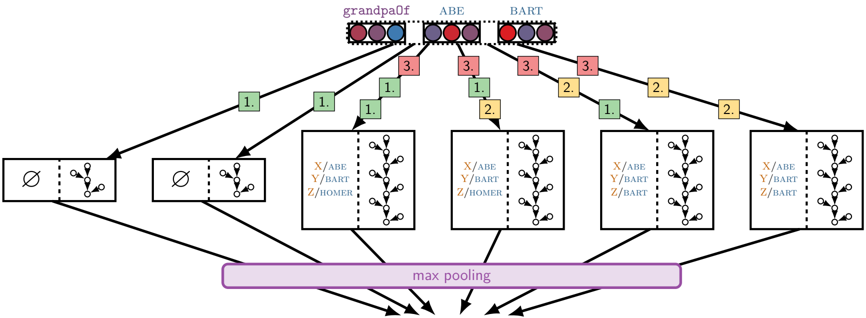
$f_\theta(\texttt{grandpaOf}(\text{ABE}, \text{BART}))$

Training Objective



- Loss: negative log-likelihood w.r.t. target proof success

Training Objective



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- Trained end-to-end using stochastic gradient descent

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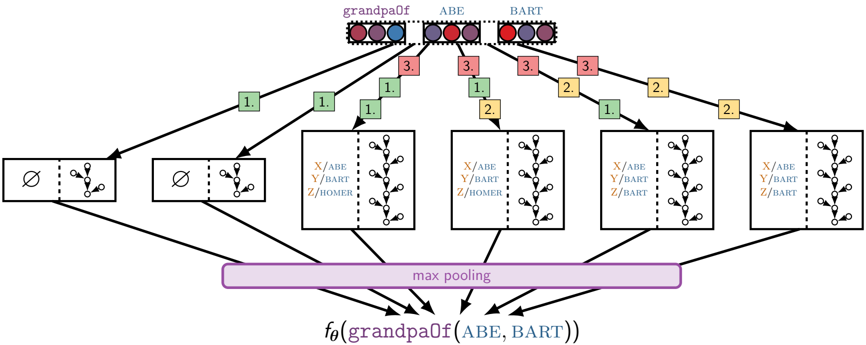
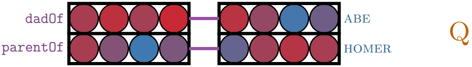


- Loss: negative log-likelihood w.r.t. target proof success
- Trained end-to-end using stochastic gradient descent
- Vectors are **learned such that proof success is high for known facts** and low for sampled negative facts

Calculation on GPU



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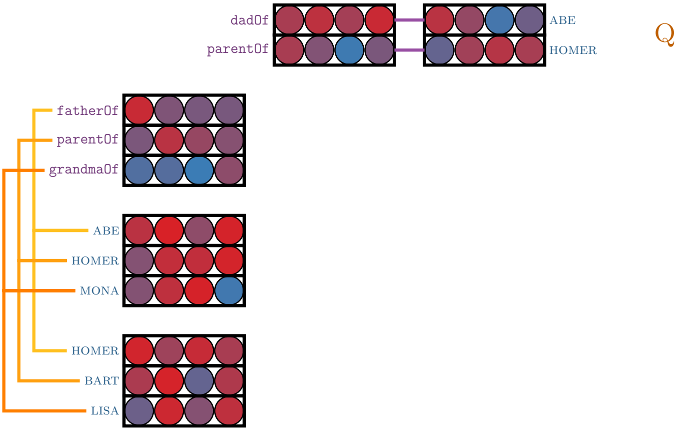

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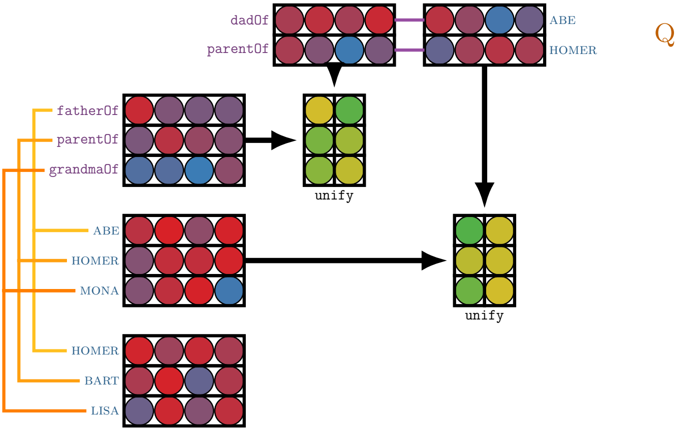

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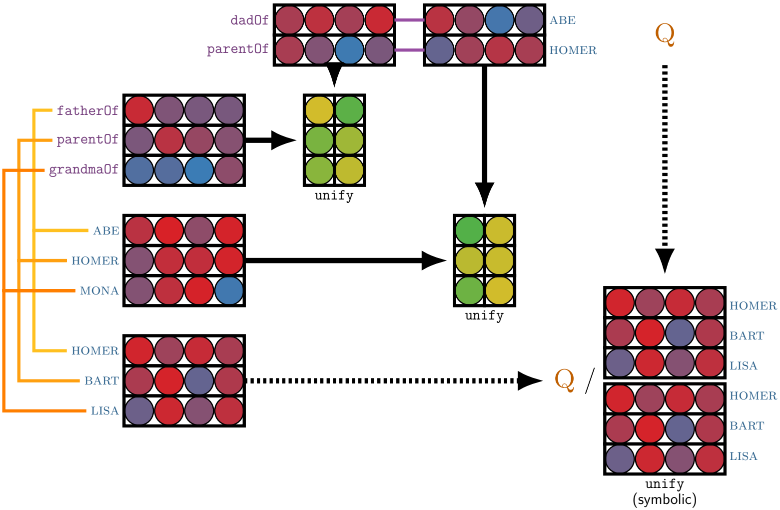

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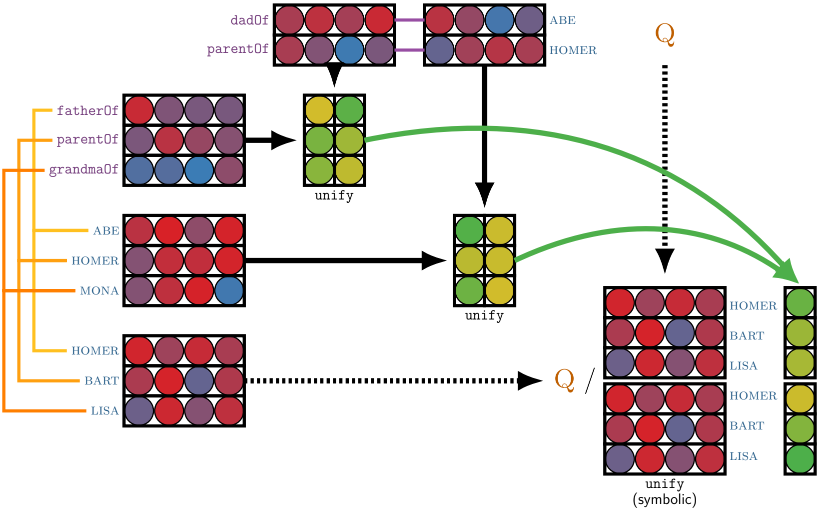
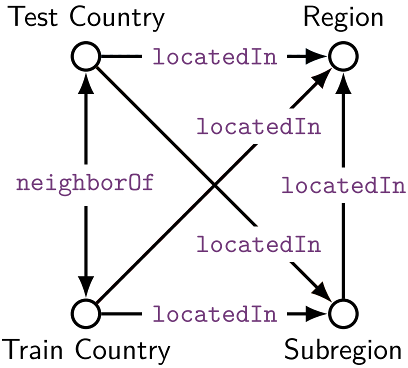
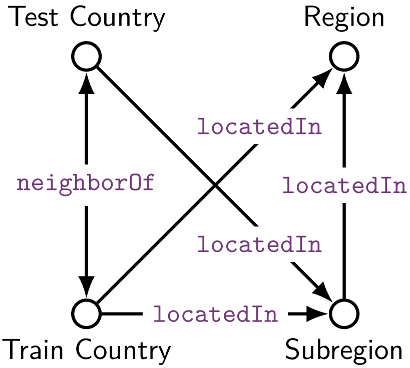


Experiments

Benchmark Knowledge Bases: **Kinship**, **Nations**, **UMLS** (Kok and Domingos, 2007), and **Countries** (Bouchard et al., 2015)





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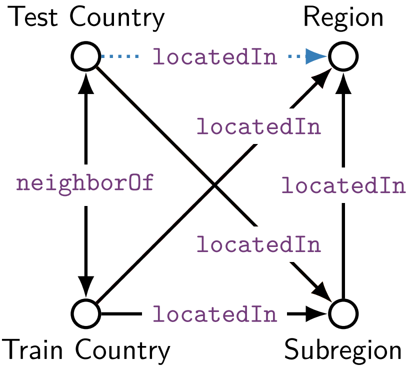

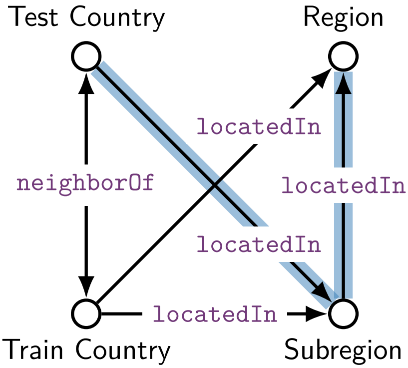

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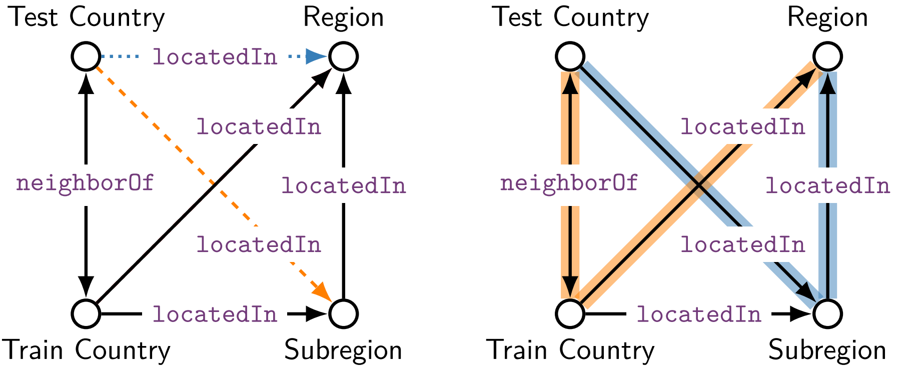

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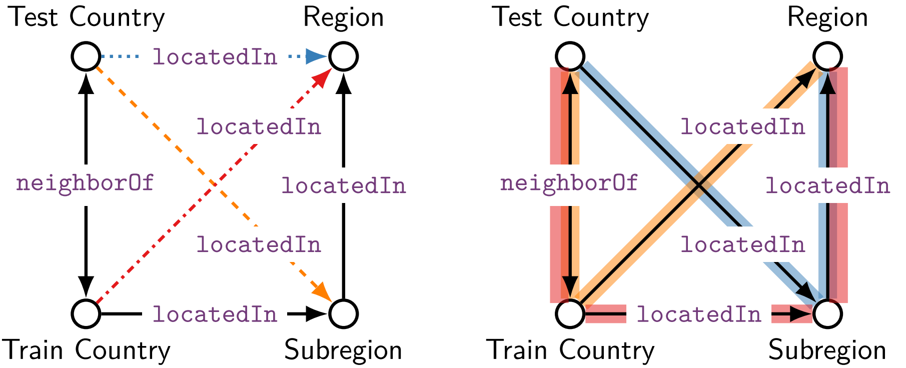

Details

- Models implemented in TensorFlow

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  ComplEx Neural link prediction model by Trouillon et al. (2016)

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  Prover End-to-end differentiable prover

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ComplEx	Neural link prediction model by Trouillon et al. (2016)
Prover	End-to-end differentiable prover
Proverλ	Same, but representations trained with ComplEx as auxiliary task

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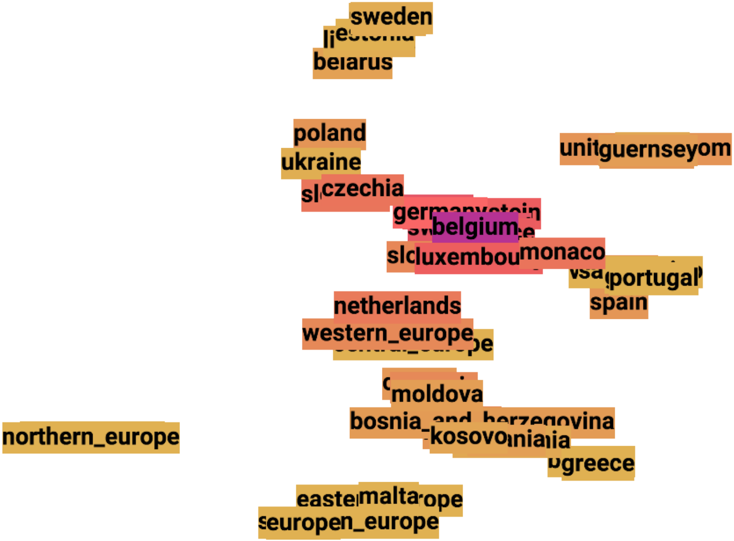
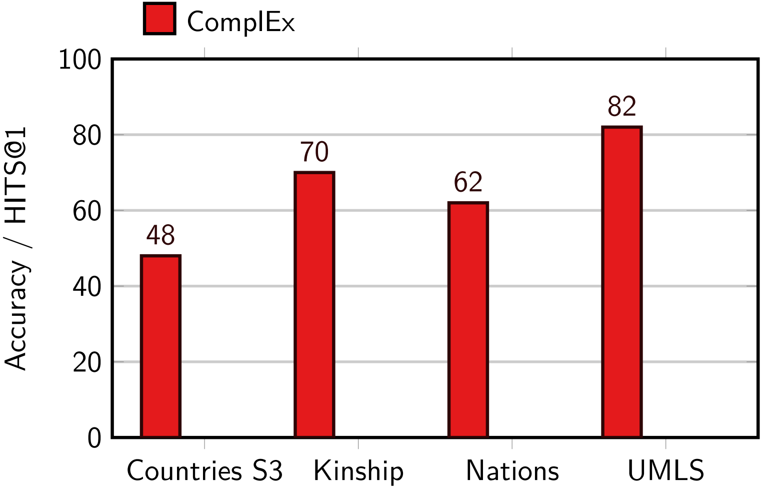
Prover	End-to-end differentiable prover
Proverλ	Same, but representations trained with ComplEx as auxiliary task

- Rule Templates:

Kinship, Nations & UMLS
20 $\#1(X, Y)$:– $\#2(X, Y)$.
20 $\#1(X, Y)$:– $\#2(Y, X)$.
20 $\#1(X, Y)$:– $\#2(X, Z), \#3(Z, Y)$.
Countries S1
3 $\#1(X, Y)$:– $\#1(Y, X)$.
3 $\#1(X, Y)$:– $\#2(X, Z), \#2(Z, Y)$.
Countries S2
3 $\#1(X, Y)$:– $\#2(X, Z), \#3(Z, Y)$.
Countries S3
3 $\#1(X, Y)$:– $\#2(X, Z), \#3(Z, W), \#4(W, Y)$.

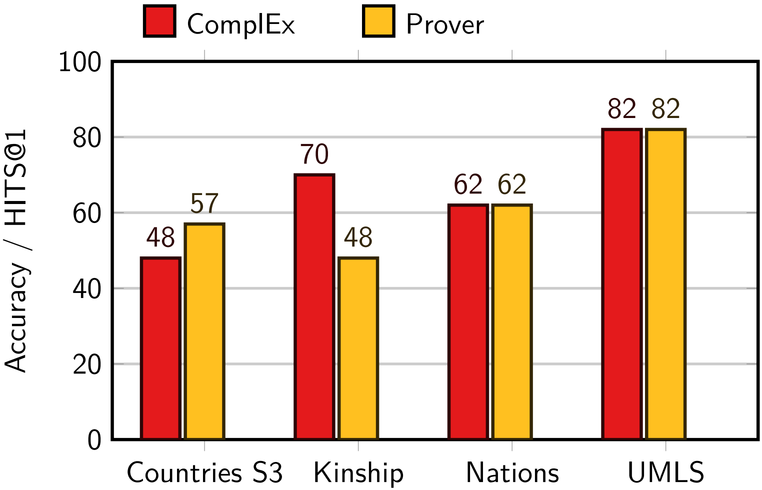

sweden
belarus
poland
ukraine
czechia
belgium
monaco
guernsey
portugal
spain
netherlands
western_europe
moldova
kosovo
greece
northern_europe
malta

Results



ComplEx
Accuracy / HITS@1
100
80
60
40
20
0
48
70
62
82
Countries S3
Kinship
Nations
UMLS

Results



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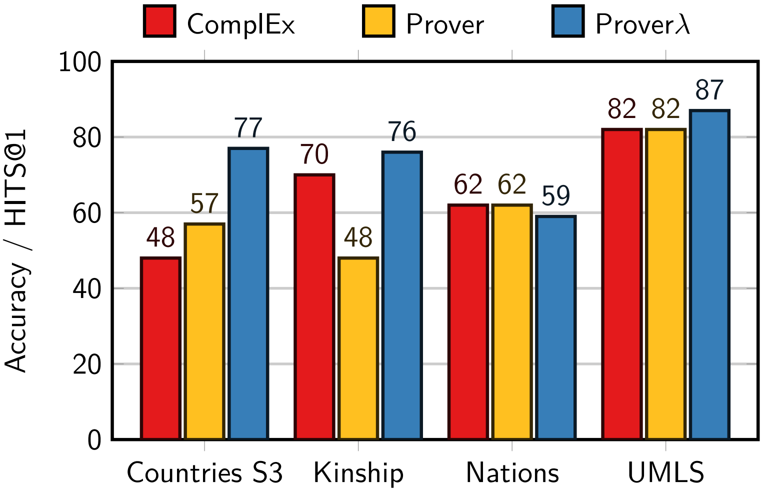
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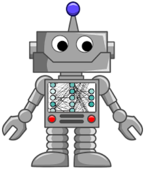
Examples of Induced Rules

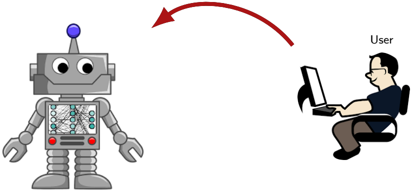
Corpus		Induced rules and their confidence
Countries	S1	0.90 `locatedIn`(X,Y) :– `locatedIn`(X,Z), `locatedIn`(Z,Y).
	S2	0.63 `locatedIn`(X,Y) :– `neighborOf`(X,Z), `locatedIn`(Z,Y).
	S3	0.32 `locatedIn`(X,Y) :– `neighborOf`(X,Z), `neighborOf`(Z,W), `locatedIn`(W,Y).
Nations		0.68 `blockpositionindex`(X,Y) :– `blockpositionindex`(Y,X).
		0.46 `expeldiplomats`(X,Y) :– `negativebehavior`(X,Y).
		0.38 `negativecomm`(X,Y) :– `commonbloc0`(X,Y).
		0.38 `intergovorgs3`(X,Y) :– `intergovorgs`(Y,X).
UMLS		0.88 `interacts_with`(X,Y) :– `interacts_with`(X,Z), `interacts_with`(Z,Y).
		0.77 `isa`(X,Y) :– `isa`(X,Z), `isa`(Z,Y).
		0.71 `derivative_of`(X,Y) :– `derivative_of`(X,Z), `derivative_of`(Z,Y).

Outlook



Outlook

Question
My patient is not responding after three days of codeine treatment. What could have happened?



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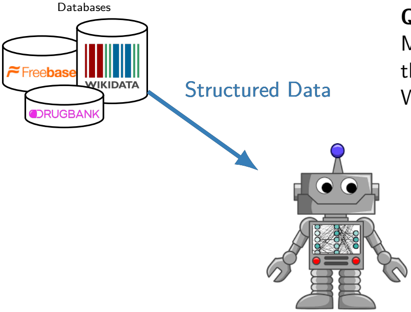

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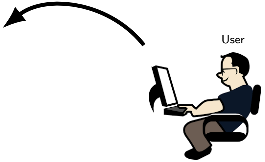

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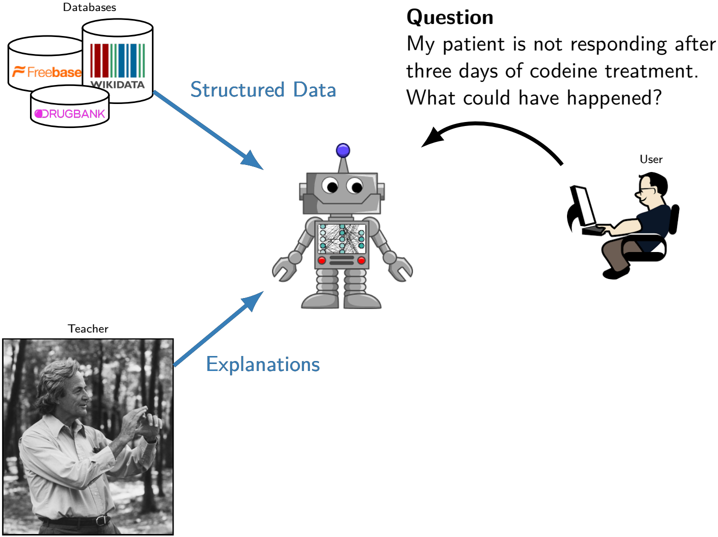
Databases
Freebase
WIKIDATA
DRUGBANK
Structured Data
Question
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User
Teacher
Explanations

Outlook

Databases

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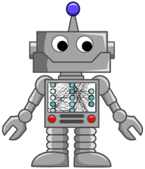
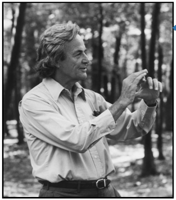
Text



Teacher



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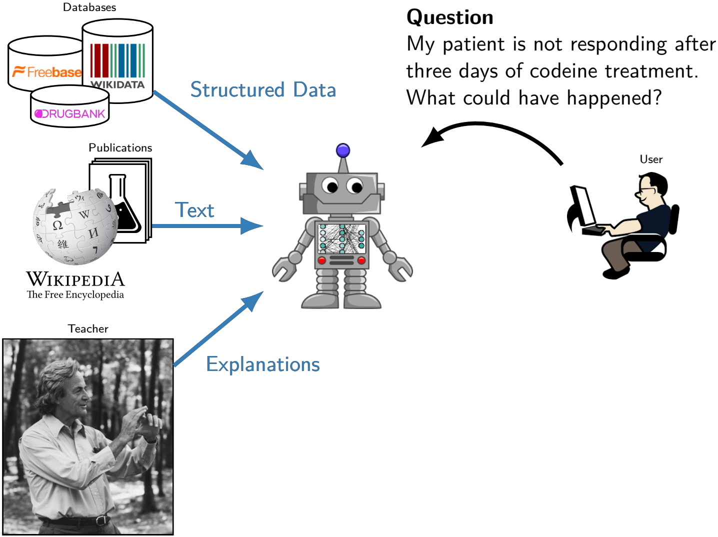
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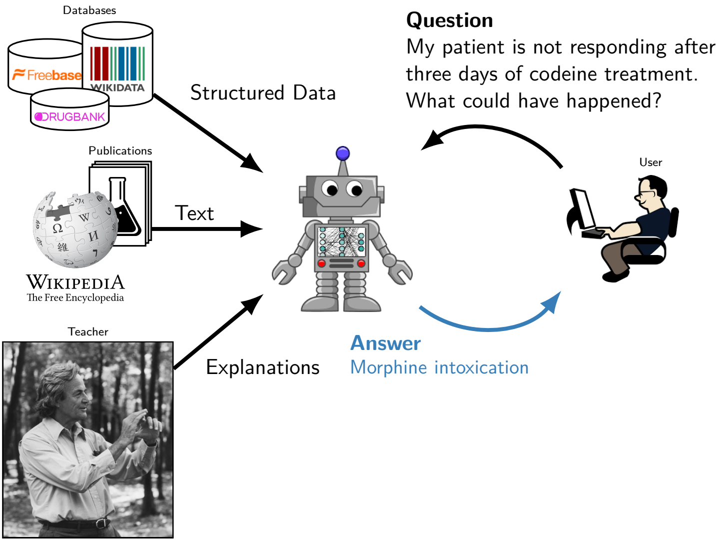
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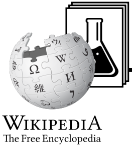
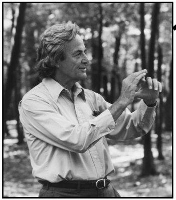


Text

Teacher



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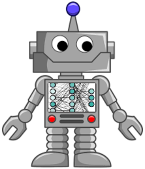

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User

Answer
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Proof

- Codeine is metabolized to morphine
- Mutation in CYP2D6 can cause ultrarapid metabolization
- Ultrarapid metabolization can lead to morphine overdose
- Morphine overdose is an intoxication

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Thank you!

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Twitter: @_rockt

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