From Specialists to Generalists

Structure, Attributes and Causality

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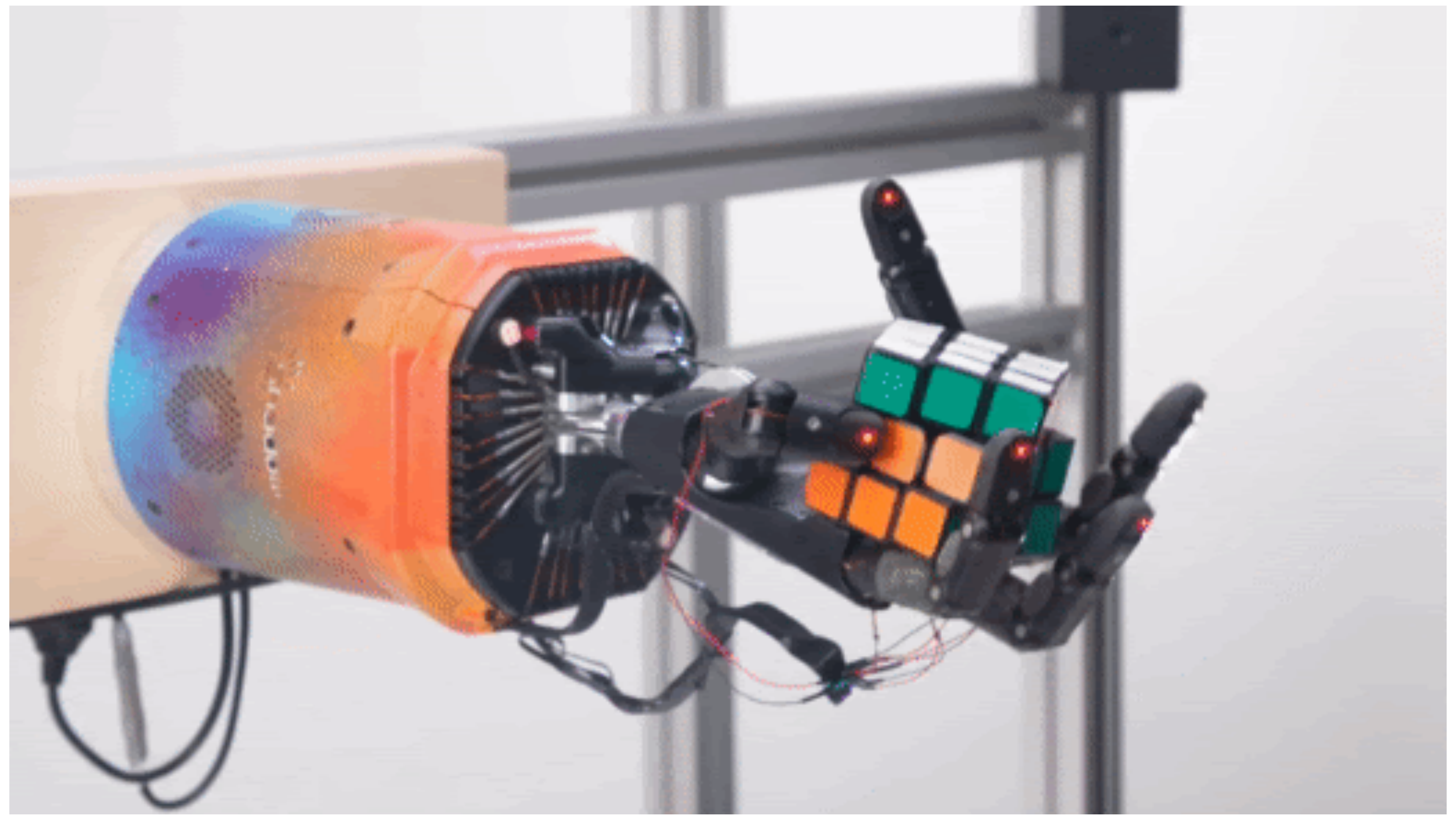
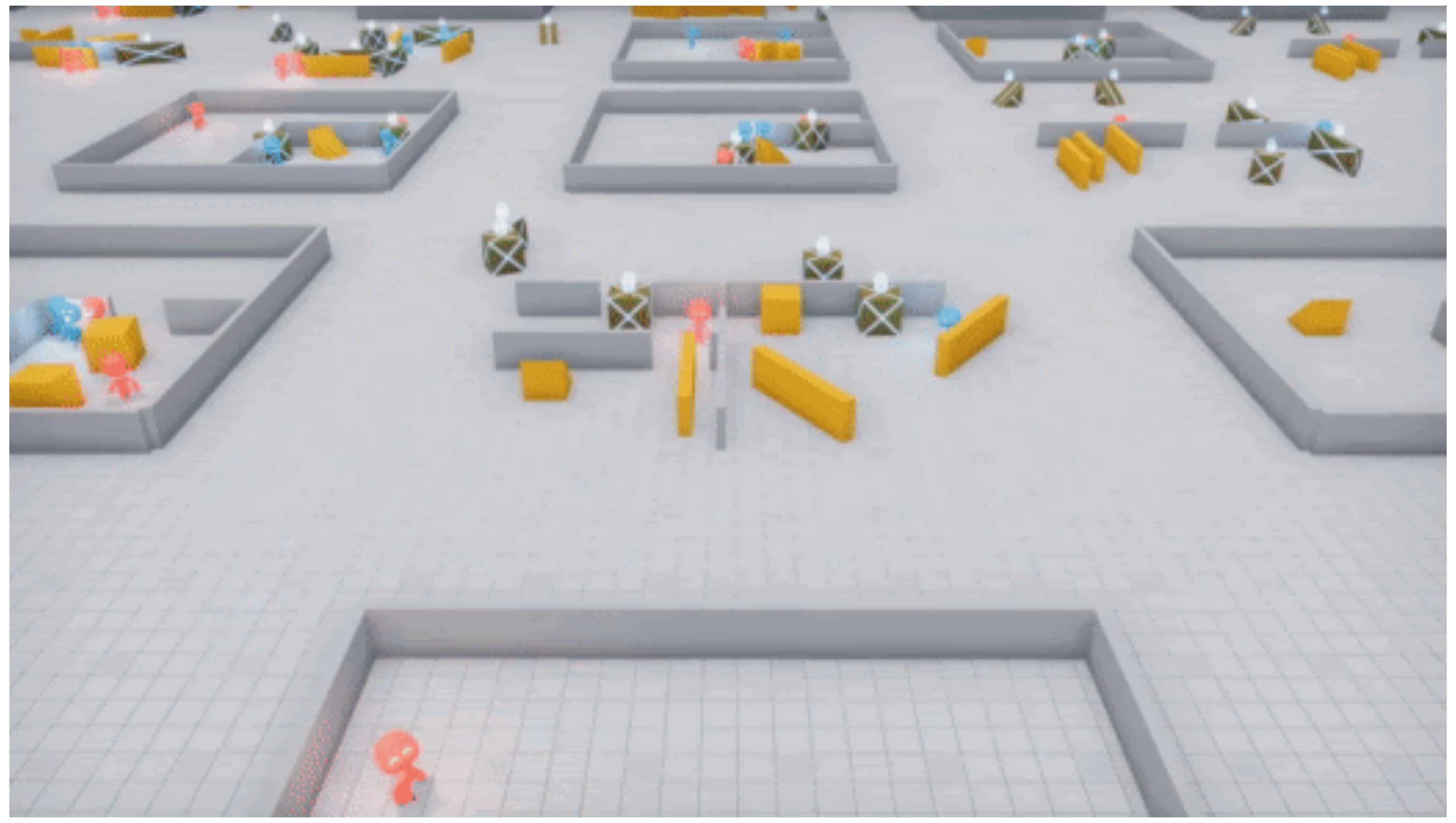
Training “Specialists” using Deep Networks



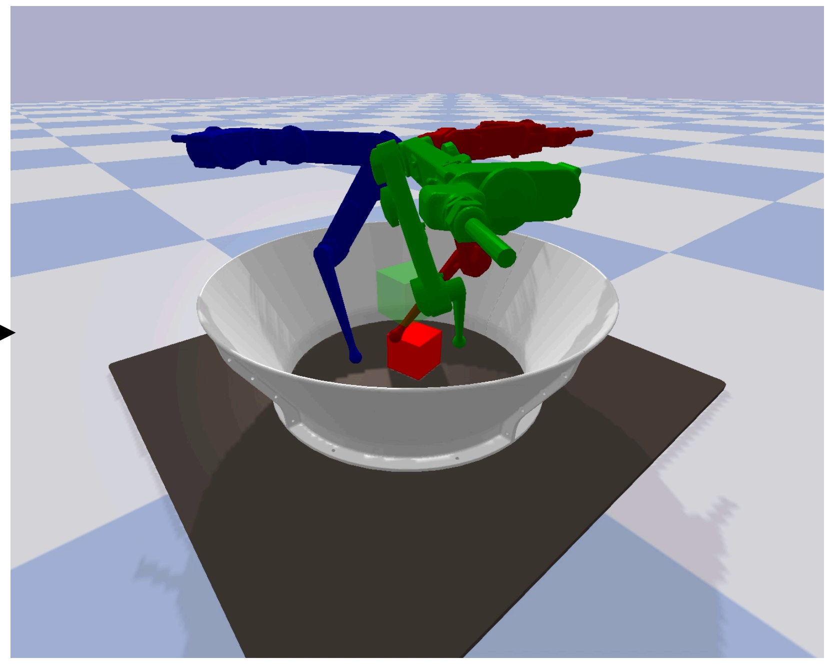


Training “Generalists” using Deep Networks

Specialists

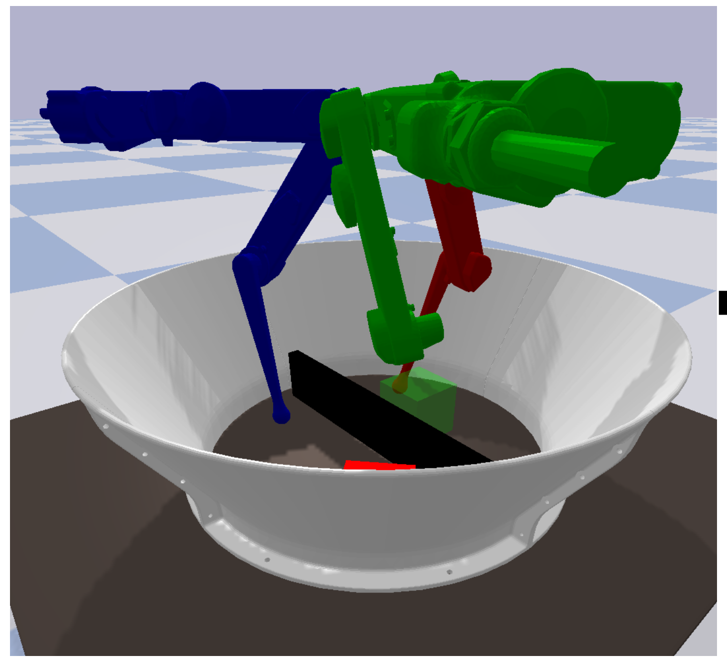
Picking

Train

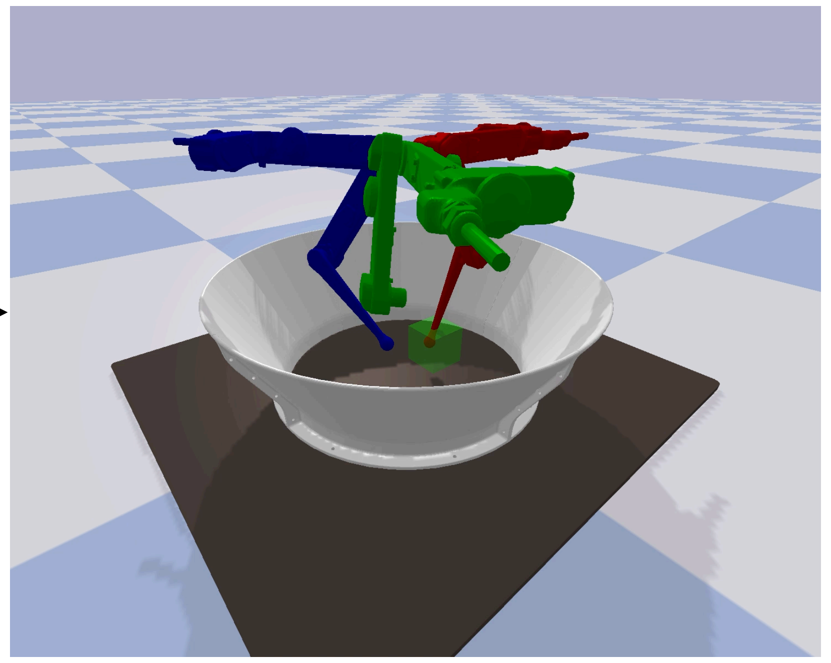


Test

Pick and Place



Train

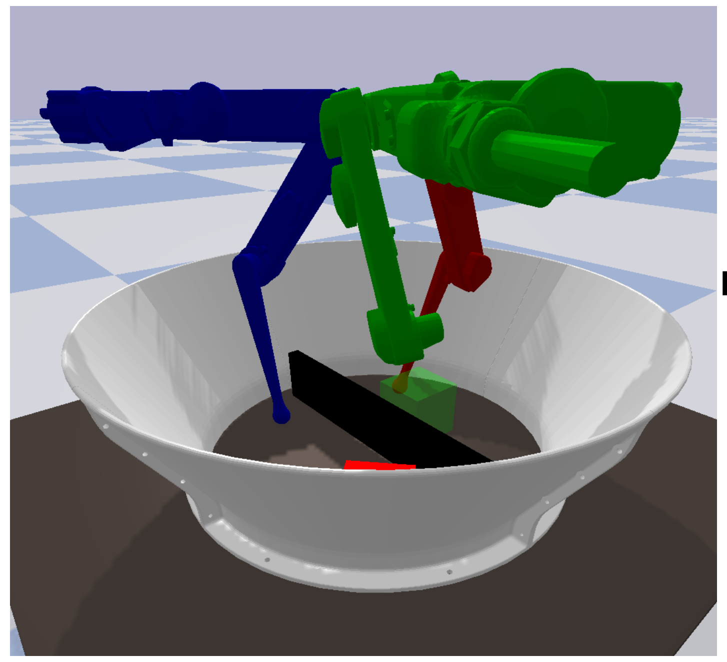


Test

Generalists

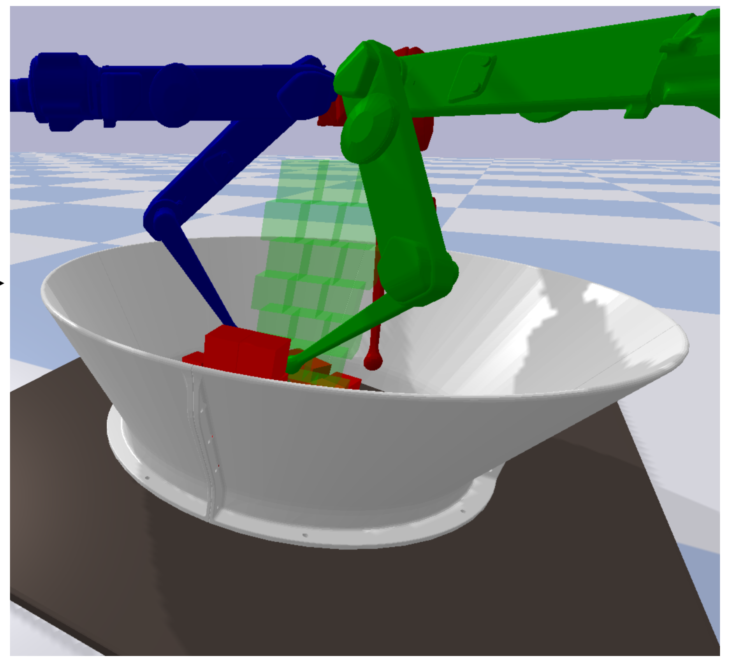
Picking

Pick and Place



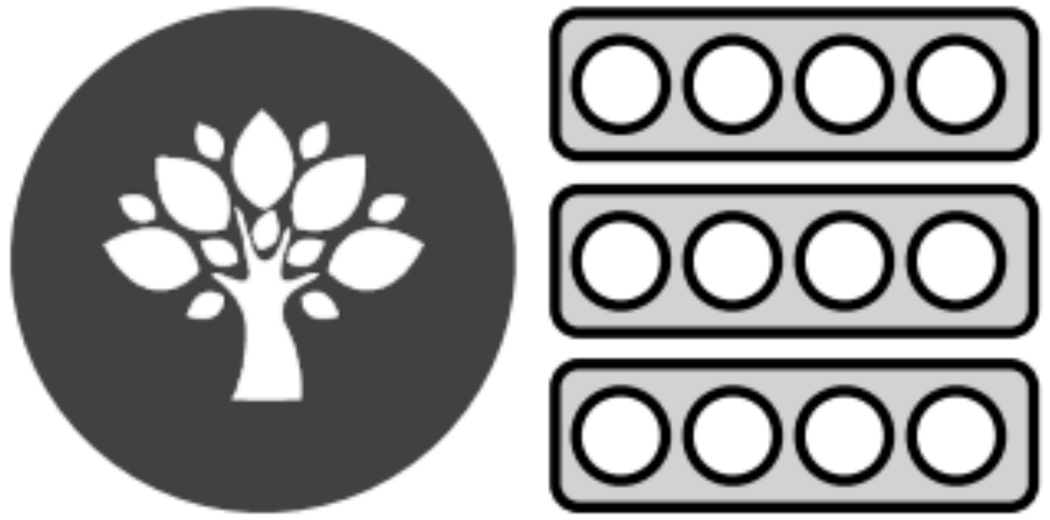
Training tasks

Stacked Blocks



Test/Transfer task

Quickly adapt to the transfer task.



Representation Model

(Learning causal structures which reflect the dynamics of the environment)

1. *Inductive Biases for Deep Learning of Higher Level Cognition:* **Goyal** and Bengio (arXiv:2011.15091)
2. *Coordination among Neural Modules through a Shared Workspace:* **Goyal** et al (**ICLR'22, Oral**)
3. *Learning to combine Top Down and Bottom Up Signals in RNN with attention over modules:* Mittal, Lamb, **Goyal** et al, **ICML'20 (Spotlight)**
4. *Object Files and Schemata: Factorizing Declarative and Procedural Knowledge in Dynamical Systems :* **Goyal** et al, **ICLR'21**
5. ***Neural Production Systems:* Goyal et al, NeurIPS'21**
6. Spatially Structured Recurrent Modules: Rahaman, **Goyal** et al, ICLR'21
7. Fast and Slow learning of Recurrent Independent Mechanisms*:* Madan, Ke, **Goyal**, et al ICLR'21
8. A meta-transfer objective for learning to disentangle causal mechanisms: Bengio […], **Goyal**, ICLR'20
9. Systematic Evaluation of Causal Discovery in Visual Model Based Reinforcement Learning: Ke […], **Goyal** et al, NeurIPS'21

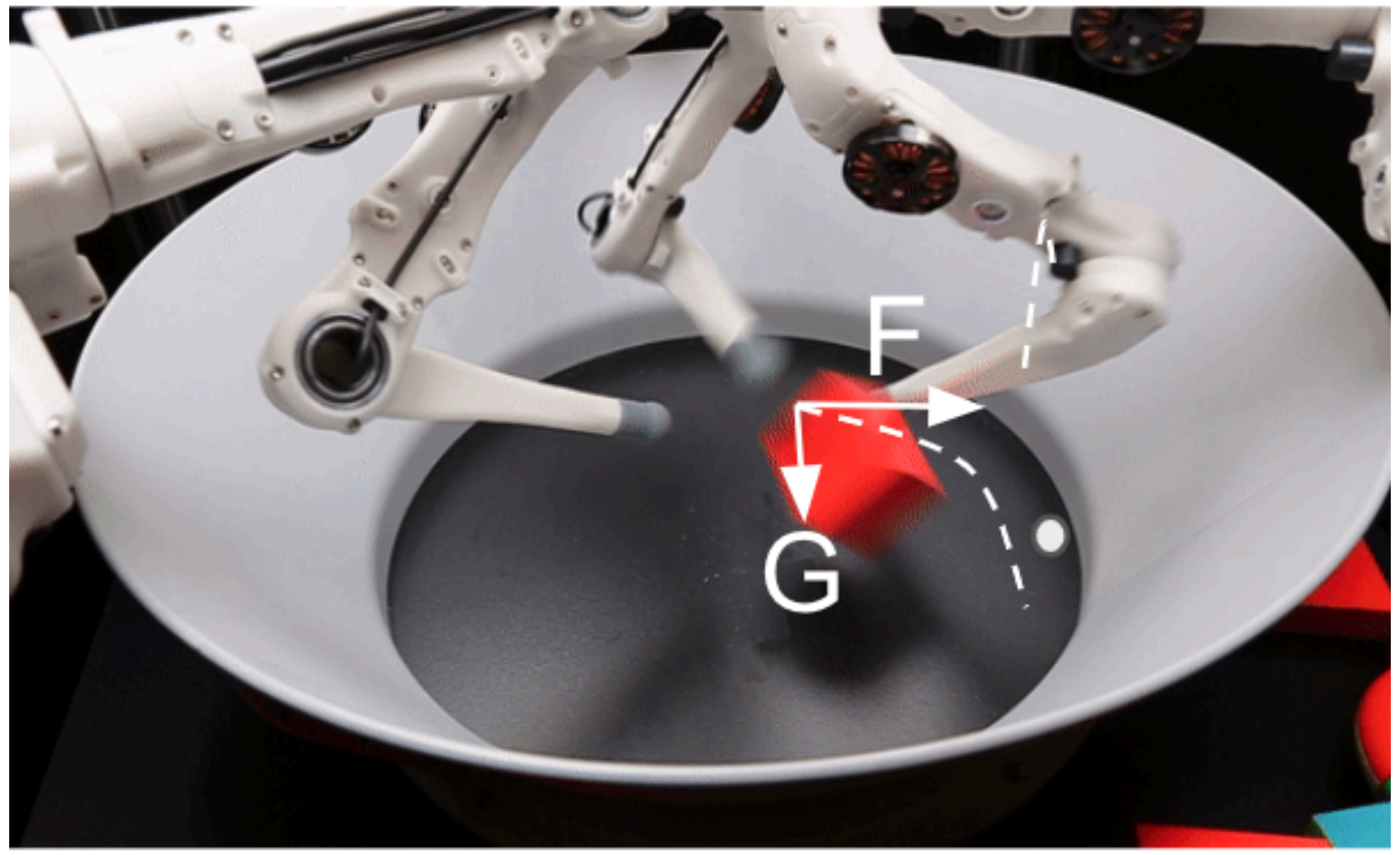
Prediction v/s Scientific Discovery

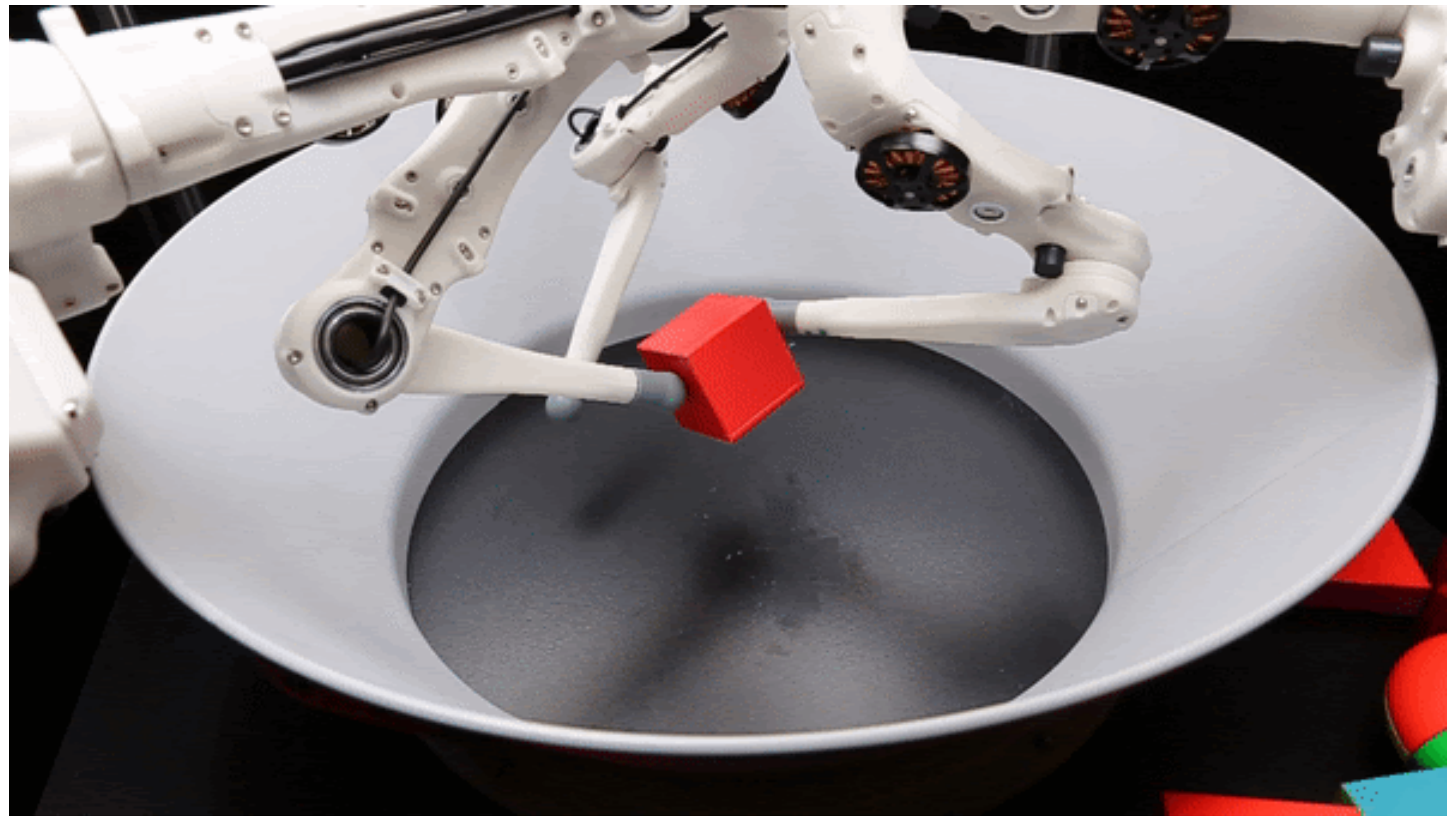
Where will the cube land ?

$$F = ma$$

$$a = \frac{d}{dt}v(t)$$

$$v = \frac{d}{dt}s(t)$$





What if the cube were green ? ***Color has no effect!***

Abstractions and Systematicity

```
int add(int a, int b){
    int c = a + b;
    return c;
}
add(4,2); // 6
add(1024, 2048); // 3072
```

Typed argument function in C++. Here, function ***add*** can be applied to any two entities as long as their type matches the expected types (in this case, integer).

Logical Rules applied to Symbolic Concepts

Discovery of Variables and Functions from Visual Input

Program state: a, b, c, d, e, g, x, y

$$z = f_i(a, g)$$

Program state: $z, a, b, c, d, e, g, x, y$

```cpp
int add(int a, int b){
    int c = a + b;
    return c;
}
add(4,2); // 6
add(1024, 2048); // 3072
```

Typed argument function in C++. Here, function ***add*** can be applied to any two entities as long as their type matches the expected types (in this case, integer).

- **Discovering High level causal variables:** How is raw sensory data mapped to high level causal variables ? (i.e., what are "a, b, c, d, e, g, x, y")
- **Relationship between these causal variables**: How do these high level variables interact with each other ?
- **Promotes systematicity:** We can apply the knowledge of the same (function) as long as the type of "input" matches the type of the input "function" expects.

Correct Knowledge Decomposition Leads to Faster Adaptation

- Random variables A and B, **where A causes B.**

- Assume the correct causal model decomposes as

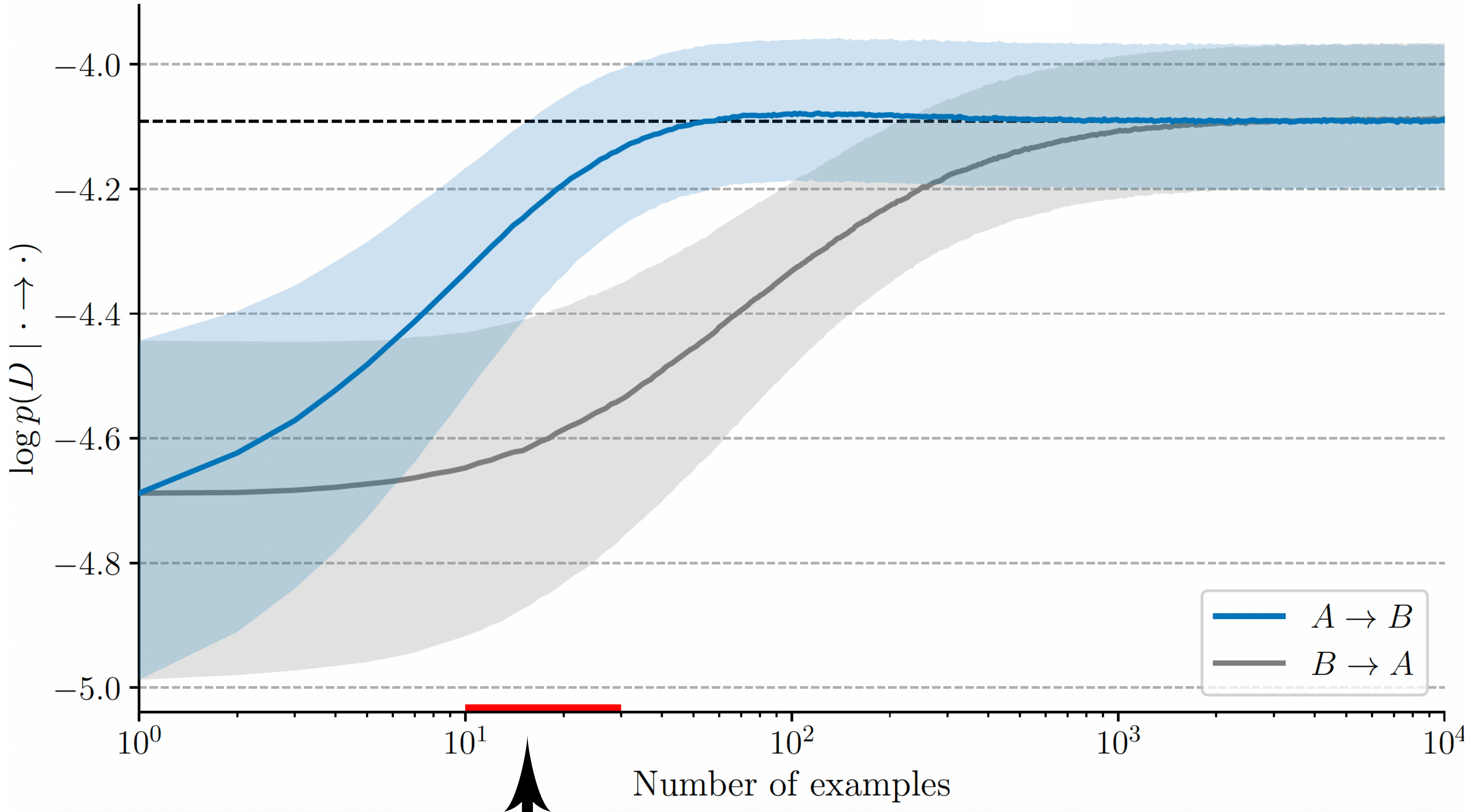
$$p(A, B) = p(A)p(B \mid A)$$

- Consider two distributions, where **only $p(A)$ changes** and $p(B \mid A)$ remains unchanged (covariate shift)
  - A **training** distribution p
  - A **transfer** distribution $\tilde{p}$

- With the wrong factorization $p(B)p(A \mid B)$, a change in p(A) influences all the modules.

Wrong factorization causes poor transfer, catastrophic forgetting.

Correct causal structure: 

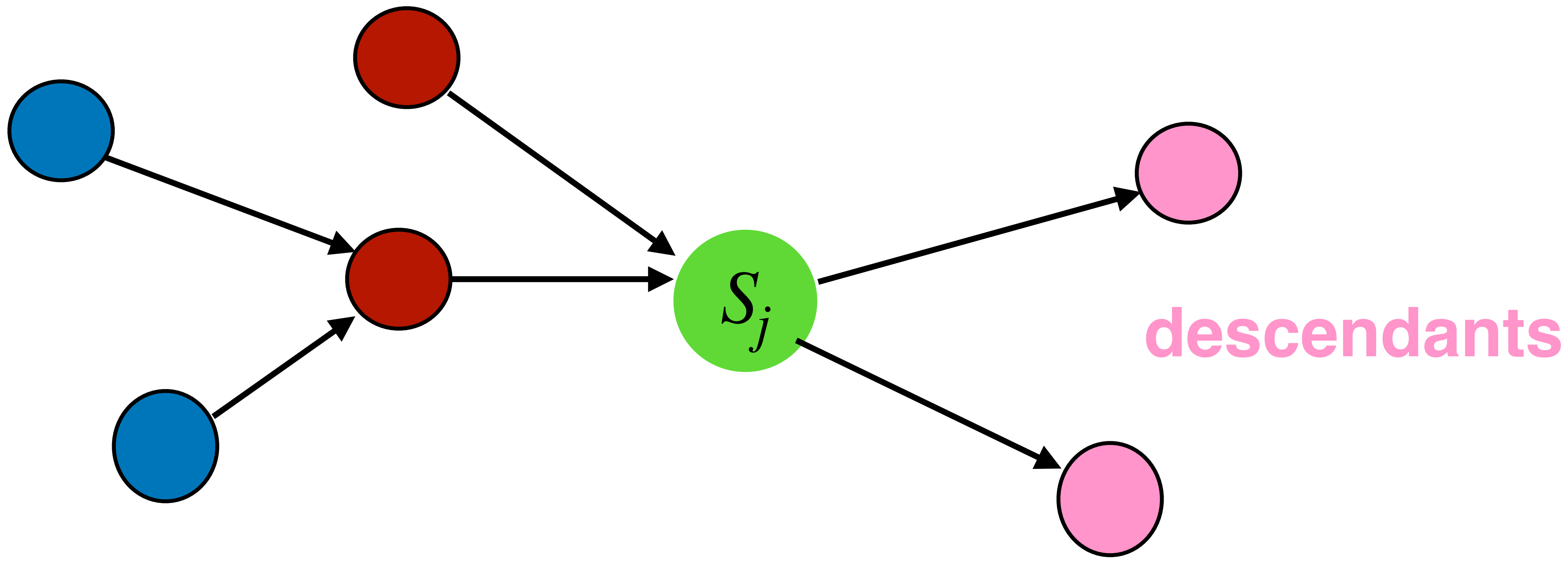


- **Faster online adaptation to modified distribution.**
- **Effect most evident using few samples from modified distribution.**

A meta transfer objective to disentangle causal mechanisms, Bengio et. al, ICLR'21

Learning Reusable Independent Mechanisms

Parents (causes) of S_j $\mathbf{PA_j}$ refers to parents of S_j.



Assumption: Set of observables $S_1 \ldots S_n$

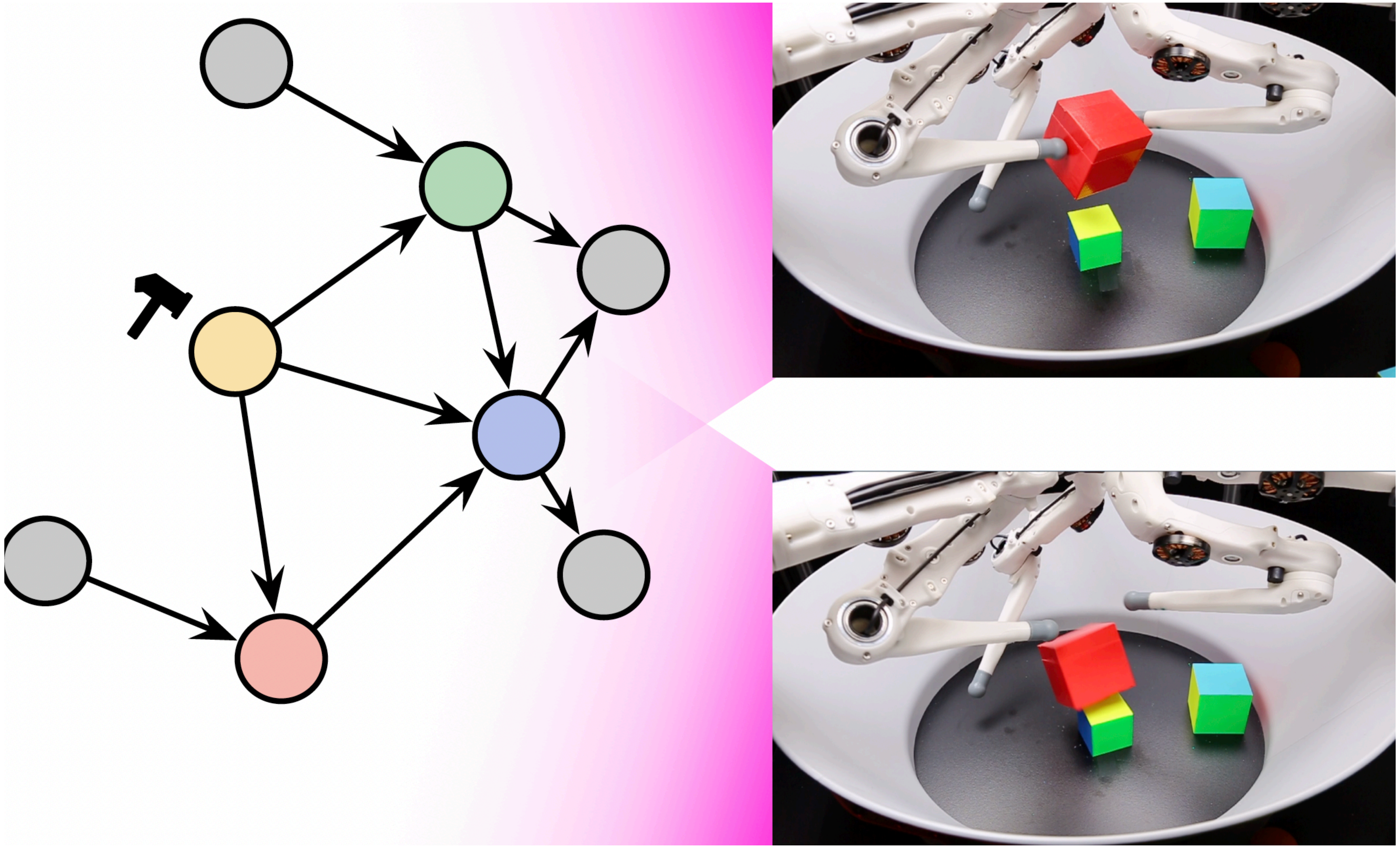
- **Causal Factorization**:

$$P(S_1, \ldots, S_n) = \prod_{i=1}^{n} P(S_i \mid \mathbf{PA}_i)$$

- **Changing one "mechanism" $p(S_i \mid \mathbf{PA_i})$ does not influence another "mechanism" $p(S_j \mid \mathbf{PA_j})$.**

Independence is not between the random variables being processed but *between the parametrization of the mechanisms*

Sparse Change in Correct Causal Factorization



*Changes in the environment tend to manifest themselves in a **sparse way** in the causal factorization.*

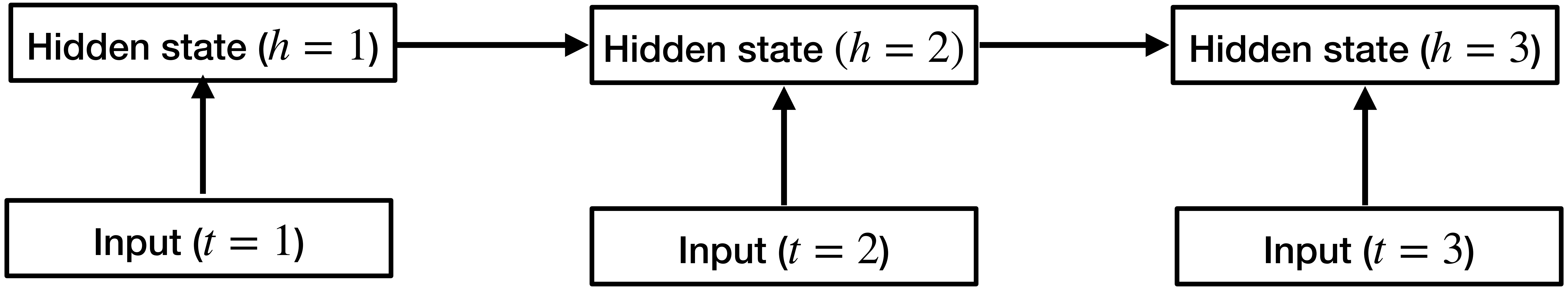
Change in the environment can often change a large fraction of the pixels (even all the pixels).

We change the position of one finger (shown by hammer), and as a consequence the object falls.

Towards Causal Representation learning, Scholkopf et. al, 2021

Deep Learning has the **Opposite** Inductive Bias

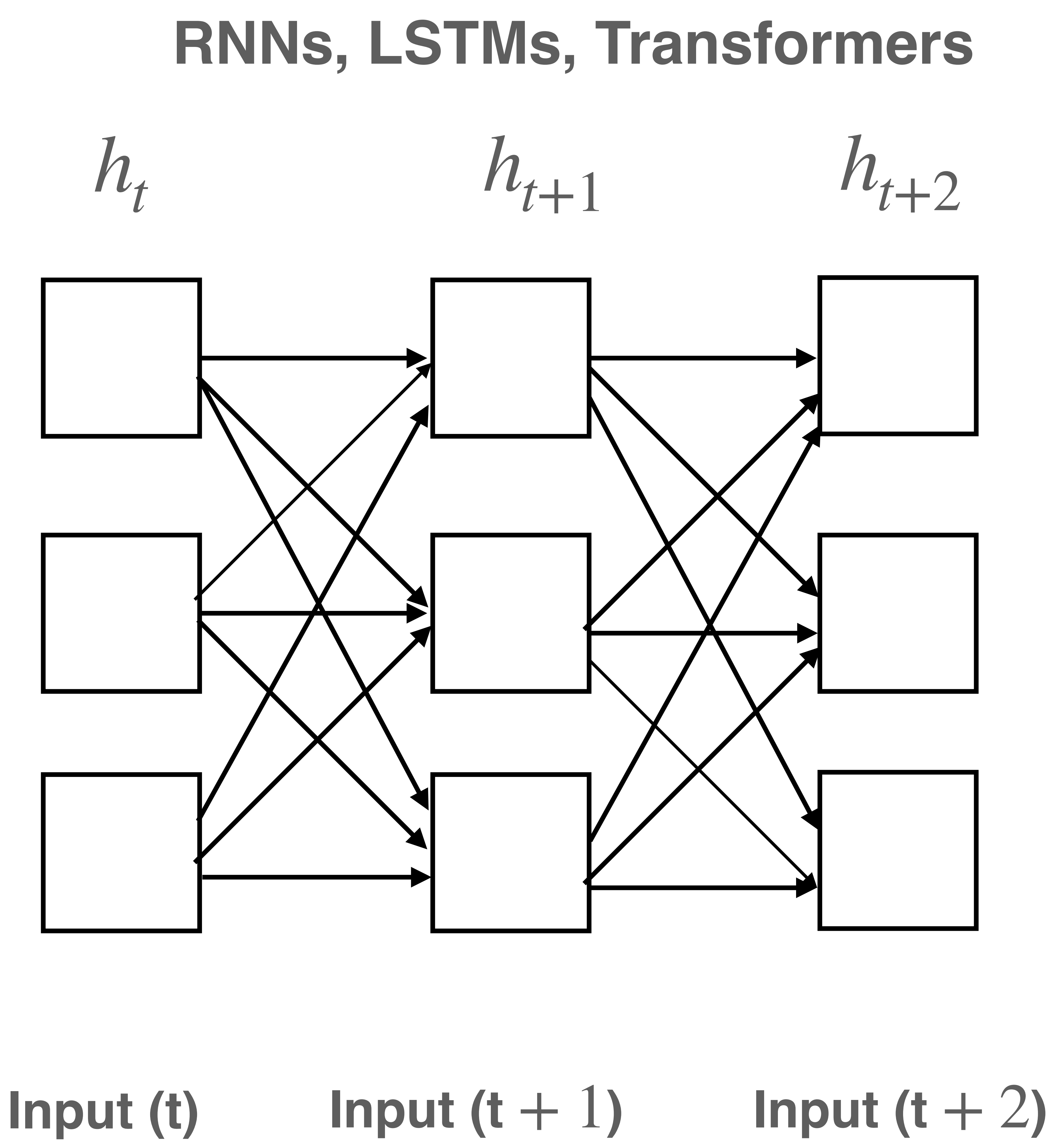
All ***sub-systems*** are constantly interacting through one big procedure.

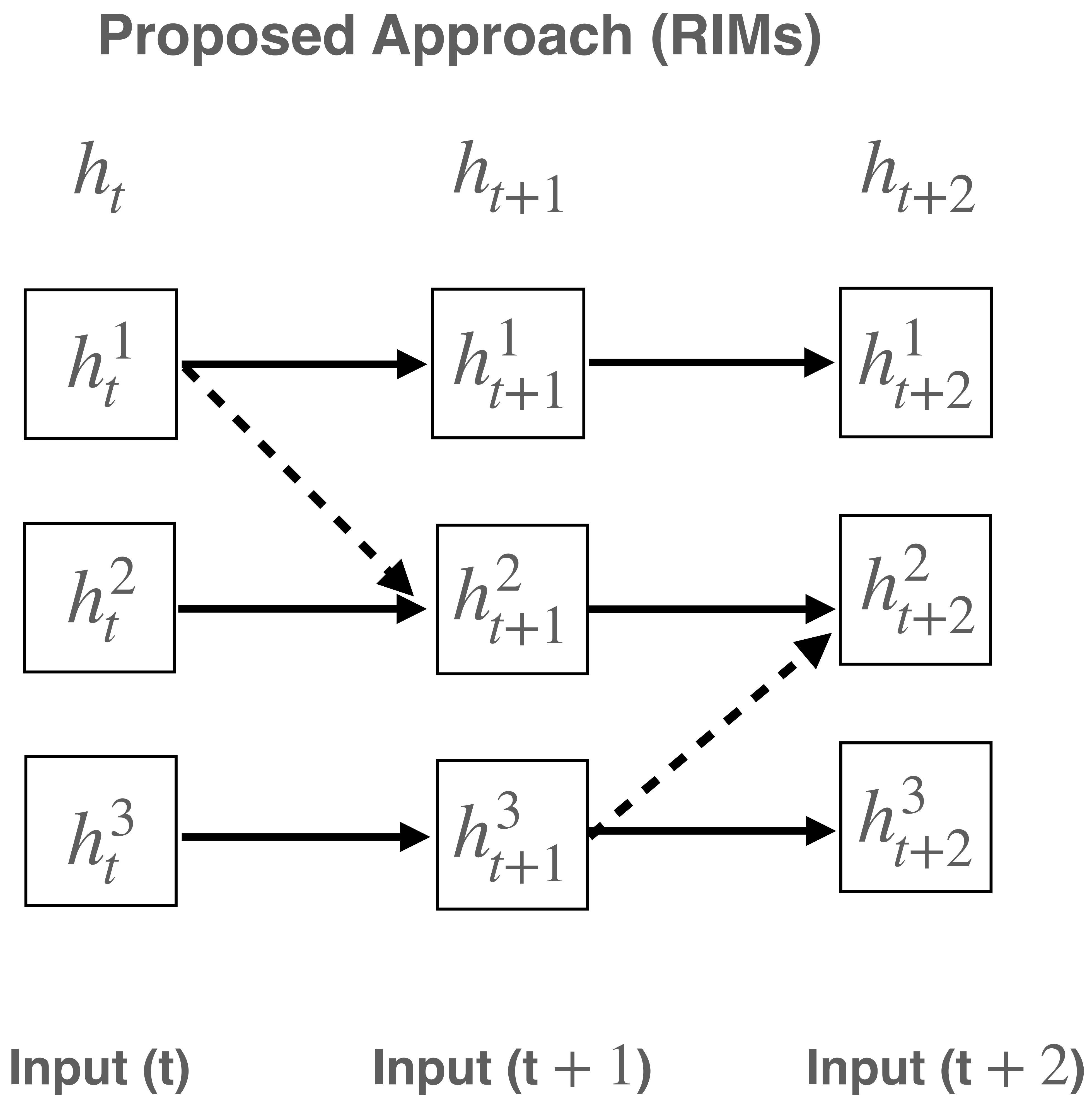


RNNs, LSTMs, Transformers

For hidden states to truly compartmentalize k different processes, a fraction $\dfrac{k-1}{k}$ of the connections may need to be set to zero weight.

Recurrent Independent Mechanisms



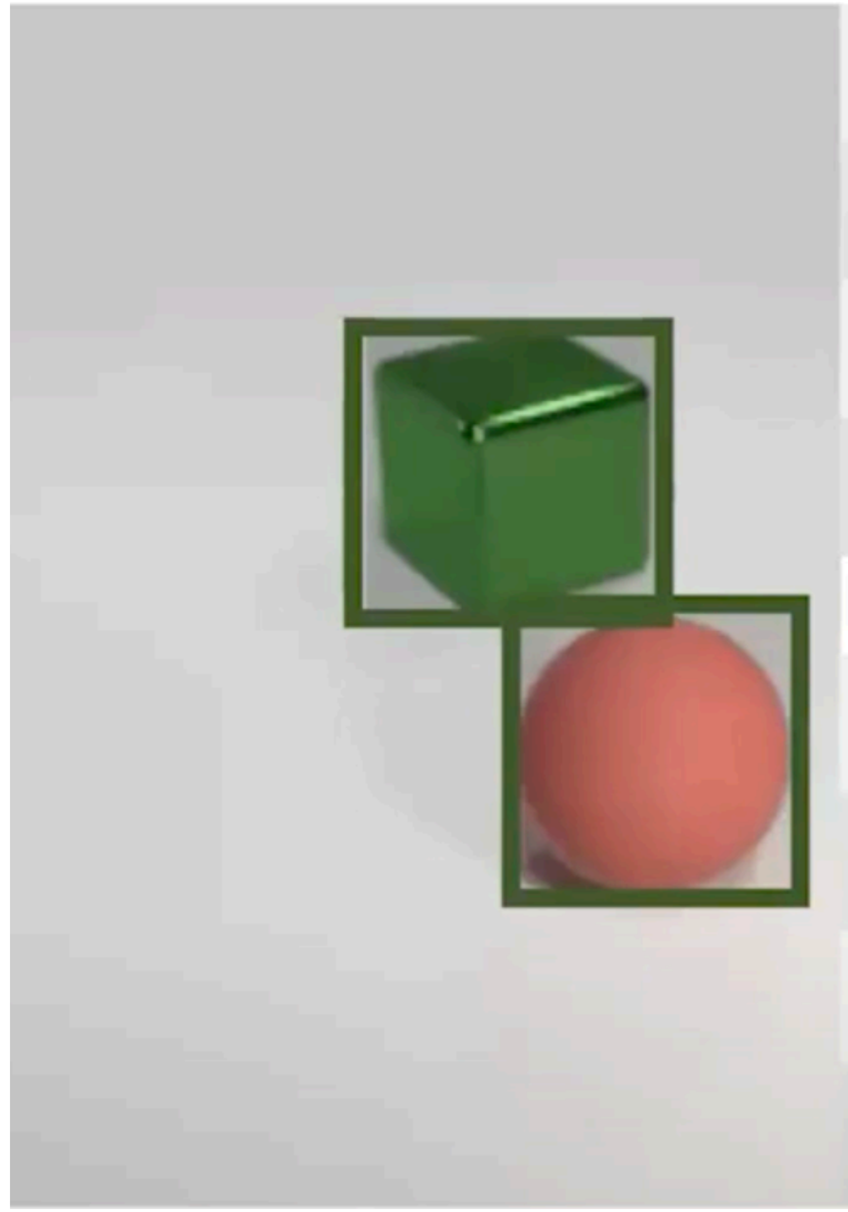


Input dependent dynamic connectivity

Object Files and Physical Reasoning System

Object Files
(Treisman, 1992; Kahneman, Treisman, & Gibbs 1992)

- Maintains representation of **attributes** over time.
  (location, trajectory, color, history)
  - State updates even when features are not visible.



Color	Green
Shape	Cube
Material	Metal
……	……

Color	Red
Shape	Sphere
Material	Rubber
……	……

Physical Reasoning System

- To ensure ***systematicity***, set of functions which operates on entities and encapsulate ***causal interactions*** between entities.

Use the idea of independent (causal) mechanisms as an inductive bias for learning.

Object Files and Physical Reasoning System

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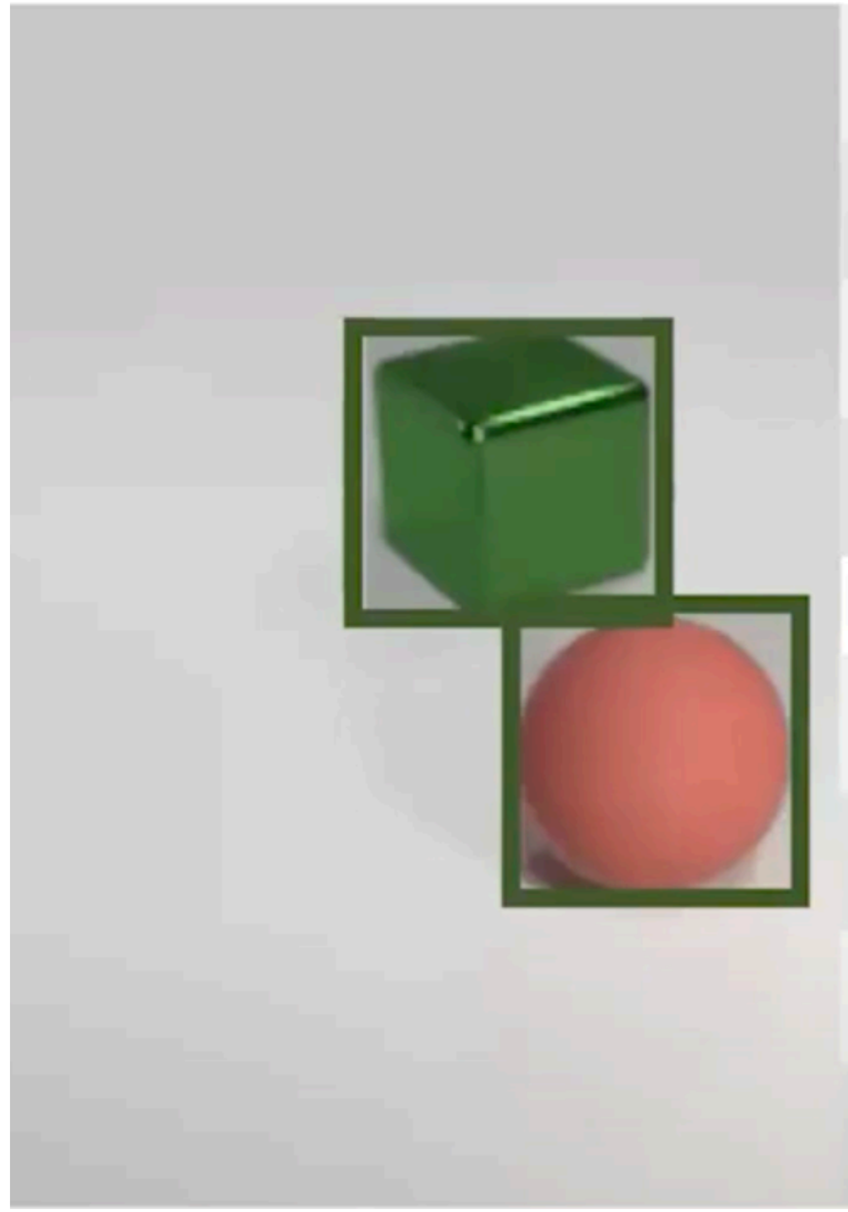

Color	Green
Shape	Cube
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Shape	Sphere
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……	……

Physical Reasoning System

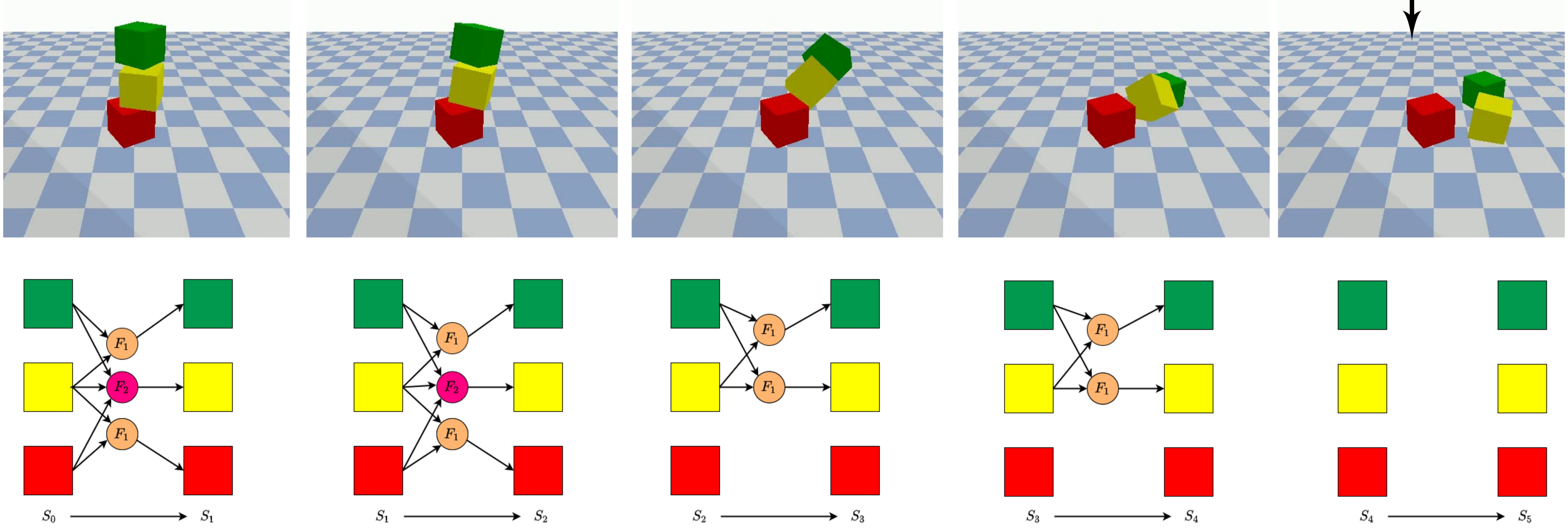
- Set of functions which operates on entities and encapsulate ***causal interactions*** between entities.

Use the idea of independent (causal) mechanisms as an inductive bias for learning.

Object Files and Physical Reasoning System

Different functions encapsulate different interactions between entities

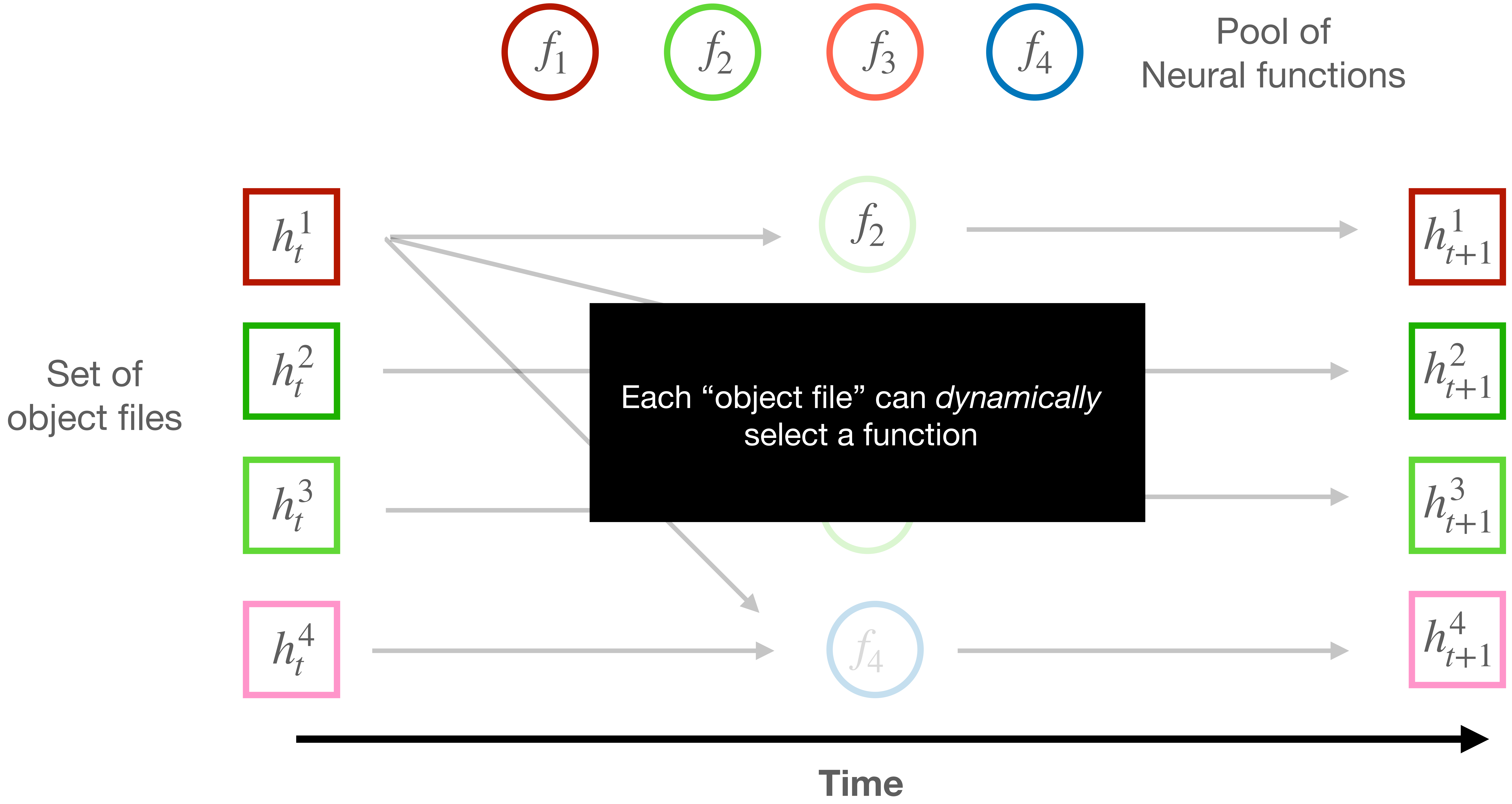
No interaction between entities.



Object Files: Track state (relevant attribute information) of different entities.

Object Files and Schemata, Goyal et. al, ICLR'21

Dynamic binding between object files and functions

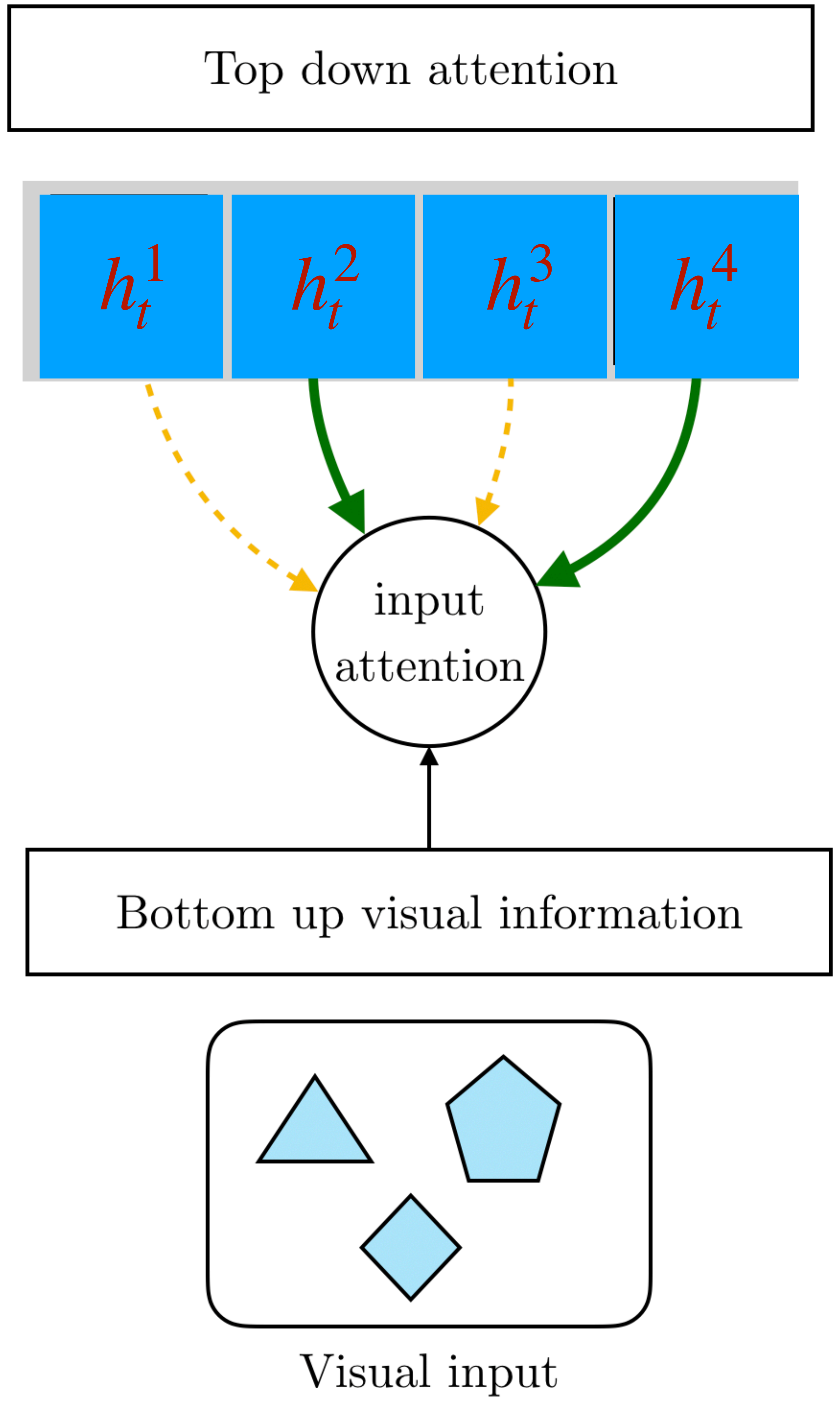


Competition Leads to Specialization

Object files compete to explain visual input.

$$\tilde{h}_{t+1}^{k} = f_{index}(h_t^k, A_t^k; \theta_{index})$$

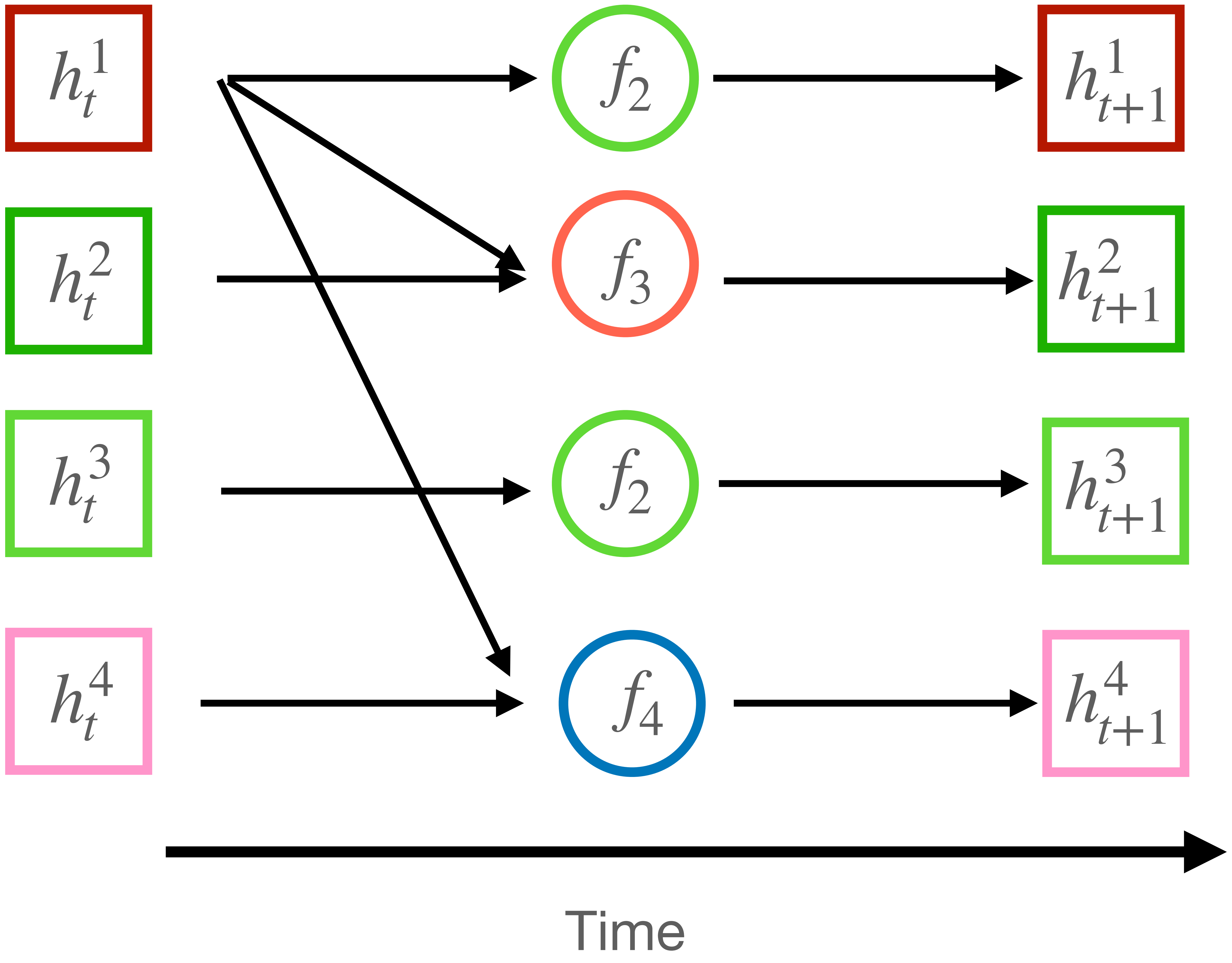
Different modules compete to organize visual information



Le Roux et al., 2011, Eslami et al., 2016, Greff et al., 2016, Raposo et al., 2017, Van Steenkiste et al., 2018, Kosiorek et al., 2018, Engelcke et al., 2019, Burgess et al., 2019, Greff et al., 2019, Locatello et al., 2020, Ahmed et al., 2020, Goyal et al., 2019, Zablotskaia et al., 2020, Rahaman et al., 2020, Du et al., 2020, Ding et al., 2020, Goyal et al., 2020, Ke et al., 2021

Dynamic binding between object files and functions

Condition and action specified by each function f_1 f_2 f_3 f_4

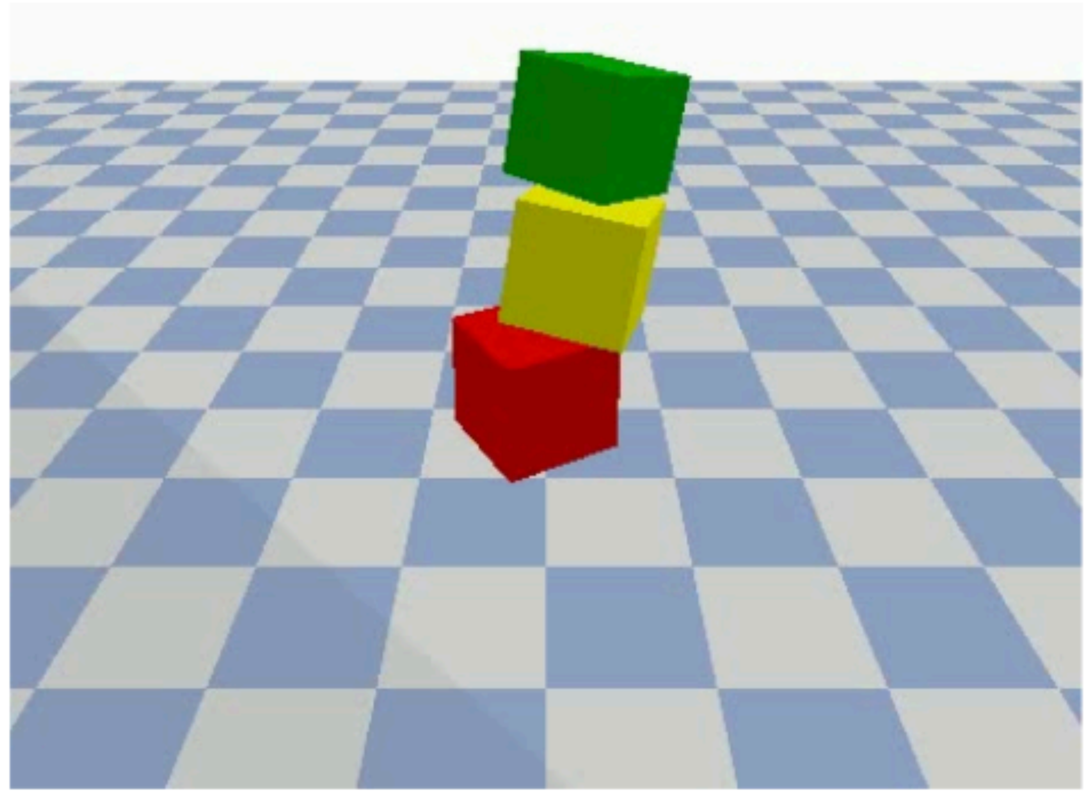


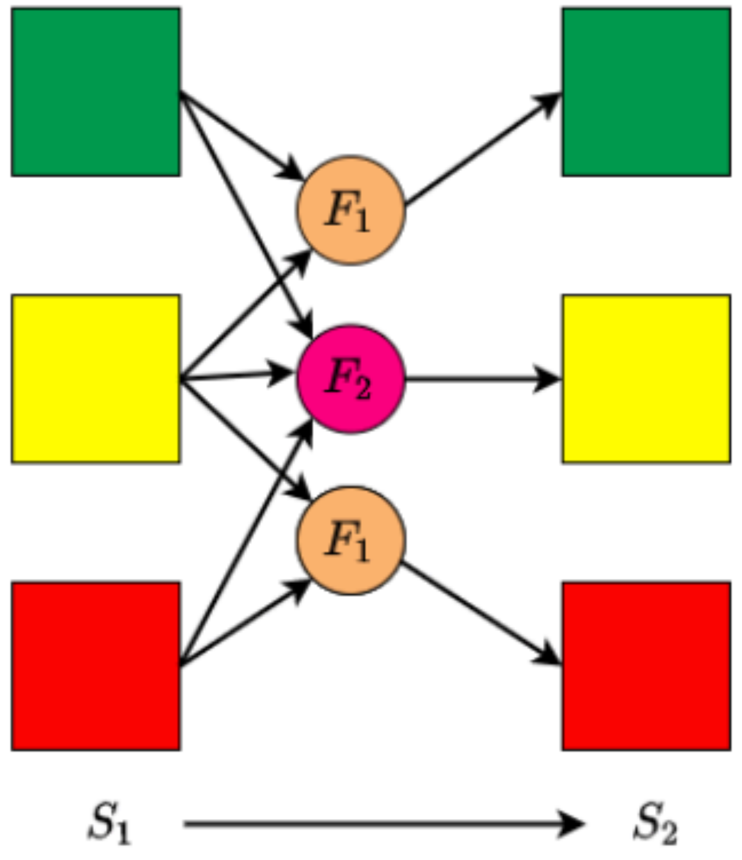
$$h_{t+1}^1 = f_2(h_t^1)$$

$$h_{t+1}^2 = f_3(h_t^2, h_t^1)$$

$$h_{t+1}^3 = f_2(h_t^3)$$

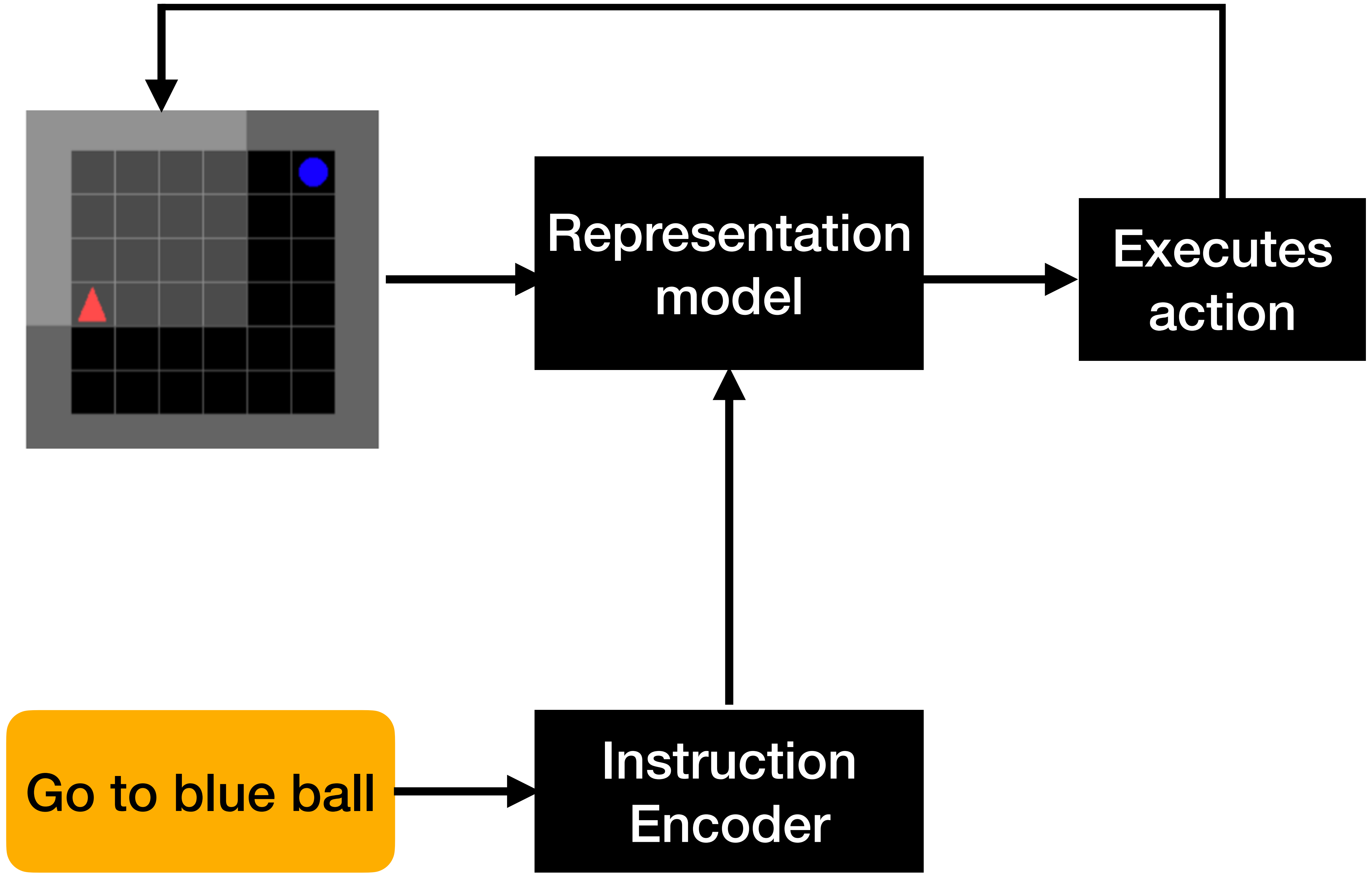
$$h_{t+1}^4 = f_4(h_t^4, h_t^1)$$





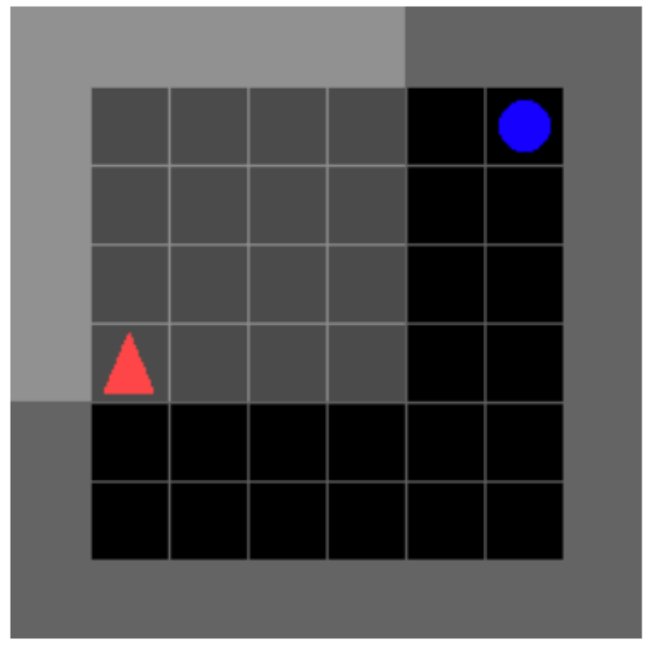
Neural Production Systems, Goyal et. al, NeurIPS'21

Problem Setup: Instruction Following

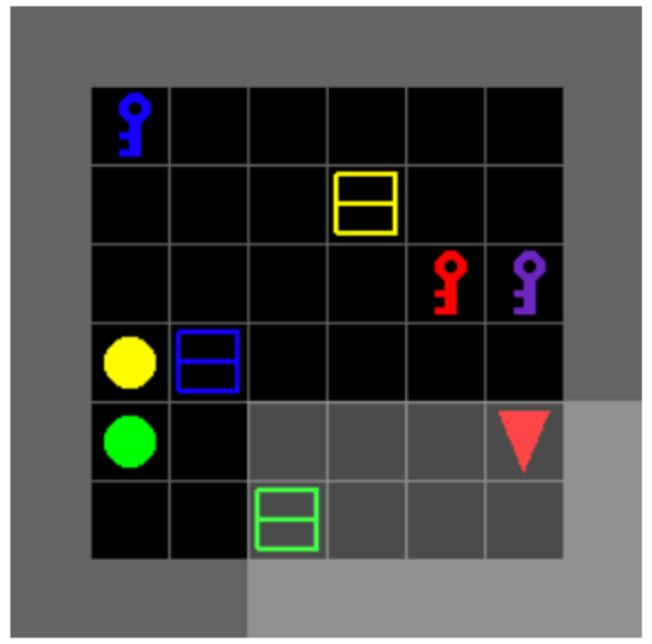


	ROOM	DISTR-BOX	DISTR	MAZE	UNBLOCK	UNLOCK	IMP-UNLOCK	GOTO	OPEN	PICKUP	PUT	LOC	SEQ
GoToObj	x												
GoToRedBallGrey	x	x											
GoToRedBall	x	x	x										
GoToLocal	x	x	x					x					
PutNextLocal	x	x	x								x		
PickupLoc	x	x	x							x		x	
GoToObjMaze	x			x									
GoTo	x	x	x	x				x					
Pickup	x	x	x	x						x			
UnblockPickup	x	x	x	x	x					x			
Open	x	x	x	x					x				
Unlock	x	x	x	x		x			x				
PutNext	x	x	x	x							x		
Synth	x	x	x	x	x	x		x	x	x	x		
SynthLoc	x	x	x	x	x	x		x	x	x	x	x	
GoToSeq	x	x	x	x				x					x
SynthSeq	x	x	x	x	x	x		x	x	x	x	x	x
GoToImpUnlock	x	x	x	x			x	x					
BossLevel	x	x	x	x	x	x	x	x	x	x	x	x	x

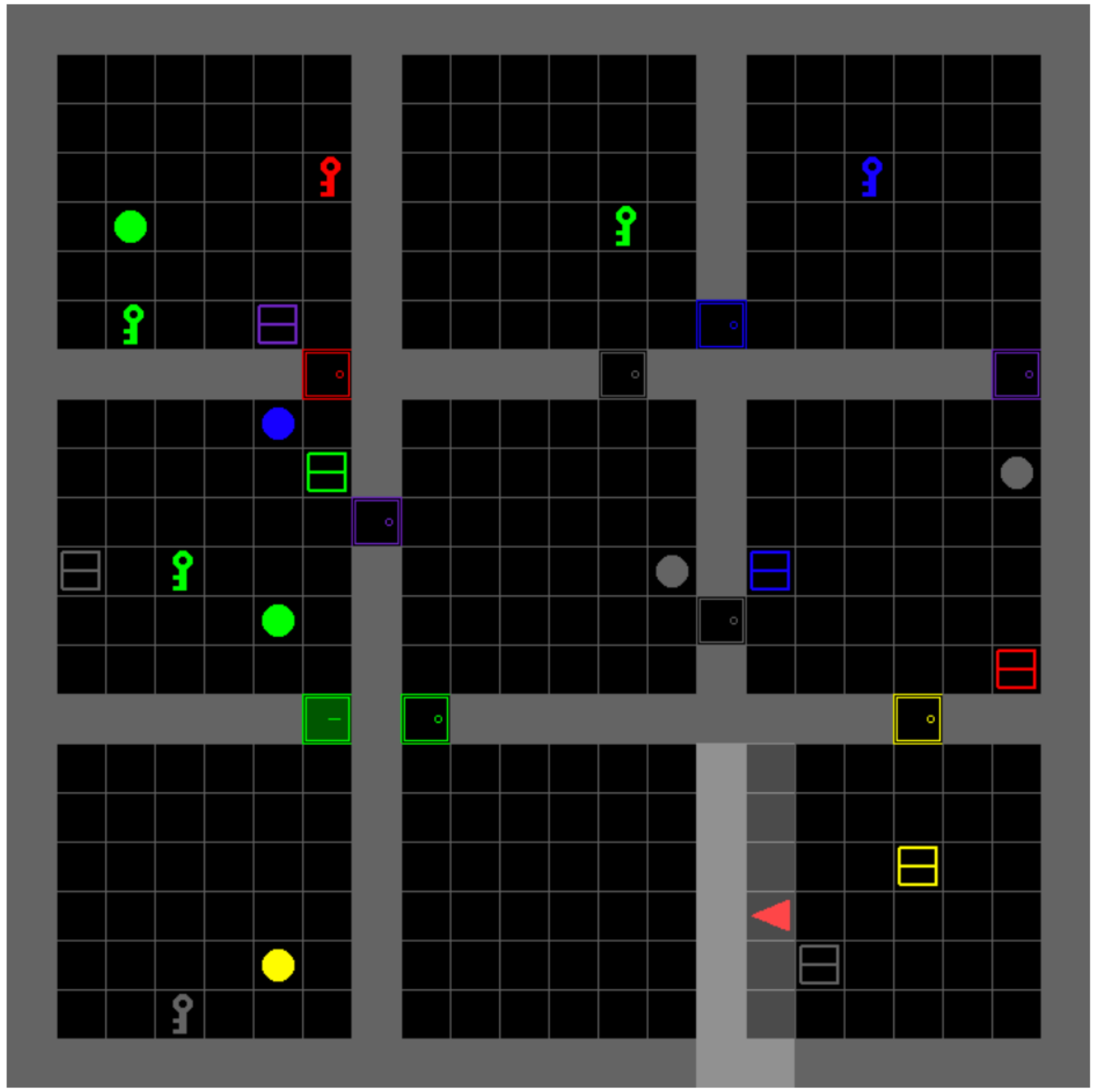
High Level Concepts: Stationary Property of the Model



(a) GoToObj: "go to the blue ball"



(b) PutNextLocal: "put the blue key next to the green ball"

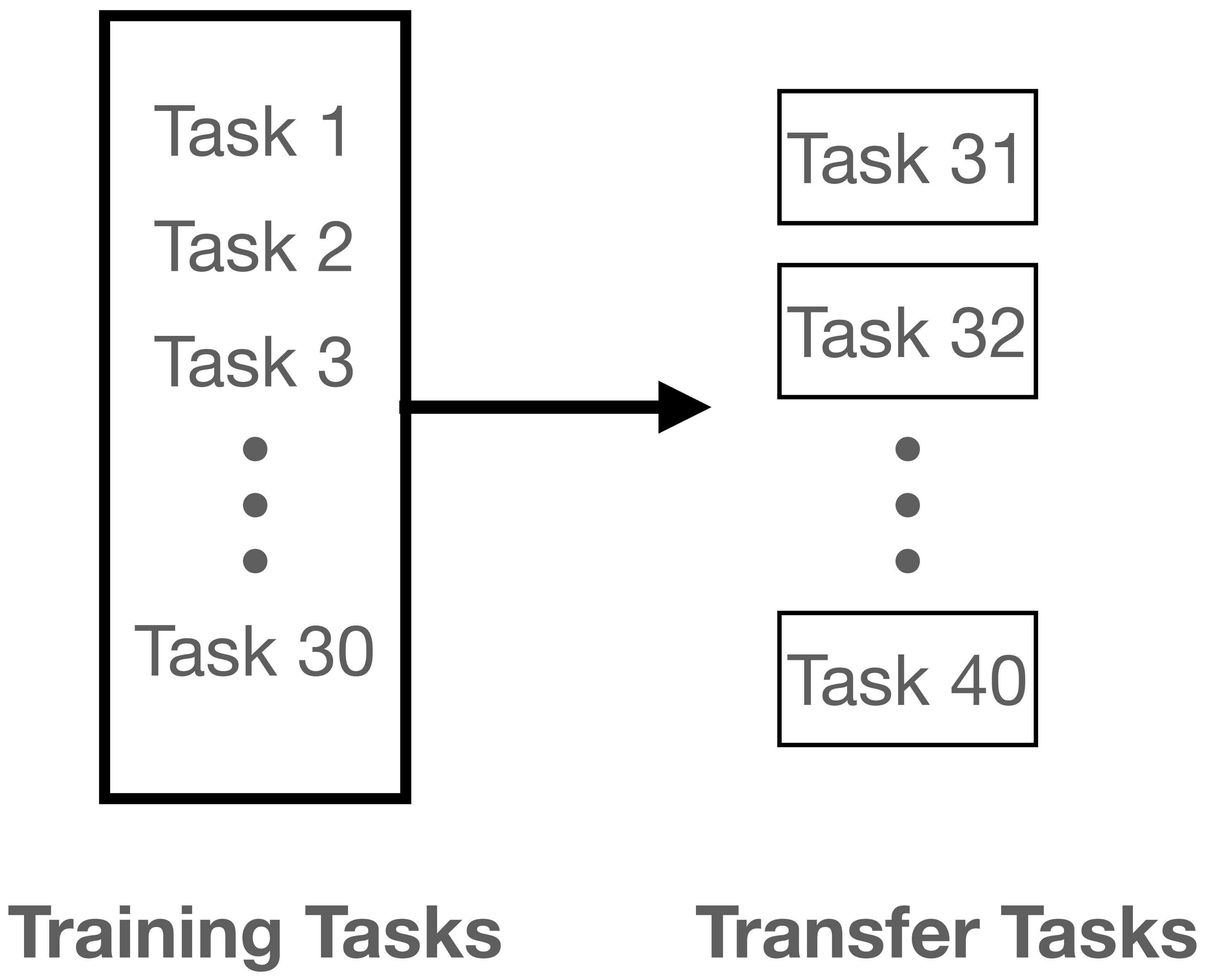


(c) BossLevel: "pick up the grey box behind you, then go to the grey key and open a door". Note that the green door near the bottom left needs to be unlocked with a green key, but this is not explicitly stated in the instruction.

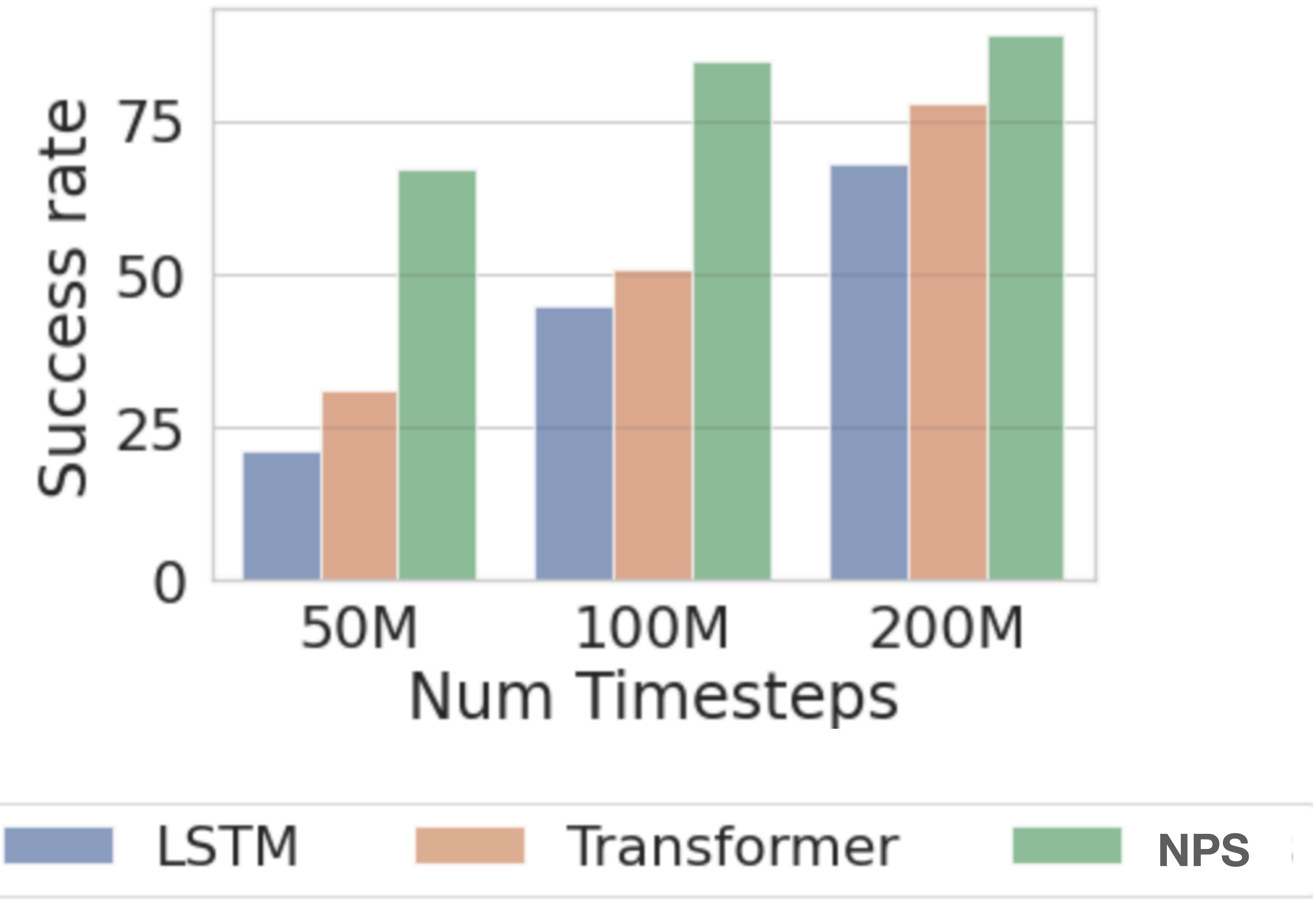
- Knowledge of entities remain same (i.e., key, door, balls etc) across tasks.
- Dynamics of the different modules are changing across different time-steps.

Results: Instruction Following

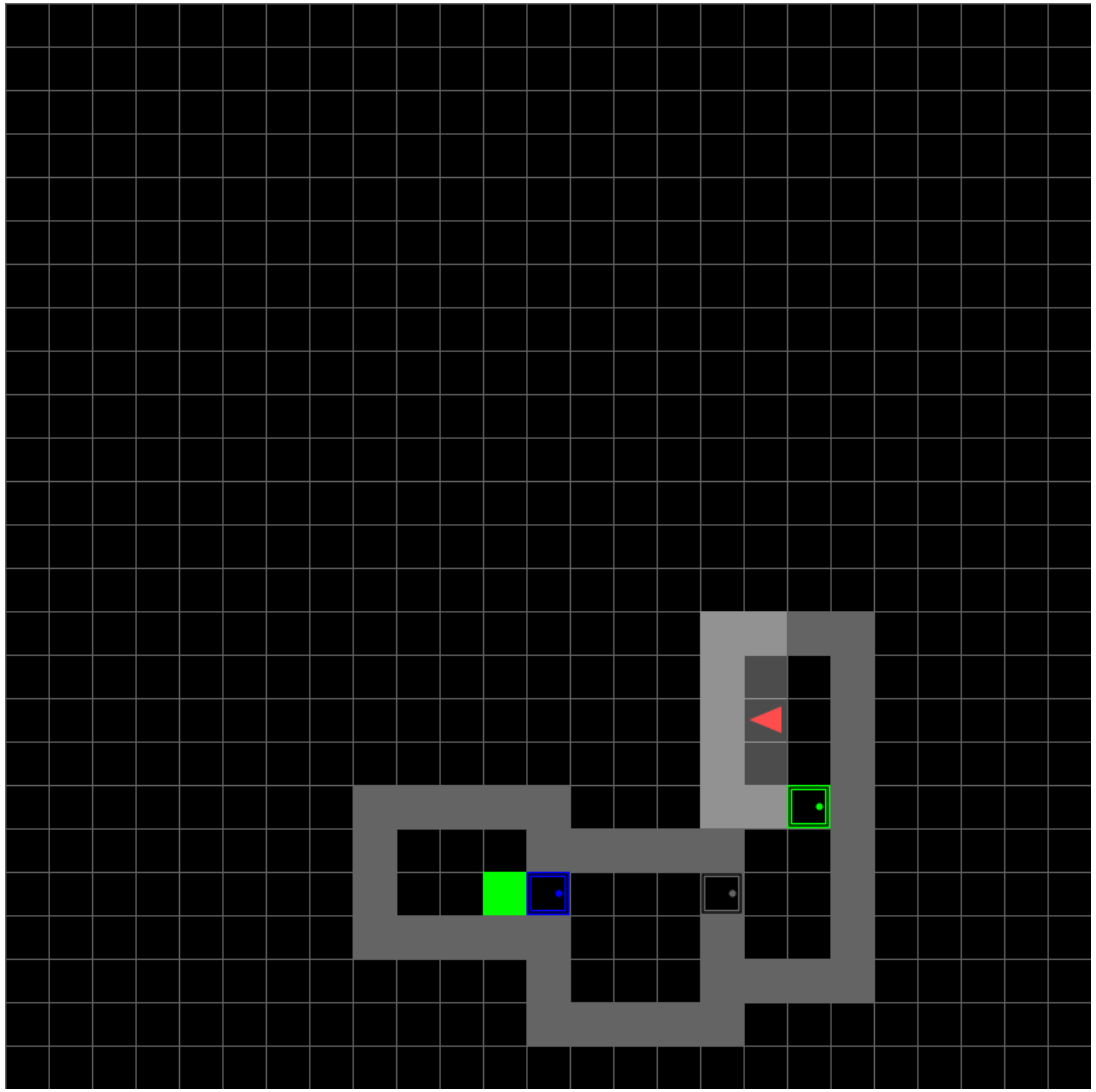
First training on training tasks, and then "adaptation" on the transfer tasks.



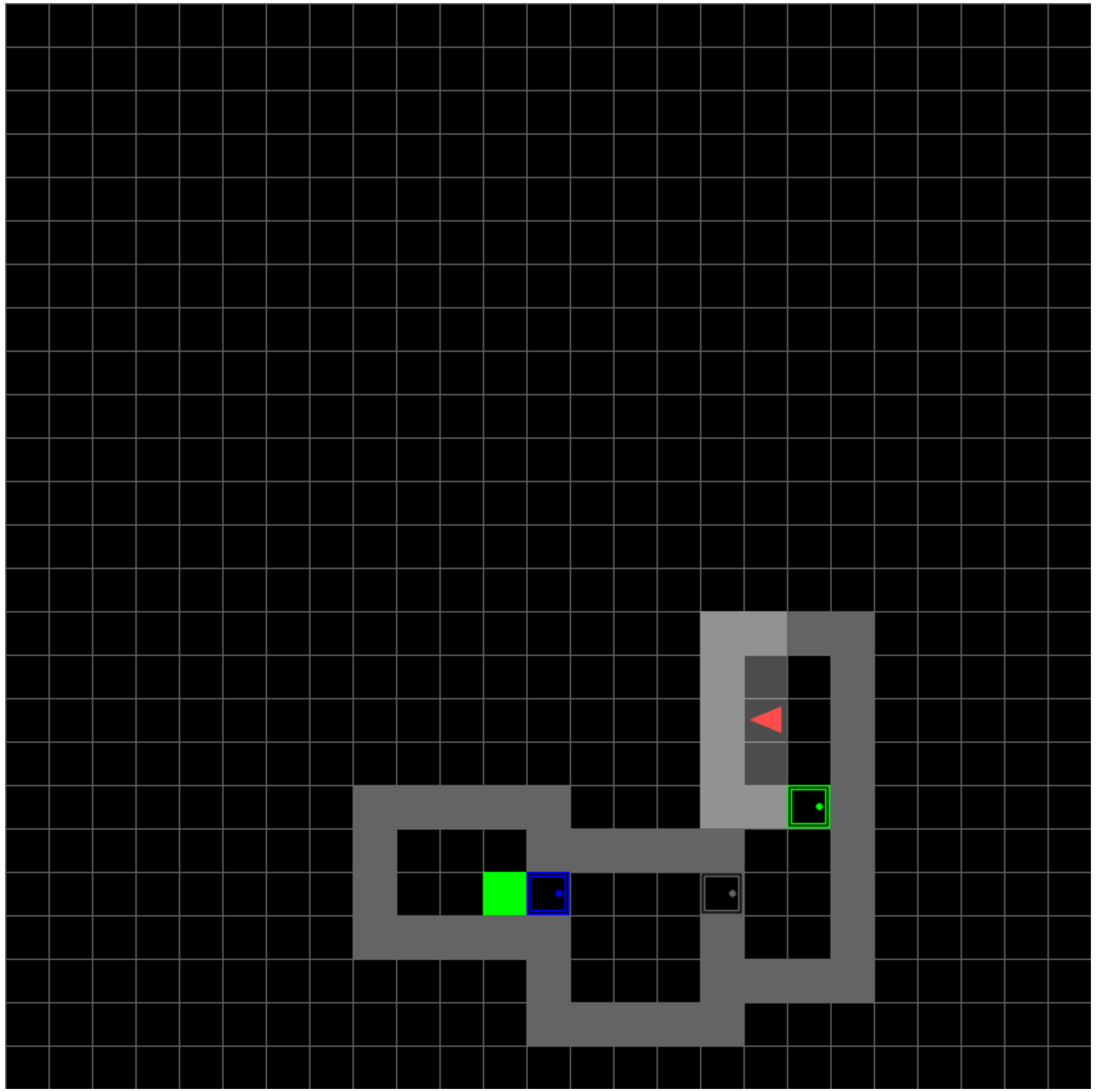
Mean success rate (10 different tasks)



Results: Instruction Following



Baseline



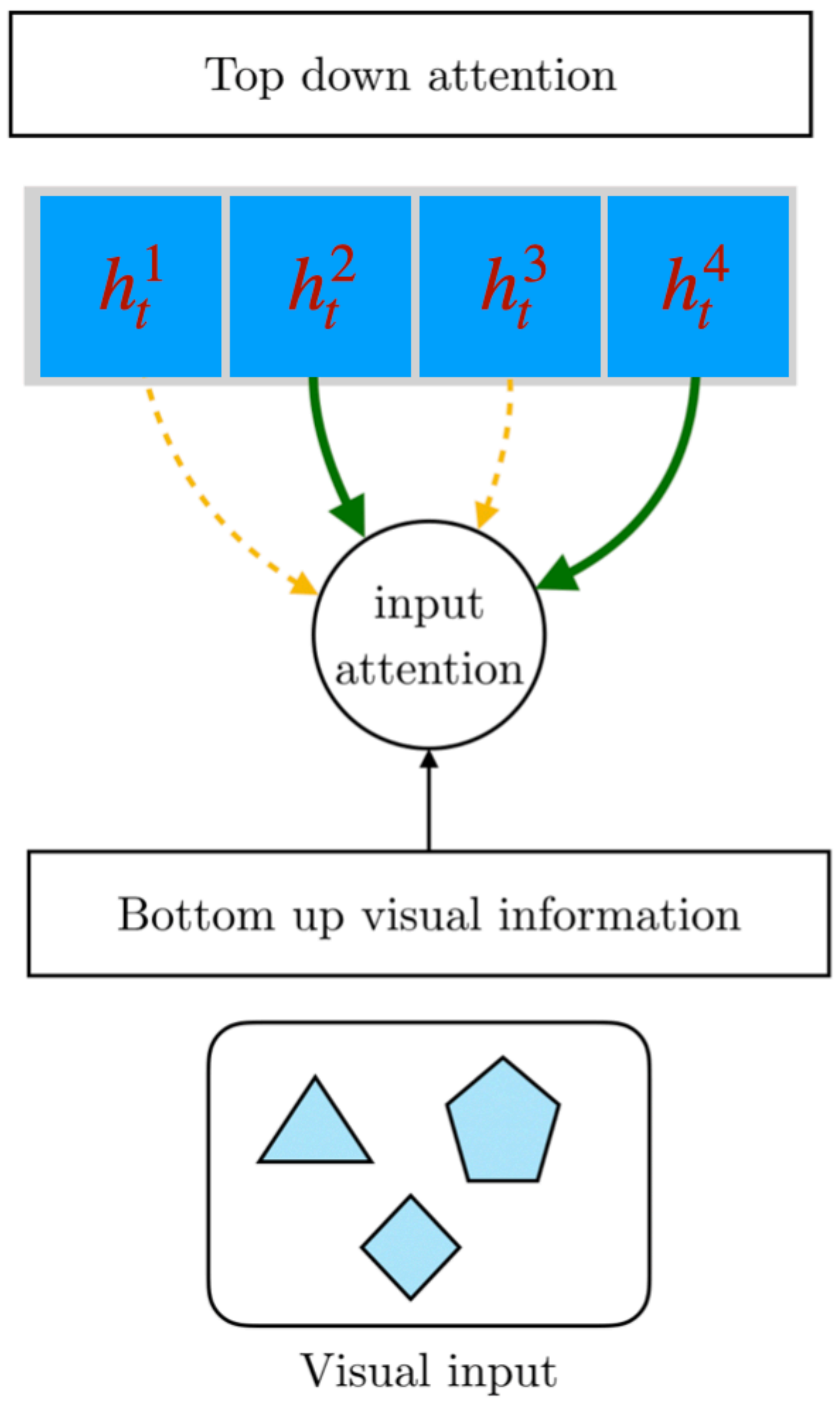
Proposed Method

Takeaway Lesson

Correct Knowledge Factorization leads to faster adaptation

The causal generative process of a system's variables is composed of causal modules that do not inform or influence each other.

Independent Causal Mechanisms



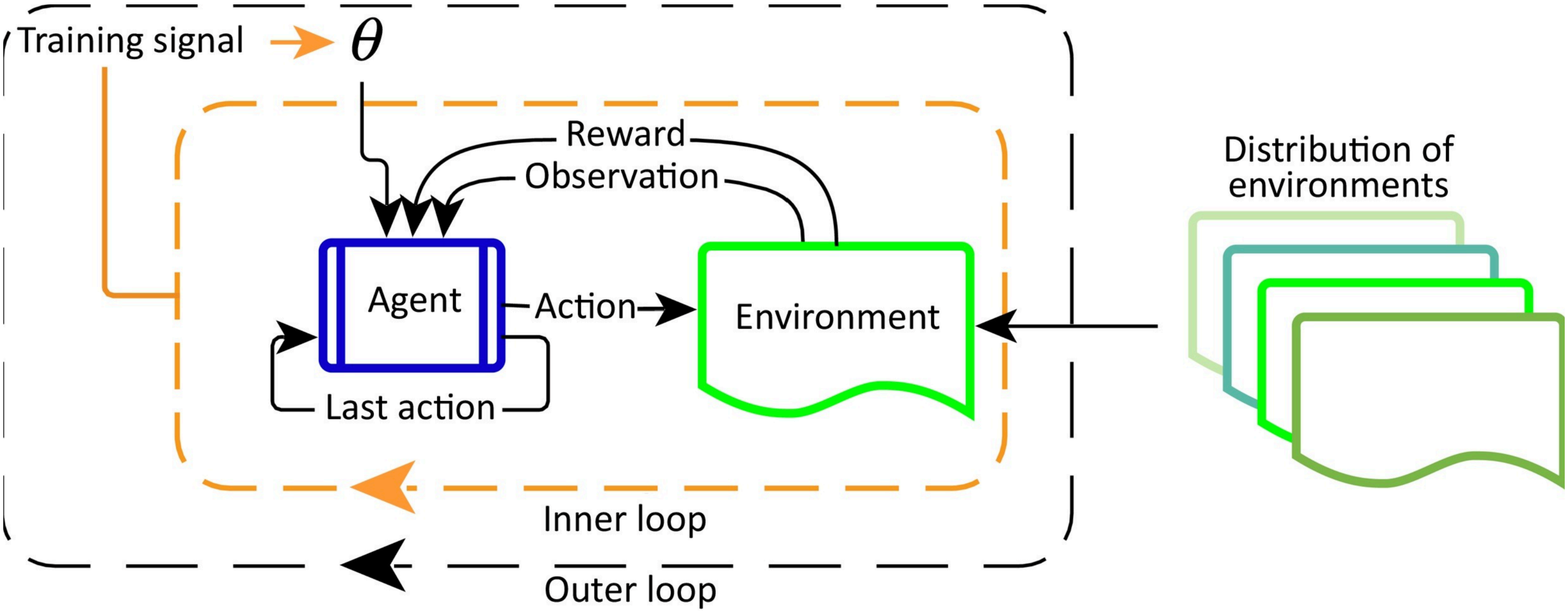
Small distribution changes tend to manifest themselves in a sparse way in the causal factorization.

Sparse Change Hypothesis

Towards Causal Representation Learning, arXiv:2102.11107

So what’s next?

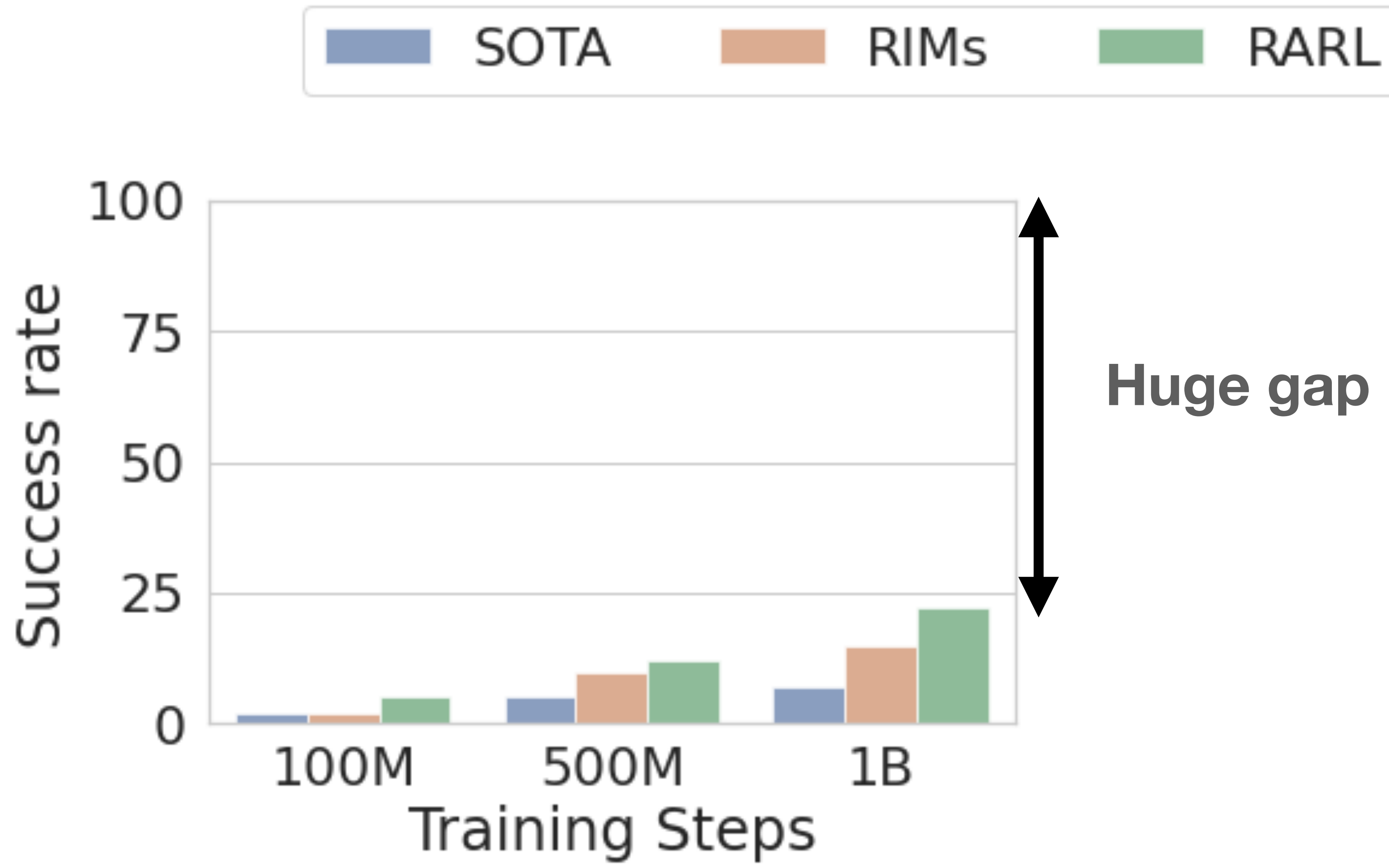
Objectives that Promote Reuse of Neural Functions

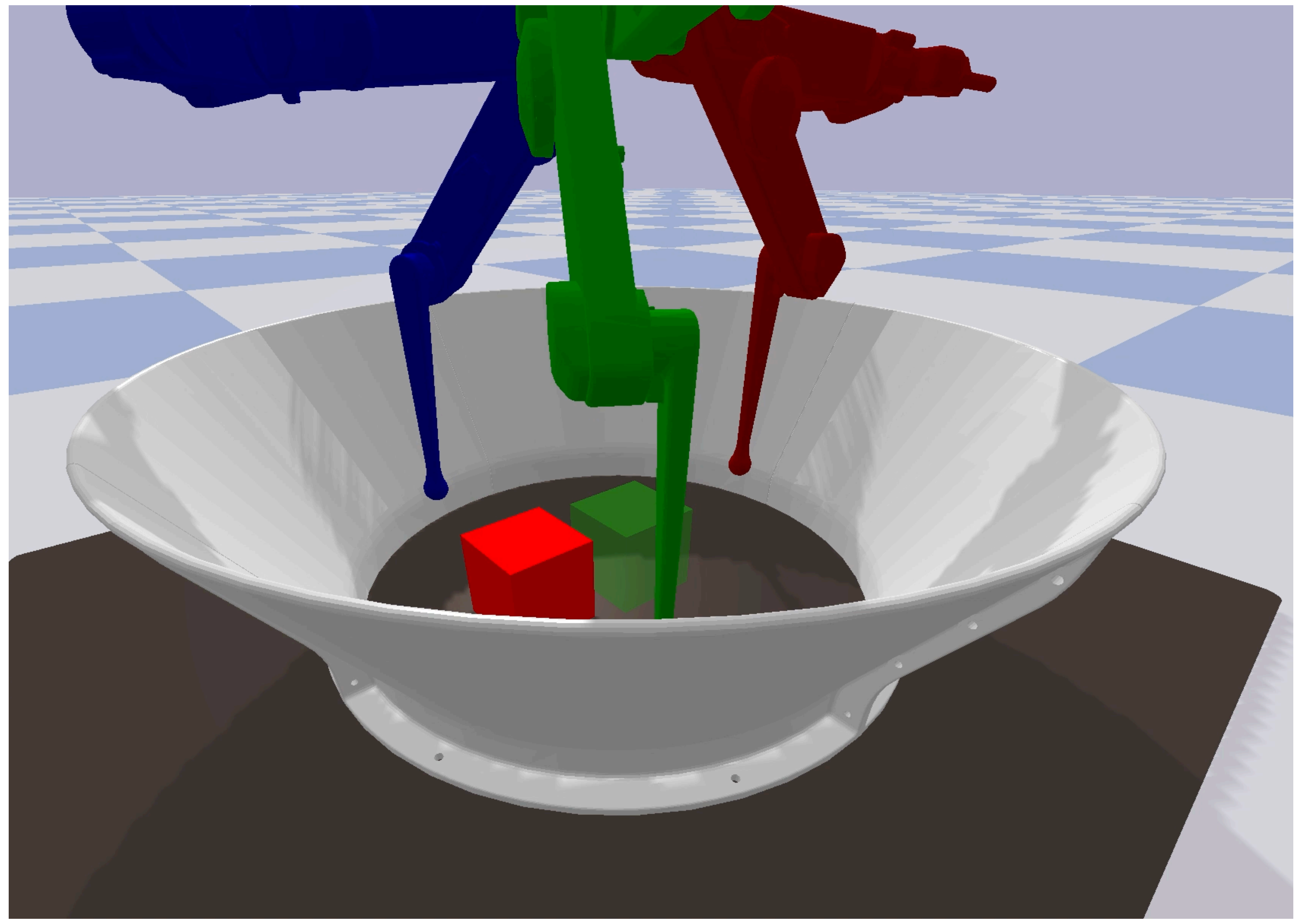


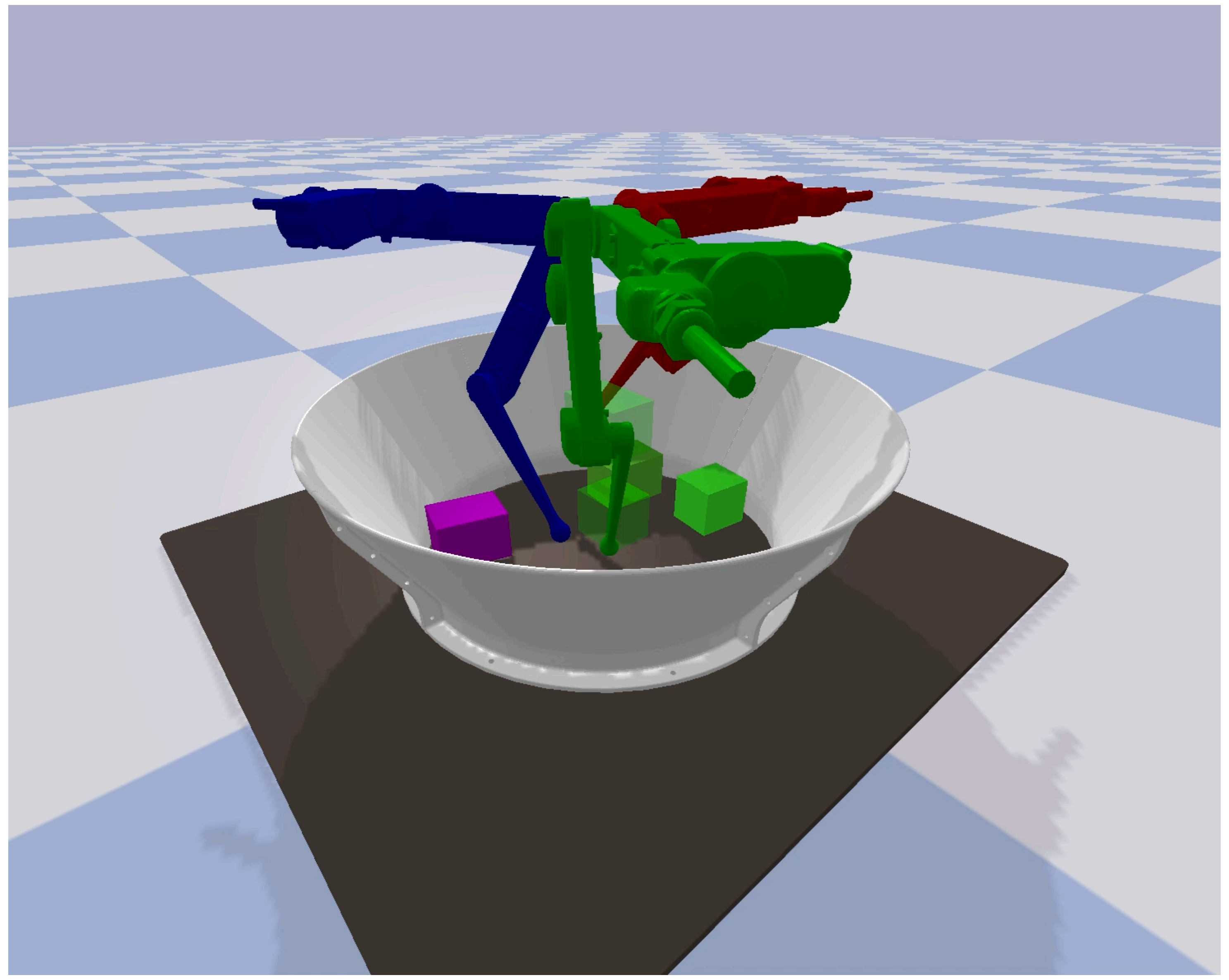
Agent learns at two levels, each associated with different time scales: Rapid learning (inner loop) occurs within an environment. This learning is guided by knowledge accrued more gradually across tasks (outer loop)

Fast and Slow Learning of RIMs, Madan et. al (ICLR'21)

Challenges Ahead: From Simulation to Real-World







Ongoing work

- **Exploration:** How can agents behave in an meaningful way in the case of sparse reward task (for ex. just a goal image).
- **Planning:** How good is a robot at building these shapes?
- **Meta-Transfer Objectives:** How well can an agent transfer and generalise to other shapes, physical properties ?
- **Synchonization:** How can different “systems” [planning, motor-control, exploration, language etc] coordinate with each other to solve a given task ?

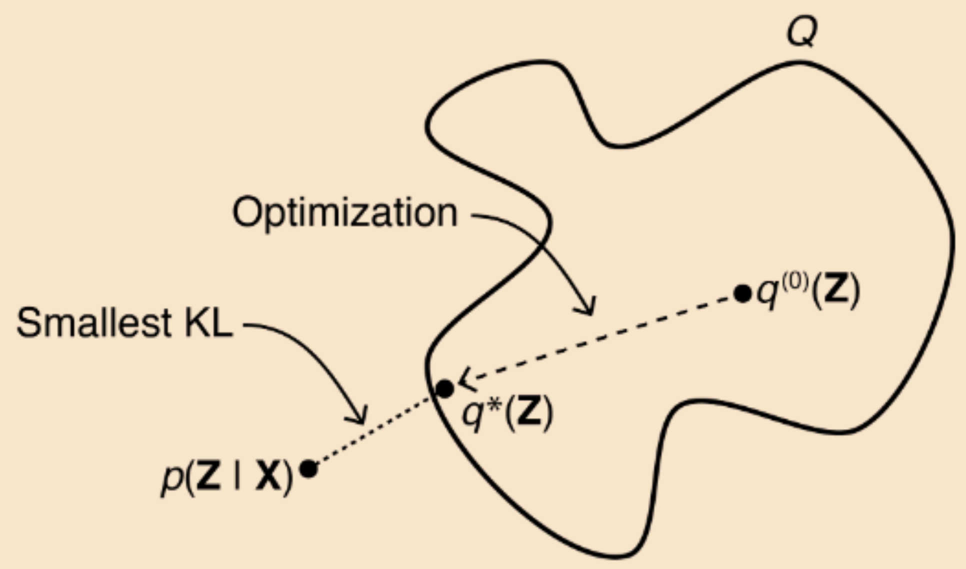
Deep Learning for Causality/ Causality for Deep Learning

A **Modelling functional relationships (causal mechanisms)**

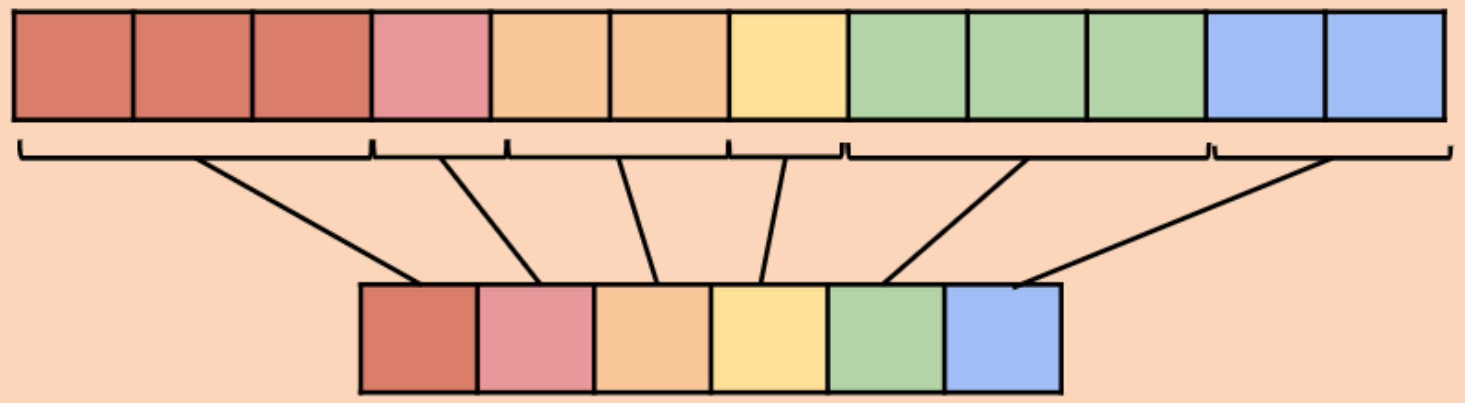
$$X_i = f_i\left(X_{pa(i,\mathbf{G})}, U_i\right)$$

$$X_{pa(i,\mathbf{G})} \rightarrow \boxed{\text{NN}} \rightarrow X_i$$

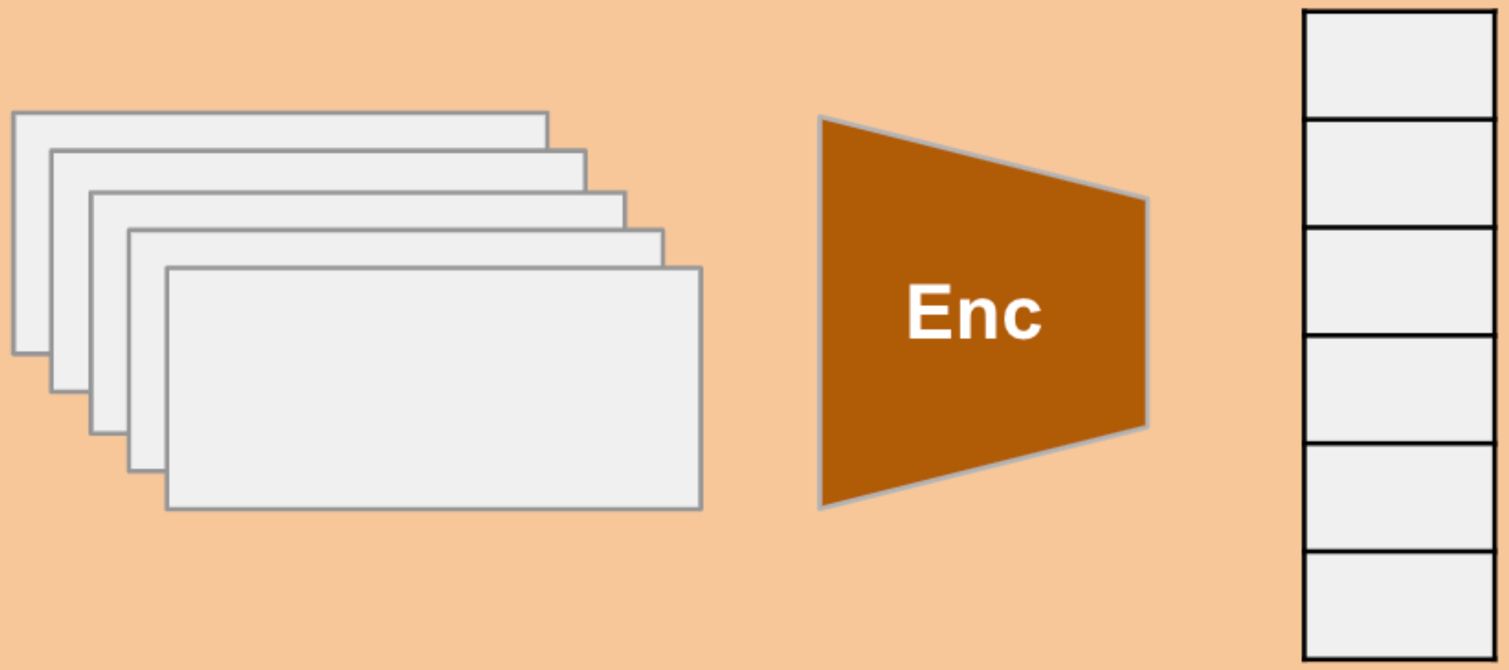
B **Learn a distribution over graphs**



C **Learn representations of causal variables as rich compositions of learned features**

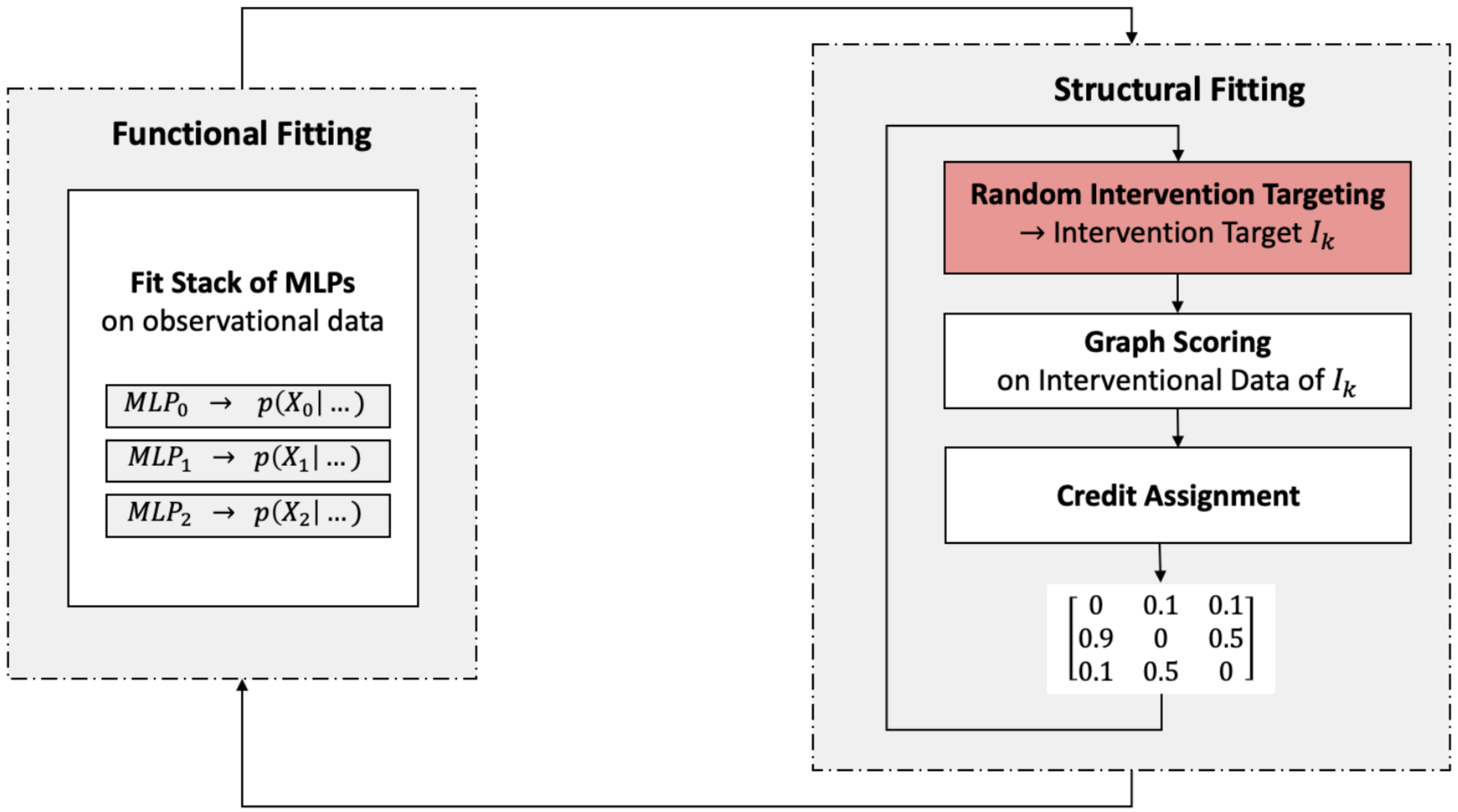


D **Learn latent causal variables**



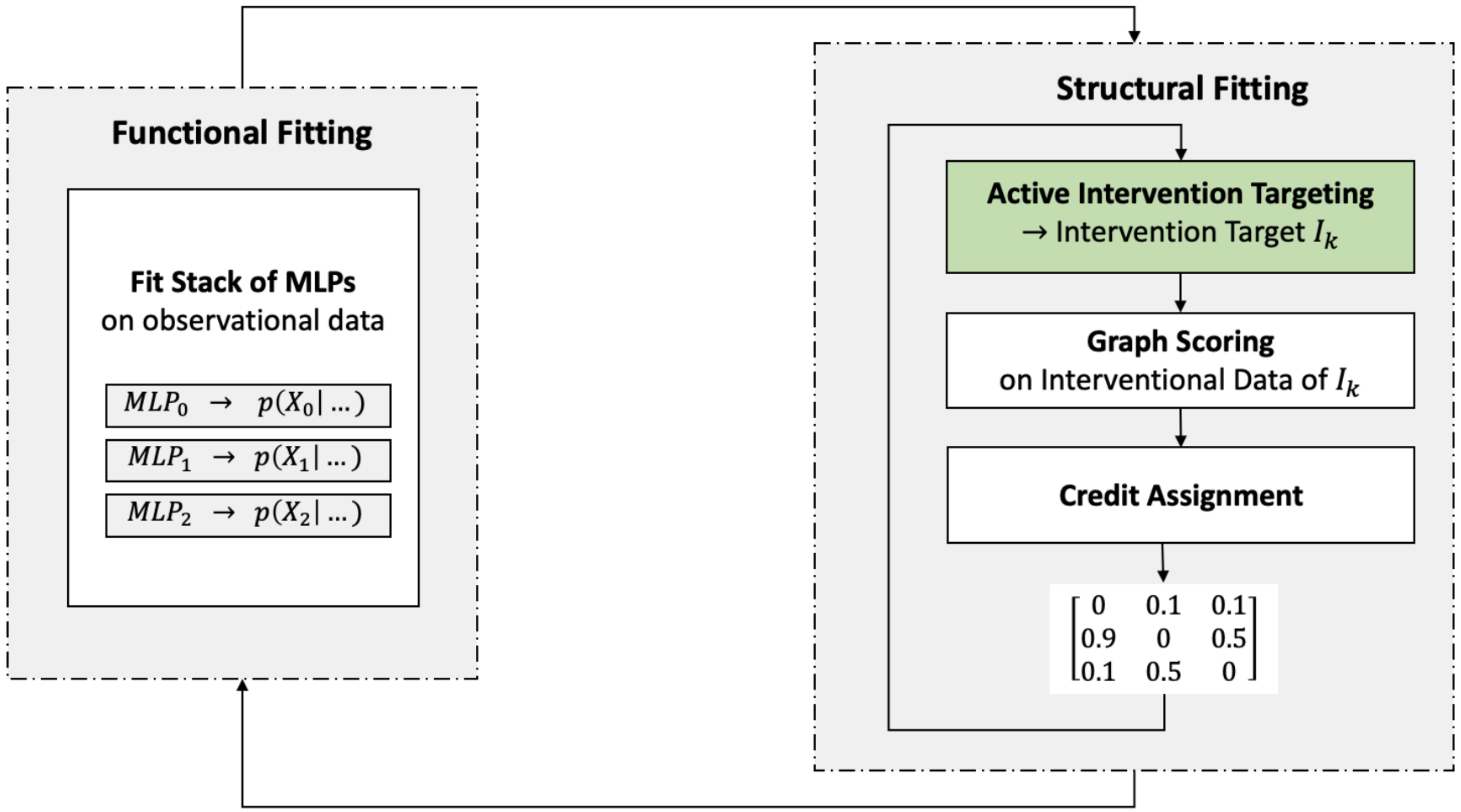
Neural Causal Models

Structure Discovery from Unknown Interventions



Learning Neural Causal Models from Unknown Interventions
Ke et. al, 2019

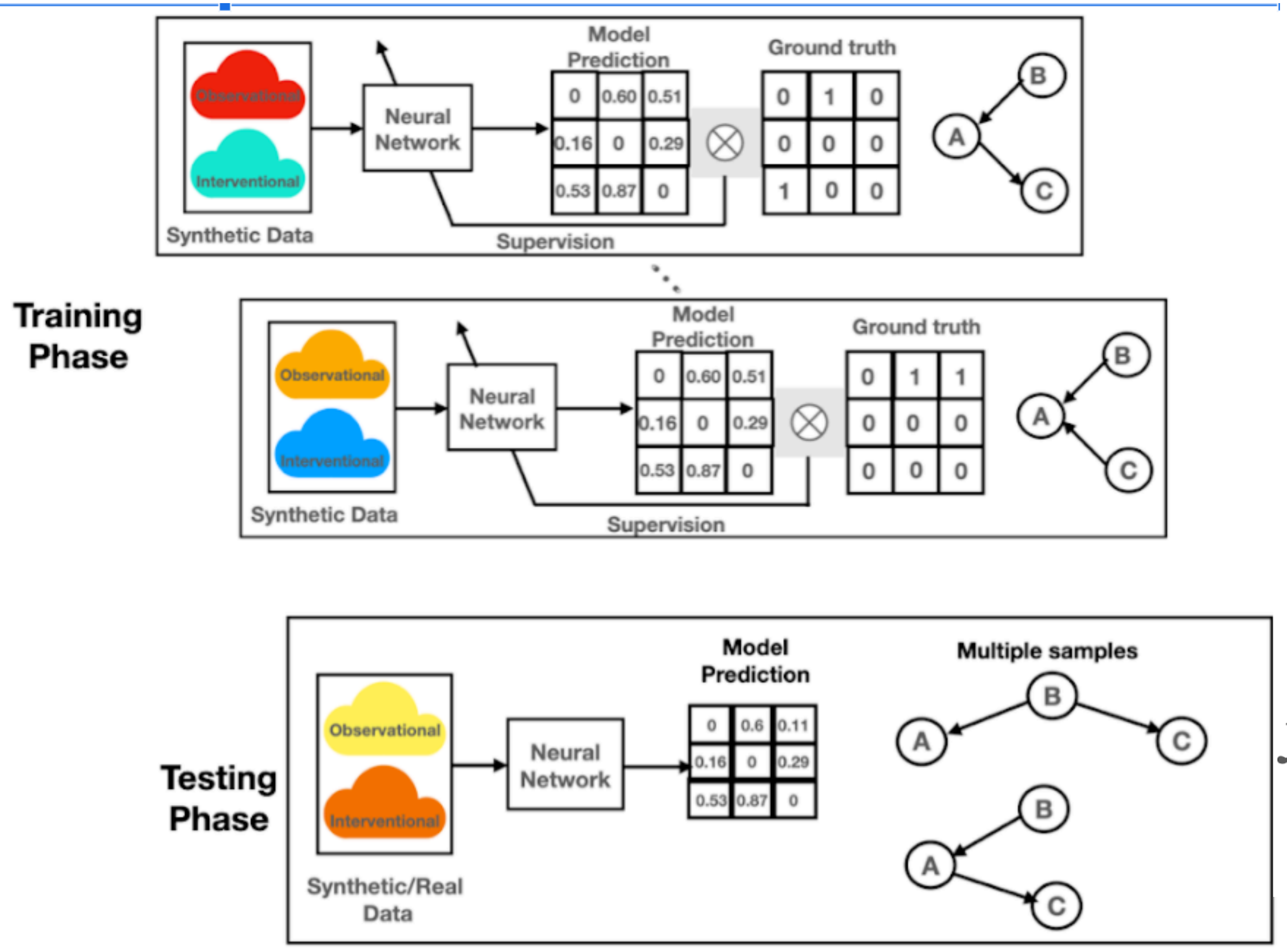
Structure Discovery from Active Interventions



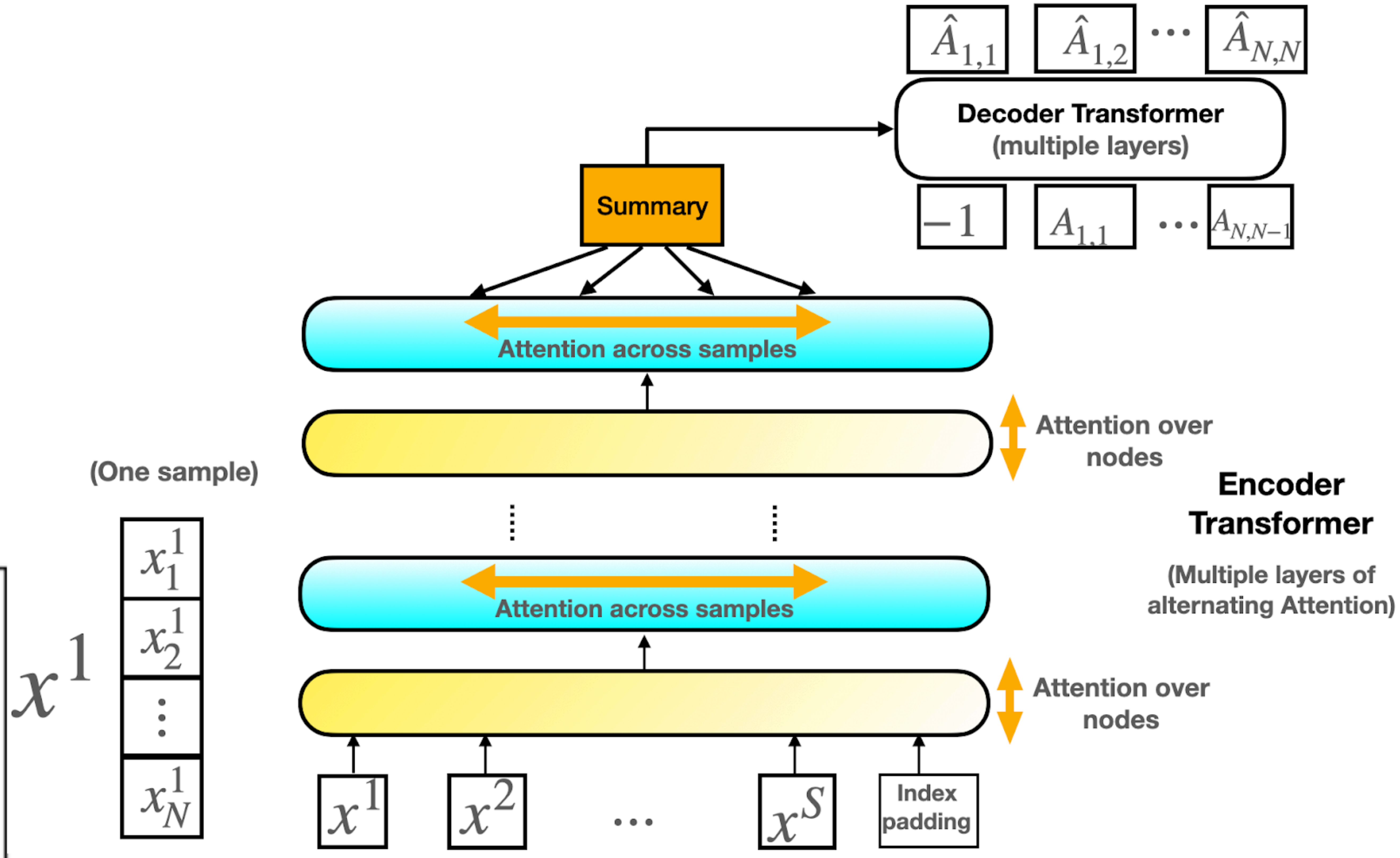
Learning Neural Causal Models from Active Interventions
Scherrer et. al, 2021

See also: Brouillard et al., 2020, Lippe et al, 2021

Learning to Induce Causal Structure: Implicit Bayesian Inference



(B). CSIvA



Learning to Induce Causal structure, Ke et. al, 2022

Yoshua Bengio, Alex Lamb, Rosemary Ke, Aniket Didolkar, Dianbo Liu, Riashat Islam, Guillaume Lajoie, Kanika Madan, Jonathan Binas, Phanideep Gampa, Shagun Sodhani, Kartikeya Badola, Sarthak Mittak, Guillaume Dumas, Kanika Madan, Sarthak Mittal, Olexa Bilaniux

Bernhard Schölkopf, Nasim Rahaman, Frederick Trauble, Stefan Bauer, Francesco Locatello

Sergey Levine

Michael Mozer, Hugo Larochelle

David Silver, Timothy Lillicrap, Nicolas Heess, Theophane Weber, Charles Blundell, Matthew Botvinick, Andrea Banino, Abe Friesen, Arthur Guez, Michael Valko, Simon Osindero, Murray Shanahan

Inductive Biases for Deep Learning of Higher Level Cognition*: Goyal* and Bengio (arXiv:2011.15091)

1. ***Inductive Biases for Deep Learning of Higher Level Cognition:*** **Goyal** and Bengio (arXiv:2011.15091)
2. *Coordination among Neural Modules through a Shared Workspace:* **Goyal** et al (ICLR'22, Oral)
3. *Learning to combine Top Down and Bottom Up Signals in RNN with attention over modules:* Mittal, Lamb, **Goyal** et al, ICML'20
4. *Object Files and Schemata: Factorizing Declarative and Procedural Knowledge in Dynamical Systems :* **Goyal** et al, ICLR'21
5. *Neural Production Systems:* **Goyal** et al, NeurIPS'21
6. Spatially Structured Recurrent Modules: Rahaman, **Goyal** et al, ICLR'21
7. ***Fast and Slow learning of Recurrent Independent Mechanisms:*** **Madan, Ke, Goyal, et al ICLR'21**
8. ***A meta-transfer objective for learning to disentangle causal mechanisms*****: Bengio […], Goyal, ICLR'20**
9. Systematic Evaluation of Causal Discovery in Visual Model Based Reinforcement Learning: Ke […], **Goyal** et al, NeurIPS'21
10. *InfoBot: Transfer and Exploration using information bottleneck:* Goyal et al, ICLR'20
11. *Variational Bandwidth Bottleneck […]:* **Goyal,** Bengio, Botvinick, Levine al, ICLR'21
12. *RL using competitive ensemble of information constrained primitives:* **Goyal** et al, ICLR'21
13. *Sparse Attentive Backtracking: Temporal Credit Assignment through Reminding:* Ke, **Goyal** et al, NeurIPS'18
14. *Untangling Tradeoffs between recurrence and self-attention in neural networks: Kerg, Kanuparthi,* **Goyal** et al, NeurIPS'20
15. *Recall Traces: BackTracking Model for efficient Reinforcement Learning,* **Goyal** et al, ICLR'19
16. ***Recurrent Independent Mechanisms*****, Goyal et al, ICLR'21**
17. **Retrieval Augmented Reinforcement Learning, Goyal et. al, ICML'22**