Recurrent Deep Learning Models and its applications

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Contents

1	Inti	roducti	on					
2	Background and Literature Review							
	2.1	Evolut	tion of Deep Learning and Recurrent Neural Networks					
	2.2	·						
		2.2.1	Backpropagation Through Time					
		2.2.2	Activation Function					
		2.2.3	Gradient vanishing and gradient exploring					
		2.2.4	Long short-term memory (LSTM)					
		2.2.5	Gated Recurrent Unit (GRU)					
		2.2.6	Deep recurrent neural networks (DRNNs)					
		2.2.7	Hidden Markov Model					
		2.2.8	Word representation					
3	Pro	iect G	oals and Objectives					
J	3.1	•	et Goals					
	3.2		tives					
	0.2	3.2.1	Implement Existing RNN Architectures					
		3.2.2	Apply the Models on a Benchmark NLP Dataset					
		3.2.3	Compare Model Performances					
		3.2.4	Analyze the Impact of Architectural Differences					
		0.2.4	Thatyze the impact of Architectural Differences					
4	Res		Plan / Methodology					
	4.1		ture Review					
	4.2	Data (Collection and Preprocessing					
		4.2.1	Data Collection					
		4.2.2	Data Preprocessing					
	4.3	Model	Architecture					
		4.3.1	Model 1 (Vanilla RNN)					
		4.3.2	Model 2 (Long short-term memory)					
		4.3.3	Model 3 (Gated recurrent unit)					
	4.4							
		4.4.1	Model Hyperparameters and Setup					
		4.4.2	Training Loop Overview					
		4.4.3	Pseudocode Description					

1 Introduction

With the rise of the Generative Artificial Intelligence, the development of AI has already made remarkable strides in processing sequential data. In understanding and producing sequential data. It has applications ranging from Natural Language Processing (NLP) to music composition to video generation. Especially NLP, has emerged as a pivotal field in artificial intelligence, enable machines to understand, interpret and generate in human readable format. Some famous Artificial Intellience assistence for example, Siri, Alexa and Bixby have shown the possibility. Everyone can communicate with those machines, which make the reasonable response back to user.

Recurrent Neural Networks (RNNs) have been a foundational architecture in this domain, Unlike the traditional Artificial Neural Network, RNNs do not treat each input independently, RNNs handle each input by considering the information from previous inputs. Conceptually this architecture able to retain the information. Thus, this architecture is suitable for handling sequential data. Unfortunately, early RNNs had limitation in training of networks over long sequence. vanishing and exploding gradient problems significantly affect the training process of RNN (Bengio et al., 1994). Eliminating many practical applications of RNNs. After that, (Hochreiter & Schmidhuber, 1997) introduced Long Short-Term Memory (LSTM) networks and are responsible for the breakthrough in how to solve these challenges. Specificized gating mechanisms were introduced in LSTMs to regulate the flow of the information, minimize the vanishing gradient problem and learn the long-term dependencies. This advanced made RNNs much more performant on tasks like a language modeling, machine translation and speech recognition tasks.

Further improvements were achieved with Gated Recurrent Units (GRUs) by (Cho et al., 2014) which diminished the LSTM architecture's complexity, but still provided the same performance. GRUs performed comparably but used fewer parameters, making it computationally and more tractably trainable.

Since the craze of AI has been revived by generative AI, natural language processing to time series prediction and speech recognition have once again aroused people's interest in RNN. This report aims to:

- Explore the theoretical foundations of recurrent deep learning models.
- Investigate their diverse applications in solving sequential data tasks.
- Analyze their performance, strengths, and inherent limitations.

2 Background and Literature Review

2.1 Evolution of Deep Learning and Recurrent Neural Networks

In the past few decades, thank to the rapidly development of technology, the computing resource has a incredible increase. Thus, substantially deep learning architecture have improved, from simple architectures, which only able to capture simple information from data to sophisticated models that are able to learn complex, abstract representations. This was before the early neural networks like perceptrons and multilayer perceptrons (MLPs) laid the footwork of neural computation that first came in the picture, but were

burdened by the lack of ability to model sequential dependencies. This however imposed a limit on the feed forward paradigm, which prompted the development of recurrent neural networks (RNNs) that extend the old stalactite of feed forward paradigm with cyclic connections. Through these connection, RNNs are capable to keep a hidden state that represents information over time steps thereby effectively capture temporal dynamics. RNNs have been a decisive step in the evolution of deep learning, as they are able to do tasks that require memory of previous events, including problems of natural language processing and time series modeling. Despite that, early RNNs models suffered from serious problems for example, vanishing gradients and exploding gradients, which prevented these RNN models from learning long ranged dependencies. This stimulated the building of more refined architectures intended to side step these obstacles.

2.2 Literature Review

2.2.1 Backpropagation Through Time

BPTT is one of the most important algorithms used for training RNNs. Dating back to the original effort to expand the typical backpropagation algorithm, BPTT has been formulated to handle the difficulties of temporal sequences that are inherent in sequential data (Werbos, 1990). This algorithm allows RNNs in learning sequence dependent data by unfold the network over time steps and then updating weights matrix through the gradient of loss function with respect to the variable (Rumelhart et al., 1986).

Conceptual Framework of BPTT

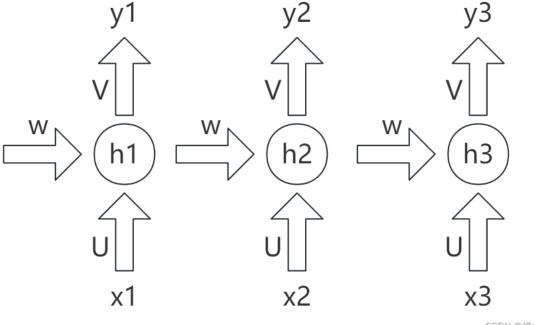
BPTT works based on the technique of treating an RNN as a deep feedforward network for across multiple time steps. In the forward pass, the RNN, like other artificial neuronal network, applies operation over the data input in sequence, bringing changes in its own state variables at every time step, depending on the input and the previous state of its general working state or hidden state. This sequential processing produces outputs and stores the internal states of the network in any period (Werbos, 1990).

This unfolds the RNN to construct a traditional Feedforward Neural Network where we can apply backpropagation through time. Below is the conceptual idea of BPTT in RNN.

Notation	Meaning	Dimension
U	Weight matrix for input to hidden state	$input\ size \times hidden\ unites$
W	Weight matrix for hidden to hidden state	$hidden\ units \times hidden\ unites$
V	Weight matrix for hidden state to output state	$hidden\ units \times number\ of\ class$
x_t	Input vector at time t	$input\ size \times 1$
h_t	Hidden state output at time t	$hidden\ units \times 1$
b_h	Bias term for hidden state	$hidden\ units \times 1$
b_y	Bias term for output state	$number\ of\ class \times 1$
\hat{o}_y	Output at time t	$number\ of\ class \times 1$
$\hat{y_t}$	Output at time t	$hidden\ units \times 1$
\mathcal{L}	Loss at time t	scalar

Table 1: Unfolded RNN

Forward Pass



CSDN @修炼室

Figure 1: Unfolded RNN

During the forward pass, the RNN processes the input sequence sequentially, computing hidden states and output at each timestep:

$$h_t = f(U^T x_t + W^T h_{t-1} + b_h) (1)$$

$$\hat{y}_t = f(V^T h_t + b_y) \tag{2}$$

Computing the loss function

Assuming the loss is computed only at the final timestep t:

$$\mathcal{L}_t = L(y_t, \hat{y}_t) \tag{3}$$

In order to do backpropagation through time to tune the parameters in RNN, we need to calculate the partial derivative of loss function \mathcal{L} with respect to the differently parameters.

Backward pass using the chain rule

Using the chain rule for computing the gradient.

Partial derivative of loss function \mathcal{L} with respect to W (hidden to hidden state) at time 2.

$$\frac{\partial \mathcal{L}_2}{\partial W} = \frac{\partial \mathcal{L}_2}{\partial y_2} \cdot \frac{\partial y_2}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial W}$$
 (4)

By mathematic induction

$$\frac{\partial \mathcal{L}_t}{\partial W} = \frac{\partial \mathcal{L}_t}{\partial y_t} \cdot \frac{\partial y_t}{\partial h_t} \cdot \left(\sum_{i=1}^t \frac{\partial h_t}{\partial h_i} \cdot \frac{\partial h_i}{\partial W}\right) \tag{5}$$

Where

$$\frac{\partial h_t}{\partial h_i} = \prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}} \tag{6}$$

Partial derivative of loss function \mathcal{L} with respect to U (input to hidden state) at time 2.

$$\frac{\partial \mathcal{L}_2}{\partial U} = \frac{\partial \mathcal{L}_2}{\partial y_2} \cdot \frac{\partial y_2}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial U}$$
 (7)

By mathematic induction

$$\frac{\partial \mathcal{L}_t}{\partial U} = \frac{\partial \mathcal{L}_t}{\partial y_t} \cdot \frac{\partial y_t}{\partial h_t} \cdot \left(\sum_{i=1}^t \frac{\partial h_t}{\partial h_i} \cdot \frac{\partial h_i}{\partial U}\right) \tag{8}$$

Where

$$\frac{\partial h_t}{\partial h_i} = \prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}} \tag{9}$$

Partial derivative of loss function \mathcal{L} with respect to V (hidden to output state) at time 2.

$$\frac{\partial \mathcal{L}_2}{\partial V} = \frac{\partial \mathcal{L}_2}{\partial y_2} \cdot \frac{\partial y_2}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial V}$$
 (10)

By mathematic induction

$$\frac{\partial \mathcal{L}_t}{\partial V} = \frac{\partial \mathcal{L}_t}{\partial y_t} \cdot \frac{\partial y_t}{\partial h_t} \cdot \left(\sum_{i=1}^t \frac{\partial h_t}{\partial h_i} \cdot \frac{\partial h_i}{\partial V}\right) \tag{11}$$

Where

$$\frac{\partial h_t}{\partial h_i} = \prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}} \tag{12}$$

Partial derivative of loss function \mathcal{L} with respect to b_h (bias term in hidden state) at time 2.

$$\frac{\partial \mathcal{L}_2}{\partial b_h} = \frac{\partial \mathcal{L}_2}{\partial y_2} \cdot \frac{\partial y_2}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial b_h}$$
(13)

By mathematic induction

$$\frac{\partial \mathcal{L}_t}{\partial b_h} = \frac{\partial \mathcal{L}_t}{\partial y_t} \cdot \frac{\partial y_t}{\partial h_t} \cdot \left(\sum_{i=1}^t \frac{\partial h_t}{\partial h_i} \cdot \frac{\partial h_i}{\partial b_h}\right) \tag{14}$$

Where

$$\frac{\partial h_t}{\partial h_i} = \prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}} \tag{15}$$

Partial derivative of loss function \mathcal{L} with respect to b_y (bias term in output state) at time 2.

$$\frac{\partial \mathcal{L}_2}{\partial b_y} = \frac{\partial \mathcal{L}_2}{\partial y_2} \cdot \frac{\partial y_2}{\partial h_2} \cdot \frac{\partial h_2}{\partial h_1} \cdot \frac{\partial h_1}{\partial b_y}$$
 (16)

By mathematic induction

$$\frac{\partial \mathcal{L}_t}{\partial b_y} = \frac{\partial \mathcal{L}_t}{\partial y_t} \cdot \frac{\partial y_t}{\partial h_t} \cdot \left(\sum_{i=1}^t \frac{\partial h_t}{\partial h_i} \cdot \frac{\partial h_i}{\partial b_y}\right) \tag{17}$$

Where

$$\frac{\partial h_t}{\partial h_i} = \prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}} \tag{18}$$

parameters updates

$$W \leftarrow W - \alpha \frac{\partial \mathcal{L}}{\partial W} \tag{19}$$

$$U \leftarrow U - \alpha \frac{\partial \mathcal{L}}{\partial U} \tag{20}$$

$$V \leftarrow V - \alpha \frac{\partial \mathcal{L}}{\partial V} \tag{21}$$

$$b_h \leftarrow b_h - \alpha \frac{\partial \mathcal{L}}{\partial b_h} \tag{22}$$

$$b_y \leftarrow b_y - \alpha \frac{\partial \mathcal{L}}{\partial b_y} \tag{23}$$

Pseudocode of BPTT (Wikipedia, 2023)

```
Algorithm 1 Backpropagation Through Time (BPTT)
```

```
1: Input:
        Sequence of input data \{x_1, x_2, \ldots, x_T\}
 2:
        Sequence of target outputs \{y_1, y_2, \dots, y_T\}
 3:
        Learning rate \eta
 4:
        Number of time steps to unroll N
 5:
 6: Initialize: Model parameters \theta, hidden state h_0 = 0
 7: Forward Pass:
 8: for t = 1 to T do
       Compute hidden state: h_t = f(h_{t-1}, x_t; \theta)
 9:
       Compute output: \hat{y}_t = g(h_t; \theta)
10:
11:
       Compute loss for time step t: L_t = \mathcal{L}(\hat{y}_t, y_t)
12: end for
13: Backward Pass (BPTT):
14: Set total loss: L = \sum_{t=1}^{T} L_t
15: for t = T down to 1 do
       Compute gradient of loss with respect to output: \frac{\partial L_t}{\partial \hat{y}_t}
16:
       Backpropagate through output layer to obtain: \frac{\partial L_t}{\partial h_t}
17:
       Accumulate gradients for parameters: \frac{\partial L}{\partial \theta}
18:
       for k = 1 to N do
19:
20:
          Backpropagate through time for N steps:
          Compute gradient contribution from step t - k: \frac{\partial L_t}{\partial h_{t-1}}
21:
22:
       end for
23: end for
24: Update Parameters:
25: \theta = \theta - \eta \cdot \frac{\partial L}{\partial \theta}
26: Output: Updated parameters \theta
```

2.2.2 Activation Function

Activation functions, particularly the sigmoid function, are fundamental components of recurrent neural networks (RNNs). They transform input data into output data. A key property of these functions is their differentiability. Differentiability is crucial for the backpropagation through time (BPTT) algorithm, enabling the application of the chain rule during training.

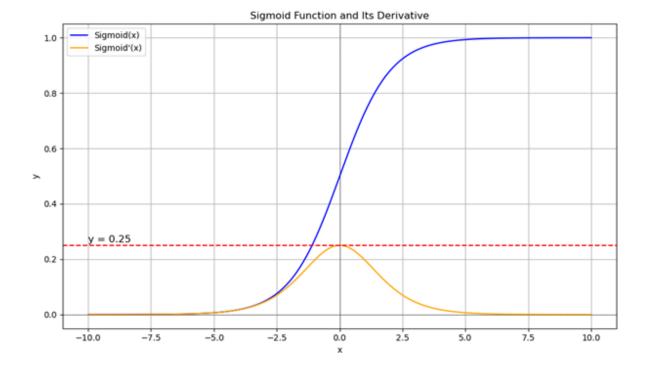
Sigmoid activation function

The main role of the sigmoid activation function is to normalize candidate values and convert the cell state to a hidden state when performing cell state updates. It limits the output between [0,1] because it has a smooth gradient, which is important for discovering long-range dependencies.

$$Sigmoid(x) = \frac{1}{1 + e^{-x}} \tag{24}$$

$$Sigmoid'(x) = Sigmoid(x)(1 - Sigmoid(x))$$
 (25)

Below is the sigmoid function and its derivative.



$$Domain(Sigmoid(x)) = \mathbb{R}, \quad Codomain(Sigmoid(x)) = (0, 1)$$

 $Domain(Sigmoid'(x)) = \mathbb{R}, \quad Codomain(Sigmoid'(x)) = [0, 0.5]$

Hyperbolic tangent activation function

The main role of the hyperbolic tangent (tanh) activation function is to normalize candidate values and convert the cell state to a hidden state when performing cell state updates. It limits the output between [-1,1] because it has a stable gradient, which is important for discovering long-range dependencies.

$$tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$
 (26)

$$tanh'(x) = 1 - tanh^2(x) \tag{27}$$

Below is the Hyperbolic tangent activation function and its derivative.

$$Domain(tanh(x)) = \mathbb{R}, \quad Codomain(tanh(x)) = [-1, 1]$$

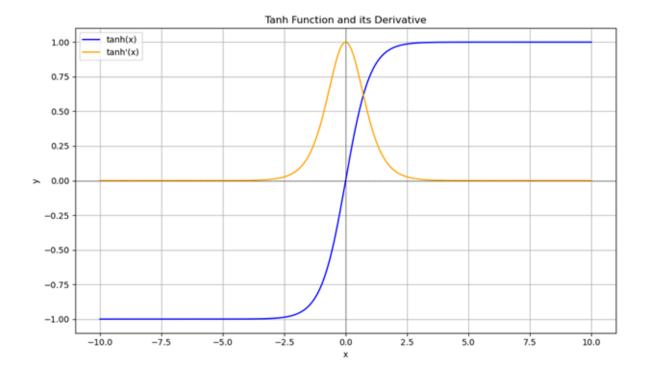
 $Domain(tanh'(x)) = \mathbb{R}, \quad Codomain(tanh'(x)) = [0, 1]$

2.2.3 Gradient vanishing and gradient exploring

When training the RNN, BPTT was used to update the weight matrix. As the number of time steps increase, the problem of gradient instability of often encountered, and this problem is gradient vanishing and gradient exploring (Bengio et al., 1994).

Vanishing Gradients

Generally, sigmoid activation function is used commonly in RNNs, has a maximum derivative of 0.25. When doing BPTT in long time steps, this multiplication results in exponentially diminishing gradients as the sequence length increases. Consequently, the shallow



neural receive very small gradient updates, making it difficult to adjust the parameters effectively. This leads to the model struggling to learn long time dependencies.

Exploding Gradients

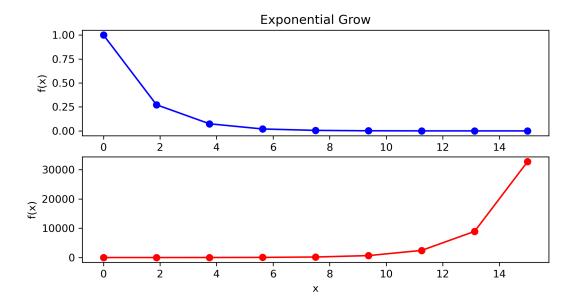
When we are doing the feedforward and get super large value computed by loss function. Then when updating the parameters. The updates to the weights will also be large. Resulting in higher loss and larger gradients in the next iterations. This will lead to exploding gradients.

We have introduce the backpropagation through time. This is the method to update the parameters in RNNs. When calculating, for example, the partial derivative of loss function with respect to W. Assume the time t go to infinity large. We will get this term. $\prod_{j=i+1}^t \frac{\partial h_j}{\partial h_{j-1}}, \text{ and it will lead to exponential problem. if } \frac{\partial h_j}{\partial h_{j-1}} > 1. \text{ Then the product of all term will increase exponentially, then exploding gradients occur. On the contrary, if } \frac{\partial h_j}{\partial h_{j-1}} < 1. \text{ Then the result will decrease exponentially, then vanishing gradients occur.}$

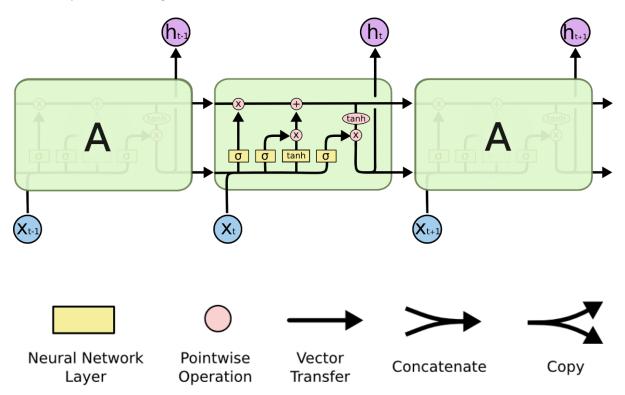
2.2.4 Long short-term memory (LSTM)

Long short-term memory proposed by (Hochreiter & Schmidhuber, 1997). LSTM is designed for handling long time step problems. The architecture of LSTM can prevent vanishing gradient and exploring gradient. The main difference between LSTM and RNN is the number of gates. LSTM introduced input, forget and output gates. This allows LSTM to manage the flow of information more effectively, retaining important information over longer sequences.

Architecture



LSTMs introduce a memory cell that can maintain information over long time steps the cell is controlled by three gates, input gate, output gate, and forget gate. Each cell of LSTMs inside has 3 sigmoid and 1 tanh layer. Below graph unfolds the LSTM hence we can analyze different gates.



Forget gate:

The forget gate is a component of the LSTM, designed to manage the flow of information within the cell state. The function of forget gate is to determine which information should be retained in memory cell (Hochreiter & Schmidhuber, 1997).

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \tag{28}$$

Input gate:

The input gate controls how much new information from the current time step is allowed to enter the cell (Hochreiter & Schmidhuber, 1997). For the \tilde{C}_t , the purpose is to suggest updates for the cell state.

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_c) \tag{29}$$

$$\widetilde{C}_t = tanh(W_c \cdot [h_{t-1}, x_t] + b_c) \tag{30}$$

Cell State Update:

The forget gate will drop the meaningless information and add some potential information.

$$C_t = f_t * C_{t-1} + i_t * \widetilde{C}_t \tag{31}$$

Output gate:

The output gate is able to control how much or what information from the cell state should be passed to the next layer or used in predictions.

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \tag{32}$$

Hidden State Update:

The hidden state is influenced by output value and current cell state.

$$h_t = o_t * tanh(C_t) \tag{33}$$

 $n = number of features in the input vector <math>x_t$. m = number of units in LSTM.

Notation	Meaning	Dimension
x_t	x_t Input vector at time t	
h_t	h_t Hidden state output at time t	
C_t	C_t Cell state at time t	
f_t	f_t Forget gate output at time t	
$egin{array}{c} f_t \ i_t \end{array}$	Input gate output at time t	$m \times 1$
	Output gate output at time t	$m \times 1$
\widetilde{C}_t	Candidate memory cell at time t	$m \times 1$
W_f	Weight matrix for the forget gate	$m \times (m+n)$
W_i	Weight matrix for the input gate	$m \times (m+n)$
W_C	Weight matrix for the candidate memory cell	$m \times (m+n)$
W_o	W_o Weight matrix for the output gate	
b_f	Bias vector for the forget gate	$m \times 1$
b_i		
b_C	b_C Bias vector for the candidate memory cell	
b_o	b_o Bias vector for the output gate	

Table 2: Unfolded RNN

Number of parameters:

1. Weights matrix for the input

• Forget gate: $n \times m$

• Input gate: $n \times m$

• Cell gate: $n \times m$

• Output gate: $n \times m$

2. Weight matrix for the hidden state

• Hidden state for forget gate: $m \times m$

• Hidden state for input gate: $m \times m$

• Hidden state for cell gate: $m \times m$

• Hidden state for output gate: $m \times m$

3. Bias term

• Bias for forget gate: $1 \times m$

• Bias for input gate: $1 \times m$

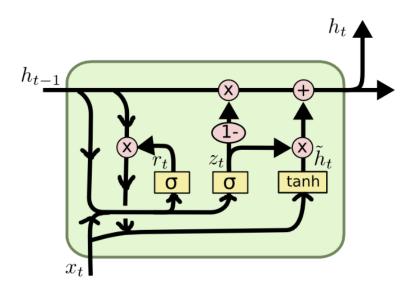
• Bias for cell gate: $1 \times m$

• Bias for output gate: $1 \times m$

Total parameters: $4 \times (n + m + 1) \times m$

2.2.5 Gated Recurrent Unit (GRU)

The gated recurrent unit (GRU) was proposed by (Cho et al., 2014) to make each recurrent unit to adaptively capture dependencies of different time scales. The GRU has 2 gates, update gate and reset gate. Update gate:



The update gate determines how much of the past information should be retained in the current hidden state.

$$z_t = \sigma(W_z \cdot [h_{t-1}, x_t] + b_z) \tag{34}$$

Reset gate:

The reset gate is similar with the update gate, but the candidate hidden state is influenced by the reset gate.

$$r_t = \sigma(W_r \cdot [h_{t-1}, x_t] + b_r)$$
 (35)

Candidate hidden state:

The candidate hidden state combined with previous hidden state and current input to form the potential new information that can be added to the current hidden state.

$$\widetilde{h_t} = tanh(W_h \cdot [r_t * h_{t-1}, x_t] + b_h) \tag{36}$$

Final hidden state

The final hidden state of the GRU at time t is a linear interpolation between the previous final hidden state and the candidate hidden state.

$$h_t = (1 - z_t) * h_{t-1} + z_t * \widetilde{h}_t \tag{37}$$

Notation	Meaning	Dimension
x_t	x_t Input vector at time t	
h_t	Hidden state output at time t	$m \times 1$
r_t	Reset gate output at time t	$m \times 1$
z_t	Update gate output at time t	$m \times 1$
W_z	Weight matrix for the update gate	$m \times (m+n)$
W_r	Weight matrix for the candidate memory cell	$m \times (m+n)$
W_h	Weight matrix for the output gate	$m \times (m+n)$
b_z	Bias vector for the input gate	$m \times 1$
b_r	b_r Bias vector for the candidate memory cell	
b_h	b_h Bias vector for the output gate	

Number of parameters:

1. Weights matrix for the input

• Update gate: $n \times m$

• Reset gate: $n \times m$

• Candidate hidden state: $n \times m$

2. Weight matrix for the hidden state

• Hidden state for update gate: $m \times m$

• Hidden state for reset gate: $m \times m$

• Hidden state candidate hidden state: $m \times m$

3. Bias term

• Bias for update: $1 \times m$

• Bias for reset: $1 \times m$

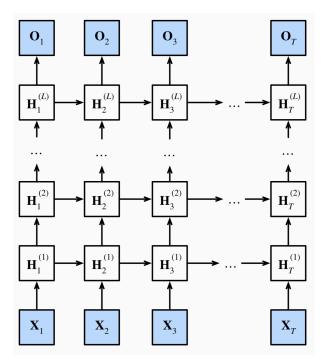
• Bias for candidate hidden state: $1 \times m$

Total parameters: $3 \times (n + m + 1) \times m$

2.2.6 Deep recurrent neural networks (DRNNs)

Deep architecture networks with multiple layers that can hierarchically learn complex representations (Bengio, 2009). By extending of this concept, stacking recurrent layers to form Deep Recurrent Neural Networks aligns with this principle. A number of research papers have been prove that the performance of DRNNs is out-performance then conventional RNNs. (Delalleau & Bengio, 2011; Le Roux & Bengio, 2010; Pascanu et al., 2013)

The architecture of DRNNs are similar with conventional RNNs. We simply stack the recurrent layers vertically. For the first layer, this layer receives the input and combines it with its previous hidden state h_{t-1} (Equation 38). The second layer receive the hidden state of the first layer and treat as the input of the layer 2 (Equation 39). We can extend this concept to L layers (Equation 40).



$$h_t^{(1)} = f(W_{xh}^{(1)} x_t + W_{hh}^{(1)} h_{t-1}^{(1)} + b_h^{(1)})$$
(38)

$$h_t^{(2)} = f(W_{xh}^{(2)} h_t^{(1)} + W_{hh}^{(2)} h_{t-1}^{(2)} + b_h^{(2)})$$
(39)

$$h_t^{(L)} = f(W_{xh}^{(L)} h_t^{(L-1)} + W_{hh}^{(L)} h_{t-1}^{(L)} + b_h^{(L)})$$
(40)

$$o_t = W_{hy} h_t^{(L)} + b_y \tag{41}$$

$$y_t = g(o_t) (42)$$

Where x_t is the input at time t. $h_t^{(l)}$ is the hidden state for the l layer at time t. $W_{xh}^{(l)}, W_{hh}^{(l)}$ are the weight matrices for the input to hidden and hidden to hidden connections in layer l, respectively. W_{hy} is weight matrix for the output layer. $b_h^{(l)}$ is the bias vector for the l layer (except output layer), b_y is the bias vector for output layer. $g(\cdot)$ and $f(\cdot)$ are an activation function.

2.2.7 Hidden Markov Model

Before reviewing Hidden Markov Model (HMM), it is essential to understand what Markov models is, or Markov chains. Markov chains are fundamental models in probability theory and statistic, and it is a stochastic process describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event. This property known as the Markov property (L. Rabiner & Juang, 1986; Roberts & Rosenthal, 2004). In rigorous terms. Let the state space be defined as:

$$S = \{s_1, s_2, \dots, s_N\}. \tag{43}$$

$$P(s_{t+1} \mid s_t, s_{t-1}, s_{t-2}, \cdots, s_1) = P(s_{t+1} \mid s_t)$$
(44)

The state transition probability is denoted by:

$$P_{ij} = P(s_{t+1} = s_j \mid s_t = s_i). (45)$$

Given an initial state s_1 with probability $P(s_1)$, the joint probability of a state sequence $\{s_1, s_2, \ldots, s_T\}$ can be written as:

$$P(s_1, s_2, \dots, s_T) = P(s_1) \cdot P(s_2 \mid s_1) \cdot P(s_3 \mid s_2) \cdots P(s_T \mid s_{T-1})$$
(46)

We can simply the joint probability of a state sequence as equestion 47.

$$P(s_1, s_2, \dots, s_T) = P(s_1) \prod_{t=1}^{T-1} P(s_{t+1} \mid s_t)$$
(47)

Then it is essential to discuss marginal probability in a Markov model because it provides critical information about the likelihood of being in particular state s_j at a specific time t. The marginal probability of being in state s_j at time t defined as:

$$\pi_t(s_j) = P(s_t = s_j) \tag{48}$$

It is the probability of the system being in state s_j at time t, irrespective of how the system transitioned to s_j . We can obtain by summing over all possible transition probability P_{ij} where s_i belong in state space.

$$\pi_{t+1}(s_j) = \sum_{s_i \in S} \pi_t(s_i) \cdot P_{ij} \tag{49}$$

If Markov chain is irreducible and aperiodic, the stationary distribution defined as below:

$$\pi_j = \sum_{i=1}^n \pi_i P_{ij} \tag{50}$$

Hidden markov model

Hidden Markov Model (HMMs) is a statistical model that extends the Markov chains by introducting a layer of latent (unobservable) variables. And connecting them to observable outputs (emission probability). In contrast to standard Markov chains, hidden states are never be observed directly. Instead, we observe a sequence of data (observations) that are probabilitically generated by these hidden state. This structure has proven useful for applications in speech recognition, biological sequence analysis, and signal processing

(L. R. Rabiner, 1989). Lets the hidden states be denoted by X_t , where X_t is the hidden state at time t. The hidden state space is defined as:

$$\mathcal{X} = \{s_1, s_2, \cdots, s_n\} \tag{51}$$

where \mathcal{X} is finite set of size n, and each $s_i \in \mathcal{X}$ represents a specific possible hidden state. Then for the observable space represents the possible outcomes (observations) that are generated by the hidden state, we have discuss previously. Let the observations at time t be denoted by Y_t . The observable space is defined as:

$$\mathcal{Y} = \{o_1, o_2, \cdots, o_m\} \tag{52}$$

where \mathcal{Y} is finite set of size m, and each $o_i \in \mathcal{Y}$ represents a specific possible observation. Then for the transition probability matrix (P), the probability of transitioning between hidden states denoted as:

$$P_{n \times n} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix}$$

$$(53)$$

$$p_{ij} = P(X_{t+1} = s_i \mid X_t = s_i) \tag{54}$$

where $s_i, s_i \in \mathcal{X}$.

For emission probability matrix (B), the probabilities of generating an observation given a hidden state.

$$B_{n \times n} = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{mm} \end{bmatrix}$$

$$(55)$$

$$b_{ik} = P(Y_t = o_k \mid X_t = s_i) \tag{56}$$

where $s_i \in \mathcal{X}, o_k \in \mathcal{Y}$.

And the goal of hidden markov model is the maximize the joint probability P(X,Y) given the initial probability $P(X_1)$.

$$P(X,Y) = P(X_1) \cdot \prod_{t=1}^{T-1} P(X_{t+1} = s_j \mid X_t = s_i) \cdot \prod_{t=1}^{T} P(Y_t = o_k \mid X_t = s_i)$$
 (57)

For the NLP tasks, there may have some unobservable data, for example the implicit sentiment, user intent, emotional state. (L. R. Rabiner & Juang, 1993) proposes the hidden Markov model (HMM), the assumption is the existence of the latent process follows a Markov chain from which observations X are generated. In other word, there would exists an unobserved state sequence $Z = \{z_1, z_2 \cdots, z_T\}$ in observed sequence $X = \{x_1, x_2, \cdots, x_T\}$ (Sengupta et al., 2023). Where the hidden states, z_t belonging to state-space $Q = \{q_1, q_2, \cdots, q_M\}$ follow a Markov chain governed by:

• A state-transition probability matrix $A = [a_{ij}] \in \mathbb{R}^{M \times M}$ where $a_{ij} = p(z_{t+1} = q_j | z_t = q_i)$

• Initial state matrix $\pi = [\pi_i] \in \mathbb{R}_{1 \times M}$ with $\pi_i = p(z_1 = q_i)$

Furthermore, for the hidden state z_t , corresponding to the observe data x_t is release by emission process $B = [b_j(x)]$ where $b_j(x) = p(x|z = q_i)$. We can assume $b_j(x)$ is follows the Gaussian mixture model (GMM).

$$p(x_t|z=q_j) = \sum_{l=1}^k c_{jl} \mathcal{N}(x_t|\mu_{jl}, \Sigma_{jl})$$
(58)

where $\sum_{l=1}^k c_{jl} = 1$, $\forall j = \{1, \dots, M\}$, k is the number of Gaussian mixture components and $\mathcal{N}(x_t|\mu_{jl}, \Sigma_{jl})$ denotes a Gaussian probability density with mean μ_{jl} and covariance Σ_{jl} for state j and mixture component l. The number of hidden states (M) and mixture component (k) are the two hyperparameters of the model which have to be provided apriori.

Therefore, the joint probability probability density function of the observation X can be expressed as:

$$p(X) = p(z_1) \prod_{t=1}^{T-1} p(z_{t+1}|z_t) \prod_{t=1}^{T} p(x_t|z_t)$$
(59)

The optimal parameters $[A, B, \pi]$, which maximize the likelihood of the observation sequence X (Equation 39), are determined using the Baum-Welch algorithm, an expectation-maximization method (L. R. Rabiner & Juang, 1993). Additionally, the probability of the system in a specific hidden state z_t corresponding to the observation x_t is calculated using the Viterbi algorithm.

2.2.8 Word representation

In RNN, the due to the architecture, the model can only handle vector, it is important that convert the word into machine readable format. By translating words into vectors, these representations capture semantic meanings, relationships and contexts. (Mikolov et al., 2013) proposed 2 model architectures for leaning distributed representations of words.

Continuous Bag of Words model

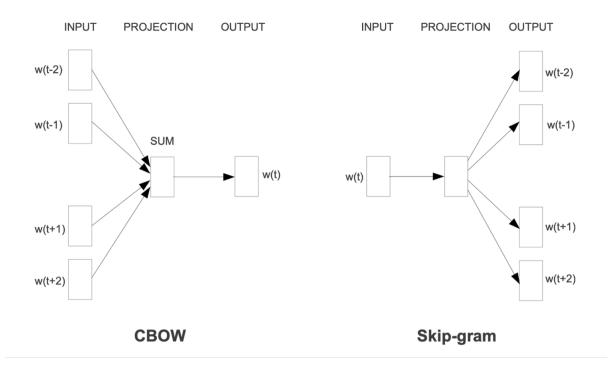
CBOW operates by taking context words around a target word, it is flexible to adjust the window size which mean that we can control how many words around our target word. Hence aggregating their embeddings and passing to hidden layer to produce a probability distribution. Capture the semantic meanings and the relationship more effectively.

$$Q = N \times D + D \times loq_2(V) \tag{60}$$

Continuous Skip gram model

The continuous skip gram model operates in opposite direction compare with CBOW. The model takes the surrounding word to predict the target word. In other word, treat the current word as an input to a log-linear classifier with continuous projection layer, and predict the probability distribution of surrounding words.

$$Q = C \times (D + D \times log_2(V)) \tag{61}$$



3 Project Goals and Objectives

3.1 Project Goals

The primary goal of this report is to deeply review on RNN and how it can apply in natural language processing (NLP) tasks. And by comparing the performance of different models. this report aims to provide a detailed comparative analysis of the following RNN-based models:

- Vanilla RNN
- Long Short-Term Memory (LSTM)
- Gated Recurrent Unit (GRU)

3.2 Objectives

3.2.1 Implement Existing RNN Architectures

Develop models using state-of-the-art deep learning framework, PyTorch, to implement each of the above RNNs model. This includes setting up the network layers, loss functions, and appropriate optimization methods.

3.2.2 Apply the Models on a Benchmark NLP Dataset

Utilize a selected NLP dataset to train and evaluate the performance of each RNN-based model. The dataset will be preprocessed (e.g., tokenization, padding, embedding initialization) to suit sequential data modeling.

3.2.3 Compare Model Performances

Compare different RNN-based models on metrics relevant to the target NLP taskquantitatively and qualitatively. Accuracy, F1, training time scores be used.

3.2.4 Analyze the Impact of Architectural Differences

Identify and discuss the strengths and limitations of each model architecture through both experimental results and theoretical insights. For example, compare how LSTM and GRU architectures mitigate vanishing gradients and exploding gradients using gating mechanisms relative to a vanilla RNN.

4 Research Plan / Methodology

To achieve the project goals and objectives, this report will follow the step as below:

4.1 Literature Review

Since this report require some knowledge related on RNN and NLP. So it is necessary to review the foundemental of those area. Different architecture of RNNs-based model for instance, vanilla RNN, LSTM, GRU. And understand the limitation of RNN, vanishing/exploding gradients. Also, it is essential to understand natural language processing (NLP).

4.2 Data Collection and Preprocessing

4.2.1 Data Collection

In this report, ACL-IMDB (Maas et al., 2011) was experiment. This is a dataset for binary sentiment classification containing substantially more data than previous benchmark datasets. This dataset provide a set of 25,000 highly polar movie reviews for training, and 25,000 for testing. I preporcess the dataset by text cleaning and tokenization.

4.2.2 Data Preprocessing

1. Lowercasing:

All text was converted to lowercase to ensure consistency and avoid treadting words like "Good" and "good" as different tokens.

2. Handing Abbreviations:

I hard code a dictionary in python, and marjority of common abbreviations were included and replaced with their full forms. For example:

- "u" -> "you"
- "pls" -> "please"
- 3. Removing HTML Tags:

HTML tags were removed using regular expression

where variable "sentence" is movie review.

4. Removing Special Characters

Non-alphanumeric characters (e.g. punctuation) were removed using the regular expression

import re re.sub(r'[
a
a-zA-Z0-9\s]', '', sentence)

5. Removing Extra Whitespace

Leading and trailing whitespaces were stripped.

6. Removing Stop Words

Stop words (e.g., "is", "the", "and") were removed to reduce noise in the text. The NLTK library's stop word list was used. Words not in the stop word list were retained.

7. Tokenization

The cleaned text was split into individual tokens, I use white space and the criterion to split the word.

Once the text was preprocessed, a vocabulary was constructed from the dataset. The vocabulary mapping each word to a unique index. Words not found in the vocabulary are replaced with an "unknown" token. I reserved index 0 as unknown token. So that if the word can not map to corresponding index. Then the token should be 0. This is a good way to handle Out-of-vocabulary words (Mikolov et al., 2013).

Word	Index
<unk></unk>	0
acting	1
good	2
movie	3
amazing	4
performance	5
bad	6
terrible	7
excellent	8

Table 4: Word to Index Mapping Table

4.3 Model Architecture

In this section, i will describe the model architecture, i will list out all of the model i have used and the detail information of those models. For mathematical notation, i will define all of the variables precisely and clearly. And because this project mainly focusing on natural language processing task. So that the classification model consists of an embedding layer, this is just like a look-up table to convert token to vector. First, the sequence of words (w_1, w_2, \dots, w_T) are passed through an embedding layer, which is the look-up table to convert those words in vector format. In other words, the look-up

table map the word in a high-demensional space (v_1, v_2, \dots, v_T) (Table 5), where $v_t \in \mathbb{R}^d$. And the dimension of the vector space is depends on how we define the hidden size of the model. Next, the forward of RNN based model will processes these word vectors v_t in the forward directions, updating corresponding hidden states at each time step t.

Word	Index	Embedding Vector
<unk></unk>	0	$\begin{bmatrix} 0.01 & -0.02 \cdots 0.03 & 0.04 \end{bmatrix}$
acting	1	$\begin{bmatrix} 0.12 & 0.23 \cdots - 0.11 & 0.05 \end{bmatrix}$
good	2	$\begin{bmatrix} 0.03 & -0.15 \cdots 0.08 & 0.07 \end{bmatrix}$
movie	3	$\begin{bmatrix} 0.10 & 0.05 \cdots - 0.09 & -0.01 \end{bmatrix}$
amazing	4	$\begin{bmatrix} 0.25 & -0.12 \cdots 0.18 & 0.30 \end{bmatrix}$
performance	5	$\begin{bmatrix} -0.10 & -0.20 \cdots 0.15 & -0.05 \end{bmatrix}$
bad	6	$\begin{bmatrix} 0.40 & 0.35 \cdots - 0.10 & 0.50 \end{bmatrix}$
terrible	7	$\begin{bmatrix} 0.30 & 0.25 \cdots - 0.11 & 0.40 \end{bmatrix}$
excellent	8	$\begin{bmatrix} 0.32 & 0.38 \cdots - 0.90 & 0.70 \end{bmatrix}$

Table 5: Word to Index Matching with Lookup Table Embeddings

4.3.1 Model 1 (Vanilla RNN)

This is the vanilla RNN model, with 1 layer. We just use the last output to calculate the loss function and do the backpropagation.

$$h_t = f(W_{ih}^T v_t + W_{hh} h_{t-1} + b_h) (62)$$

where W_{ih} is input to hidden matrix, v_t is the word vector at time step t, W_{hh} is hidden to hidden matrix. h_t is hidden state at time t. b_h is biased term for hidden state. For the output at time t, we will pass the hidden state output to an activation function defined as below.

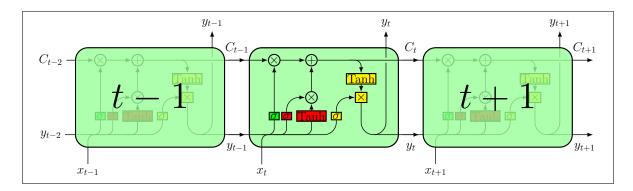
$$\hat{y}_t = f(W_{ho}^T h_t + b_y) \tag{63}$$

where y_t is the output at time step t and W_{ho} is the hidden to output matrix and b_y is biased term for output. And $f(\cdot)$ is an activation function. Then we calculate the loss function by the last output.

$$Loss = \mathcal{L}(\hat{y}, y) \tag{64}$$

4.3.2 Model 2 (Long short-term memory)

For the LSTM model, I use 1 layer:



For an LSTM, the overall structure is similar to the Vanilla RNN shown in the diagram, but the hidden state computation is replaced by the LSTM's more complex gating mechanism. Using its gating mechanisms to control how information flows through time. Let us consider an input sequence $\{v_1, v_2, \ldots, v_T\}$, where v_t represents the input vector at time step t. Here's how the LSTM processes the input:

Step 1: Initialize Hidden and Cell States At the beginning of the sequence, the LSTM initializes the hidden state h_0 and cell state C_0 . For our model, we use 0 matrix as h_0 and C_0 :

$$h_0 = \mathbf{0}, \quad C_0 = \mathbf{0} \tag{65}$$

Step 2: Process Each Input Vector For each time step t, LSTM processes the current input v_t along with the previous hidden state h_{t-1} and cell state C_{t-1} to compute:

- The forget gate f_t , determine which information should be retained in memory cell C_{t-1} .
- The **input gate** i_t , controls how much new information from the current time step is allowed to enter the cell.
- The **cell candidate** \tilde{C}_t , represents the new information to be added to the cell state.
- The updated **cell state** C_t , which combines the retained information from C_{t-1} and the new candidate \tilde{C}_t .
- The **output gate** o_t , control how much or what information from the cell state should be passed to the next layer or used in predictions.
- The updated hidden state h_t , summarizes the information at time t.

Step 3: Compute Forget Gate The forget gate f_t is computed as:

$$f_t = \sigma(W_f v_t + U_f h_{t-1} + b_f) \tag{66}$$

where:

- σ is the sigmoid activation function.
- W_f is the input to hidden weight matrix for the forget gate.
- \bullet U_f is the hidden to hidden weight matrix for the forget gate.
- b_f is the bias term for the forget gate.

The forget gate determines which parts of the previous cell state C_{t-1} to retain.

Step 4: Compute Input Gate The input gate i_t is computed as:

$$i_t = \sigma(W_i v_t + U_i h_{t-1} + b_i) \tag{67}$$

where:

• W_i , U_i , and b_i are the weight matrices and bias for the input gate.

The input gate determines how much new information to add to the cell state.

Step 5: Compute Cell Candidate The cell candidate \tilde{C}_t is computed as:

$$\tilde{C}_t = \tanh(W_c v_t + U_c h_{t-1} + b_c) \tag{68}$$

where:

- tanh is the hyperbolic tangent activation function.
- W_c , U_c , and b_c are the weight matrices and bias for the cell candidate.

The cell candidate represents potential new information to add to the cell state.

Step 6: Update Cell State The cell state C_t is updated as:

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \tag{69}$$

where \odot represents element-wise multiplication. The updated cell state combines retained information from C_{t-1} (via f_t) and new information from \tilde{C}_t (via i_t).

Step 7: Compute Output Gate The output gate o_t is computed as:

$$o_t = \sigma(W_o v_t + U_o h_{t-1} + b_o) \tag{70}$$

where W_o , U_o , and b_o are the weight matrices and bias for the output gate.

Step 8: Compute Hidden State The hidden state h_t is computed as:

$$h_t = o_t \odot \tanh(C_t) \tag{71}$$

The hidden state summarizes the information at time t and is passed to the next time step.

Step 9: Use Final Hidden State for Output After processing all time steps, the final hidden state h_T is used as the input to a fully connected layer for classification:

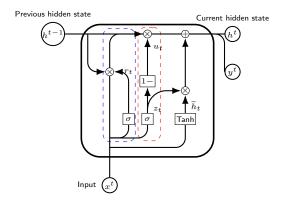
$$\hat{y} = f(W_{ho}^T h_T + b_y) \tag{72}$$

where W_{ho} and b_y are the weight matrix and bias for the output layer, and f is the activation function. Then we calculate the loss function by the last output.

$$Loss = \mathcal{L}(\hat{y}, y) \tag{73}$$

4.3.3 Model 3 (Gated recurrent unit)

For the GRU model, I use 1 layer. This architecture is similar with LSTM but reduce the among of parameters. Let us consider an input sequence $\{v_1, v_2, \ldots, v_T\}$, where v_t represents the input vector at time step t. Here's how the GRU processes the input:



Step 1: Initialize Hidden State At the beginning of the sequence, the GRU initializes the hidden state h_0 to zero:

$$h_0 = \mathbf{0} \tag{74}$$

Step 2: Process Each Input Vector For each time step t, the GRU processes the current input v_t along with the previous hidden state h_{t-1} to compute:

- The **reset gate** r_t , which determines how much of the previous hidden state h_{t-1} to forget.
- The **update gate** z_t , which determines how much of the previous hidden state h_{t-1} to retain
- The candidate hidden state \tilde{h}_t , which represents the new information to be combined with the previous hidden state.
- The updated hidden state h_t , which summarizes the information at time t.

Step 3: Compute Reset Gate The reset gate r_t is computed as:

$$r_t = \sigma(W_r v_t + U_r h_{t-1} + b_r) \tag{75}$$

where:

- σ is the sigmoid activation function.
- W_r is the input to hidden weight matrix for the reset gate.
- U_r is the hidden to hidden weight matrix for the reset gate.
- b_r is the bias term for the reset gate.

The reset gate determines how much of the previous hidden state h_{t-1} to use when computing the candidate hidden state.

Step 4: Compute Update Gate The update gate z_t is computed as:

$$z_t = \sigma(W_z v_t + U_z h_{t-1} + b_z) \tag{76}$$

where:

- W_z is the input to hidden weight matrix for the update gate.
- U_z is the hidden to hidden weight matrix for the update gate.
- b_z is the bias term for the update gate.

The update gate determines how much of the previous hidden state h_{t-1} to retain and how much of the new candidate hidden state to use.

Step 5: Compute Candidate Hidden State The candidate hidden state \tilde{h}_t is computed as:

$$\tilde{h}_t = \tanh(W_h v_t + U_h(r_t \odot h_{t-1}) + b_h)$$
 (77)

where:

- tanh is the hyperbolic tangent activation function.
- $r_t \odot h_{t-1}$: The reset gate modulates the contribution of the previous hidden state h_{t-1} .
- W_h , U_h , and b_h are the weight matrices and bias for the candidate hidden state.

Step 6: Update Hidden State The updated hidden state h_t is computed as:

$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t \tag{78}$$

where:

- z_t : The update gate decides how much of the previous hidden state h_{t-1} to retain.
- $(1-z_t)$: The complement of the update gate decides how much of the candidate hidden state \tilde{h}_t to use.

Step 7: Use Final Hidden State for Output After processing all time steps, the final hidden state h_T is used as the input to a fully connected layer for classification:

$$\hat{y} = f(W_{ho}^T h_T + b_y) \tag{79}$$

where:

- ullet W_{ho} and b_y are the weight matrix and bias for the output layer.
- ullet f is the activation function (e.g., sigmoid for binary classification).

Then we calculate the loss function by the last output.

$$Loss = \mathcal{L}(\hat{y}, y) \tag{80}$$

4.4 Training, Hyperparameter Tuning, and Evaluation

In my experiments, I implemented the training loop using PyTorch. The following details describe the key components of my training code, which are designed to ensure robust model optimization and fair evaluation:

4.4.1 Model Hyperparameters and Setup

The following hyperparameters were chosen based on preliminary experiments and standard practices for sentiment classification tasks:

• Architecture Hyperparameters:

- Number of layers: no_layers = 1
- Vocabulary size: $vocab_size = len(vocab) + 1$ (the extra one is for unknown word)
- Embedding dimension: embedding_dim = 100
- Hidden dimension: hidden_dim = 50
- Output dimension: output_dim = 1
- Dropout probability: drop_prob = 0.5
- Batch size: batch_size = 50

• Optimization Hyperparameters:

- Learning rate: lr = 0.001
- Loss Function: Binary Cross Entropy Loss
- Optimizer: Adam with predefined learning rate.

In order to keep the fair experiment. I train 3 RNN model with the same hyperparameters

4.4.2 Training Loop Overview

- Mini-Batch Training with Hidden State Initialization: At the start of each epoch, the model is set to training mode using model.train(). For each mini-batch from the training data:
 - 1. The model's hidden state is initialized with zero matrix.
 - 2. Before the forward pass, gradients are zeroed via model.zero_grad() and optimizer.zero_grad().
 - 3. The forward pass is executed, producing outputs and an updated hidden state.
 - 4. The hidden state is detached from the computation graph using h.detach() to avoid backpropagating through all previous batches.
 - 5. The loss is computed using binary cross entropy.
 - 6. Backpropagation is performed via loss.backward().
 - 7. The gradients are clipped using nn.utils.clip_grad_norm_ with the specified clip value to mitigate exploding gradients.

- 8. Finally, the optimizer updates the model parameters using optimizer.step().
- Validation Stage: After each epoch, the model is switched to evaluation mode using model.eval() and evaluated on the validation set. Similar to training, the hidden state is updated parameters and the model will use that parameters to make the prediction. And the accuracy is computed and recorded.
- Performance Monitoring and Checkpointing: At the end of each epoch, the mean training and validation losses, as well as accuracy, are calculated. The validation loss is compared against the best loss seen so far. If the current validation loss is lower than the lowerest one, then the model's state dictionary is saved as the best model in .pth format.

4.4.3 Pseudocode Description

The following Python pseudocode summarizes the training procedure implemented in my experiment:

Listing 1: Training Loop Pseudocode

```
clip = 5
epochs = 5
valid_loss_min = np.inf
epoch_tr_loss, epoch_vl_loss = [], []
epoch_tr_acc, epoch_vl_acc = [], []
for epoch in range (epochs):
    train_losses = []
    train_acc = 0.0
    model.train()
    \# Initialize the hidden state for the first mini-batch
    h = model.init_hidden(batch_size)
    for inputs, labels in train_loader:
        inputs, labels = inputs.to(device), labels.to(device)
        model.zero_grad()
        optimizer.zero_grad()
        output, h = model(inputs, h)
        h = h.detach()
        loss = criterion (output, labels.float())
        loss.backward()
        train_losses.append(loss.item())
        accuracy = acc(output, labels)
        train_acc += accuracy
        nn.utils.clip_grad_norm_(model.parameters(), clip)
        optimizer.step()
```

```
val_h = model.init_hidden(batch_size)
val_losses = []
val_acc = 0.0
model.eval()
for inputs, labels in valid_loader:
    inputs, labels = inputs.to(device), labels.to(device)
    output, val_h = model(inputs, val_h)
    val_loss = criterion(output.squeeze(), labels.float())
    val_losses.append(val_loss.item())
    accuracy = acc(output, labels)
    val_acc += accuracy
epoch_train_loss = np.mean(train_losses)
epoch_val_loss = np.mean(val_losses)
epoch_train_acc = train_acc / len(train_loader.dataset)
epoch_val_acc = val_acc / len(valid_loader.dataset)
epoch_tr_loss.append(epoch_train_loss)
epoch_vl_loss.append(epoch_val_loss)
epoch_tr_acc.append(epoch_train_acc)
epoch_vl_acc.append(epoch_val_acc)
print ( f 'Epoch - { epoch +1} ')
print(f'train_loss \cdot: \{epoch_train_loss\} \cdot val_loss \cdot: \{epoch_val_loss\}')
print(f'train_accuracy::{epoch_train_acc*100}-val_accuracy::{epoch_
if epoch_val_loss <= valid_loss_min:</pre>
    torch.save(model.state_dict(), './working/state_dict.pt')
    print('Validation loss decreased ({:.6f}-->-{:.6f}). Saving model
          .format(valid_loss_min, epoch_val_loss))
    valid_loss_min = epoch_val_loss
print (25 * '==')
```

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