Sequence Modeling: Recurrent Neural Networks

High Dimensional and Deep Learning – juliette.chevallier@insa-toulouse.fr
N7 & INSA Toulouse, 5th year ModIA

Sequence Modeling

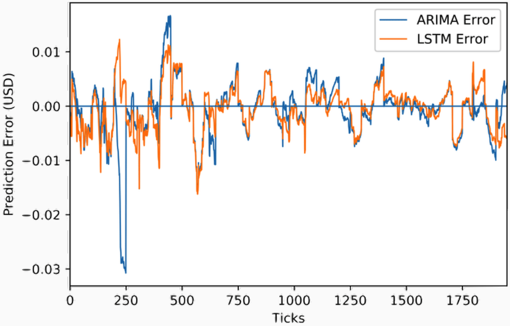
Sequential Data

Sequence $\leftrightarrow$ Explicit order on the observations that must be preserved when training models and making predictions.

- **Sequence *Prediction***: Weather forecasting, Stock market prediction, Product recommendation
- **Sequence *Classification***: DNA seq. classification, Anomaly detection, Sentiment analysis;
- **Sequence *Generation***: Text generation, Handwriting prediction, Music generation;
- **Sequence-to-Sequence *Prediction***: Multi-Step time series forecasting, Text summarization, Program execution.

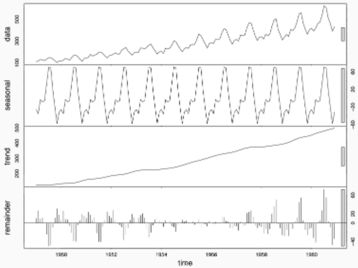
From: Vinyals, Toshev, Bengio, Erhan. Show and tell: A neural image caption generator. *CVPR* 2015

Do not get rid of traditional models too quickly!



Baughman, Haas, Wolski, Foster, Chard. *Predicting Amazon Spot Prices with LSTM Networks*. 2018.

Sequence Modeling



AR Autoregressive

MA Moving average

ARMA Autoregressive moving average

ARIMA Autoregressive integrated moving average

SARIMA Seasonal autoregressive integrated moving average

- Describing temporal dynamics in great detail;
- Realization of a stochastic process;
- Decomposition: trend, seasonality and (stochastic) reminder.

ARIMA *vs.* (Recurrent) Neural Network

ARIMA:	**Neural Network:**
+ Out-perform deep learning methods for forecasting **short-term** + Out-perform deep learning methods for forecasting on **univariate** data	

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$\rightsquigarrow$ **Neural Networks**

Naive approaches

Sequential Data: Audio, Speech, Language, Videos with time context, Time series

Question: *How can we integrate this context in neural networks?*

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Time series prediction $\longleftrightarrow$ Regression problem: x_{t+1} as a function of x_t

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Feed the whole sequence to a huge network

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Outline

Recurrent Neural Networks

Information Persistence – Parameter-Sharing

- Humans don't start their thinking from scratch every second:
  While reading, each word is understood according to your previous ones.
  Your thoughts have persistence.

- Traditional neural networks can't do this.

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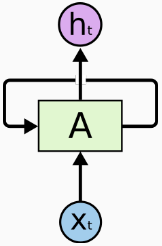


 # Input x_t at time t

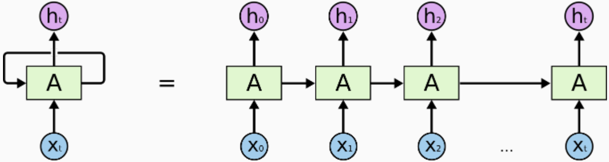
 # Output h_t at time t

 # Loop allows information to be passed from one step of the network to the next

Little (1974), Hopfield (1982),
Rumelhart, Hinton & Williams (1986), Elman (1990)

Unfolding Computational Graphs

- RNN $\equiv$ Multiple copies of the **same** network,
  each passing a message to its successor: $h_t = \boldsymbol{f}(h_{t-1}, x_t; \theta)$.



- **Advantages of the unfoldingprocess:**
  - Whatever the sequence length, the learned model always has the same input size,
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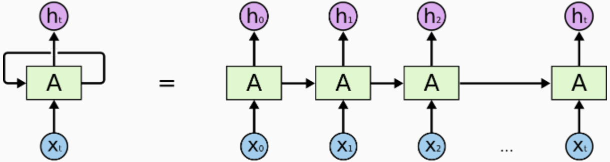

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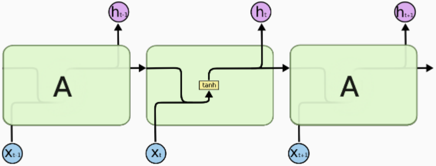
$\leadsto$ *A single model f that operates*

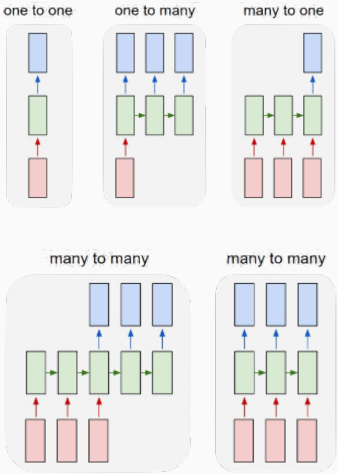
- *on all time steps,*
- *and all sequence lengths.*



Standard Recurrent Neural Networks

Different types of RNN's:

- One-to-one *e.g.* Image classification,
- One-to-Many *e.g.* Image captioning,
- Many-to-One *e.g.* Sentiment analysis,
- Many-to-Many *e.g.* Machine translation.



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RNNs are Turing-Complete

RNN:

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Programming terms: Running a fixed program with certain inputs and some internal variables

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RNNs are Turing-Complete

They can simulate arbitrary programs (with proper weights)

- Similar to universal approximation theorems for neural nets
- Shouldn't read too much into this.

Siegelmann and Sontag (1992)

Recurrent Neural Networks

Bidirectional RNNs

- All the recurrent networks we have considered so far have a causal structure:

  State at time t captures only information from the past $x_1, \ldots, x_{t-1}$, and the present input x_t

- In many *applications*, however, we want to output a prediction of y_t that may depend on the whole input sequence

  Handwriting recognition, Speech recognition, Bio-informatics, *etc.*

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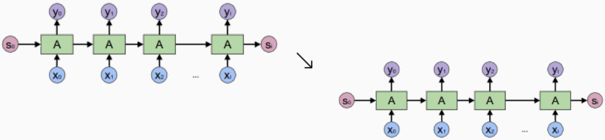

Schuster & Paliwal (1997), Graves (2012)

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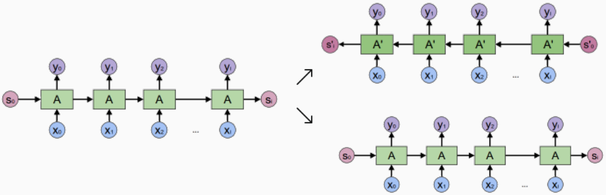

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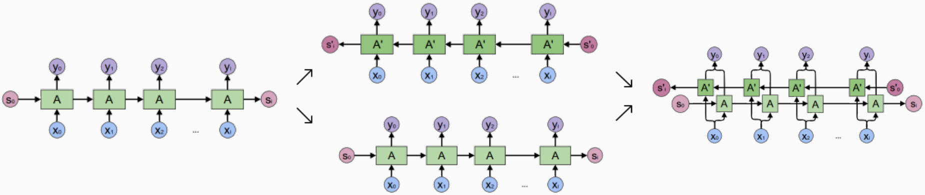

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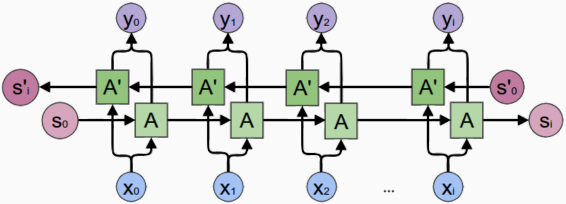

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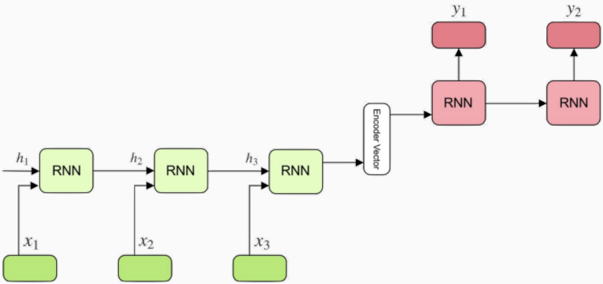
Sequence-to-Sequence Model

The model consists of **3 parts**: Encoder, Context (encoder vector) and Decoder.



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Encoder:

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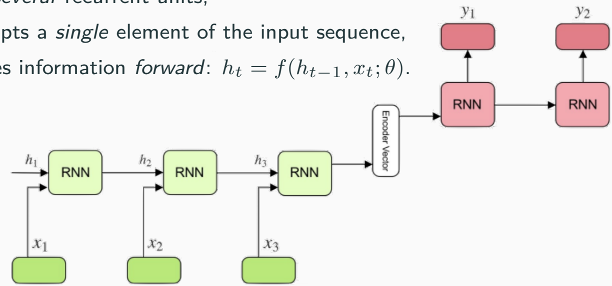

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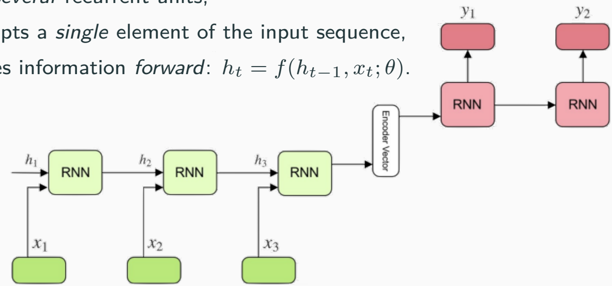

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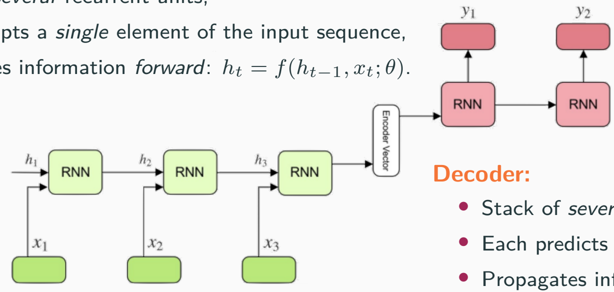

Decoder:

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Deep Recurrent Networks

RNN: Three blocks of parameter/transformations:

1. `Input` $x_t \longmapsto$ `Hidden state` h_t
2. Previous `hidden state` $h_t \longmapsto$ Next `hidden state` h_{t+1}
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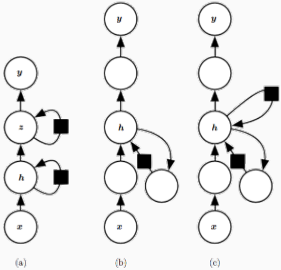
$\rightsquigarrow$ ***We can introduce depth into each of these operations!***



Deep Learning, Goodfellow, Bengio, Courville (2016)
§ 10.5 Deep Recurrent Networks

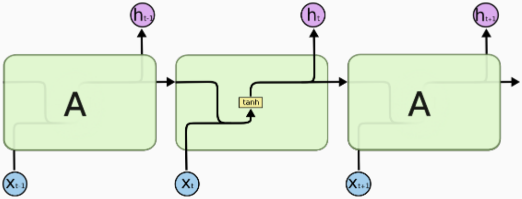
www.deeplearningbook.org

Training Recurrent Networks

Forward Propagation (Input & output of same length)

Weight matrices: Connections between the different states

Activation functions:



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3. `Hidden-to-Output`: $\boldsymbol{V}$

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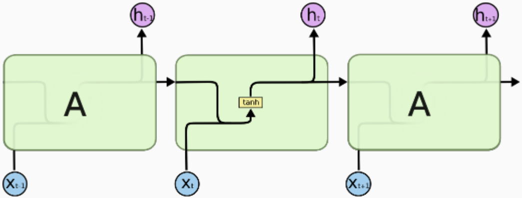

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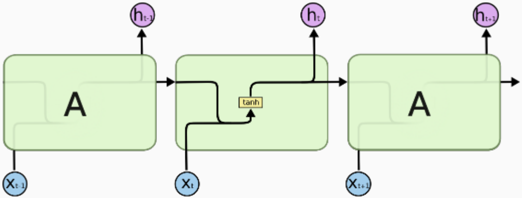
1. `Input-to-Hidden`: Hyperbolic tangent activation function
2. Assume that the output is discrete.
   Outputs $\longleftrightarrow$ Unnormalized probabilities of each possible value
   $\rightsquigarrow$ Softmax aftivation function to obtain normalized probabilities



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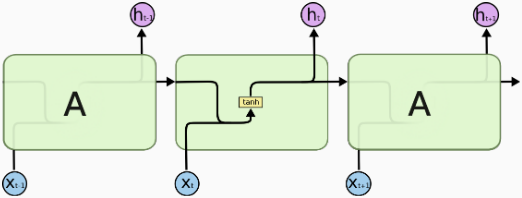

Given initial state h_0,
For each step $t \in [\![1, T]\!]$:

$$\boxed{\begin{aligned} h_t &= \tanh\left(W h_{t-1} + U x_t + b\right) \\ \hat{y}_t &= \operatorname{softmax}\left(V h_t + c\right) \end{aligned}}$$

Training Recurrent Networks

Computing the Gradient in a Recurrent Neural Network

Total loss function for a given sequence values x paired with a sequence of y

$$\begin{aligned}\mathcal{L}\left(\{x_1,\ldots,x_T\},\{y_1,\ldots,y_T\};\theta\right) &= \sum_{t=1}^{T} L_t(\theta) \quad ; \quad \theta = (U, V, W, b, c) \\ &= \sum_{t=1}^{T} -\log p_{\text{model}}(y_t|\{x_1,\ldots,x_t\};\theta)\end{aligned}$$

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Gradient of this loss function expensive operation:

1. A **forward** propagation pass moving left to right,
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$\Longrightarrow$ $\boxed{\text{Runtime} = O(T)}$ and cannot be reduced by parallelization...

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$\Longrightarrow$ $\boxed{\text{Runtime} = O(T)}$ and cannot be reduced by parallelization...

Moreover, states computed in the forward pass must be stored until they are reused during the backward pass

$\Longrightarrow$ $\boxed{\text{Memory cos} = O(T)}$

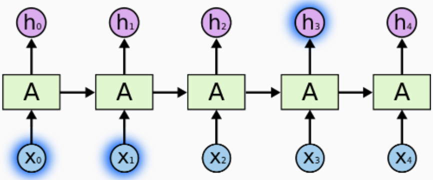
For an example: *Deep Learning*, Goodfellow et al. (2016), § 10.2.2

Training Recurrent Networks

Long-Term Dependencies

Strenght of RNNs: Being able to connect previous information to the present task

If the gap between relevant information and where it is needed is small, RNNs work "perfectly"



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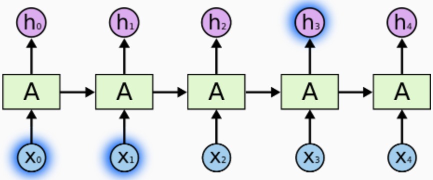
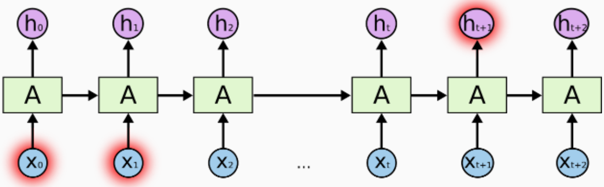


☹ Unfortunately, as this gap widens, RNNs become unable to learn to connect information...

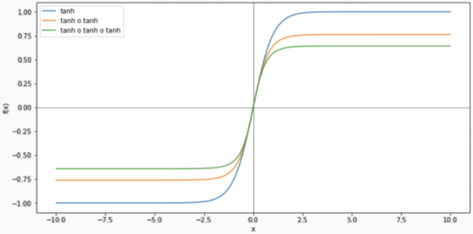


A Short Memory Model

- The hyperbolic tangent tends to *smash* the values taken as input.
- Information coming from x_1 passes t times through $\tanh$

  $\rightsquigarrow$ x_1 *is very crushed.*
- At the same time, the one from x_t passes through $\tanh$ only once

  $\rightsquigarrow$ x_t *is preserved overall.*



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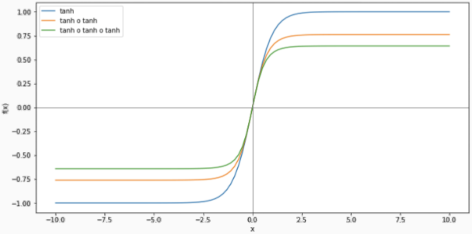

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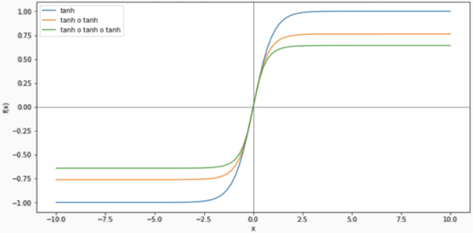

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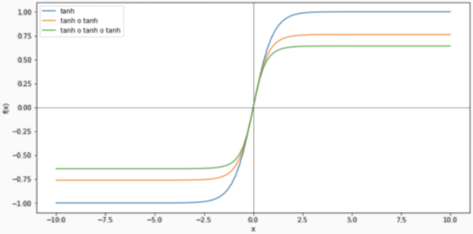

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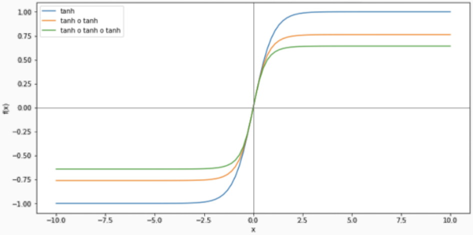

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$\rightsquigarrow$ **LSTM, GRU, ...**

Vanishing of the Gradients

Basic problem: Gradients propagated over many stages

- **vanish** (most of the time)
- or **explode** (rarely, but with much damage to the optimization)

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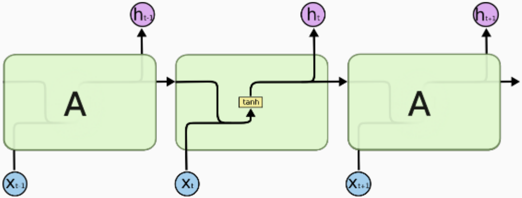
Remark: **Problem particular to recurrent networks**, due to the multiple composition of same function

Hochreiter(1991), Bengio, Simard & Frasconi (1994)

Summary of the RNN Framework



Given initial state h_0,
For each step $t \in [\![1, T]\!]$:

$$h_t = \tanh\left(W h_{t-1} + U x_t + b\right)$$
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Advantages of RNN:

- Performance not significantly affected from *missing values*;
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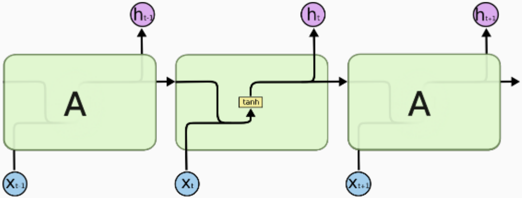

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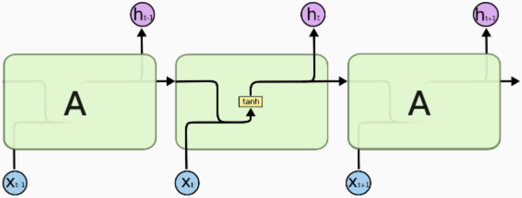
Disadvantages of RNN:

- When trained on long time series, RNNs suffer from the vanishing gradient or exploding gradient problem;
- Weak memory unable to take into account several elements of the past in the prediction of the future;
- Training of a Recurrent Neural Network hard to parallelize and computationally expensive.



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Optimization for Long-Term Dependencies

Clipping gradient: avoids gradient explode but **NOT** gradient vanish.

- Mikolov (2012): Clip the parameter gradient from a mini-batch element-wise,
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Remarks: These techniques are *not* quite useful nowadays: Most of the time using LSTM will solve the long-term dependency problem.

Take-Home Message:

It is often much easier to design a model that is easy to optimize than it is to design a more powerful optimization algorithm.

Challenge of Long-Term Dependencies

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First idea: Design a model that operates at multiple time scales

(i) Some parts operate at *fine-grained* time scales
  $\rightsquigarrow$ Handle small details,

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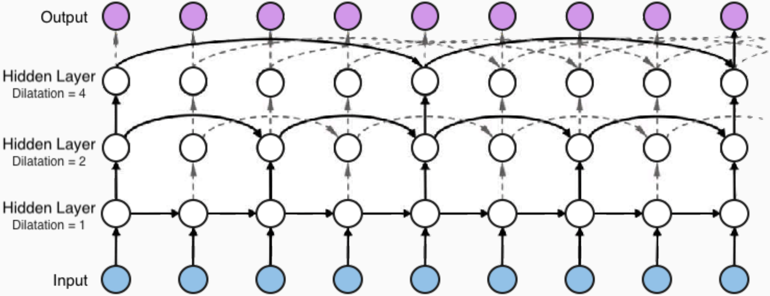

$\rightsquigarrow$ Gradients decrease exponentially with rate $\frac{T}{d}$ rather than T.

Lin, Horne, Tino and Giles (1996).

Strategies for MultipleTime Scales

Leaky Units: Mozer (1992); El Hihi & Bengio (1996).

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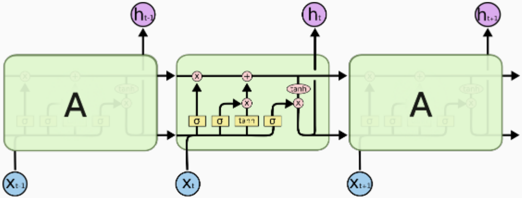
- **Idea**: Actively removing length-one connections and replacing them with longer connections.
- *Removing connections* $\neq$ *Skipping connections*:
  - *Removing connections*: Units forced to operate on along time scale;
  - *Skip connections*: Units may learn on a long time scale but may also focus on their other, short-term connections.

Gated Recurrent Neural Network

Long-Short-Term-Memory Neural Networks

"Special kind of RNN's, capable of learning long-term dependencies."

Hochreiter & Schmidhuber (1997).



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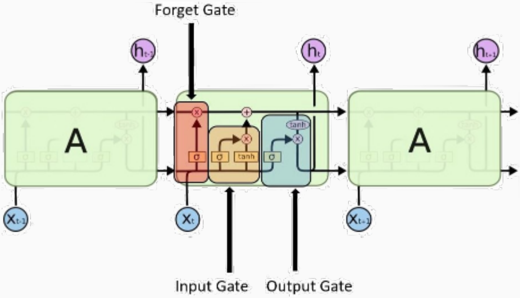

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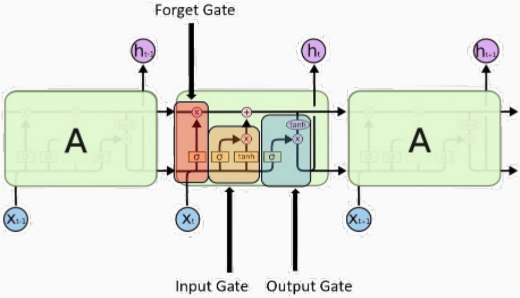

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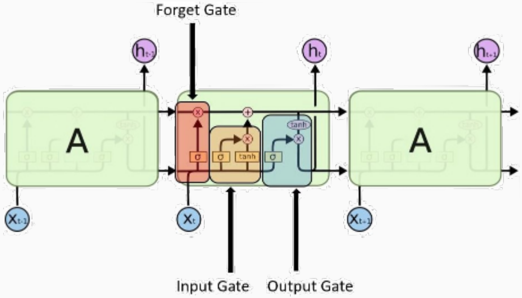

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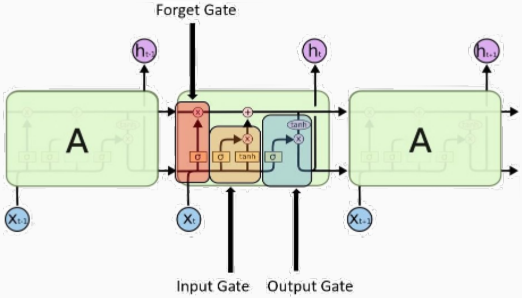

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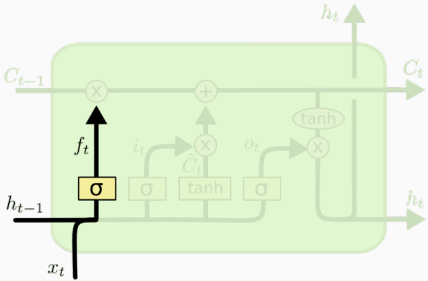
Forget Gate

"Decides how much of the past you should remember."



$$\boxed{f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)}$$

Input:

- Previous state h_{t-1},
- Content input x_t.

Layer:

- Dense layer.

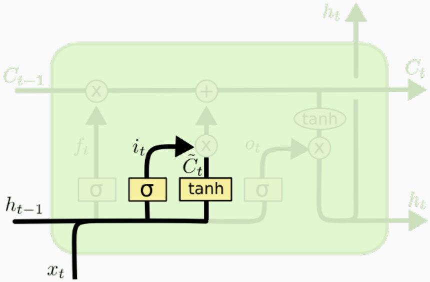
Output:

- A number between 0 (omit this) and 1 (keep this) for each number in the cell state C_{t-1}.

$\rightsquigarrow$ **Forget gate** $\equiv$ **filter** to "forget" some information of the cell state.
Term to term multiplication between f_t and C_{t-1}

$\implies$ cancellation of components of C_{t-1} whose counterparts on f_t are near 0.

"Decides how much of this unit is added to the current state."



$$\boxed{i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] + b_i\right)}$$

$$\boxed{\tilde{C}_t = \tanh\left(W_C \cdot [h_{t-1}, x_t] + b_C\right)}$$

$$\boxed{C_t = f_t \otimes C_{t-1} + i_t \otimes \tilde{C}_t}$$

Input:

- Previous state h_{t-1},
- Content input x_t.

Output:

- Cell state C_t.

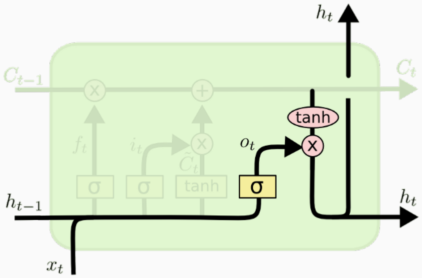
Remarks

- Input gate $i_t \equiv$ Filter,
- $\tilde{C}_t \equiv$ *Candidate* vector to update the cell state,

$\rightsquigarrow$ *Update vector* of the cell state.

Output Gate

"Decides which part of the current cell makes it to the output."



$$\boxed{o_t = \sigma\left(W_o \cdot [h_{t-1}, x_t] + b_o\right)}$$

$$\boxed{h_t = o_t \otimes \tanh(C_t)}$$

Input:

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- Content input x_t,
- Cell state C_t,

Output:

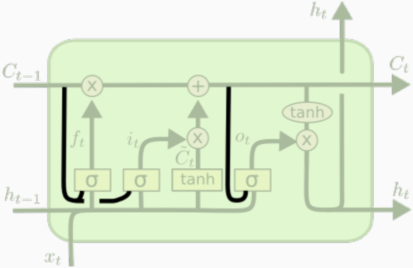
- Current state h_t.

Remarks

- Output gate $o_t \equiv$ Filter,
- New output $\equiv$ Weighted cell filtration.

Gated Recurrent Neural Network

LSTM Augmented by "Peephole Connection"



Gers & Schmidhuber (2000).

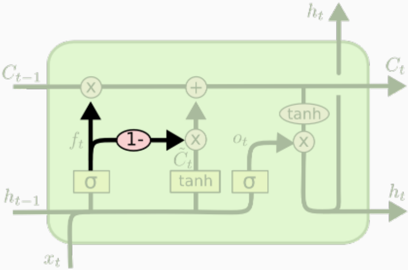
- "Peephole connections": Let the gate layers look at the cell state;
- Diagram adds peepholes to all the gates, but we can give some peepholes and not others.

$$
\begin{cases}
f_t = \sigma\left(W_f \cdot [\mathbf{C_{t-1}}, h_{t-1}, x_t] + b_f\right) \\
i_t = \sigma\left(W_i \cdot [\mathbf{C_{t-1}}, h_{t-1}, x_t] + b_i\right) \\
\tilde{C}_t = \tanh\left(W_C \cdot [h_{t-1}, x_t] + b_C\right) \\
C_t = f_t \otimes C_{t-1} + i_t \otimes \tilde{C}_t \\
o_t = \sigma\left(W_o \cdot [\mathbf{C_t}, h_{t-1}, x_t] + b_o\right) \\
h_t = o_t \otimes \tanh(C_t)
\end{cases}
$$

Other Minor Variants

- Coupled Input and Forget gates: $f_t = 1 - i_t$

- Full gate recurrence $f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t, C_t, f_{t-1}, i_{t-1}, o_{t-1}] + b_f\right)$



LSTM: A Search Space Odyssey (Greff et al., 2015)

- Tested the following variants, using Peephole LSTM as standard:

NIG No Input Gate,

NFG No Forget Gate,

NOG No Output Gate,

NIAF No Input Activation Function,

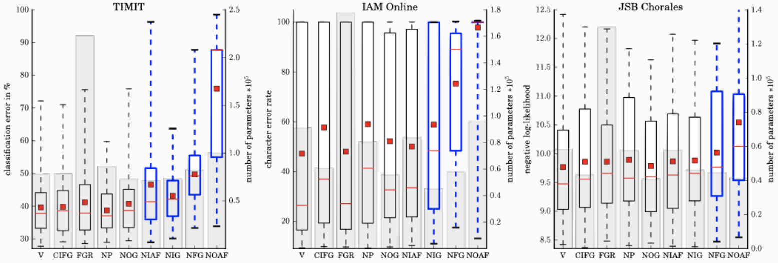
NOAF No Output Activation Function,

NP No Peepholes,

CIFG Coupled Input and Forget Gate,

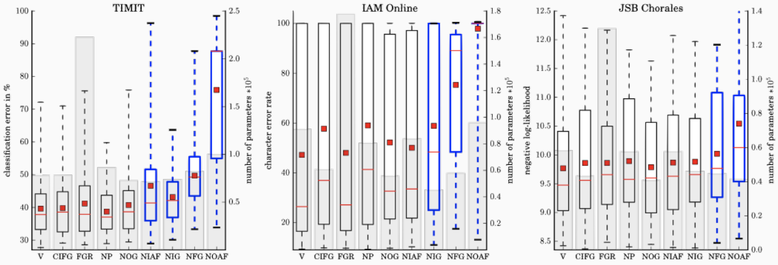
FGR Full Gate Recurrence;

- On the tasks of:
  - Timit Speech Recognition: Audio frame to 1 of 61 phonemes,
  - IAM Online Handwriting Recognition: Sketch to characters,
  - JSB Chorales: Next-step music frame prediction.



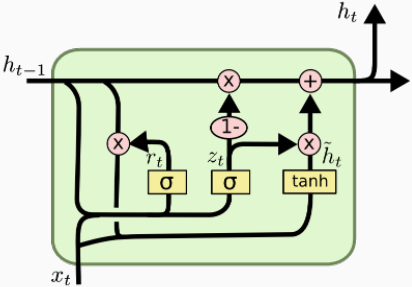
LSTM: A Search Space Odyssey (Greff et al., 2015)

- Standard LSTM performed reasonably well on multiple datasets and *none of the modifications significantly improved the performance*;
- Coupling gates and removing peephole connections simplified the LSTM without hurting performance much;
- The forget gate and output activation are crucial;
- Found interaction between learning rate and network size to be minimal – indicates calibration can be done using a small network first.



Gated Recurrent Neural Network

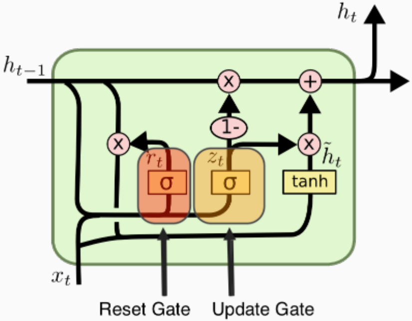
"Another special kind of RNN's, designed to solve the vanishing gradient problem."



Cho, et al. (2014).

Gated Recurrent Unit

"Another special kind of RNN's, designed to solve the vanishing gradient problem."



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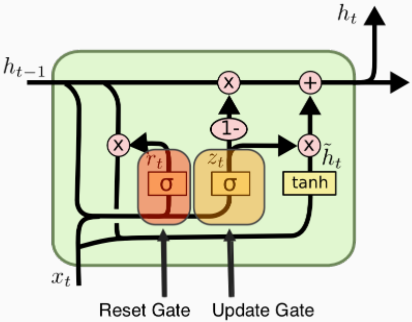

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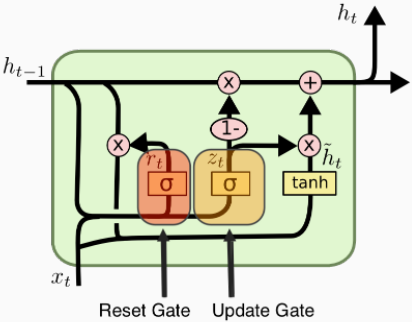

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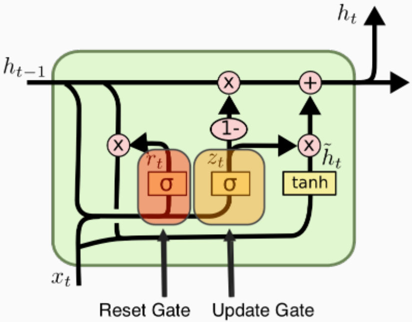

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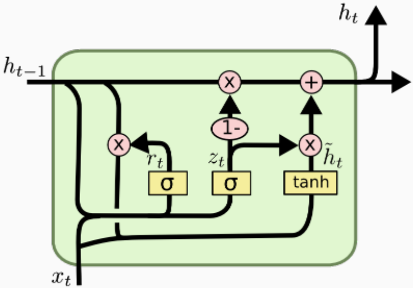
- A GRU unit is composed of:

Reset gate How much information from the previous steps can be forgotten;

Update gate How much information from the previous time steps must be saved;

Current memory Provides information throughout the sequence,
Represents the memory of the network.

Gates: Reset and Update



Cho, Van Merriënboer, Gulcehre, Bahdanau, Bougares, Schwenk & Bengio (2014).

Reset gates:

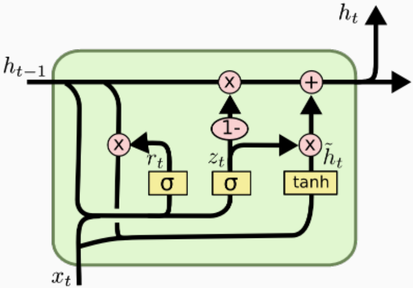
- How to combine the new input with the previous memory?
- How much information from previous time steps can be forgotten?

$$\boxed{r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t] + b_i\right)}$$

Update gates:

- How much information from previous time steps needs to be passed along to the future.

$$\boxed{z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t] + b_i\right)}$$



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Current memory content:

- Store the relevant information from the past

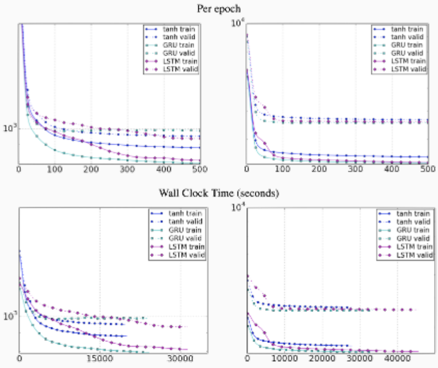
$$\boxed{\tilde{h}_t = \tanh\left(W \cdot [r_t \otimes h_{t-1}, x_t] + b_i\right)}$$

Final memory (at current time step):

- What to collect from the current memory content $\tilde{h}_t$ and what from the previous steps h_{t-1}.

$$\boxed{h_t = \sigma\left((1 - z_t \otimes h_{t-1} + z_t \otimes \tilde{h}_t\right)}$$

Vanilla RNN *vs.* LSTM *vs.* GRU



(a) Nottingham Dataset
(b) MuseData Dataset

			RNN	GRU	LSTM
Next step Music prediction	Nottingham	train	3.22	2.79	3.08
		test	**3.13**	3.23	3.20
	JSB Chorales	train	8.82	6.94	8.15
		test	9.10	**8.54**	8.67
	MuseData	train	5.64	5.06	5.18
		test	6.23	**5.99**	6.23
	Piano-midi	train	5.64	4.93	6.49
		test	9.03	**8.82**	9.03
Speech recognition	Ubisoft dataset A	train	6.29	2.31	1.44
		test	6.44	3.59	**2.70**
	Ubisoft dataset B	train	7.61	0.38	0.80
		test	7.62	**0.88**	1.26

- GRU has fewer tensor operations
  $\rightsquigarrow$ Little speedier to train than LSTM.
- No clear winner between LSTM & GRU
  $\rightsquigarrow$ Try both to determine which one works better for the considered case.

Junyoung, Caglar, KyungHyun & Bengio (2014).

A Profusion of RNN Variants

- Only a few of the most notable LSTM variants.
  Which of these variants is best? Do the differences matter?

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- All architectures are evaluated on 3 problems:

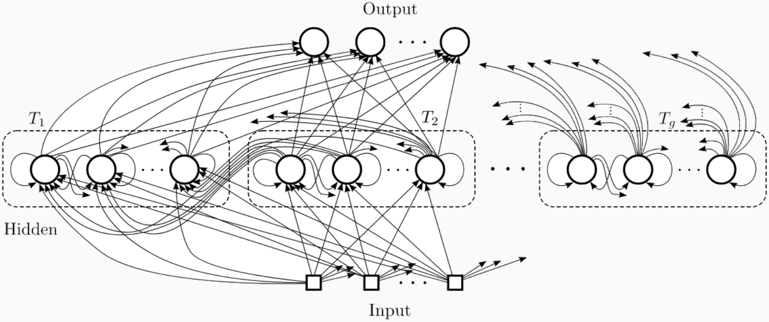
  Arithmetic Compute sum/difference of two numbers, with distractors
  3e36d9 - h1h39f94eeh43keg3c = 3369 – 13994433 = -13991064;

  XML Modeling Predict next character in valid XML modeling;

  Language Modeling Predict distributions over words (Penn.

- There are also completely different strategies: *Cf.* Clockwork RNN (Koutnik, Greff, Gomez & Schmidhuber, 2014)

Clockwork Recurrent Neural Network



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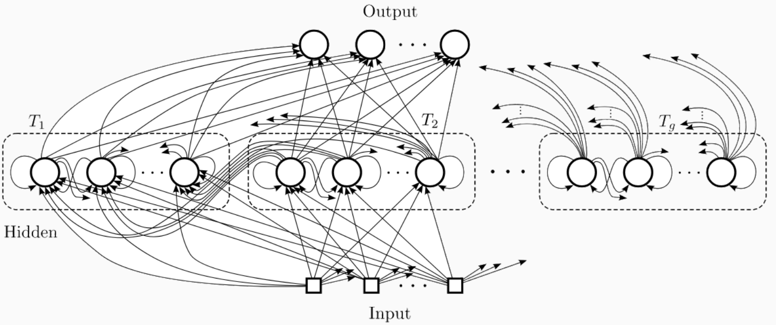

- *"Better memory" than LSTMs:* Structured hidden layer that does not enforce representing the mean of all inputs (running average in case of the LSTM).

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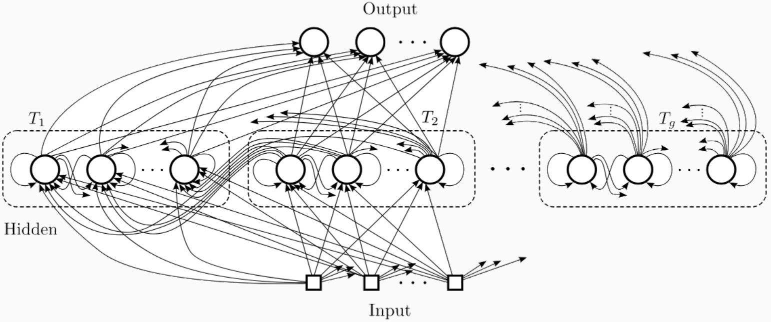

- *"Better memory" than LSTMs:* Structured hidden layer that does not enforce representing the mean of all inputs (running average in case of the LSTM).

- *But not really used in practice:* Need to know the numbers of modules to partition the hidden layer,
  - Depends most likely on the data,
  - No literature that suggests how to do this properly.

(Koutnik, Greff, Gomez & Schmidhuber, 2014)

Explicit Memory

Memory Networks : Pushing Further the Idea of Memory in Neural Networks

- Neural networks excel at storing *implicit knowledge*.
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$\leadsto$ *Introduction of an* ***explicit memory*** *component*.

1. **Memory networks** (Weston, Chopra & Bordes, 2014)
   - Set of memory cells that can be accessed via an addressing mechanism,
   - *But* requires a supervision signal instructing them how to use their memory cells.
2. **Neural Turing Machine** (NTM) (Graves, Wayne & Danihelka, 2014) : able to learn to *read* from and *write* arbitrary content to memory cells without explicit supervision about which actions to undertake.

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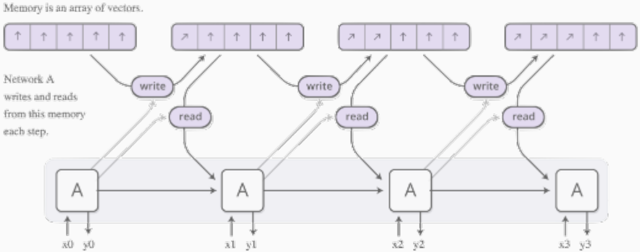
- *Memory cell in NTM* $\longleftrightarrow$ *Memory cells in LSTMs and GRUs.*
  NTM outputs an internal state that chooses which cell to read from or write to, (think of memory accesses in a computer read from or write to a specific address).

Explicit Memory

Neural Turing Machines

- Designed such that every component of the architecture is differentiable, making it straight forward to train with gradient descent.



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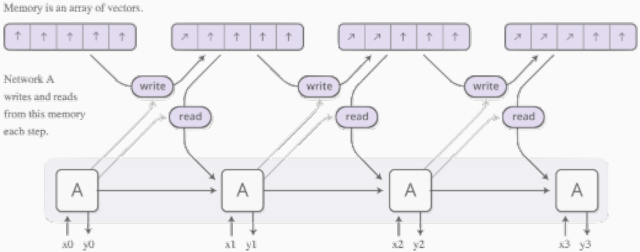

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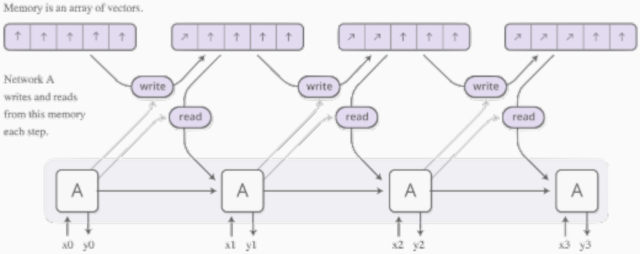

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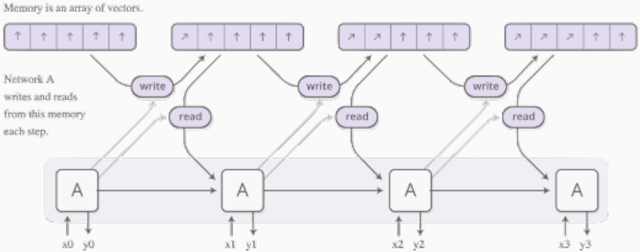
- Reading head: Convex combination of the row-vectors M_t in memory: $r_t = W_t \otimes M_t$.
- Writting head: Two parts:
  1. *Erase* $\leftrightarrow$ Forget gate of LSTM. Given an *erase* vector, e_t: $\tilde{M}_t = M_{t-1}\,(\mathbb{1} - W_t e_t)$,
  2. *Add* $\leftrightarrow$ Input gate of LSTM. Given an *add* vector, a_t: $M_t = \tilde{M}_t + W_t a_t$.



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Even Longer-Term Memory

Experiments: Copy a sequence of binary vectors, of size between 1 and 20.

Focus:

- Can NTM store and recall a long sequence of arbitrary information?
- And, in particular, is it able to overcome longer delays than LSTMs?

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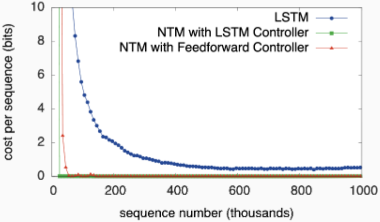


Figure 3: Copy Learning Curves.

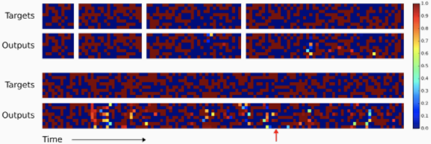


Figure 4: NTM Generalisation on the Copy Task.

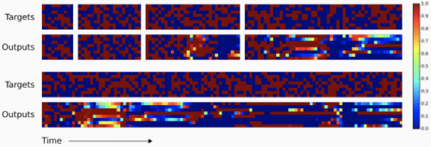


Figure 5: LSTM Generalisation on the Copy Task.

Graves, Wayne & Danihelka (2014)

But: How to know *where* to read and write? $\leadsto$ ***Attention mechanism***

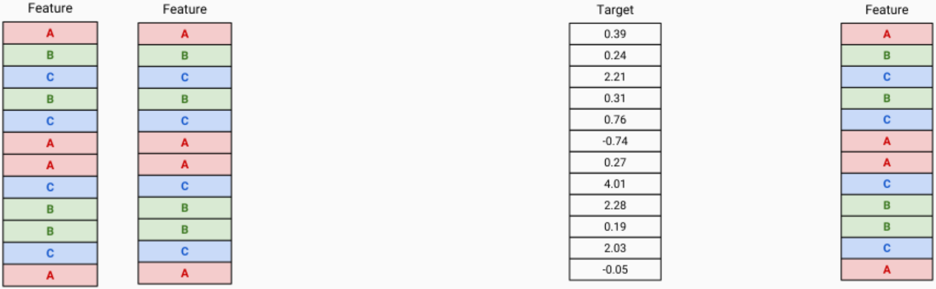
Appendix: Categorical Variable Encoding

Encoding: Convert a categorical variable to numerical values for machine learning model building.

Different types of Encoding:

Micci-Barreca (2001)

- Label Encoding
- One Hot Encoding
- Target Encoding



Credit: Brendan Hasz blog post

An others: Word2Vec, BERT (Bidirectional Encoder Representations from Transformers), . .

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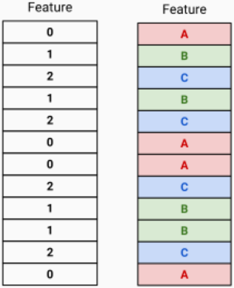

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Feature
0
1
2
1
2
0
0
2
1
1
2
0

Feature_A	Feature_B	Feature_C
1	0	0
0	1	0
0	0	1
0	1	0
0	0	1
1	0	0
1	0	0
0	0	1
0	1	0
0	1	0
0	0	1
1	0	0

Target
0.39
0.24
2.21
0.31
0.76
-0.74
0.27
4.01
2.28
0.19
2.03
-0.05

Feature
A
B
C
B
C
A
A
C
B
B
C
A

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Feature
0
1
2
1
2
0
0
2
1
1
2
0

Feature_A	Feature_B	Feature_C
1	0	0
0	1	0
0	0	1
0	1	0
0	0	1
1	0	0
1	0	0
0	0	1
0	1	0
0	1	0
0	0	1
1	0	0

Target
0.39
0.24
2.21
0.31
0.76
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4.01
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0.19
2.03
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Feature
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