



Neural Models with Symbolic Representations for Perceptuo-Reasoning Tasks

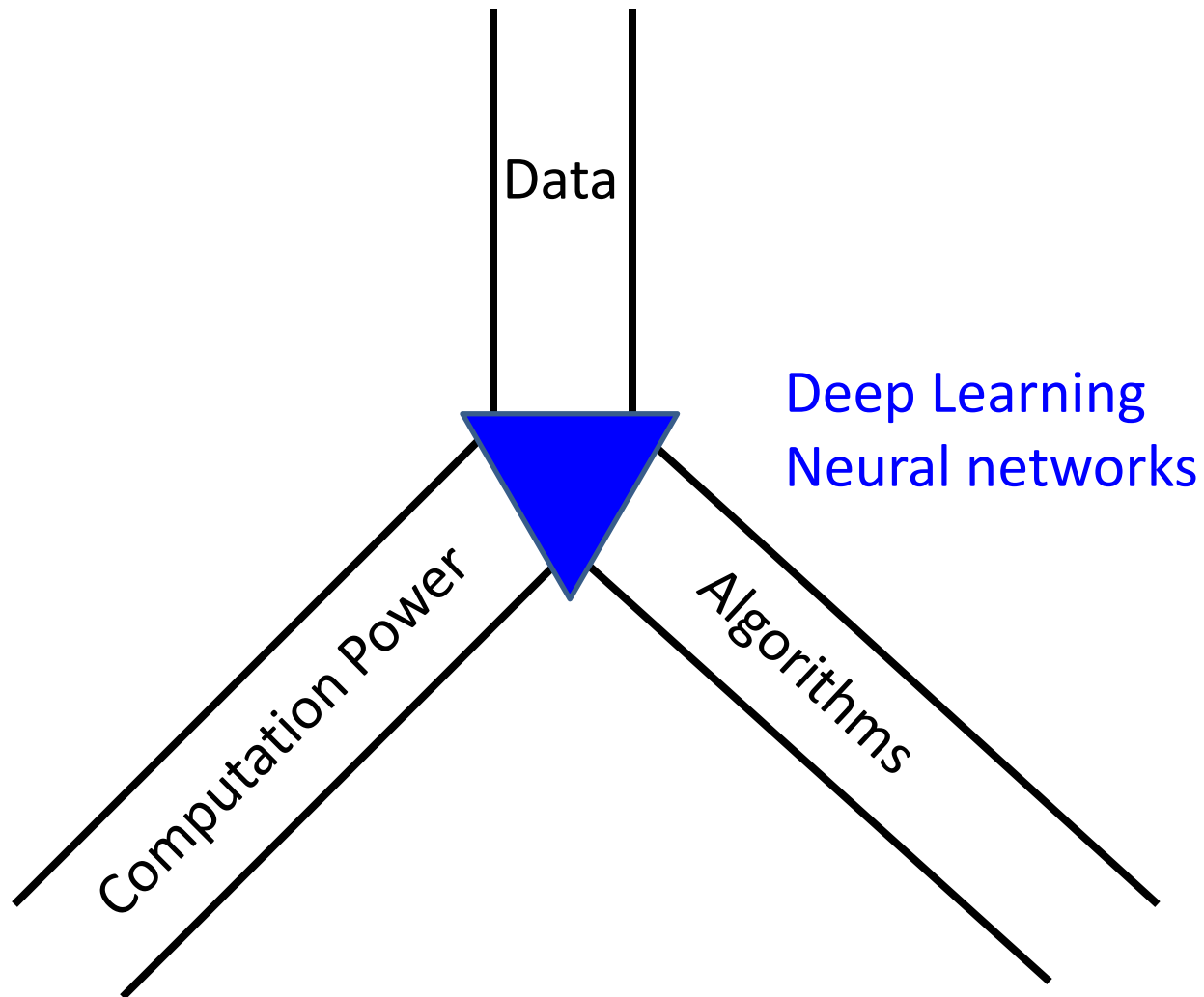
Mausam

Professor, Computer Science & Engg
Head, Yardi School of Artificial Intelligence
Indian Institute of Technology, Delhi

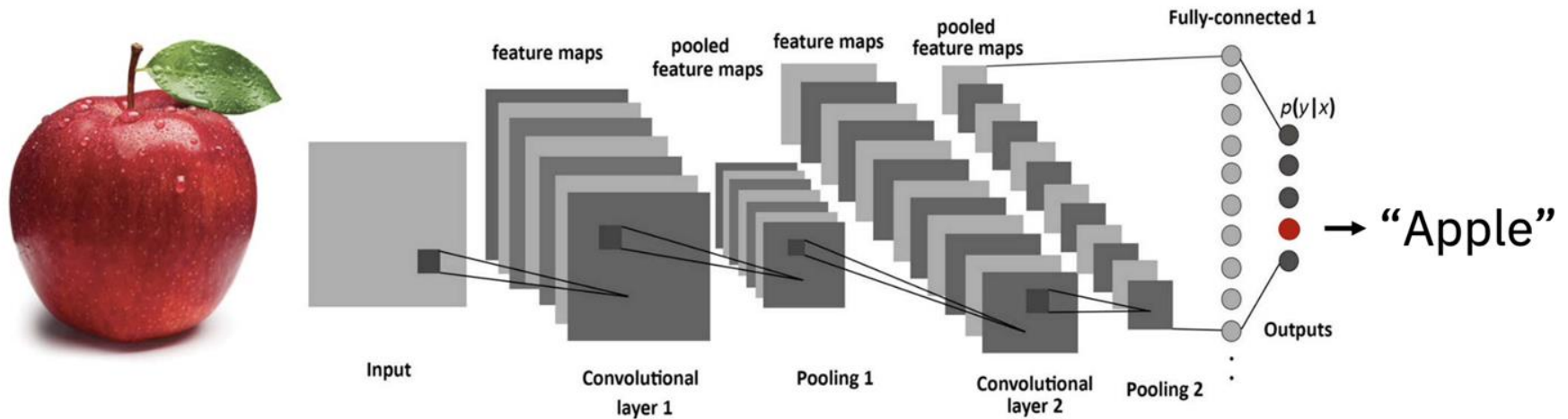
Primary joint work with Parag Singla, Yatin Nandwani, Vishal Sharma
Daman Arora, Aniket Bajpai, Sankalp Garg, Abhishek Pathak, Rishabh Ranjan

Other joint work with Soumen Chakrabarti, NM Anoop Krishnan, Danish Contractor, Keshav Kolluru, Vaibhav Adlakha, Tanishq Gupta, Vidit Jain, Barun Patra, Vipul Rathore, Mohd Zaki

The A.I. Revolution



Deep Learning for Perception



Source:

http://introtodeeplearning.com/2020/slides/6S191_MIT_DeepLearning_L7.pdf

Deep Learning

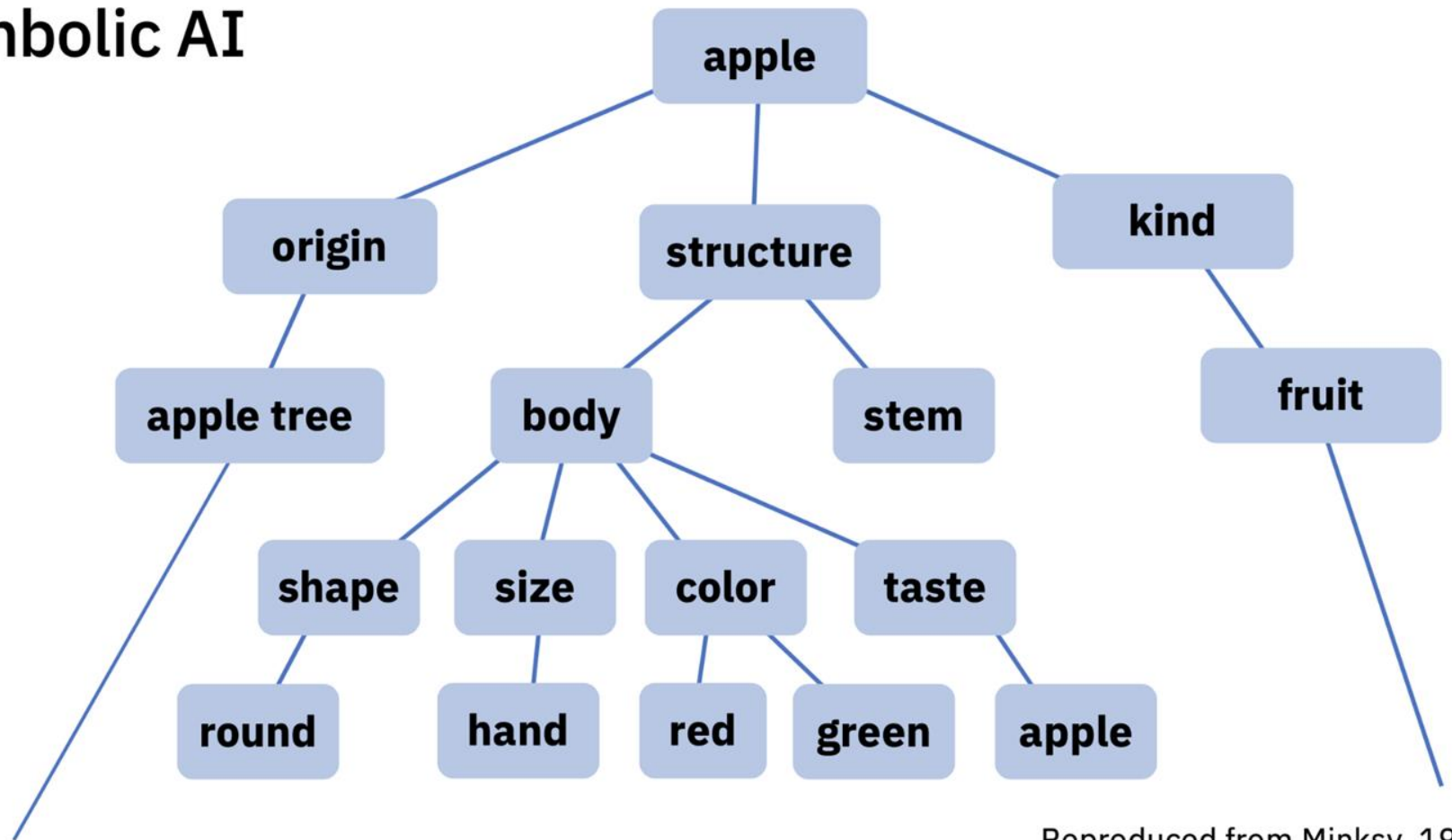
- Strengths
 - universal approximators: learn non-trivial functions
 - compositional models ~similar to human brain
 - universal representation across modalities
 - discover features automagically
 - in a task-specific manner
 - features not limited by human creativity

Deep Learning

- Weaknesses
 - annotated data hungry
 - compute hungry at train time
 - no guarantees on output
 - uninterpretable
 - ...

Symbolic AI / GOFAI

Symbolic AI



Reproduced from Minsky, 1991

Symbolic AI

- Symbolic AI methods based on high-level symbolic representations.
- Symbolic representations
 - Symbols for concepts
 - Expressions: structures that combine symbols
 - Processes: manipulation of expressions
- Examples
 - Formal logic
 - Math/Algebra
 - Graph Theory

Deep Learning

- Features
 - annotated data hungry
 - compute hungry at train
 - no guarantees on output
 - uninterpretable
 - ...
- Pros/Cons
 - Perception/Reasoning

Symbolic AI

- Features
 - often need less/no data
 - compute hungry at test
 - guarantees on output
 - human-understandable
 - ...
- Pros/Cons
 - Reasoning/Perception

Bridging Gap: Neural & Symbolic

- Neuro-Symbolic AI
 - combine benefits of neural and symbolic AI
- What can be Symbolic inside Neural AI?
 - features or constraints provided by human
 - domain theory provided by human
 - intermediate symbolic representation induced by model
 - symbolic algorithm in conjunction with neural
 -
- What can be Neural inside Symbolic AI?
 - Learnt heuristics, pattern recognition subroutines, e.g. AlphaGo, AlphaZero, Alexa, Google Search

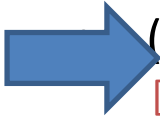
Outline

- Motivation
- (Human) Features within Neural AI (domain insight, better learning)
[Contractor JNLE'21, Gupta ArXiv'22]
- (Human) Constraints within Neural AI (dom. insight, learning, guarantees?)
[Nandwani NeurIPS'19, Kolluru EMNLP'20, Contractor JNLE'21, Gupta ArXiv'22]
- (Human) Symbolic Theory \rightarrow Neural AI (scalability)
[Bajpai NeurIPS'18, Garg ICAPS'19, Garg ICML'20, Sharma UAI'22]
- (Human) Incomplete Symbolic Theory \rightarrow Neural AI (scalability)
[Nandwani ICLR'21, Nandwani ICLR'22]
- Neural AI \rightarrow (Machine) Symbolic Theory (interpretability, scalability)
[Nandwani NeurIPS'22]
- Neural AI \rightarrow (Machine) Symbolic Explanation (explanations)
[Nandwani AKBC'20]

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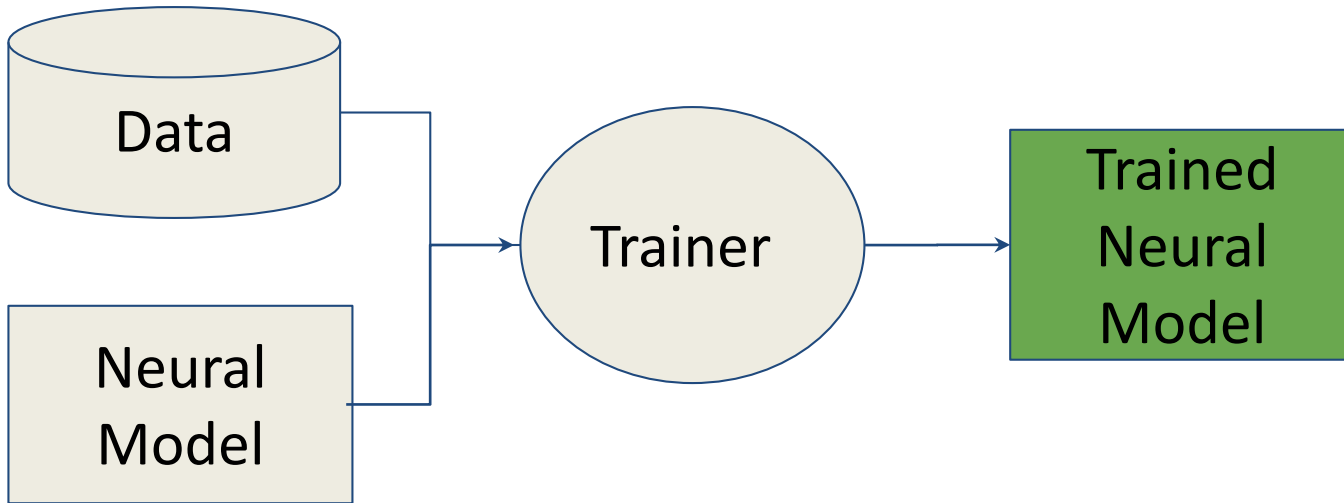
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(Human) Constraints within Neural AI

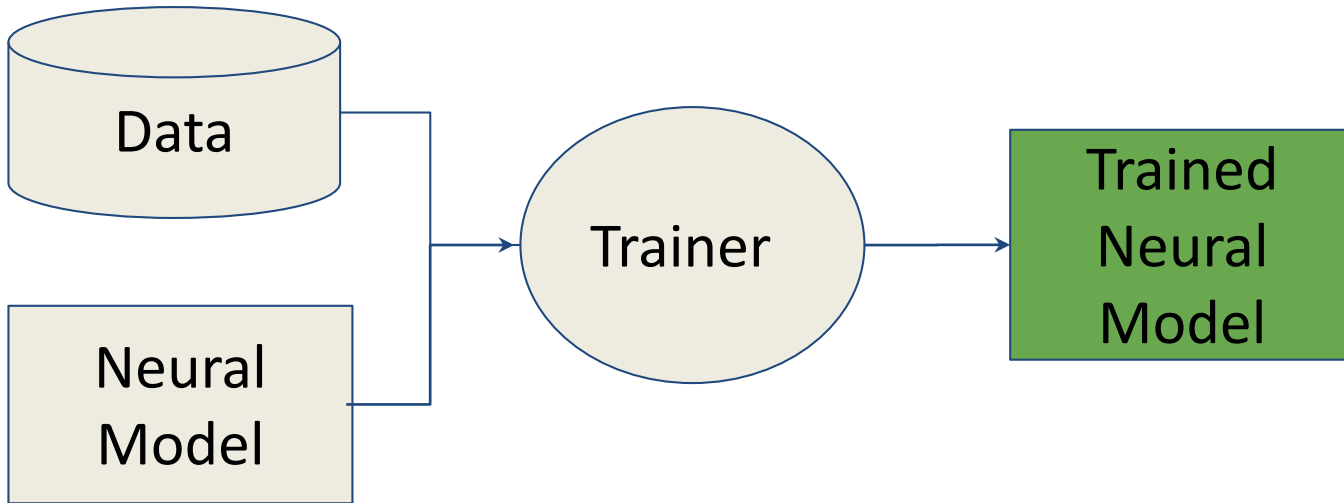
Standard Neural AI

Training

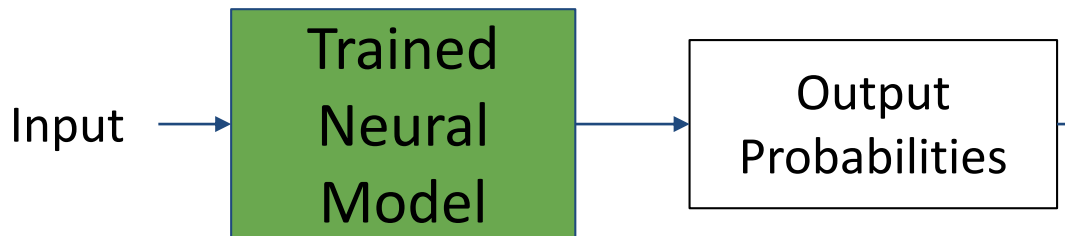


Standard Neural AI

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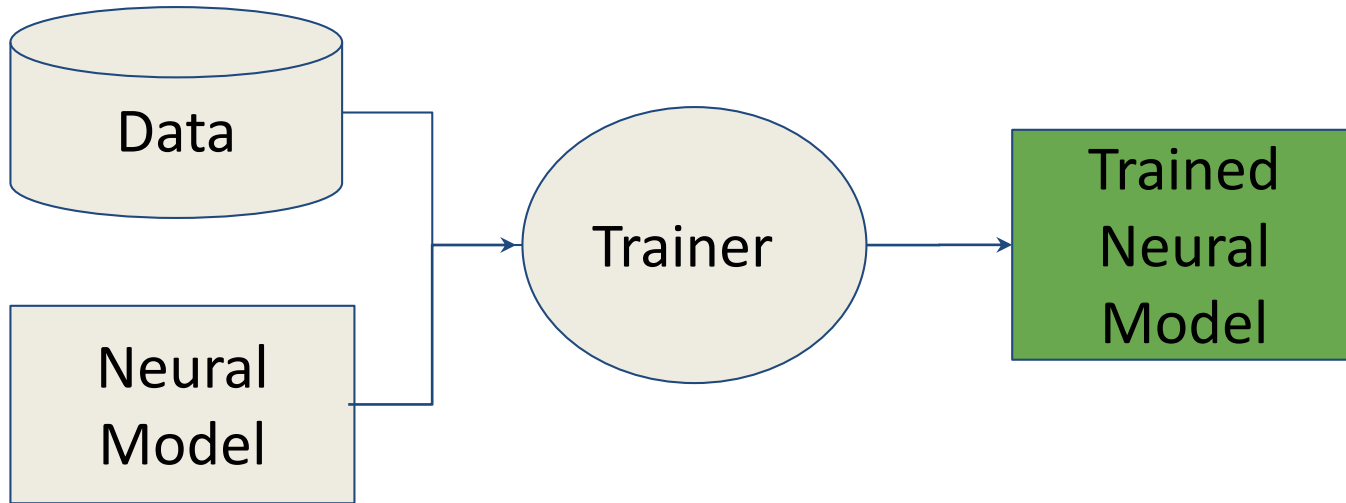


Testing

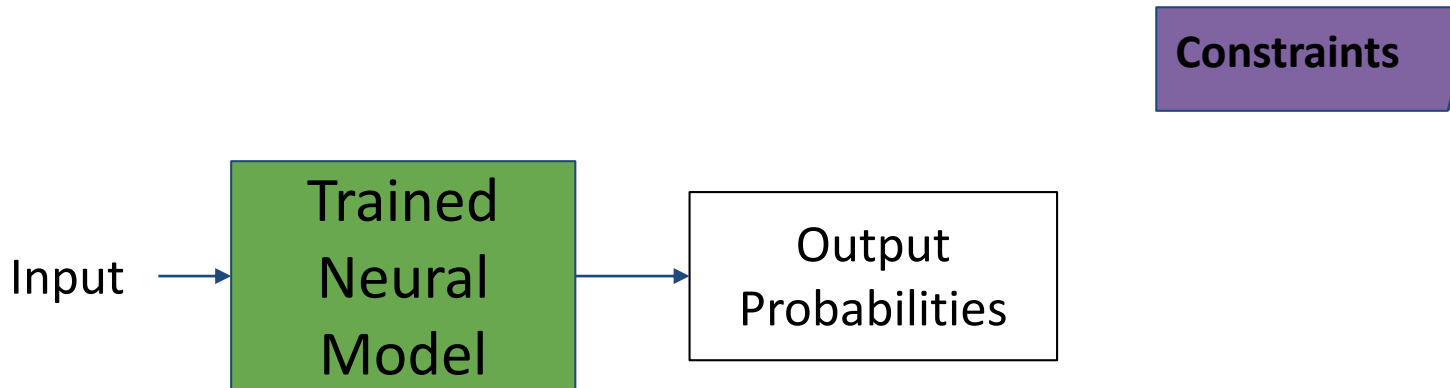


Constraints over Output Space

Training

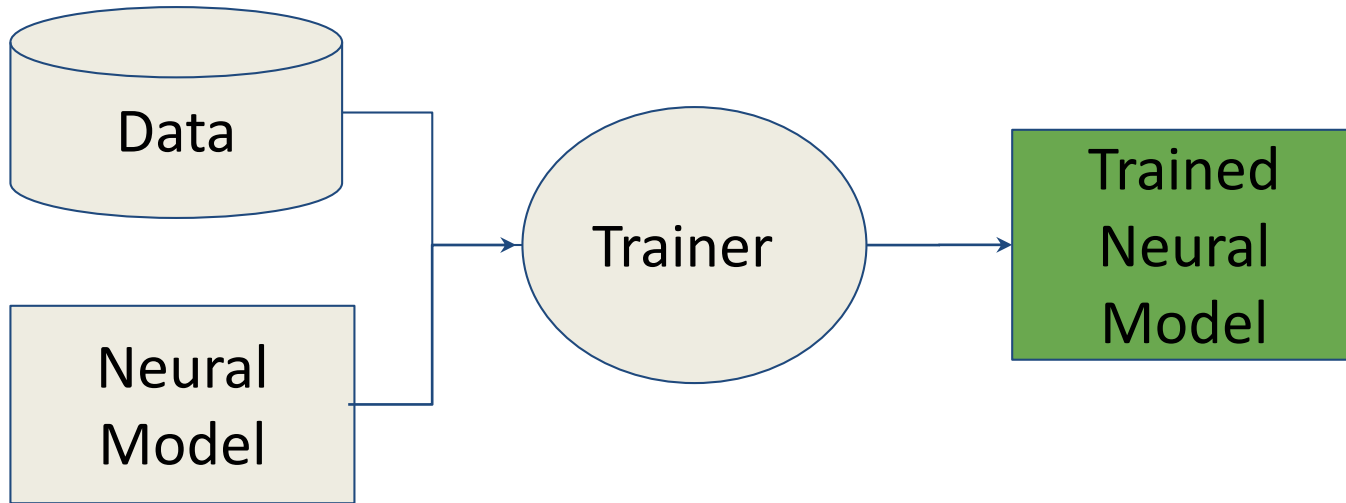


Testing

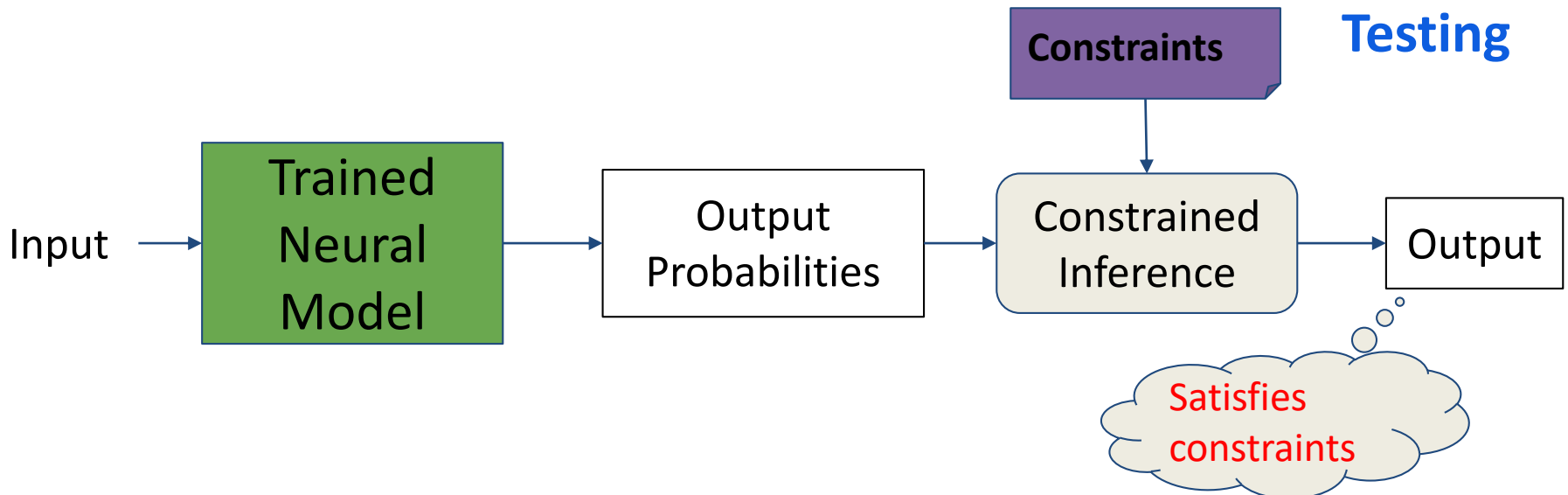


Reasoning at Inference

Training

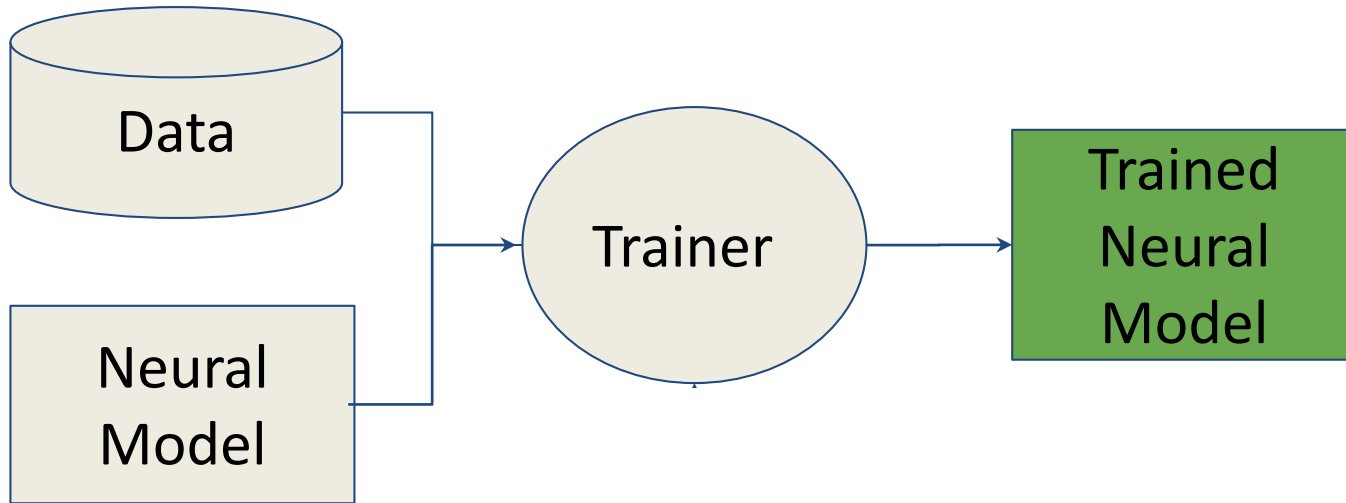


Testing



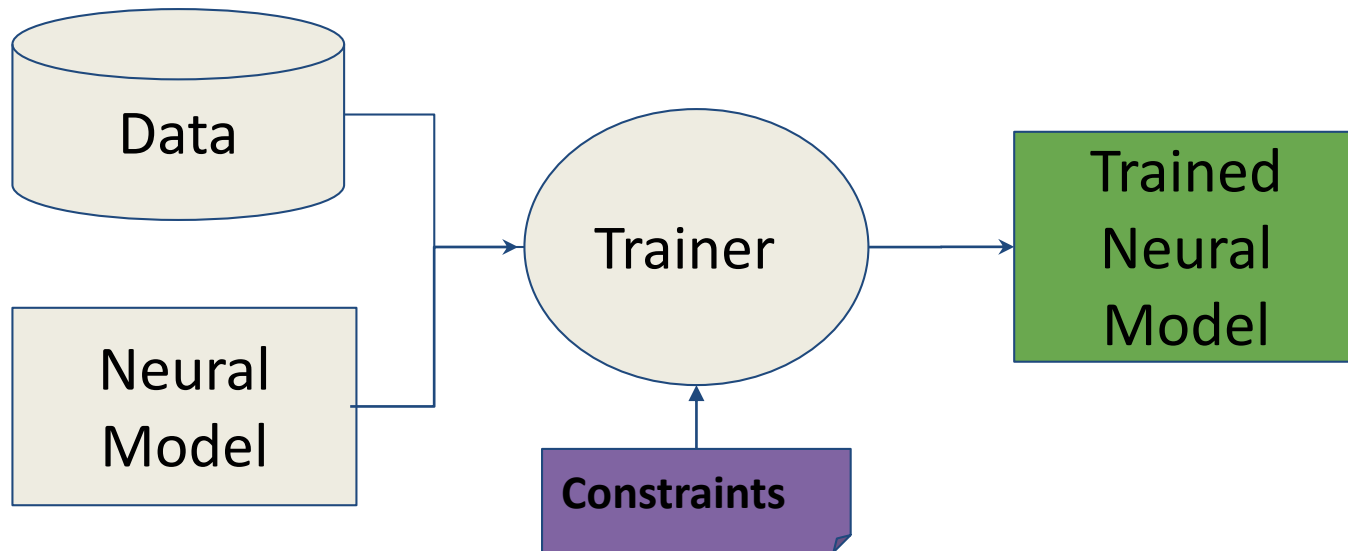
Reasoning within Learning

Training



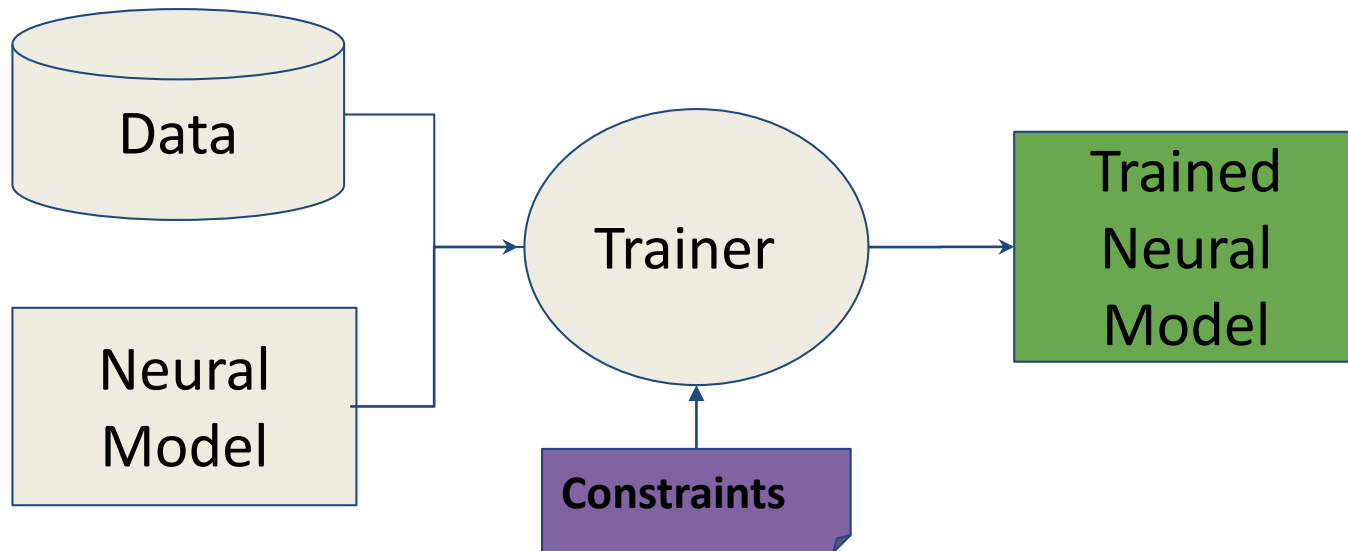
Reasoning within Learning

Training

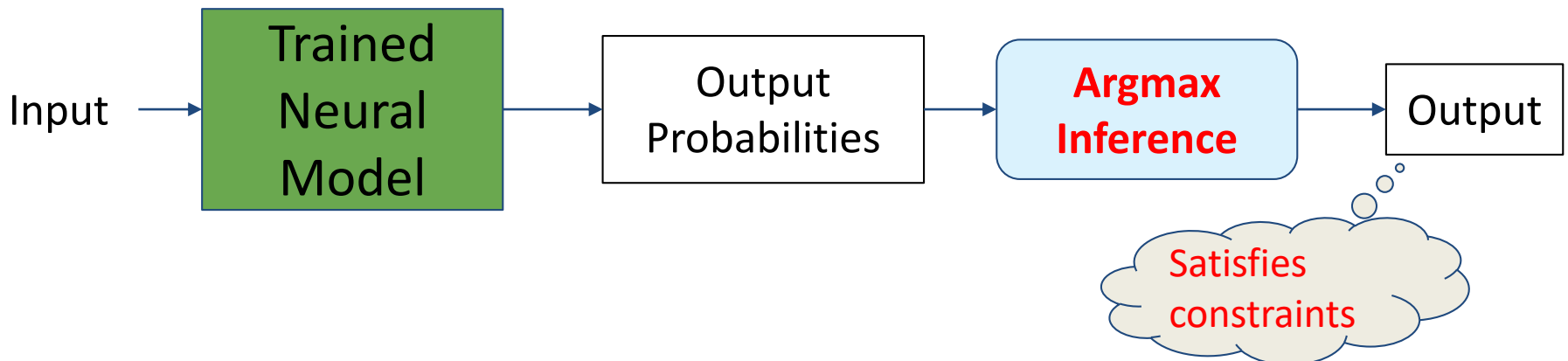


Reasoning within Learning

Training



Testing



Human-Provided Output Constraints

- Fine-Grained Type Prediction (FIGER)
- Constraints
 - $\text{Scientist}_{\text{FIGER}} \rightarrow \text{Person}_{\text{FIGER}}$
 - $\text{Scientist}_{\text{FIGER}} \rightarrow \neg \text{Vehicle}_{\text{FIGER}}$
 - ...

Human-Provided Output Constraints

- POS Tagging
- Constraints
 - There must be a verb in the sentence

Human-Provided Output Constraints

- Multi-task Constraints between
 - Named Entity Recognition
 - Part of Speech Tagging
- Constraints
 - $\text{Person}_{\text{NER}} \rightarrow \text{NNP}_{\text{POS}}$
 - $\text{Org}_{\text{NER}} \rightarrow \text{NNP}_{\text{POS}}$
 - $\text{Time}_{\text{NER}} \rightarrow \{\text{NNP}, \text{CD}, \text{JJ}, \text{IN}\}_{\text{POS}}$
 - ...

Output Constraints →

Constraints on Output Probabilities

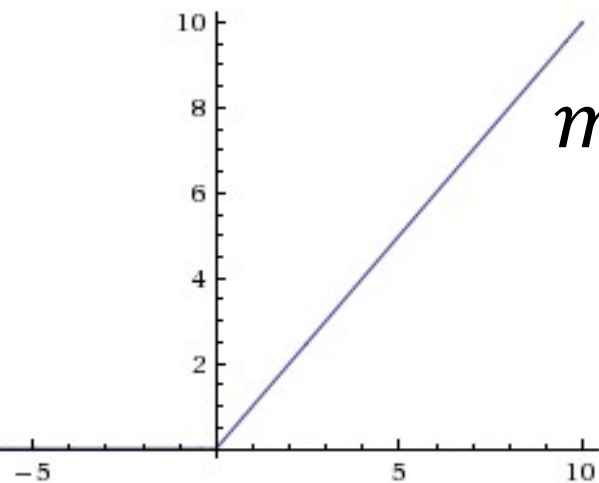
Constraints

- Person → NNP
- Time → {NNP, CD, JJ, IN}

Converted Constraints

- $p(\text{Person}) \leq p(\text{NNP})$
 - $p(\text{PERSON}) - p(\text{NNP}) \leq 0$
- $p(\text{Time}) \leq p(\text{NNP}) + p(\text{CD}) + p(\text{JJ}) + p(\text{IN})$
 - $p(\text{TIME}) - p(\text{NNP}) - p(\text{CD}) - p(\text{JJ}) - p(\text{IN}) \leq 0$

Optimization Problem



$$\min_w L(w) = CE(y^*, z^* | x; w)$$

$$\text{s.t } C(y, z | x; w) \leq 0$$

$$\text{s.t. Hinge}(C(y, z | x; w)) = 0$$

Solved by Lagrangian relaxation

Iterating over updating weights and Lagrange variables

$h_k(w)$

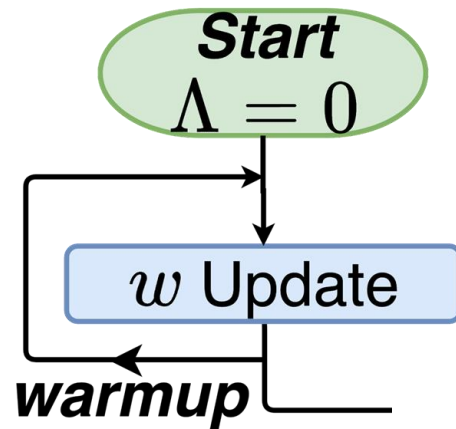
Lagrangian Formulation

$$\min_w L(w) \quad \text{subject to} \quad h_k(w) = 0; \quad \forall 1 \leq k \leq K$$

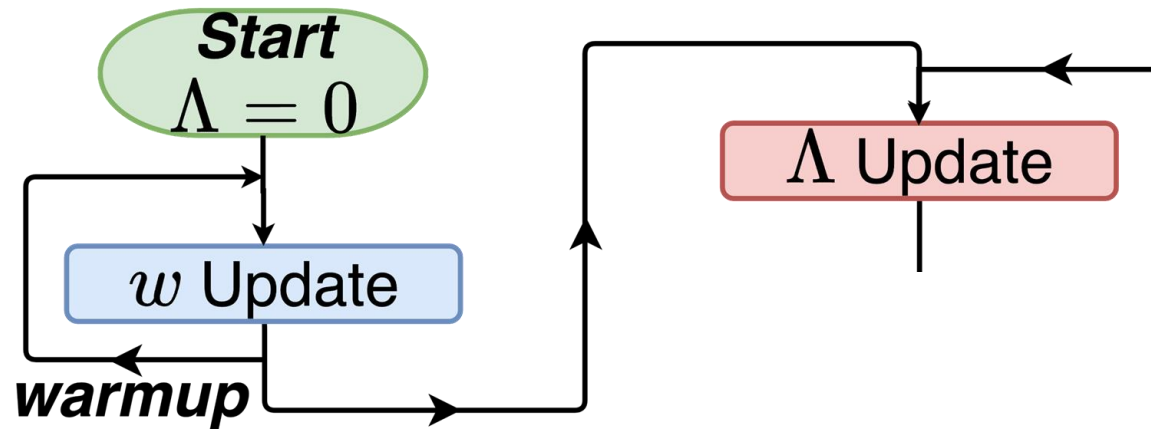
Lagrangian

$$\mathcal{L}(w; \Lambda) = L(w) + \sum_{k=1}^K \lambda_k h_k(w)$$

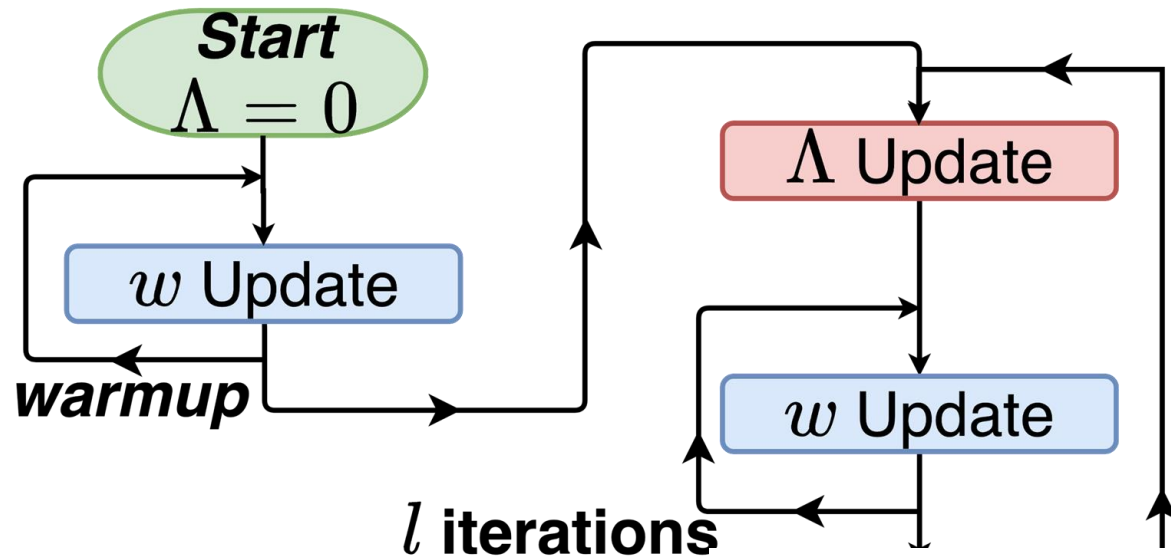
Training Algorithm



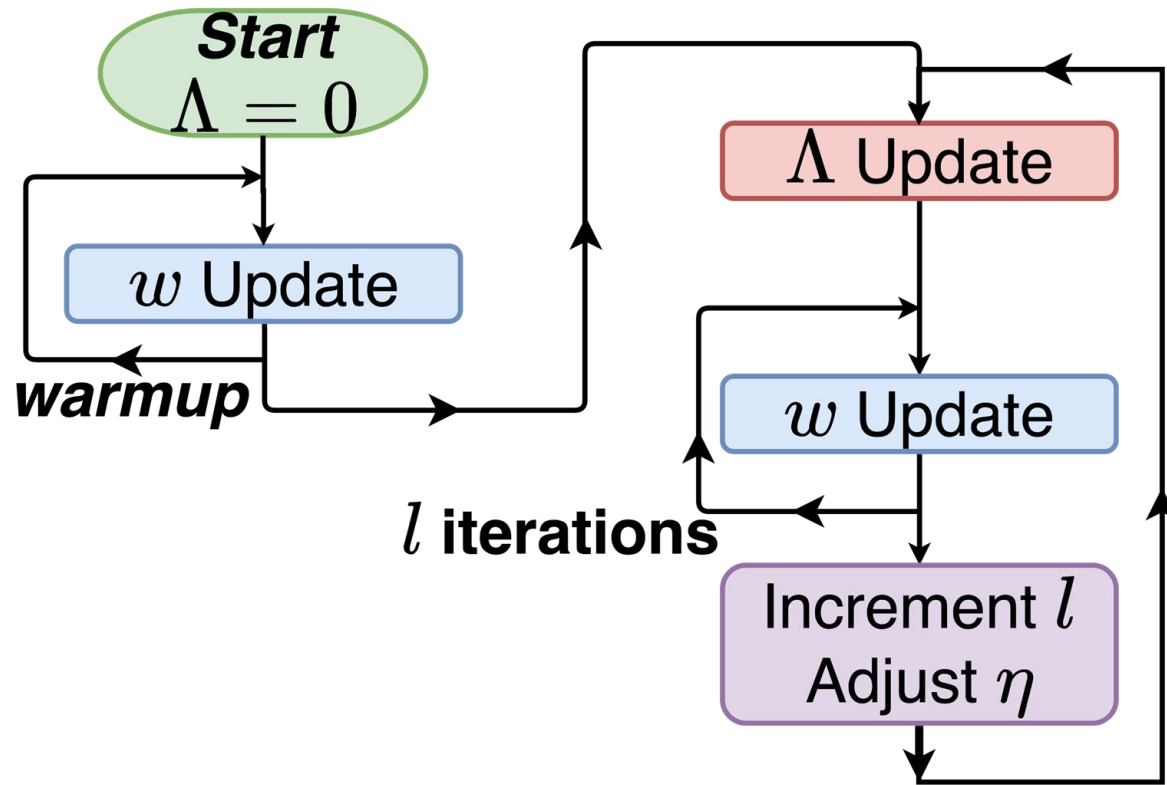
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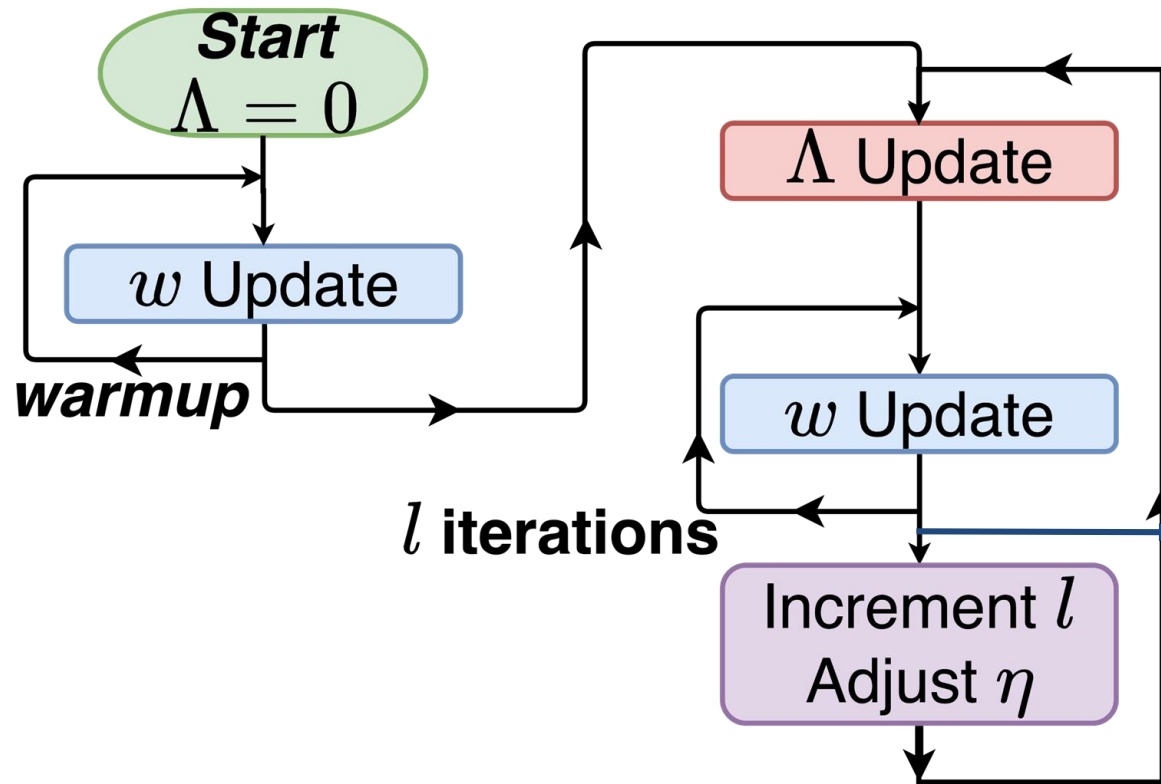
Training Algorithm



Training Algorithm



Training Algorithm



Semi-Supervised Learning

- Supervised Data

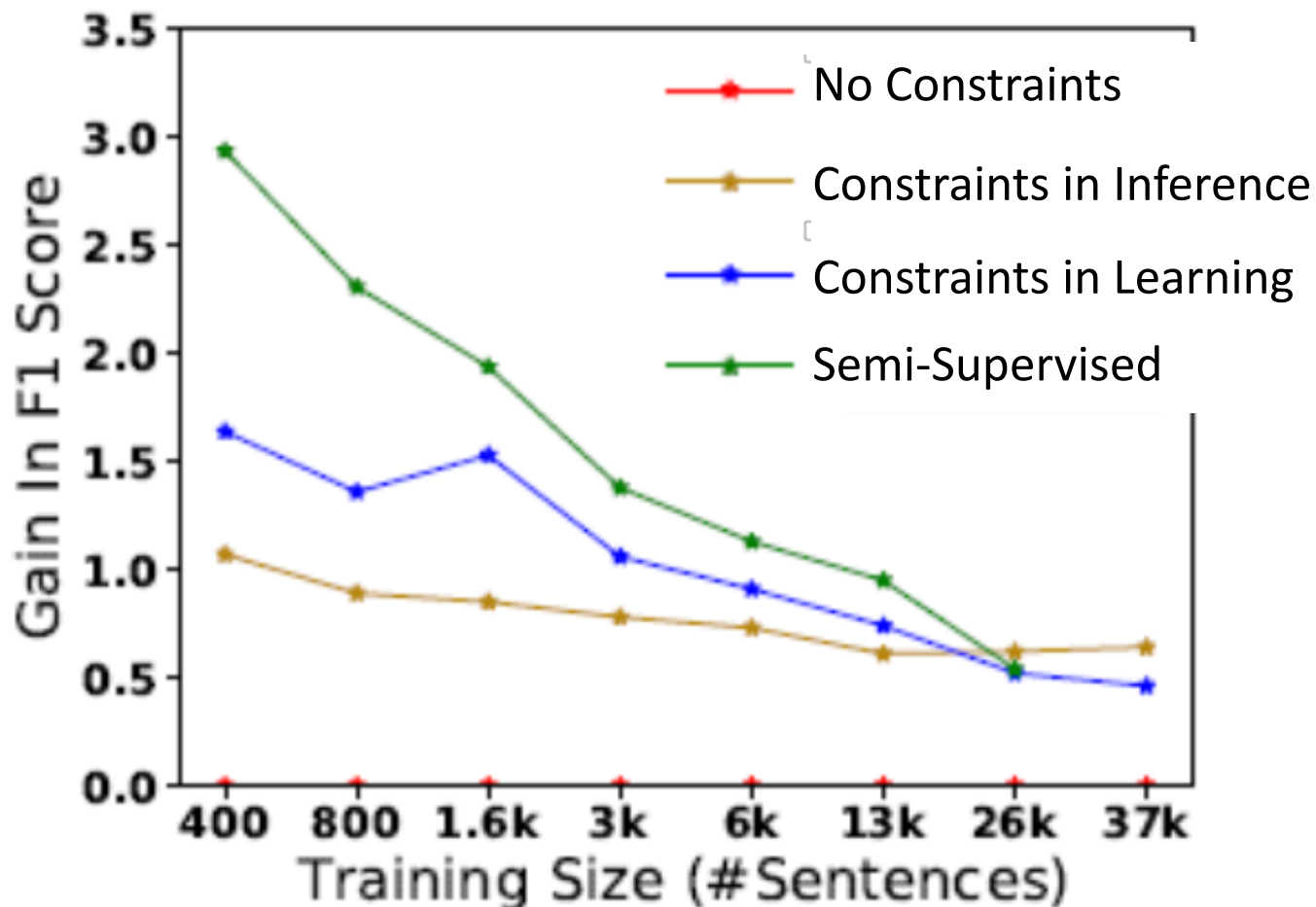
$$\mathcal{L}(w; \Lambda) = L(w) + \sum_{k=1}^K \lambda_k h_k(w)$$

- Unsupervised Data

$$\mathcal{L}(w; \Lambda) = \sum_{k=1}^K \lambda_k h_k(w)$$

Results (Multi Task NER-POS)

[Nandwani et al, NeurIPS 2019]

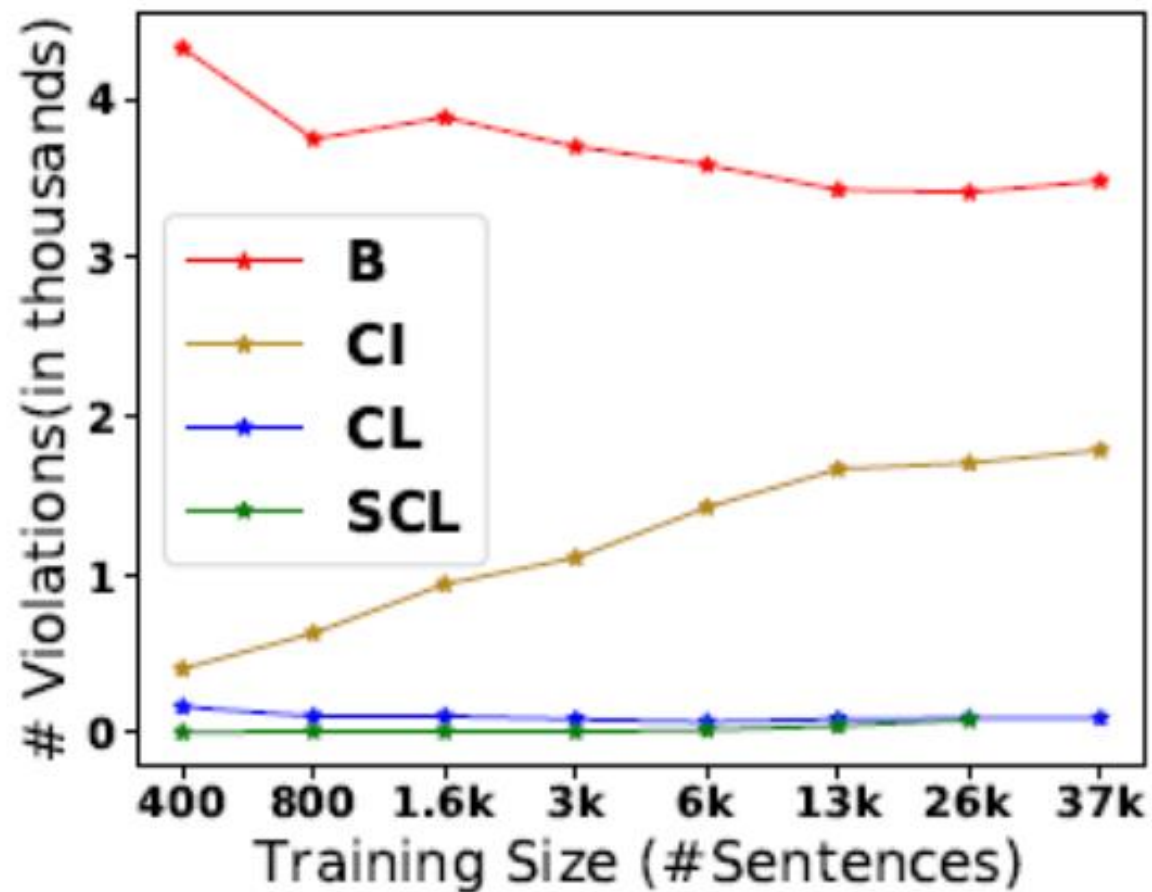


(a) Avg. Gain in F1 Score Over Baseline.

Test Time

	Test Time
Constraints in Training	115 sec
Constraints in Inference	2,895 sec

Num. of Constraint Violations



(b) Avg. number of Constrained Violations

More Results

[Nandwani et al, NeurIPS 2019]

- Fine-Grained Entity Typing

% Data	5%	10%	100%	5%	10%	100%
Baseline	68.6	69.2	70.5	22,715	21,451	22,359
Const. L	78.4	80.6	83.5	186	95	97

- Semantic Role Labeling

% Data	1%	5%	10%	1%	5%	10%
Baseline	62.7	72.6	75.3	19,317	11,718	10,570
Const. L	66.0	73.7	76.0	9,231	6,436	6,140

Soft Constraints

[Kolluru et al, EMNLP 2020, Gupta et al, ArXiv 2022]

- Open Information Extraction

Algos	AUC	F1
Baseline	33.7	52.4
Constrained Learning	35.7	54

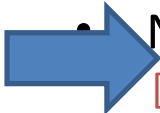
- Info. Extraction from Tables in Research Papers

Algos	ID F1	Tuple F1	Mat. F1
GNN	78.7	69.3	60.9
Constrained Learning of GNN	82.4	70.1	63.5

Take Home

- Low Data Settings
 - Encode human insight as output constraints
- To get guarantees
 - Use hard constraints: solve using Lagrangian
- Availability of unsupervised data
 - Use constraint loss to regularize the model

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Neural AI → (Machine) Symbolic Theory

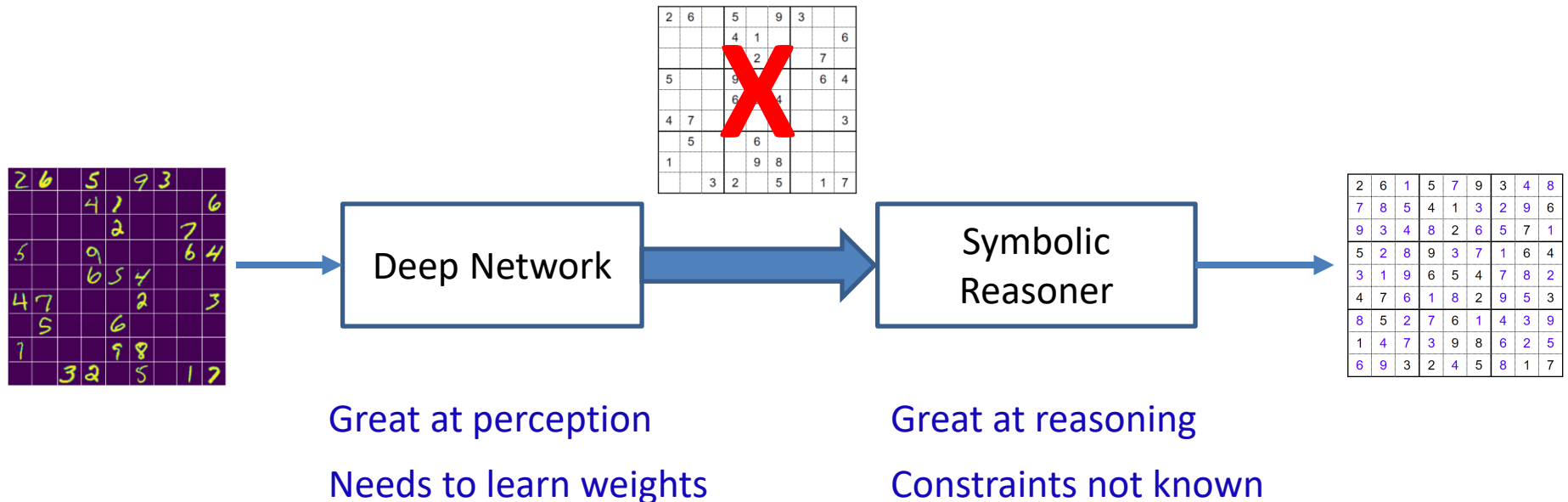
Visual Reasoning Tasks

2	6		5		9	3		
			4	7				6
				2			7	
5			9				6	4
			6	5	4			
4	7				2			3
	5			6				
7				9	8			
		3	2		5		1	7



2	6	1	5	7	9	3	4	8
7	8	5	4	1	3	2	9	6
9	3	4	8	2	6	5	7	1
5	2	8	9	3	7	1	6	4
3	1	9	6	5	4	7	8	2
4	7	6	1	8	2	9	5	3
8	5	2	7	6	1	4	3	9
1	4	7	3	9	8	6	2	5
6	9	3	2	4	5	8	1	7

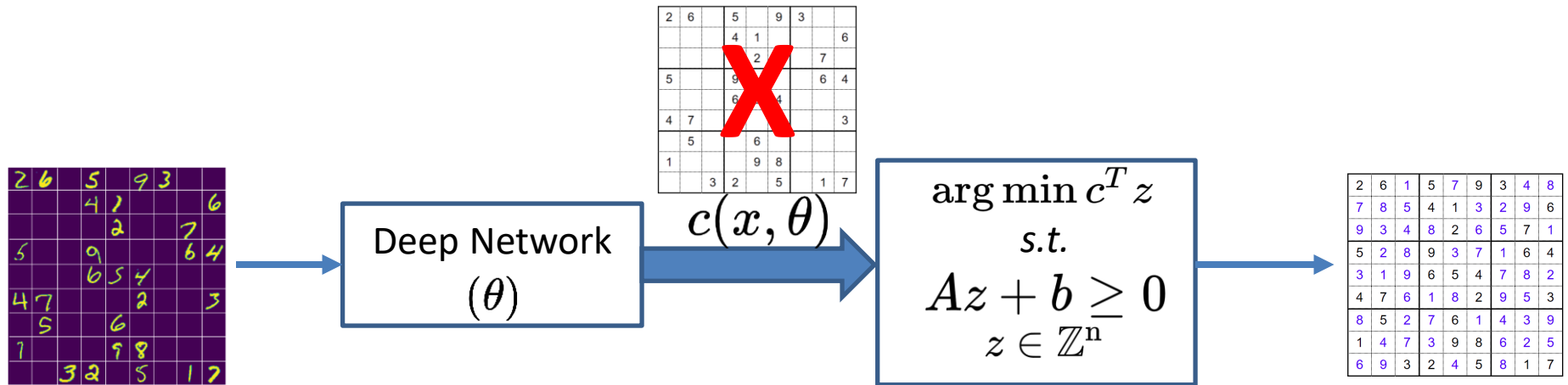
Perception with Reasoning



Challenge: no intermediate supervision!

Benefit: Explicit representation of symbolic constraints in the language of the symbolic solver.

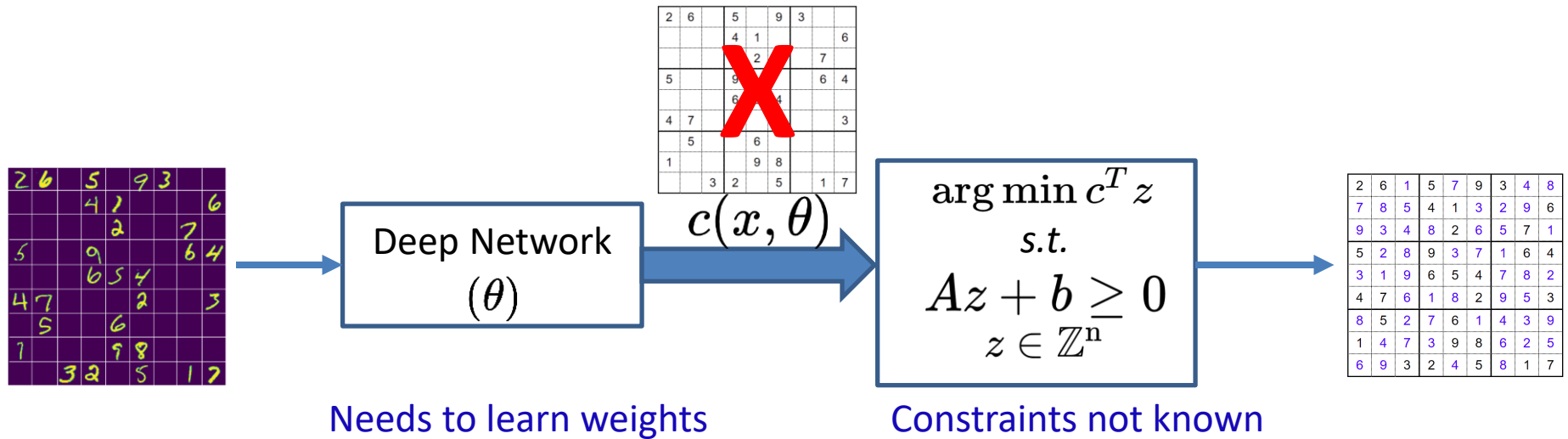
Neural-ILP Architecture



Forward Pass: Generate + solve an optimization problem (ILP)

Backward Pass: Define derivatives w.r.t. A , b and c

Neural-ILP Architecture: Bottleneck



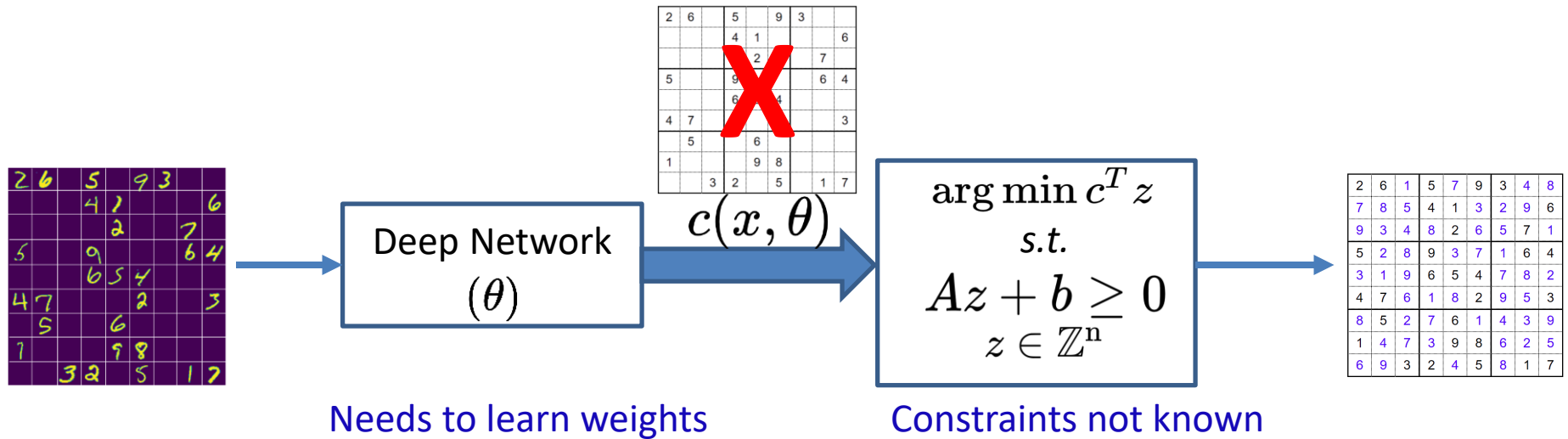
Training Bottleneck:

existing works call ILP solver (expensive)

in each learning iteration for computing the gradients

[Paulus et al. ICML 2021: “CombOptNet: Fit the Right NP-Hard Problem by Learning Integer Programming Constraints.”]

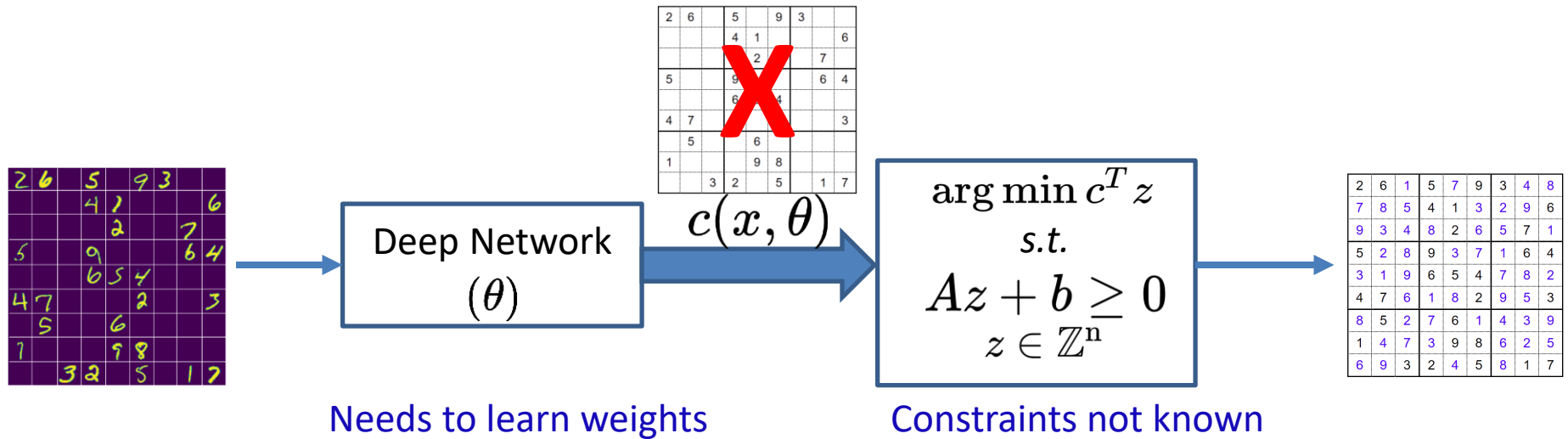
Neural-ILP Architecture: Solution



Our Solution:

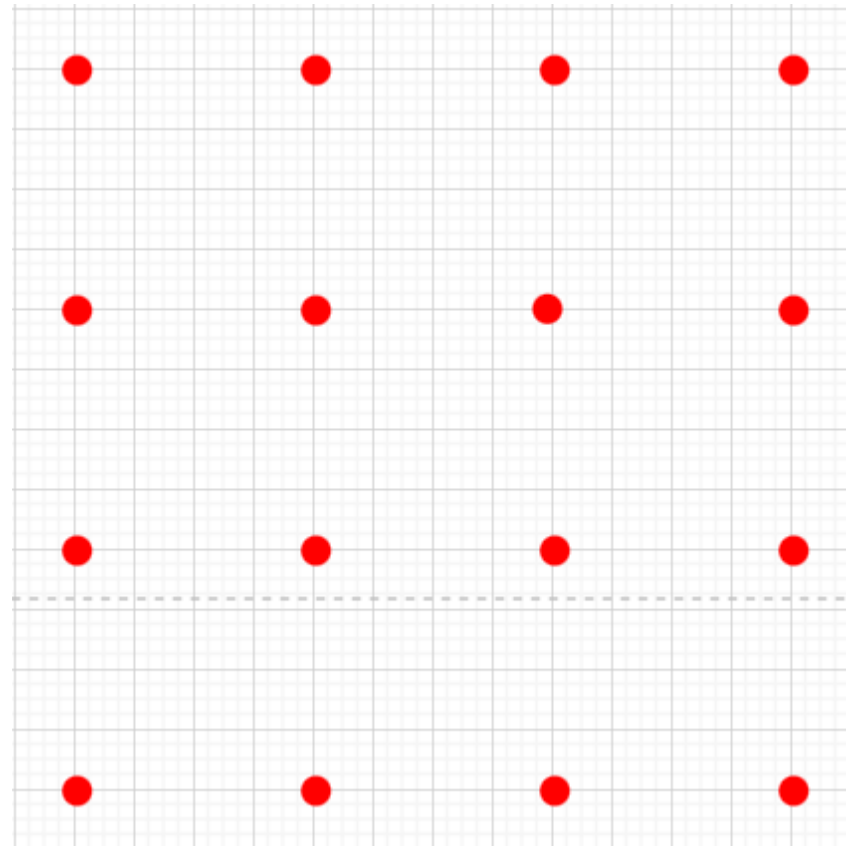
A solver-free Framework for Scalable Learning in Neural ILP architectures

Neural-ILP Architecture: Solution



Treat linear constraints as Binary Linear Classifiers
separating gold targets from the negatives (rest of the space)!

Learning Constraints



Learning Constraints

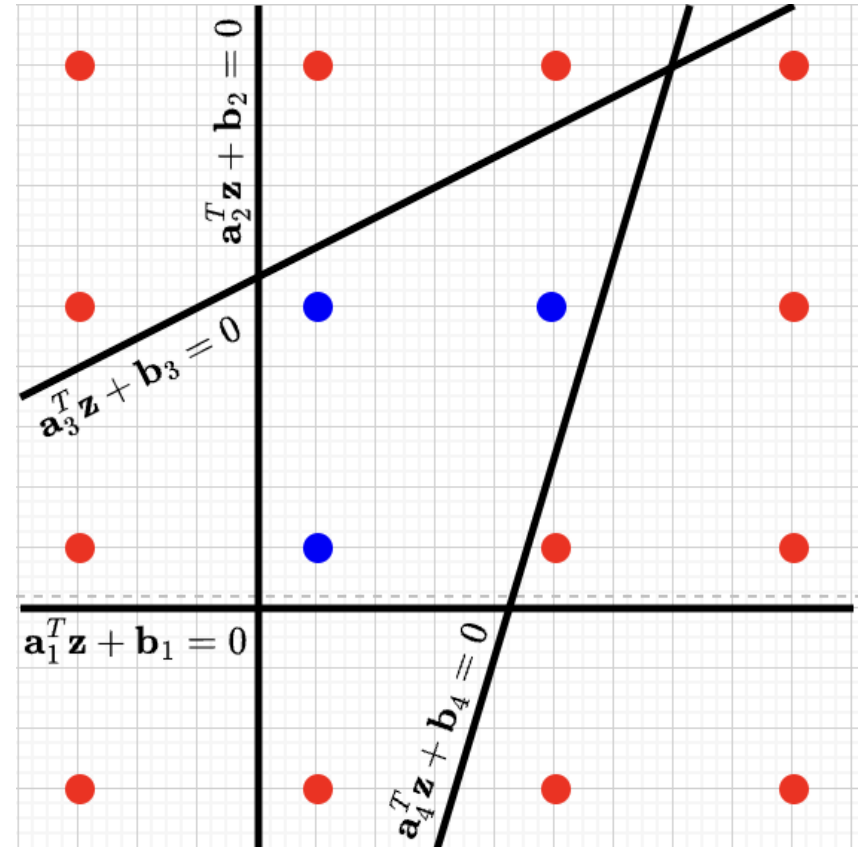
- 4 learnable constraints

$$\mathbf{a}_1^T \mathbf{z} + \mathbf{b}_1 \geq 0$$

$$\mathbf{a}_2^T \mathbf{z} + \mathbf{b}_2 \geq 0$$

$$\mathbf{a}_3^T \mathbf{z} + \mathbf{b}_3 \geq 0$$

$$\mathbf{a}_4^T \mathbf{z} + \mathbf{b}_4 \geq 0$$



Learning Constraints

- 4 learnable constraints

$$\mathbf{a}_1^T \mathbf{z} + \mathbf{b}_1 \geq 0$$

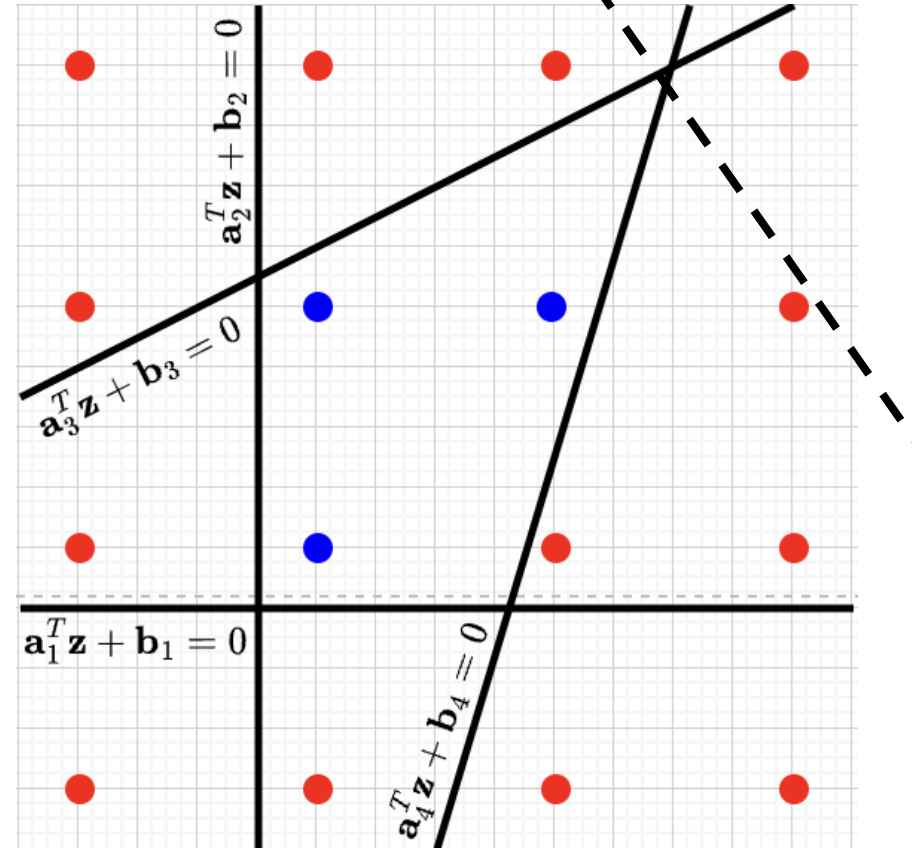
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$$\mathbf{a}_4^T \mathbf{z} + \mathbf{b}_4 \geq 0$$

- One objective function

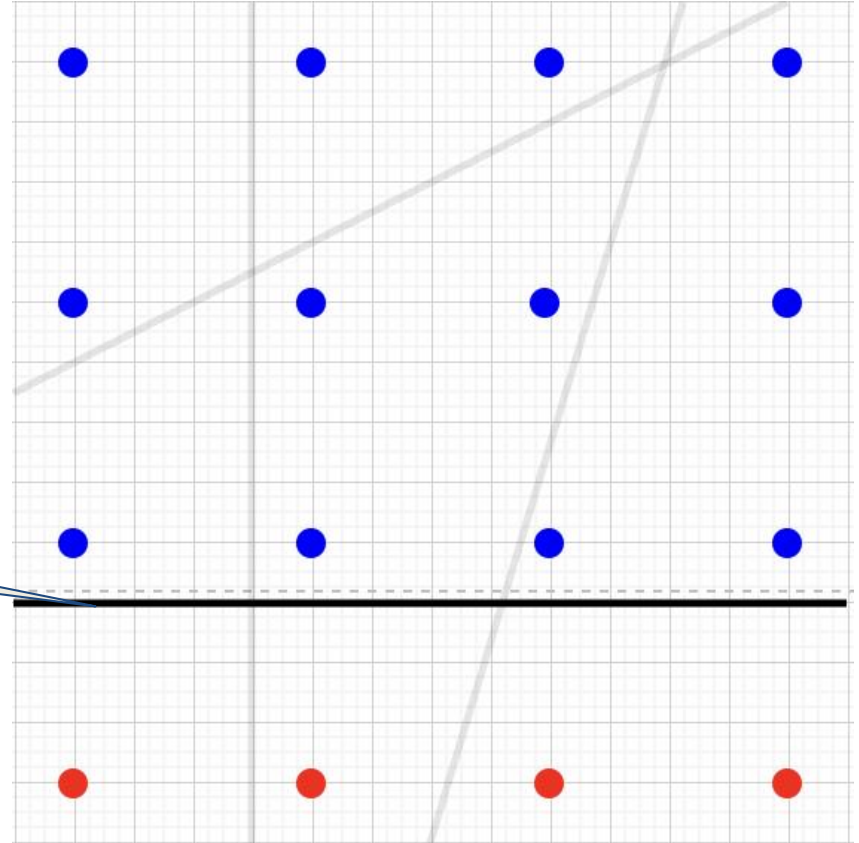
$$\arg \min c^T \mathbf{z}$$



Learning Constraints

- 4 learnable constraints
- Each constraint is a binary-classifier

Binary classifier separating +ve points (blue) from -ves (red)

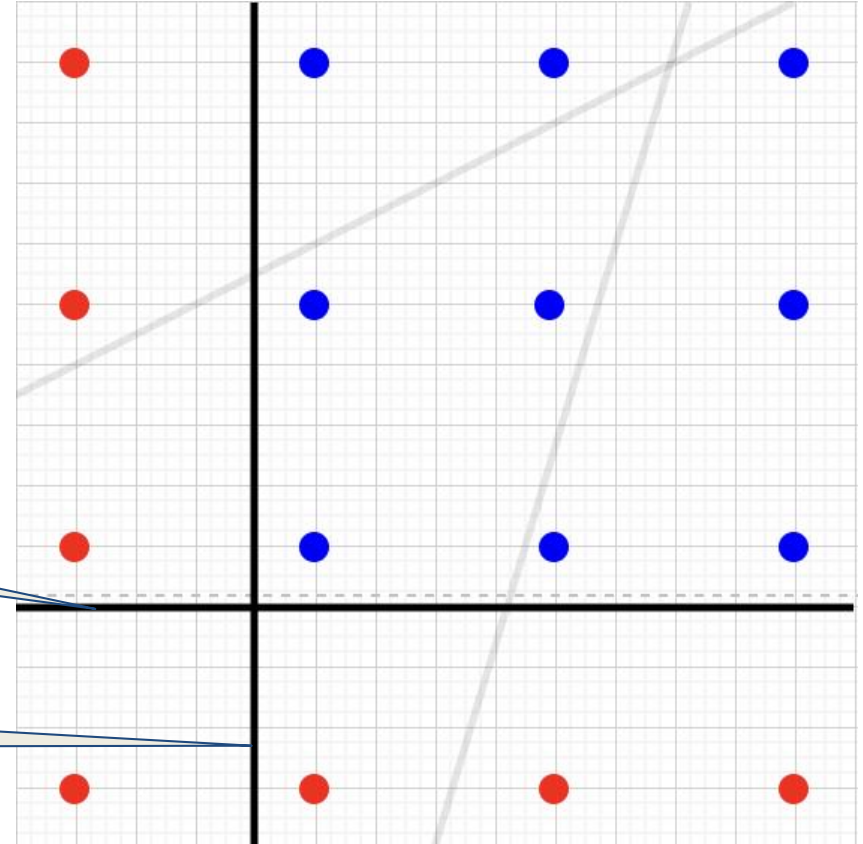


Learning Constraints

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Binary classifier separating +ve points (blue) from -ves (red)

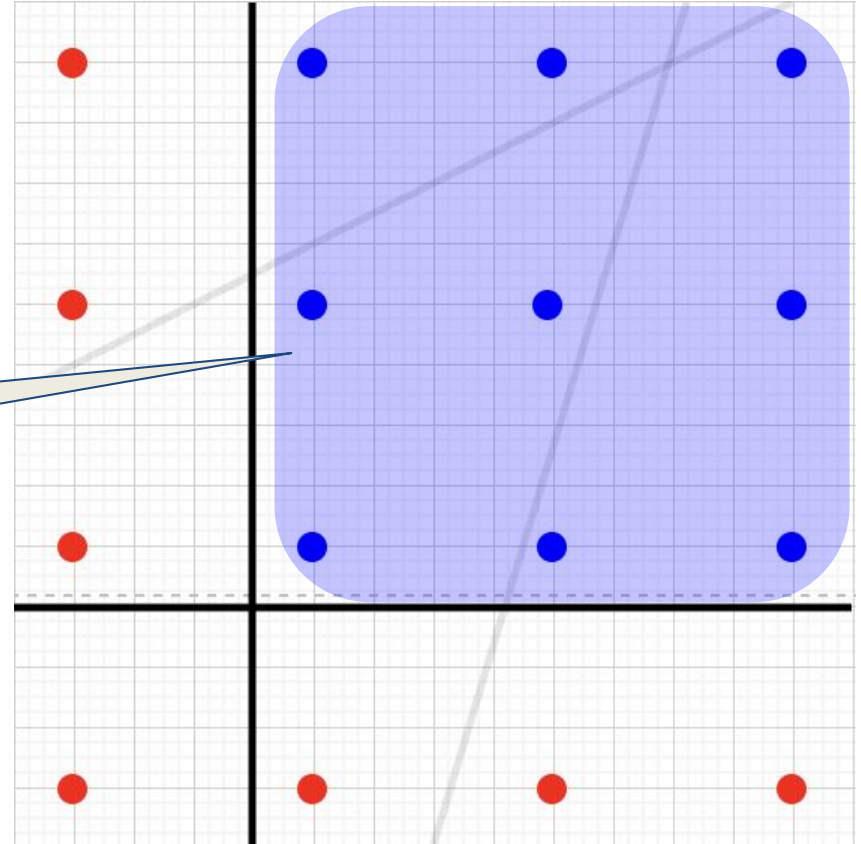
Another classifier



Learning Constraints

- 4 learnable constraints
- Each constraint is a binary-classifier

+ve points are +ve for both classifiers

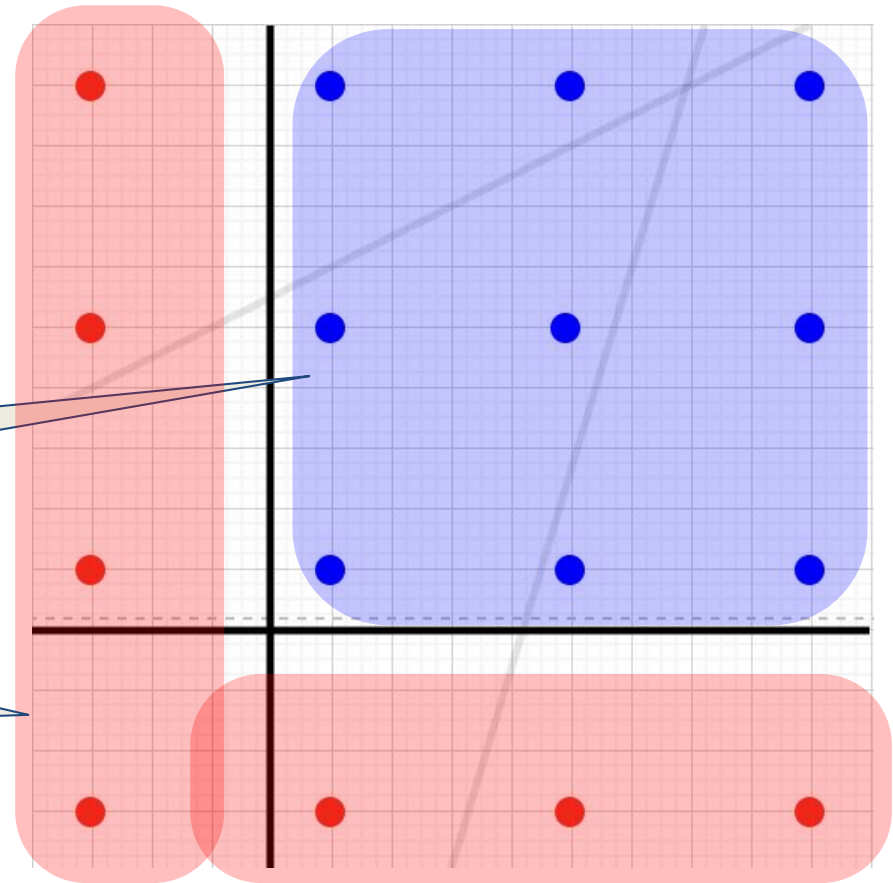


Learning Constraints

- 4 learnable constraints
- Each constraint is a binary-classifier

+ve points are +ve for both classifiers

-ve points are -ve for at least one of the classifiers

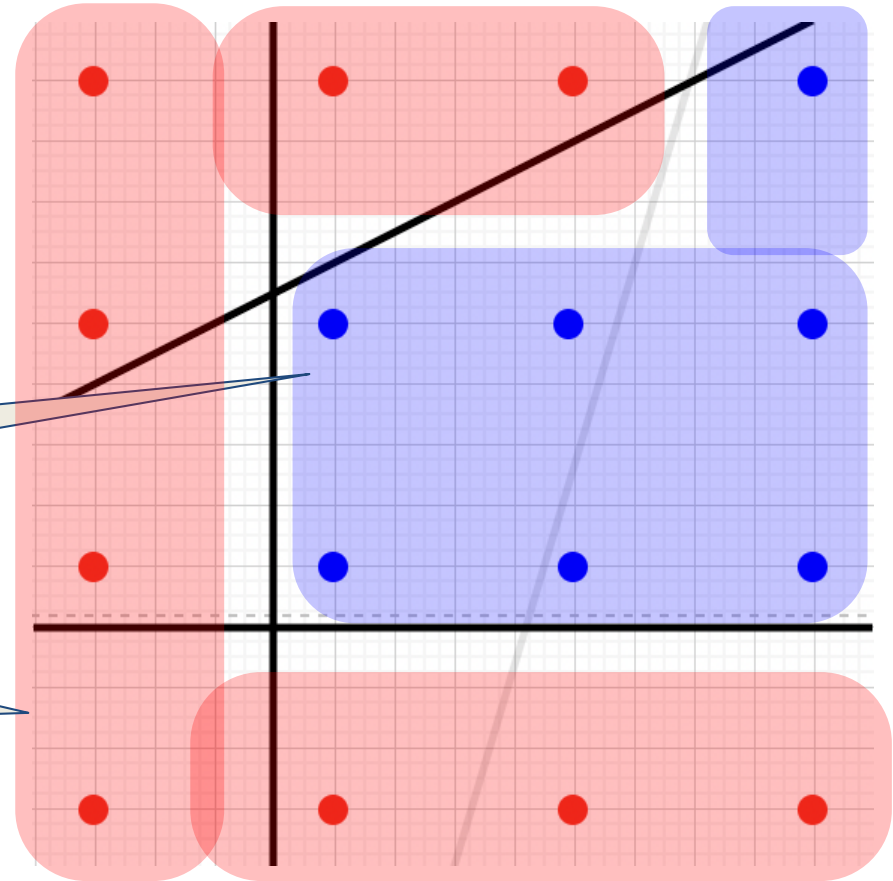


Learning Constraints

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+ve points are +ve for all classifiers

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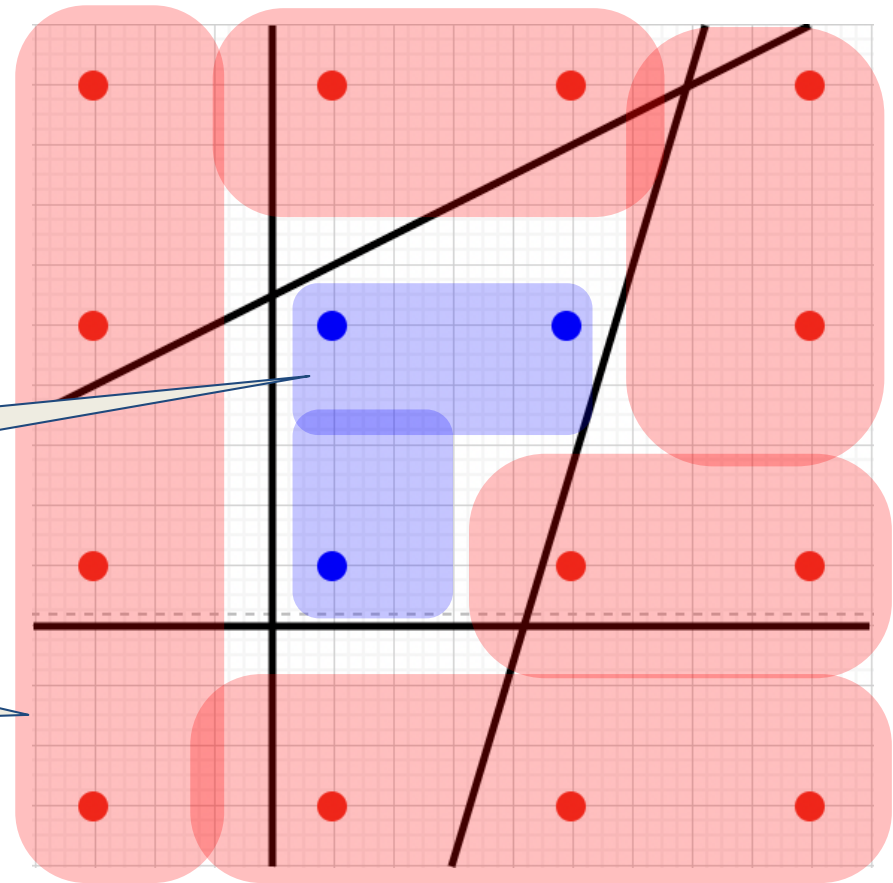


Learning Constraints

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Learning Cost

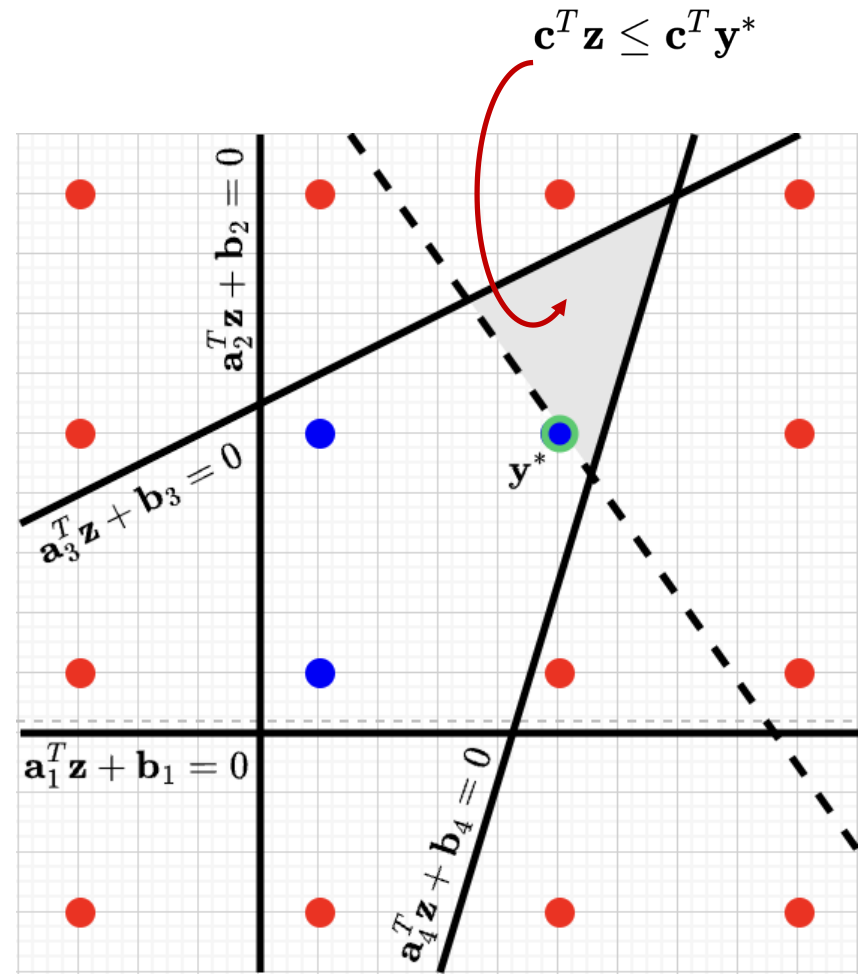
For a given $(\mathbf{x}, \mathbf{y}^*)$ in training data

- Convert corresponding cost vector \mathbf{c} to a constraint. \mathbf{y}^* has optimal cost, i.e.

- Only \mathbf{y}^* in the polytope satisfies

$$\mathbf{c}^T \mathbf{z} \leq \mathbf{c}^T \mathbf{y}^*$$

- All other points in the polytope are -ve for this constraint



Learning Constraints & Cost

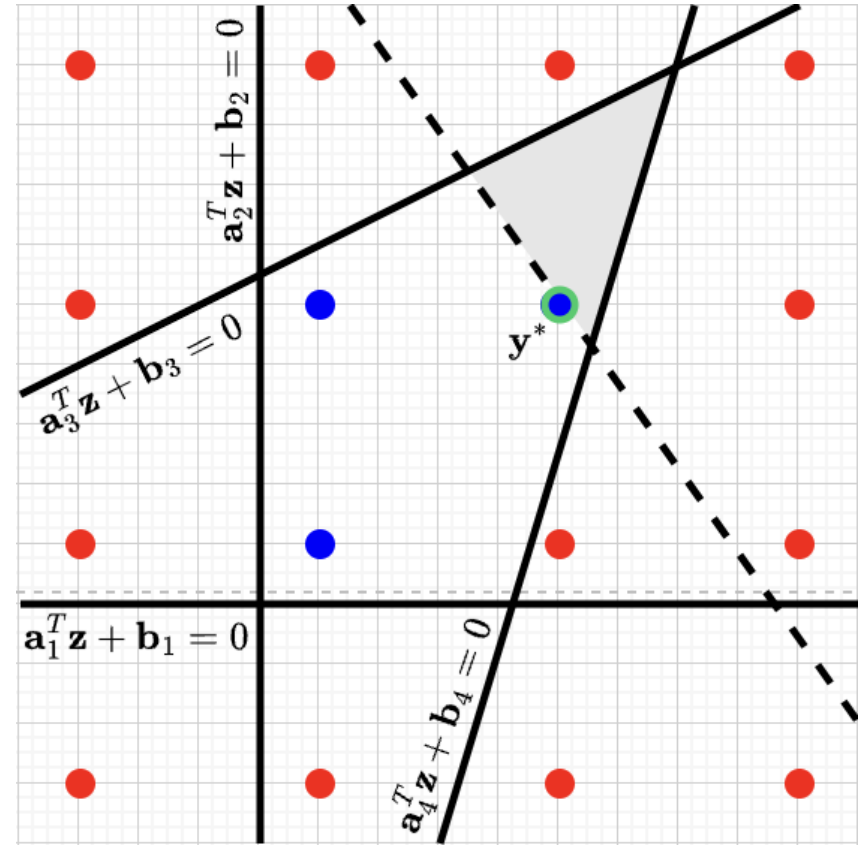
Original ILP:

$$\arg \min_{\mathbf{z}} \mathbf{c}^T \mathbf{z} \text{ subject to } \mathbf{A}\mathbf{z} + \mathbf{b} \geq 0, \mathbf{z} \in \mathbb{Z}^n$$

Modified ILP:

$$\arg \min_{\mathbf{z}} 1 \text{ subject to } \mathbf{A}\mathbf{z} + \mathbf{b} \geq 0, \mathbf{z} \in \mathbb{Z}^n \\ \mathbf{c}^T \mathbf{z} \leq \mathbf{c}^T \mathbf{y}^*$$

\mathbf{y}^* is the **only** point feasible
for the modified ILP.



Other Details

- **Negative Sampling**

For a given (x, y^*)

*sample k -hop neighbors of y^**

use positive samples of other examples in the batch

- **Loss**

encourages each positive example to satisfy each constraint

encourages each negative example to fail on some constraint

Results

[Nandwani et al, NeurIPS 2022]

Visual Sudoku

	Accuracy	Training Time (m)
Neural (RRN)	71.1	97
SATNet	17.8	205
Neuro-Symb (CombOptNet)	0.0	Timeout
Neuro-Symb (Ours)	98.3	92

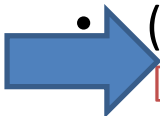
Textual Knapsack

Test size	10	15	20	25	30
CombOptNet	63.2	48.2	30.1	2.6	0.0
Ours	71.4	58.5	48.7	41.0	28.4

Take Home

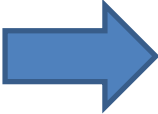
- Symbolic representations can be outputted by a neural model without supervision
- Symbolic algorithms can be explicitly used at test time
 - Especially useful for perception+reasoning tasks
- Notice the System1+System2 analogy!

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- Neural AI \rightarrow (Machine) Symbolic Explanation (explanations)
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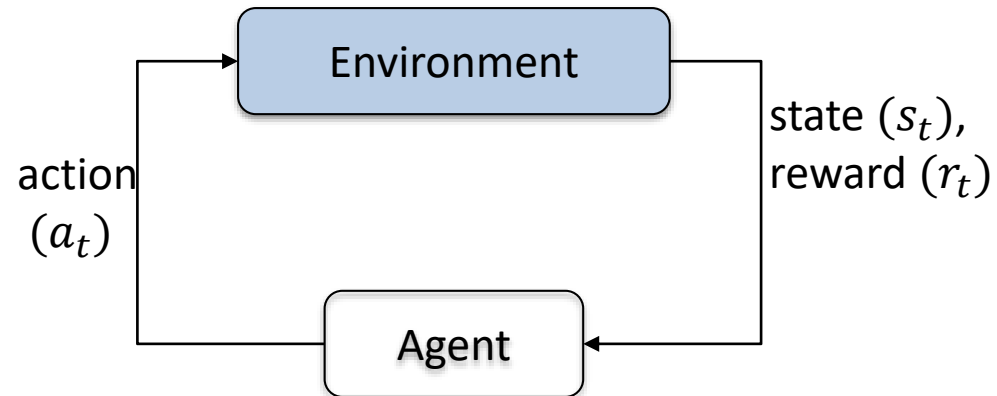
(Human) Symbolic Theory → Neural AI

GOFAI(++)

- Logical theory provided by domain designer
 - satisfiability
 - planning
- Probabilistic theory provided by domain designer
 - weighted maxsat
 -  – probabilistic planning
- Learn *generalized solution* for a GOFAI++ domain
 - train on small instances of a domain
 - transfer onto a new larger test instance of the same domain

Markov Decision Processes

- **MDP**: Markov Decision Process
 - S : States
 - A : Actions
 - T : Transition Function
 - R : Reward Function
 - H : Horizon
 - s_0 : Initial State
 - γ : Discount Factor

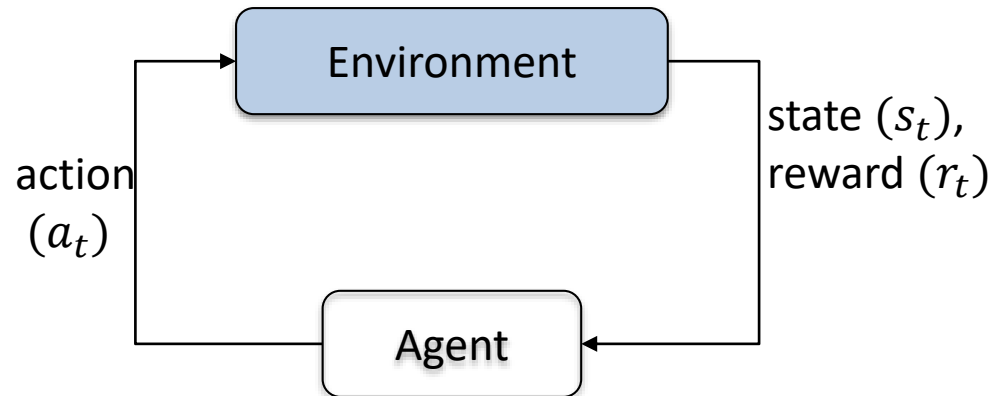


Goal of the Agent:

Learn a **policy** $\pi(a_t|s_t)$ that maximizes the expected long-term reward.

Relational MDPs

- **RMDP**: A factored Markov Decision Process in first-order form
 - C : Class types of objects
 - O : Objects
 - SP : State Predicates
 - AP : Action Predicates
 - T : Transition Function
 - R : Reward Function
 - H : Horizon
 - s_0 : Initial State
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Goal of the Agent:

Learn a **policy** $\pi(a_t|s_t)$ that maximizes the expected long-term reward.

RDDL for Relational MDPs

- **RMDP**: A factored Markov Decision Process in first-order form

- C : Class types of objects
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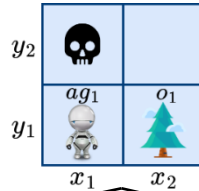
- **RDDL**: Relational Dynamic Influence Diagram Language [Sanner '10]

Domain Description
(C, SF, NF, A, T, R)

Instance Description
(O, H, s_o, γ)

- | | |
|---|------------------------------|
| • C : Class types of objects | • O : Objects |
| • SF : State Fluent Predicates | • H : Horizon |
| • NF : Non-Fluent Predicates | • s_o : Initial State |
| • AP : Action Predicates | • γ : Discount Factor |
| • T : Transition Function (1 st ord) | |
| • R : Reward Function (1 st ord) | |

Running Example



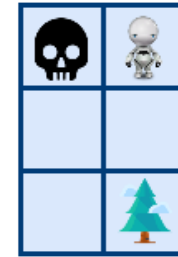
Domain Description

- ***C***: $x, y, object, agent, tool$
- ***SF***: $agentAt(agent, x, y), damaged(tool), waterChecked(obj), \dots$
- ***NF***: $objAt(obj, x, y), isUp(x_1, x_2), \dots, hazard(x, y), cameraTool(tool)$
- ***AP***: $goUp(agent), \dots, repair(agent, tool), useToolOn(agent, tool, obj)$
- ***T* and *R***: Set of first order formulas



Instance Description

- ***O***: $\{x_1, x_2\} \rightarrow x$
 $\{y_1, y_2\} \rightarrow y$
 $\{t_1, t_2\} \rightarrow tool$
 $\{o_1\} \rightarrow object$
 $\{ag_1\} \rightarrow agent$
- ***H***: 40
- ***s_o***: Initial State
- ***γ***: Discount Factor



Instance Description

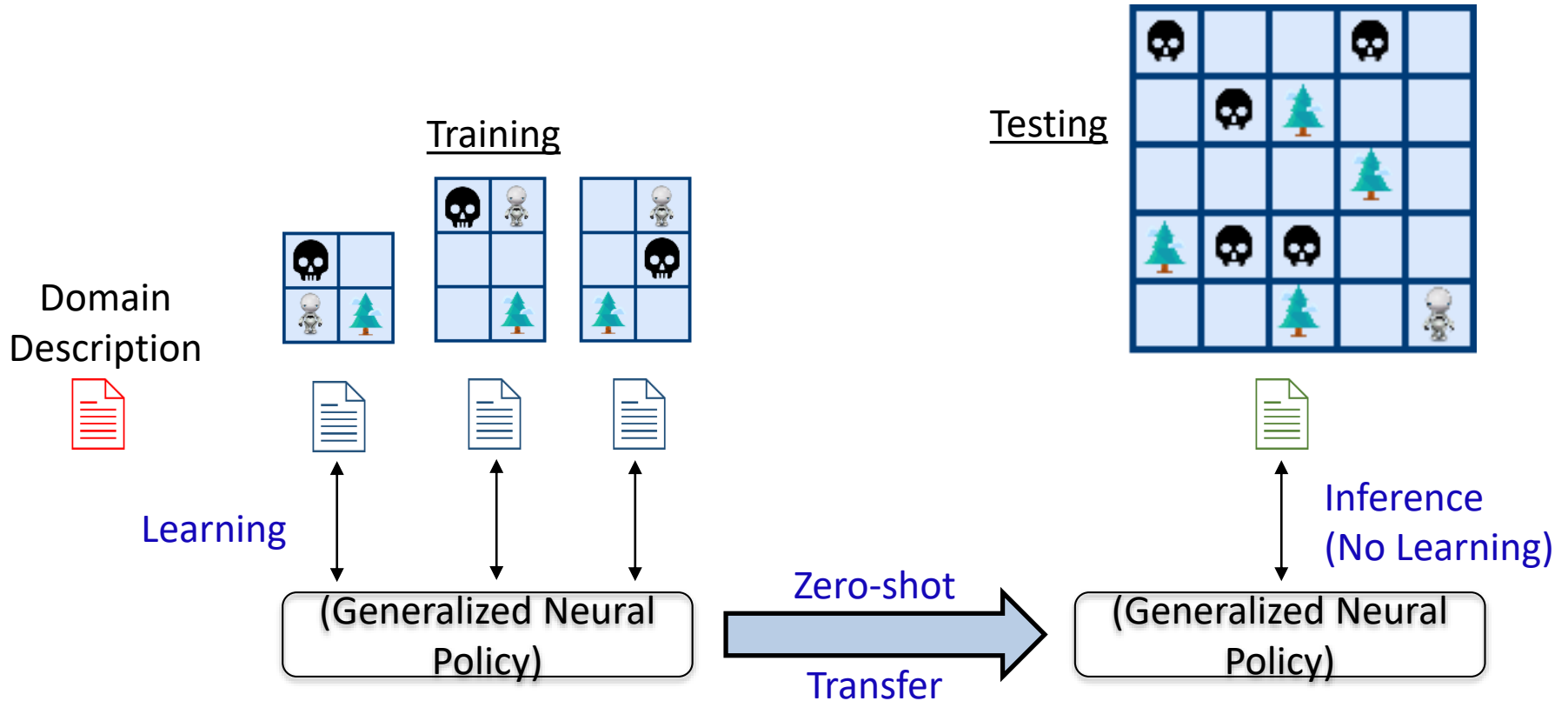
- ***O***: $\{x_1, x_2\} \rightarrow x$
 $\{y_1, y_2, y_3\} \rightarrow y$
 $\{t_1, t_2\} \rightarrow tool$
 $\{o_1\} \rightarrow object$
 $\{ag_1\} \rightarrow agent$
- ***H***: 40
- ***s_o***: Initial State
- ***γ***: Discount Factor

First-order representation → Infinite number of problem instances.

Relational MDPs: 1999-2010s

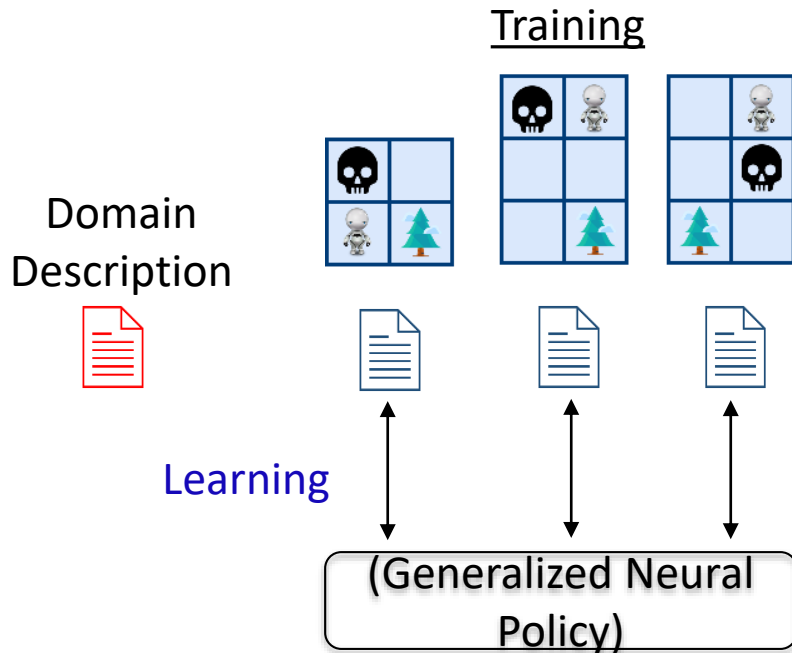
- Introduced by [Boutilier, Reiter, Price 1999]
- Followed the theme of stat. relational learning
- Several papers written until early 2010s
 - First order value iteration
 - First order representations of policy/value function
 - Machine learning approaches
 - approximations via linear basis-functions
- Vision broadly unsuccessful
 - problem too hard; representations not powerful

Transfer Learning for RMDPs



Generalized Neural Policy: A neural network representing a policy applicable on any instance of the domain.

Challenges



1. **Symbolic state:** a vector representing values of each state variable

$$agentAt(ag_1, x_1, y_1) = True$$

$$objAt(o_1, x_1, y_2) = True$$

2. **Variable state space:** Each instance has different number of state variables

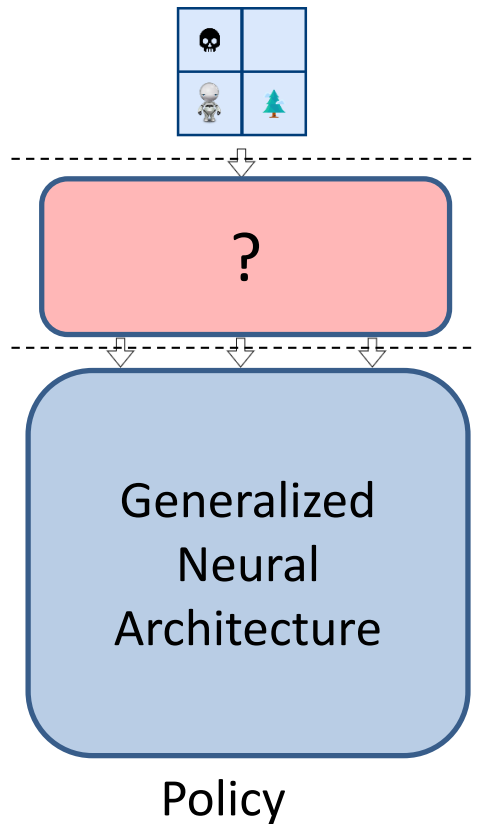
$$agentAt(agent, x, y)$$

3. **Variable action space:** actions are parameterized

$$useToolOn(agent, tool, obj)$$

Solution Approach

[Garg et al, ICML 2020]



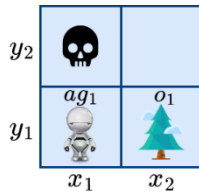
RDDL Instance (Symbolic)

Representation?

Graphs with
shared params

How to make it size invariant?

Instance Graphs → Nodes



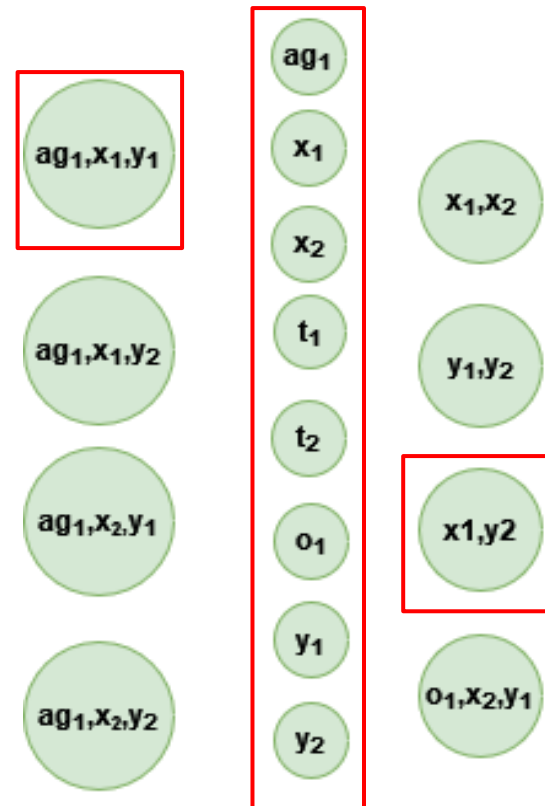
1. **Object-tuple Nodes:** A node for each unique argument of any predicate
2. **Singleton Object Nodes:** A node for each unique object

- Objects: $x_1, y_1, \dots, ag_1, t_1, t_2, o_1$
- State Fluents: **can change**

agentAt(ag_1, x_1, y_1) ...
damaged(t_1) ...
waterChecked(o_1)

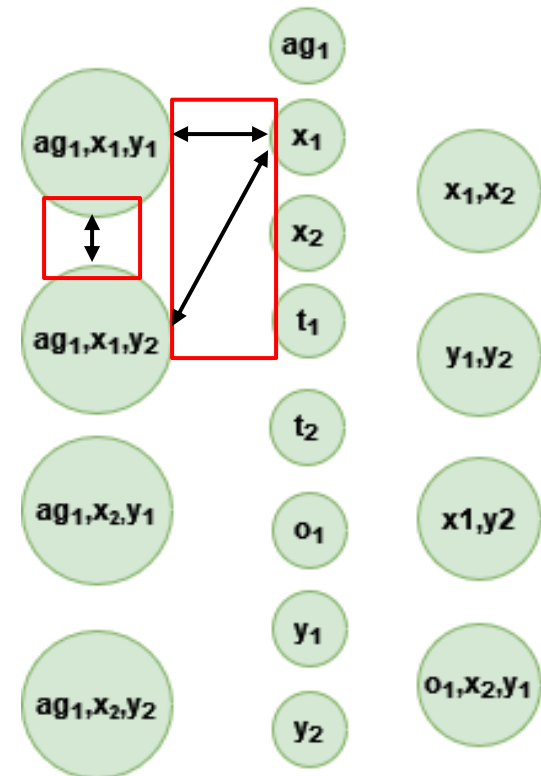
- Non Fluents: **can not change**

objAt(o_1, x_1, y_1), ...
lifeTool(t_1) ...
damageProb(t_1) ...
hazard(x_1, y_2) ...

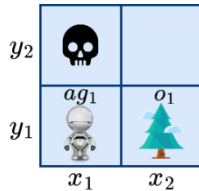


Instance Graphs \rightarrow Nodes

1. Add $u \rightarrow v$ if,
some state fluent with argument u affects
some other state fluent with argument v
2. Add $u \leftrightarrow v$ if,
 u occurs at position i in tuple v



Instance Graphs → Features



1. A feature for each (un)parameterized State-Fluent

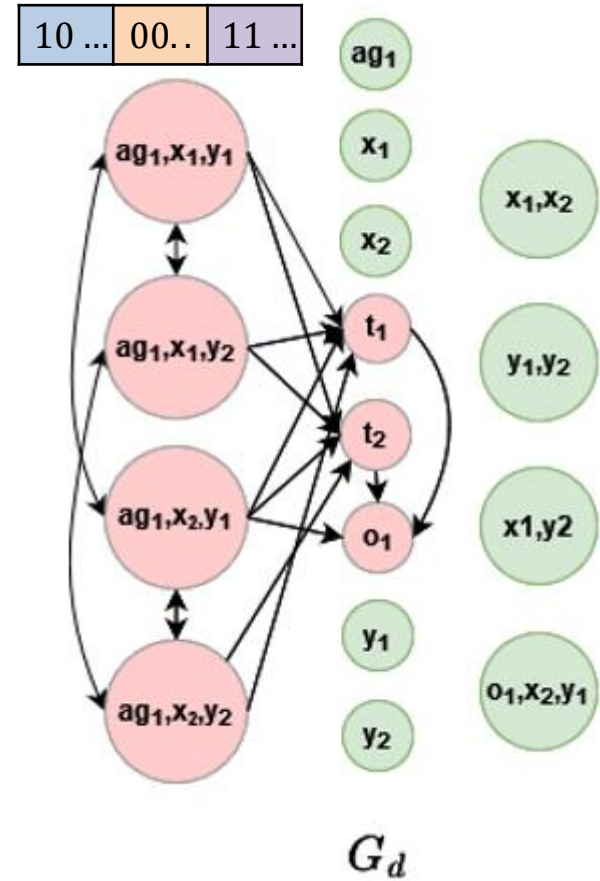
<i>agentAt(...)</i>	<i>damagedTool(...)</i>	...
---------------------	-------------------------	-----

2. A feature for each (un)parameterized Non-Fluent

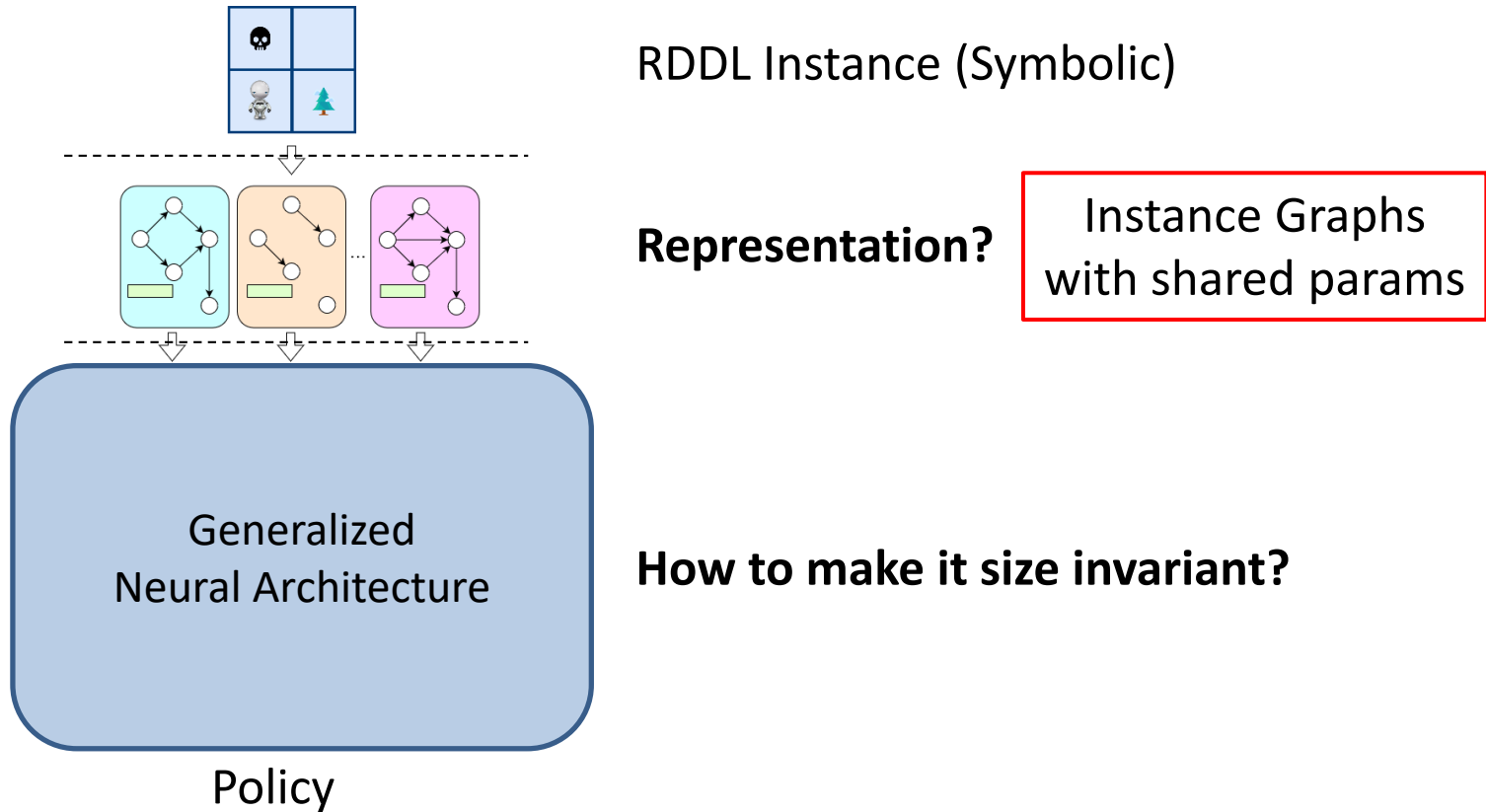
<i>lifeTool(...)</i>	<i>waterTool(...)</i>	...
----------------------	-----------------------	-----

3. A boolean vector for type signature of node

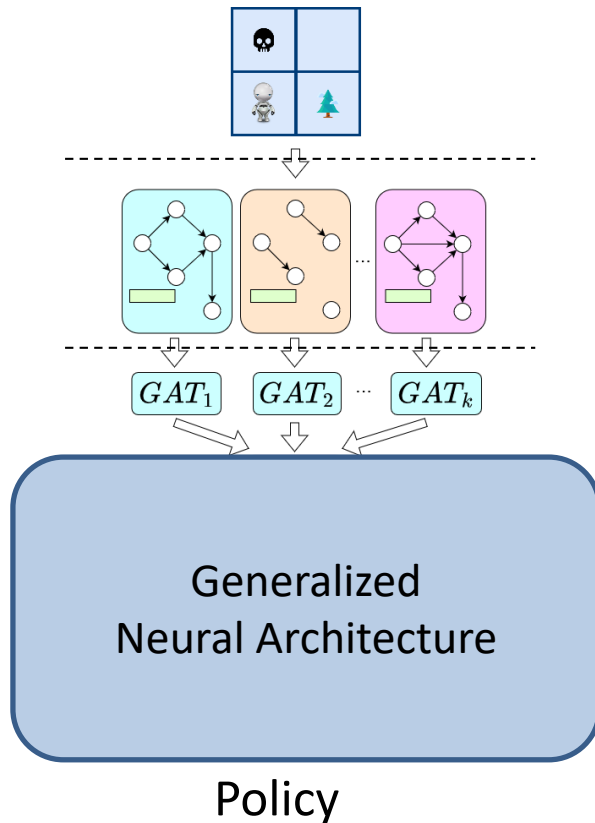
<i>type(object₁)</i>	<i>type(object₂)</i>	...
---------------------------------	---------------------------------	-----



Solution Approach



Solution Approach



RDDL Instance (Symbolic)

Representation?

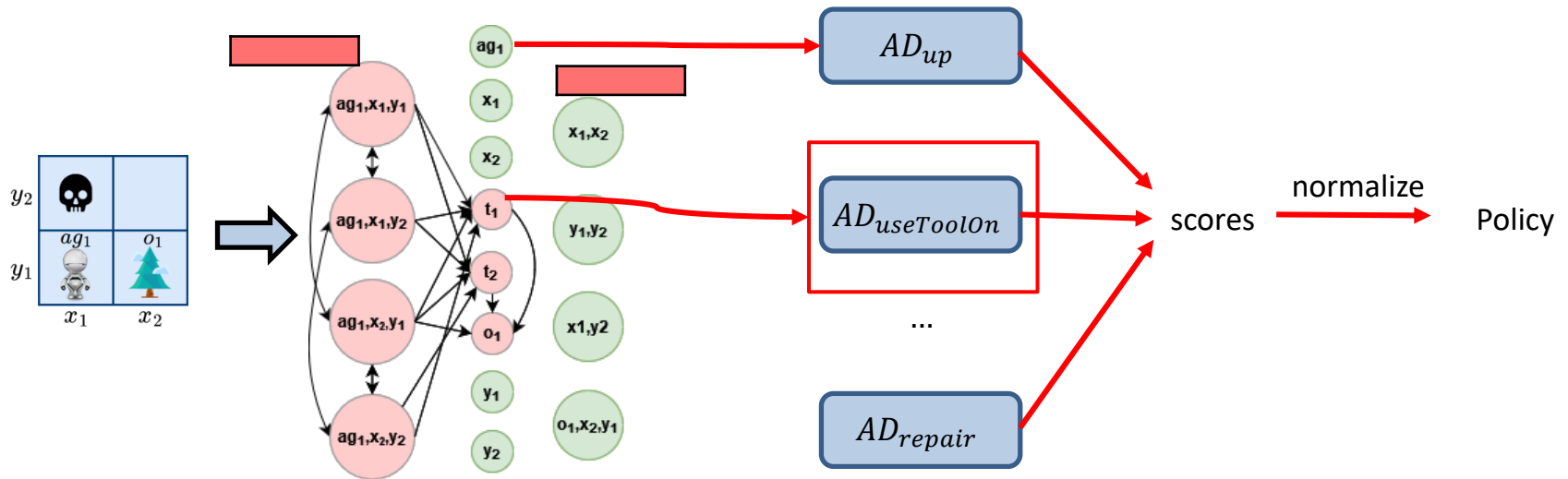
Instance Graphs
with shared params

Consolidate information

- Message Passing: What is in my neighbourhood?
(Graph Attention Networks [Veličković ICLR'18])
- A single graph with merged node embeddings (ne)
- Global Embedding: $s = \maxpool_{i \in nodes}(ne_i)$

Action Decoders

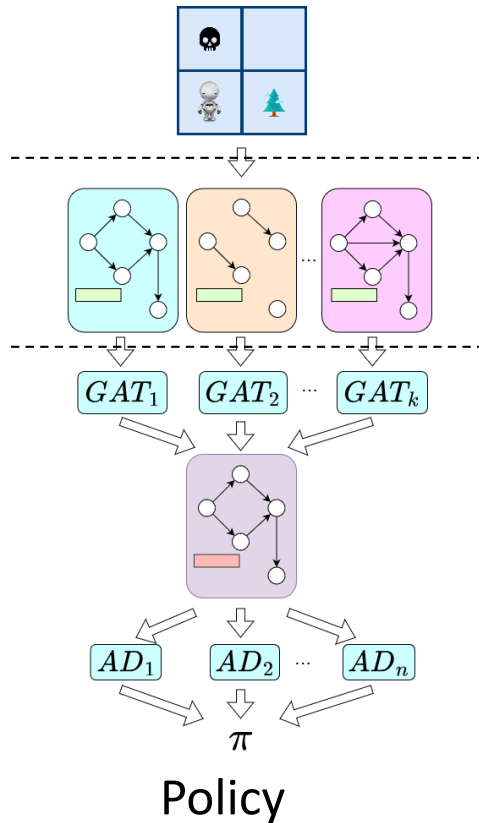
- A feed forward network for each action predicate type.
- Input:
 - Node embedding of each parameter
 - Node embeddings corresponding to the State-Fluents affected by the action
 - Global embedding



$$useToolOn(ag_1, t_1, o_1) \rightarrow damaged(t_1)$$

$$AD_{useToolOn}(ne_{ag_1}, ne_{t_1}, ne_{o_1}, ne_{t_1} || s)$$

Solution Approach



RDDL Instance (Symbolic)

Representation?

Instance Graphs
with shared params

Message Passing using GAT

Weight shared
so generalizable

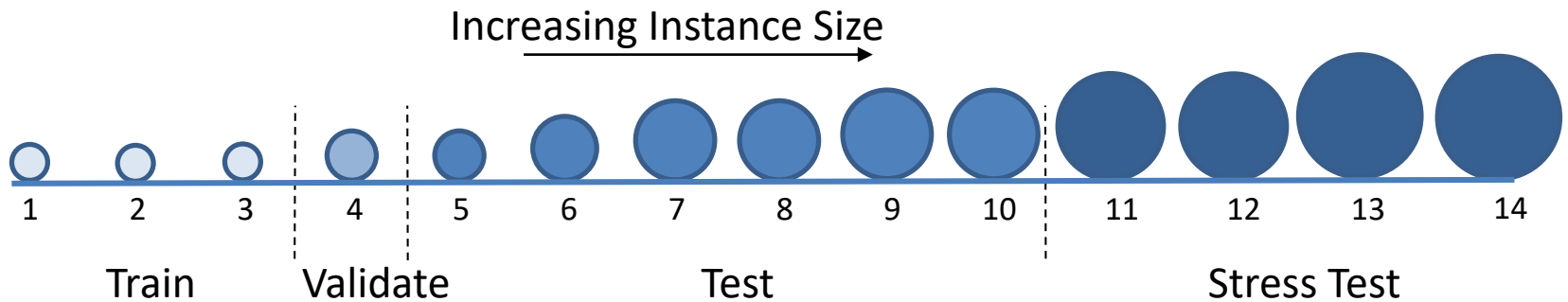
Action Decoders for each action type

Policy

Experimental Setting

Test Suite:

- 12 International Probabilistic Planning Competition (IPPC) domains



Training Algorithm

Phase 1: Dataset Generation

1. For each training instance:
 1. Generate a set of trajectories using PROST [Keller ICAPS'12]

Phase 2: Neural Learning

1. Randomly shuffle training instances
2. Train using supervised loss

Baselines:

1. PROST: MCTS based online planner
2. Random policy

Performance Metrics

- Performance of algorithm m on instance i

$$\alpha(i, m) = \frac{rew_{max}^i - rew_m^i}{rew_{max}^i - rew_{rand}^i} \in (-\infty, 1]$$

0 \rightarrow Random Policy

1 \rightarrow Best policy

- Performance on all Test instances

$$\alpha(m) = \frac{1}{m} \sum_{i \in \text{test instances}} \alpha(i, m)$$

Results-IPPC

[Sharma et al, UAI 2022]

IPPC Test Instances 5-10													
Model	TT	CT	Acad	Elev	Tam	Nav	GoL	Skill	Sys	Wild	Traffic	Recon	Mean
PROST	0.53	0.86	0.47	1.00	0.94	0.88	1.00	1.00	0.65	0.70	1.00	0.99	0.84
SYMNET	0.81	0.95	0.82	0.44	0.92	0.47	0.29	0.43	0.94	0.77	0.28	0.30	0.62
Larger Instances													
Model	TT	CT	Acad	Elev	Tam	Nav	GoL	Skill	Sys	Wild	Traffic	Recon	Mean
PROST	0.09	0.55	0.39	1.00	0.90	0.44	0.91	1.00	0.36	1.00	1.00	0.78	0.70
SYMNET	0.95	0.89	0.77	0.19	0.94	0.95	0.84	0.34	0.46	0.20	0.39	0.32	0.60

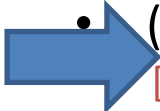
1. IPPC Instances:

1. **Zero-Shot capability:** We are better than random in all 12 domains
2. **Better than the teacher (PROST):** In 5 domains

2. Larger Instances:

1. Performance Drop in SymNet < Drop in PROST
2. Better than teacher (PROST) in 6 domains

Outline

- Motivation
- (Human) Features within Neural AI (domain insight, better learning)
[Contractor JNLE'21, Gupta ArXiv'22]
- (Human) Constraints within Neural AI (dom. insight, learning, guarantees?)
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First-Order Reasoning Problems

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9



5	3	4	6	7	8	9	1	2
6	7	2	1	9	5	3	4	8
1	9	8	3	4	2	5	6	7
8	5	9	7	6	1	4	2	3
4	2	6	8	5	3	7	9	1
7	1	3	9	2	4	8	5	6
9	6	1	5	3	7	2	8	4
2	8	7	4	1	9	6	3	5
3	4	5	2	8	6	1	7	9

Goal

[Nandwani et al, ICLR 2022]

- Can we get a size-invariant reasoner?
- Learn *generalized solver* for Sudoku
 - using small instances
- Challenge
 - Solution Space (digits of solution) changes across problems
 - Contribution: Invariance over Solution Cardinality

Take Home

- Neural models are excellent at generalization
 - Useful on tasks represented in first-order language
 - Can train on small instances
 - Applicable on larger instances

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Conclusions

- Neural AI is here to stay
- Symbolic AI also offers tremendous value
- **Neuro-Symbolic AI is useful**
 - In low data settings
 - In faster inference
 - In guaranteeing output constraints
 - In complex models requiring perception w reasoning
 - In size-invariant (first order) learning
 - In explanations of predictions
 - ...