RHEINISCH-WESTFÄLISCHE TECHNISCHE HOCHSCHULE AACHEN

Neuroinspired Computing (Prof. Dr. Abigail Morrison)

Deterministic Recurrent Neural Networks

Seminar Thesis

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Contents

1 Introduction

Machine learning has seen a rapid evolution in recent years, with neural networks emerging as a powerful tool for a wide range of applications. Initially inspired by the structure and function of the human brain, artificial neural networks have evolved into a diverse family of models, each tailored to specific tasks and data types. In particular, Recurrent Neural Networks (RNNs) have revolutionized the processing of sequential data, enabling tasks such as language modeling [12], machine translation [3], and speech recognition [6]. In this paper, we explore the architecture and operation of RNNs, with a focus on Long Short-Term Memory networks, which are designed to learn long-term dependencies more effectively than standard RNNs. We also discuss the Neural Turing Machine, which is a type of recurrent neural network that is augmented with an external memory bank.

1.1 Feedforward Neural Networks

Before delving into the realm of RNNs, it is essential to understand the foundational concepts of feedforward neural networks, which form the basis for more complex models such as RNNs. Feedforward neural networks, also known as multilayer perceptrons, are a class of neural networks that process input data through a series of interconnected layers. Each layer consists of a set of nodes, or neurons, which perform a weighted sum of the inputs followed by the application of an activation function. The output of each layer serves as the input to the next layer, ultimately producing a final output. The process of training a feedforward neural network involves adjusting the weights of the connections between neurons to minimize the difference between the predicted and actual outputs, typically using the backpropagation algorithm and gradient descent [13].

This poses a limitation on the types of data that can be processed by feedforward neural networks, as they are designed to operate on fixed-size input vectors and produce fixed-size output vectors. This constraint makes them ill-suited for tasks involving sequential data, where the length of the input and output sequences may vary. For example, in natural language processing, the length of a sentence can vary significantly, making it challenging to process using a feedforward neural network [17]. Additionally, feedforward neural networks lack an internal state, meaning they do not have the ability to remember information from previous inputs. This makes it difficult for them to capture the sequential dependencies present in many real-world datasets. To address these limitations, we turn to Recurrent Neural Networks.

2 Recurrent Neural Networks

Recurrent Neural Networks are a class of neural networks that are designed to handle sequential data by maintaining an internal state. Unlike feedforward neural networks, which process the entire input at once, RNNs process the input elements one at a time, allowing them to capture dependencies over time.

In its simplest form, the structure of an RNN is the same as a feedforward neural network, with the addition of a feedback loop to maintain an internal state, which is updated at each time step, allowing the network to remember information from previous inputs. The output of the network at each time step is influenced not only by the current input but also by the internal state. This means that, instead of having multiple layers with separate weights, RNNs have a single layer that acts as a dynamical system, changing over time. The repeating

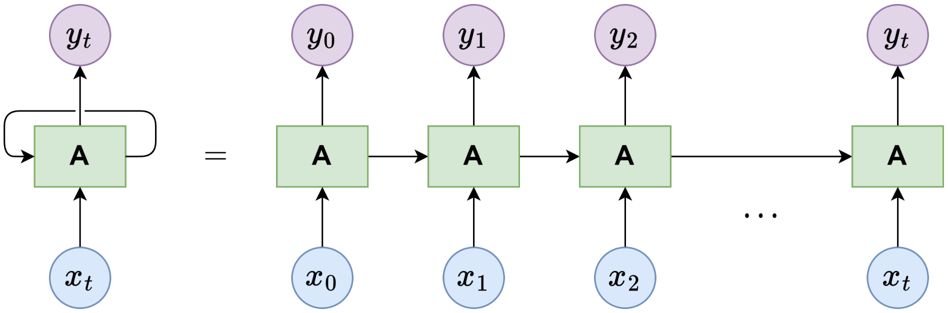


Figure 1: A recurrent neural network unrolled into a sequence of layers. The input sequence $x_0, x_1, \ldots, x_t$ is shown in blue, the network layer in green and the output sequence $y_0, y_1, \ldots, y_t$ in purple.

module in an RNN can be unrolled into a sequence of interconnected layers, allowing the network to process sequences of arbitrary length, as shown in Figure 1. This unrolling reveals that RNNs are intimately related to sequences and lists, making them a natural architecture for processing data of this form.

2.1 Categories of Applications

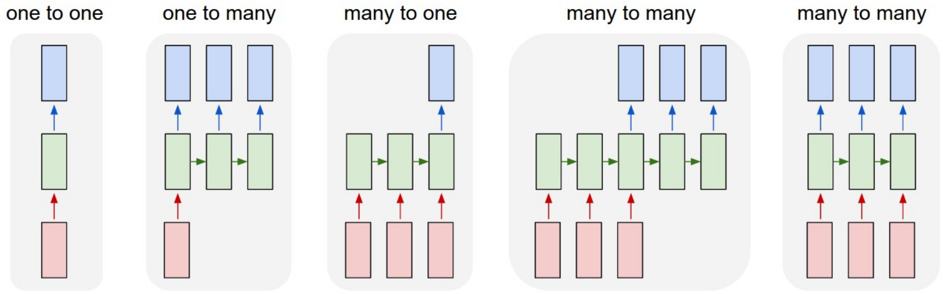


Figure 2: Ways of applying RNNs to different types of data. Both the input and output can be a fixed-size vector or a sequence of vectors. If both are sequences, the input and output vectors can either be regarded as pairs or as unrelated sequences of different lengths. [10]

The applications of RNNs can be categorized based on the length of the input and output sequences and the relationship between them, as shown in Figure 2. For example, for tasks such as image classification, where the input and output sequences are of fixed length, RNNs can be used in a manner similar to feedforward neural networks (one-to-one). They can also be used for tasks such as image captioning, where the input is a fixed-size image and the output is a sequence of words (one-to-many). Additionally, RNNs can be used for tasks such as sentiment analysis, where the input is a sequence of words and the output is a single value (many-to-one). Tasks, where both the input and output are sequences of varying lengths (many-to-many), can be categorized into two subtypes. For example, in machine translation, the input sequence is processed first, and then the output sequence is generated. In contrast, for video classification, the output is generated simultaneously with the input, allowing the network to use the previous frames as context. This demonstrates the flexibility of RNNs in handling a wide range of tasks involving sequential data.

2.2 Internal Structure

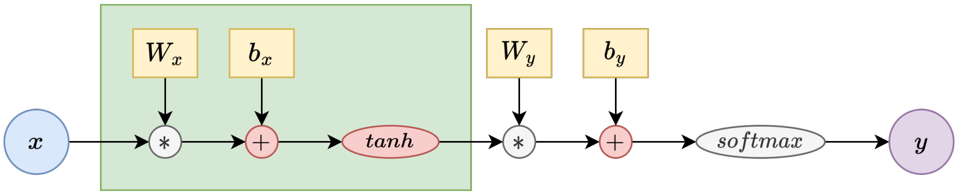


Figure 3: The internal structure of a feedforward neural network with a single layer (in green) and an example for output processing.

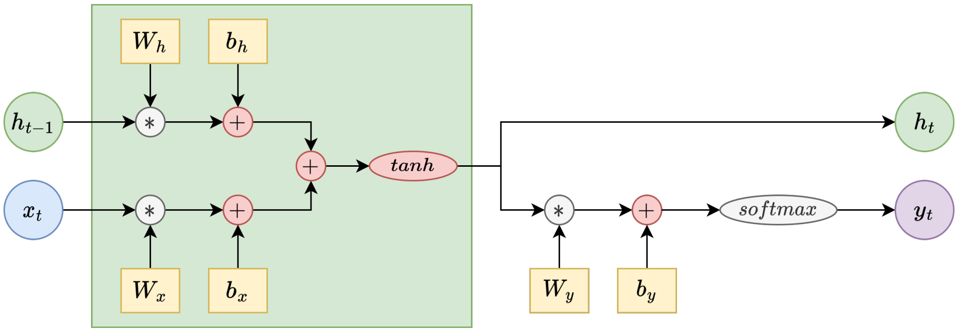


Figure 4: The internal structure of a recurrent neural network with a single layer (in green) and an example for output processing.

To understand the structure of an RNN, we compare a single layer feedforward NN with a single layer RNN. As shown in Figure 3, a feedforward NN transforms the input vector x by a linear transformation and an activation function to produce the output of a single layer. In contrast, as shown in Figure 4, an RNN first concatenates the input vector x with the previous state vector h_{t-1}, then transforms the concatenated vector in the same way as a feedforward NN. The resulting state vector h_t then serves as the input to the next time step. For the first iteration of the RNN, the previous state vector is typically initialized to a vector of zeros. However, it can also be learned as part of the training process, which can boost the performance of the network in some cases [18].

2.3 Backpropagation

The training of RNNs is typically performed using the backpropagation through time (BPTT) algorithm, which is an extension of the backpropagation algorithm used to train feedforward neural networks. As an example, consider a single layer feedforward NN, like the green box in Figure 3. Let

- x be the input vector,

- W the weight matrix,
- b the bias vector,
- y the output vector,
- t the target vector (ground truth)
- σ the activation function, and
- $L = \frac{1}{2}\sum_{i=1}^{n}(t_i - y_i)^2$ the loss function (e.g. mean squared error).

We first do a forward pass to compute the output $y = \sigma(Wx + b)$ and compare it to the target t by the loss function L. Then, we do a backward pass to compute the gradient of the loss function with respect to the weights and biases of the network. Here, we use the chain rule of calculus:

$$\begin{aligned} \frac{\partial L}{\partial W} &= \frac{\partial L}{\partial y}\frac{\partial y}{\partial W} && (1) \\ &= \frac{\partial L}{\partial y}\frac{\partial y}{\partial (Wx+b)}\frac{\partial (Wx+b)}{\partial W} && (2) \\ &= -(t-y)\cdot \sigma'(Wx+b)\cdot x^T && (3) \end{aligned}$$

The gradient for the bias vector $\frac{\partial L}{\partial b}$ can be computed similarly. For a network with multiple layers, the gradients are computed layer by layer using the chain rule, starting from the output layer and moving backwards through the network. In the final step, the weights and biases are updated in the direction that minimizes the loss: $W \leftarrow W - \alpha\frac{\partial L}{\partial W}$ and $b \leftarrow b - \alpha\frac{\partial L}{\partial b}$, where α is the learning rate. This is usually done using an optimization algorithm such as stochastic gradient descent.

The BPTT algorithm extends this approach to RNNs by unrolling the network into a sequence of connected layers. The forward pass is performed as usual, with the output of each time step serving as the input to the next time step. The backward pass then accumulates the gradients over the entire sequence and updates the weights and biases accordingly. This allows the network to capture the dependencies between the input elements and learn from the entire sequence, rather than just the current input. The key difference between BPTT and regular backpropagation is that the weights of the RNN are shared across time steps and the number of steps is not given by the number of layers, but by the length of the input sequence. For long sequences, this can lead to problems such as vanishing or exploding gradients, which can make training difficult [2].

2.4 The Problem of Long-Term Dependencies

One of the key challenges in training RNNs is the problem of long-term dependencies. To illustrate this, consider a simplified RNN that takes an input sequence $x_0, x_1, \ldots, x_n$ and produces a sequence of outputs/hidden states $h_0, h_1, \ldots, h_n$. It is defined by the function F for each time step $t \in \{0, 1, \ldots, n\}$:

$$h_t = F(h_{t-1}, x_t) = W_h \tanh h_{t-1} + W_x x_t + b \tag{4}$$

Then the gradient with respect to the hidden state at time step t is given by:

$$\nabla_h F(h_{t-1}, x_t) = W_h \text{diag}(\tanh'(h_{t-1})) \tag{5}$$

For the backward pass, we need to compute the gradient of the loss function, which in this case is given by

$$\partial L = \nabla_h L(h_n, x_1, \dots, x_n) \cdot \sum_{t=1}^{n} \prod_{k=n-t+1}^{n} \nabla_h F(h_{k-1}, x_k) \tag{6}$$

where each term in the sum is the gradient of the current layer. The sum can be written as:

$$\begin{aligned} &\sum_{t=1}^{n} \prod_{k=n-t+1}^{n} \nabla_h F(h_{k-1}, x_k) \\ &= \nabla_h F(h_{n-1}, x_n) \\ &+ \nabla_h F(h_{n-1}, x_n) \cdot \nabla_h F(h_{n-2}, x_{n-1}) \\ &+ \nabla_h F(h_{n-1}, x_n) \cdot \nabla_h F(h_{n-2}, x_{n-1}) \cdot \nabla_h F(h_{n-3}, x_{n-2}) \\ &+ \dots \end{aligned} \tag{7}$$

With Equation (5) and Equation (7), we can see that the gradient for time step t is predominantly influenced by W_h^{n-t+1}. If the largest singular value of W_h is less than 1, the gradient will vanish as t increases. If it is greater than 1, the gradient will explode [16]. This makes it difficult for the network to learn long-term dependencies, as the gradients become too small or too large to be useful. This is known as the problem of long-term dependencies, and it is a fundamental limitation of standard RNNs.

Multiple approaches have been proposed to address this problem, for example, clipping the gradient to prevent it from becoming too large [16]. Let $\nabla_W L$ be the gradient of the loss function and ϵ a small constant. Then the clipped gradient ∇ is

$$\nabla = \begin{cases} \nabla_W L & \text{if } ||\nabla_W L|| < \epsilon \\ \epsilon \cdot \frac{\nabla_W L}{||\nabla_W L||} & \text{otherwise} \end{cases} \tag{8}$$

This prevents the gradient from growing indefinitely, but it does not address the problem of vanishing gradients. Another approach is to use ReLU activation functions [5], which have the advantage of not saturating for positive inputs because their derivative is 1. However, the problem of vanishing gradients still remains for negative inputs. Moreover, there were methods proposed to initialize the weights of the network in a way that prevents the gradients from vanishing or exploding [11]. While these methods can mitigate the problem of long-term dependencies to some extent, they do not provide a complete solution. A more effective approach is to use Long Short-Term Memory networks, which were specifically developed to address the problem of vanishing and exploding gradients in RNNs.

3 Long Short-Term Memory Networks

Long Short-Term Memory (LSTM) networks are a special type of RNN that are designed to learn long-term dependencies more effectively than standard RNNs. They were introduced by Hochreiter and Schmidhuber in 1997 [9] and have since become a popular choice for a wide range of applications, including language generation, medical diagnosis, sentiment analysis and video processing. The key idea behind LSTMs is the use of a memory cell, which allows the network to store and access information over long time scales. In this section, we explore the architecture and operation of LSTMs, as well as some of the variants that have been developed to improve their performance.

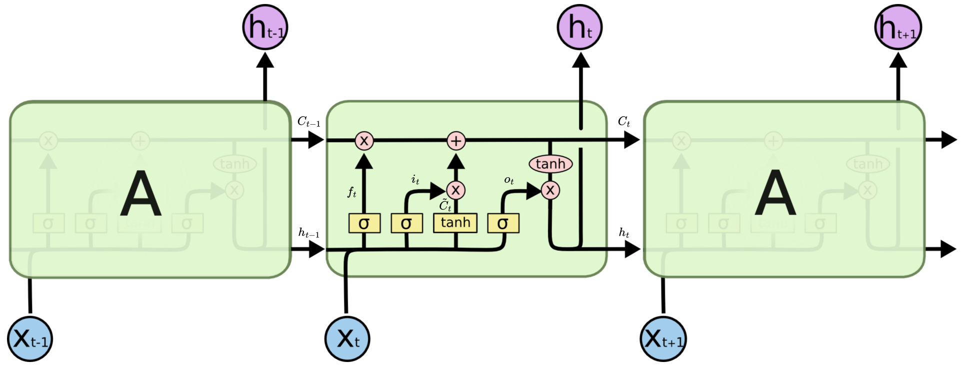


Figure 5: The repeating module of an LSTM network. Each yellow box represents a neural network layer with its activation function and the pink circles represent pointwise operations. The lines merging denote concatenation, while a line forking denotes its content being copied. The output is denoted by h_t. [14]

3.1 Architecture

The architecture of an LSTM network is based on a repeating module that contains four interacting layers, as shown in Figure 5. The key to LSTMs is the cell state C_t, which runs straight down the entire chain with only minor linear interactions. This allows information to flow along the cell state unchanged, making it easy for the network to remember information over long time scales. The cell state is regulated by structures called gates, which are composed of neural network layers and pointwise operations. The gates allow the network to remember or forget information as needed.

3.1.1 Forget Gate

The first step in the operation of an LSTM is to decide what information to forget from the cell state. This is done by a sigmoid layer, which takes the previous hidden state h_{t-1} and the current input x_t as input and outputs a number between 0 and 1 for each element in the cell state C_{t-1}. A value of 0 indicates that the corresponding element should be forgotten, while a value of 1 indicates that it should be retained. This allows the network to discard irrelevant information and focus on the most important elements.

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \tag{9}$$

3.1.2 Input Gate

The next step is to decide what new information to store in the cell state. This has two parts. First, a sigmoid layer decides which values to update. Next, a tanh layer creates a vector of new candidate values $\tilde{C}_t$ that could be added to the state. The input gate layer outputs a number between 0 and 1 for each element in the cell state, indicating how much of the new candidate values should be added to the state. This allows the network to selectively update the cell state with new information.

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i) \tag{10}$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \tag{11}$$

3.1.3 Update Cell State

The next step is to update the old cell state C_{t-1} into the new cell state C_t. First, the old state is multiplied by the forget gate f_t, forgetting the things that were decided to forget earlier. Then, the new candidate values $\tilde{C}_t$ are added to the state, scaled by how much the input gate decided to update each state value.

$$C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t \tag{12}$$

3.1.4 Output Gate

Finally, the network needs to decide what to output. This output will be based on the cell state, but will be a filtered version. First, a sigmoid layer decides what parts of the cell state should be output. Then, the cell state is put through a tanh function to push the values to be between -1 and 1, and multiplied by the output of the sigmoid gate. The result is the output of the network at the current time step h_t, which can be used for further processing or as the final output of the network.

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \tag{13}$$

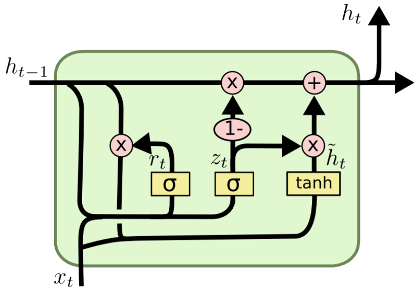
$$h_t = o_t \cdot \tanh(C_t) \tag{14}$$

3.2 Variants

LSTMs have been the subject of extensive research, leading to the development of several variants that aim to improve their performance and address specific challenges [8]. One popular variant, introduced by Gers and Schmidhuber in 2000 [4], adds peephole connections to the architecture of the LSTM. These connections allow the cell to control the gates more precisely, making it easier for the network to learn precise timings. Additionally, the output activation function is omitted, as there is no evidence that it is essential for solving the problems that LSTMs have been tested on so far.

Another variant, called Dynamic Cortex Memory (DCM), was introduced by Otte et al. in 2014 [15]. The DCM is an extension of the LSTM model that enhances the inner interplay of the gates and the error carousel due to several new and trainable connections. These connections enable a direct signal transfer from the gates to one another, allowing the network to converge faster during training than LSTM under the same training conditions. Furthermore, DCMs yield better generalization results than LSTMs, as shown for different supervised problem scenarios, including storing precise values, adding, and learning a context-sensitive grammar.

One of the most well-known variants of the LSTM architecture is the Gated Recurrent Unit (GRU), which was proposed by Cho et al. in 2014 [3]. The GRU simplifies the LSTM architecture by removing the output gate and the cell state, and combining the input and forget gates into a single update gate. This reduces the number of parameters in the network and makes it easier to train. The internal structure of a GRU network is shown in Figure 6. While the GRU has been shown to perform comparably to the LSTM on many tasks, it has the advantage of being simpler and more efficient, making it a popular choice for many applications.



$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$
$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$
$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$
$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

Figure 6: The structure of a Gated Recurrent Unit (GRU) network. [14]

4 Neural Turing Machines

While LSTMs and their variants have proven to be effective for a wide range of tasks, they are still limited in their ability to perform complex operations that require explicit memory access. To address this limitation, Graves et al. introduced the Neural Turing Machine (NTM) in 2014 [7]. The NTM is augmented with an external memory bank to combine the power of neural networks with the ability to store and retrieve information. Unlike the operations on the memory of a computer, the operations of the NTM are designed to be fully differentiable, to be trained using backpropagation and gradient-based optimization algorithms.

The approach is inspired by the structure and operation of a Turing machine, which is a theoretical model of a computer that can read from and write to an infinite tape of memory. A computer program makes use of three fundamental mechanisms: elementary operations (e.g., arithmetic operations), logical flow control (branching), and external memory, which can be written to and read from in the course of computation [19]. In human cognition, the process that shares the most similarity to algorithmic operation is known as working memory, which is understood to mean a capacity for short-term storage of information and its rule-based manipulation [1].

4.1 Architecture

The architecture of an NTM, as shown in Figure 7, consists of two main components: a controller and a memory bank. The controller is an LSTM, which is responsible for processing the input data and interacting with the memory bank. The memory bank for time step t is a matrix $\mathbf{M}_t$ of size $N \times M$, where N is the number of memory locations and M is the size of each memory location. The memory bank can be read from and written to by the controller. It interacts with the memory bank using read heads and write heads, which are responsible for reading and writing information from and to the memory bank. They use an attention mechanism to select the memory locations, allowing the network to focus on specific parts of the memory.

4.2 Addressing Mechanism

The addressing mechanism of an NTM is responsible for selecting the memory locations to read from and write to. It combines both content-based addressing and location-based addressing and consists of four main steps: content addressing, interpolation, convolutional

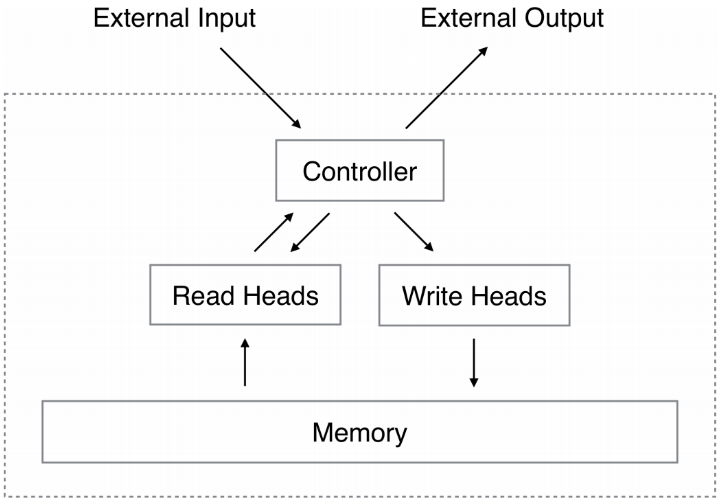


Figure 7: The architecture of a Neural Turing Machine.

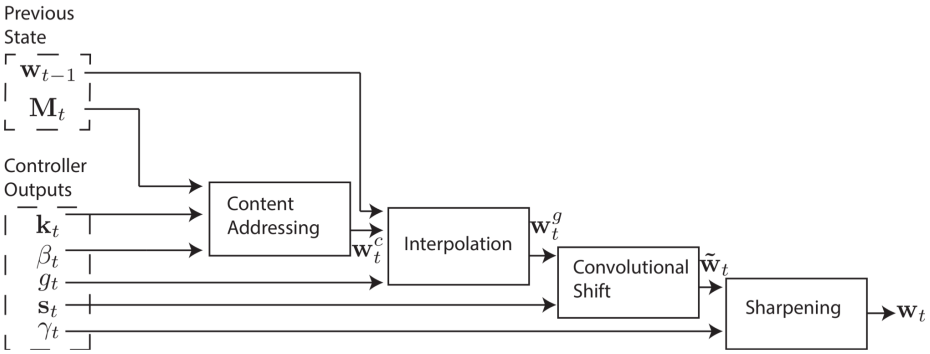


Figure 8: Flow diagram of the addressing mechanism in a Neural Turing Machine. [7]

shift, and sharpening, as shown in Figure 8. The addressing mechanism is performed at each time step, allowing the controller to interact with the memory bank in a dynamic and flexible manner.

4.2.1 Content Addressing

The first step of the addressing mechanism is content addressing, which selects memory locations based on the content of the cells. It takes the current memory bank $\mathbf{M}_t$, the key vector $\mathbf{k}_t$, and the key strength β_t as input. The key vector is used to calculate the similarity between the key and each memory location using the cosine similarity measure $K[\cdot,\cdot]$. The parameter β_t amplifies the precision of the attention weights, enforcing high sparsity in the weights.

$$\mathbf{w}_t^c = \text{softmax}(\beta_t K[\mathbf{M}_t, \mathbf{k}_t]) \tag{15}$$

4.2.2 Interpolation

The next step is interpolation, which allows the network to iteratively access subsequent memory locations. It takes the previous attention weights $\mathbf{w}_{t-1}$, the content-based attention weights $\mathbf{w}_t^c$, and the interpolation gate $g_t \in (0,1)$ as input. For a value of $g_t = 0$, the previous weights are retained, while for a value of $g_t = 1$, the current weights are used. This allows the network to blend between them based on the value of g_t.

$$\mathbf{w}_t^g = g_t \mathbf{w}_t^c + (1 - g_t)\mathbf{w}_{t-1} \tag{16}$$

4.2.3 Convolutional Shift

After interpolation, each head produces a shift weighting $\mathbf{s}_t$ that is used as the kernel for a convolutional shift operation. It convolves the new attention weights with the kernel $\mathbf{s}_t$, allowing the network to shift the attention if needed. This is useful for accessing memory locations in a flexible and dynamic manner. All indices are modulo N to ensure that the shift operation is circular.

$$\tilde{\mathbf{w}}_t(i) \leftarrow \sum_{j=0}^{N-1} \mathbf{w}_t^g(j)\mathbf{s}_t(i-j) \tag{17}$$

4.2.4 Sharpening

The final step of the addressing mechanism is sharpening, which amplifies the focus of the attention weights. It takes the convolved attention weights $\tilde{\mathbf{w}}_t$ and the sharpening parameter $\gamma_t \geq 1$ as input and applies a power function to the weights, increasing large weights and decreasing small weights. The effect of sharpening increases with higher values of γ_t.

$$\mathbf{w}_t(i) = \frac{\tilde{\mathbf{w}}_t(i)^{\gamma_t}}{\sum_j \tilde{\mathbf{w}}_t(j)^{\gamma_t}} \tag{18}$$

4.3 Comparison with LSTMs

To compare the performance of the NTM with LSTMs, Graves et al. conducted a series of experiments on a set of simple algorithmic tasks such as copying and sorting data sequences. The goal was to establish that the NTM is able to solve the problems by learning compact internal programs. The hallmark of such solutions is that they generalize well beyond the range of the training data. For example, the researchers examined if a network that had been trained to copy sequences of length up to 20 could copy a sequence of length up to 120 with no further training. The results of the experiments showed that the NTM was able to learn much faster than LSTMs and converged to a lower cost. Additionally, the NTM was able to generalize well beyond the range of the training data, while LSTMs rapidly degraded beyond length 20. This suggests that the NTM, unlike LSTMs, has learned some form of copy algorithm. The researchers also examined the interaction between the controller and the memory and concluded that the NTM has learned how to create and iterate through arrays. The focus-sharpening mechanism was also found to be essential, as the weightings would lose precision over time without it.

5 Conclusion

In this paper, we have explored the architecture and operation of Recurrent Neural Networks, Long Short-Term Memory networks and Neural Turing Machines, focusing on their ability to store and retrieve information over long time scales. We addressed their internal structure, the backpropagation algorithm used to train them, the problem of long-term dependencies in standard RNNs and introduced LSTMs as a solution to this problem. We also discussed the architecture of LSTMs and their variants and introduced the Neural Turing Machine built on top of the LSTM architecture. The results of experiments comparing the performance of LSTMs and NTMs on a set of simple algorithmic tasks were presented, showing that the NTM was able to learn these specific tasks much faster than LSTMs and converged to a lower cost. All in all, the field of RNNs and their variants is a rapidly evolving area of research, and we expect to see many more exciting developments in the future.

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