



Tutorial at KDD, August 14<sup>th</sup> 2021

# From Deep Learning to Deep Reasoning

Part C: Memory | Data efficiency | Recursive reasoning

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<https://bit.ly/37DYQn7>

# Agenda

- Reasoning with external memories
  - Memory of entities – memory-augmented neural networks
  - Memory of relations with tensors and graphs
  - Memory of programs & neural program construction.
- Learning to reason with less labels
  - Data augmentation with analogical and counterfactual examples
  - Question generation
  - Self-supervised learning for question answering
  - Learning with external knowledge graphs
- Recursive reasoning with neural theory of mind.

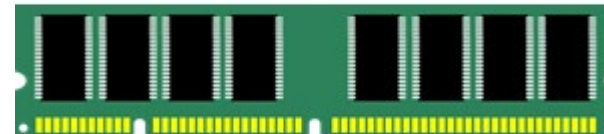
# Agenda

- **Reasoning with external memories**
  - Memory of entities – memory-augmented neural networks
  - Memory of relations with tensors and graphs
  - Memory of programs & neural program construction.
- Learning to reason with less labels:
  - Data augmentation with analogical and counterfactual examples
  - Question generation
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- Recursive reasoning with neural theory of mind.

# Introduction

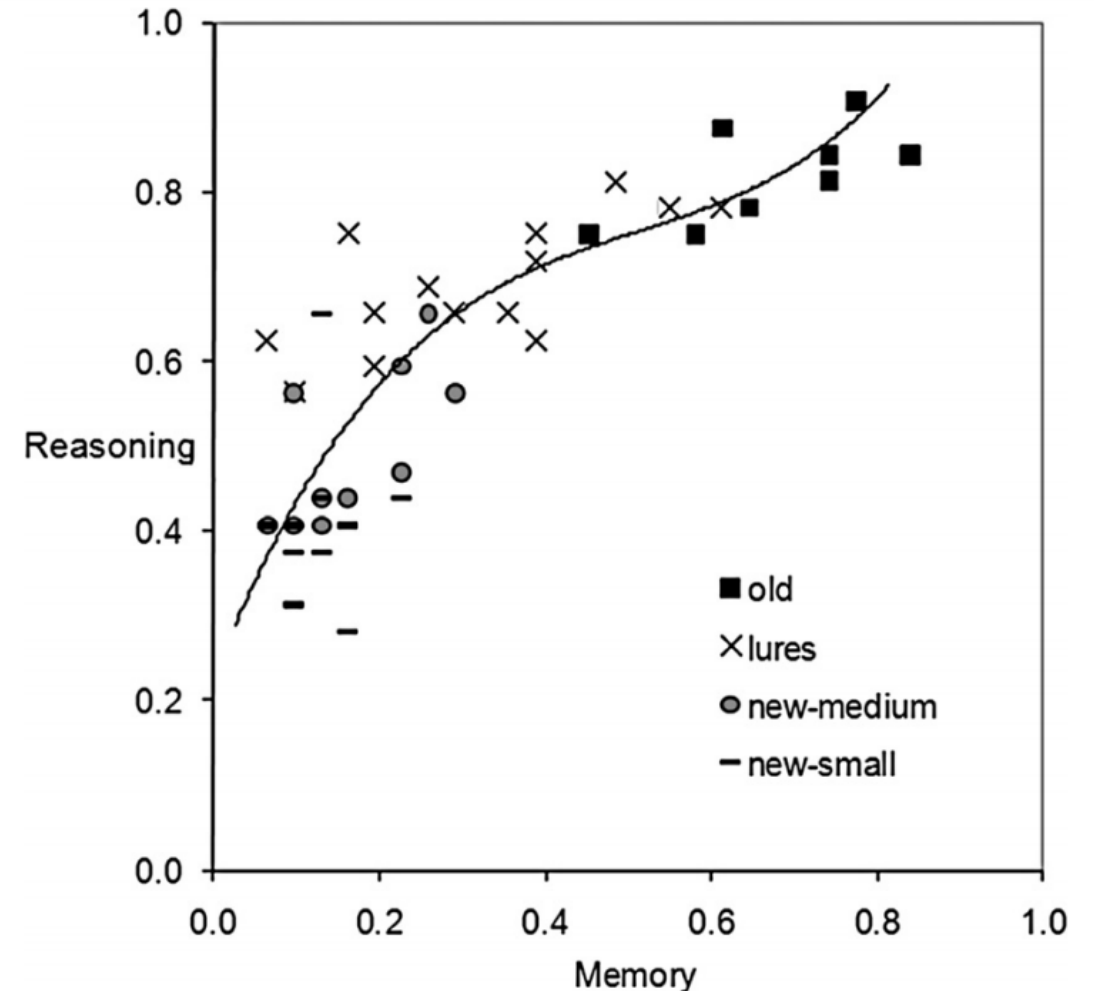
# Memory is part of intelligence

- Memory is the ability to store, retain and recall information
- Brain memory stores items, events and high-level structures
- Computer memory stores data and temporary variables



# Memory-reasoning analogy

- 2 processes: fast-slow
  - Memory: familiarity-recollection
- Cognitive test:
  - Corresponding reasoning and memorization performance
  - Increasing # premises, inductive/deductive reasoning is affected



# Common memory activities

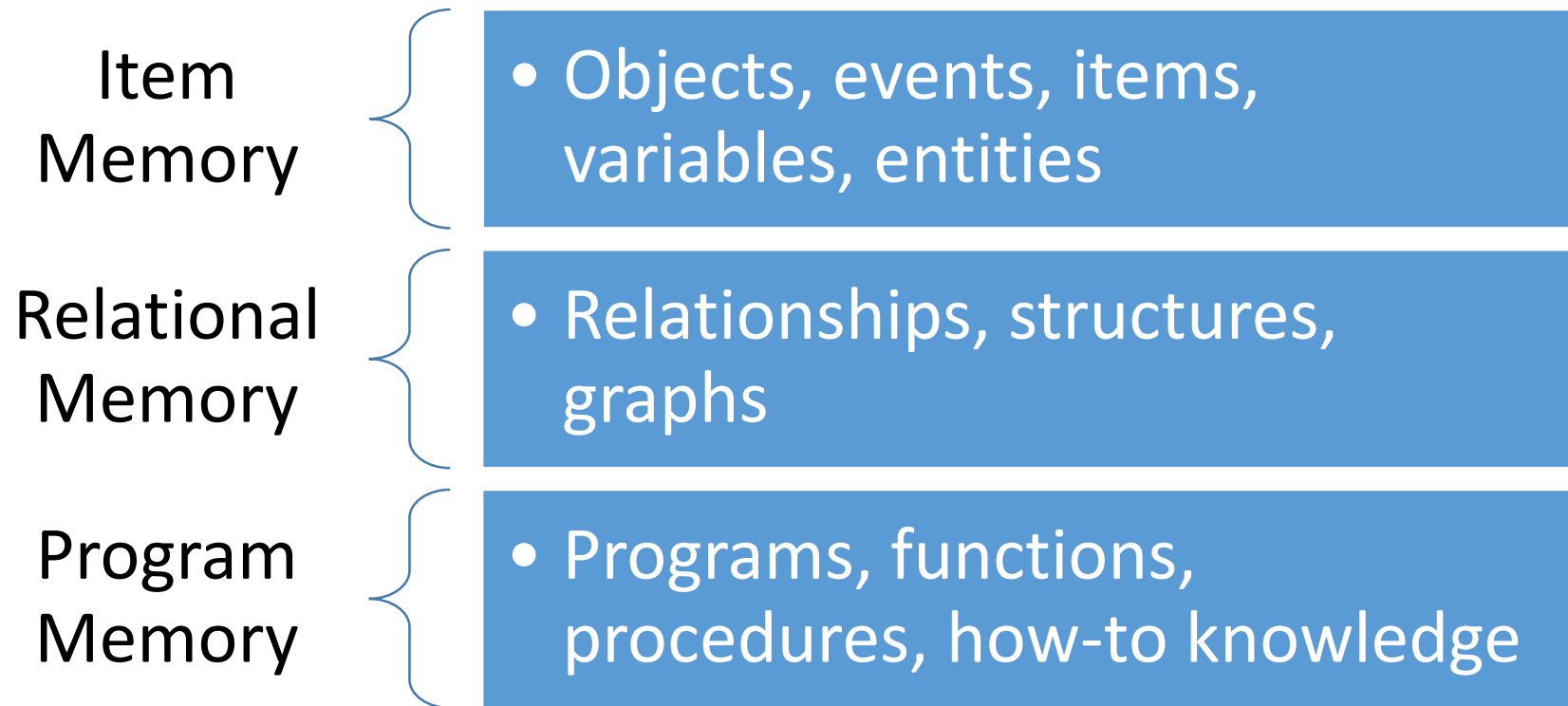
- Encode: write information to the memory, often requiring compression capability
- Retain: keep the information overtime. This is often assumed in machinery memory
- Retrieve: read information from the memory to solve the task at hand

Encode

Retain

Retrieve

# Memory taxonomy based on memory content





# Item memory

Associative memory

RAM-like memory

Independent memory

# Distributed item memory as associative memory

Language

"Green" means  
"go," but what  
does "red" mean?

Semantic  
memory

Time

birthday party on  
30<sup>th</sup> Jan

Episodic  
memory

Object

Where is my pen?  
What is the  
password?

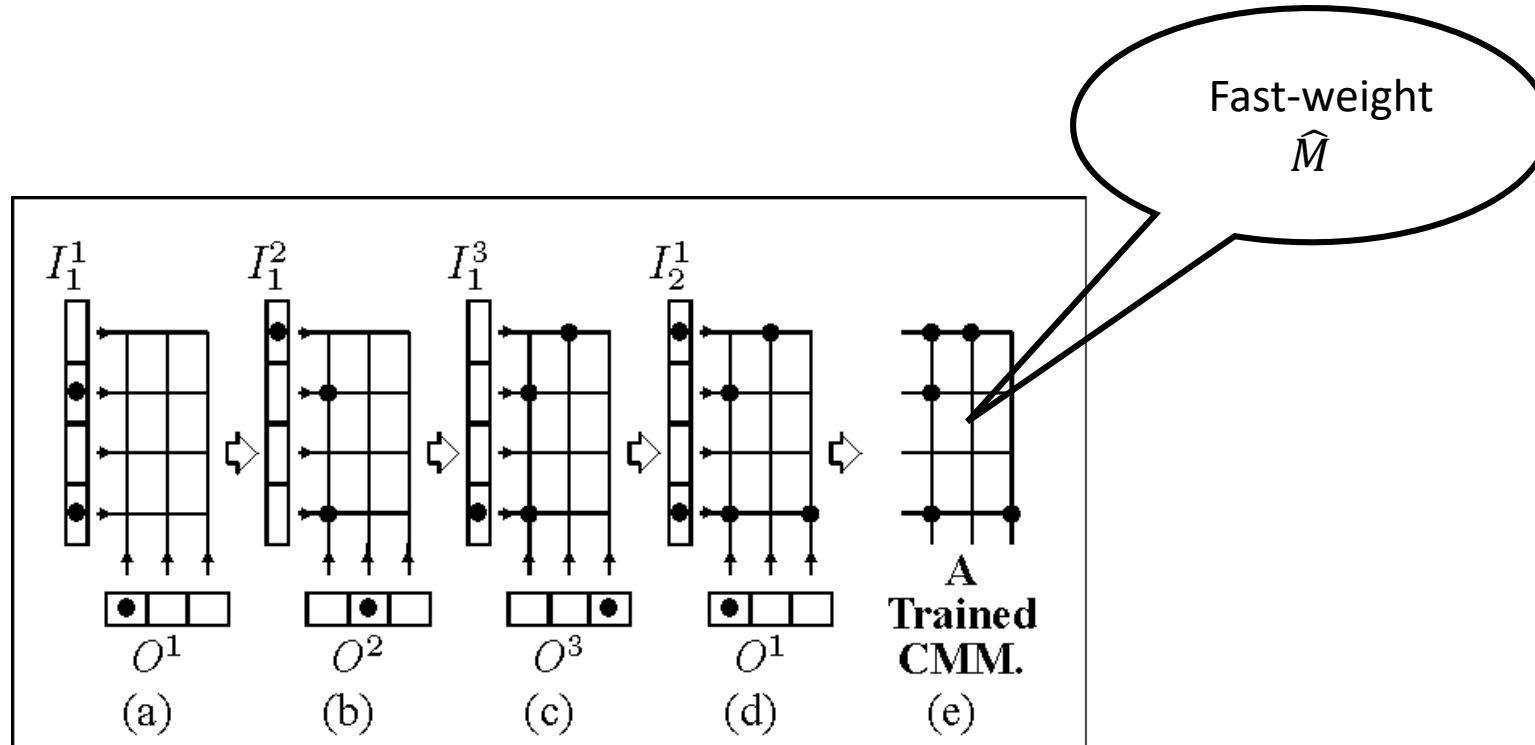
Working  
memory

Behaviour



Motor  
memory

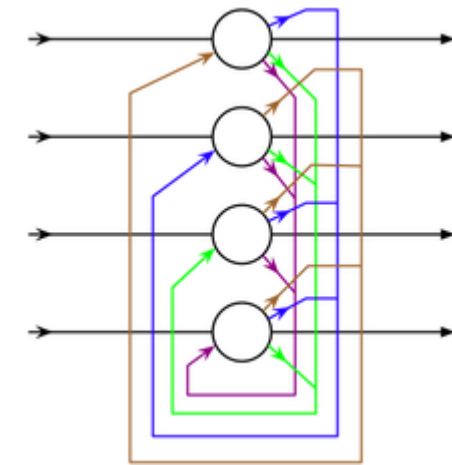
# Associate memory can be implemented as Hopfield network



Correlation matrix memory

Encode  $\hat{\mathbf{M}} = \sum_{k=1}^q \mathbf{b}_k \mathbf{a}_k^T$  Retrieve  $\mathbf{b} = \hat{\mathbf{M}} \mathbf{a}_j$

Feed-forward retrieval



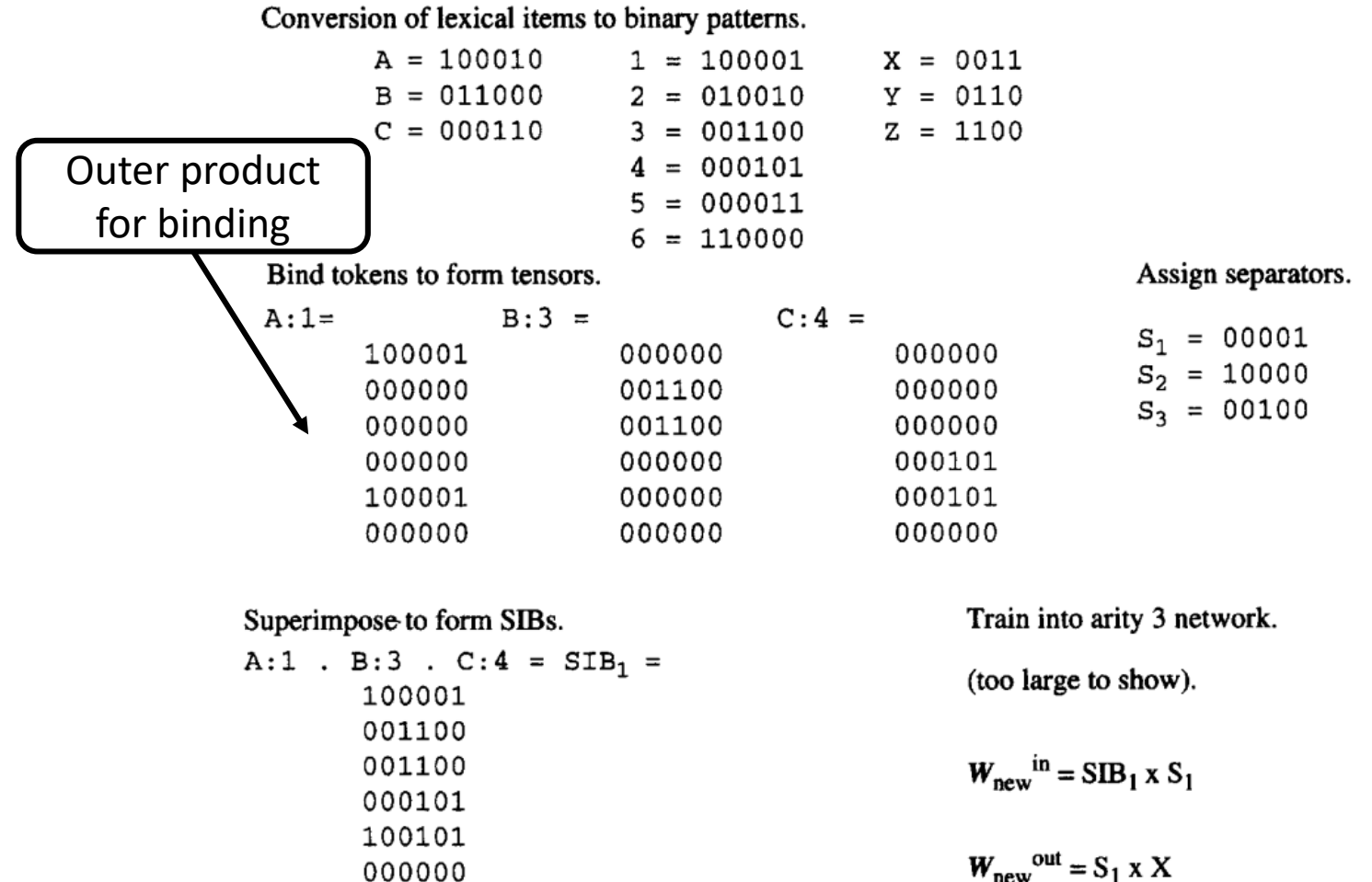
Hopfield network

Retrieve  $x_i(t+1) = \text{sign} \left( \sum_{j=1}^N w_{ij} x_j(t) \right)$

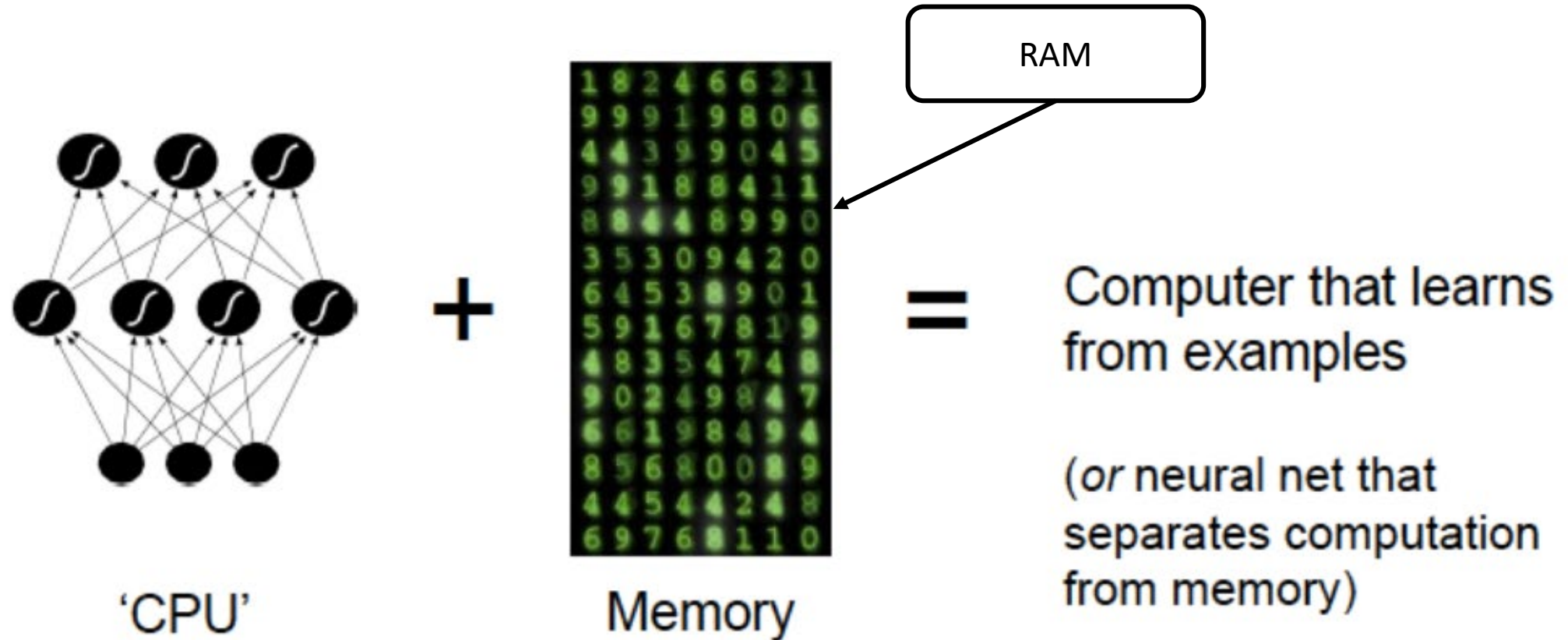
Recurrent retrieval

# Rule-based reasoning with associative memory

- Encode a set of rules:  
“pre-conditions  
→post-conditions”
- Support variable binding, rule-conflict handling and partial rule input
- Example of encoding rule “A:1,B:3,C:4→X”

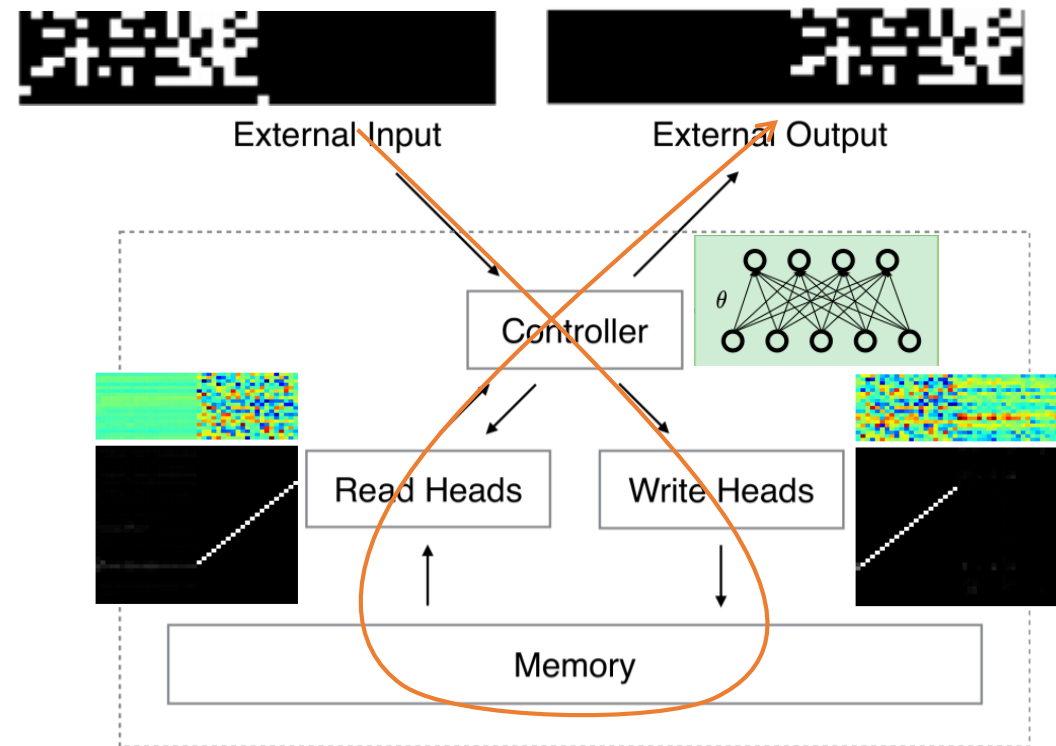


# Memory-augmented neural networks: computation-storage separation

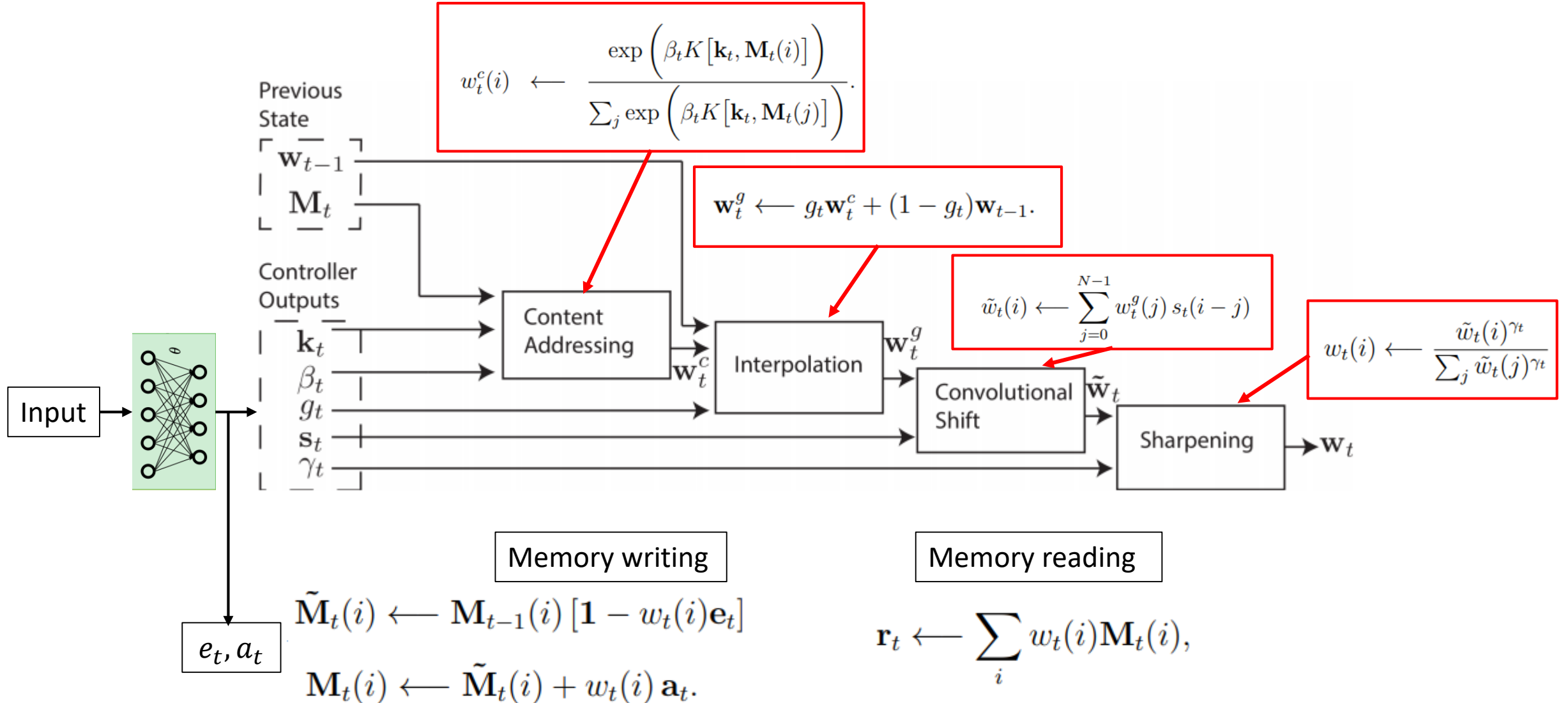


# Neural Turing Machine (NTM)

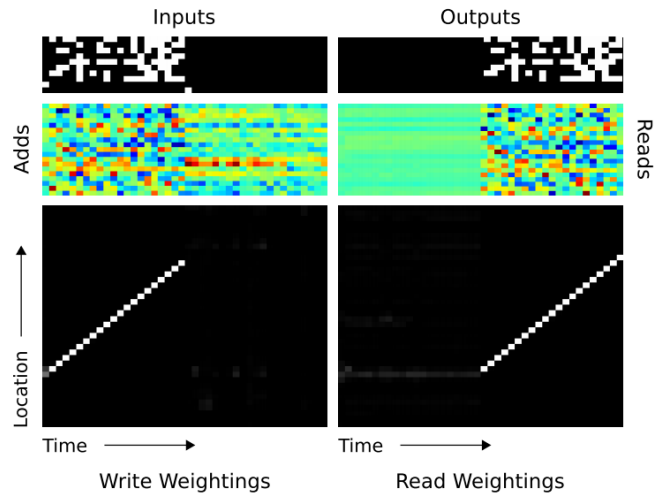
- Memory is a 2d matrix
- Controller is a neural network
- The controller read/writes to memory at certain addresses.
- Trained end-to-end, differentiable
- Simulate Turing Machine  
→ support symbolic reasoning, algorithm solving



# Addressing mechanism in NTM



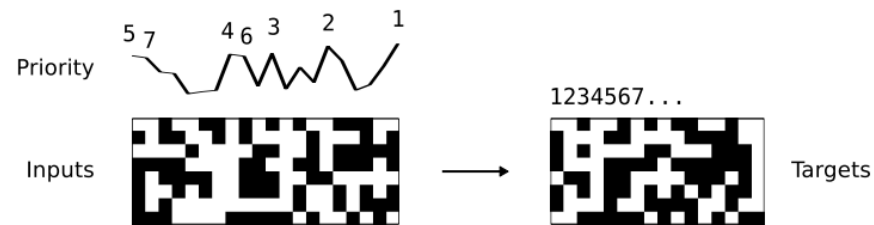
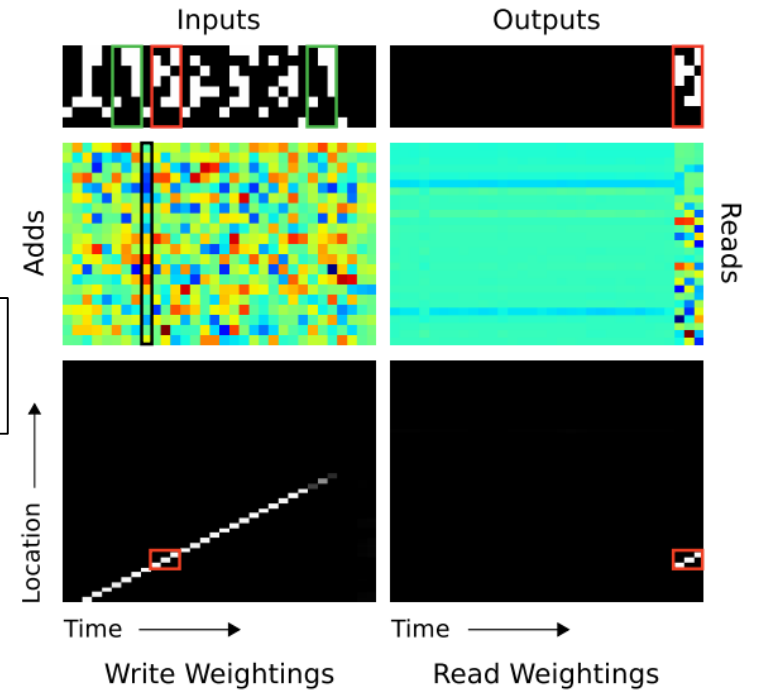
# Algorithmic reasoning



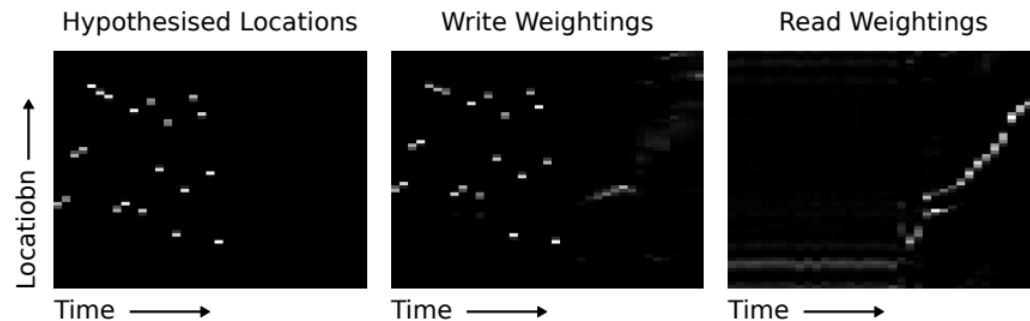
Copy

**initialise:** move head to start location  
**while** input delimiter not seen **do**  
    receive input vector  
    write input to head location  
    increment head location by 1  
**end while**  
return head to start location  
**while** true **do**  
    read output vector from head location  
    emit output  
    increment head location by 1  
**end while**

Associative recall



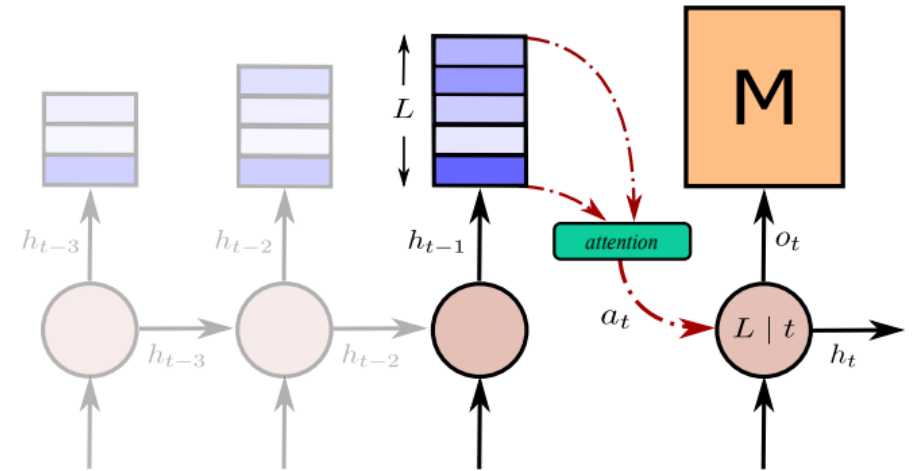
Priority sort





# Optimal memory writing for memorization

- Simple finding: writing too often deteriorates memory content (not retainable)
- Given input sequence of length  $T$  and only  $D$  writes, *when should we write to the memory?*



Uniform writing is optimal for memorization

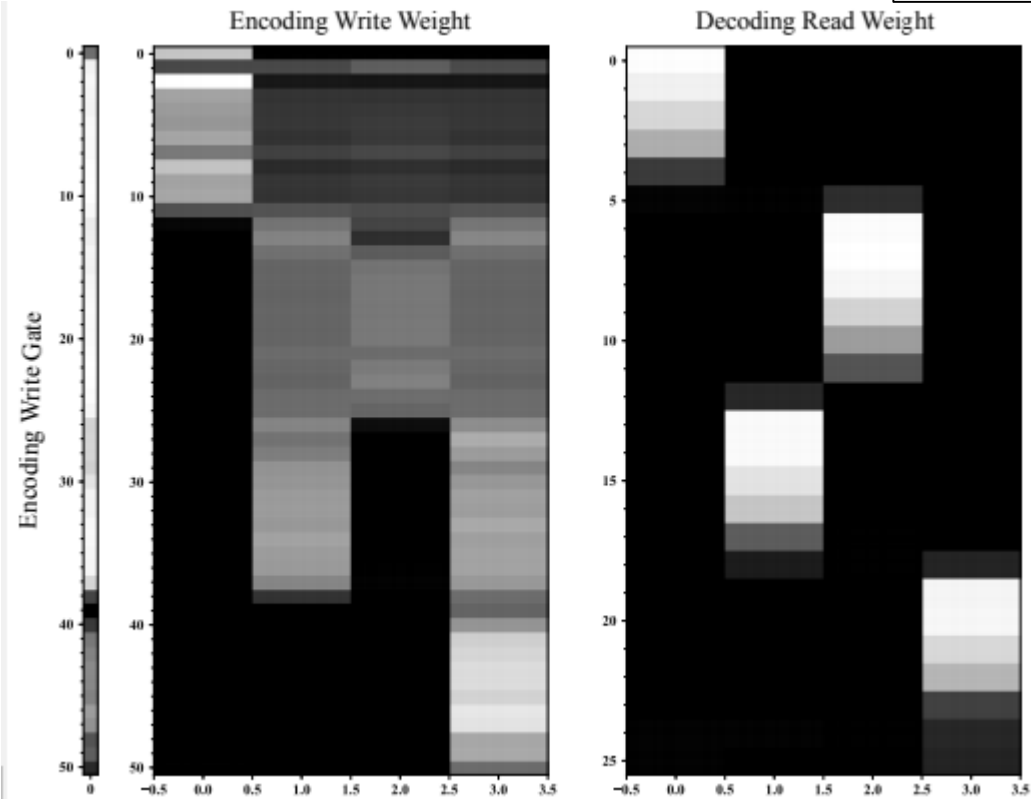
**Theorem 3.** Given  $D$  memory slots, a sequence with length  $T$ , a decay rate  $0 < \lambda \leq 1$ , then the optimal intervals  $\{l_i \in \mathbb{R}^+\}_{i=1}^{D+1}$  satisfying  $T = \sum_{i=1}^{D+1} l_i$  such that the lower bound on the average contribution  $I_\lambda = \frac{C}{T} \sum_{i=1}^{D+1} f_\lambda(l_i)$  is maximized are the following:

$$l_1 = l_2 = \dots = l_{D+1} = \frac{T}{D+1} \quad (7)$$

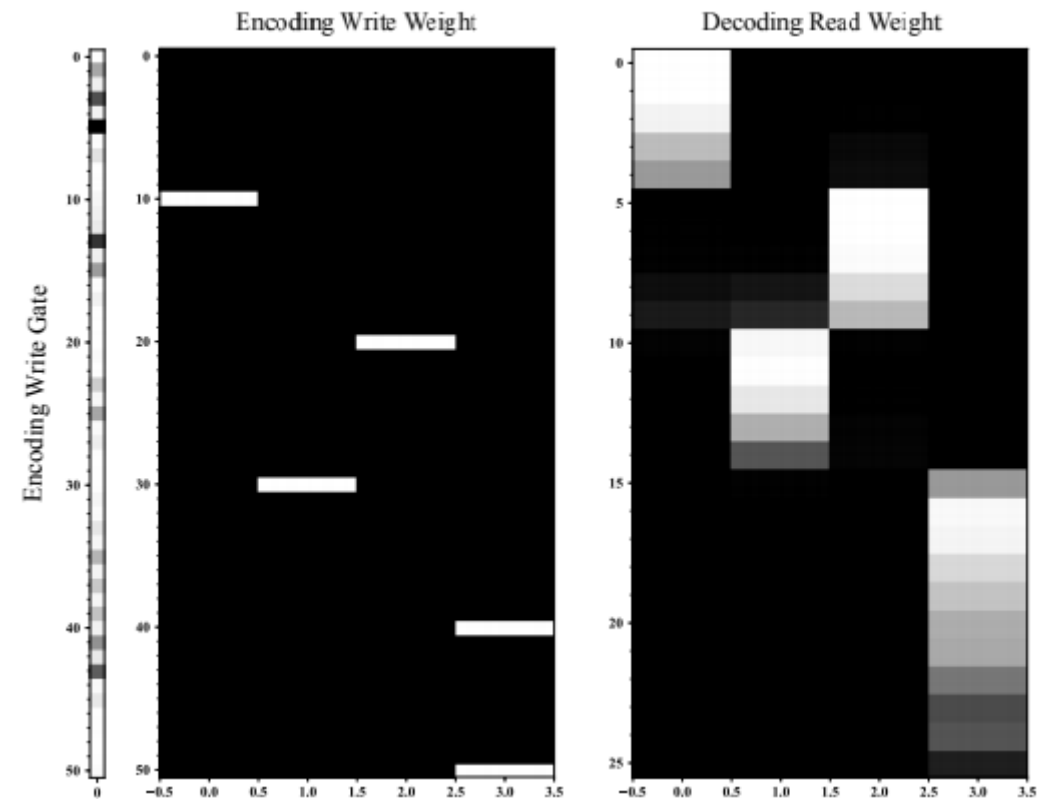
# Better memorization means better algorithmic reasoning

Max	$x_1 x_2 \dots x_T$	$\max(x_1, x_2) \max(x_3, x_4) \dots \max(x_{T-1}, x_T)$
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T=50, D=5



Regular



Uniform (cached)

# Memory of independent entities

Weston, Jason, Bordes, Antoine, Chopra, Sumit, and Mikolov, Tomas.  
Towards ai-complete question answering: A set of prerequisite toy tasks. CoRR, abs/1502.05698, 2015.

- Each slot store one or some entities
- Memory writing is done separately for each memory slot
- each slot maintains the life of one or more entities
- The memory is a set of N parallel RNNs

## Task 3: Three Supporting Facts

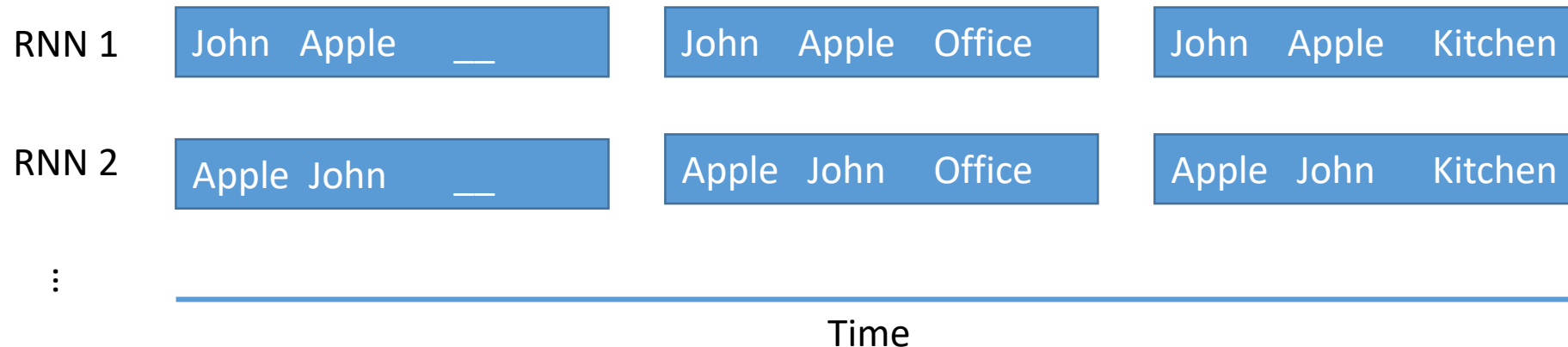
John picked up the apple.

John went to the office.

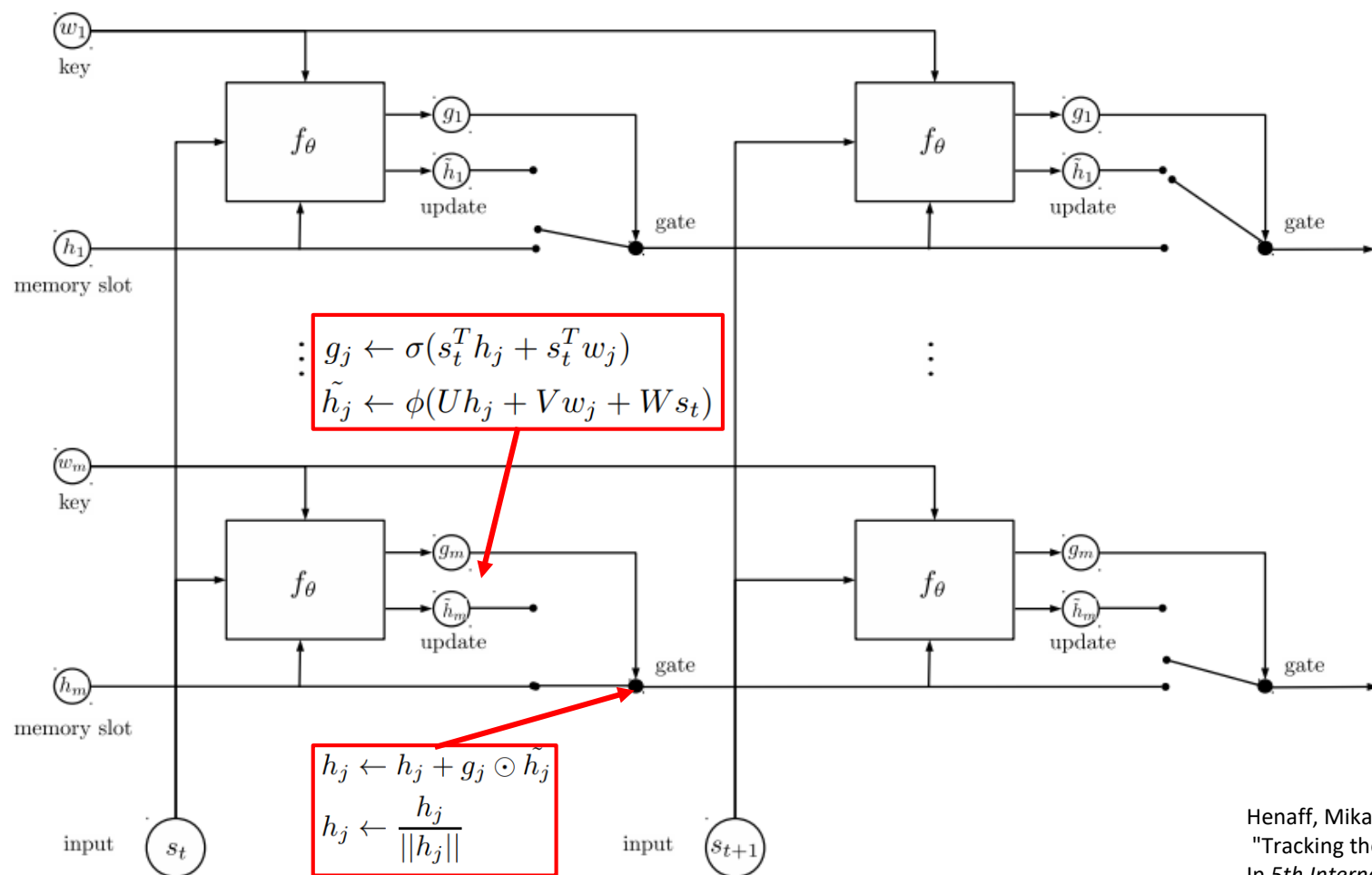
John went to the kitchen.

John dropped the apple.

Where was the apple before the kitchen? **A:office**



# Recurrent entity network



“Where is the ball?”

$$p_j = \text{Softmax}(q^T h_j)$$

$$u = \sum_j p_j h_j$$

$$y = R\phi(q + Hu)$$

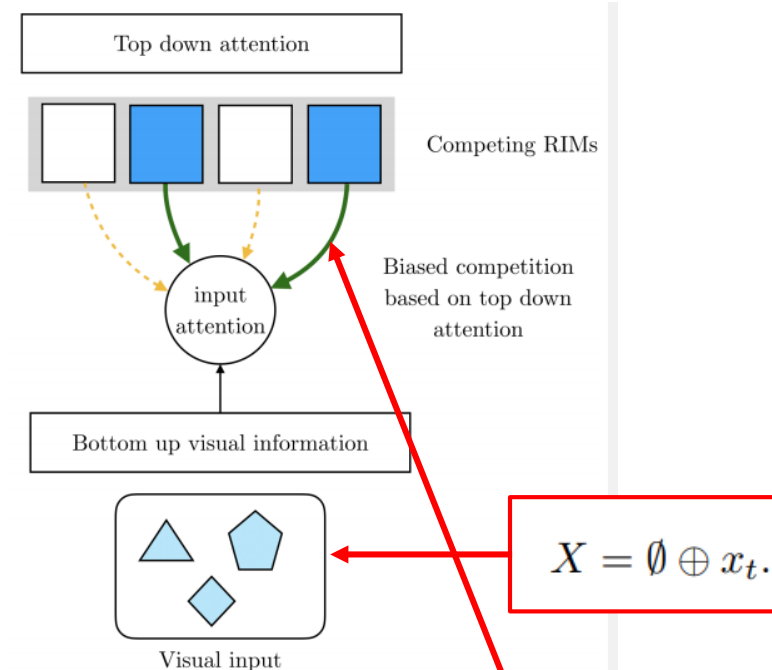
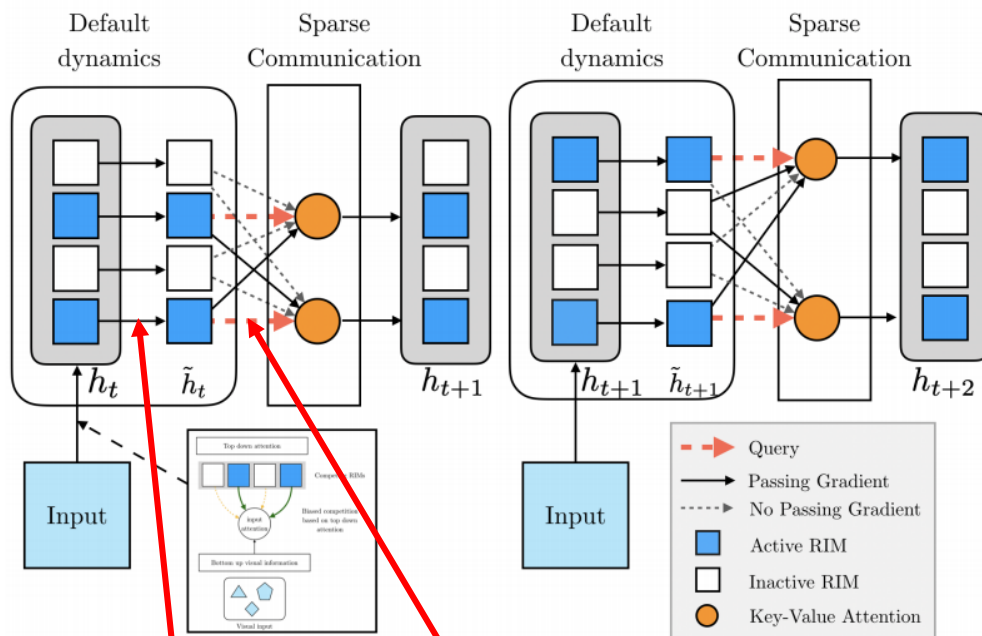
Garden

Mary picked up the ball.

Mary went to the garden.

Henaff, Mikael, Jason Weston, Arthur Szlam, Antoine Bordes, and Yann LeCun.  
 “Tracking the world state with recurrent entity networks.”  
 In *5th International Conference on Learning Representations, ICLR 2017*. 2017.

# Recurrent Independent Mechanisms



$$\tilde{h}_{t,k} = D_k(h_{t,k}) = LSTM(h_{t,k}, A_k^{(in)}; \theta_k^{(D)}) \quad \forall k \in \mathcal{S}_t$$

$$Q_{t,k} = \tilde{W}_k^q \tilde{h}_{t,k}, \forall k \in \mathcal{S}_t \quad K_{t,k} = \tilde{W}_k^e \tilde{h}_{t,k}, \forall k \quad V_{t,k} = \tilde{W}_k^v \tilde{h}_{t,k}, \forall k$$

$$h_{t+1,k} = \text{softmax} \left( \frac{Q_{t,k} (K_{t,:})^T}{\sqrt{d_e}} \right) V_{t,:} + \tilde{h}_{t,k} \quad \forall k \in \mathcal{S}_t.$$

$$A_k^{(in)} = \text{softmax} \left( \frac{h_t W_k^q (X W^e)^T}{\sqrt{d_e}} \right) X W^v,$$

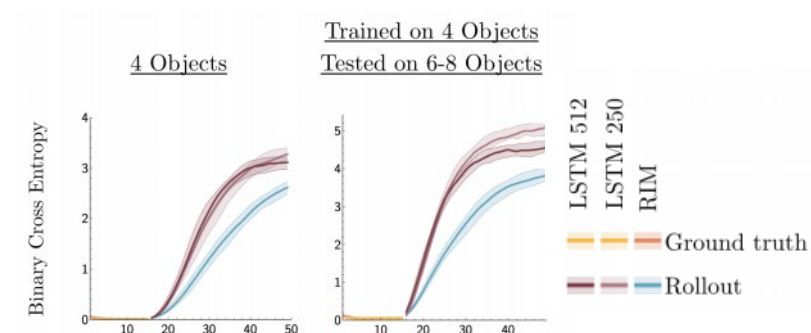
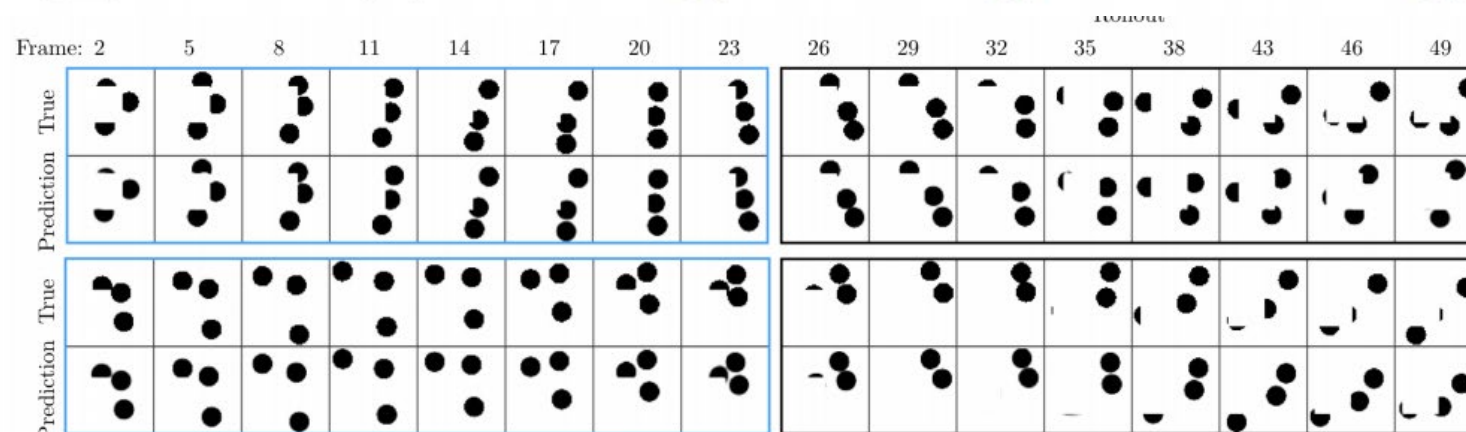
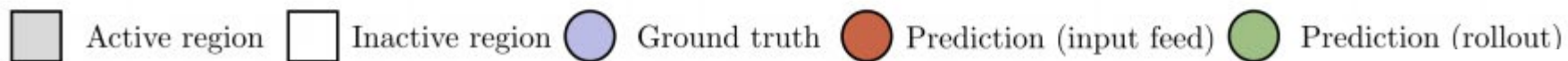
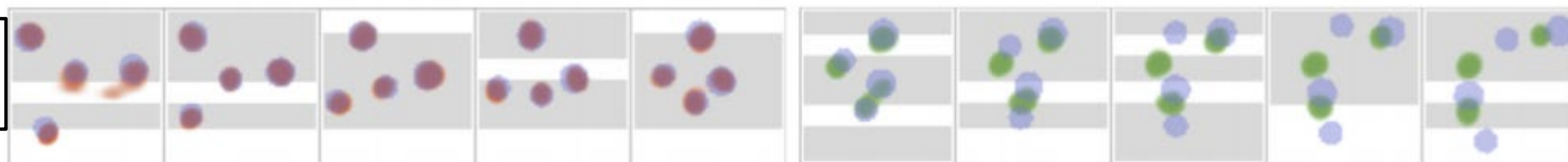
# Reasoning with independent dynamics

Copying	$k_T$	$k_A$	$h_{\text{size}}$	Train(50)	Test(200)
				CE	CE
<b>RIMs</b>	6	4	600	<b>0.00</b>	<b>0.00</b>
	6	3	600	<b>0.00</b>	<b>0.00</b>
	6	2	600	<b>0.00</b>	<b>0.00</b>
	5	2	500	<b>0.00</b>	<b>0.00</b>
<b>LSTM</b>	-	-	300	0.00	4.32
	-	-	600	0.00	3.56
<b>NTM</b>	-	-	-	0.00	2.54
<b>RMC</b>	-	-	-	0.00	0.13
<b>Transformers</b>	-	-	-	0.00	0.54

Copy



Ball dynamics

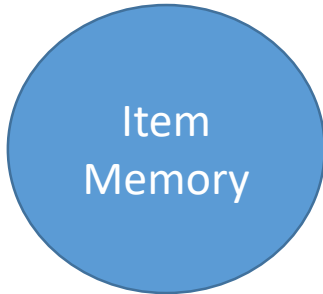


# Relational memory

Graph memory

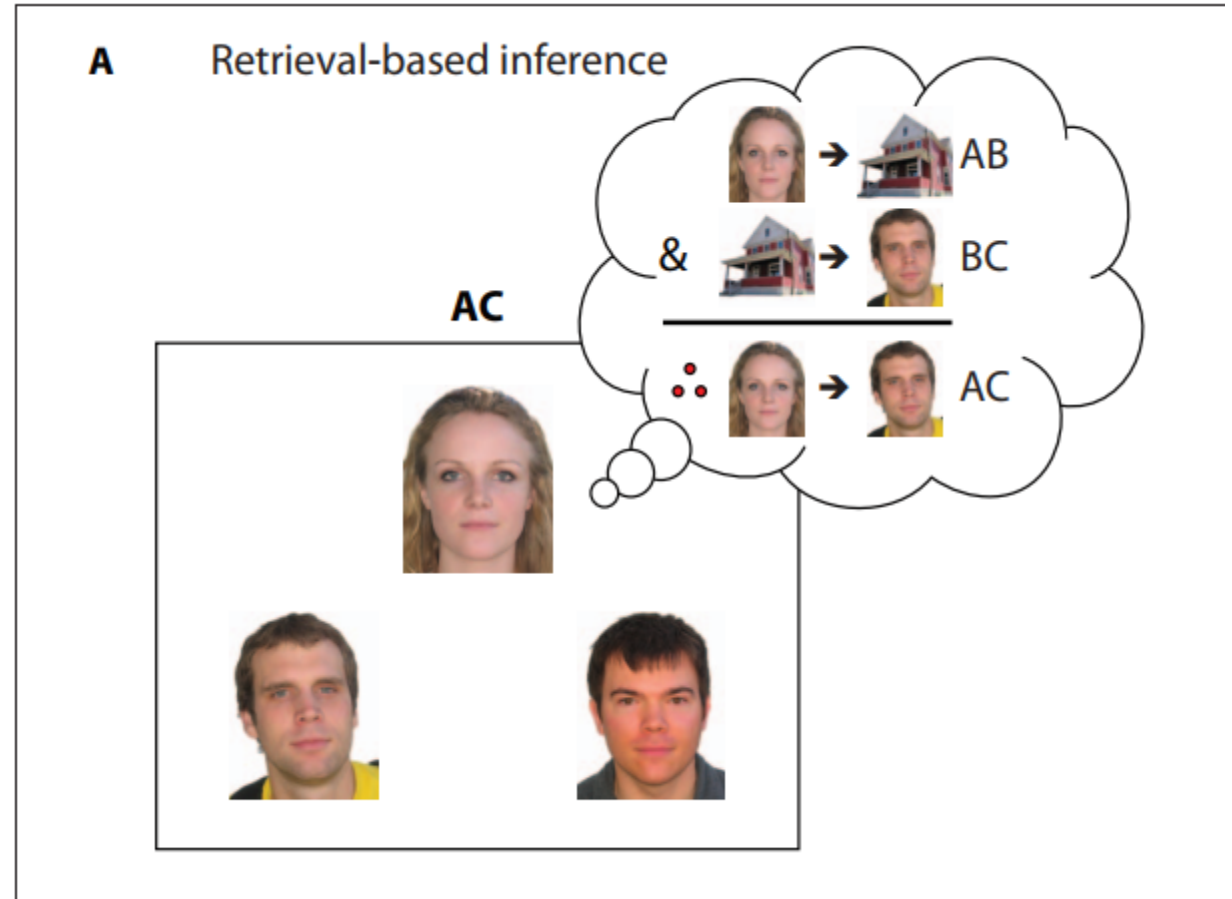
Tensor memory

# Why relational memory? Item memory is weak at recognizing relationships



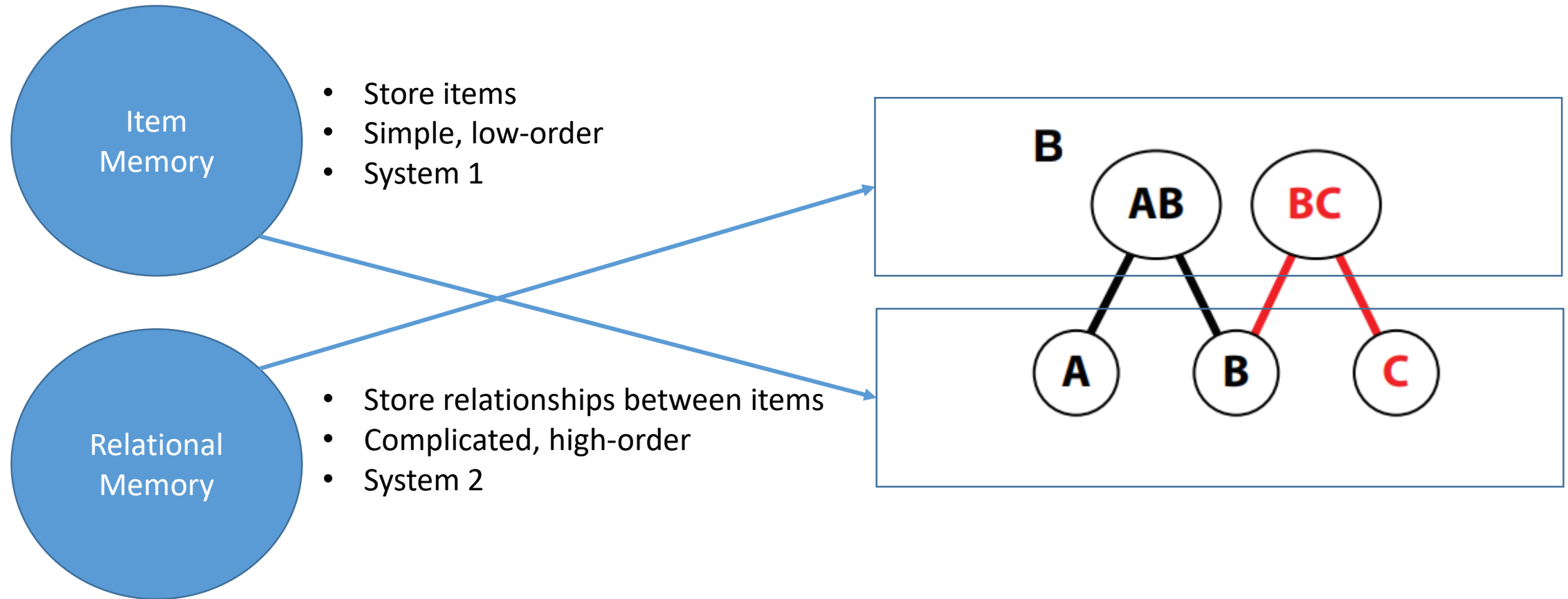
- Store and retrieve individual items
- Relate pair of items of the same time step
- Fail to relate temporally distant items

$$\hat{\mathbf{M}} = \sum_{k=1}^q \mathbf{b}_k \mathbf{a}_k^T$$





# Dual process in memory

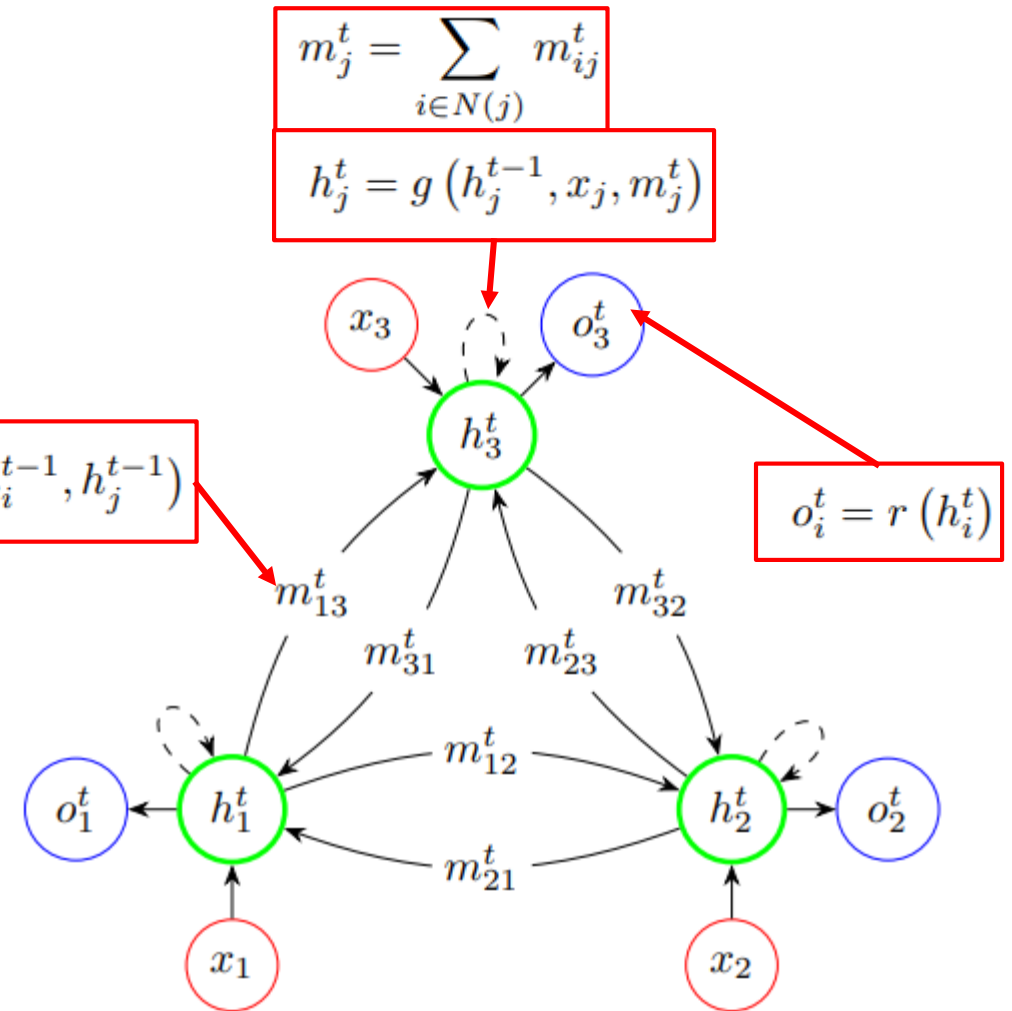


Howard Eichenbaum, *Memory, amnesia, and the hippocampal system* (MIT press, 1993).

Alex Konkelt and Neal J Cohen, "Relational memory and the hippocampus: representations and methods", *Frontiers in neuroscience* 3 (2009).

# Memory as graph

- Memory is a static graph with fixed nodes and edges
- Relationship is somehow known
- Each memory node stores the state of the graph's node
- Write to node via message passing
- Read from node via MLP



# bAbI

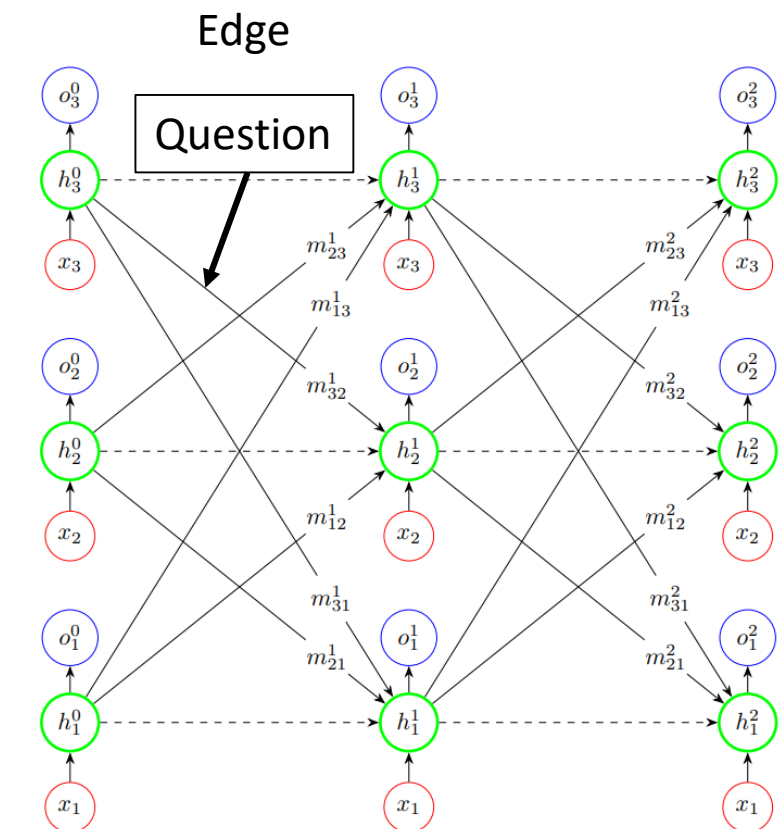
$$x_i = \text{MLP}(\text{concat}(\text{last}(\text{LSTM}_S(s_i)), \text{last}(\text{LSTM}_Q(q)), \text{onehot}(p_i + o)))$$

Node

Fact 1

Fact 2

Fact 3



$$o^t = r(\sum_i h_i^t)$$

Answer

$$m_{ij}^t = f(h_i^{t-1}, h_j^{t-1}, e_{ij})$$

Method	N	Mean Error (%)	Failed tasks (err. >5%)
RRN* (this work)	15	<b>0.46 ± 0.77</b>	<b>0.13 ± 0.35</b>

# CLEVER

$$o_i = \text{concat}(p_i, \text{onehot}(c_i), \text{onehot}(m_i))$$

$$q = \text{concat}(\text{onehot}(s), \text{onehot}(n))$$

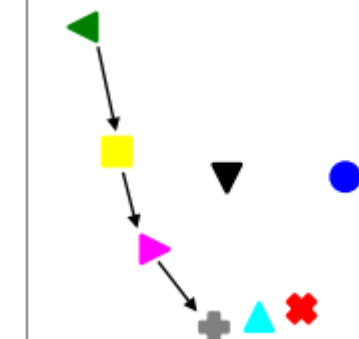
$$x_i = \text{MLP}(\text{concat}(o_i, q))$$

Node

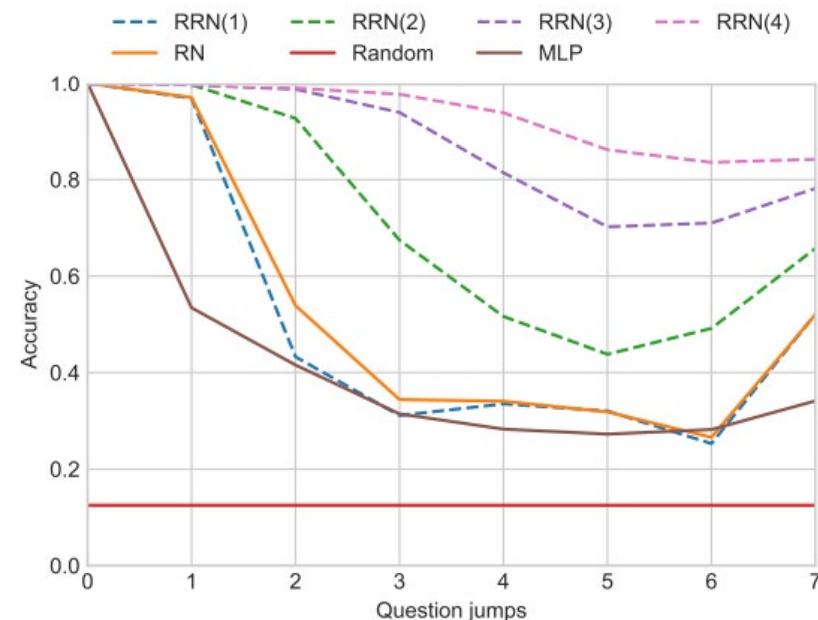
(colour, shape, position)

Edge

(distance)

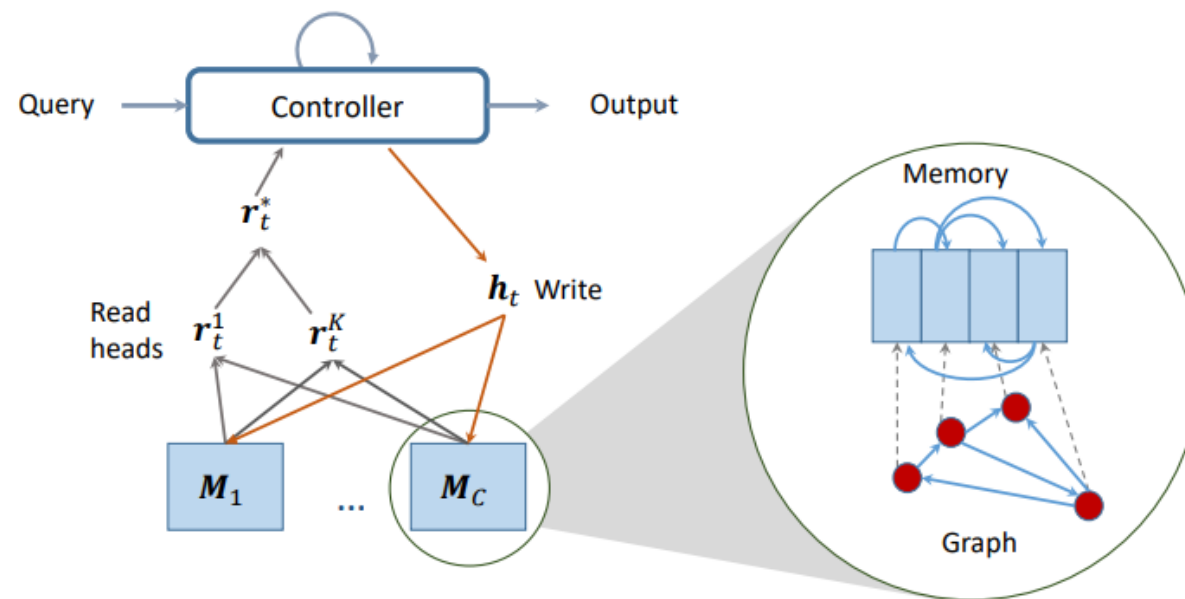


solution to the question: "green, 3 jumps", which is "plus",



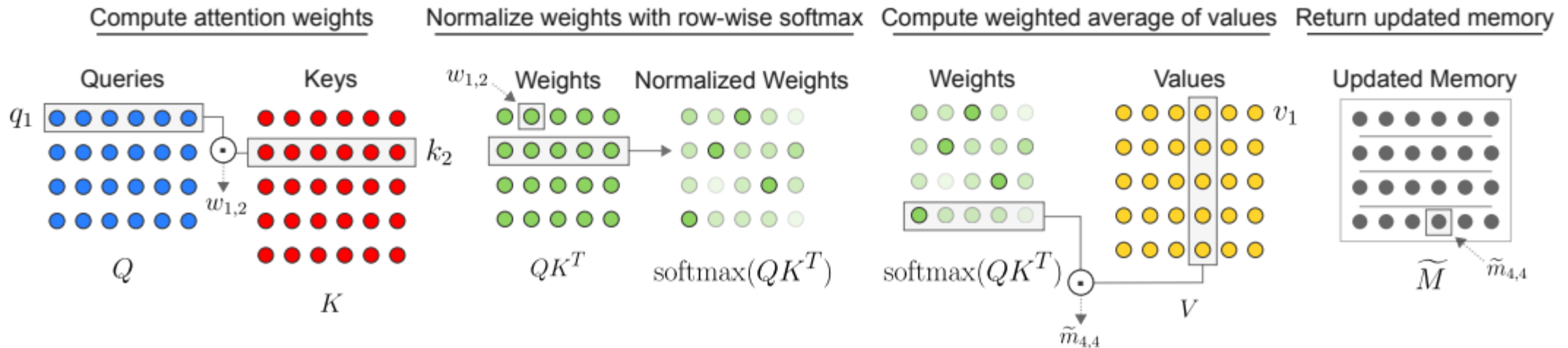
# Memory of graphs access conditioned on query

- Encode multiple graphs, each graph is stored in a set of memory row
- For each graph, the controller read/write to the memory:
  - Read uses content-based attention
  - Write use message passing
- Aggregate read vectors from all graphs to create output

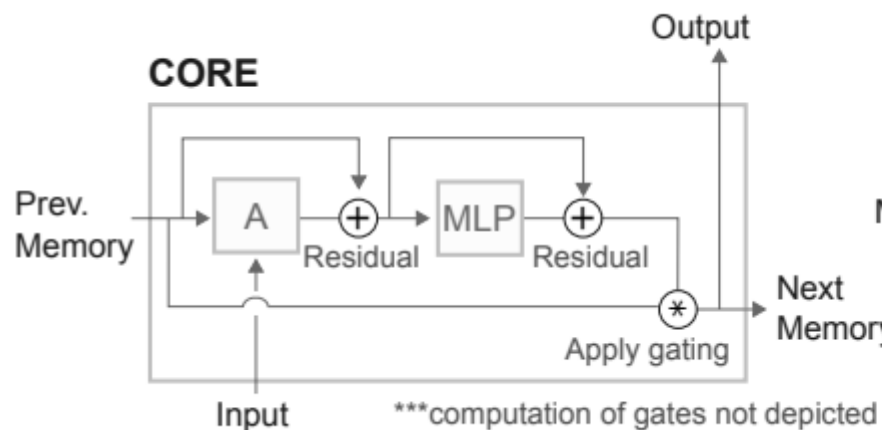


# Capturing relationship can be done via memory slot interactions using attention

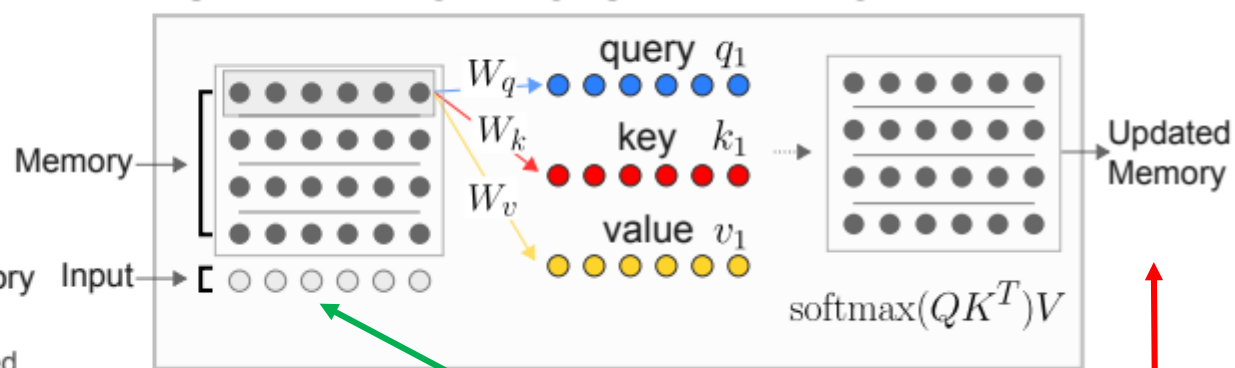
- Graph memory needs customization to an explicit design of nodes and edges
- Can we automatically learn structure with a 2d tensor memory?
- Capture relationship: each slot interacts with all other slots (self-attention)



# Relational Memory Core (RMC) operation



## MULTI-HEAD DOT PRODUCT ATTENTION



$$s_{i,t} = (h_{i,t-1}, m_{i,t-1})$$

$$f_{i,t} = W^f x_t + U^f h_{i,t-1} + b^f$$

$$i_{i,t} = W^i x_t + U^i h_{i,t-1} + b^i$$

$$o_{i,t} = W^o x_t + U^o h_{i,t-1} + b^o$$

$$m_{i,t} = \sigma(f_{i,t} + \tilde{b}^f) \circ m_{i,t-1} + \sigma(i_{i,t}) \circ \underbrace{g_\psi(\tilde{m}_{i,t})}_{\text{row/memory-wise MLP with layer normalisation}}$$

$$h_{i,t} = \sigma(o_{i,t}) \circ \tanh(m_{i,t})$$

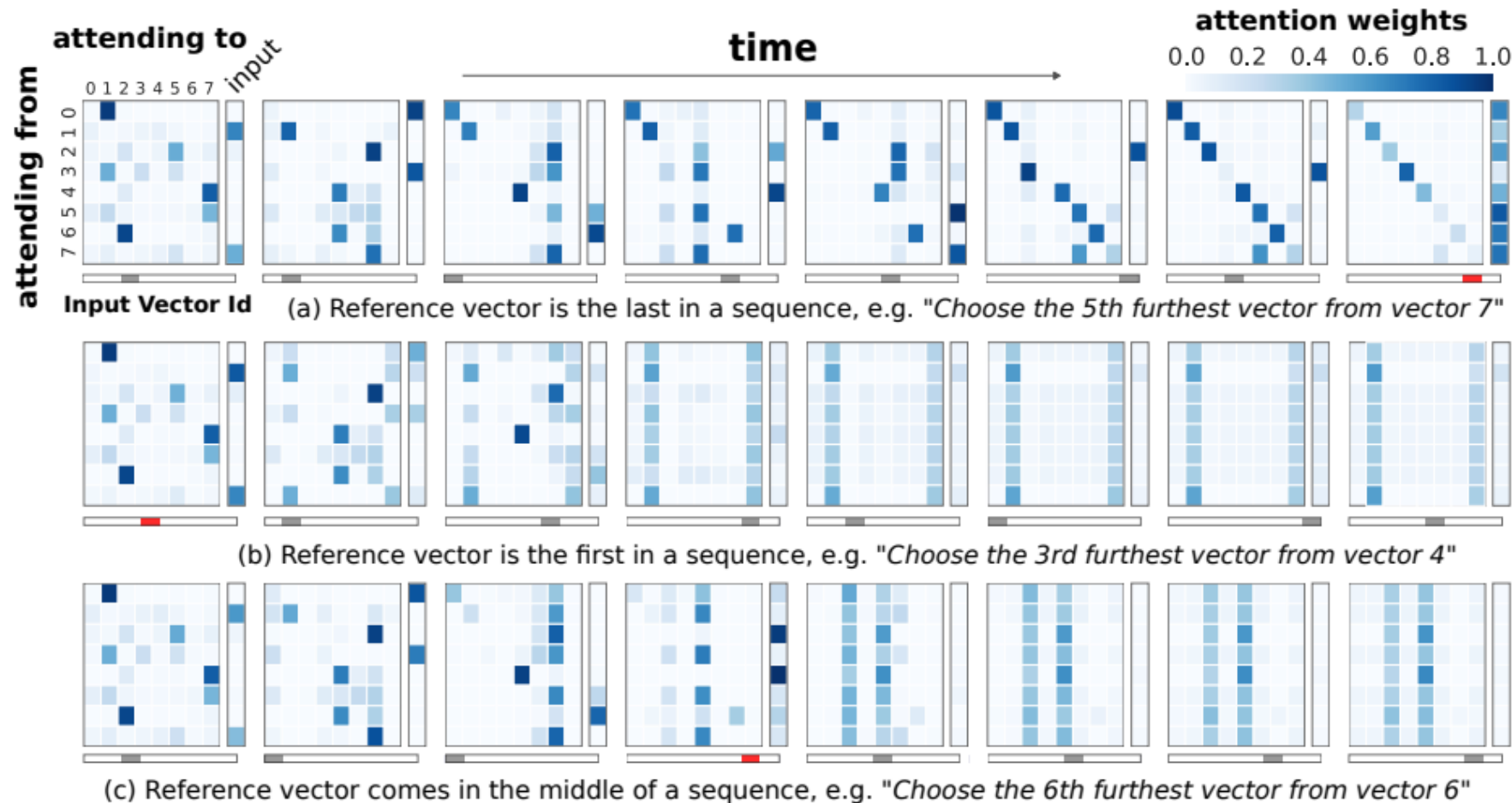
row/memory-wise MLP with layer normalisation

$$s_{i,t+1} = (m_{i,t}, h_{i,t})$$

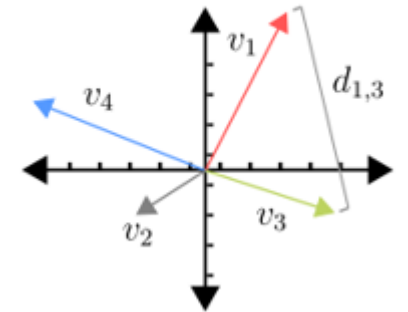
$$\tilde{M} = \text{softmax} \left( \frac{MW^q ([M; x] W^k)^T}{\sqrt{d^k}} \right) [M; x] W^v,$$

RNN-like  
Interface

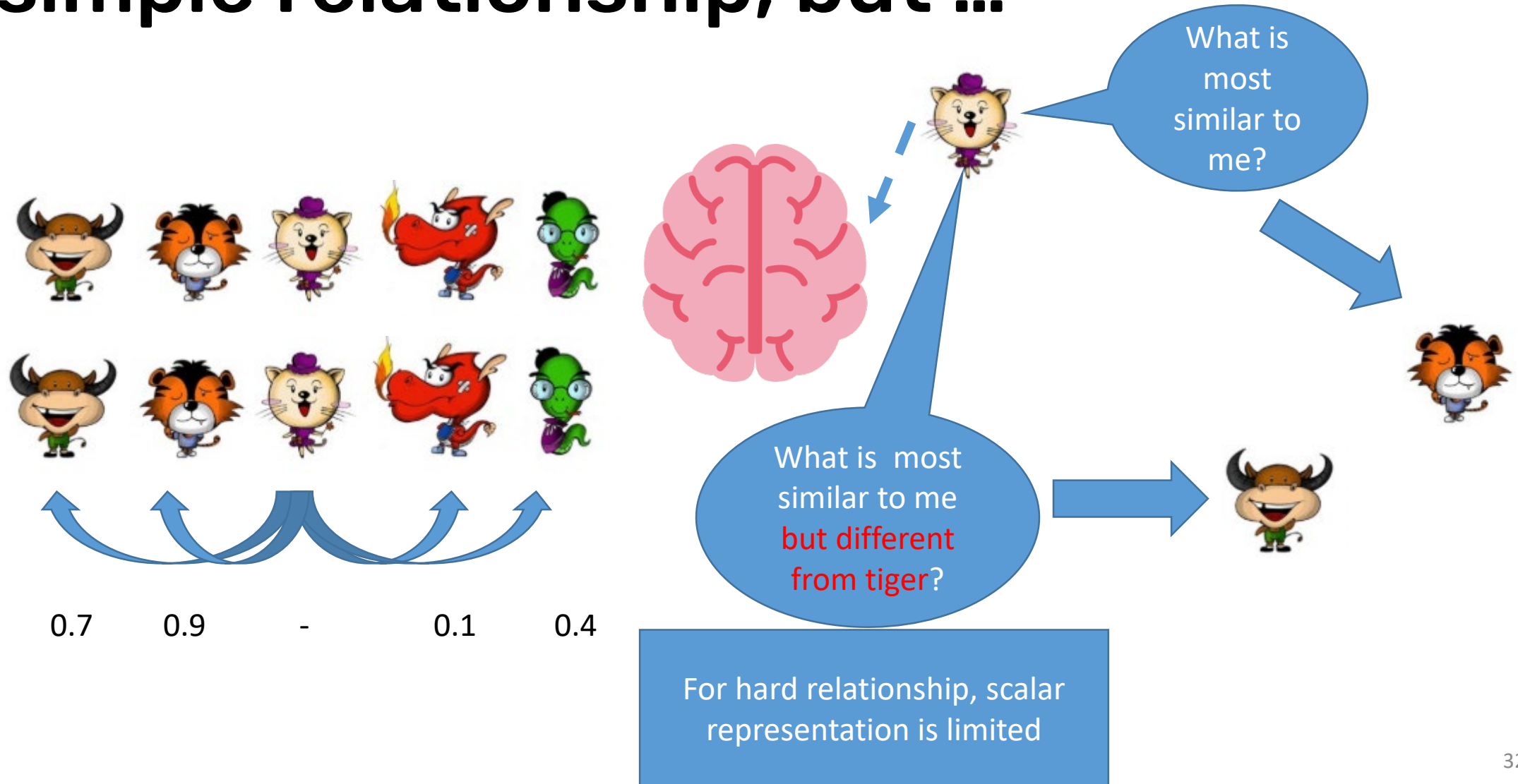
# Allowing pair-wise interactions can answer questions on temporal relationship



What is the  $N^{th}$  furthest from vector  $m$ ?

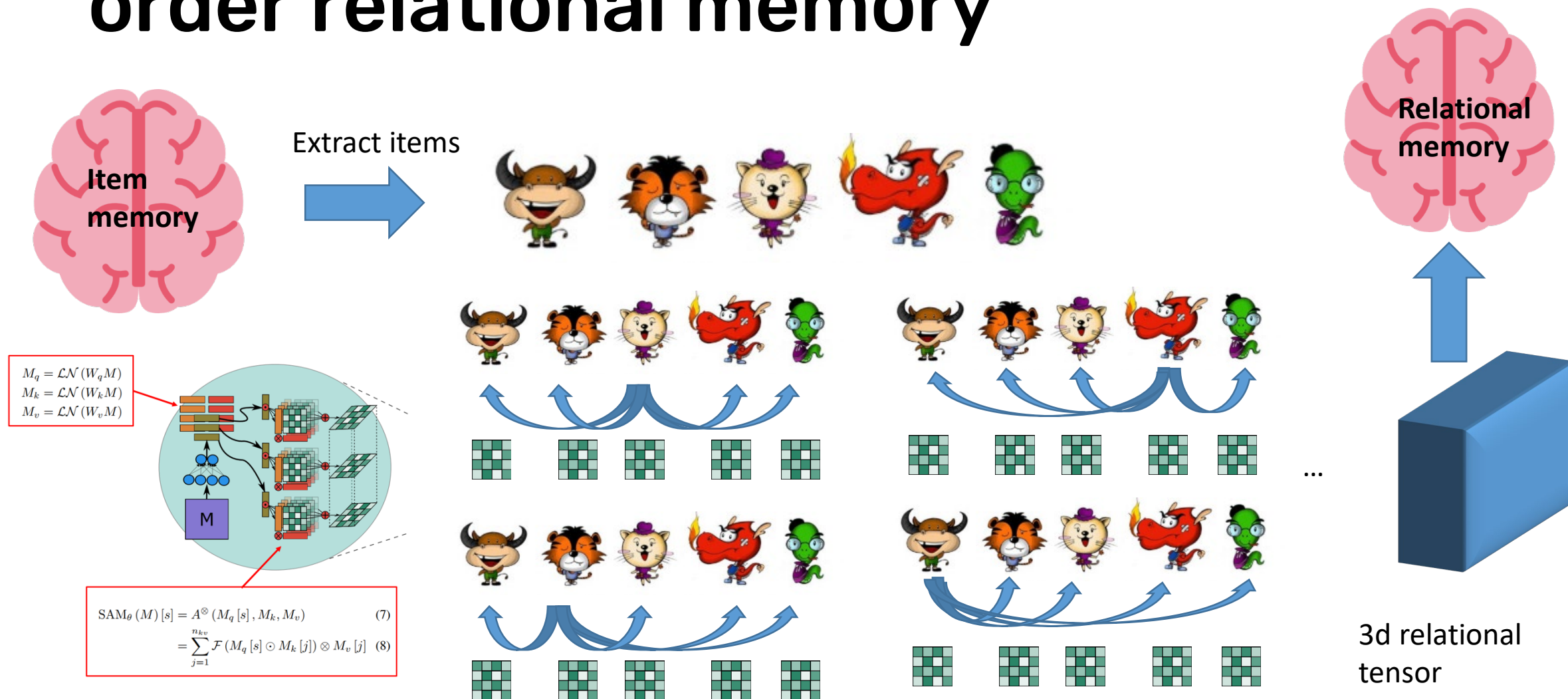


# Dot product attention works for simple relationship, but ...





# Complicated relationship needs high-order relational memory



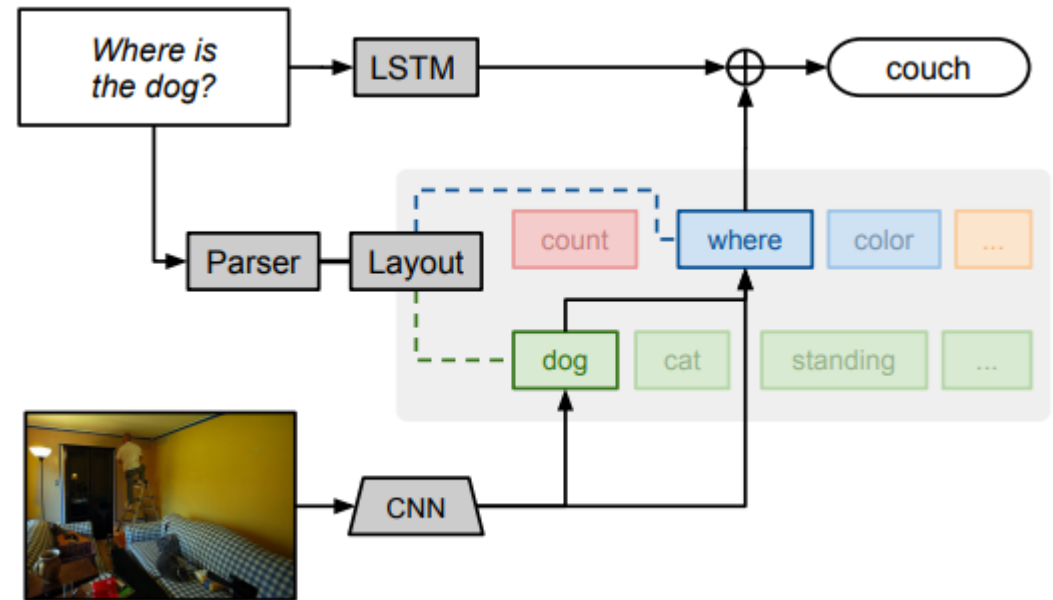
# Program memory

Module memory

Stored-program memory

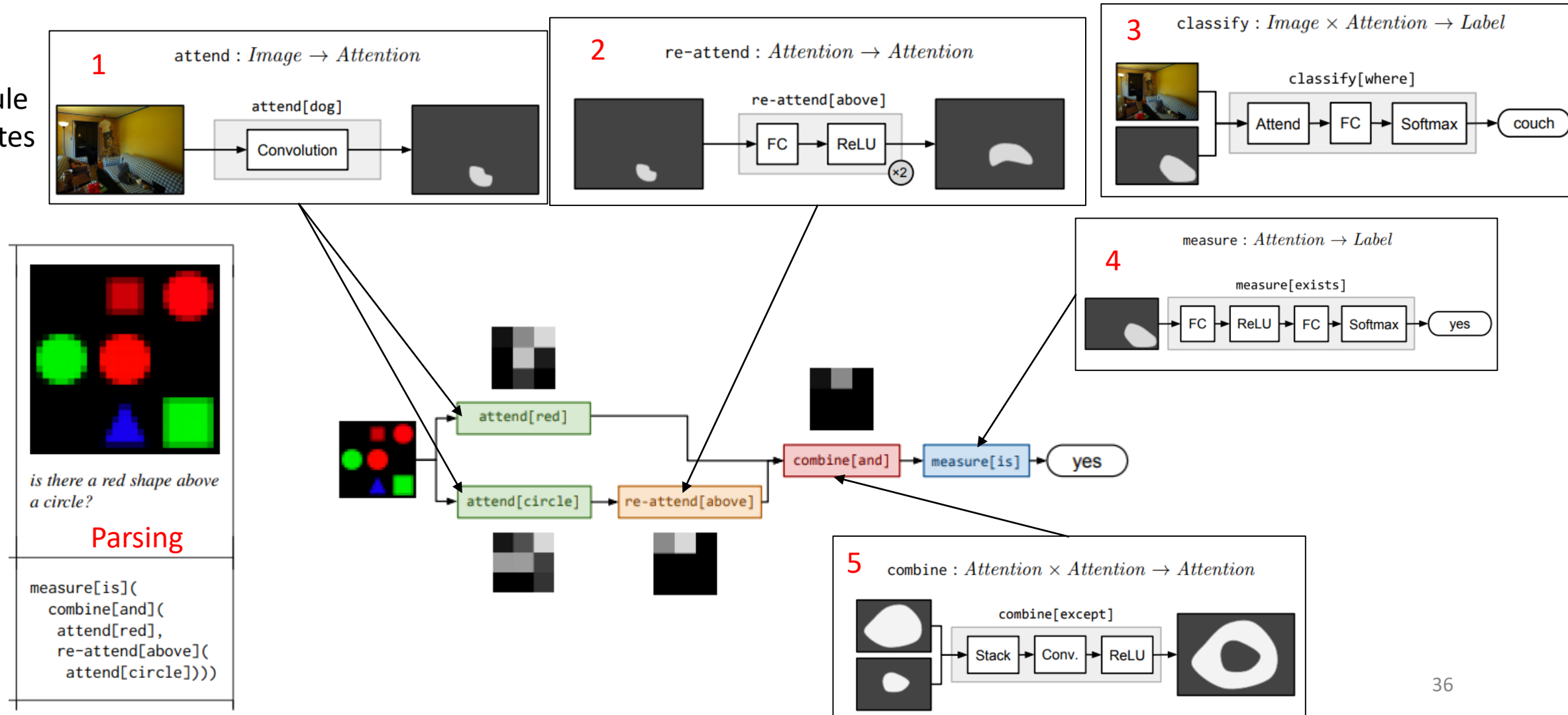
# Predefining program for subtask

- A program designed for a task becomes a module
- Parse a question to module layout (order of program execution)
- Learn the weight of each module to master the task



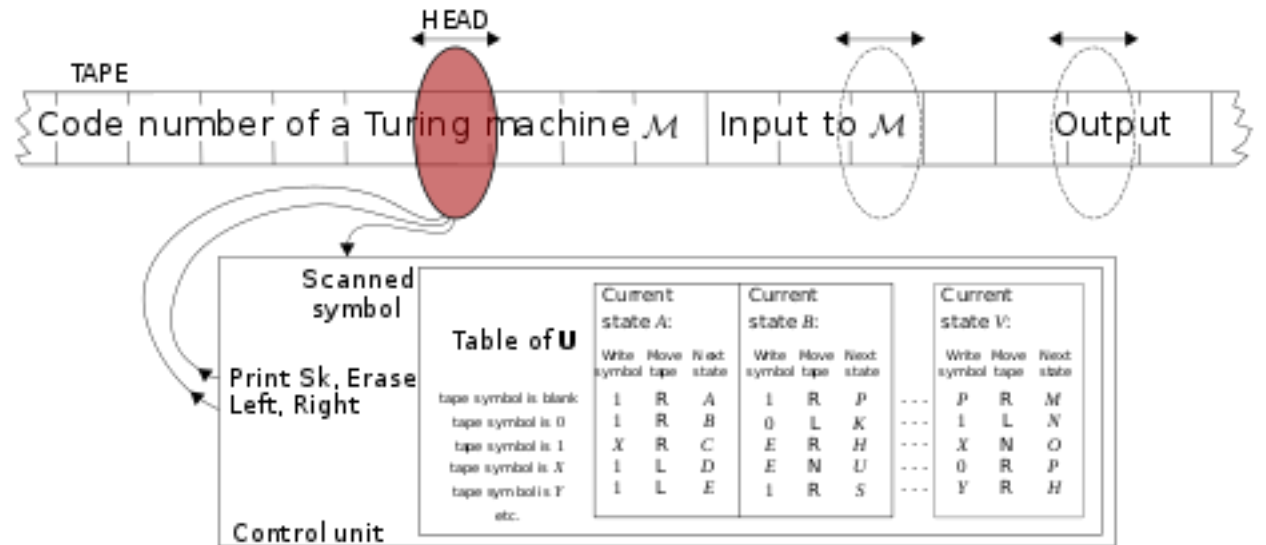
# Program selection is based on parser, others are end2end trained

5 module templates



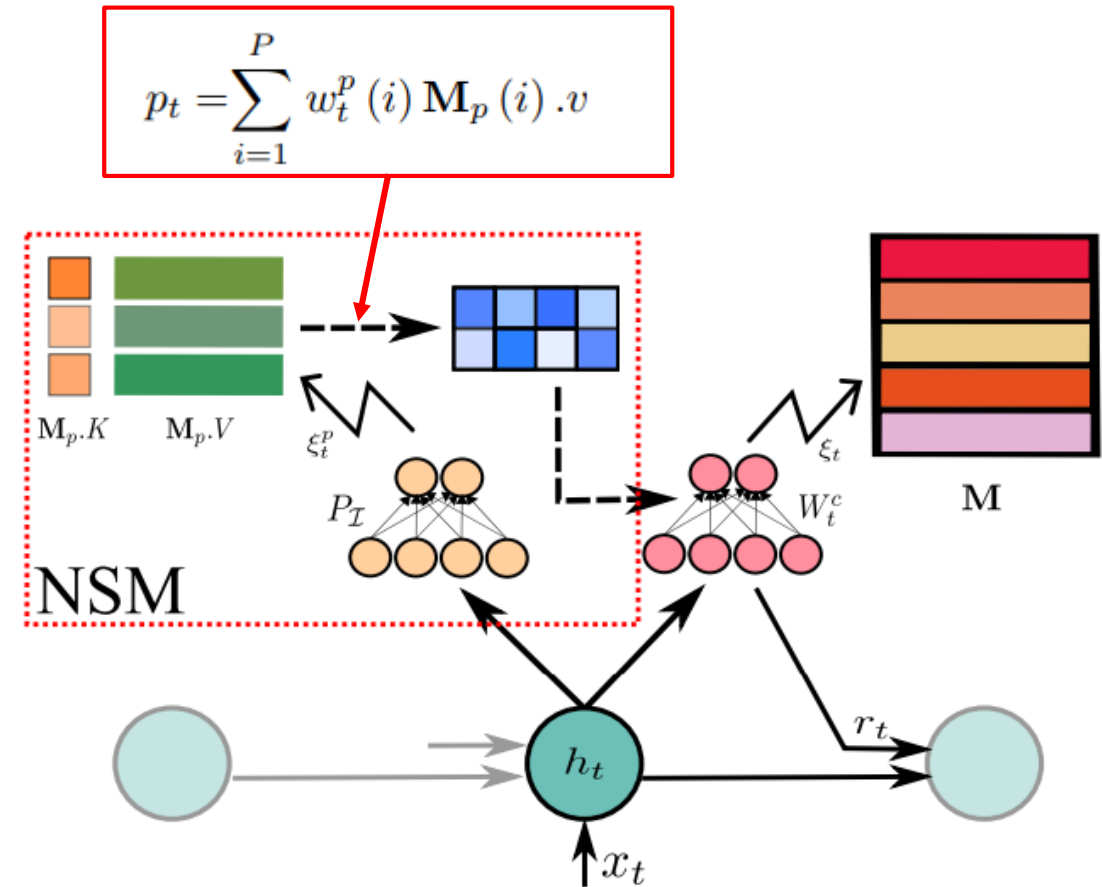
# The most powerful memory is one that stores both program and data

- Computer architecture:  
Universal Turing  
Machines/Harvard/VNM
- Stored-program principle
- Break a big task into subtasks,  
each can be handled by a  
TM/single purposed program  
stored in a program memory



# NUTM: Learn to select program (neural weight) via program attention

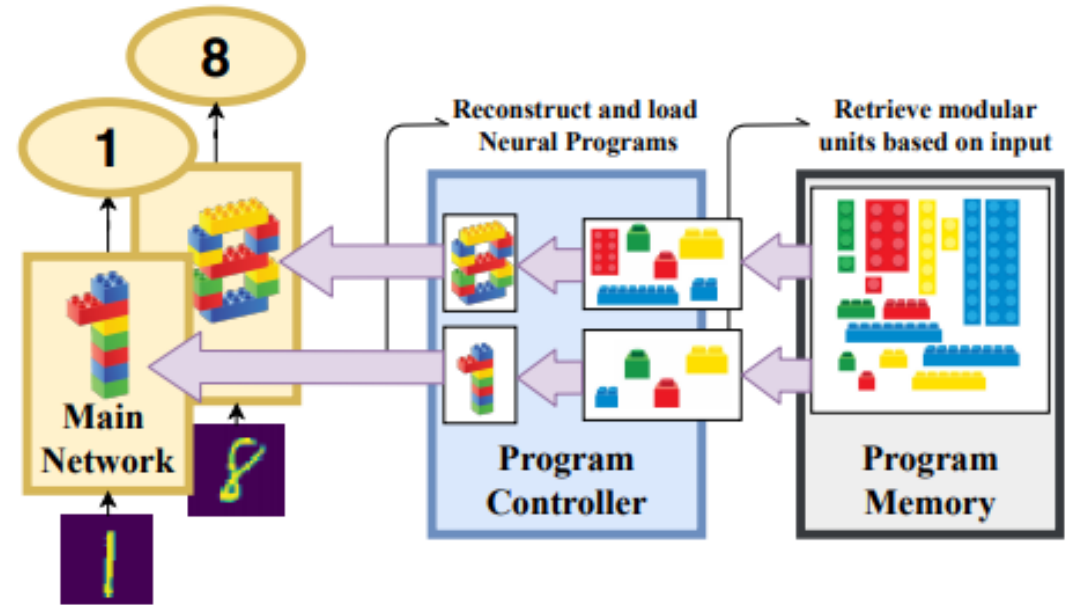
- Neural stored-program memory (NSM) stores key (the address) and values (the weight)
- The weight is selected and loaded to the controller of NTM
- The stored NTM weights and the weight of the NUTM is learnt end-to-end by backpropagation



Le, Hung, Truyen Tran, and Svetha Venkatesh. "Neural Stored-program Memory." In *International Conference on Learning Representations*. 2019.

# Scaling with memory of mini-programs

- Prior, 1 program = 1 neural network (millions of parameters)
- Parameter inefficiency since the programs do not share common parameters
- Solution: store sharable mini-programs to compose infinite number of programs

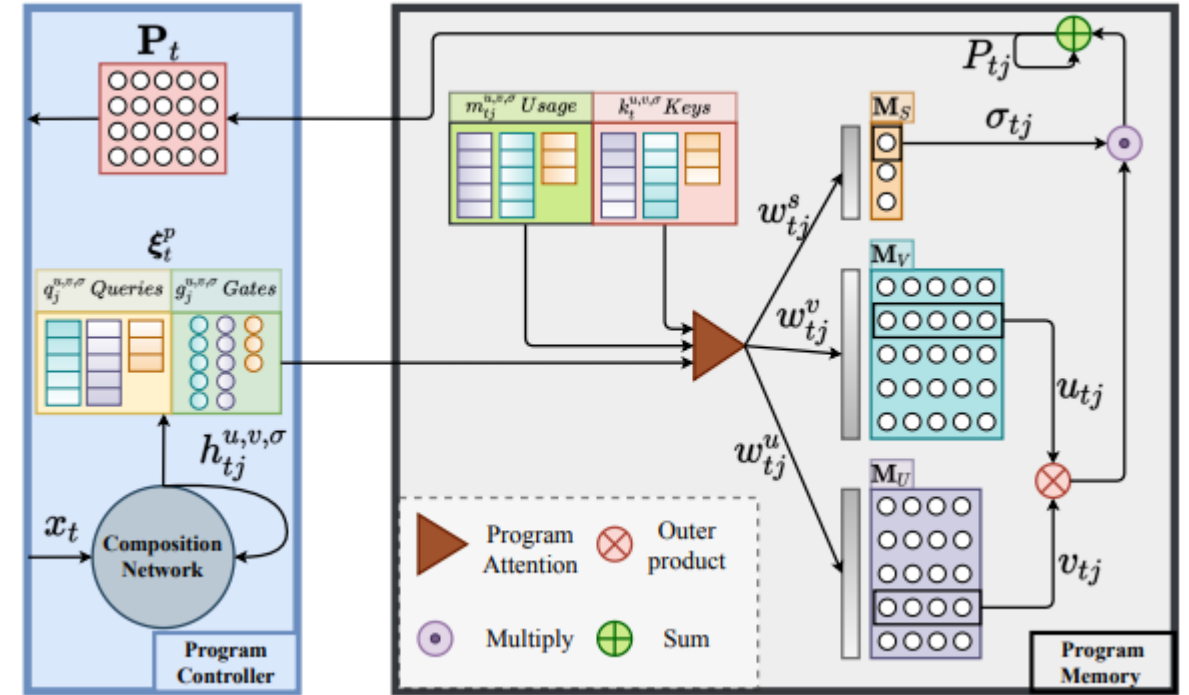


it is analogous to building Lego structures corresponding to inputs from basic Lego bricks.

# Recurrent program attention to retrieve singular components of a program

$$\begin{aligned} \mathbf{P}_t &= \mathbf{U}\mathbf{S}\mathbf{V}^T \\ &= \sum_n^{r_m} \sigma_{tn} u_{tn} v_{tn}^T \\ u_{tn} &= \sum_{i=1}^{P_u} w_{tin}^u \mathbf{M}_U(i) \\ v_{tn} &= \sum_{i=1}^{P_v} w_{tin}^v \mathbf{M}_V(i) \end{aligned}$$

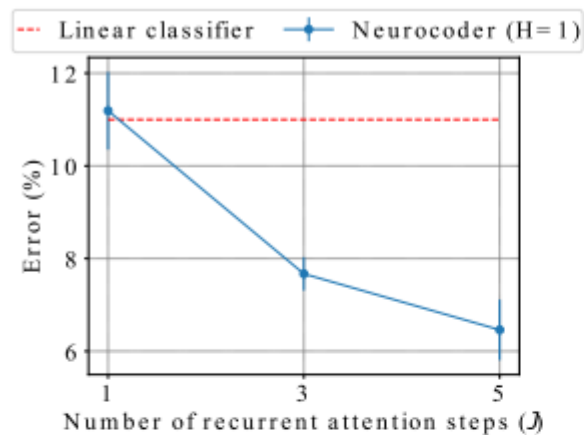
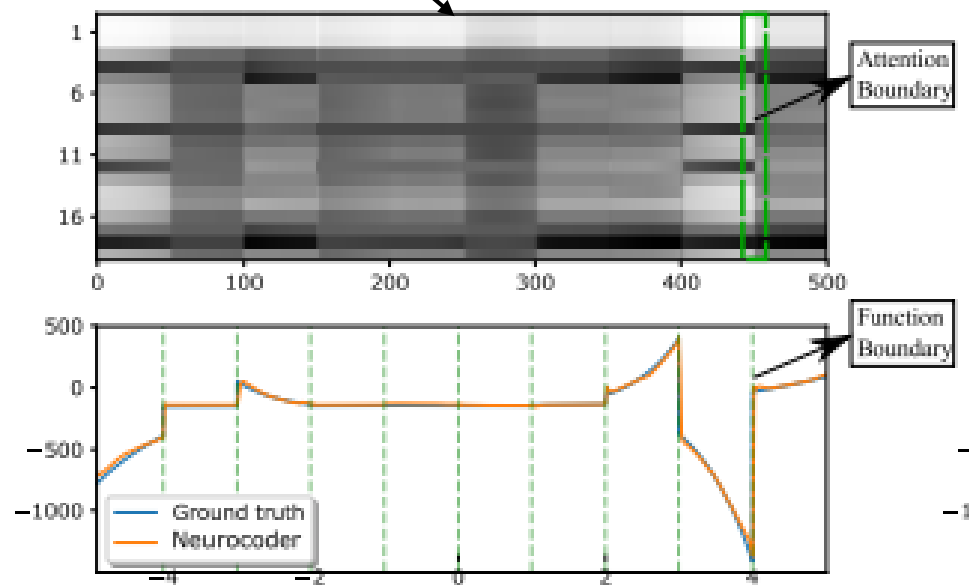
$$\sigma_{tn} = \begin{cases} \text{softplus} \left( \sum_{i=1}^{P_s} w_{tin}^\sigma \mathbf{M}_S(i) \right) & n = r_m \\ \sigma_{tn+1} + \text{softplus} \left( \sum_{i=1}^{P_s} w_{tin}^\sigma \mathbf{M}_S(i) \right) & n < r_m \end{cases}$$



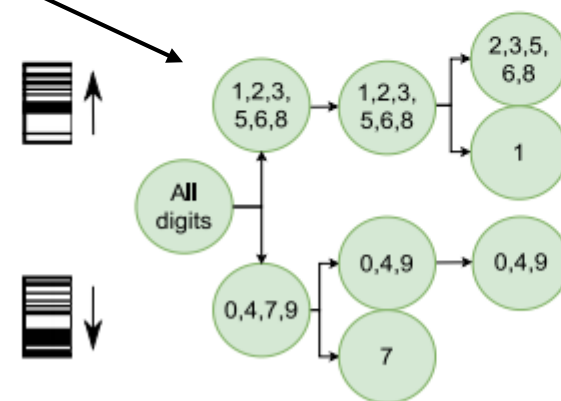


Program attention is equivalent to binary decision tree reasoning

Recurrent program attention auto detects task boundary

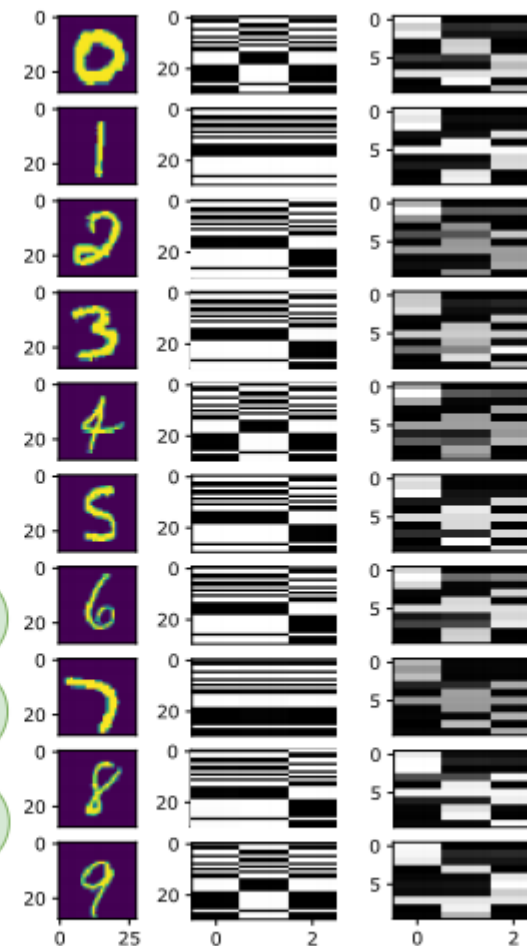


(a)



(c)

(d)

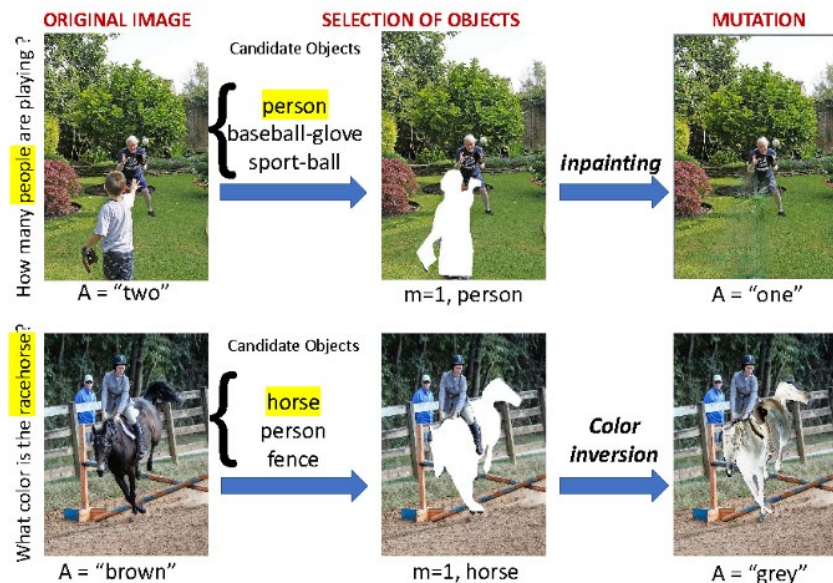


(b)

# Agenda

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  - Memory of entities – memory-augmented neural networks
  - Memory of relations with tensors and graphs
  - Memory of programs & neural program construction.
- **Learning to reason with less labels:**
  - Data augmentation with analogical and counterfactual examples
  - Question generation
  - Self-supervised learning for question answering
  - Learning with external knowledge graphs
- Recursive reasoning with neural theory of mind.

# Data Augmentation with Analogical and Counterfactual Examples



Visual counterfactual example

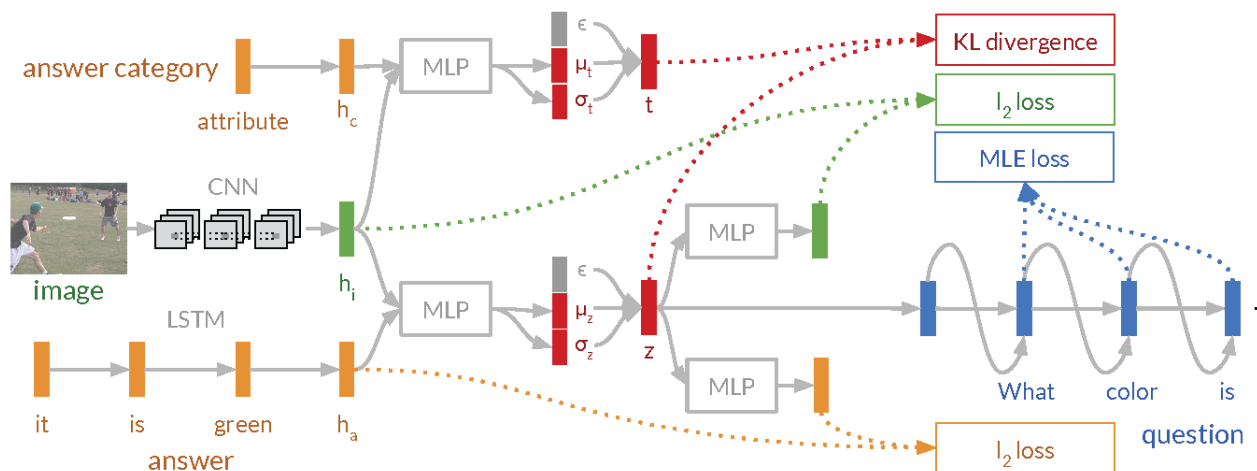
- **Poor generalization** when training under independent and identically distributed assumption.
- **Intuition:** augmenting counterfactual samples to allow machines to understand the critical changes in the input that lead to changes in the answer space.
  - Perceptually similar, yet
  - Semantically dissimilar realistic samples



Mutation Type	Question	Answer
Original	Is the lady holding the baby?	Yes
Substitution (Negation)	Is the lady not holding the baby?	No
Substitution (Adversarial)	Is the cat holding the baby?	No
Original	How many people are there?	Three
Deletion (Masking)	How many [MASK] are there?	"Number"
Original	What is the color of the man's shirt?	Blue
Substitution (Negation)	What is not the color of the man's shirt?	Magenta
Deletion (Masking)	Is the [MASK] holding the baby?	Can't say
Original	What color is the umbrella ?	Pink
Deletion (Masking)	What color is the [MASK]?	"color"

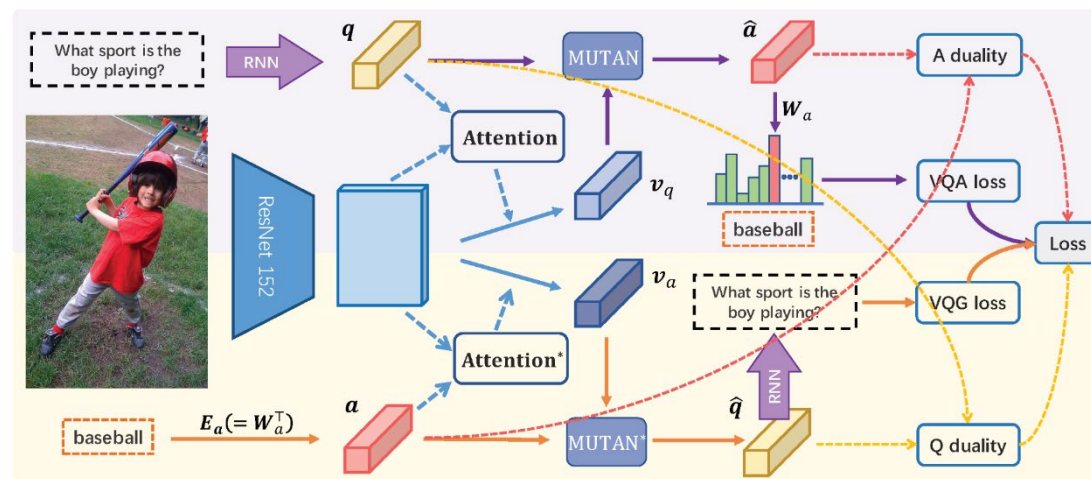
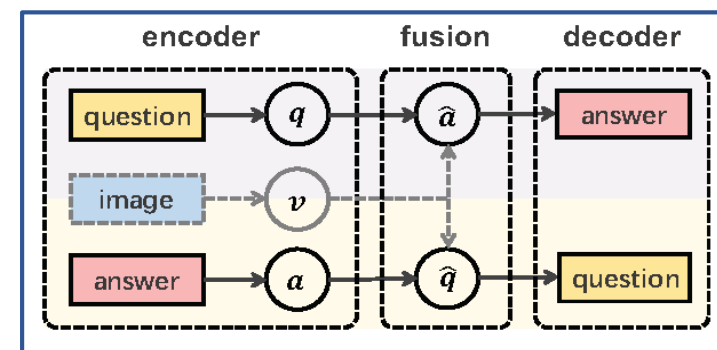
Gokhale, Tejas, et al. "Mutant: A training paradigm for out-of-distribution generalization in visual question answering." *EMNLP'20*.

# Question Generations



Krishna, Ranjay, Michael Bernstein, and Li Fei-Fei. "Information maximizing visual question generation." *CVPR*'19.

- Question answering is a zero-shot learning problem. Question generation helps cover a wider range of concepts.
- Question generation can be done with either supervised and unsupervised learning.

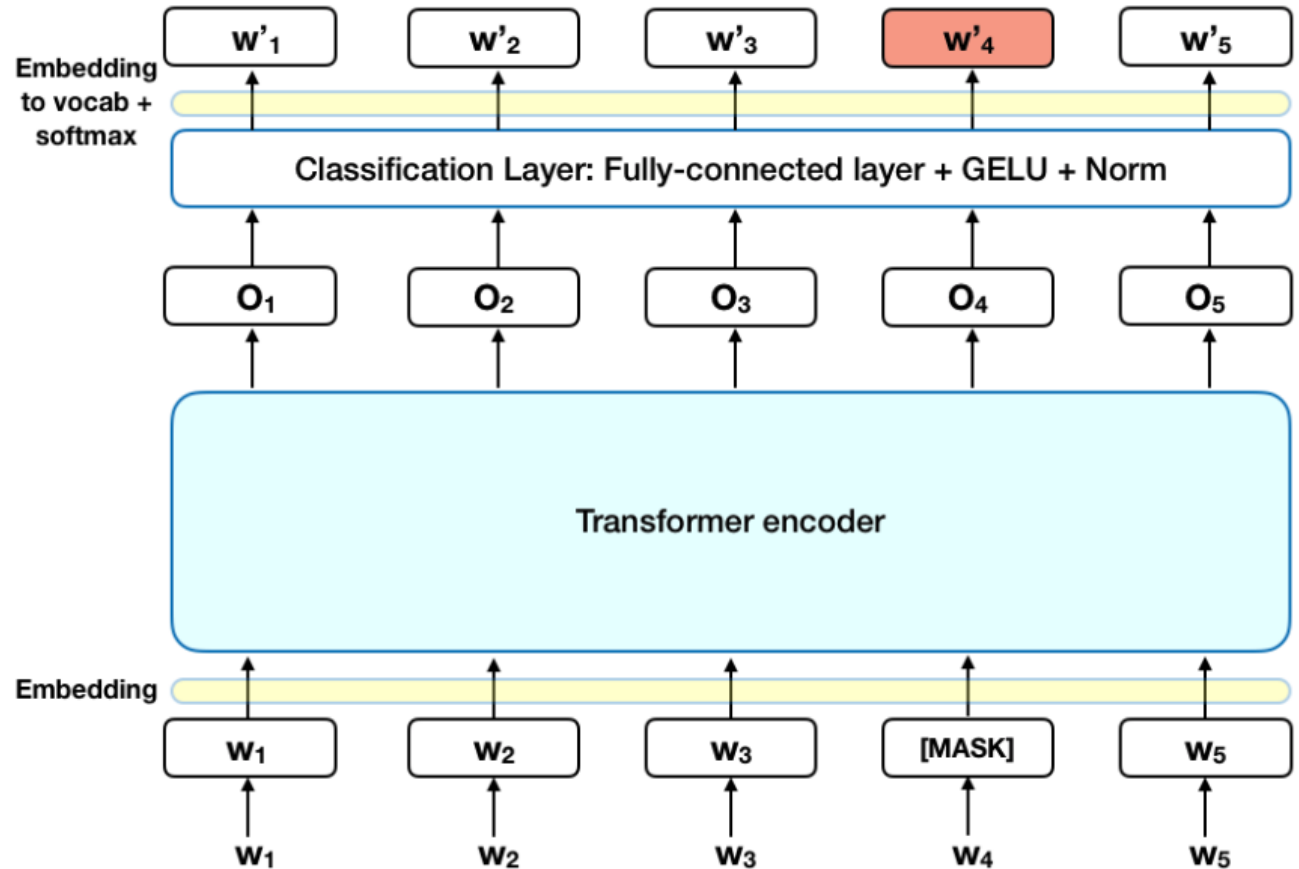


Li, Yikang, et al. "Visual question generation as dual task of visual question answering." *CVPR*'18.

# BERT: Transformer That Predicts Its Own Masked Parts

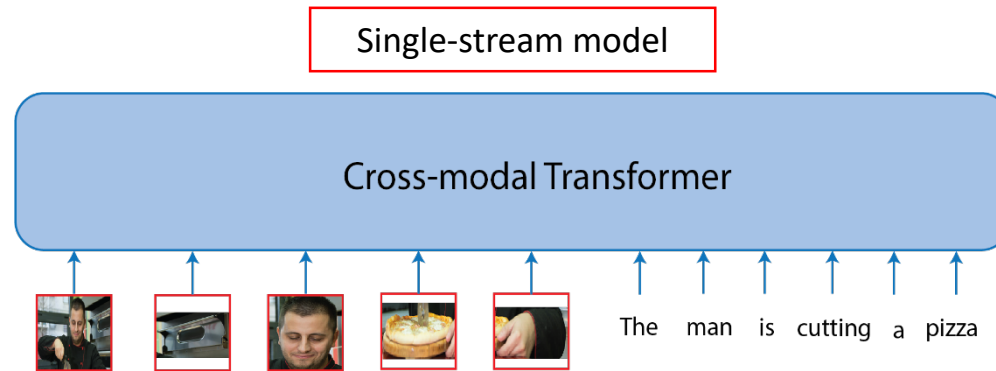
BERT is like parallel approximate pseudo-likelihood

- ~ Maximizing the conditional likelihood of some variables given the rest.
- When the number of variables is large, this converges to MLE (maximum likelihood estimate).



# Visual QA as a Down-stream Task of Visual-Language BERT Pre-trained Models

Numerous pre-trained visual language models during 2019-2021.



VisualBERT (Li, Liunian Harold, et al., 2019)

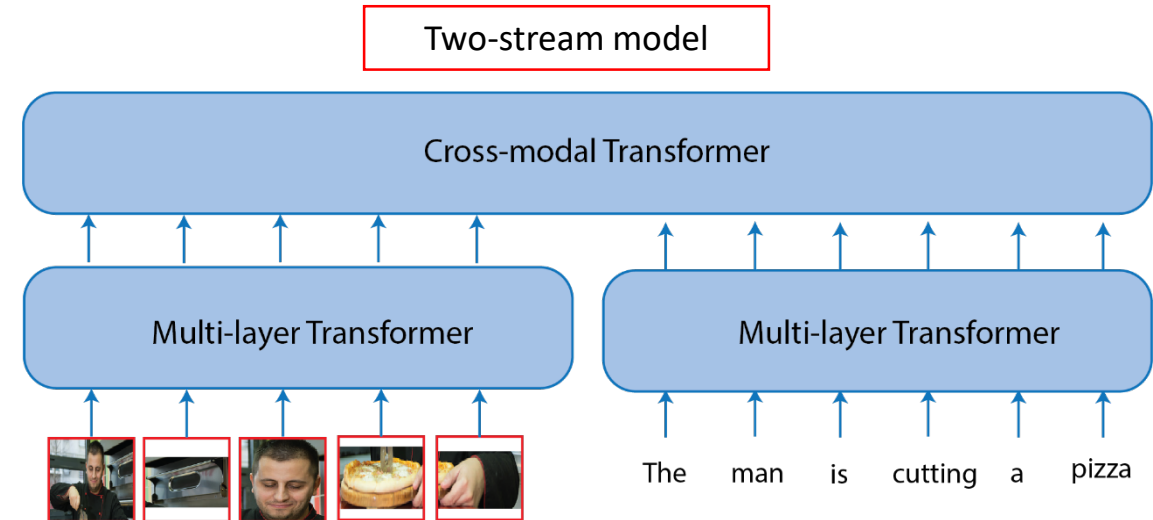
VL-BERT (Su, Weijie, et al., 2019)

UNITER (Chen, Yen-Chun, et al., 2019)

12-in-1 (Lu, Jiasen, et al., 2020)

Pixel-BERT (Huang, Zhicheng, et al., 2019)

OSCAR (Li, Xiujun, et al., 2020)



ViLBERT (Lu, Jiasen, et al., 2019)

LXMERT (Tan, Hao, and Mohit Bansal, 2019)



# Learning with External Knowledge

Why external knowledge for reasoning?

- Questions can be beyond visual recognition (e.g. firetrucks usually use a fire hydrant).
- Human's prior knowledge for cognition-level reasoning (e.g. human's goals, intents etc.)

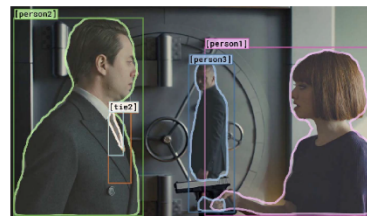


Q: What sort of vehicle uses this item?  
A: firetruck

Marino, Kenneth, et al. "Ok-vqa: A visual question answering benchmark requiring external knowledge." *CVPR'19*.



Q: What is the sports position of the man in the orange shirt?  
A: goalie/goalkeeper



Why is [person1] pointing a gun at [person2]?

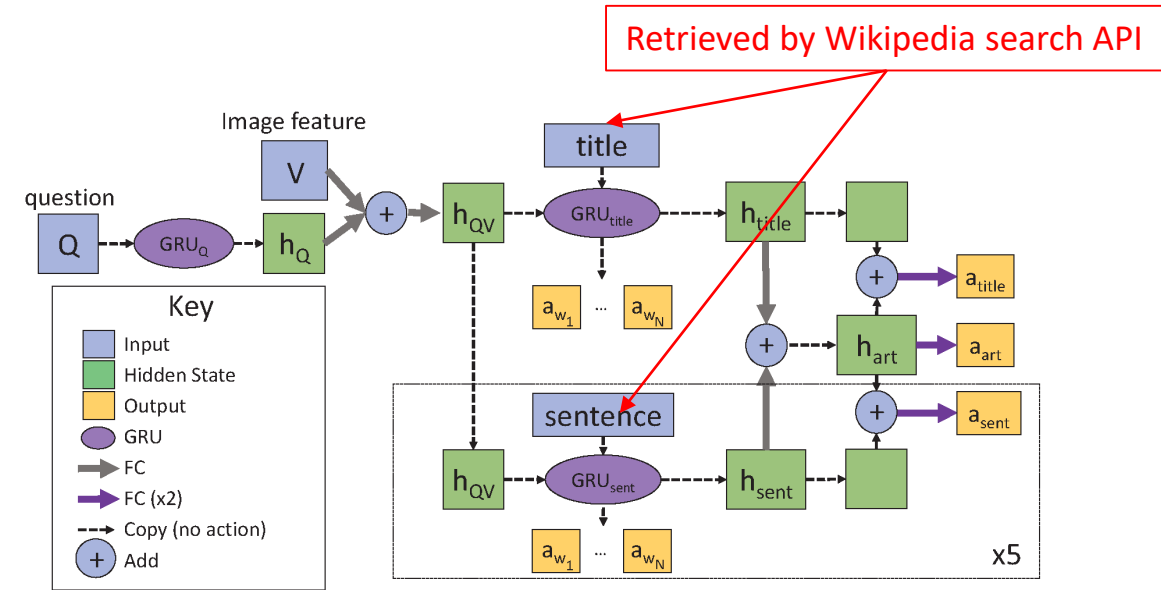
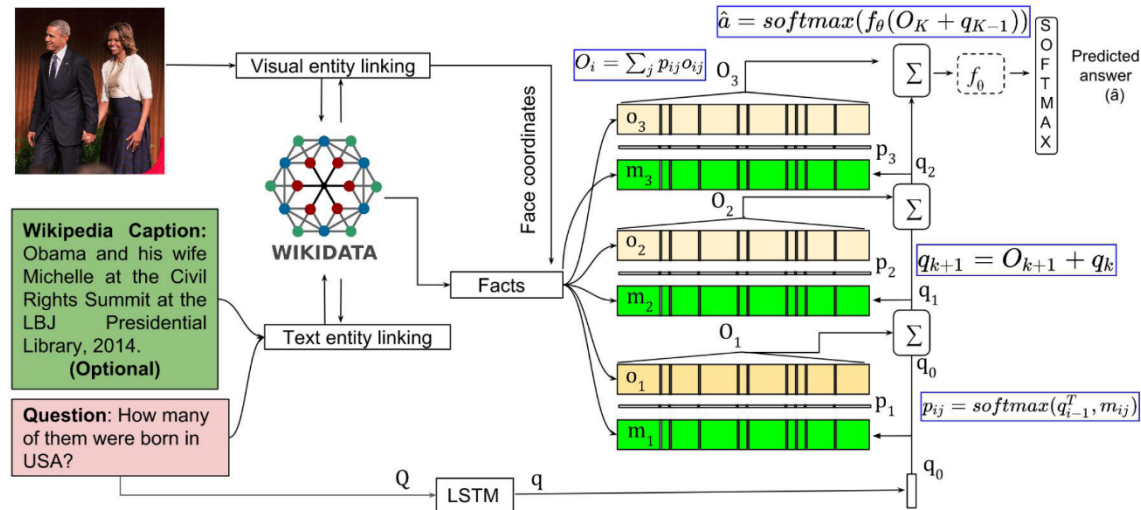
- a) [person1] wants to kill [person2]. (1%)
- b) [person1] and [person3] are robbing the bank and [person2] is the bank manager. (71%)
- c) [person2] has done something to upset [person1]. (18%)
- d) Because [person2] is [person1]'s daughter. [person1] wants to protect [person2]. (8%)

b) is right because...

- a) [person1] is chasing [person1] and [person3] because they just robbed a bank. (33%)
- b) Robbers will sometimes hold their gun in the air to get everyone's attention. (5%)
- c) The vault in the background is similar to a bank vault. [person3] is waiting by the vault for someone to open it. (49%)
- d) A room with barred windows and a counter usually resembles a bank. (11%)

# Learning with External Knowledge

Shah, Sanket, et al. "Kvqa: Knowledge-aware visual question answering." AAAI'19.

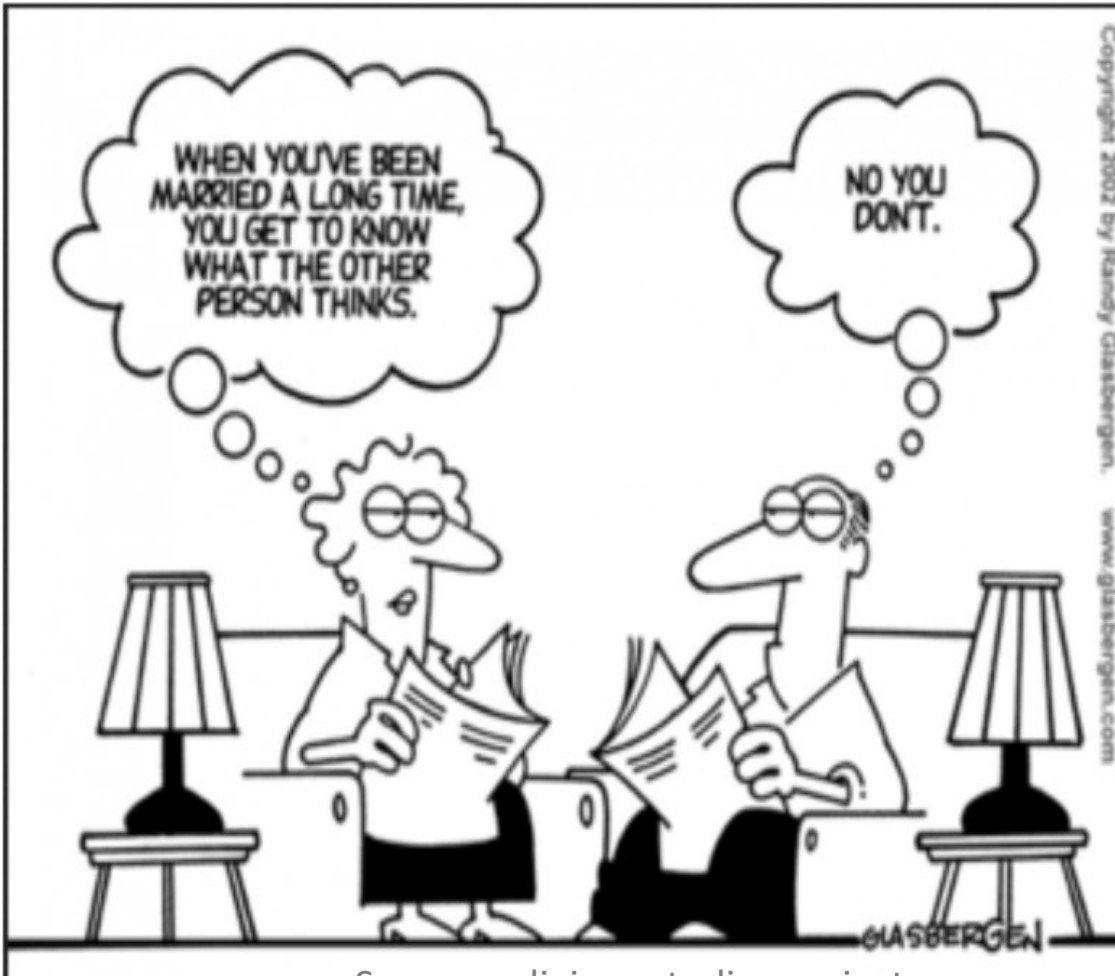


Marino, Kenneth, et al. "Ok-vqa: A visual question answering benchmark requiring external knowledge." CVPR'19.



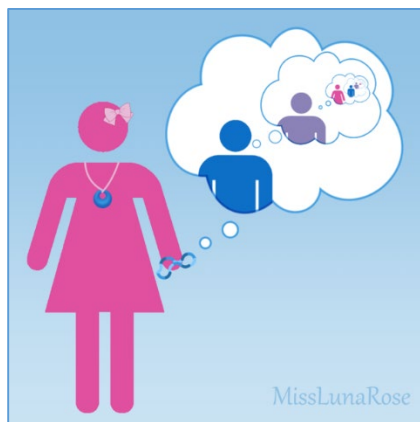
# Agenda

- Reasoning with external memories
  - Memory of entities – memory-augmented neural networks
  - Memory of relations with tensors and graphs
  - Memory of programs & neural program construction.
- Learning to reason with less labels:
  - Data augmentation with analogical and counterfactual examples
  - Question generation
  - Self-supervised learning for question answering
  - Learning with external knowledge graphs
- **Recursive reasoning with neural theory of mind.**



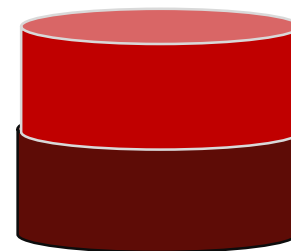
Source: religious studies project

# Core AI faculty: Theory of mind



Theory of mind  
Recursive reasoning

Memory



Facts  
Semantics  
Events and relations  
Working space

Multiple

System 1:  
Intuitive

- Fast
- Implicit/automatic
- Pattern recognition
- Multiple

Single

System 2:  
Analytical

- Slow
- Deliberate/rational
- Careful analysis
- Single, sequential



Perception



# Where would ToM fit in?

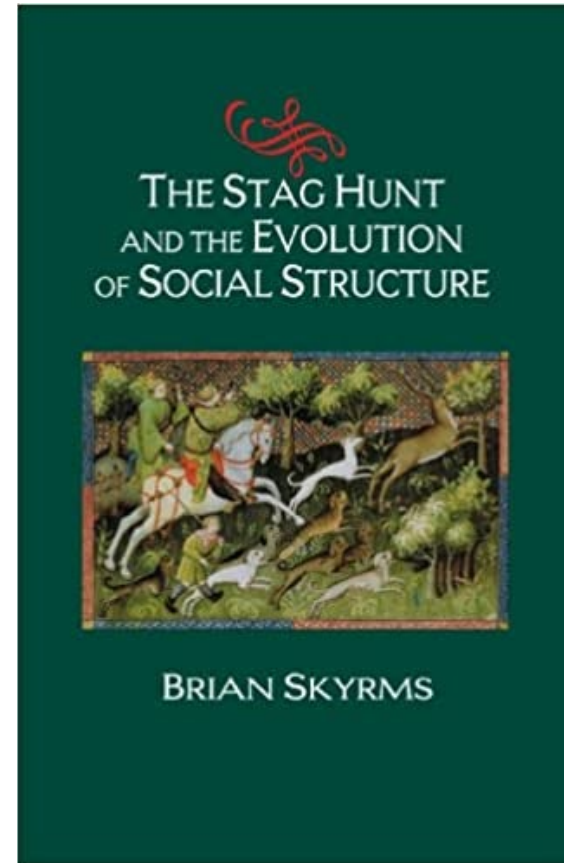
# Contextualized recursive reasoning

- Thus far, QA tasks are straightforward and objective:
  - Questioner: I will ask about what I don't know.
  - Answerer: I will answer what I know.
- Real life can be tricky, more subjective:
  - Questioner: I will ask only questions I think they can answer.
  - Answerer 1: This is what I think they want from an answer.
  - Answerer 2: I will answer only what I think they think I can.

→ We need Theory of Mind to function socially.

# Social dilemma: Stag Hunt games

- **Difficult decision:** individual outcomes (selfish) or group outcomes (cooperative).
  - Together hunt Stag (both are cooperative): Both have more meat.
  - Solely hunt Hare (both are selfish): Both have less meat.
  - One hunts Stag (cooperative), other hunts Hare (selfish): Only one hunts hare has meat.
- **Human evidence:** Self-interested but considerate of others (cultures vary).
- **Idea:** Belief-based guilt-aversion
  - One experiences loss if it lets other down.
  - Necessitates Theory of Mind: reasoning about other's mind.



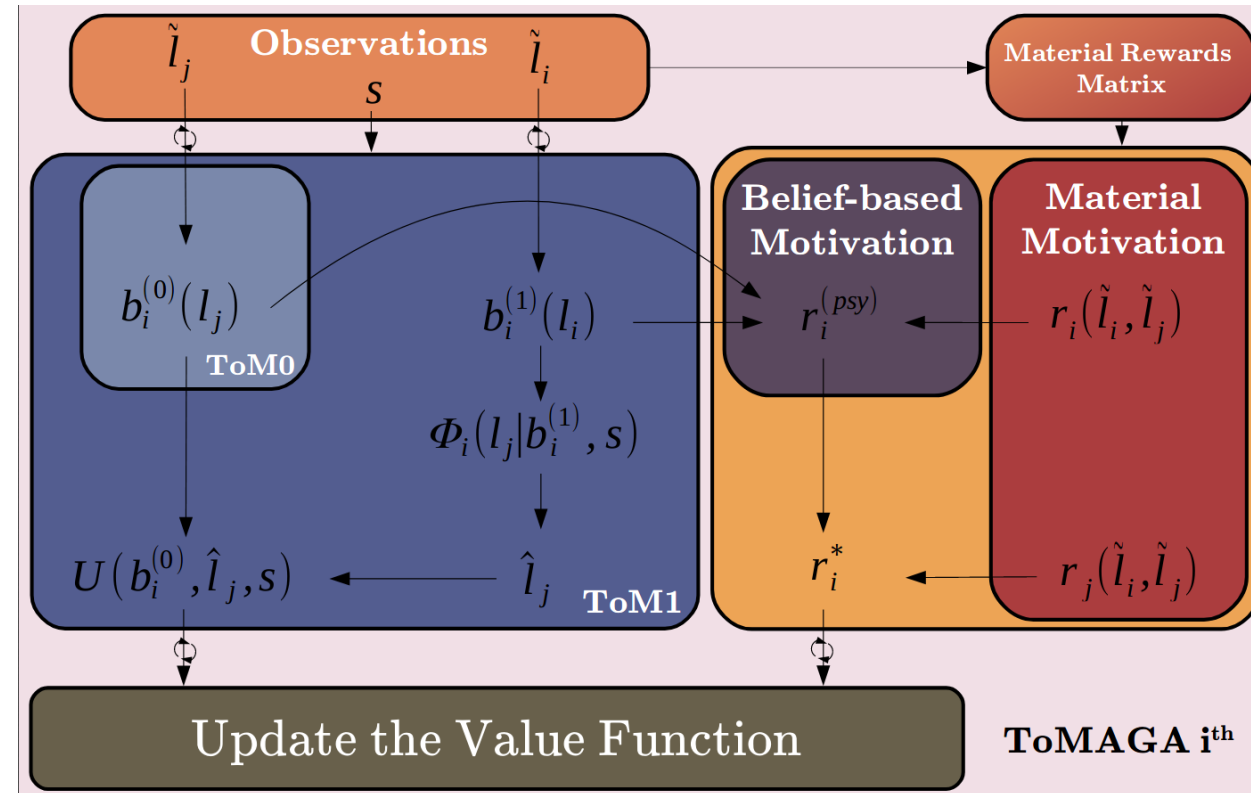
# Theory of Mind Agent with Guilt Aversion (ToMAGA)

## Update Theory of Mind

- Predict whether other's behaviour are cooperative or uncooperative
- Updated the zero-order belief (what other will do)
- Update the first-order belief (what other think about me)

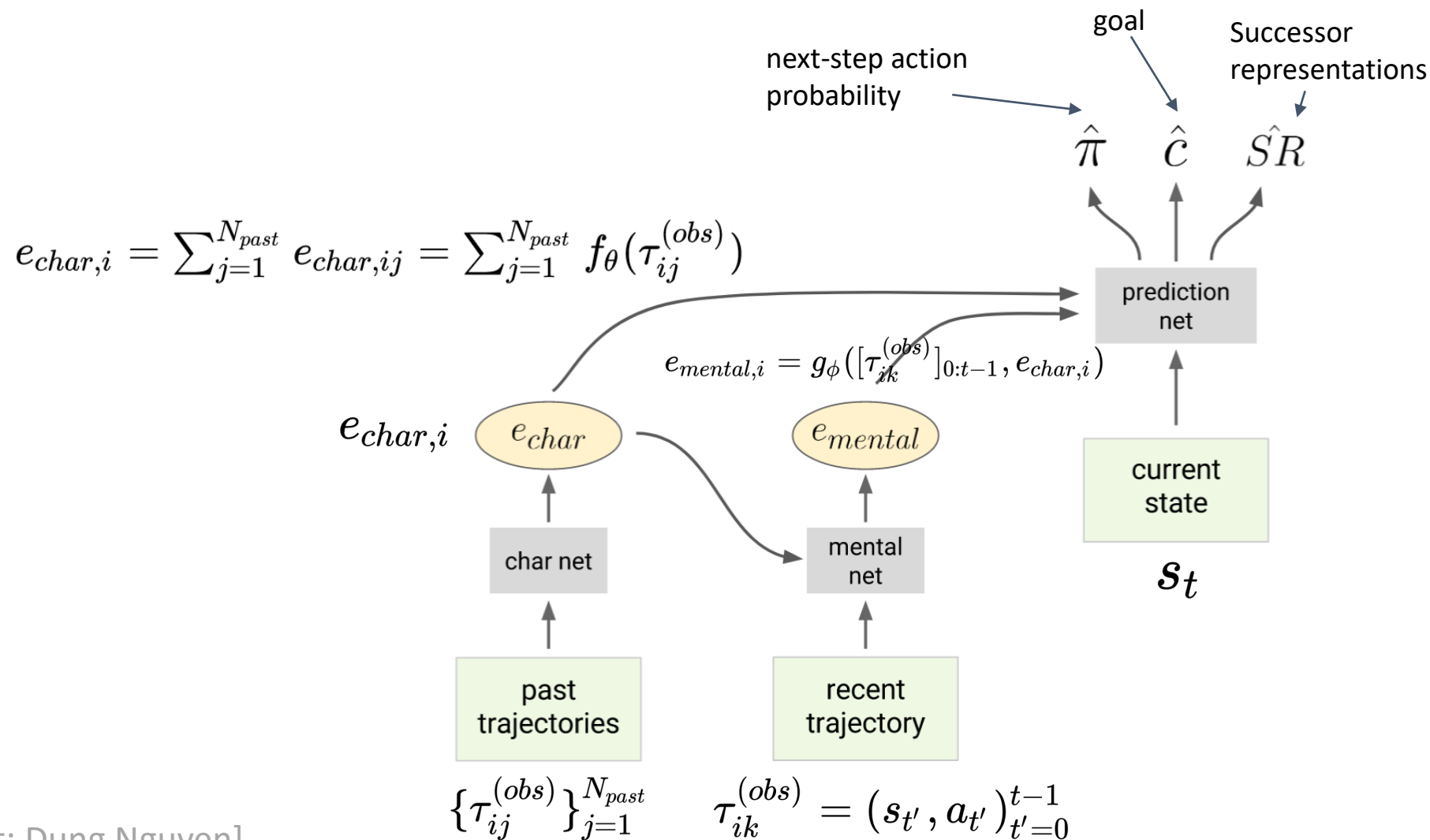
## Guilt Aversion

- Compute *the expected material reward* of other based on Theory of Mind
- Compute *the psychological rewards*, i.e. "feeling guilty"
- Reward shaping: subtract the expected loss of the other.



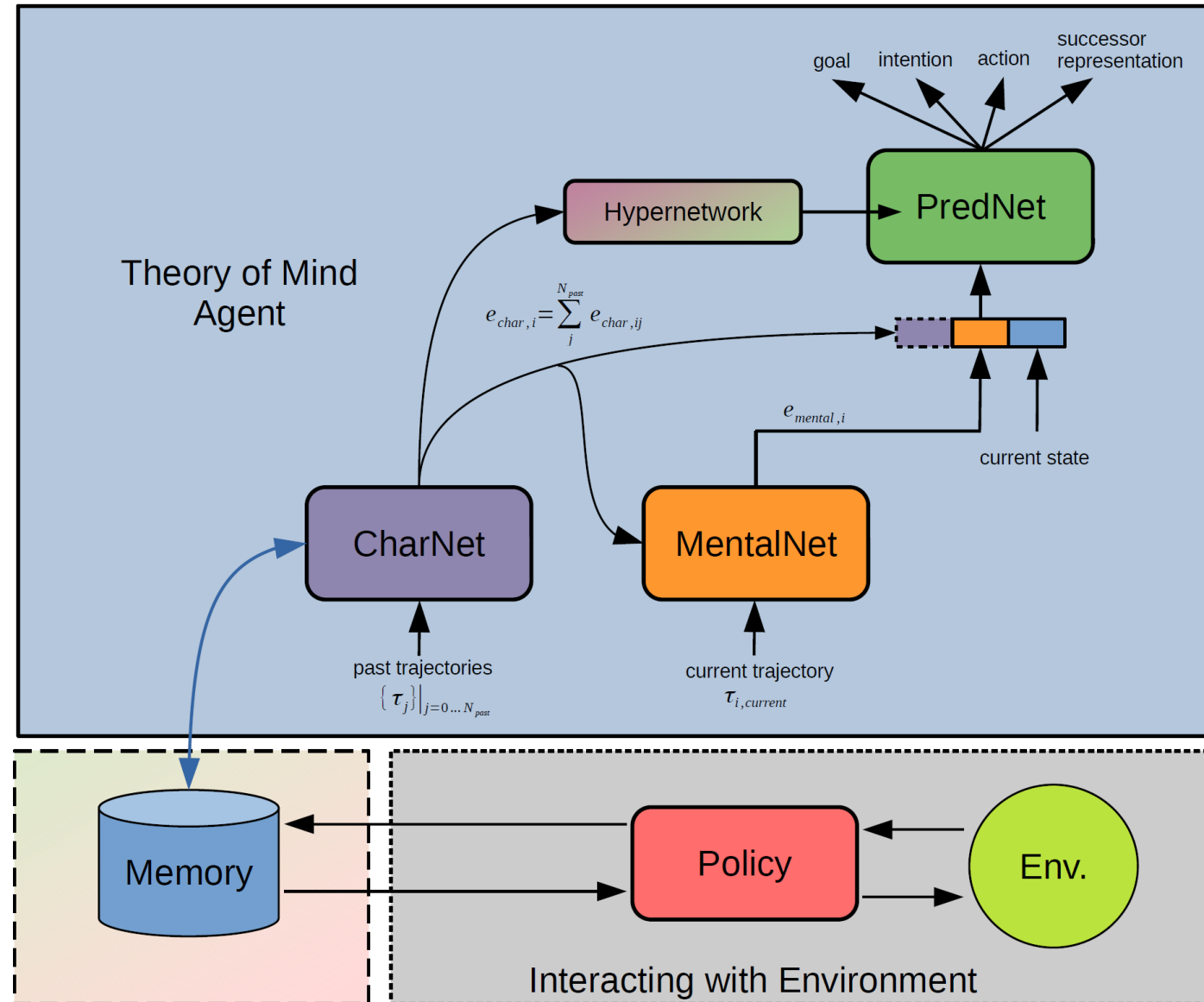
Nguyen, Dung, et al. "Theory of Mind with Guilt Aversion Facilitates Cooperative Reinforcement Learning." *Asian Conference on Machine Learning*. PMLR, 2020.

# Machine Theory of Mind Architecture (inside **the Observer**)



# A ToM architecture

- Observer maintains memory of previous episodes of the agent.
- It theorizes the “traits” of the agent.
  - Implemented as Hyper Networks.
- Given the current episode, the observer tries to infer goal, intention, action, etc of the agent.
  - Implemented as memory retrieval through attention mechanisms.

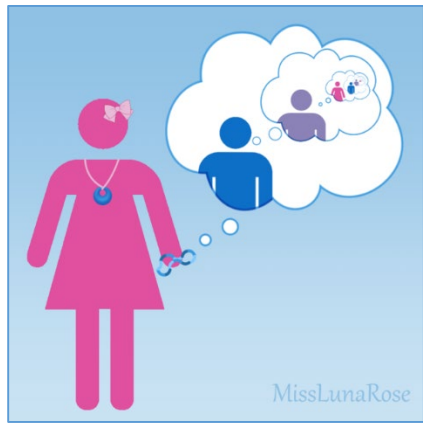




# Wrapping up

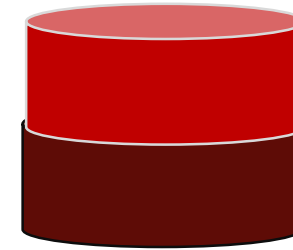
# Wrapping up

- Reasoning as the next challenge for deep neural networks
- Part A: Learning-to-reason framework
  - Reasoning as a prediction skill that can be learnt from data
  - Dynamic neural networks are capable
  - Combinatorics reasoning
- Part B: Reasoning over unstructured and structured data
  - Reasoning over unstructured sets
  - Relational reasoning over structured data
- Part C: Memory | Data efficiency | Recursive reasoning
  - Memories of items, relations and programs
  - Learning with less labels
  - Theory of mind



Theory of mind  
Recursive reasoning

Memory



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Perception



**A possible framework for learning and reasoning  
with deep neural networks**

QA

<https://bit.ly/37DYQn7>