## One Year With Deepire: Lessons Learned and Where to Go Next?

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#### Vampire

• Automatic Theorem Prover (ATP) for First-order Logic (FOL)

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• state-of-the-art saturation-based prover



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state-of-the-art saturation-based prover

#### Neural (ENIGMA-style) guidance

- targeting the clause selection decision point
- supervised learning from successful runs



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#### Neural (ENIGMA-style) guidance

- targeting the clause selection decision point
- supervised learning from successful runs
- The special bit: uses a recursive neural network (RvNN) based solely on clause derivation history

## Deepire Is One Year Old!



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## Deepire Is One Year Old!

#### The story so far:

- [AITP20] introduced the first prototype
- [CADE21] improved Vampire's theory reasoning on SMTLIB
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In this talk:

• overview of the main results, insights, and future outlooks

1 Saturation, Clause Selection, and Machine Learning

2 Recursive Neural Networks over Clause Derivations

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4 Experiments on Mizar



## 1 Saturation, Clause Selection, and Machine Learning

2 Recursive Neural Networks over Clause Derivations

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- 3 Notes on Implementation and Training
- 4 Experiments on Mizar
- 5 Conclusion

## Saturation-based Theorem Proving



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## Saturation-based Theorem Proving



At a typical successful end:  $|Passive| \gg |Active| \gg |Proof|$ 

## How is clause selection traditionally done?

#### Take simple clause evaluation criteria:

• age: prefer clauses that were generated long time ago

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• weight: prefer clauses with fewer symbols

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#### Combine them into a single scheme:

- have a priority queue ordering Passive for each criterion
- alternate between selecting from the queues using a fixed ratio

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Learn to recognize and prefer for selection clauses that look like those that contributed to a proof in past successful runs.

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- integrating the learned advice back to the saturation loop

## Adding the Learnt Advice $\mathcal M$ as Another Queue?

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#### Priority:

• sort by model's Y/N and tiebreak by age



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Logits:

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• A:4 A:5 A:6 A:2 A:3 A:1 W:8 W:3 W:6 W:3 W:3 W:4

#### Combine with the original strategy

$$\mathcal{S} \oplus \mathcal{M}^{1,0}: \begin{array}{c} 1 \\ 1 \\ 2 \\ \end{array} \begin{array}{c} A:1 \\ W:4 \\ W:3 \\ W:4 \\ W:3 \\ W:4 \\ W:4 \\ W:5 \\ W:5 \\ W:4 \\ W:5 \\ W:5 \\ W:4 \\ W:5 \\ W:5 \\ W:4 \\ W:5 \\ W:5$$

## What Worked the Best?

#### Layered Clause Selection [Tammet19,G&S20]:



## What Worked the Best?





#### Advantages of LCS:

- ullet keep using the well-tuned  ${\mathcal S}$  also for the positively classified
- allows for the lazy evaluation trick [AITP20,CADE21]
- a smooth transition from the original to the ML-boosted

## Saturation, Clause Selection, and Machine Learning

### 2 Recursive Neural Networks over Clause Derivations

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## Represent Clauses by Their Derivation History

"Don't look at what the clause says, only where it's coming from."

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"Don't look at what the clause says, only where it's coming from."



#### Focusing on the MIZAR dataset here:

- $\bullet$  a large set of axioms  ${\cal A}$  referenced by all the problems
- each problem P consists of a conjecture  $C_P$  and a  $\mathcal{A}_P \subseteq \mathcal{A}$
- a small set of inference rules labeling the internal nodes

The idea of embeddings:

• represent each clause C by a real vector  $v_C \in \mathbb{R}^n$ 

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#### Recursively compose the following neural building blocks:

- init function  $I_A \in \mathbb{R}^n$ , for every axiom type A
- deriv function  $D_R : \mathbb{R}^n \times \cdots \times \mathbb{R}^n \to \mathbb{R}^n$ , for every inference R

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• eval function  $E : \mathbb{R}^n \to \mathbb{R}$ 

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- eval function  $E : \mathbb{R}^n \to \mathbb{R}$

#### Example (Evaluating the derivation from the previous slide)

$$\begin{aligned} v_{C_2} &:= I_{\$conjecture} \\ v_{C_3} &:= I_{t_3\_subset} \\ v_{C_6} &:= D_{Resolution}(v_{C_2}, v_{C_3}) \\ v_{C_8} &:= D_{AVATAR}(v_{C_6}) \end{aligned}$$

 $C_8$  is classified positive iff  $E(v_{C_8}) \ge 0$ 

#### The idea of embeddings:

• represent each clause C by a real vector  $v_C \in \mathbb{R}^n$ 

#### Recursively compose the following neural building blocks:

- <u>init</u> function  $I_A \in \mathbb{R}^n$ , for every axiom type A
- deriv function  $D_R : \mathbb{R}^n \times \cdots \times \mathbb{R}^n \to \mathbb{R}^n$ , for every inference R
- eval function  $E : \mathbb{R}^n \to \mathbb{R}$

#### Example (Evaluating the derivation from the previous slide)

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➡ NB: Constant work per clause!

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#### 1) Axioms (and the init function)

•  $|\mathcal{A}_{\mathrm{MIZAR}}| pprox$  43K, clipped to m=0.5/1/2K most frequent ones

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- all others marked I<sub>\$unknown</sub>
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  - $\bullet\,$  but the ability to distinguish rules  $\sim\,$  extra 5% problems solved

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#### 3) Conjecture relatedness

- in each problem, we mark conjecture clauses by Isconjecture
- the network learns to incorporate the right level of goal directedness

Saturation, Clause Selection, and Machine Learning

2 Recursive Neural Networks over Clause Derivations

#### 3 Notes on Implementation and Training

4 Experiments on Mizar



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## Experience with PyTorch

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#### Training in Python $\longrightarrow$ inference from C++

- good experience with TorchScript model export
- almost any PyTorch code will get (VM-)interpreted in C++

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#### Training in Python $\longrightarrow$ inference from C++

- good experience with TorchScript model export
- almost any PyTorch code will get (VM-)interpreted in C++

#### Dynamic computational graphs:

- elegant and flexible, but
- training needs to keep building them over and over!

#### Batching

- group derivations to create similarly-sized chunks for training
- merge equivalent nodes (within problem / across problems)

## Batching and Parallel Training Setup

#### Batching

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 $\blacktriangleright$  However, this is not SIMD  $\rightarrow$  only trained on CPUs

## Batching and Parallel Training Setup

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Master-worker parallel training setup:



## Batching and Parallel Training Setup

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Master-worker parallel training setup:



► A funny "drift" effect that actually regularizes!

## Validate and Compare to the ATP Performance



(from [CADE21]: Deepire for theory reasoning on SMTLIB)

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How often is  $\mathcal{M}$  100% correct?



[CADE21]: leaning a bit positively improves ATP performance

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## Experimental Setup



#### Mizar40 benchmark [Urban&Kaliszyk15]

- 57 880 problems in the TPTP format
- MPTP export from the Mizar Mathematical Library
- the small, bushy (i.e., re-proving), version



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#### Mizar40 benchmark [Urban&Kaliszyk15]

- 57 880 problems in the TPTP format
- MPTP export from the Mizar Mathematical Library
- the small, bushy (i.e., re-proving), version



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#### Fixed for the whole experiment:

- a base strategy  $\mathcal{V}$ :
  - previously shown to work well on Mizar40
- 10 s time limit

- $\bullet \ \mathcal{V}$  was able to solve 20197 problems
- 800 MB of successful derivations (when zipped)
- 43 080 named Mizar axioms occurring in them

• largest derivation: 242 023 (merged) nodes

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#### How network size affects training:

model shorthand	$\mid \mathcal{H}^{n128}$	$\mathcal{M}^{n64}$	$\mathcal{M}^{n128}$	$\mathcal{M}^{n256}$	$\mathcal{D}^{n128}$
revealed axioms <i>m</i>	0.5K	1K	1K	1K	2K
embedding size <i>n</i>	128	64	128	256	128
training time (min/epoch)	42	32	48	74	58
model size (MB)	4.6	1.6	5.0	17.9	5.8
best validation loss		0.455	0.455	0.452	

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➡ Large capacity generalizes best!

strategy	$\mid \mathcal{V} \mid$	$\mathcal{H}^{n128}$	$\mathcal{M}^{n64}$	$\mathcal{M}^{n128}$	$\mathcal{M}^{n256}$	$\mathcal{D}^{n128}$
solved	20 197	24 581	25 484	25 805	25 287	26014
$\mathcal{V}+$	+0	+5022	+5879	+6129	+5707	+6277
$\mathcal{V}-$	-0	-638	-592	-521	-617	-460
NN-eval.time	0%	37.1 %	32.9 %	37.7 %	48.6 %	36.7 %

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#### Num.probs solved by $\ensuremath{\mathcal{V}}$ and its RvNN boosted variants

#### Points to note:

•  $\mathcal{D}^{n128}$  solves almost 30 % more problems than  $\mathcal{V}$ 

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#### Points to note:

- $\mathcal{D}^{n128}$  solves almost 30 % more problems than  $\mathcal V$
- Could be even more greedy about the revealed axioms (m)
- Going over the embedding size (n = 128) makes it too slow
- It's fine to spend 40% of time *just thinking what the next clause should be* if it results in a good enough advice!

## Looping and a Comparison to ENIGMA

## Looping [Jakubův&Urban19]

- iterate the learning and solving phases
- keep learning also from the newly discovered proofs
- ➡ There: boosted tree learner over hand-crafted features

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## Performance comparison

	ENIGMA [J&U19] Deepire			e	
loop	solved	$+\mathcal{S}\%$	solved	$+\mathcal{V}\%$	note
0	14933	0.0	20 197	0.0	
1	20 366	35.8	26 014	28.8	m = 2000
2	22 839	52.3	27 348	35.4	<i>m</i> = 3000
3	23 467	56.5	28 947	43.3	m = 5000
4	23753	58.4			
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#### Points to note:

• both show the effect of diminishing returns

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#### Points to note:

- both show the effect of diminishing returns
- ENIGMA climbs higher (relatively) from lower numbers

Saturation, Clause Selection, and Machine Learning

2 Recursive Neural Networks over Clause Derivations

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④ Experiments on Mizar



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#### Summary

• Deepire explores ENIGMA-style clause selection guidance deliberately focusing on just derivation history

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#### Open

 positive example selection is more tricky than it seems (AVATAR, LRS, but already in DISCOUNT)

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- classification vs regression
- What did the model actually learn? (XAI)

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- looping is the first step towards RL
- general ATP knowledge rather than benchmark-specific!

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## Thank you for attention!