

Deep Prolog: End-to-end Differentiable Proving in Knowledge Bases

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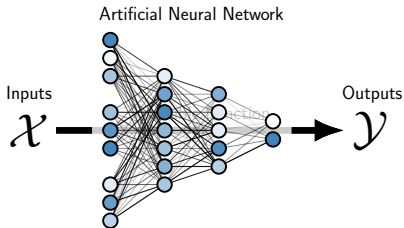
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Overview

Machine Learning

Deep Learning



First-order Logic

“Every father of a parent is a grandfather.”

```
grandfatherOf(X, Y) :-  
    fatherOf(X, Z),  
    parentOf(Z, Y).
```

- Behavior learned automatically
- Strong generalization
- Needs a lot of training data
- Behavior not interpretable

- Behavior defined manually
- No generalisation
- Needs no training data
- Behavior interpretable

Outline

- 1 Reasoning with Symbols
 - Knowledge Bases
 - Prolog: Backward Chaining
- 2 Reasoning with Neural Representations
 - Symbolic vs. Neural Representations
 - Neural Link Prediction
 - Computation Graphs
- 3 Deep Prolog: Neural Backward Chaining
- 4 Optimizations
 - Batch Proving
 - Gradient Approximation
 - Regularization by Neural Link Predictor
- 5 Experiments
- 6 Summary

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Notation

- **Constant:** HOMER, BART, LISA etc. (lowercase)
- **Variable:** X, Y etc. (uppercase, universally quantified)
- **Term:** constant or variable
- **Predicate:** fatherOf, parentOf etc.
function from terms to a Boolean
- **Atom:** predicate and terms, e.g., parentOf(X, BART)
- **Literal:** negated or non-negated atom, e.g.,
not parentOf(BART, LISA)
- **Rule:** head :- body.
head: literal
body: (possibly empty) list of literals representing conjunction
- **Fact:** ground rule (no free variables) with empty body, e.g.,
parentOf(HOMER, BART).

Example Knowledge Base

```
1  fatherOf(ABE, HOMER).
2  parentOf(HOMER, LISA).
3  parentOf(HOMER, BART).
4  grandpaOf(ABE, LISA).
5  grandfatherOf(ABE, MAGGIE).
6  grandfatherOf(X1, Y1) :-
    fatherOf(X1, Z1),
    parentOf(Z1, Y1).
7  grandparentOf(X2, Y2) :-
    grandfatherOf(X2, Y2).
```

Backward Chaining

```
1 def or(KB, goal,  $\Psi$ ):
2     for rule head :- body in KB do
3          $\Psi' \leftarrow \text{unify}(\text{head}, \text{goal}, \Psi)$ 
4         if  $\Psi' \neq \text{failure}$  then
5             for  $\Psi''$  in and(KB, body,  $\Psi'$ ) do
6                 yield  $\Psi''$ 
7
8 def and(KB, subgoals,  $\Psi$ ):
9     if subgoals is empty then return  $\Psi$ ;
10    else
11        subgoal  $\leftarrow \text{substitute}(\text{head}(\text{subgoals}), \Psi)$ 
12        for  $\Psi'$  in or(KB, subgoal,  $\Psi$ ) do
13            for  $\Psi''$  in and(KB, tail(subgoals),  $\Psi'$ ) do yield  $\Psi''$  ;
```

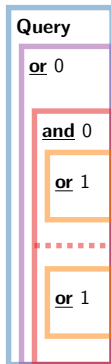
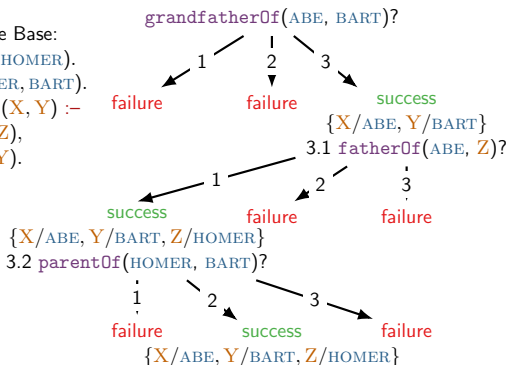
Unification

```
1 def unify(A, B,  $\Psi$ ):
2   if  $\Psi = failure$  then return failure;
3   else if A is variable then
4     return unifyvar(A, B,  $\Psi$ )
5   else if B is variable then
6     return unifyvar(B, A,  $\Psi$ )
7   else if A =  $[a_1, \dots, a_N]$  and B =  $[b_1, \dots, b_N]$  are atoms then
8      $\Psi' \leftarrow unify([a_2, \dots, a_N], [b_2, \dots, b_N], \Psi)$ 
9     return unify( $a_1, b_1, \Psi'$ )
10  else if A = B then return  $\Psi$ ;
11  else return failure;
```


Example

Example Knowledge Base:

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



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Symbolic Representations

- Symbols (constants and predicates) do not share any information:
`grandpaOf` \neq `grandfatherOf`
- No notion of similarity:
`APPLE` \sim `ORANGE`, `professorAt` \sim `lecturerAt`
- No generalization beyond what can be symbolically inferred:
`isFruit`(`APPLE`), `APPLE` \sim `ORGANGE`, `isFruit`(`ORANGE`)?
- But... leads to powerful inference mechanisms and proofs for predictions:
`fatherOf`(`ABE`, `HOMER`). `parentOf`(`HOMER`, `LISA`).
`parentOf`(`HOMER`, `BART`).
`grandfatherOf`(`X`, `Y`) :- `fatherOf`(`X`, `Z`), `parentOf`(`Z`, `Y`).
`grandfatherOf`(`ABE`, `Q`)? {`Q/LISA`}, {`Q/BART`}
- Fairly easy to debug and trivial to incorporate domain knowledge:
just change/add rules
- Hard to work with language, vision and other modalities
‘‘is a film based on the novel of the same name by’’(`X`, `Y`)

Neural Representations

- Lower-dimensional fixed-length vector representations of symbols (predicates and constants):

$$\mathbf{v}_{\text{APPLE}}, \mathbf{v}_{\text{ORANGE}}, \mathbf{v}_{\text{fatherOf}}, \dots \in \mathbb{R}^k$$

- Can capture similarity and even semantic hierarchy of symbols: $\mathbf{v}_{\text{grandpaOf}} = \mathbf{v}_{\text{grandfatherOf}},$

$$\mathbf{v}_{\text{APPLE}} \sim \mathbf{v}_{\text{ORANGE}}, \mathbf{v}_{\text{APPLE}} < \mathbf{v}_{\text{FRUIT}}$$

- Can be trained from raw task data (e.g. facts)

- Can be compositional

$$\mathbf{v}_{\text{“is the father of”}} = \text{RNN}_{\theta}(\mathbf{v}_{\text{is}}, \mathbf{v}_{\text{the}}, \mathbf{v}_{\text{father}}, \mathbf{v}_{\text{of}})$$

- But... need large amount of training data

- No direct way of incorporating prior knowledge

$$\mathbf{v}_{\text{grandfatherOf}}(X, Y) :- \mathbf{v}_{\text{fatherOf}}(X, Z), \mathbf{v}_{\text{parentOf}}(Z, Y).$$

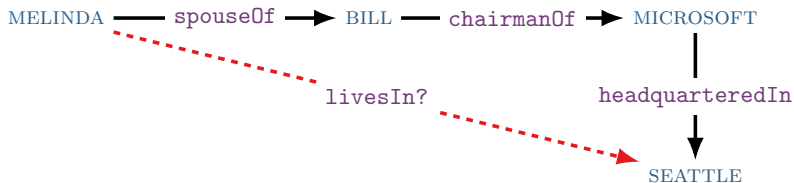
Related Work

- Fuzzy Logic (Zadeh, 1965)
- Probabilistic Logic Programming, e.g.,
 - IBAL (Pfeffer, 2001), BLOG (Milch et al., 2005), **Markov Logic Networks** (Richardson and Domingos, 2006), ProbLog (De Raedt et al., 2007) ...
- Inductive Logic Programming, e.g.,
 - Plotkin (1970), Shapiro (1991), Muggleton (1991), De Raedt (1999) ...
 - **Statistical Predicate Invention** (Kok and Domingos, 2007)
- Neural-symbolic Connectionism
 - Propositional rules: EBL-ANN (Shavlik and Towell, 1989), KBANN (Towell and Shavlik, 1994), C-LIP (Garcez and Zaverucha, 1999)
 - First-order inference (no training of symbol representations): **Unification Neural Networks** (Holldöbler, 1990; Komendantskaya 2011), SHRUTI (Shastri, 1992), **Neural Prolog** (Ding, 1995), CLIP++ (Franca et al. 2014), Lifted Relational Networks (Sourek et al. 2015)

Neural Link Prediction

Real world knowledge bases (like Freebase) are incomplete!

- `placeOfBirth` attribute is missing for 71% of people!
- Commonsense knowledge often not stated explicitly
- Weak logical relationships that can be used for inferring facts



Predict `livesIn(MELINDA, SEATTLE)` using local scoring function

$$f(\mathbf{v}_{\text{livesIn}}, \mathbf{v}_{\text{MELINDA}}, \mathbf{v}_{\text{SEATTLE}})$$

State-of-the-art Neural Link Prediction

$$f(\mathbf{v}_{\text{livesIn}}, \mathbf{v}_{\text{MELINDA}}, \mathbf{v}_{\text{SEATTLE}})$$

DistMult (Yang et al., 2014)

$$\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j \in \mathbb{R}^k$$

$$\begin{aligned} f(\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j) &= \mathbf{v}_s^\top (\mathbf{v}_i \odot \mathbf{v}_j) \\ &= \sum_k \mathbf{v}_{sk} \mathbf{v}_{ik} \mathbf{v}_{jk} \end{aligned}$$

Complex (Trouillon et al., 2016)

$$\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j \in \mathbb{C}^k$$

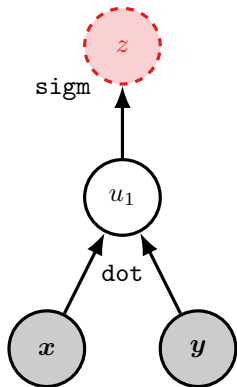
$$\begin{aligned} f(\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j) &= \\ & \text{real}(\mathbf{v}_s)^\top (\text{real}(\mathbf{v}_i) \odot \text{real}(\mathbf{v}_j)) \\ & + \text{real}(\mathbf{v}_s)^\top (\text{imag}(\mathbf{v}_i) \odot \text{imag}(\mathbf{v}_j)) \\ & + \text{imag}(\mathbf{v}_s)^\top (\text{real}(\mathbf{v}_i) \odot \text{imag}(\mathbf{v}_j)) \\ & - \text{imag}(\mathbf{v}_s)^\top (\text{imag}(\mathbf{v}_i) \odot \text{real}(\mathbf{v}_j)) \end{aligned}$$

Training Loss

$$\mathcal{L} = \sum_{r_s(e_i, e_j), y \in \mathcal{T}} -y \log(\sigma(f(\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j))) - (1 - y) \log(1 - \sigma(f(\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j)))$$

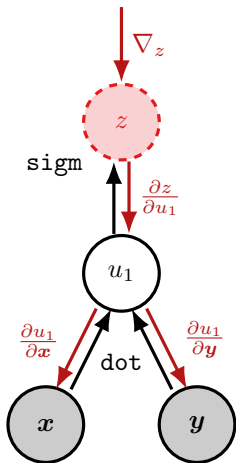
- Gradient-based optimization for learning $\mathbf{v}_s, \mathbf{v}_i, \mathbf{v}_j$ from data
- How do we calculate gradients $\nabla_{\mathbf{v}_s} \mathcal{L}, \nabla_{\mathbf{v}_i} \mathcal{L}, \nabla_{\mathbf{v}_j} \mathcal{L}$?

Computation Graphs



- Example: $z = f(\mathbf{x}, \mathbf{y}) = \sigma(\mathbf{x}^\top \mathbf{y})$
- Nodes represent variables (inputs or parameters)
- Directed edges to a node correspond to a differentiable operation

Backpropagation



- Chain Rule of Calculus:
Given function $z = f(\mathbf{a}) = f(g(\mathbf{b}))$
$$\nabla_{\mathbf{a}} z = \left(\frac{\partial \mathbf{b}}{\partial \mathbf{a}} \right)^\top \nabla_{\mathbf{b}} z$$
- Backpropagation is efficient recursive application of the Chain Rule
- Gradient of $z = \sigma(\mathbf{x}^\top \mathbf{y})$ w.r.t. \mathbf{x}
$$\nabla_{\mathbf{x}} z = \frac{\partial z}{\partial \mathbf{x}} = \frac{\partial z}{\partial u_1} \frac{\partial u_1}{\partial \mathbf{x}} = \sigma(u_1)(1 - \sigma(u_1))\mathbf{y}$$
- Given upstream supervision on z , we can learn \mathbf{x} and \mathbf{y} !

Deep Learning = “Large” differentiable computation graphs

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Aims

“We are attempting to replace symbols by vectors so we can replace logic by algebra.” — Yann LeCun

- End-to-end-differentiable proving
- Calculate gradient of proof success w.r.t. symbol representations
- Train symbol representations from facts and rules in a knowledge base via gradient descent
- Use similarity of symbol representations during proofs
- Induce rules of predefined structure via gradient descent

Neural Knowledge Base

Symbolic Representation

- 1 `fatherOf(ABE, HOMER).`
- 2 `parentOf(HOMER, LISA).`
- 3 `parentOf(HOMER, BART).`
- 4 `grandpaOf(ABE, LISA).`
- 5 `grandfatherOf(ABE, MAGGIE).`
- 6 `grandfatherOf(X1, Y1) :-
 fatherOf(X1, Z1),
 parentOf(Z1, Y1).`
- 7 `grandparentOf(X2, Y2) :-
 grandfatherOf(X2, Y2).`

Neural-Symbolic Representation

- 1 `vfatherOf(vABE, vHOMER).`
- 2 `vparentOf(vHOMER, vLISA).`
- 3 `vparentOf(vHOMER, vBART).`
- 4 `vgrandpaOf(vABE, vLISA).`
- 5 `vgrandfatherOf(vABE, vMAGGIE).`
- 6 `vgrandfatherOf(X1, Y1) :-
 vfatherOf(X1, Z1),
 vparentOf(Z1, Y1).`
- 7 `vgrandparentOf(X2, Y2) :-
 vgrandfatherOf(X2, Y2).`

Neural Unification

Soft-matching: $\tau_{A,B} = e^{-\|\mathbf{v}_A - \mathbf{v}_B\|_2} \in [0, 1]$

```
1 def unify(A, B,  $\Psi$ ,  $\tau$ ):
2   if  $\Psi = \text{failure}$  then return failure, 0;
3   else if A is variable then
4     return unifyvar(A, B,  $\Psi$ ),  $\tau$ 
5   else if B is variable then
6     return unifyvar(B, A,  $\Psi$ ),  $\tau$ 
7   else if A =  $[a_1, \dots, a_N]$  and B =  $[b_1, \dots, b_N]$  are atoms then
8      $\Psi', \tau' \leftarrow \text{unify}([a_2, \dots, a_N], [b_2, \dots, b_N], \Psi, \tau)$ 
9     return unify( $a_1, b_1, \Psi', \tau'$ )
10  else if A and B are symbol representations then return  $\Psi, \min(\tau, \tau_{A,B})$ ;
11  else return failure, 0;
```

Example: unify $\mathbf{v}_{\text{grandfatherOf}}(X, \mathbf{v}_{\text{BART}})$ with $\mathbf{v}_{\text{grandpaOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{BART}})$

$\Psi = \{X/\mathbf{v}_{\text{ABE}}\}, \quad \tau = \min(e^{-\|\mathbf{v}_{\text{grandfatherOf}} - \mathbf{v}_{\text{grandpaOf}}\|_2}, e^{-\|\mathbf{v}_{\text{BART}} - \mathbf{v}_{\text{BART}}\|_2})$

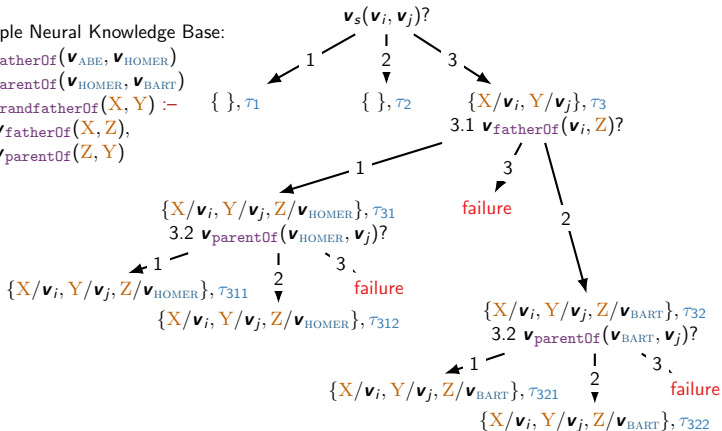
Compiling a Computation Graph using Backward Chaining

```
1 def or(KB, goal,  $\Psi$ ,  $\tau$ , D):  
2   for rule head :- body in KB do  
3      $\Psi'$ ,  $\tau'$   $\leftarrow$  unify(head, goal,  $\Psi$ ,  $\tau$ )  
4     if  $\Psi' \neq$  failure then  
5       for  $\Psi''$ ,  $\tau''$  in and(KB, body,  $\Psi'$ ,  $\tau'$ , D) do  
6         yield  $\Psi''$ ,  $\tau''$   
  
7 def and(KB, subgoals,  $\Psi$ ,  $\tau$ , D):  
8   if subgoals is empty then return  $\Psi$ ,  $\tau$ ;  
9   else if D = 0 then return failure;  
10  else  
11    subgoal  $\leftarrow$  substitute(head(subgoals),  $\Psi$ )  
12    for  $\Psi'$ ,  $\tau'$  in or(KB, subgoal,  $\Psi$ ,  $\tau$ , D - 1) do  
13      for  $\Psi''$ ,  $\tau''$  in and(KB, tail(subgoals),  $\Psi'$ ,  $\tau'$ , D) do yield  
         $\Psi''$ ,  $\tau''$  ;
```

Example

Example Neural Knowledge Base:

1. $\mathbf{v}_{\text{fatherOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{HOMER}})$
2. $\mathbf{v}_{\text{parentOf}}(\mathbf{v}_{\text{HOMER}}, \mathbf{v}_{\text{BART}})$
3. $\mathbf{v}_{\text{grandfatherOf}}(X, Y) :-$
 - $\{ \}, \tau_1$
 - $\mathbf{v}_{\text{fatherOf}}(X, Z),$
 - $\mathbf{v}_{\text{parentOf}}(Z, Y)$



Training

Proof Aggregation

$$\Psi, \tau = \text{or}(KB, Q, \{\}, 1, D)$$

$$\tau_Q = \max \tau$$

Supervision Signal

$$y_Q = \begin{cases} 1.0 & \text{if } Q \in \mathcal{F} \\ 0.0 & \text{otherwise} \end{cases}$$

Masking Unification for Training Facts

$$\tilde{\tau}_{Q,B} = \begin{cases} 0.0 & \text{if } Q \in \mathcal{F} \text{ and } Q = B \\ \tau_{Q,B} & \text{otherwise} \end{cases}$$

Loss

$$\mathcal{L} = \sum_{Q \in \mathcal{T}} -y_Q \log(\tau_Q) - (1 - y_Q) \log(1 - \tau_Q)$$

Neural Inductive Logic Programming

- 1 $\mathbf{v}_{\text{fatherOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{HOMER}})$.
- 2 $\mathbf{v}_{\text{parentOf}}(\mathbf{v}_{\text{HOMER}}, \mathbf{v}_{\text{LISA}})$.
- 3 $\mathbf{v}_{\text{parentOf}}(\mathbf{v}_{\text{HOMER}}, \mathbf{v}_{\text{BART}})$.
- 4 $\mathbf{v}_{\text{grandpaOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{LISA}})$.
- 5 $\mathbf{v}_{\text{grandfatherOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{MAGGIE}})$.
- 6 $\theta_1(\mathbf{X}_1, \mathbf{Y}_1) :-$
 $\theta_2(\mathbf{X}_1, \mathbf{Z}_1),$
 $\theta_3(\mathbf{Z}_1, \mathbf{Y}_1)$.
- 7 $\theta_4(\mathbf{X}_2, \mathbf{Y}_2) :-$
 $\theta_5(\mathbf{X}_2, \mathbf{Y}_2)$.

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Batch Proving: Utilizing GPUs

Let $\mathbf{A} \in \mathbb{R}^{N \times k}$ be a matrix of N symbol representations that are to be unified with M other symbol representations $\mathbf{B} \in \mathbb{R}^{M \times k}$

$$\tau_{\mathbf{A}, \mathbf{B}} = e^{-\sqrt{\mathbf{A}^{sq} + \mathbf{B}^{sq} - 2\mathbf{A}\mathbf{B}^T} + \epsilon} \in \mathbb{R}^{N \times M}$$

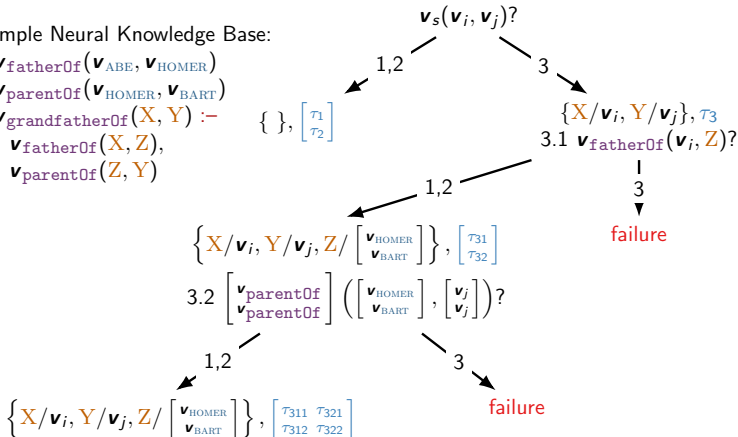
$$\mathbf{A}^{sq} = \begin{bmatrix} \sum_{i=1}^k \mathbf{A}_{1i}^2 \\ \vdots \\ \sum_{i=1}^k \mathbf{A}_{Ni}^2 \end{bmatrix} \mathbf{1}_M^T \in \mathbb{R}^{N \times M}$$

$$\mathbf{B}^{sq} = \mathbf{1}_N \begin{bmatrix} \sum_{i=1}^k \mathbf{B}_{1i}^2 \\ \vdots \\ \sum_{i=1}^k \mathbf{B}_{Mi}^2 \end{bmatrix}^T \in \mathbb{R}^{N \times M}$$

Batch Proving Example

Example Neural Knowledge Base:

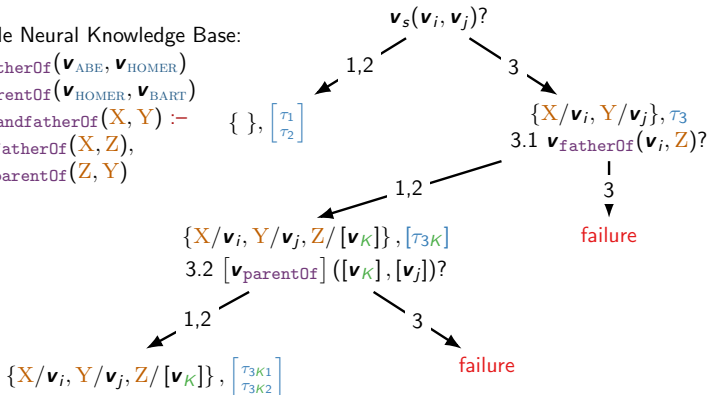
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3. $\mathbf{v}_{\text{grandfatherOf}}(X, Y) :-$ $\{ \}, [\tau_1, \tau_2]$
 $\mathbf{v}_{\text{fatherOf}}(X, Z),$
 $\mathbf{v}_{\text{parentOf}}(Z, Y)$



Gradient Approximation with K max Proofs

Example Neural Knowledge Base:

1. $\mathbf{v}_{\text{fatherOf}}(\mathbf{v}_{\text{ABE}}, \mathbf{v}_{\text{HOMER}})$
2. $\mathbf{v}_{\text{parentOf}}(\mathbf{v}_{\text{HOMER}}, \mathbf{v}_{\text{BART}})$
3. $\mathbf{v}_{\text{grandfatherOf}}(X, Y) :- \{ \}, [\tau_1, \tau_2]$
 $\mathbf{v}_{\text{fatherOf}}(X, Z),$
 $\mathbf{v}_{\text{parentOf}}(Z, Y)$



Regularization by Neural Link Predictor

- Train jointly with neural link prediction method
- Share symbol representations
- Neural link prediction model quickly learns similarities between symbols
- Let p_Q be score by neural link prediction model (DistMult or ComplEx), and τ_Q be the proof success
- Multi-task training loss:

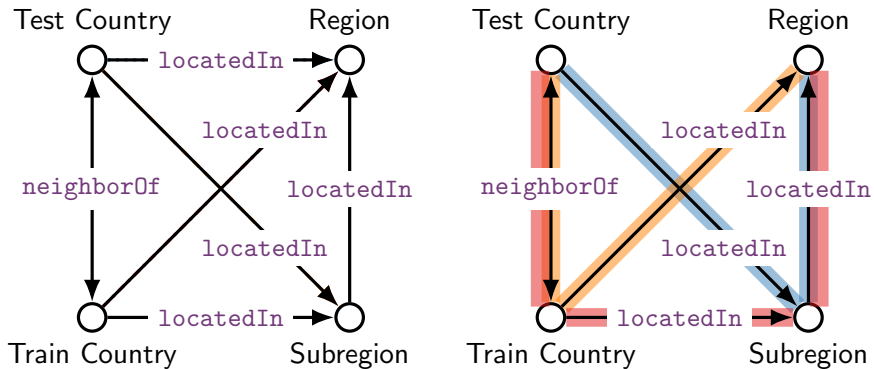
$$\mathcal{L} = \sum_{Q \in \mathcal{T}} -y_Q(\log(\tau_Q) + \log(p_Q)) - (1 - y_Q)(\log(1 - \tau_Q) + \log(1 - p_Q))$$

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Experiments

Countries Knowledge Base (Bouchard et al., 2015)



Models

NTP: prover is trained alone

DistMult: neural link prediction model by [Yang et al. \(2014\)](#)

NTP DistMult: jointly training prover and DistMult, and use maximum prediction at test time

NTP DistMult λ : only prover is used at test time; DistMult acts as a regularizer

Complex: neural link prediction model by [Trouillon et al. \(2016\)](#)

NTP Complex: jointly training prover and Complex, and use the maximum prediction at test time

NTP Complex λ : only prover is used at test time; Complex acts as a regularizer

Rule Templates

S1 $\theta_1(\mathbf{X}, \mathbf{Y}) :- \theta_2(\mathbf{Y}, \mathbf{Z}).$

$\theta_1(\mathbf{X}, \mathbf{Y}) :- \theta_2(\mathbf{X}, \mathbf{Z}), \theta_2(\mathbf{Z}, \mathbf{Y}).$

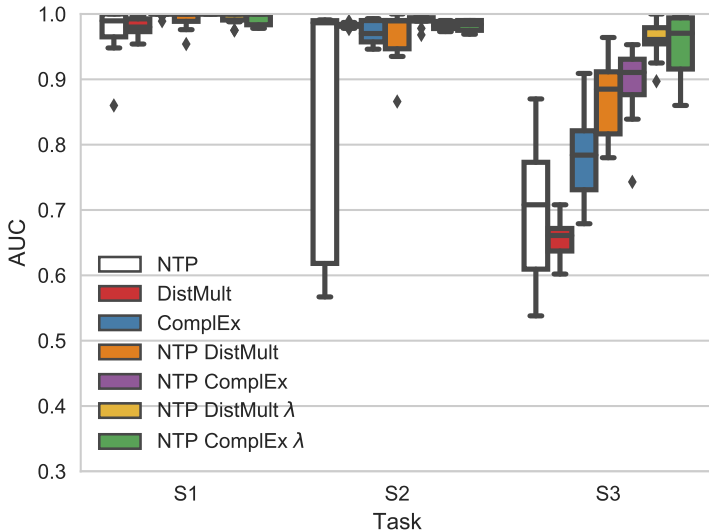
S2 $\theta_1(\mathbf{X}, \mathbf{Y}) :- \theta_2(\mathbf{X}, \mathbf{Z}), \theta_3(\mathbf{Z}, \mathbf{Y}).$

S3 $\theta_1(\mathbf{X}, \mathbf{Y}) :- \theta_2(\mathbf{X}, \mathbf{Z}), \theta_3(\mathbf{Z}, \mathbf{W}), \theta_4(\mathbf{W}, \mathbf{Y}).$

Results

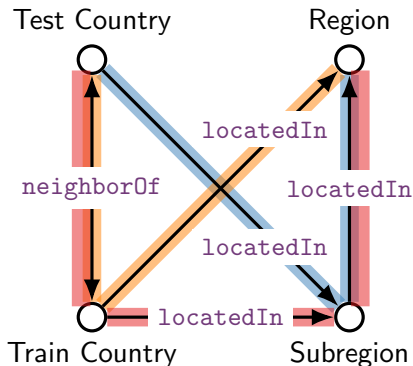
Model	S1	S2	S3
Random	32.3	32.3	32.3
Frequency	32.3	32.3	30.8
ER-MLP (Dong et al., 2014)	96.0	74.5	65.0
Rescal (Nickel et al., 2012)	99.7	74.5	65.0
HolE (Nickel et al., 2015)	99.7	77.2	69.7
TARE (Wang et al., 2017)	99.4	90.6	89.0
NTP	97.3	83.7	70.0
DistMult (Yang et al., 2014)	98.1	98.3	65.5
NTP DistMult	99.2	96.7	87.0
NTP DistMult λ	99.4	98.3	95.9
Complex (Trouillon et al., 2016)	99.9	97.1	78.6
NTP Complex	100.0	98.9	89.1
NTP Complex λ	99.3	98.2	95.1

Results



Induced Logic Programs

Task	Confidence	Rule
S1	0.999	<code>neighborOf(X, Y) :- neighborOf(Y, X).</code>
	0.767	<code>locatedIn(X, Y) :- locatedIn(X, Z), locatedIn(Z, Y).</code>
S2	0.998	<code>neighborOf(X, Y) :- neighborOf(Y, X).</code>
	0.995	<code>locatedIn(X, Y) :- locatedIn(X, Z), locatedIn(Z, Y).</code>
	0.705	<code>locatedIn(X, Y) :- neighborOf(X, Z), locatedIn(Z, Y).</code>
S3	0.891	<code>neighborOf(X, Y) :- neighborOf(Y, X).</code>
	0.750	<code>locatedIn(X, Y) :- neighborOf(X, Z), neighborOf(Z, W), locatedIn(W, Y).</code>



Summary

- Prolog's backward chaining can be used as a recipe for recursively constructing a neural network
- Proof success differentiable w.r.t. symbol representations
- Can learn vector representations of symbols and rules of predefined structure
- Various optimizations: batch proving, gradient approximation
- Outperforms neural link prediction models on a medium-sized knowledge base
- Induces interpretable rules

Thank you!

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