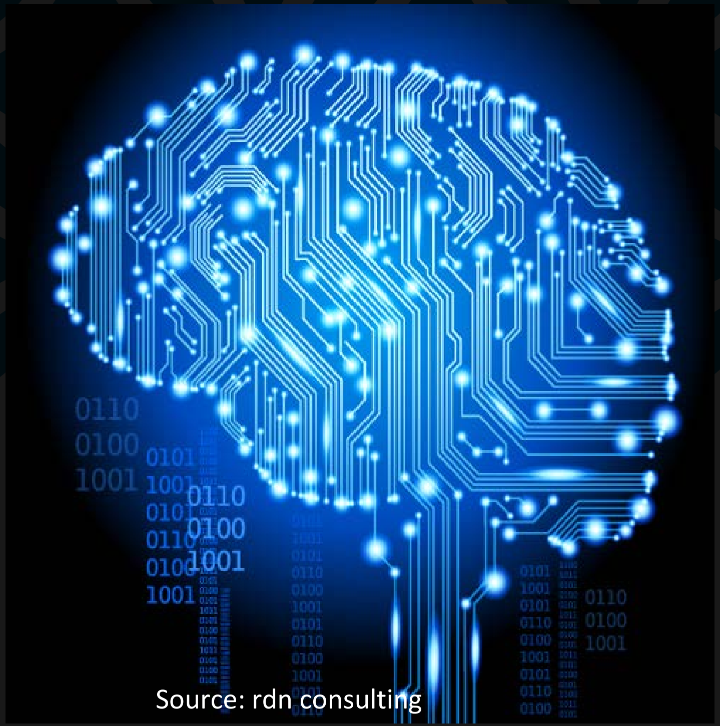
Advances in Neural Turing Machines



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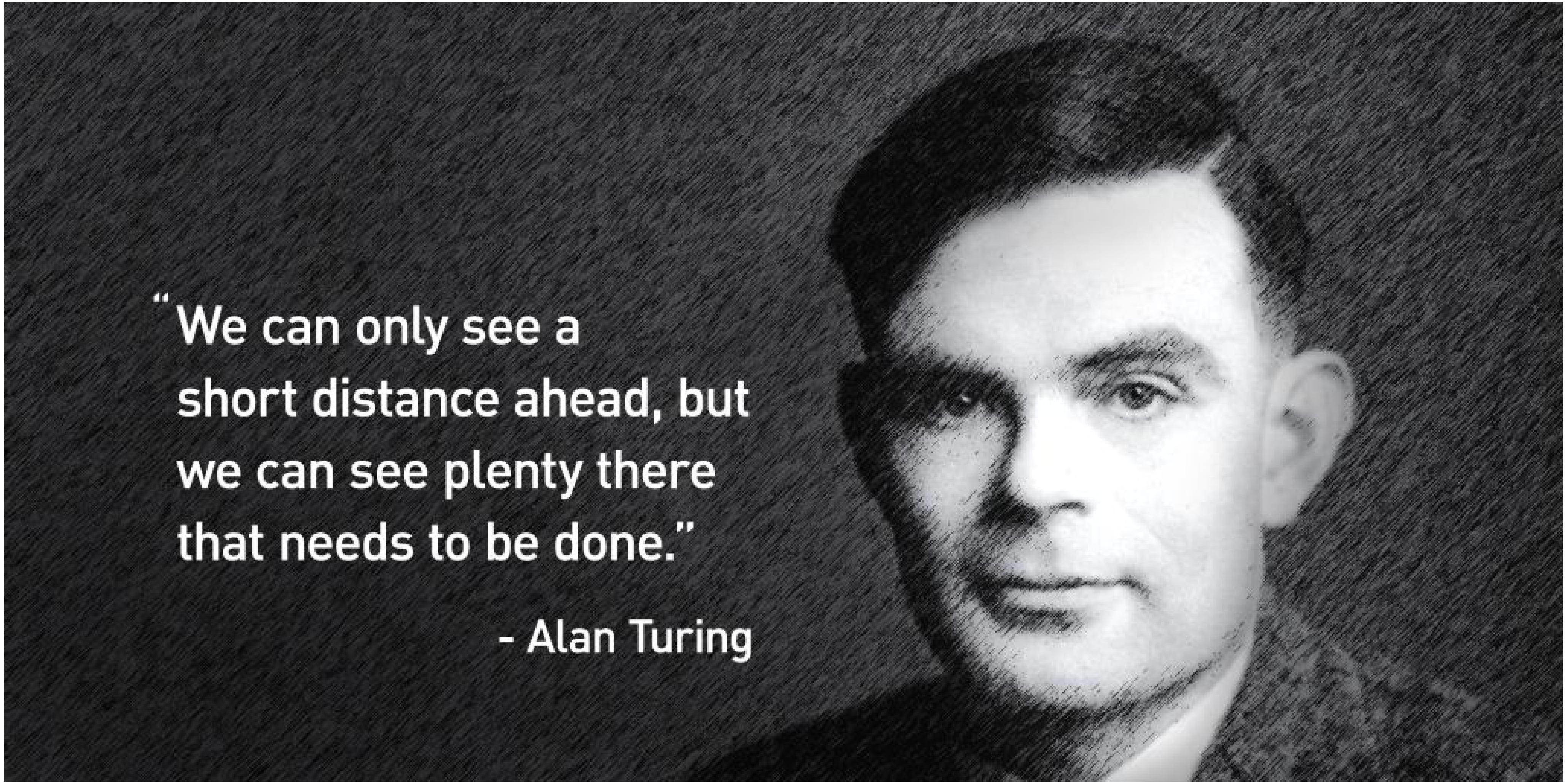
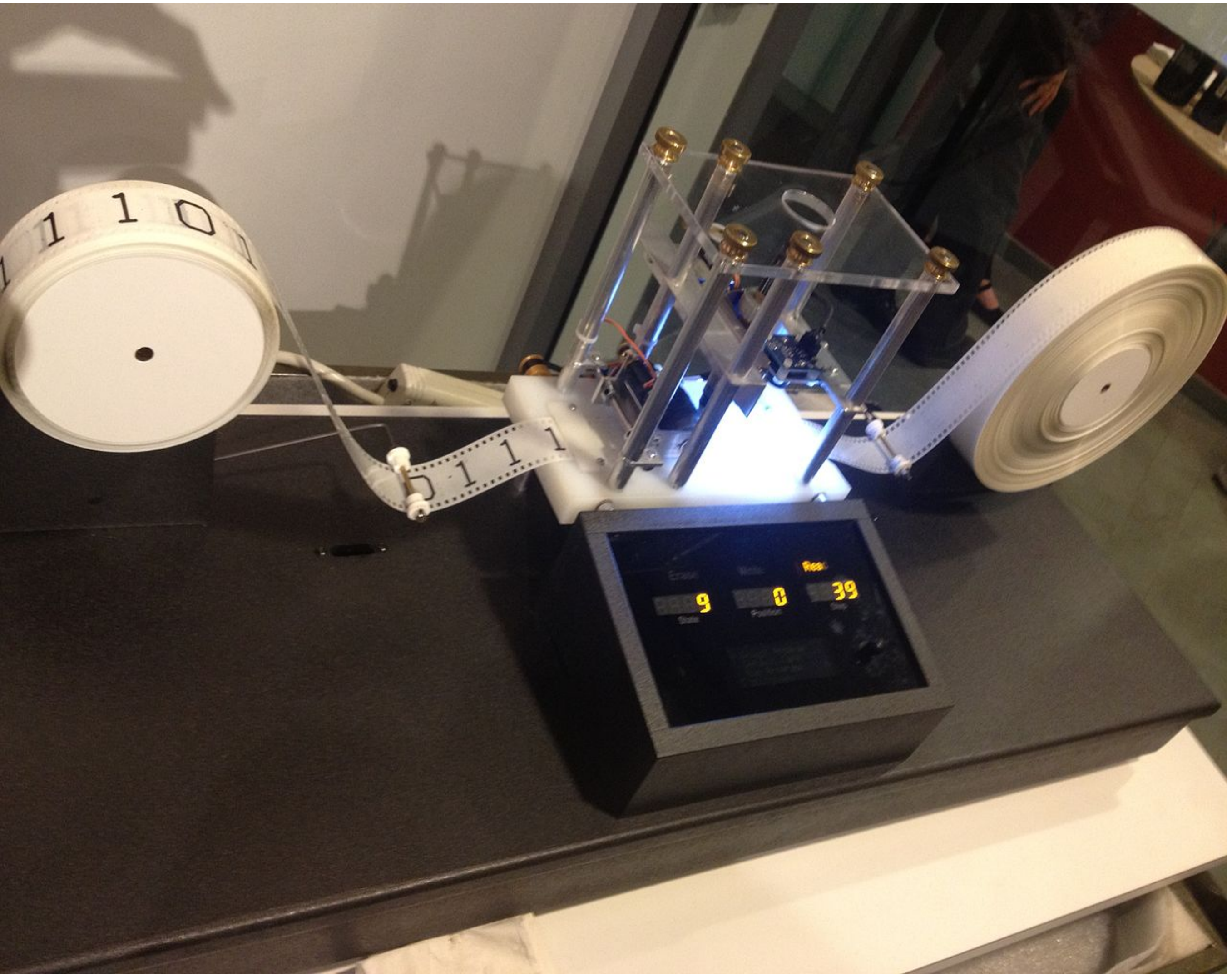
CafeDSL, Aug 2018



https://twitter.com/nvidia/status/1010545517405835264



(Real) Turing machine

It is possible to invent a *single machine* which can be used to compute *any* computable sequence. If this machine **U** is supplied with the tape on the beginning of which is written the string of quintuples separated by semicolons of some computing machine **M**, then **U** will compute the same sequence as **M**.

Wikipedia

Can we learn from data a model that is as powerful as a Turing machine?

Agenda

Brief review of deep learning

Neural Turing machine (NTM)

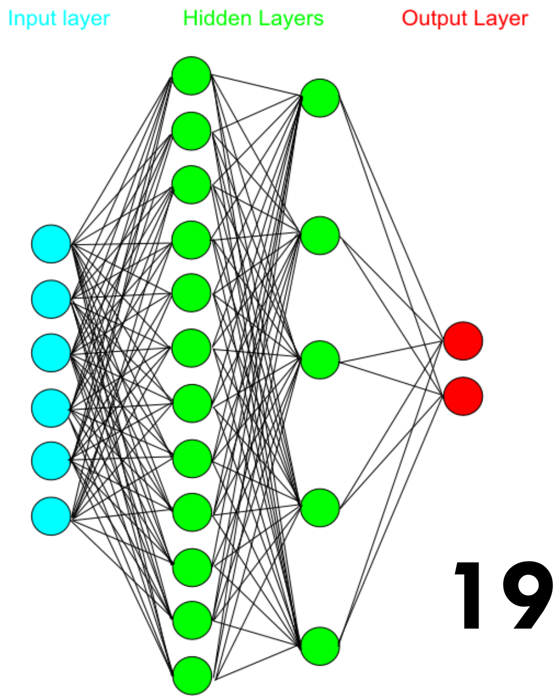
Dual-controlling for read and write (PAKDD’18)

Dual-view in sequences (KDD’18)

Bringing variability in output sequences (NIPS’18 ?)

Bringing relational structures into memory (IJCAI’17 WS+)

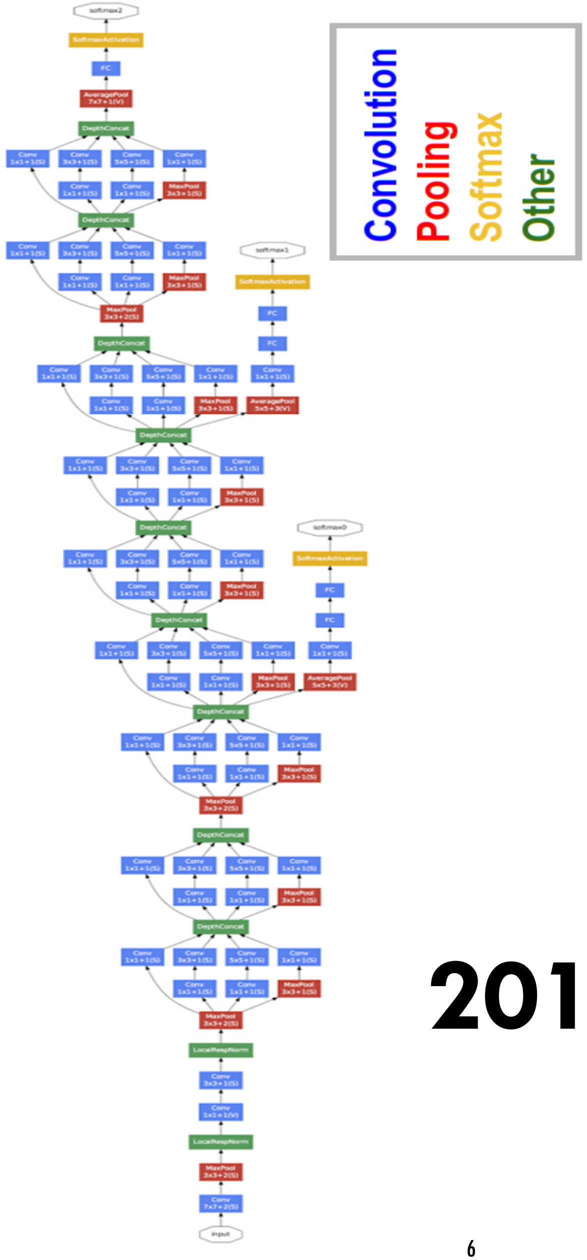
Deep learning in a nutshell



1986

http://blog.refu.co/wp-content/uploads/2009/05/mlp.png

2012



2016

Let’s review current offerings

Feedforward nets (FFN)

Recurrent nets (RNN)

Convolutional nets (CNN)

Message-passing graph nets (MPGNN)

Universal transformer

…..

Work surprisingly well on LOTS of important problems

Enter the age of differentiable programming

BUTS …

No storage of intermediate results.

Little choices over what to compute and what to use

Little support for complex chained reasoning

Little support for rapid switching of tasks

Searching for better priors

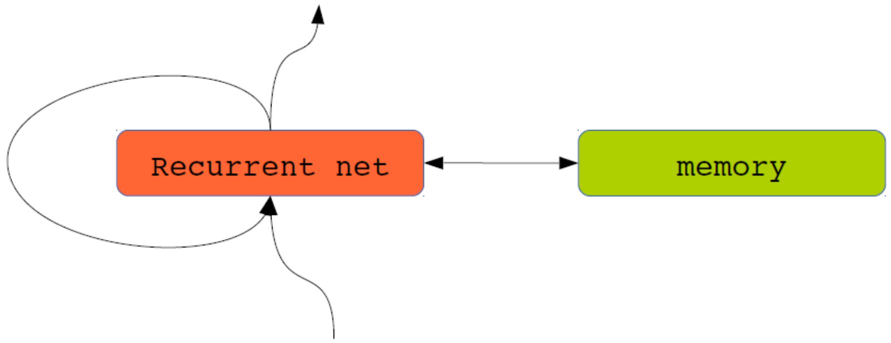
Translation invariance in CNN

Recurrence in RNN

Permutation invariance in attentions and graph neural networks

Memory for complex computation

→ Memory-augmented neural networks (MANN)



(LeCun, 2015)

What is missing? A memory

Use multiple pieces of information

Store intermediate results (RAM like)

Episodic recall of previous tasks (Tape like)

Encode/compress & generate/decompress long sequences

Learn/store programs (e.g., fast weights)

Store and query external knowledge

Spatial memory for navigation

Rare but important events (e.g., snake bite)

Needed for complex control

Short-cuts for ease of gradient propagation = constant path length

Division of labour: program, execution and storage

Working-memory is an indicator of IQ in human

Example: Code language model

```
FileWriter writer = new FileWriter(file);
writer.write(``This is an example'');
int count = 0;
System.out.prinltln(``Long gap'');
    ......

writer.flush();
writer.close();
```

$$P(s) = P(w_1) \prod_{t=2}^{k} P\left(w_t \mid \boldsymbol{w}_{1:t-1}\right)$$

Still needs a better memory for:

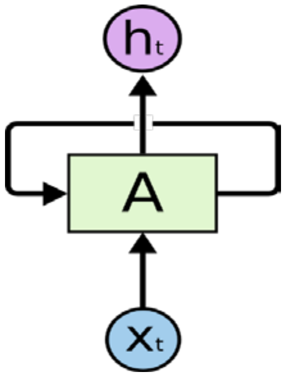
Repetitiveness

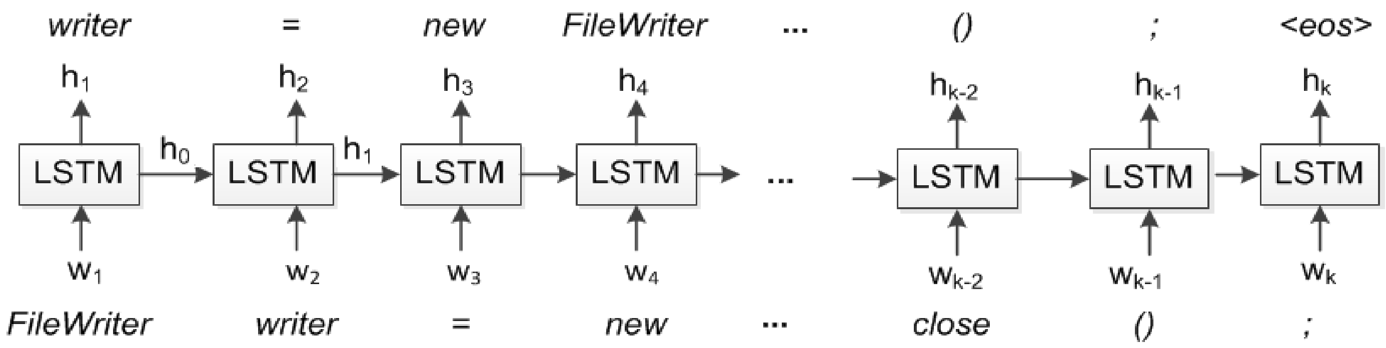
E.g. for (int i = 0; i < n; i++)

Localness

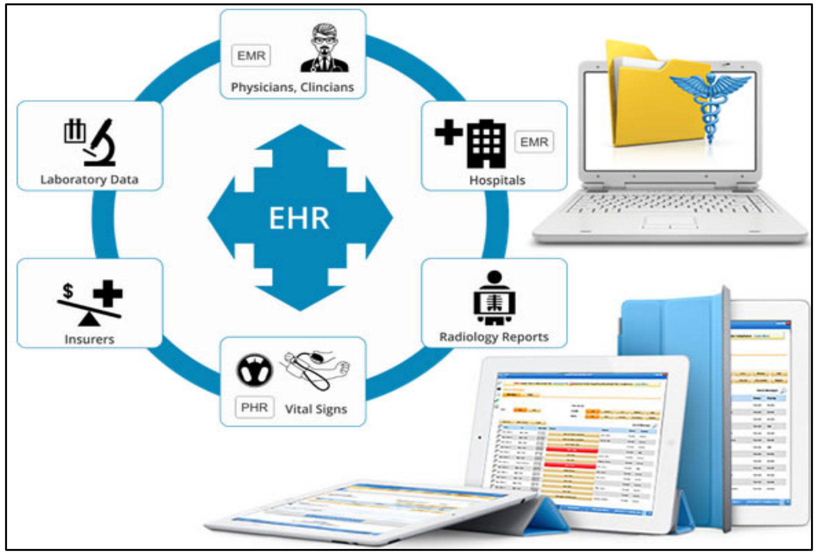
E.g. *for (int size* may appear more often that *for (int i* in some source files.

Very long sequence (big file, or char level)



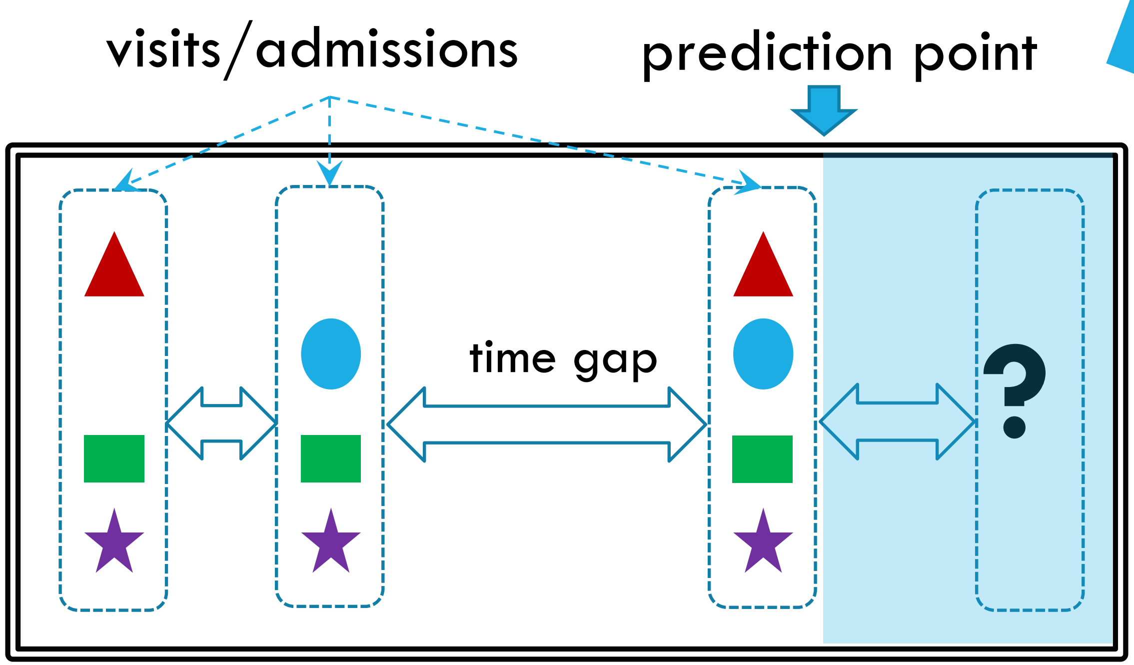


Example: Electronic medical records



Source: medicalbillingcodings.org

Abstraction

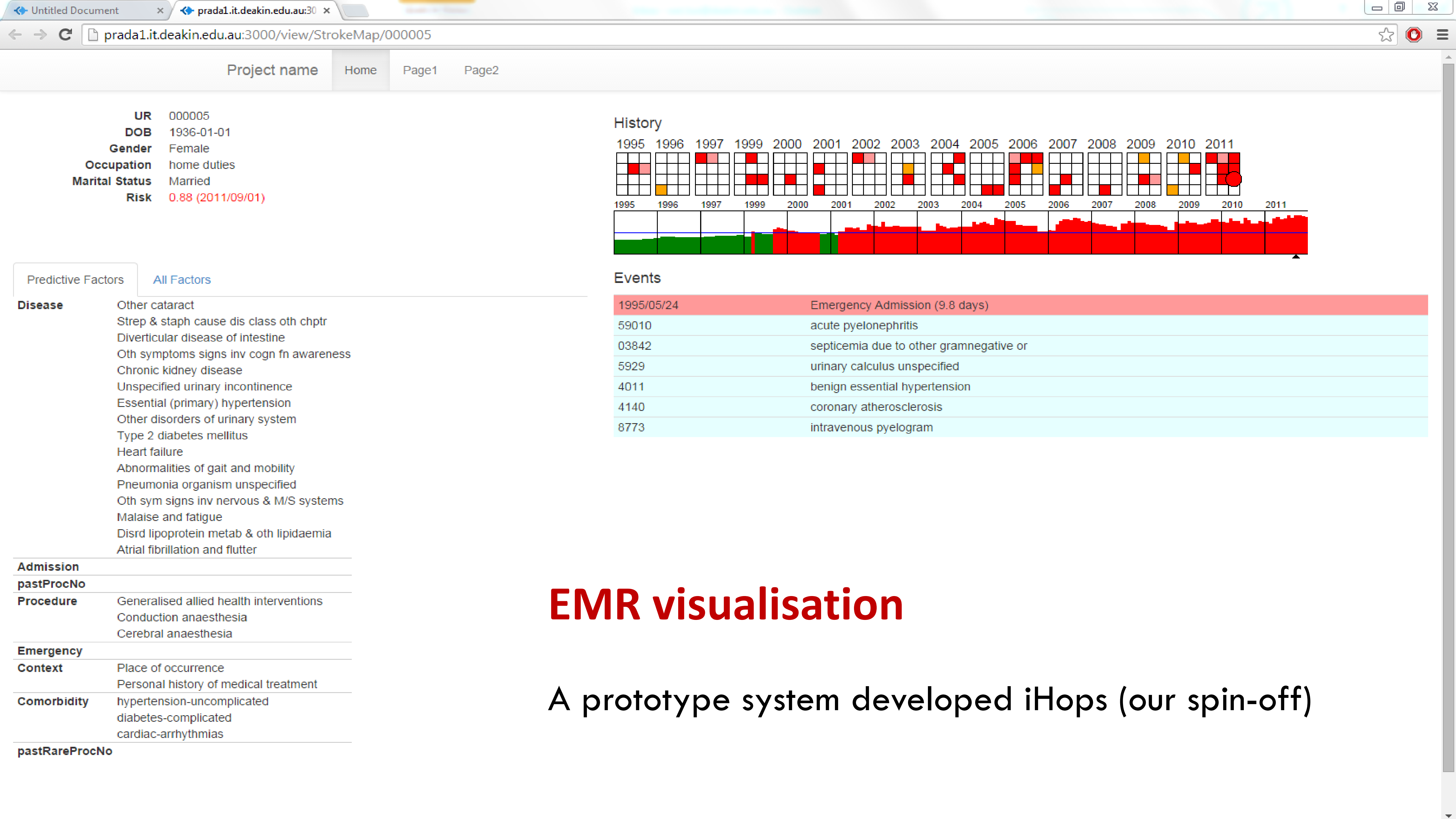


Modelling

Three interwoven processes:

- Disease progression
- Interventions & care processes
- Recording rules

Need memory to handle thousands of events



EMR visualisation

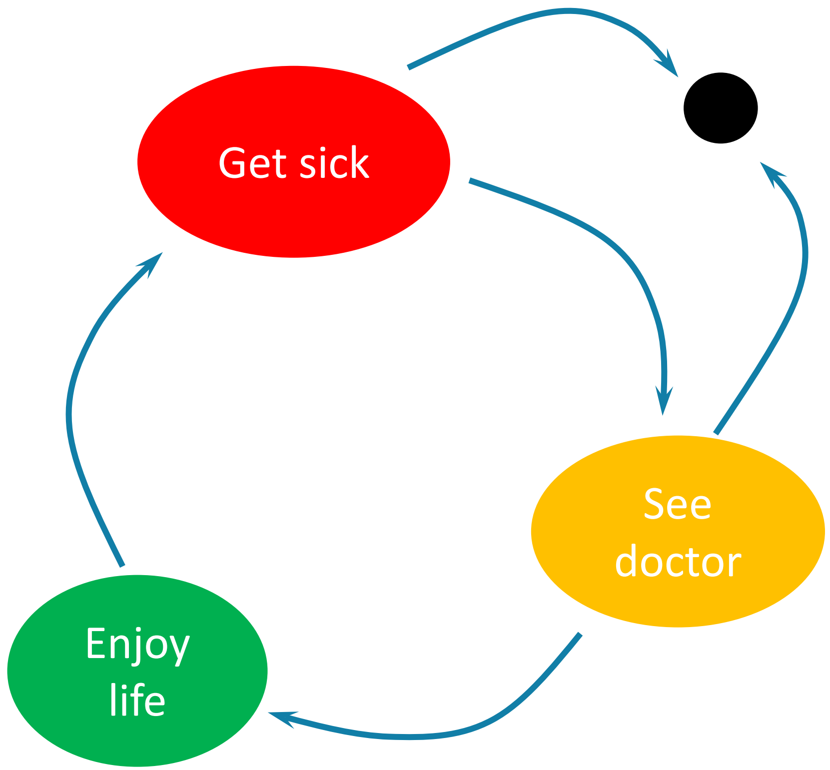
A prototype system developed iHops (our spin-off)

Conjecture: Healthcare is Turing computational

Healthcare processes as executable computer program obeying hidden "grammars"

The "grammars" are learnable through observational data

With "generative grammars", entire health trajectory can be simulated.



Other possible applications of memory

Video captioning

QA, VQA

Machine translation

Machine reading (stories, books, DNA)

Business process continuation

Software execution

Code generation

Graph as sequence of edges

Event sequences

Graph traversal

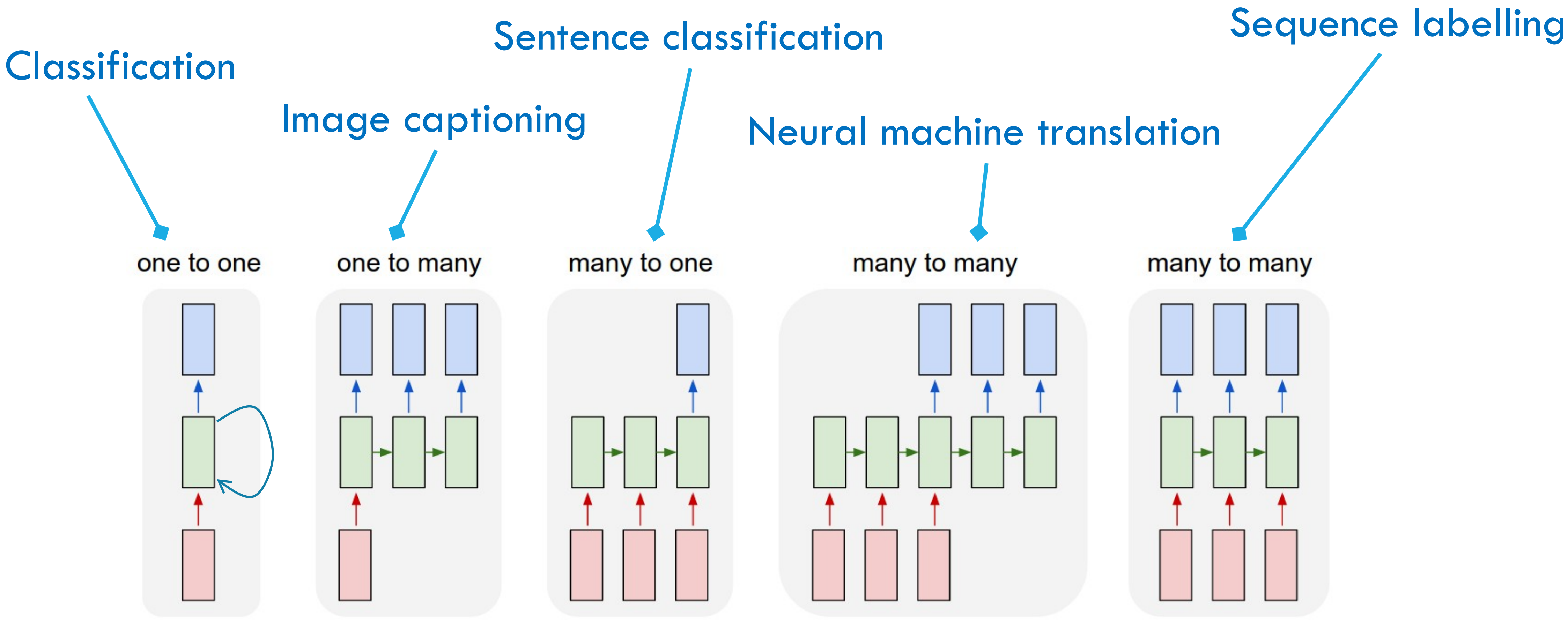
Algorithm learning (e.g., sort)

Dialog systems (e.g., chat bots)

Reinforcement learning agents

Neural Turing machine (NTM)

RNN: theoretically powerful, practically limited



Source: http://karpathy.github.io/assets/rnn/diags.jpeg

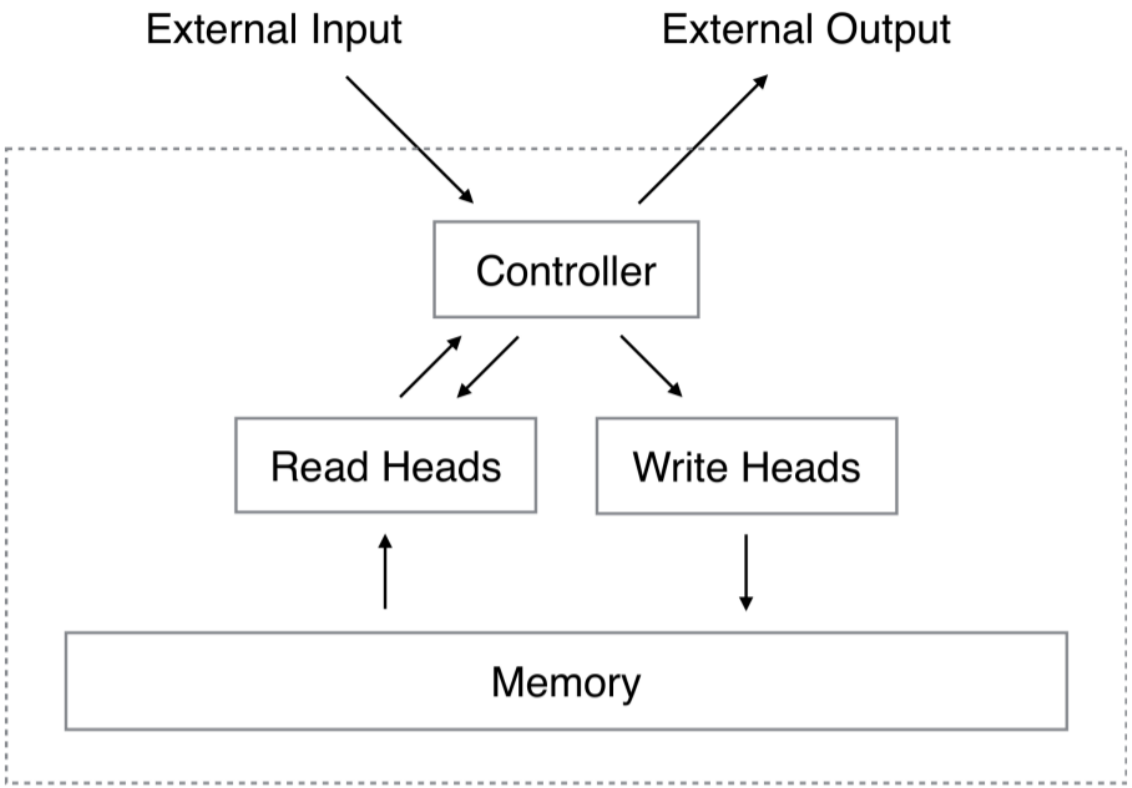
Neural Turing machine (NTM)

A controller that takes input/output and talks to an external memory module.

Memory has read/write operations.

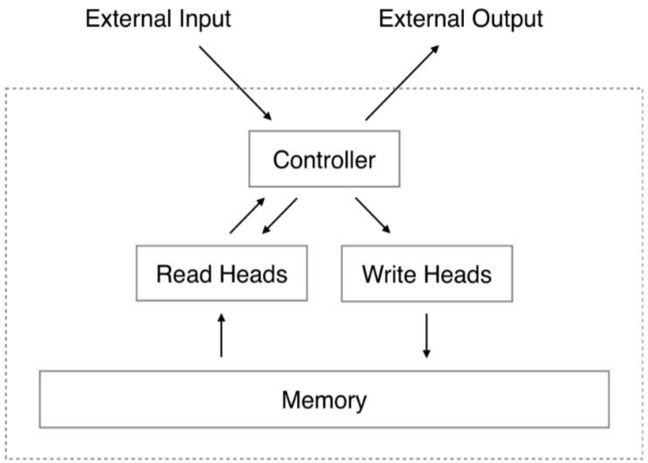
The main issue is where to write, and how to update the memory state.

All operations are differentiable.



https://rylanschaeffer.github.io/content/research/neural_turing_machine/main.html

NTM operations



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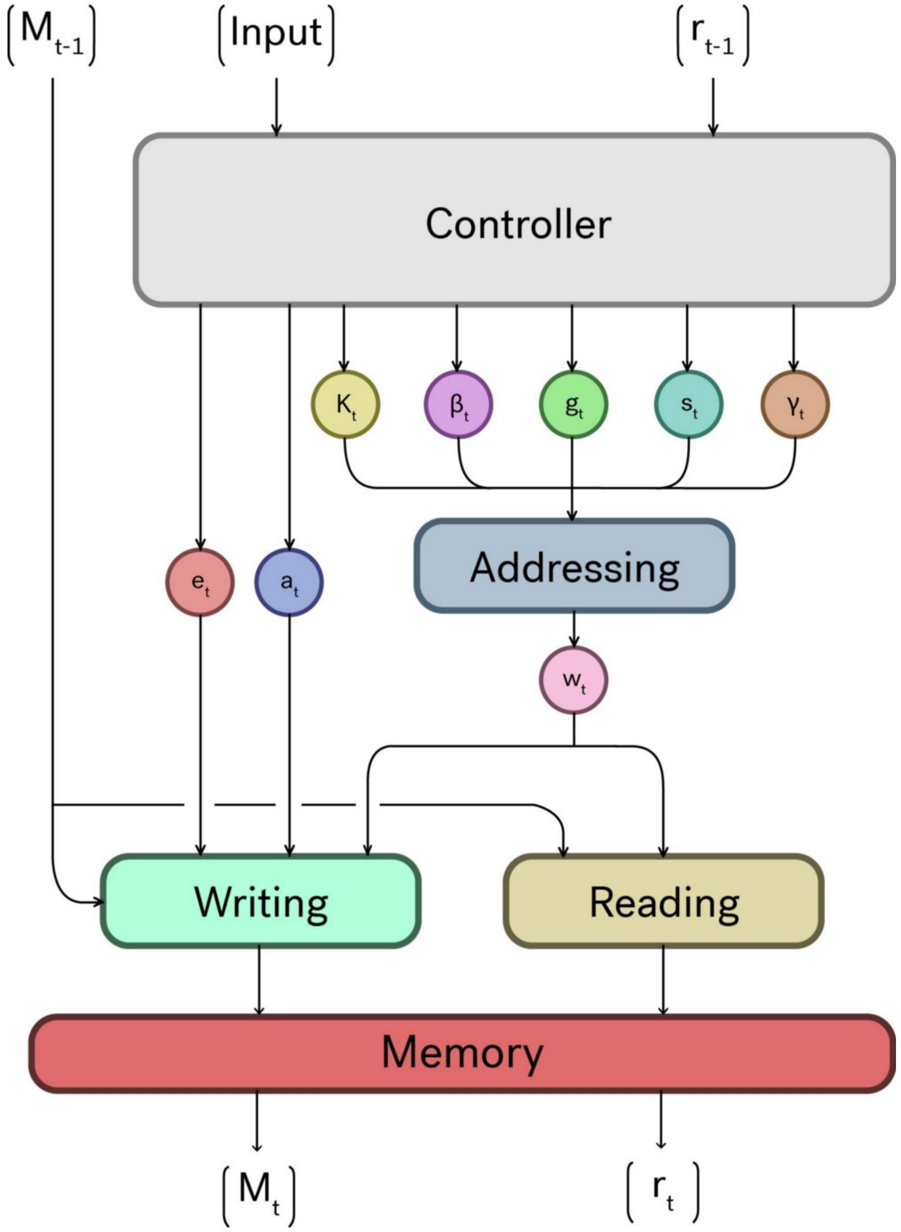
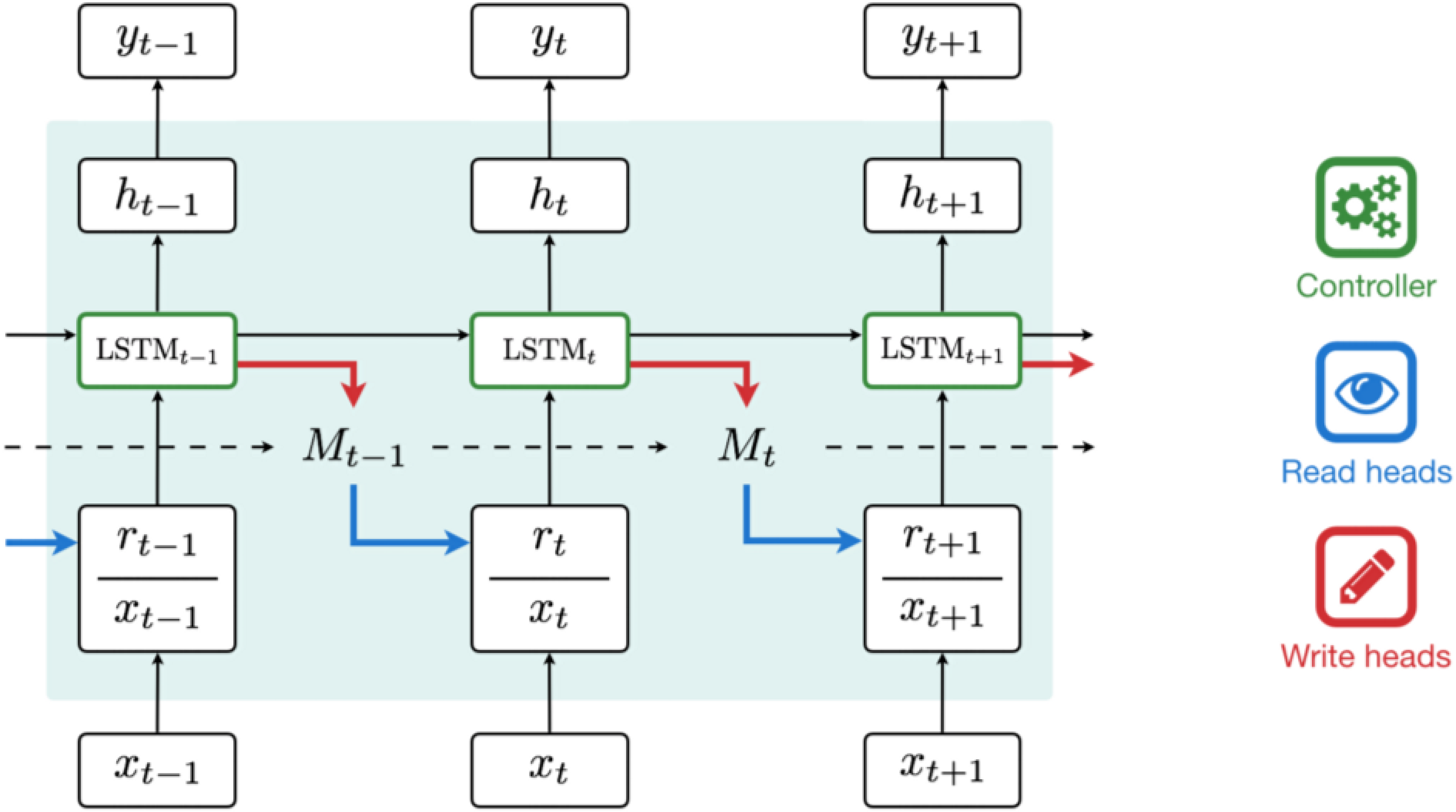


https://medium.com/@aidangomez/the-neural-turing-machine-79f6e806c0a1

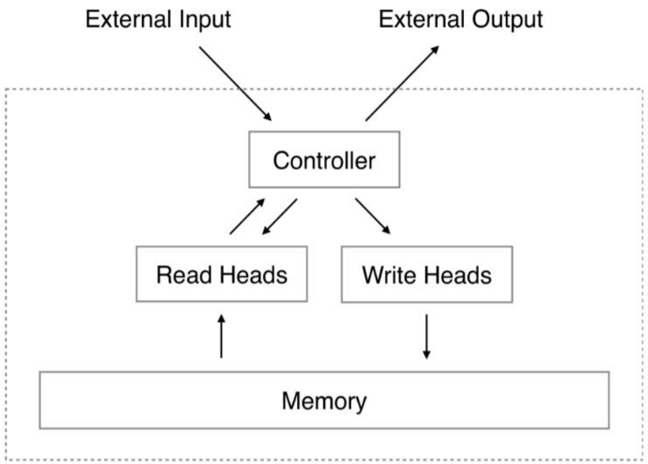


NTM unrolled in time with LSTM as controller

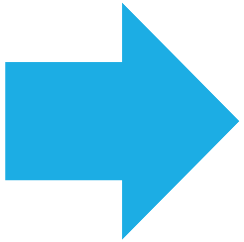
#Ref: https://medium.com/snips-ai/ntm-lasagne-a-library-for-neural-turing-machines-in-lasagne-2cdce6837315

Differentiable neural computer (DNC)

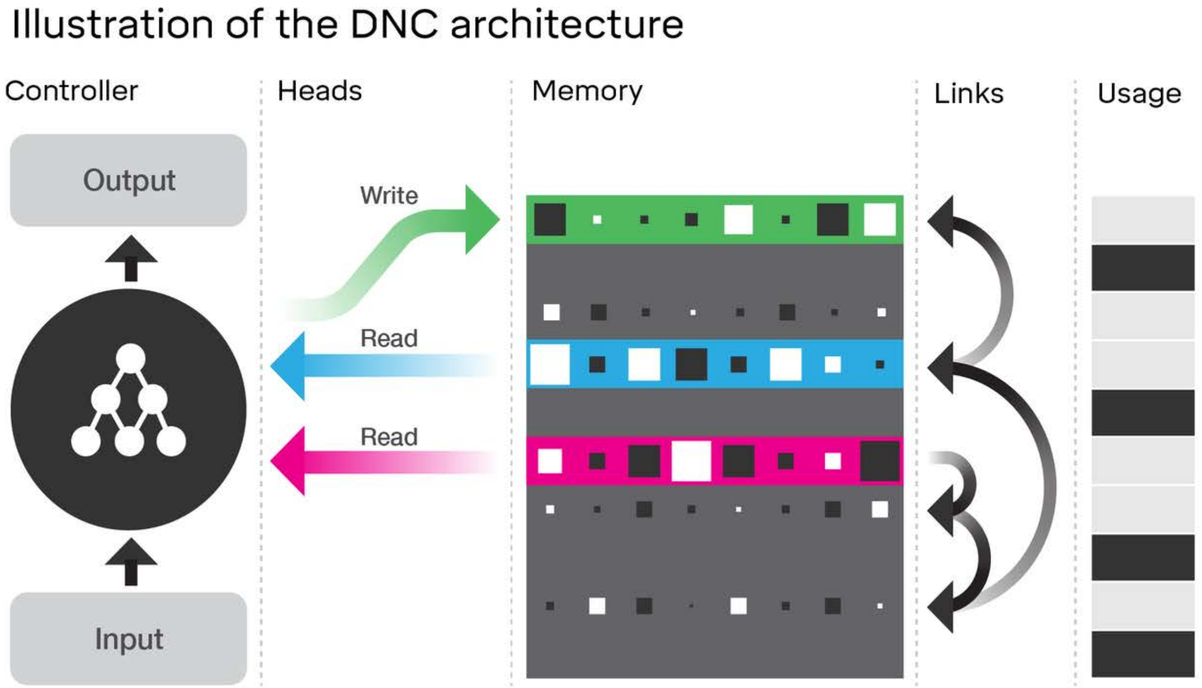
2014



https://rylanschaeffer.github.io



2016



Source: deepmind.com

#REF: Graves, Alex, et al. "Hybrid computing using a neural network with dynamic external memory." *Nature* 538.7626 (2016): 471-476.

Dual-controlling for read and write

Hung Le, Truyen Tran & Svetha Venkatesh

PAKDD'18

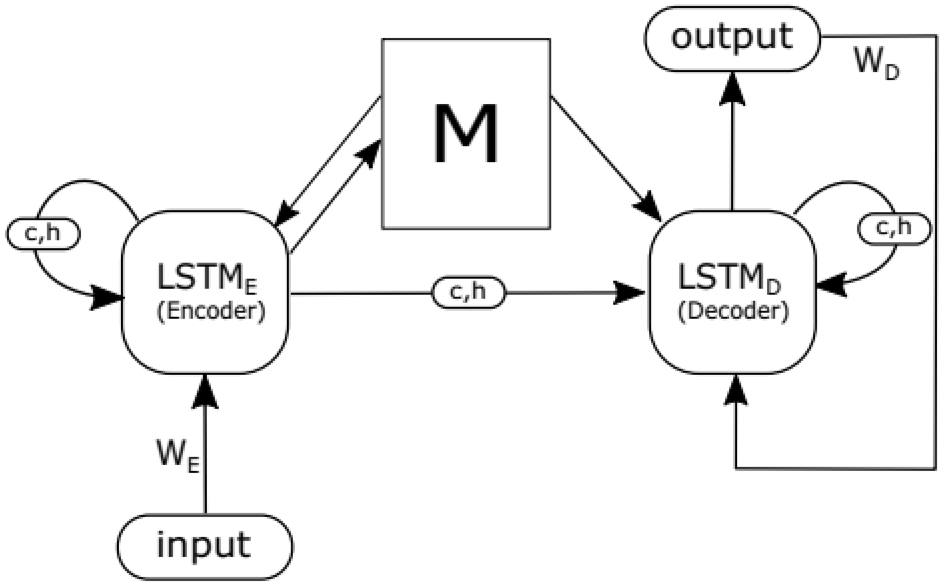
MANN with dual control (DC-MANN)

Two controllers, for input & output

The encoder reads the input sequence is encoded into memory

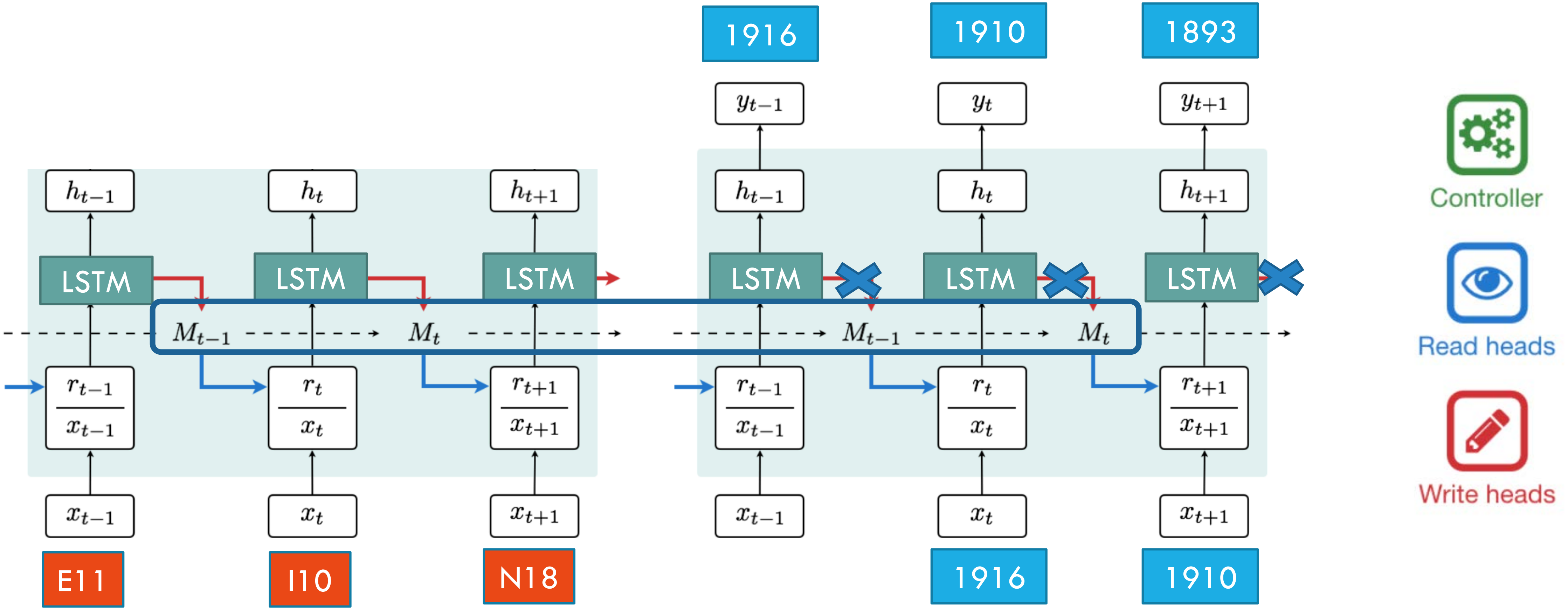
The decoder reads the memory and produces a sequence of output symbols

During decoding, the memory is write-protected (DCw-MANN)



#REF: Hung Le, Truyen Tran, and Svetha Venkatesh. "Dual Control Memory Augmented Neural Networks for Treatment Recommendations", PAKDD18.

DC-MANN



#Ref: https://medium.com/snips-ai/ntm-lasagne-a-library-for-neural-turing-machines-in-lasagne-2cdce6837315

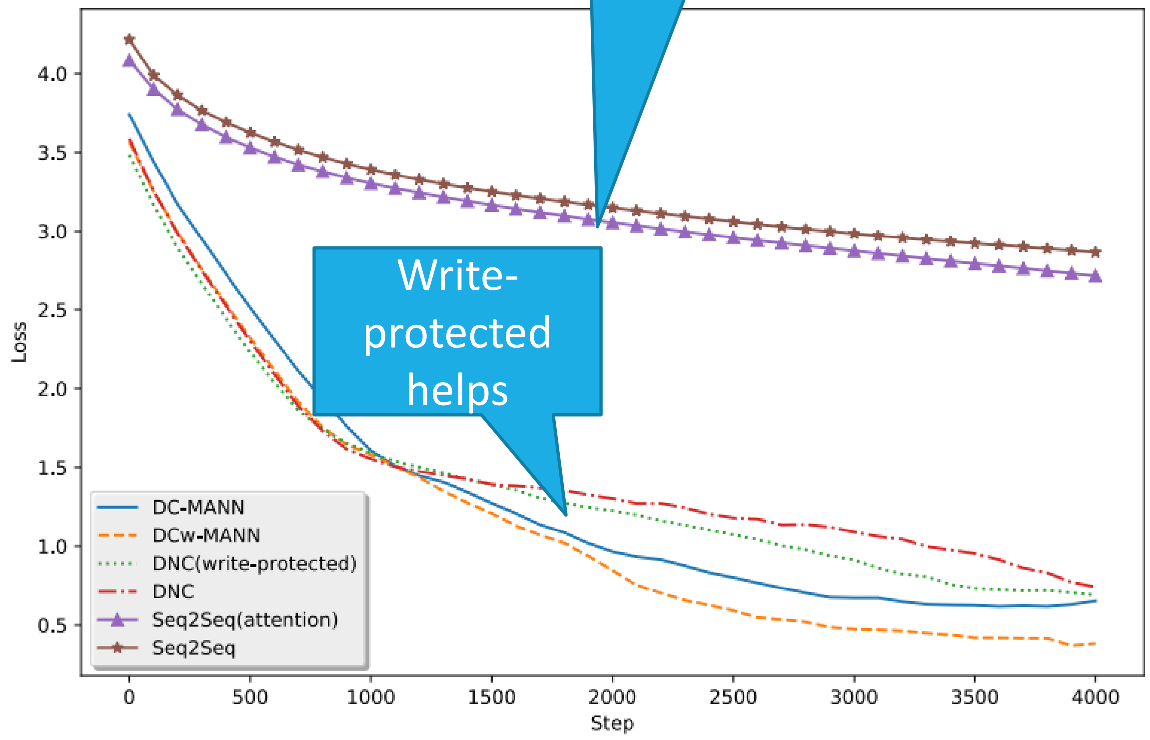
Result: Odd-Even Sequence Prediction

- Input: a sequence of random odd numbers → output: a sequence of even numbers
- Output:

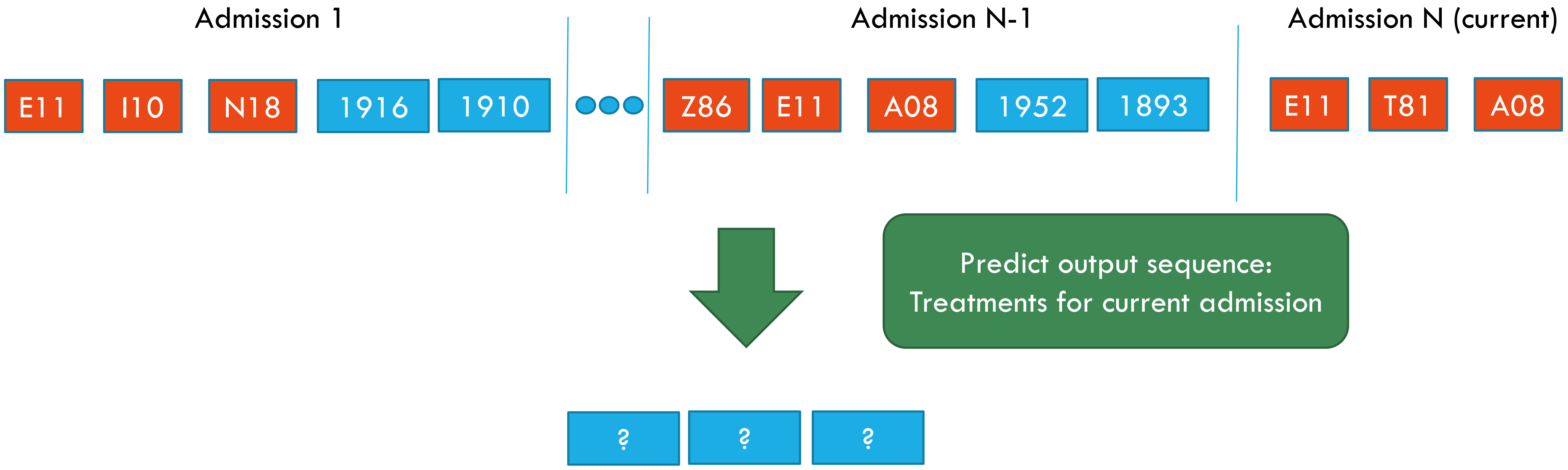
$$y_n = \begin{cases} 2x_n & n \le \lfloor \frac{L}{2} \rfloor \\ y_{n-1} + 2 & n > \lfloor \frac{L}{2} \rfloor \end{cases}$$

Model	NLD
Seq2Seq	0.679
Seq2Seq with attention	0.637
DNC	0.267
DNC (write-protected)	0.250
DC-MANN	0.161
DCw-MANN	**0.082**

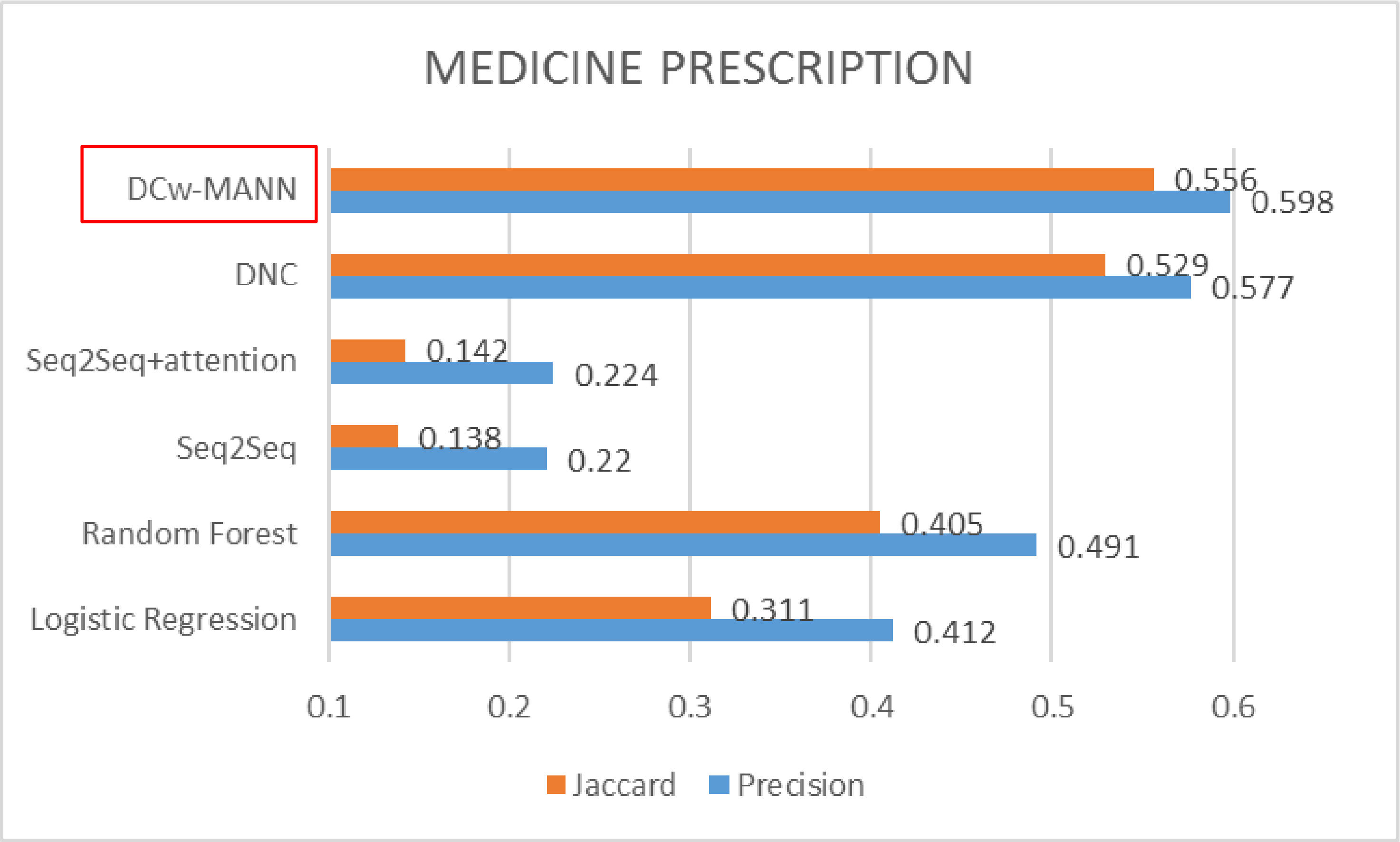
Without memory, LSTMs fail the task



Treatment recommendation



Result: Medicine prescription



Compared to DNC

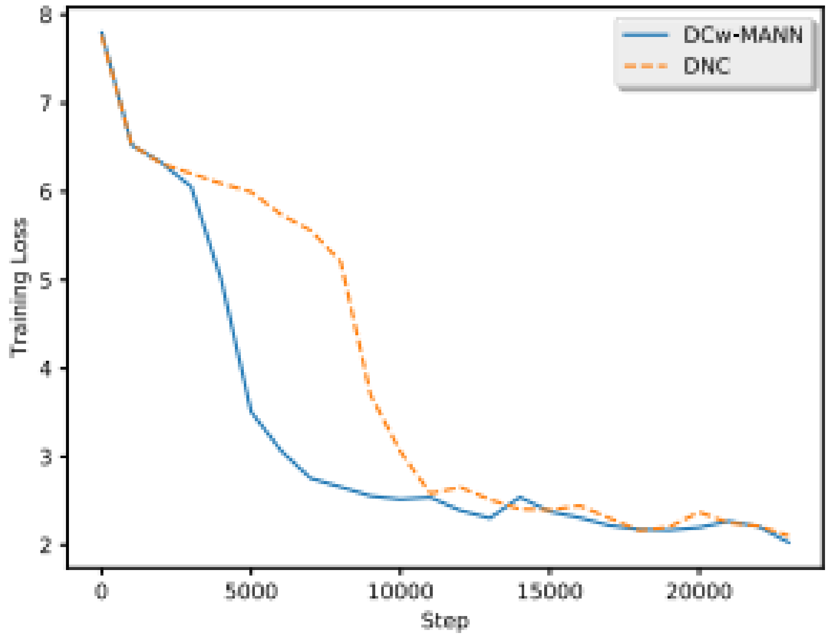


Fig. 5. Training Loss of Drug Prescription Task

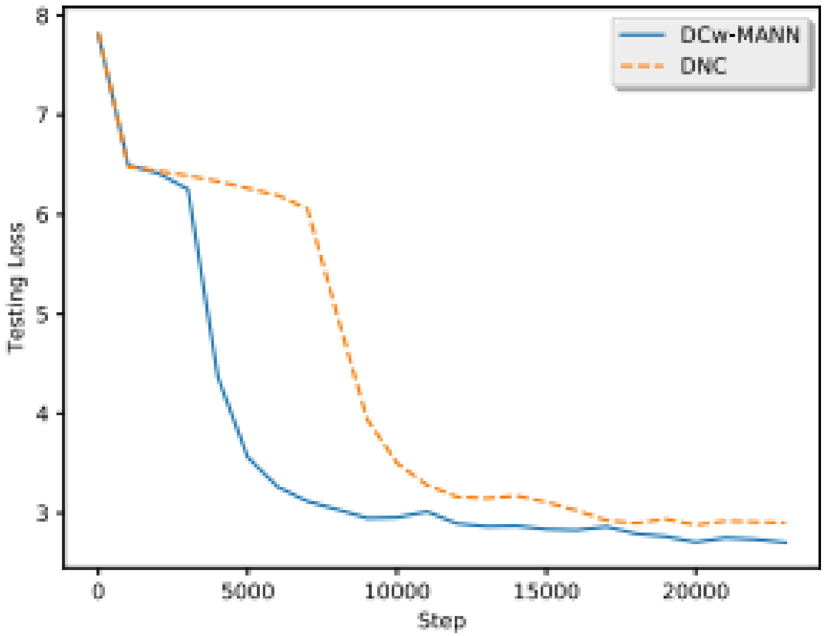


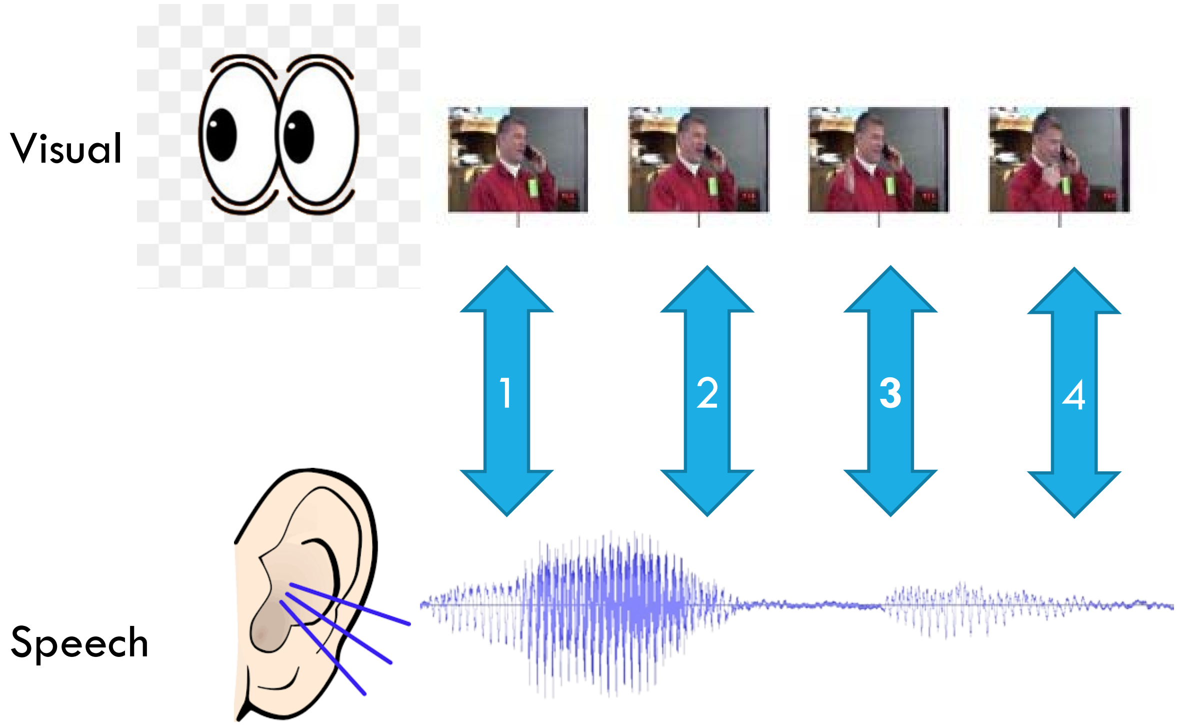
Fig. 6. Testing Loss of Drug Prescription Task

Dual-view sequential problems

Hung Le, Truyen Tran & Svetha Venkatesh

KDD'18

Synchronous two-view sequential learning



Asynchronous two-view sequential learning Healthcare: medicine prescription

Diagnoses

E11 I10 N18 Z86 E11

1916 1910 1952 1893

Procedures

Medicines

DOCU100L ACET325

Asynchronous two-view sequential learning Healthcare: disease progression

Previous diagnoses

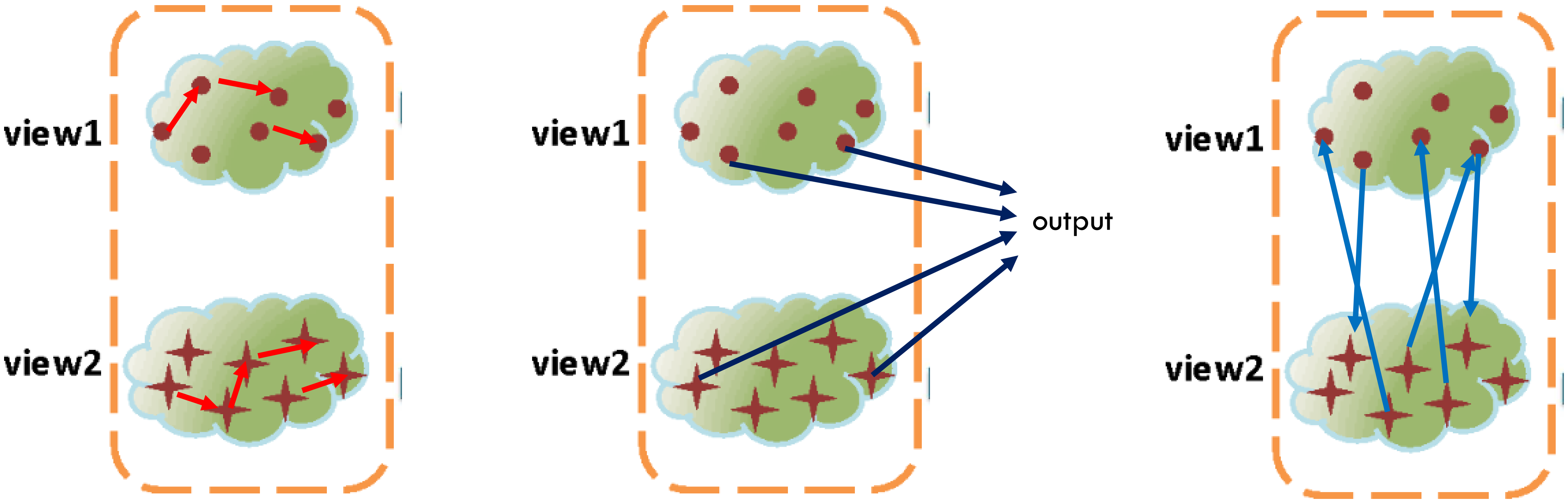
Future diagnoses ???

E11 I10 N18 Z86 E11

1916 1910 ACET325 DOCU100L

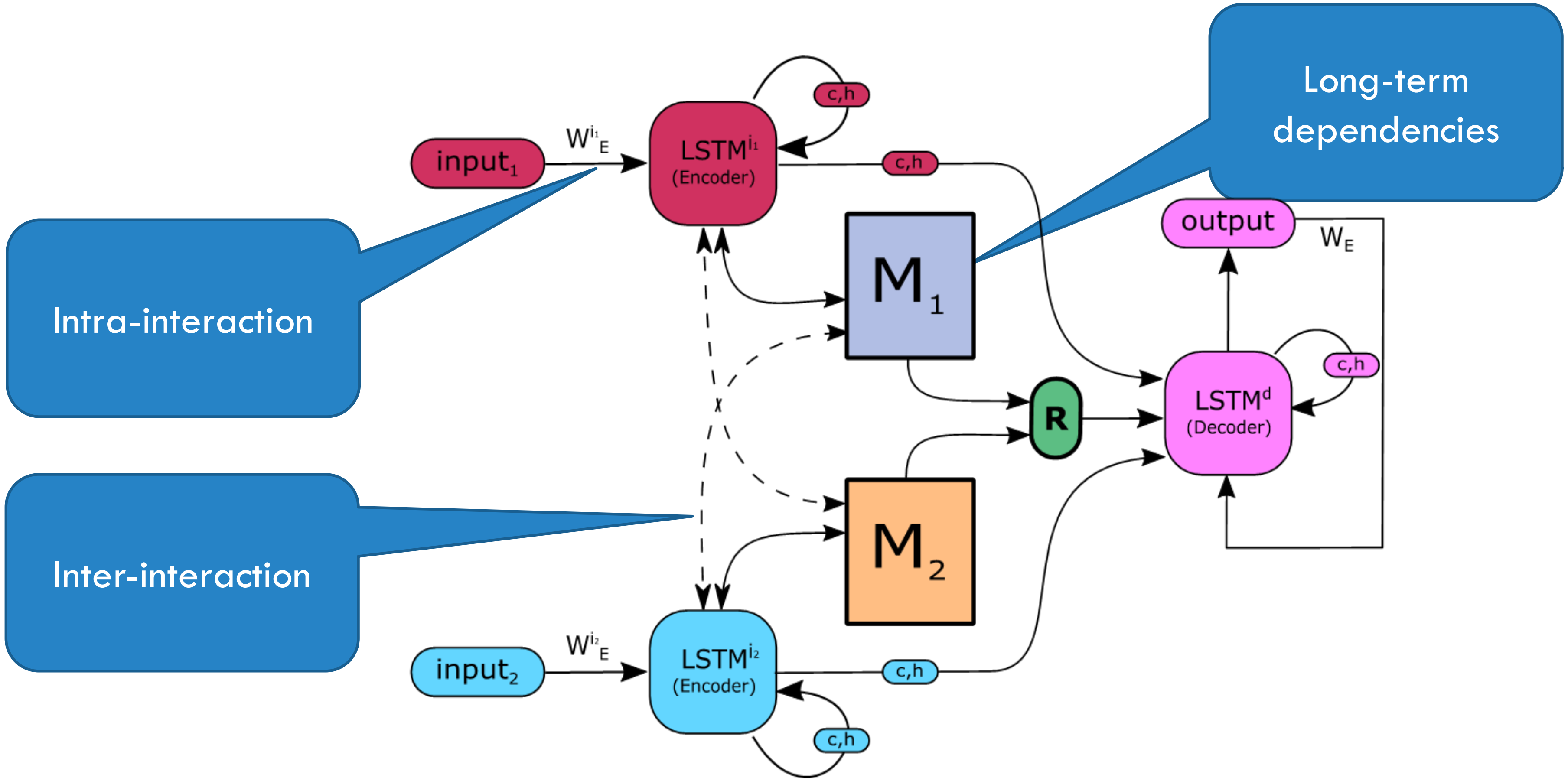
Previous interventions

Intra-view & inter-view interactions



#Ref: Le, Hung, Truyen Tran, and Svetha Venkatesh. "Dual Memory Neural Computer for Asynchronous Two-view Sequential Learning." *KDD18*.

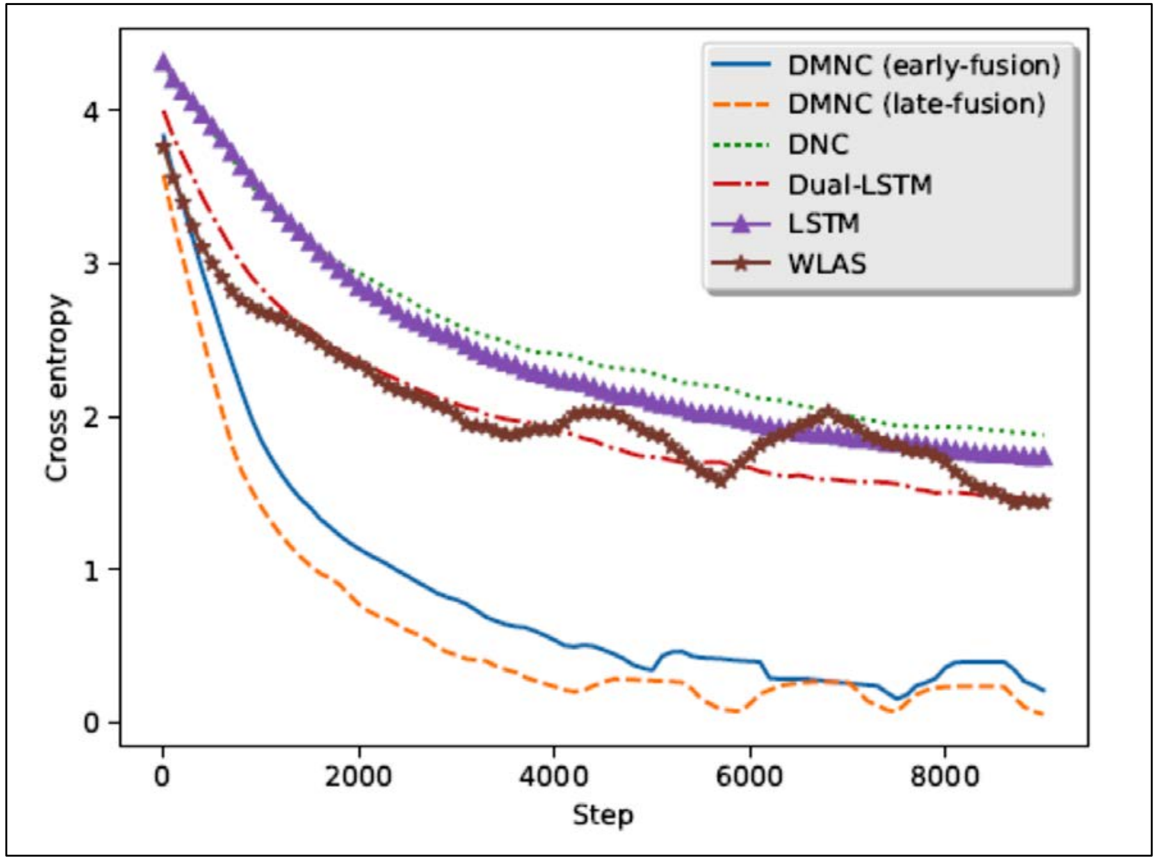
Dual architecture



Dual Memory Neural Computer (DMNC)*. There are two encoders and one decoder implemented as LSTMs. The dash arrows represent cross-memory accessing in early-fusion mode*

Simple sum, but distant, asynchronous

$$\{y_i = x_i^1 + x_{L+1-i}^2\}_{i=1}^{L}$$

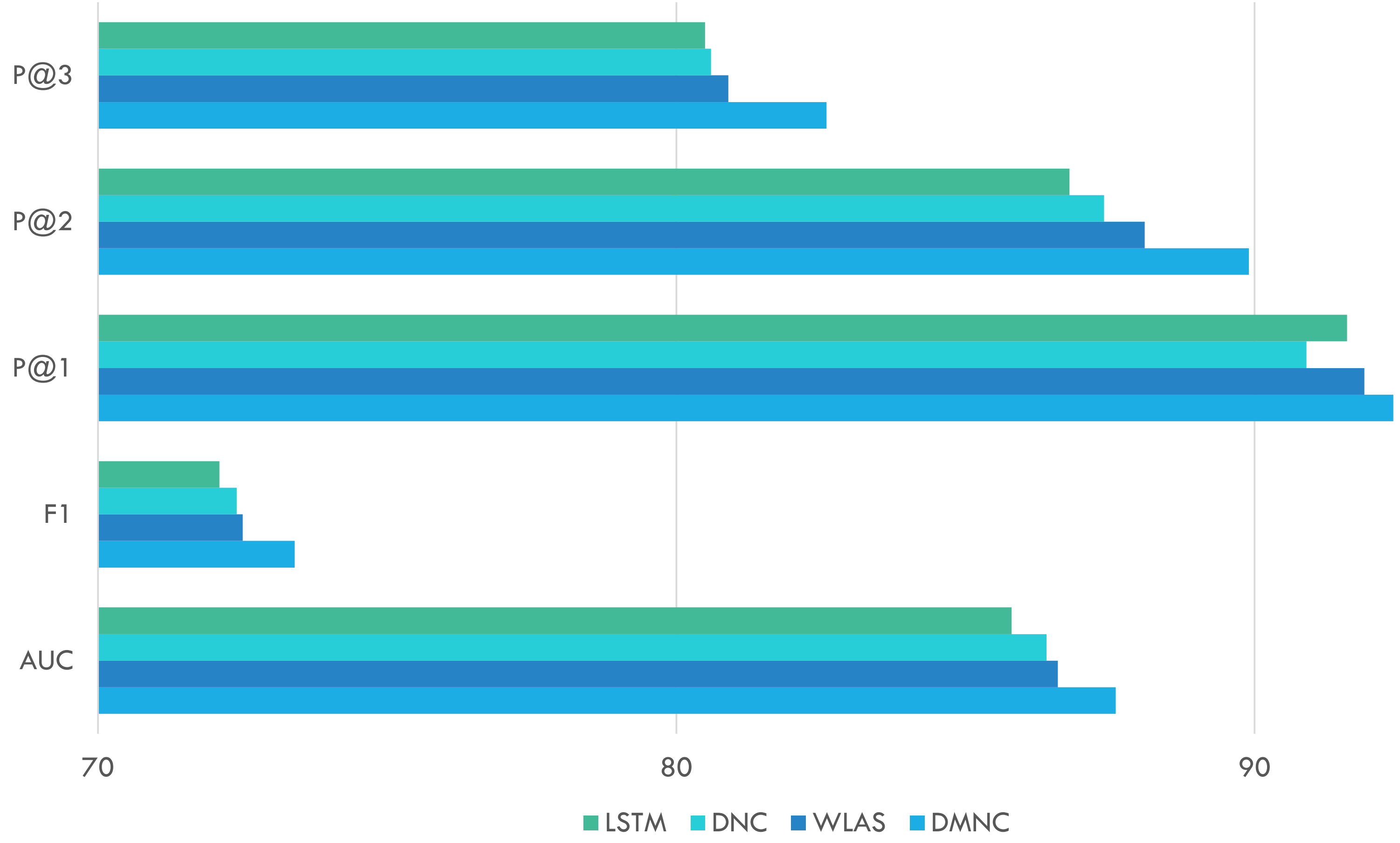


Learning curve

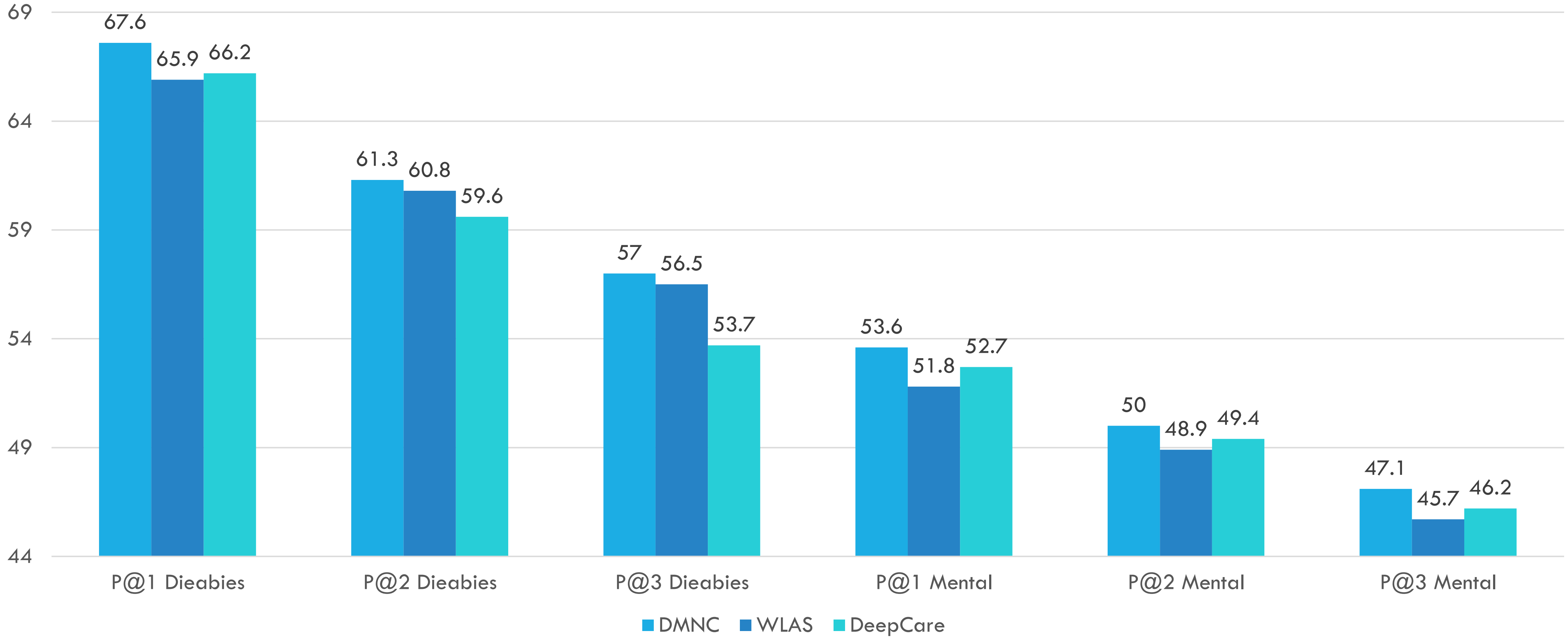
Accuracy

DMNC	Others
≈ 99%	<55%

Medicine prescription performance (data: MIMIC-III)



Disease progression performance (data: MIMIC-III)



Bringing variability in output sequences

Hung Le, Truyen Tran & Svetha Venkatesh

Submitted to NIPS'18

Motivation: Dialog system

A dialog system needs to maintain the history of chat (e.g., could be hours)

- → Memory is needed

The generation of response needs to be flexible, adapting to variation of moods, styles

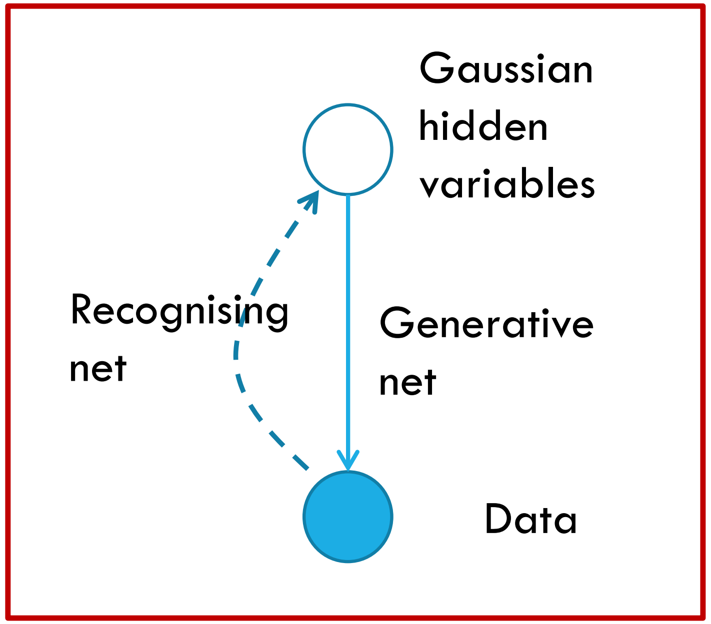
- Current techniques are mostly based on LSTM, leading to “stiff” default responses (e.g., “I see”).

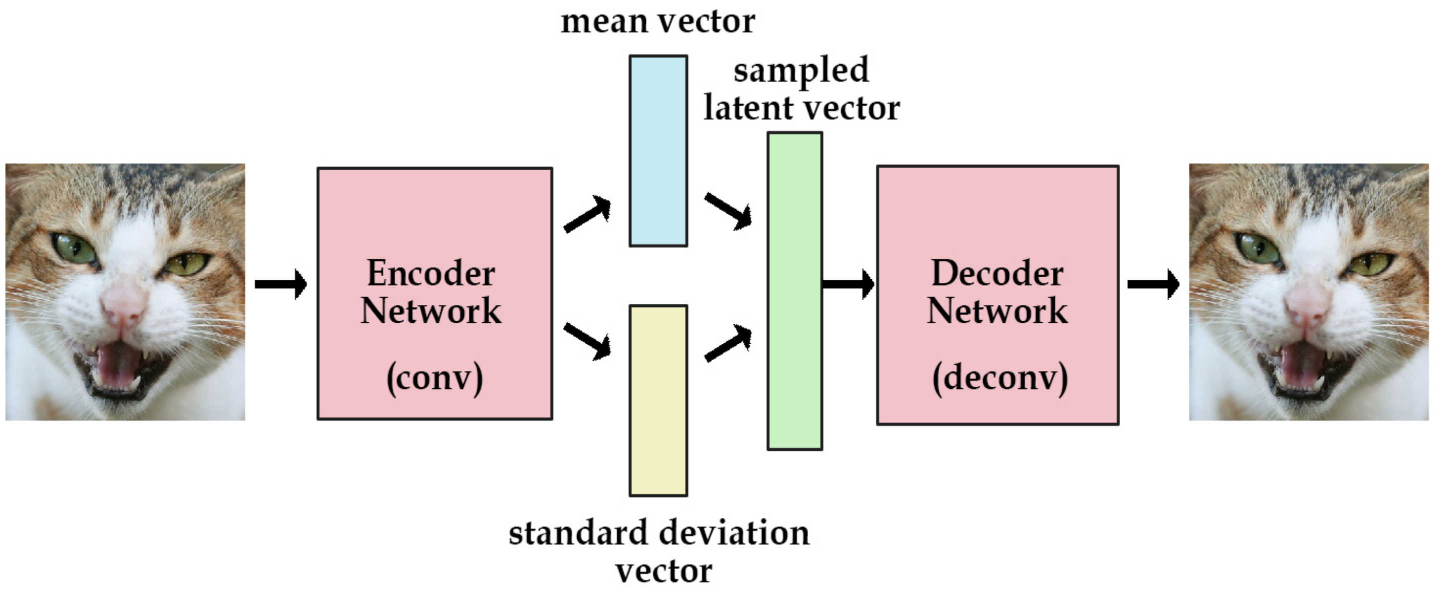
There are many ways to express the same thought

- → Variational generative methods are needed.

Variational Auto-Encoder (VAE)
(Kingma & Welling, 2014)

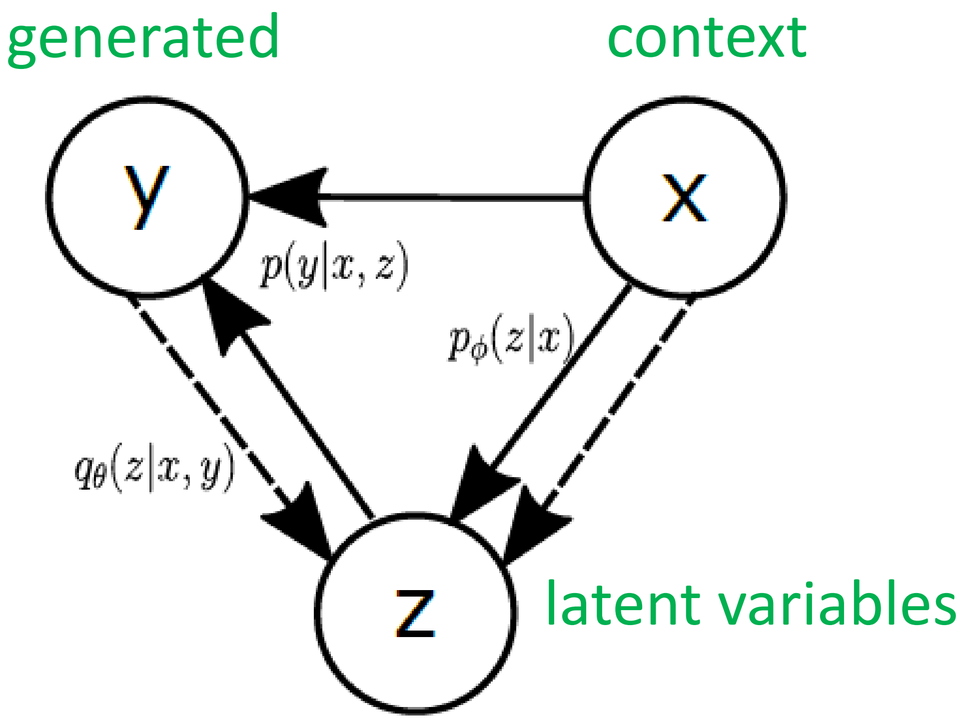
Two separate processes: generative (hidden → visible) versus recognition (visible → hidden)



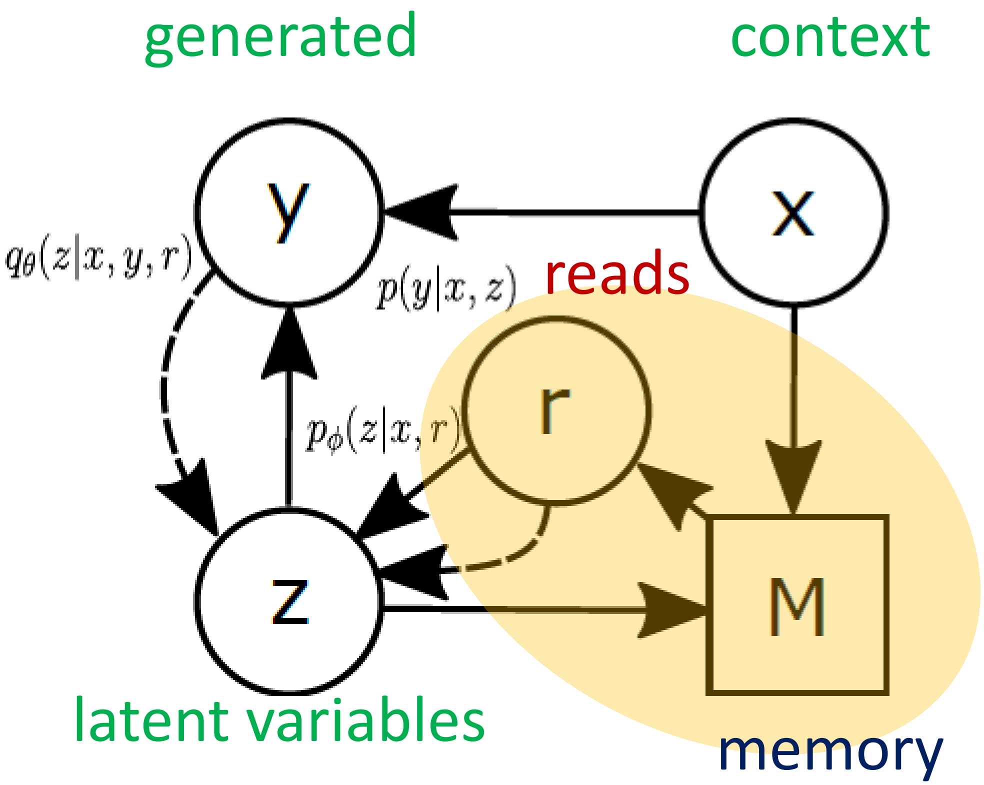


http://kvfrans.com/variational-autoencoders-explained/

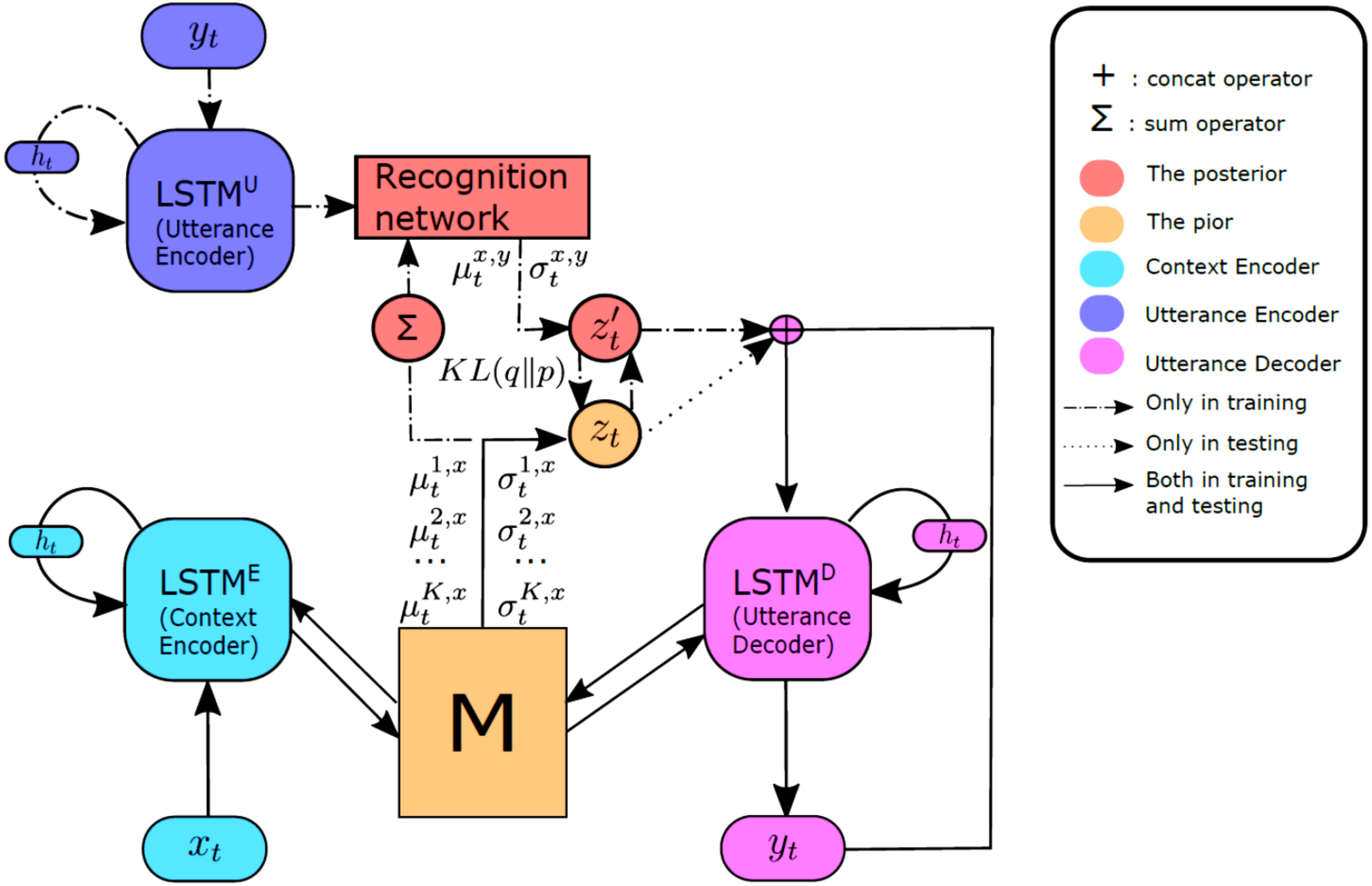
Variational memory encoder-decoder (VMED)



Conditional Variational Auto-Encoder



VMED


y_t
h_t
LSTM^U (Utterance Encoder)
Recognition network
$\mu_t^{x,y}$ $\sigma_t^{x,y}$
Σ
z'_t
$KL(q\|p)$
z_t
$\mu_t^{1,x}$ $\mu_t^{2,x}$ … $\mu_t^{K,x}$
$\sigma_t^{1,x}$ $\sigma_t^{2,x}$ … $\sigma_t^{K,x}$
h_t
LSTM^E (Context Encoder)
M
LSTM^D (Utterance Decoder)
h_t
x_t
y_t
+ : concat operator
Σ : sum operator
The posterior
The pior
Context Encoder
Utterance Encoder
Utterance Decoder
Only in training
Only in testing
Both in training and testing

Sample response

Input context	Response
Reddit comment: What is your favorite scene in film history ? Mine is the restaurant scene in the Godfather.	**Seq2Seq:** The scene in **Seq2Seq-att:** The final **DNC:** The scene in **CVAE:** Inception god! Not by a shark /*/ Amour great /*/ Pro thing you know 3 dead **VMED (K=3):** The opening scene from history movie /*/ The scene in a shot nights! Robin movie /*/ The psycho scene in fight from
Reddit comment: What actor will win an Oscar in the next 10 years ?	**Seq2Seq:** Colin **Seq2Seq-att:** Liam Neeson **DNC:** Tom Gyllenhaal **CVAE:** Daryl and Aaron /*/ Carefully count Alfred Deniro /*/ Ponyo Joker posible **VMED (K=3):** Edward or Leo Dicaprio goes on /*/ Dicaprio will /*/ Dicaprio Tom has actually in jack on road

Sample response (2)

LJ user: Your very pretty and your is very cute. May i add ya to my friends list ?	**Seq2Seq:** I! Add and too you back **Seq2Seq-att:** I did may! Away back **DNC:** Sure you added **CVAE:** Sure ! I can add you /*/ Thank cool of surely /*/ Thank hi of sure! **VMED (K=3):** Thank cool for sure /*/ Add definitely! Sure surely friends /*/ Thank girl go ahead
Cornell movies: Nobody can murder someone with their feelings . I mean that is crazy ?	**Seq2Seq:** Yes you are **Seq2Seq-att:** Really not is it **DNC:** Managing the truth **CVAE:** Sure not to be in here /*/ Oh yes but i know! /*/ That to doing with here and **VMED (K=4):** You are right! /*/ That is crazy /*/ You can't know Jimmy
OpenSubtitle: I'm obliged for your hospitality. I appreciate it and your husband too.	**Seq2Seq:** That is have got coming about these **Seq2Seq-att:** May you not what nothing nobody **DNC:** Yes i am taking this **CVAE:** No . that for good! And okay /*/ All in the of two thing /*/ Sure. Is this! **VMED (K=3):** I know. I can afford /*/ I know nothing to store for you pass /*/ I know. Doing anymore you father

Bringing relational structures into memory

Trang Pham, Truyen Tran & Svetha Venkatesh

IJCAI’17 WS+

NTM as matrix machine

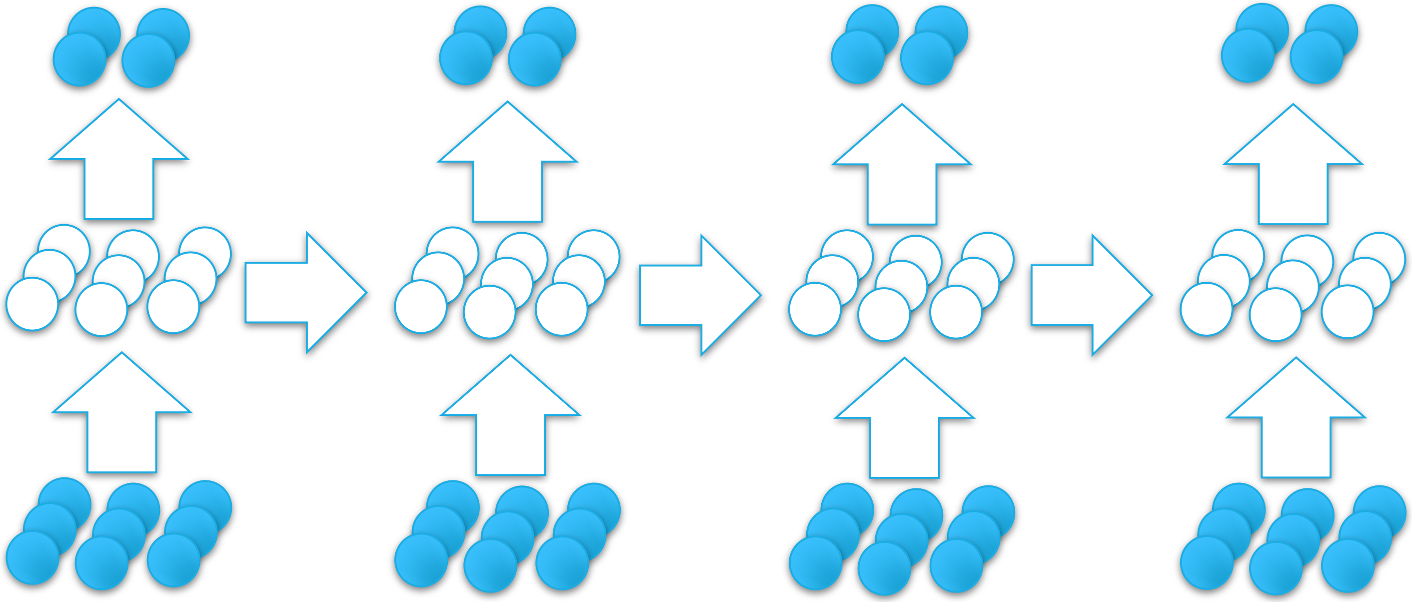
Controller and memory operations can be conceptualized as matrix operations

- **Controller is a vector changing over time**
- **Memory is a matrix changing over time**

#REF: Kien Do, Truyen Tran, Svetha Venkatesh, “Learning Deep Matrix Representations”, *arXiv preprint arXiv:*1703.01454

Recurrent dynamics

$$\boxed{H_t = \sigma(U_x^\top X_t V_x + U_h^\top H_{t-1} V_h + B)}$$



Idea: Relational memory

Independent memory slots not suitable for relational reasoning

Human working memory sub-processes seem inter-dependent

Relational structure

Transformation

$$\boxed{H_t = \sigma(U_x^\intercal X_t V_x + U_h^\intercal H_{t-1} V_h + B)}$$

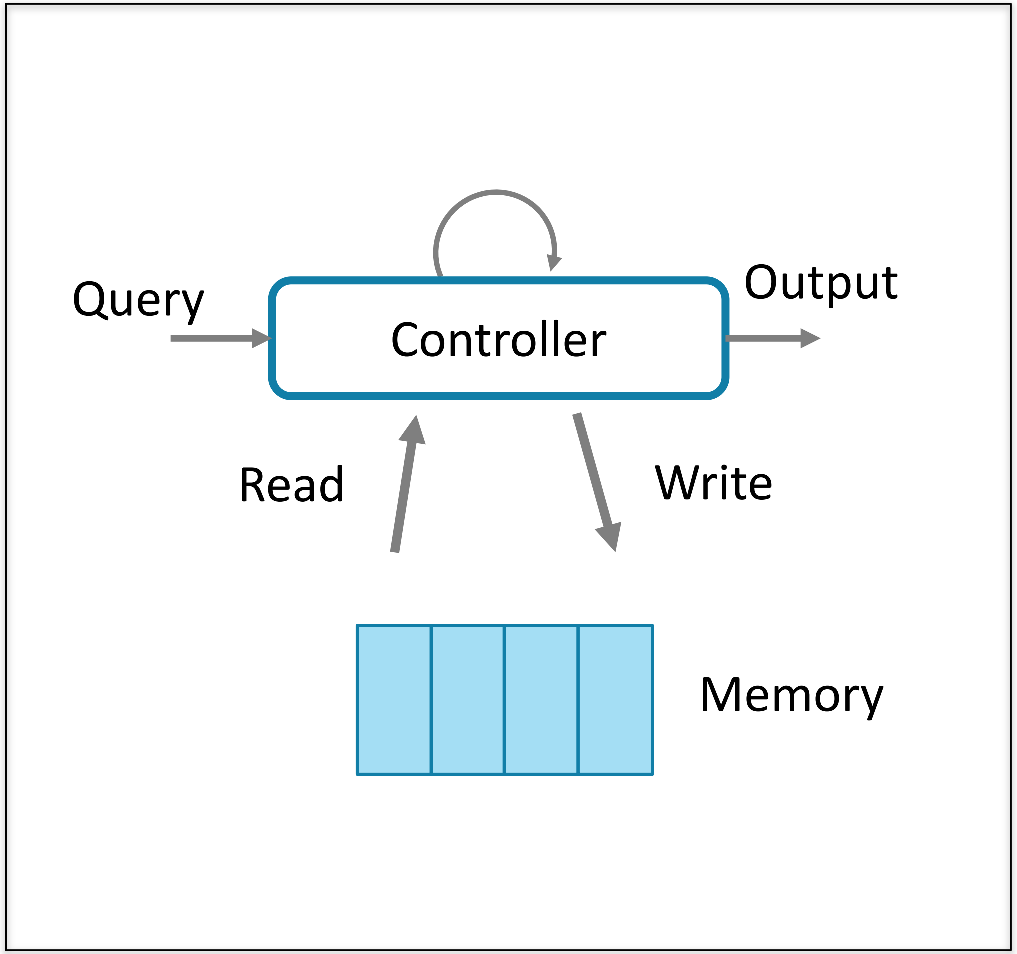
Old memory

Time-aware bias

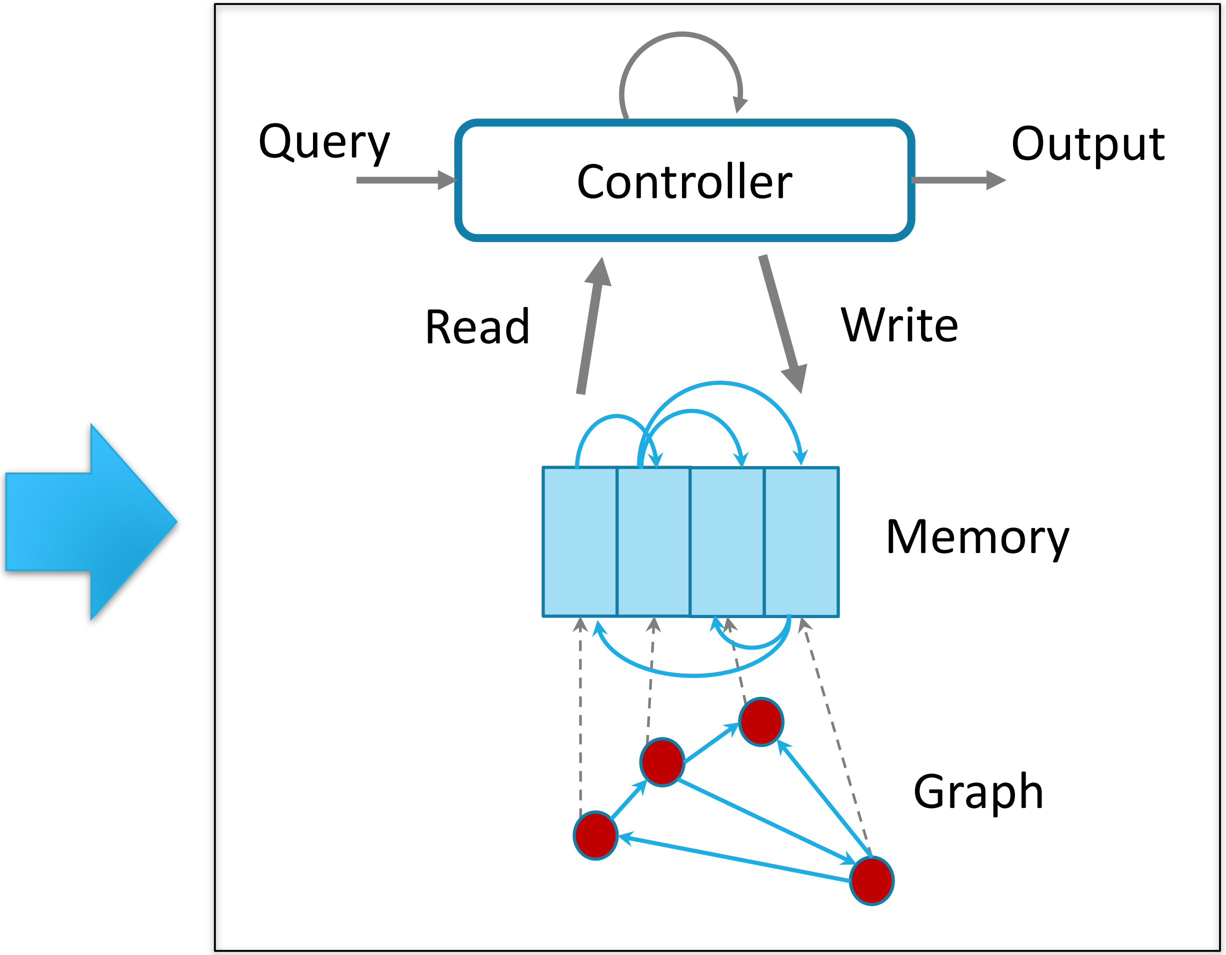
New information

New memory proposal

Relational Dynamic Memory Network (DMNN)

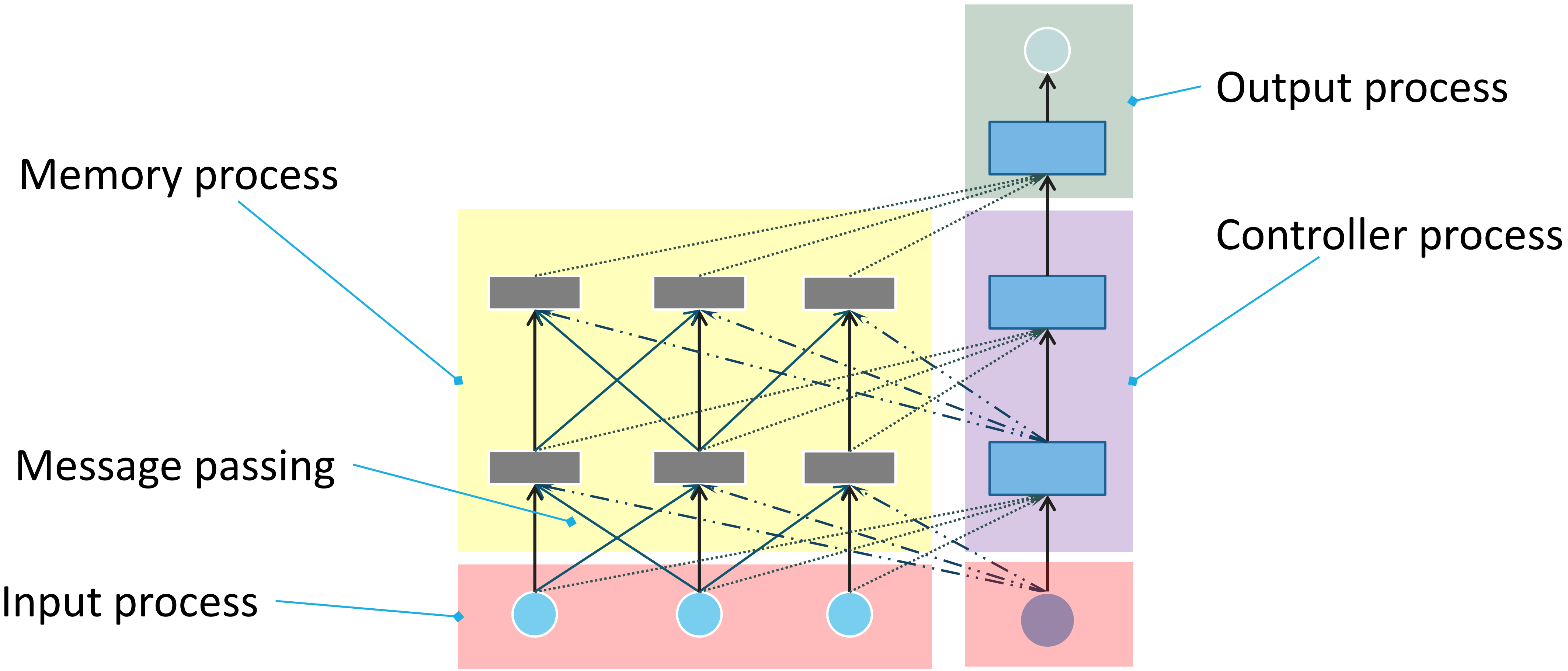


NTM



Relational Dynamic Memory Network

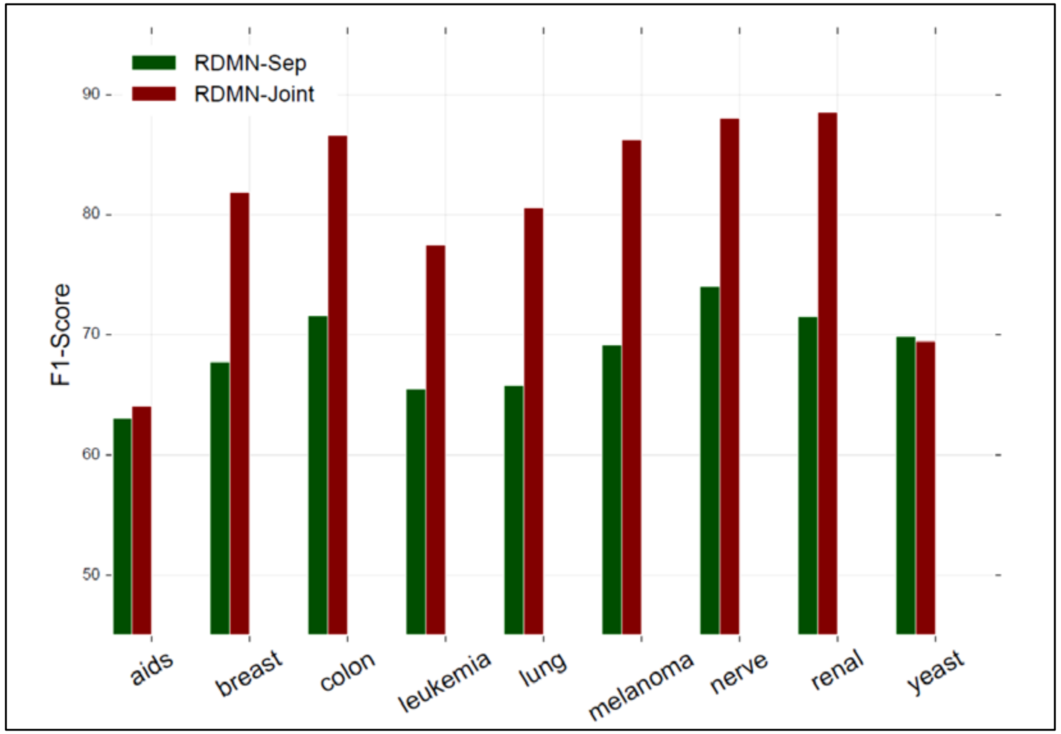
RDMN unrolled

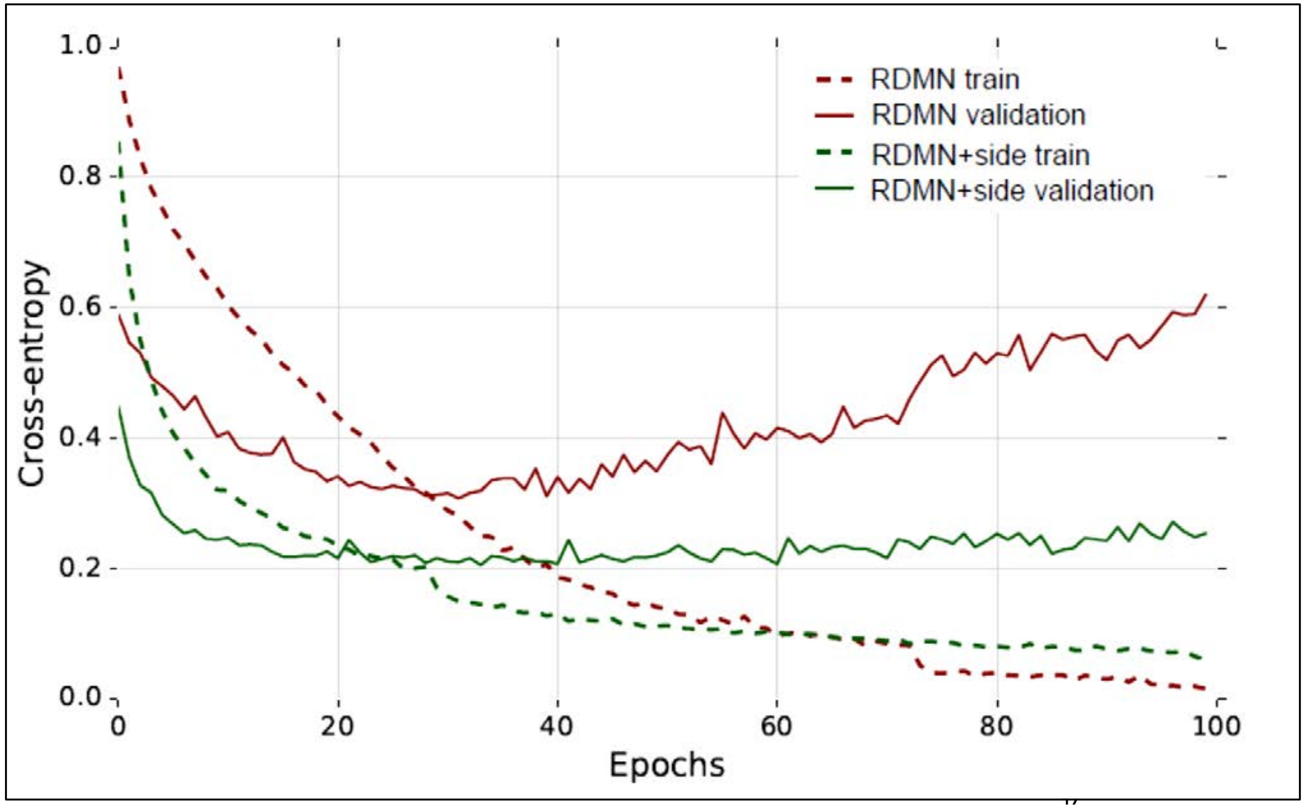


Drug-disease response

Molecule → Bioactivity

Model	MicroF1	MacroF1	Average AUC
SVM	66.4	67.9	85.1
RF	65.6	66.4	84.7
GB	65.8	66.9	83.7
NeuralFP [19]	68.2	67.6	85.9
MT-NN [51]	75.5	78.6	90.4
RDMN	77.8	80.3	92.1





Chemical reaction

Molecules → Reaction

	CCI900		CCI800	
	AUC	F1-score	AUC	F1-score
Random Forests	94.3	86.4	98.2	94.1
Highway Networks	94.7	88.4	98.5	94.7
DeepCCI [38]	96.5	92.2	99.1	97.3
RDMN	96.6	92.6	99.1	97.4
RDMN+multiAtt	97.3	93.4	99.1	97.8
RDMN+FP	97.8	93.3	99.4	98.0
RDMN+multiAtt+FP	98.0	94.1	99.5	98.1
RDMN+SMILES	98.1	94.3	99.7	97.8
RDMN+multiAtt+SMILES	**98.1**	**94.6**	**99.8**	**98.3**

Team @ Deakin (A2I2)

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