Recurrent Neural Networks, Transformers, and Attention

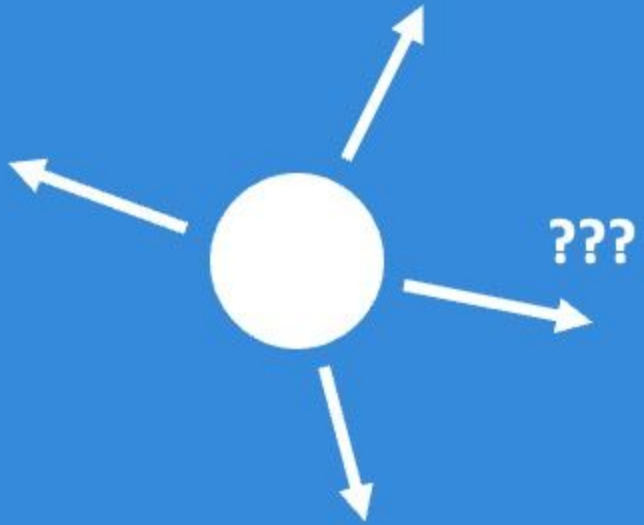
Prof. Dr. Patrick Terrematte (IMD / UFRN)

UFRN
UNIVERSIDADE FEDERAL DO RIO GRANDE DO NORTE

RNNs and Transformers

- Deep sequence modeling
- Intuition and Applications of RNNs
- Drawbacks of RNNs
- Self-Attention and Transformers

Given an image of a ball, can you predict where it will go next?



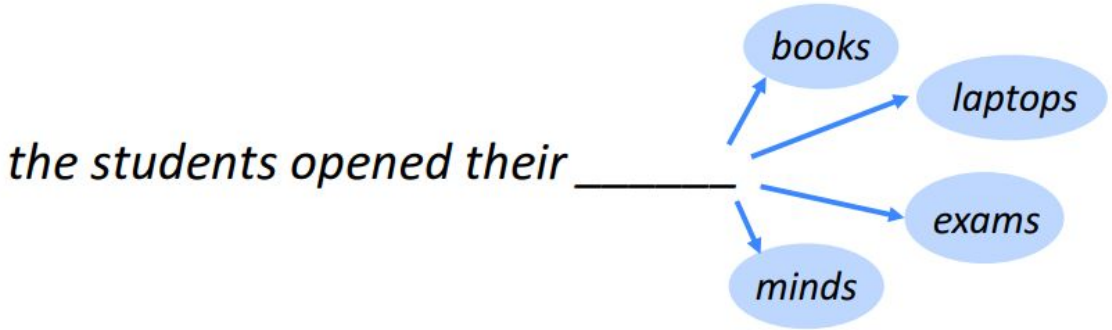
https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Given an image of a ball,
can you predict where it will go next?

https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Language Modeling

Language modeling is the task of predicting what word comes next.

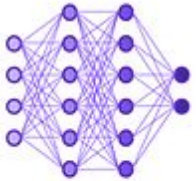


Language Modeling

Language modeling is the task of predicting what word comes next.

The cat likes to sleep in the

Input



Neural Network (LLM)

Word	Probability
ability	0.002
bag	0.071
box	**0.085**
...	...
zebra	0.001

Output

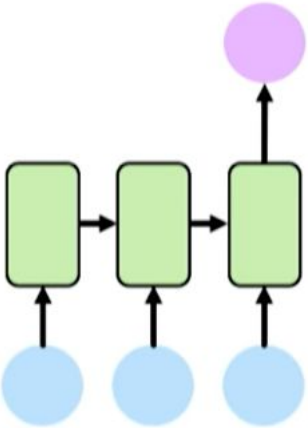
Sequence Modeling

One to One

Binary Classification

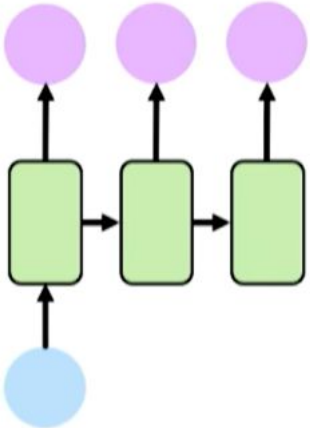
"Will I pass this class?"

Student → Pass?



Many to One

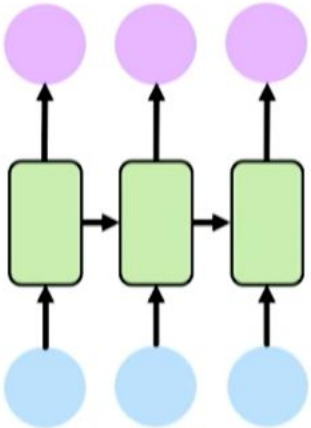
Sentiment Classification



One to Many

Image Captioning

"A baseball player throws a ball."



Many to Many

Machine Translation

https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Attention Timeline

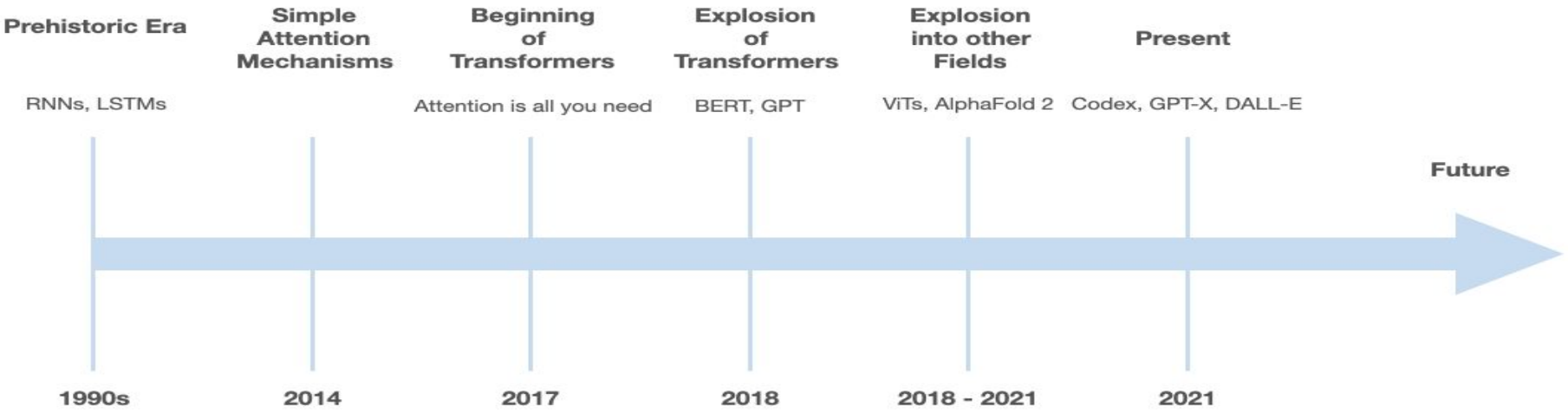
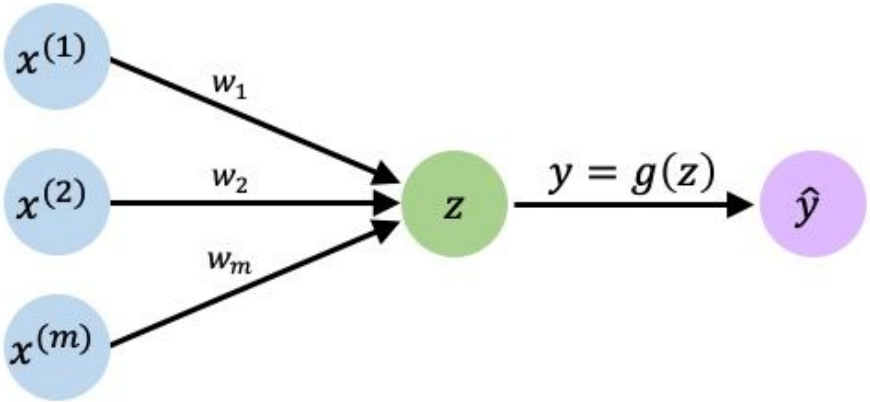


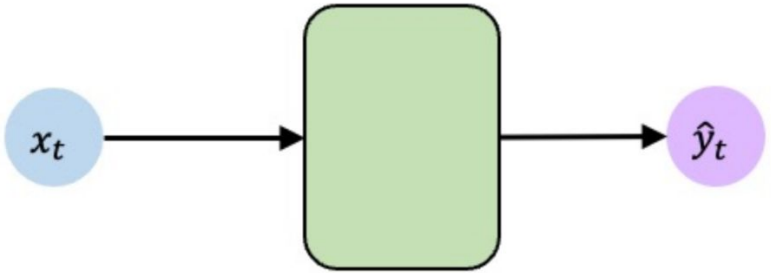
Figure adapted from Transformer United Course by Stanford.

Perceptron



https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Perceptron

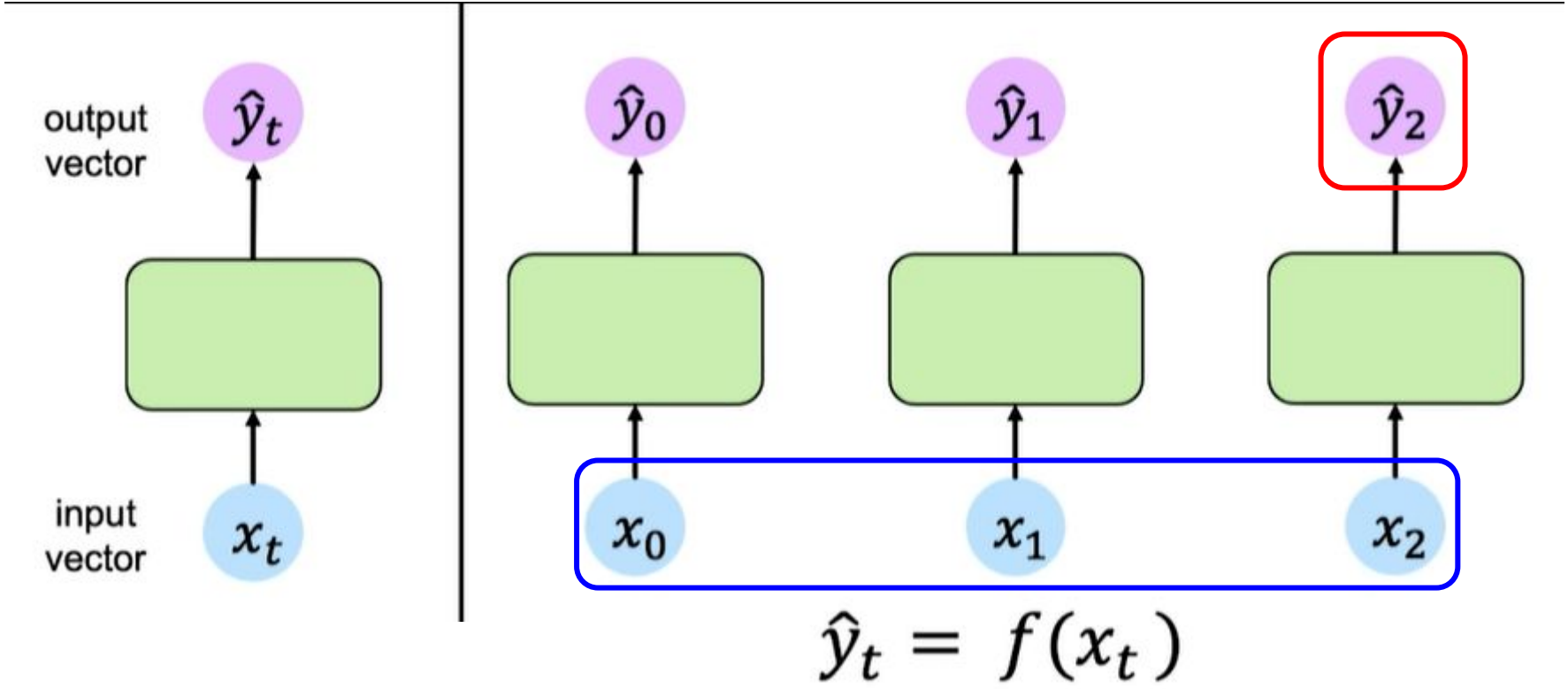


$$\boldsymbol{x_t} \in \mathbb{R}^m$$

$$\hat{\boldsymbol{y}}_t \in \mathbb{R}^n$$

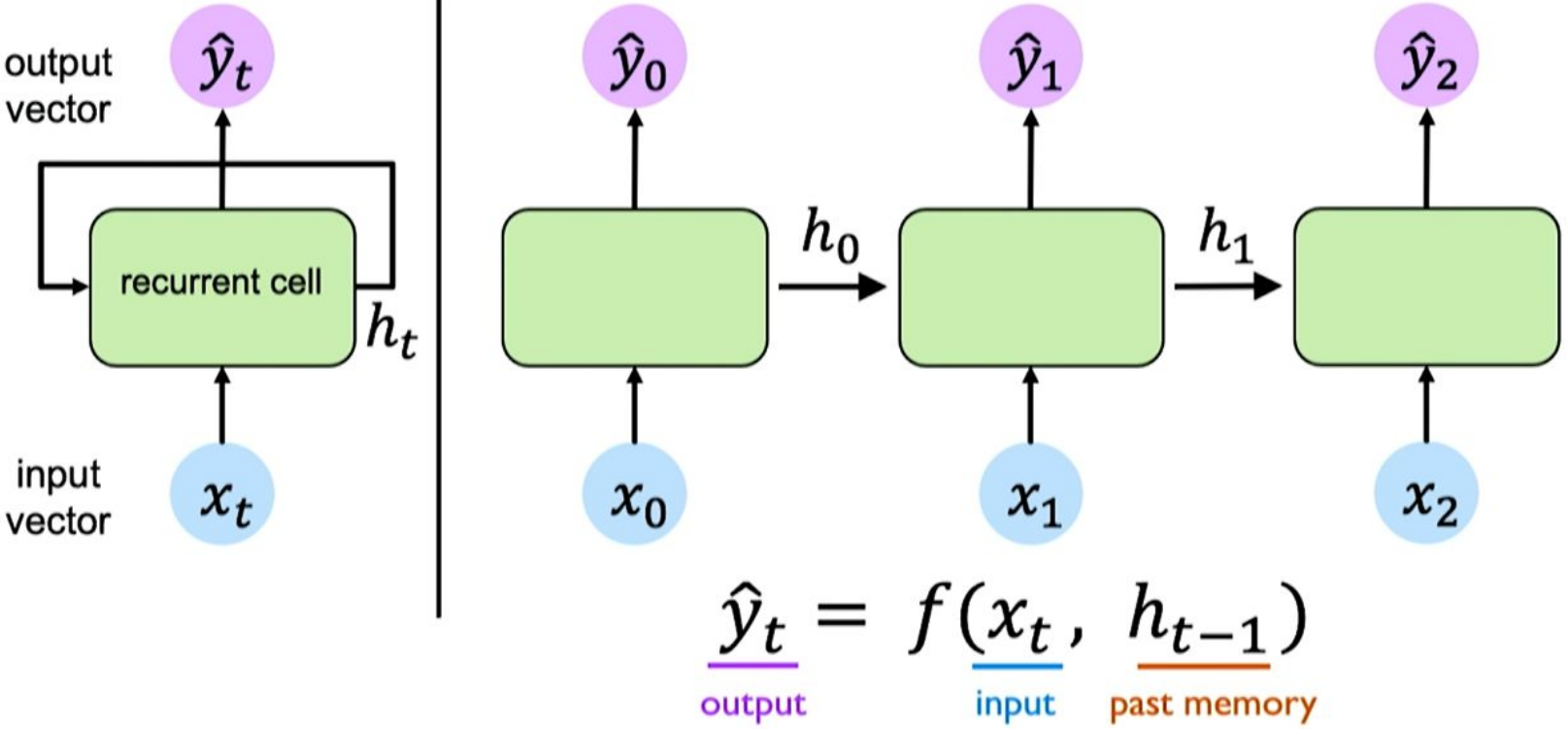
https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Time steps



https://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L2.pdf

Neuron with Recurrence

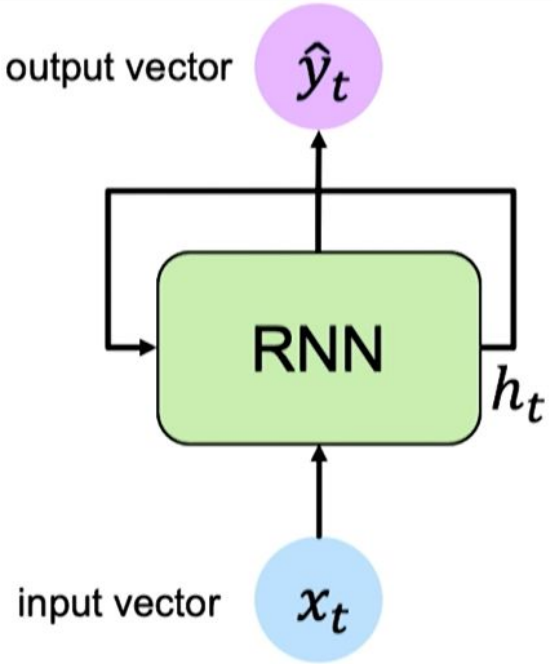


$$\hat{y}_t = f(x_t, h_{t-1})$$

output input past memory

Recurrent Neural Networks (RNNs)

Recurrent Neural Networks



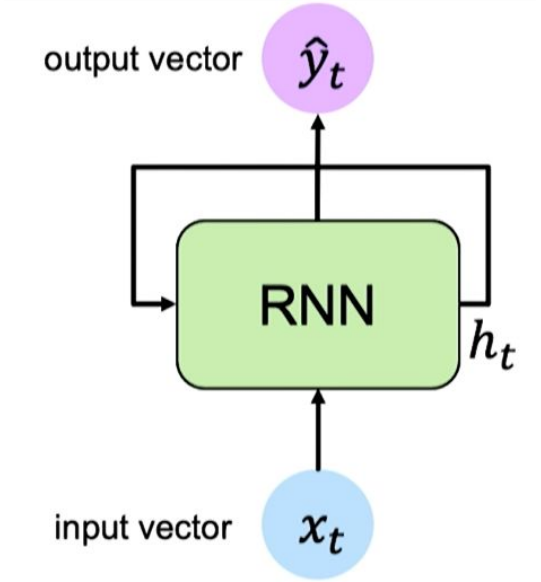
$$h_t = f_W(x_t, h_{t-1})$$

cell state | function with weights W | input | old state

RNNs have a state h_t that is updated at each time step as a sequence is processed.

RNN Intuition

```
my_rnn = RNN()
hidden_state = [0, 0, 0, 0]

sentence = ["I", "love", "recurrent", "neural"]

for word in sentence:
    prediction, hidden_state = my_rnn(word, hidden_state)

next_word_prediction = prediction
# >>> "networks!"
```



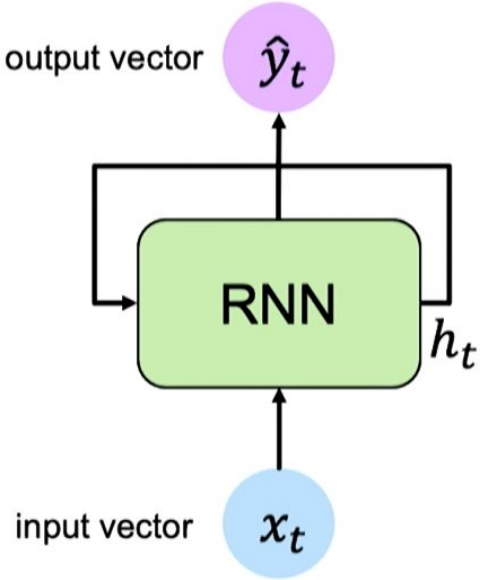
Perplexity

Perplexity measures language model quality

- "It's raining outside"
- "It's raining bananas"
- "It's raining piouw;kcj pwepoiut"

$$\exp\left(-\frac{1}{n}\sum_{t=1}^{n}\log P(x_t \mid x_{t-1}, \ldots, x_1)\right)$$

- Inverse of the geometric mean of the number of actual choices we have when deciding which token to choose next.
  - Best case, the model always perfectly estimates the probability of the target token as 1.
  - Worst case, the model always predicts the probability of the target token as 0. In this situation, the perplexity is positive infinity.
- If the model predicts a uniform distribution over all available tokens in the vocabulary, the perplexity is equal to the number of unique tokens in the vocabulary.



Output Vector

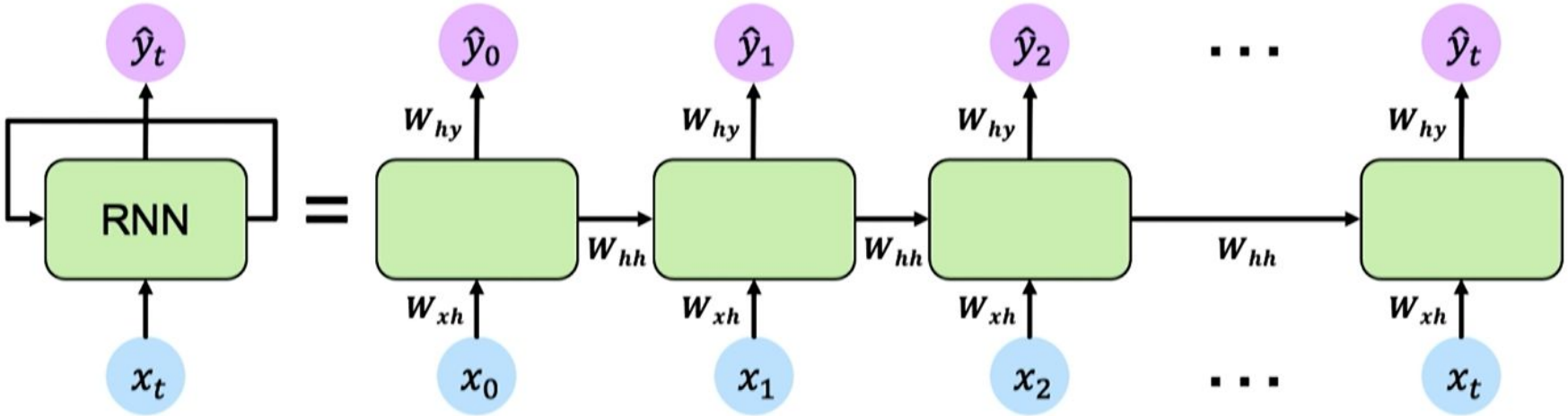
$$\hat{y}_t = \boldsymbol{W}_{\boldsymbol{hy}}^{\boldsymbol{T}} h_t$$

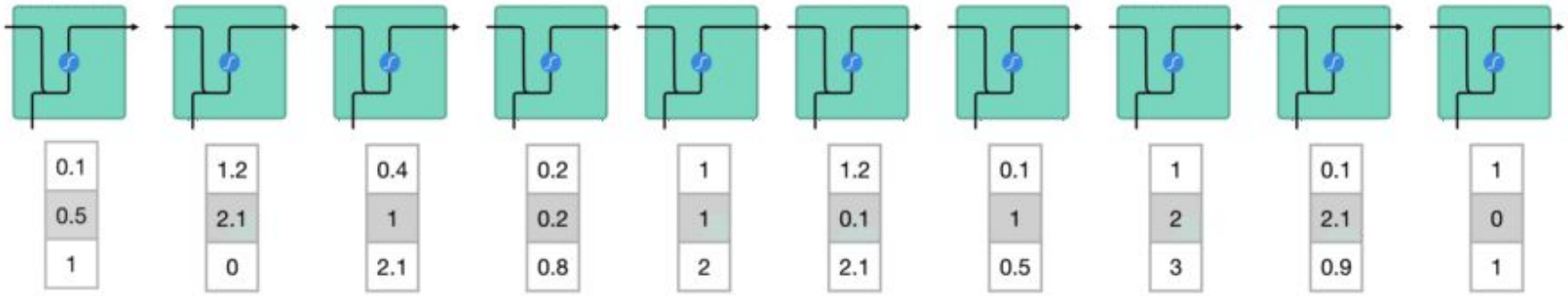
Update Hidden State

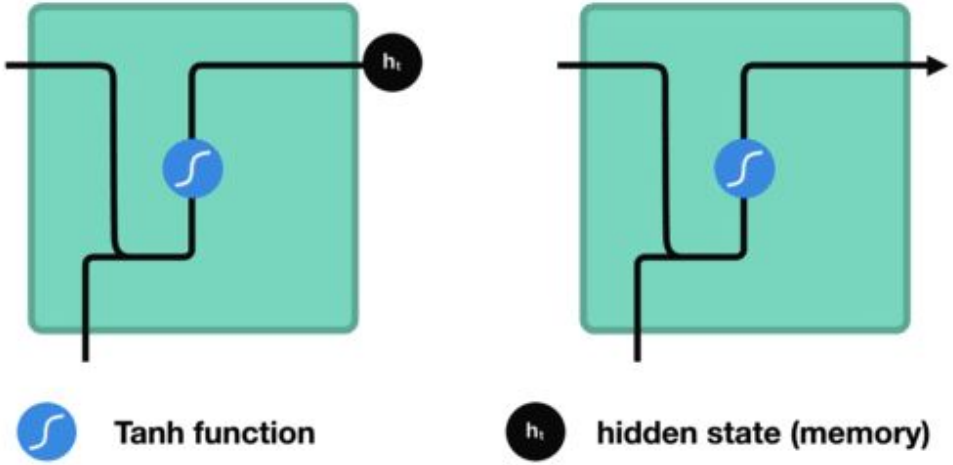
$$h_t = \tanh(\boldsymbol{W}_{\boldsymbol{hh}}^{\boldsymbol{T}} h_{t-1} + \boldsymbol{W}_{\boldsymbol{xh}}^{\boldsymbol{T}} x_t)$$

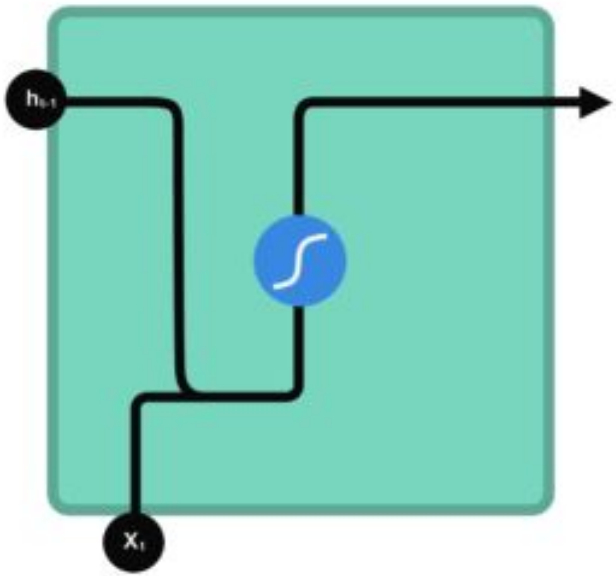
Input Vector

$$x_t$$


$\hat{y}_t$
RNN
x_t
=
$\hat{y}_0$
W_{hy}
W_{xh}
x_0
W_{hh}
$\hat{y}_1$
W_{hy}
W_{xh}
x_1
W_{hh}
$\hat{y}_2$
W_{hy}
W_{xh}
x_2
W_{hh}
. . .
. . .
$\hat{y}_t$
W_{hy}
W_{xh}
x_t


0.1
0.5
1
1.2
2.1
0
0.4
1
2.1
0.2
0.2
0.8
1
1
2
1.2
0.1
2.1
0.1
1
0.5
1
2
3
0.1
2.1
0.9
1
0
1


h_t
Tanh function
h_t
hidden state (memory)



Tanh function

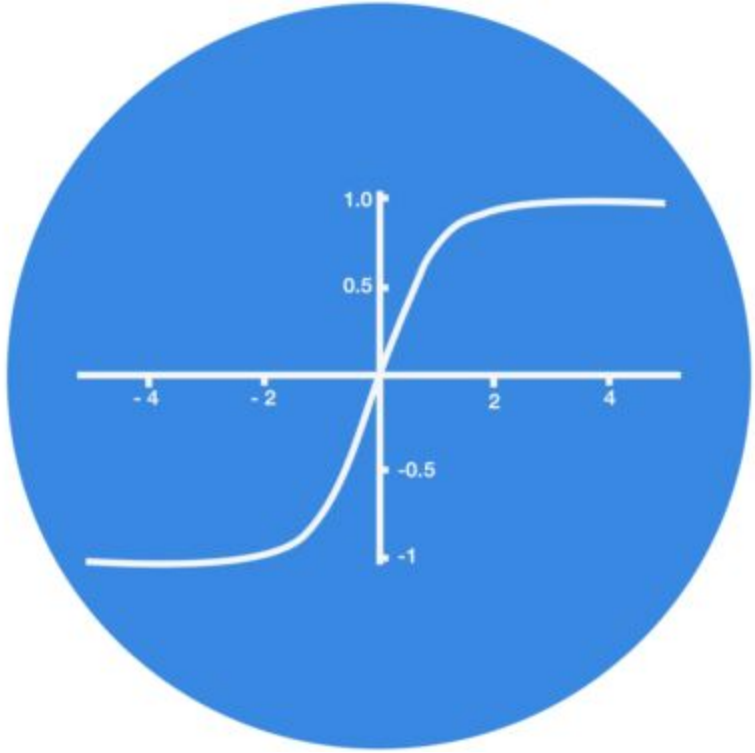
h_t new hidden state

h_{t-1} previous hidden state

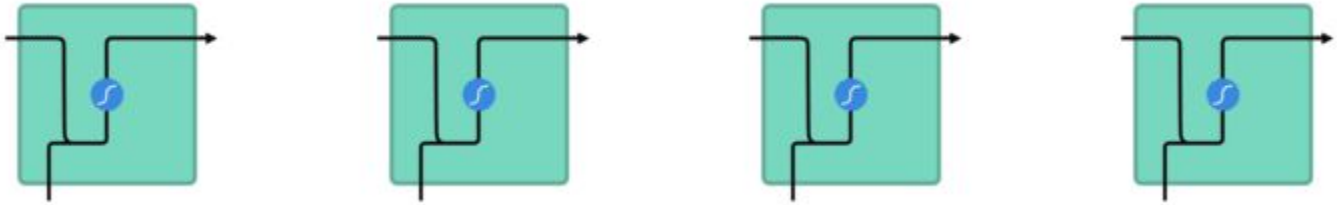
X_t input

concatenation

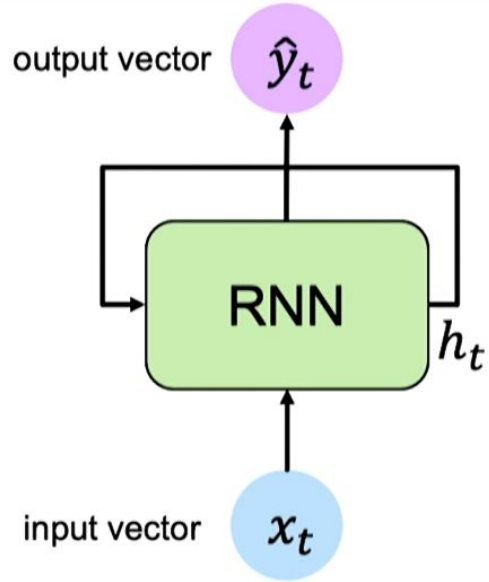
5
0.1
-0.5



5
0.01
-0.5

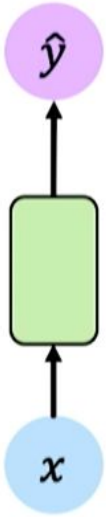


```python
class MyRNNCell(tf.keras.layers.Layer):
  def __init__(self, rnn_units, input_dim, output_dim):
    super(MyRNNCell, self).__init__()

    # Initialize weight matrices
    self.W_xh = self.add_weight([rnn_units, input_dim])
    self.W_hh = self.add_weight([rnn_units, rnn_units])
    self.W_hy = self.add_weight([output_dim, rnn_units])

    # Initialize hidden state to zeros
    self.h = tf.zeros([rnn_units, 1])

  def call(self, x):
    # Update the hidden state
    self.h = tf.math.tanh( self.W_hh * self.h + self.W_xh * x )

    # Compute the output
    output = self.W_hy * self.h

    # Return the current output and hidden state
    return output, self.h
```

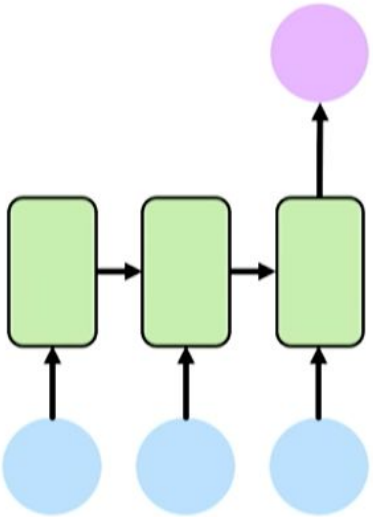



```python
tf.keras.layers.SimpleRNN(rnn_units)
```

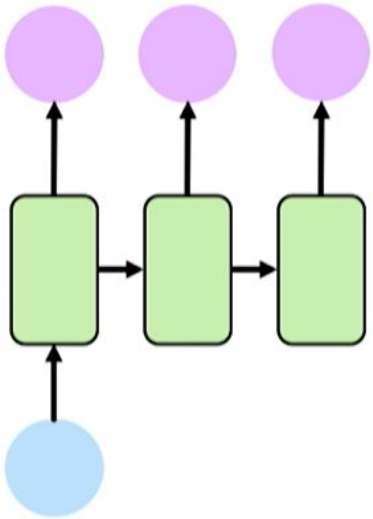
Sequence Modeling



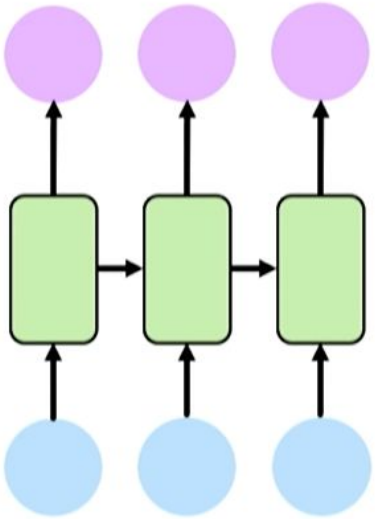
One to One
"Vanilla" NN
Binary classification



Many to One
Sentiment Classification



One to Many
Text Generation
Image Captioning



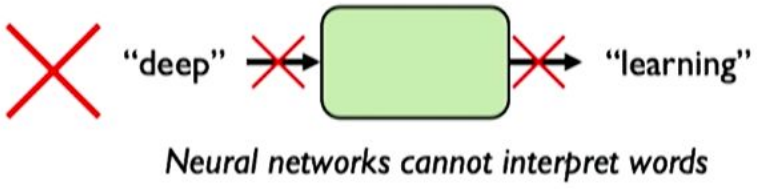
Many to Many
Translation & Forecasting
Music Generation

Sequence Modeling

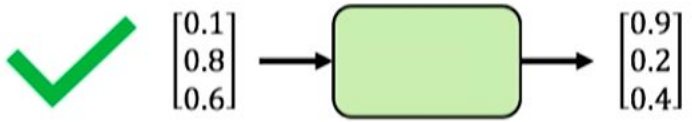
1. Handle variable-length sequences
2. Track long-term dependencies
3. Maintain information about order
4. Share parameters across the sequence
5. Capture differences in Sequence Order.

Sequence Modeling

Representing Language to a Neural Network



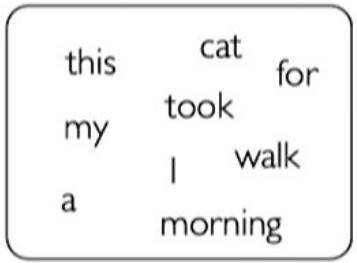
Neural networks cannot interpret words



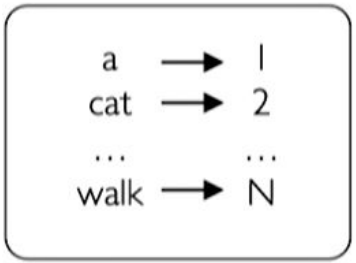
Neural networks require numerical inputs

Embedding

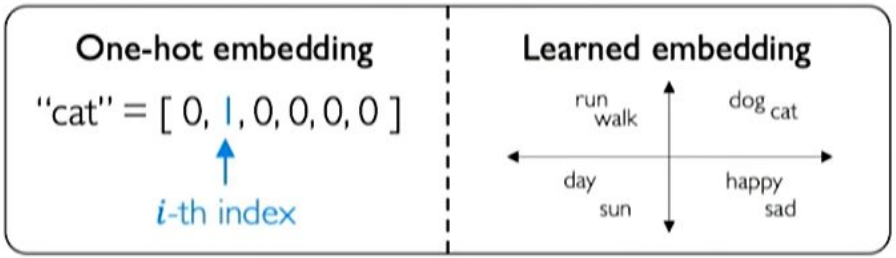
Transform indexes into a vector of fixed size.



1. Vocabulary:
Corpus of words

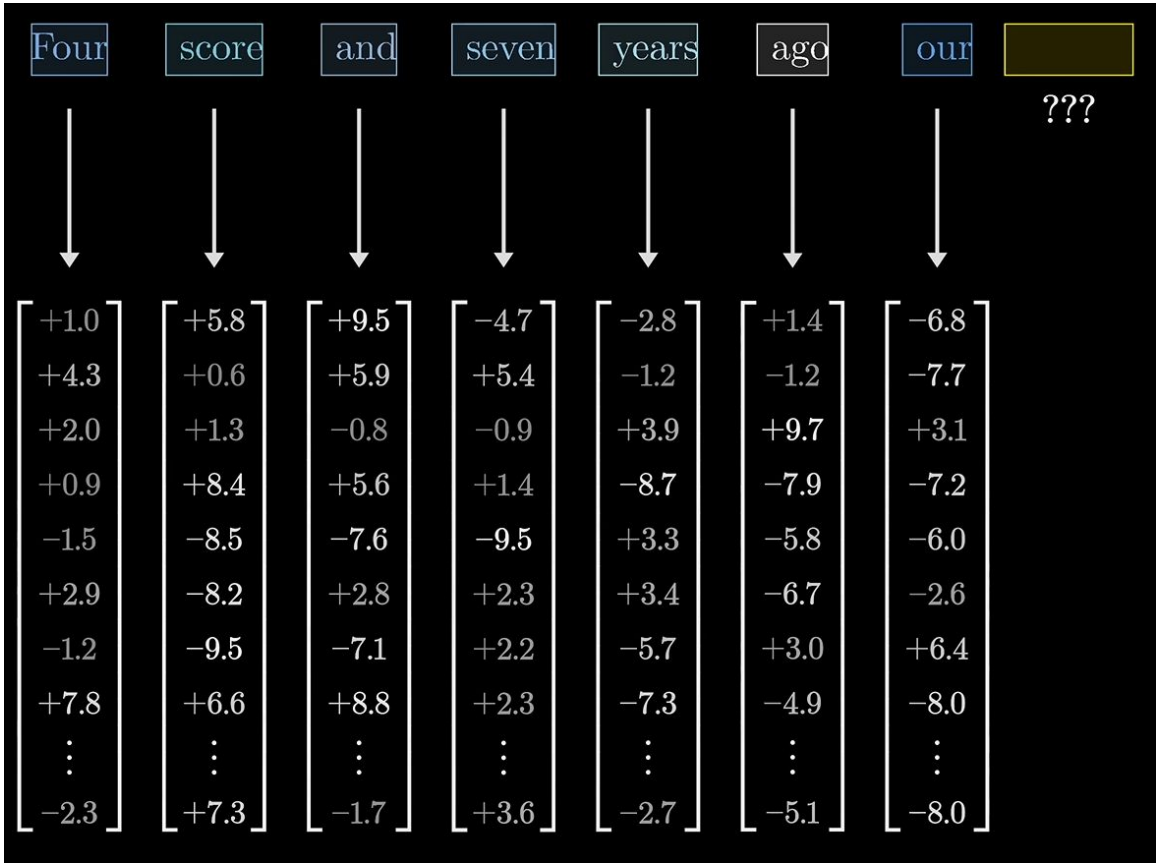


2. Indexing:
Word to index



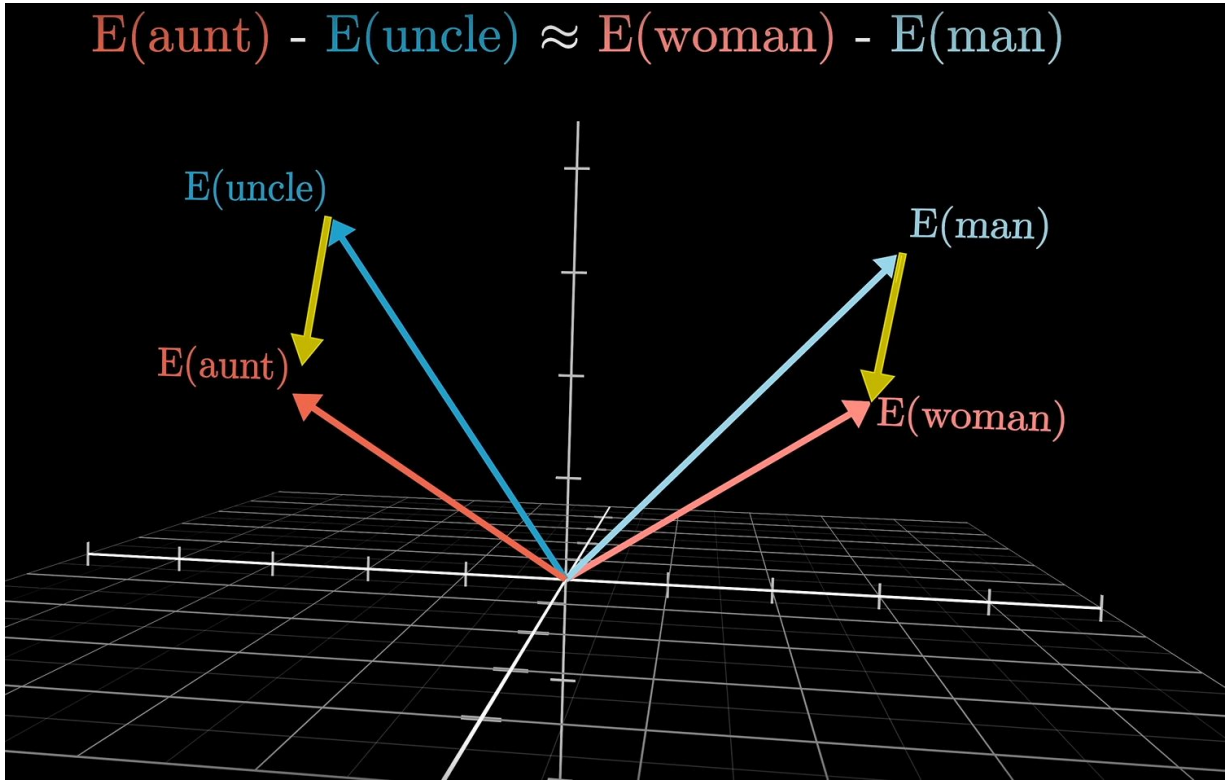
3. Embedding:
Index to fixed-sized vector

Embedding



https://youtu.be/eMlx5fFNoYc

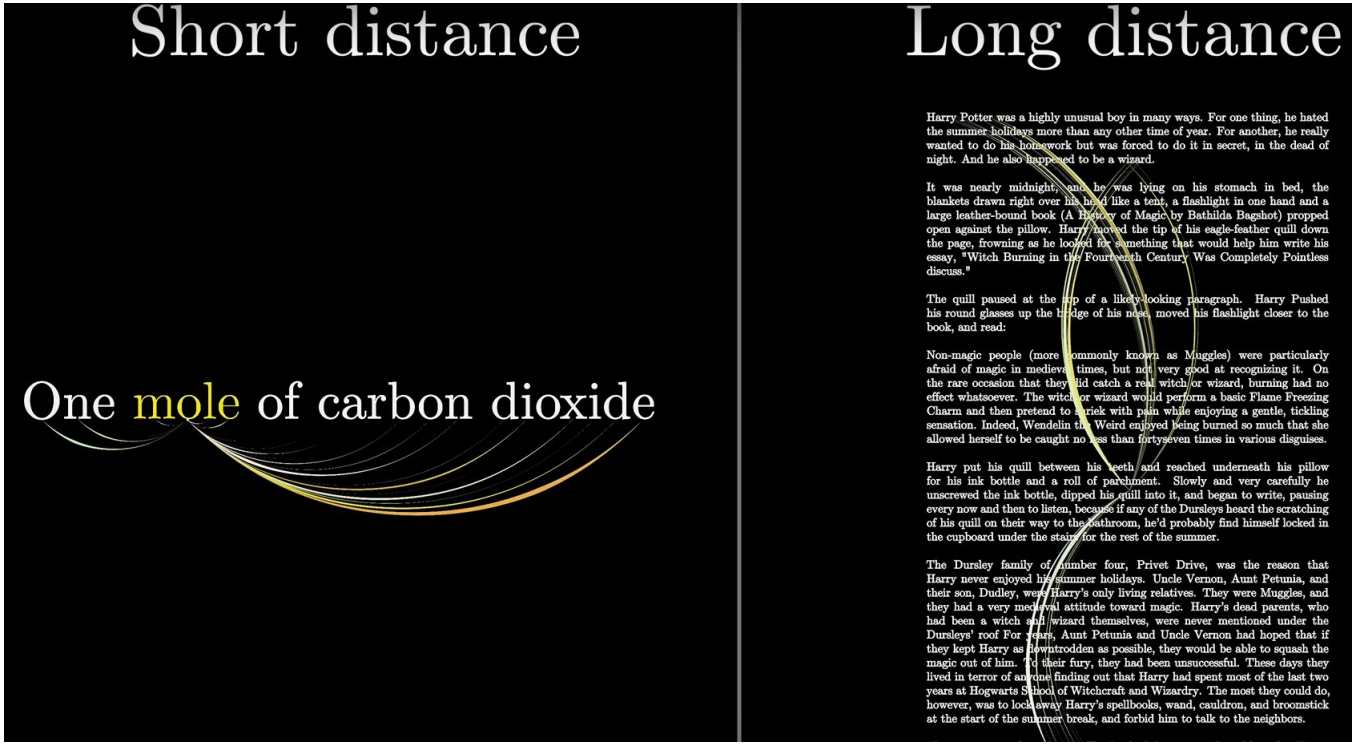
Embedding



https://youtu.be/eMlx5fFNoYc

Model Long-Term Dependencies

"France is where I grew up, but I now live in Boston. I speak fluent _____"



https://youtu.be/eMlx5fFNoYc

Share parameters

Capture differences in Sequence Order.

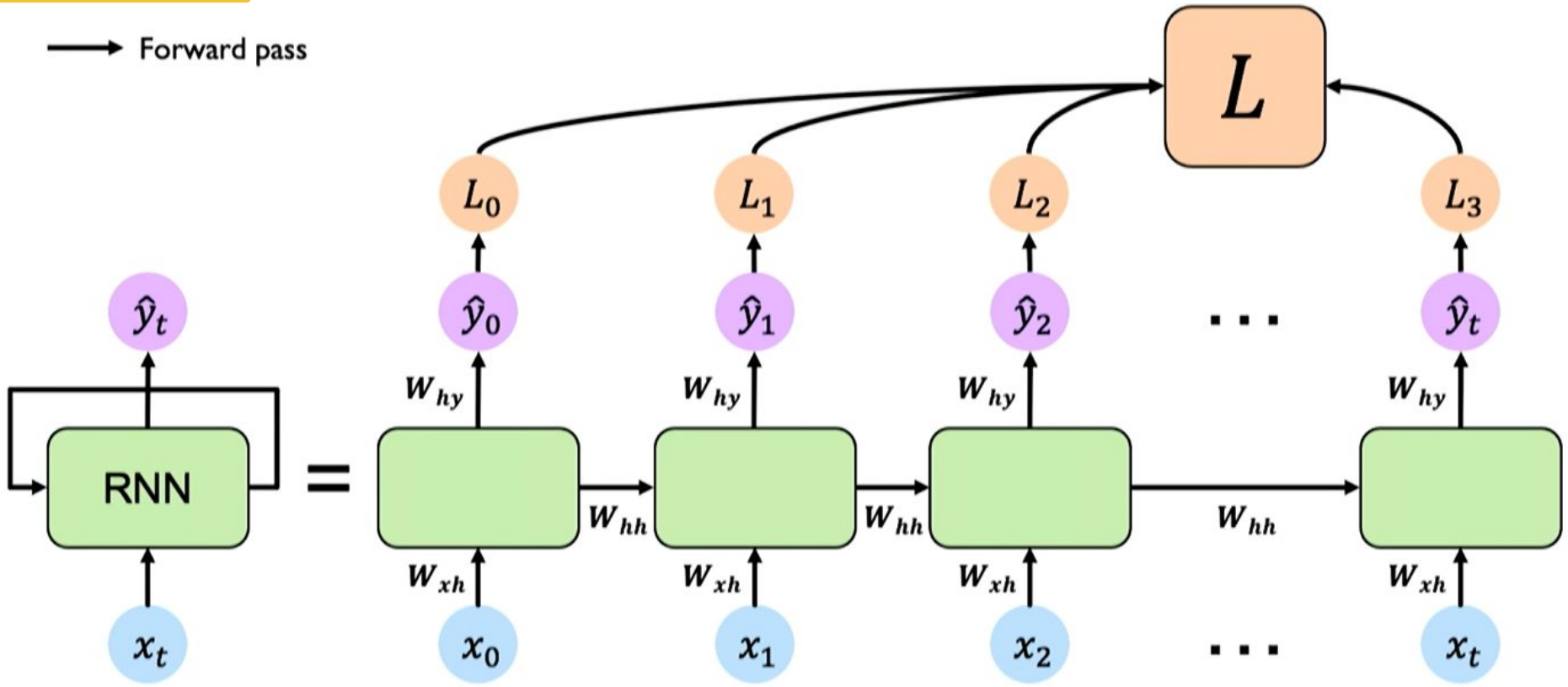
The food was good, not bad at all.

vs.

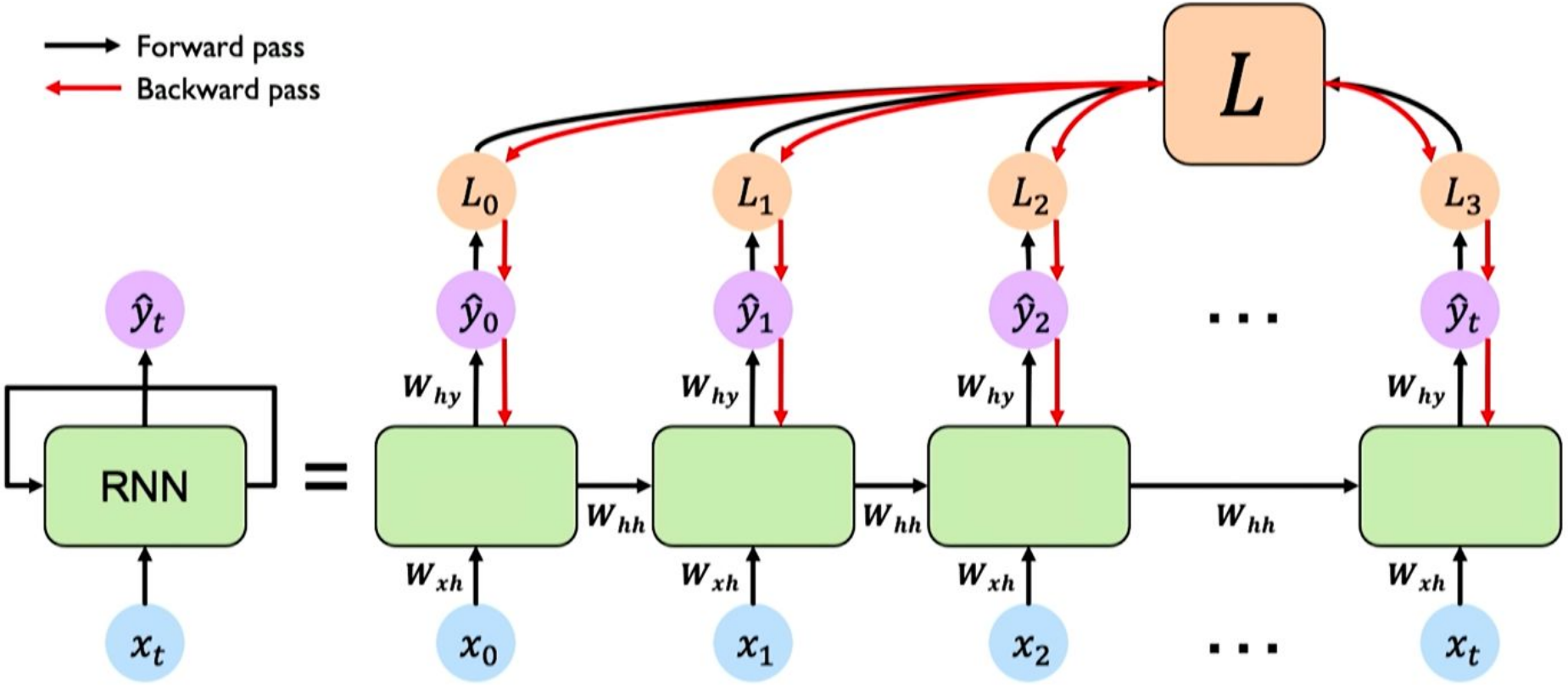
The food was bad, not good at all.

Backpropagation Through Time

Backpropagation Through Time



Backpropagation Through Time



Exploding and Vanishing

Many values > 1:
exploding gradients

Gradient clipping to scale big gradients

Many values < 1:
vanishing gradients

1. **Activation function**
2. **Weight initialization**
3. **Network architecture**

Why are vanishing gradients a problem?

Multiply many **small numbers** together

↓

Errors due to further back time steps have smaller and smaller gradients

↓

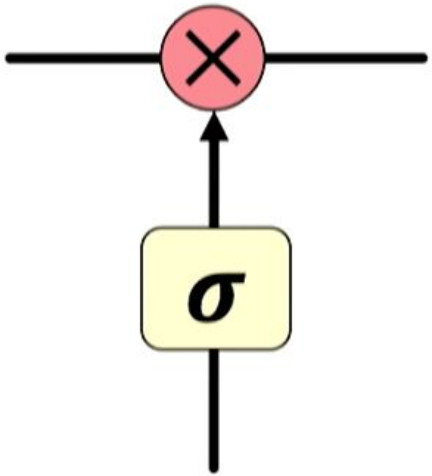
Bias parameters to capture short-term dependencies

Avoid Vanishing

Idea: use **gates** to selectively **add** or **remove** information within **each recurrent unit with**

Pointwise multiplication

Sigmoid neural net layer



gated cell

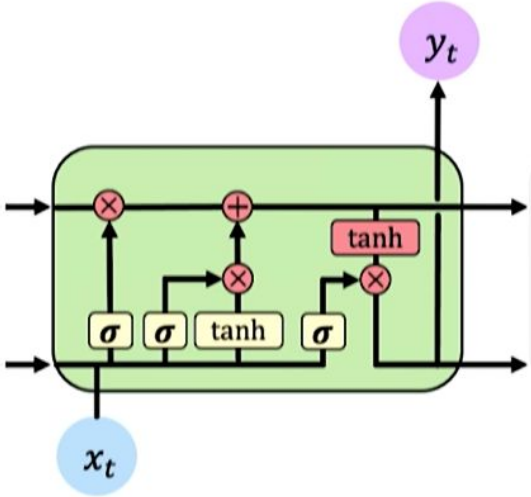
LSTM, GRU, etc.

Gates optionally let information through the cell

LSTM

Gated LSTM cells **control information flow:**

1) Forget 2) Store 3) Update 4) Output

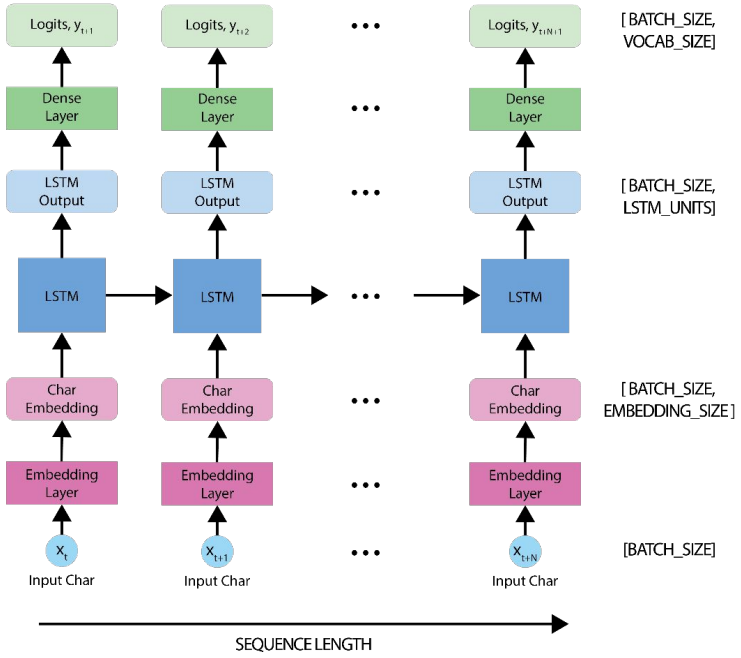


LSTM cells are able to track information throughout many timesteps

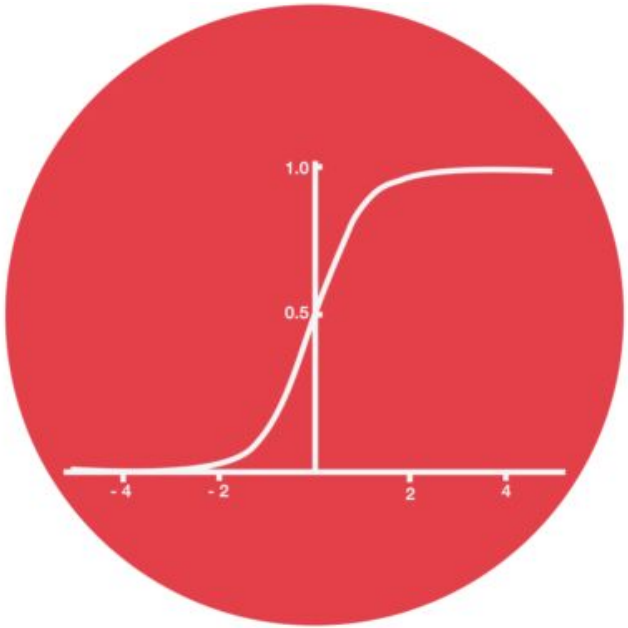
```
tf.keras.layers.LSTM(num_units)
```

LSTM

1. Maintain a cell state
2. Use gates to control the flow of information
   - Forget gate gets rid of irrelevant information
   - Store relevant information from current state
   - Selectively Update cell state
   - Output gate return a filtered version of the cell state
3. Backpropagation through time with partially uninterrupted gradient flow



Gates

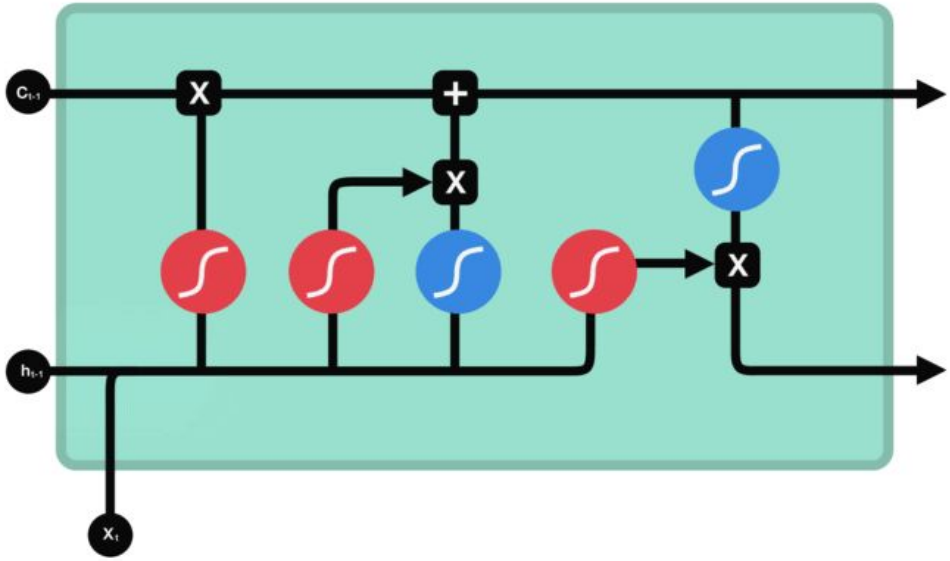


Tanh compresses
values between -1 and 1

Sigmoid compresses values betw
0 and 1

Useful for updating or
forgetting data

Forget Gate



C_{t-1} previous cell state

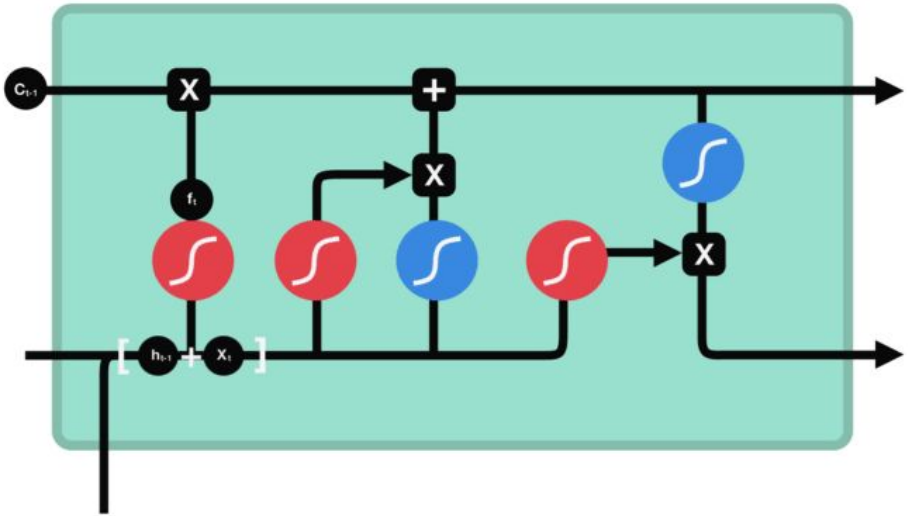
f_t forget gate output

This gate decides which information should be discarded or kept.

The information from the previous hidden state and the information from the current input are passed through the sigmoid function.

The values are between 0 and 1. Near 0 it forgets and near 1 it keeps

Input Gate



C_{t-1} previous cell state

f_t forget gate output

i_t input gate output

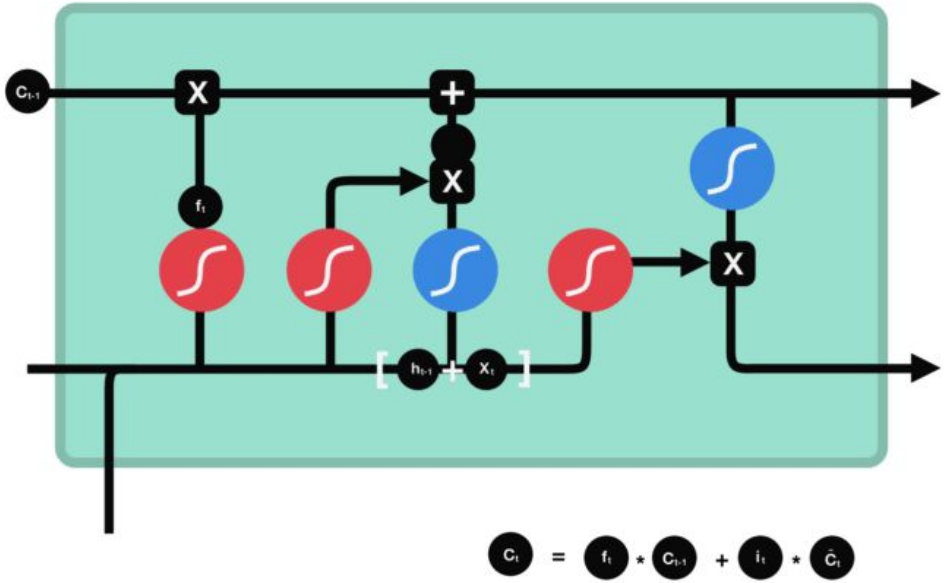
$\tilde{C}_t$ candidate

The input gate update the cell state

Previous hidden state and the current input to a sigmoid function.

Hidden state and the current input to the tanh function to compress values between -1 and 1 to help regulate the network. Then you multiply the tanh output by the sigmoid output.

Cell State



C_{t-1} previous cell state

f_t forget gate output

i_t input gate output

$\tilde{C}_t$ candidate

C_t new cell state

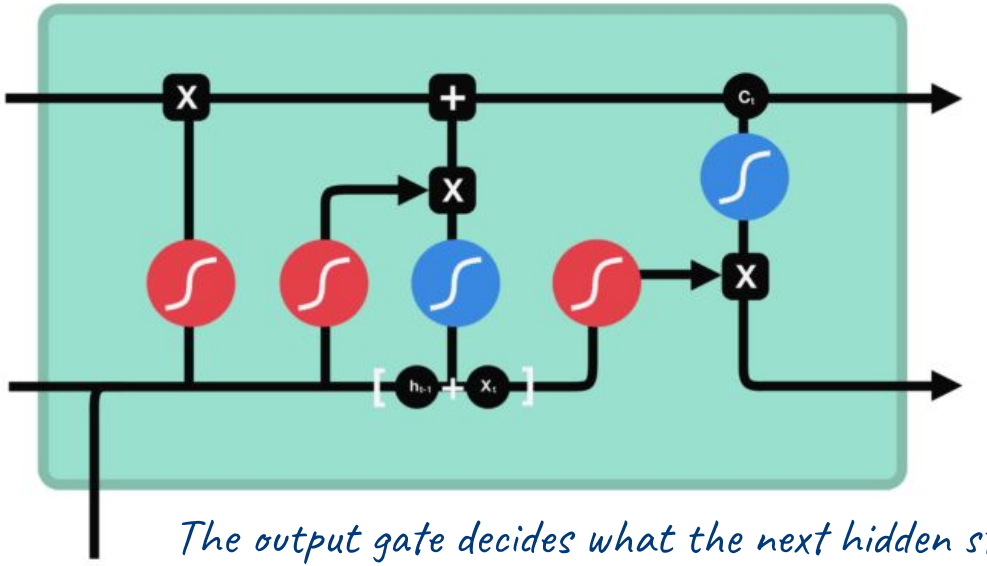
$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

The input gate update the cell state

Previous hidden state and the current input to a sigmoid function.

Hidden state and the current input to the tanh function to compress values between -1 and 1 to help regulate the network. Then you multiply the tanh output by the sigmoid output.

Output Gate



C_{t-1} previous cell state

f_t forget gate output

i_t input gate output

$\tilde{C}_t$ candidate

C_t new cell state

o_t output gate output

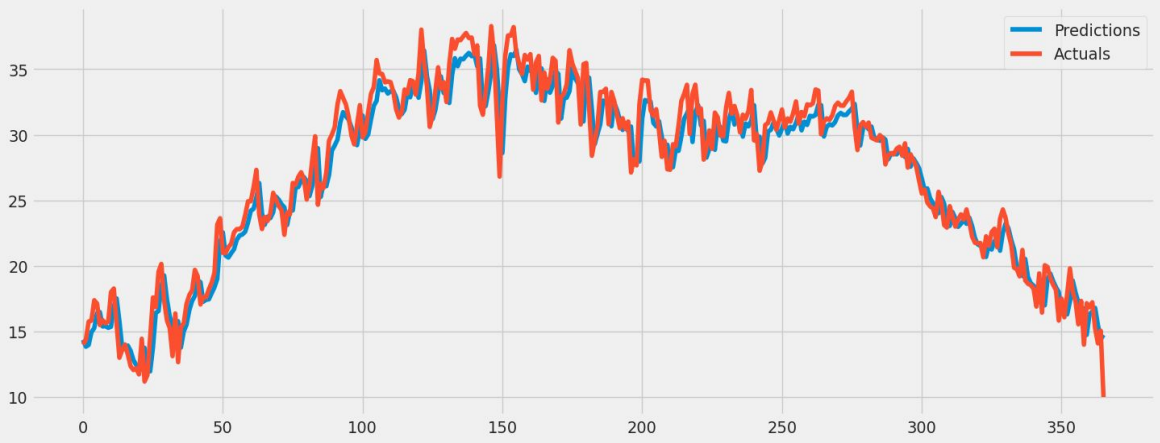
h_t hidden state

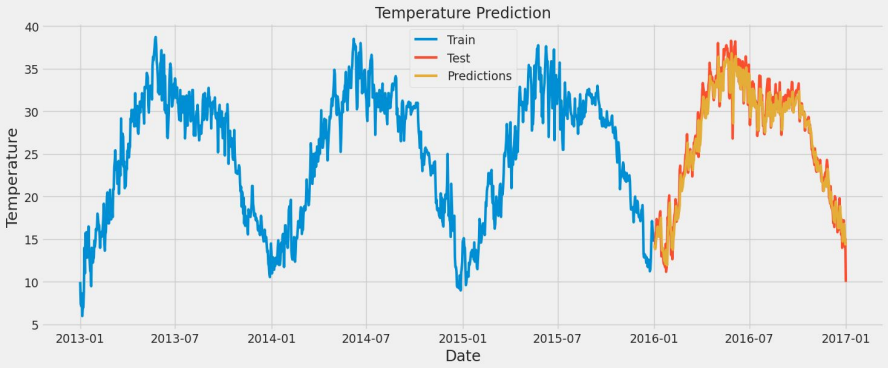
The output gate decides what the next hidden state should be.

The hidden state contains information about previous inputs.

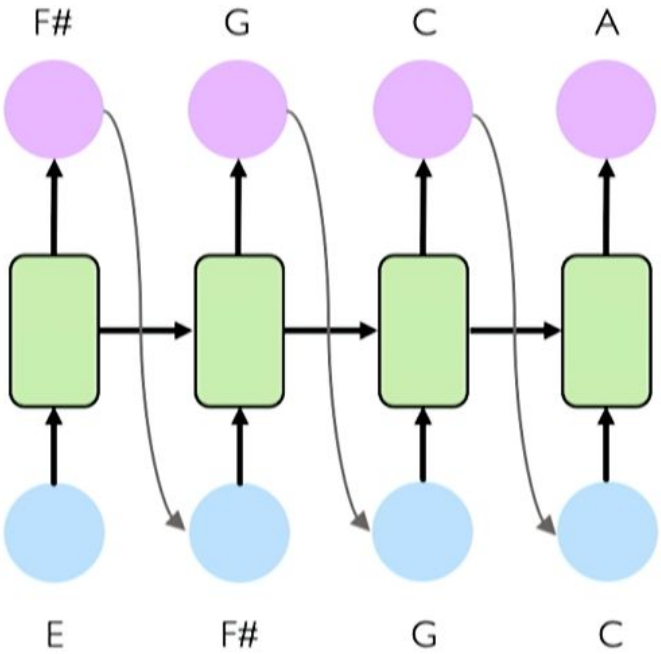
We multiply the tanh output by the sigmoid output to decide what information the hidden state should carry.

Time series

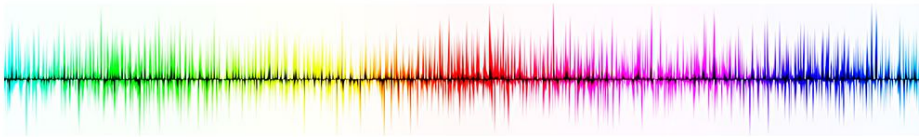

Predictions
Actuals
35
30
25
20
15
10
0
50
100
150
200
250
300
350


Temperature Prediction
Train
Test
Predictions
Temperature
40
35
30
25
20
15
10
5
2013-01
2013-07
2014-01
2014-07
2015-01
2015-07
2016-01
2016-07
2017-01
Date

LSTM: Music Generation

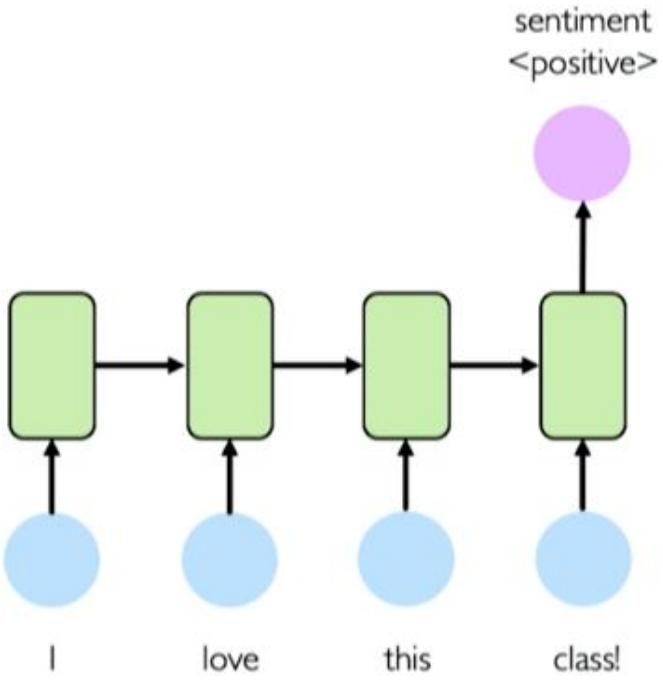


MIT 6.S191 Lab 1: Intro to TensorFlow and Music Generation with RNNs



https://github.com/aamini/introtodeeplearning/tree/master/lab1

Sentiment Classification



Tweet sentiment classification

Ivar Hagendoorn
@IvarHagendoorn
Follow

The @MIT Introduction to #DeepLearning is definitely one of the best courses of its kind currently available online introtodeeplearning.com

12:45 PM · 12 Feb 2018

Angels-Cave
@AngelsCave
Follow

Replying to @Kazuki7048

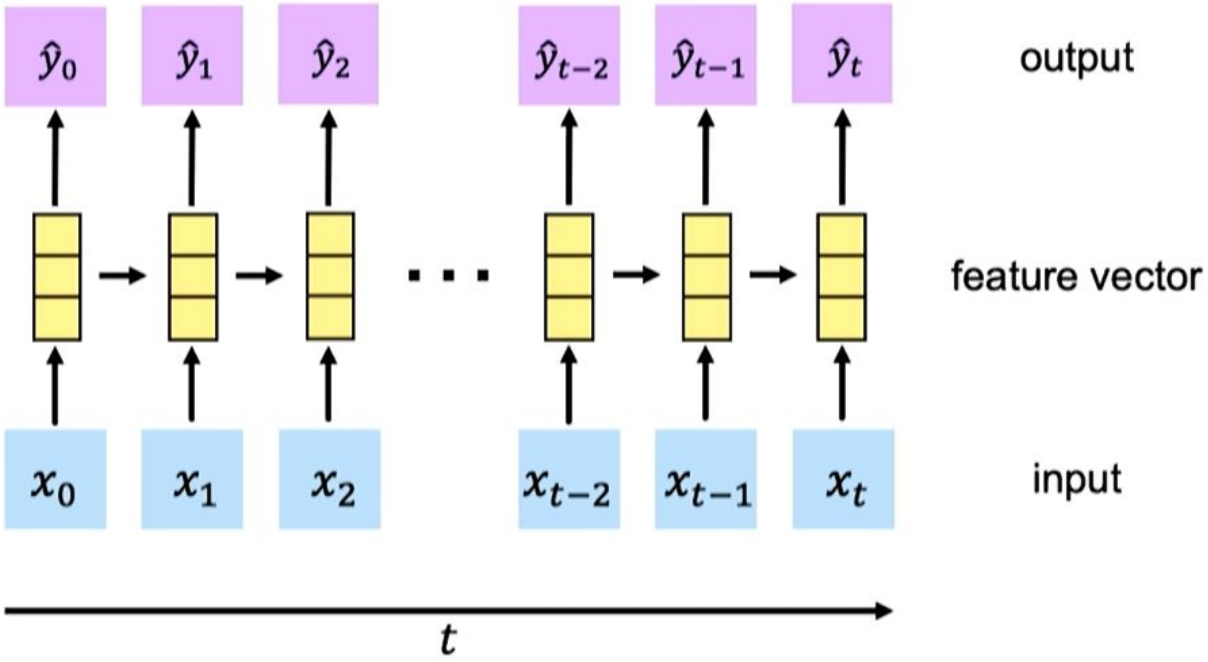
I wouldn't mind a bit of snow right now. We haven't had any in my bit of the Midlands this winter! :(

2:19 AM · 25 Jan 2019

Limitations of RNN

Limitations of RNNs

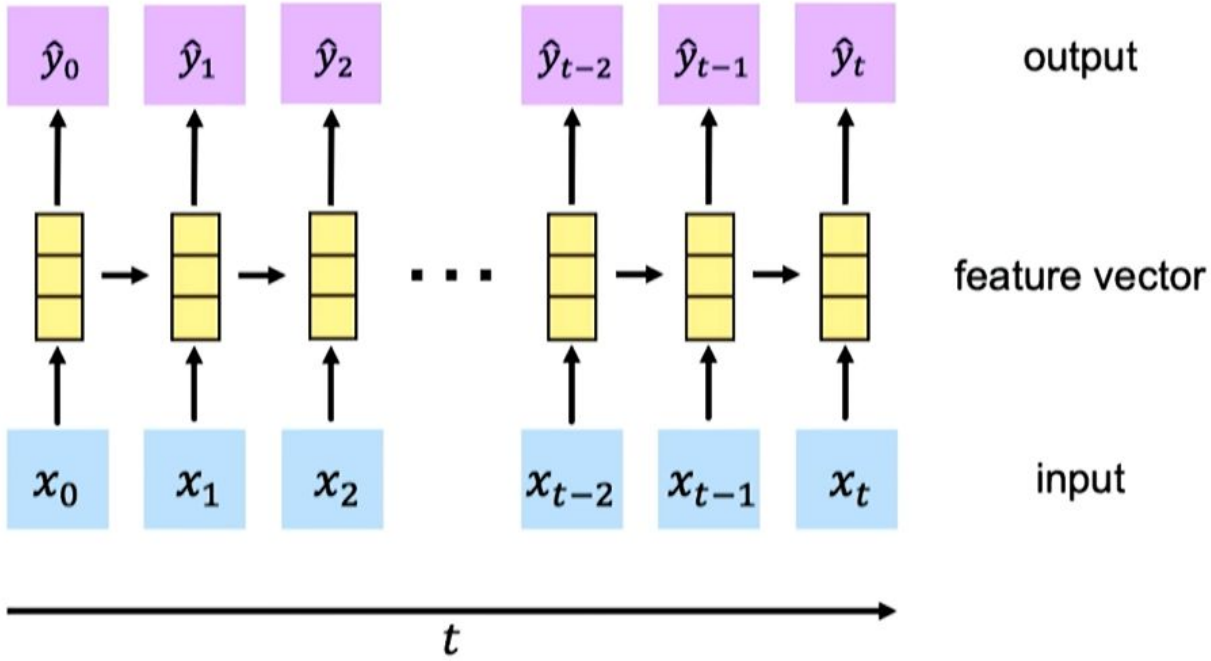
- Encoding bottleneck
- Slow, no parallelization
- Not long memory



Limitations of RNN

Desired Capabilities

- Continuous stream
- Parallelization
- Long memory



Attention Is All You Need

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

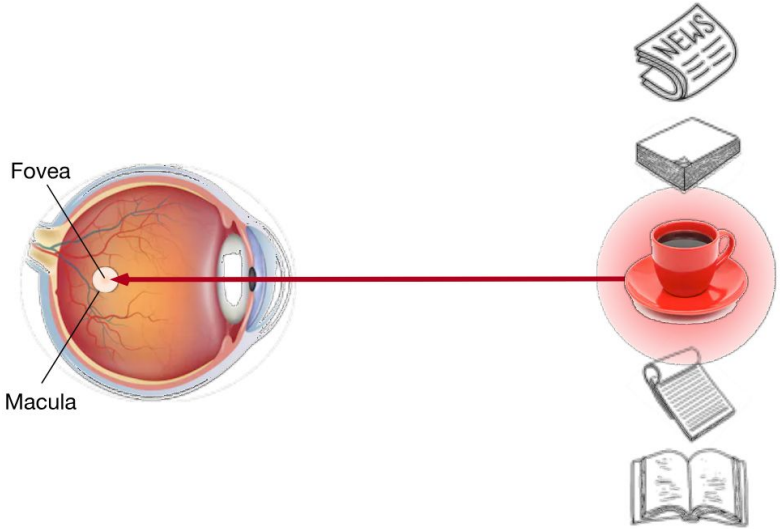
Łukasz Kaiser* Google Brain lukaszkaiser@google.com

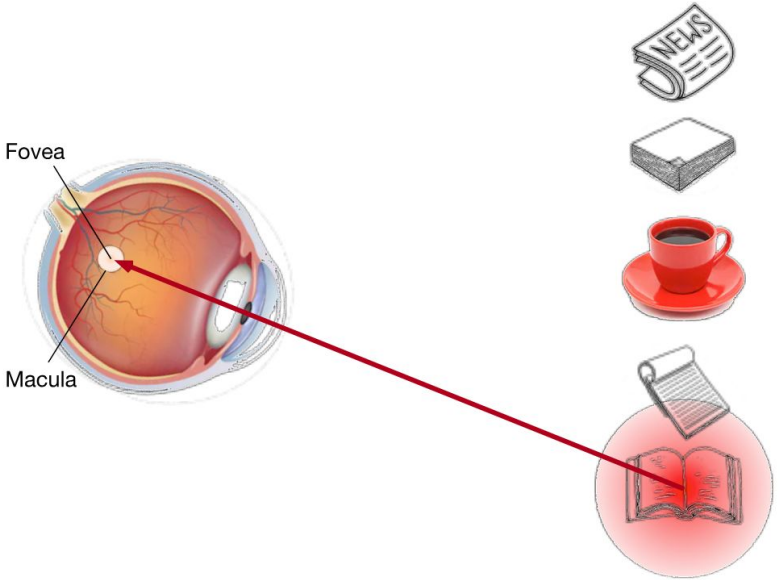
Illia Polosukhin* † illia.polosukhin@gmail.com

Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.0 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature.

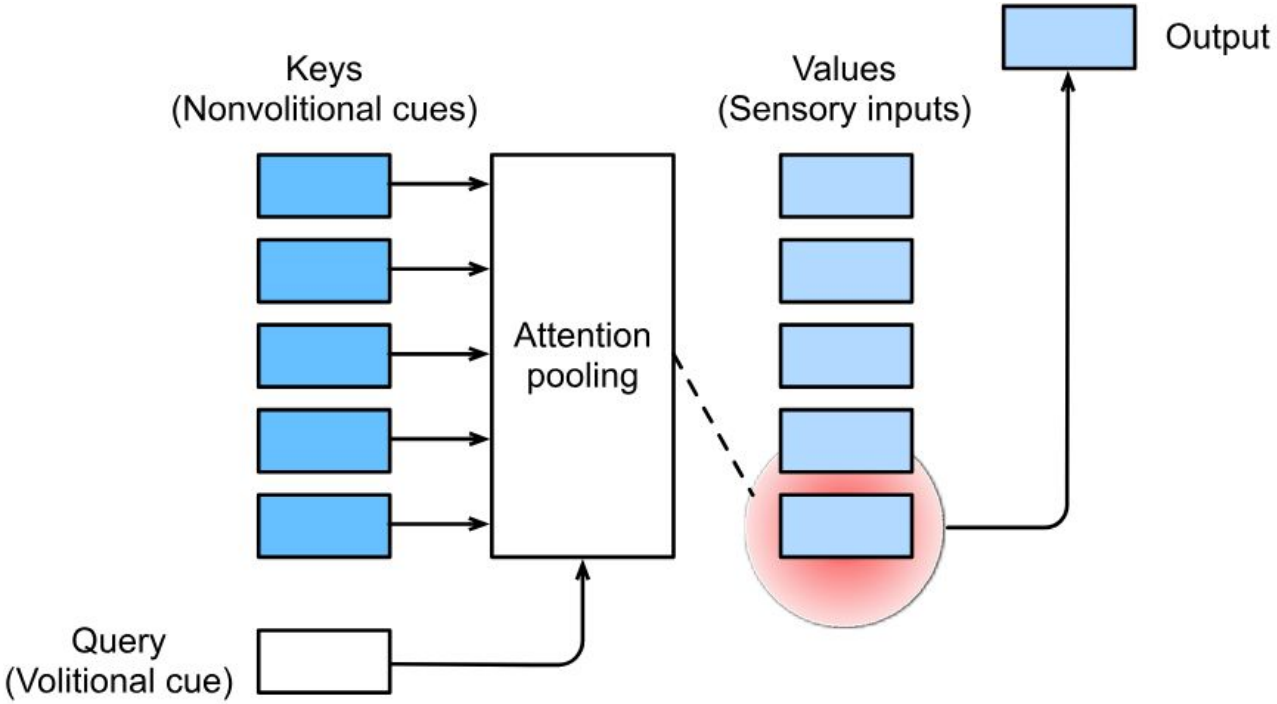
Attention Is All You Need





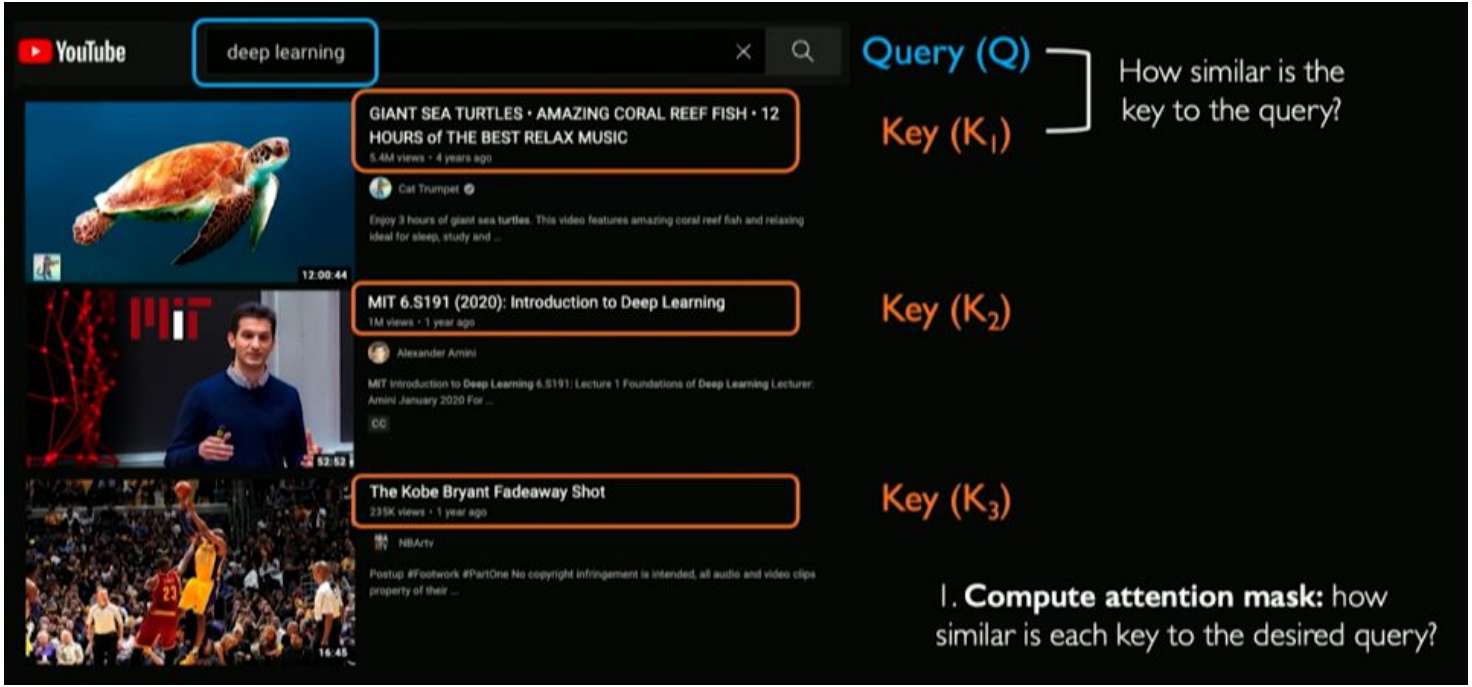
1. Identify which parts to attend to
2. Extract the features with high attention

Attention Is All You Need



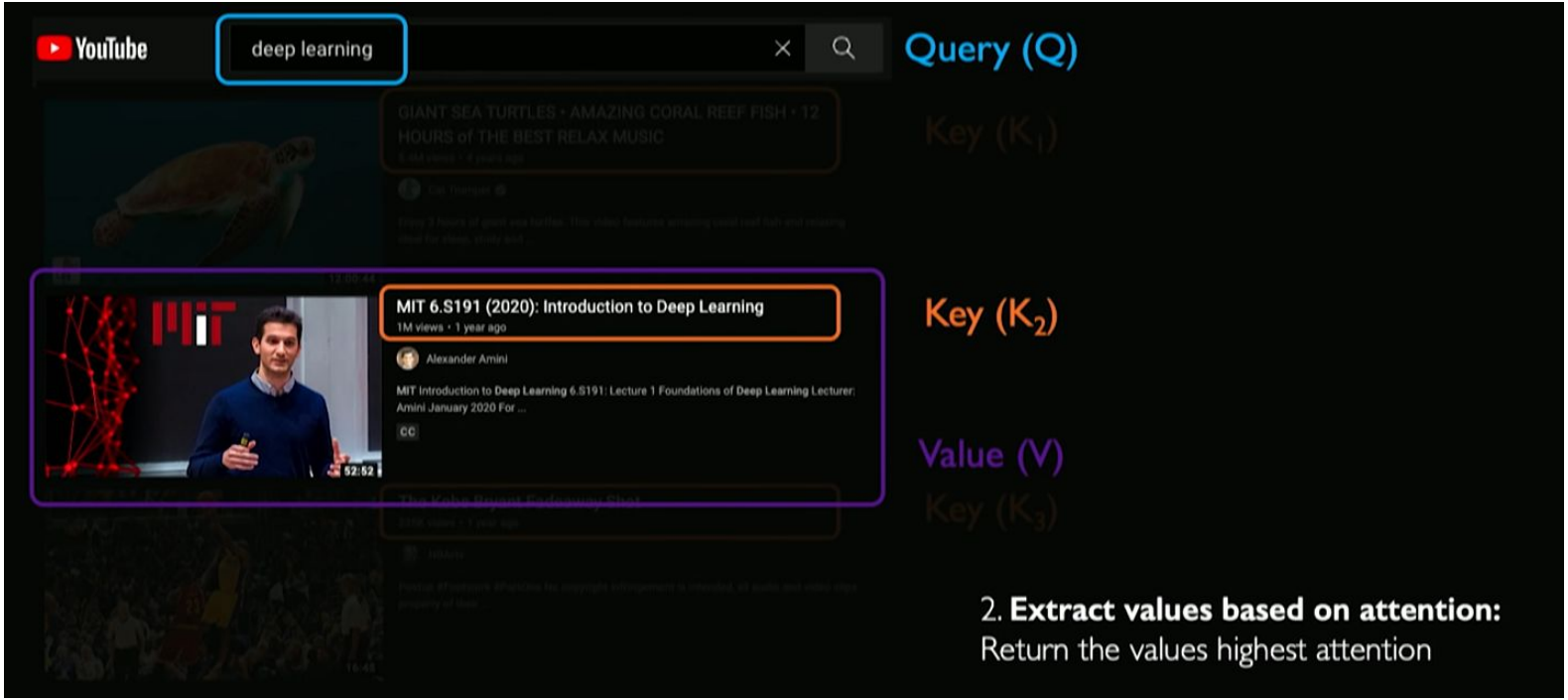
Attention Is All You Need

$$\text{Attention}(\mathbf{q}, \mathcal{D}) \stackrel{\text{def}}{=} \sum_{i=1}^{m} \alpha(\mathbf{q}, \mathbf{k}_i)\mathbf{v}_i$$



Attention Is All You Need

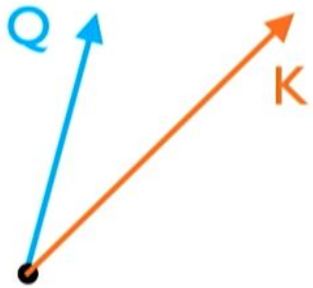
$$\text{Attention}(\mathbf{q}, \mathcal{D}) \stackrel{\text{def}}{=} \sum_{i=1}^{m} \alpha(\mathbf{q}, \mathbf{k}_i)\mathbf{v}_i$$



Self-Attention

Goal: identify and attend to most important features in input.

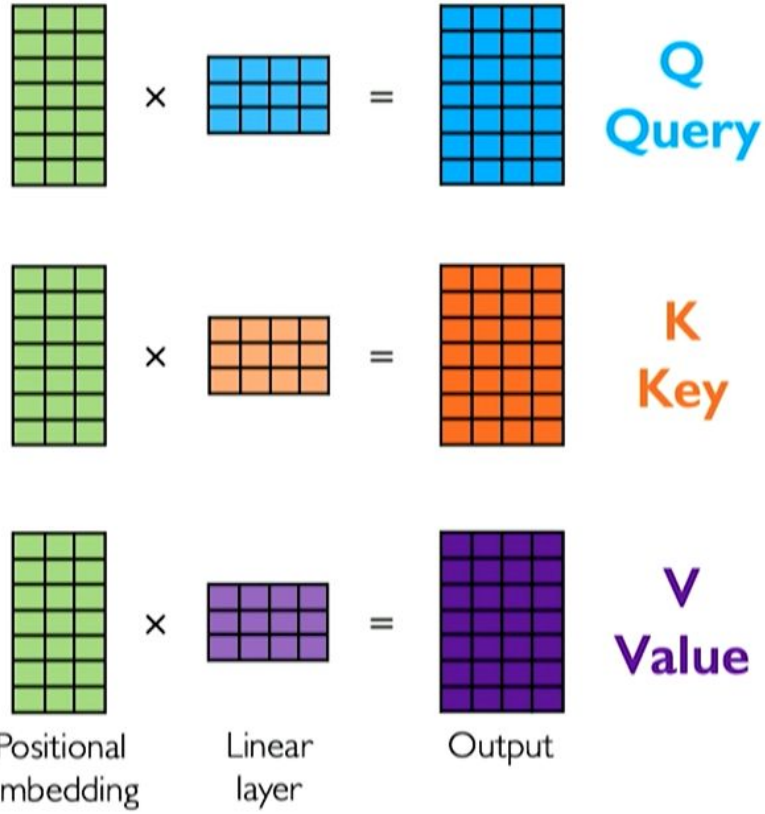
1. Encode **position** information
2. Extract **query, key, value** for search



Dot product

Scale

$$\frac{Q \cdot K^T}{\text{scaling}}$$

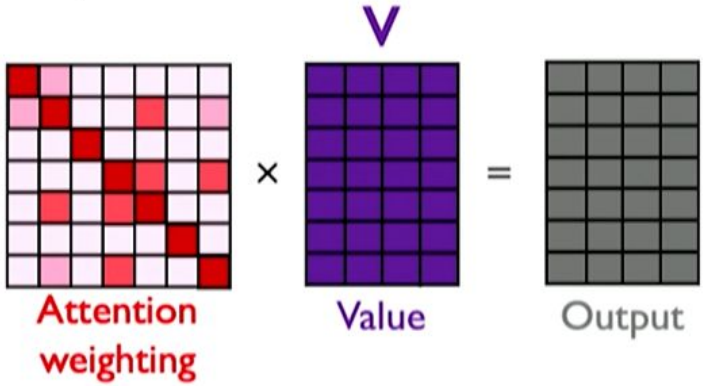


Self-Attention

Goal: identify and attend to most important features in input.

1. Encode **position** information
2. Extract **query, key, value** for search
3. Compute **attention weighting**
4. Extract **features with high attention**

Last step: self-attend to extract features

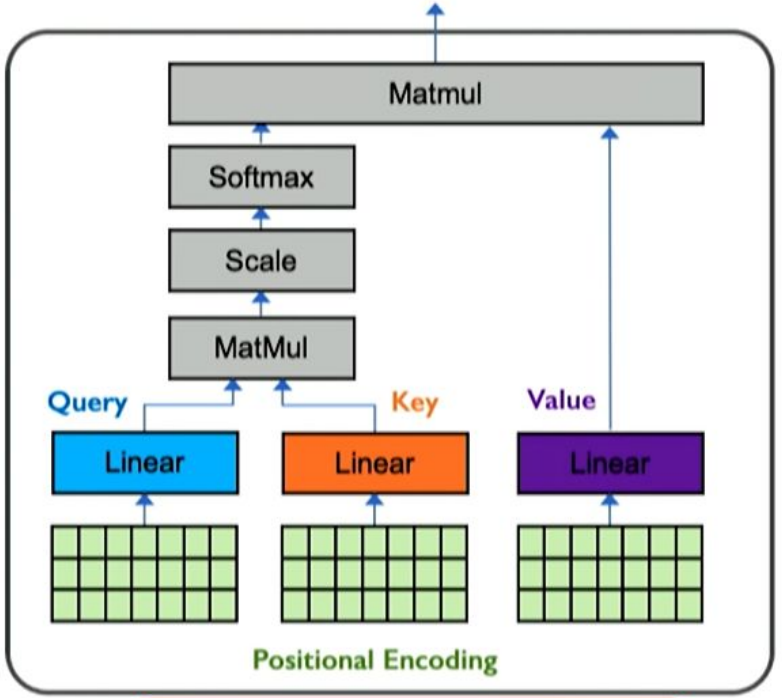


$$softmax\left(\frac{Q \cdot K^T}{scaling}\right) \cdot V = A(Q, K, V)$$

Self-Attention with NN

Goal: identify and attend to most important features in input.

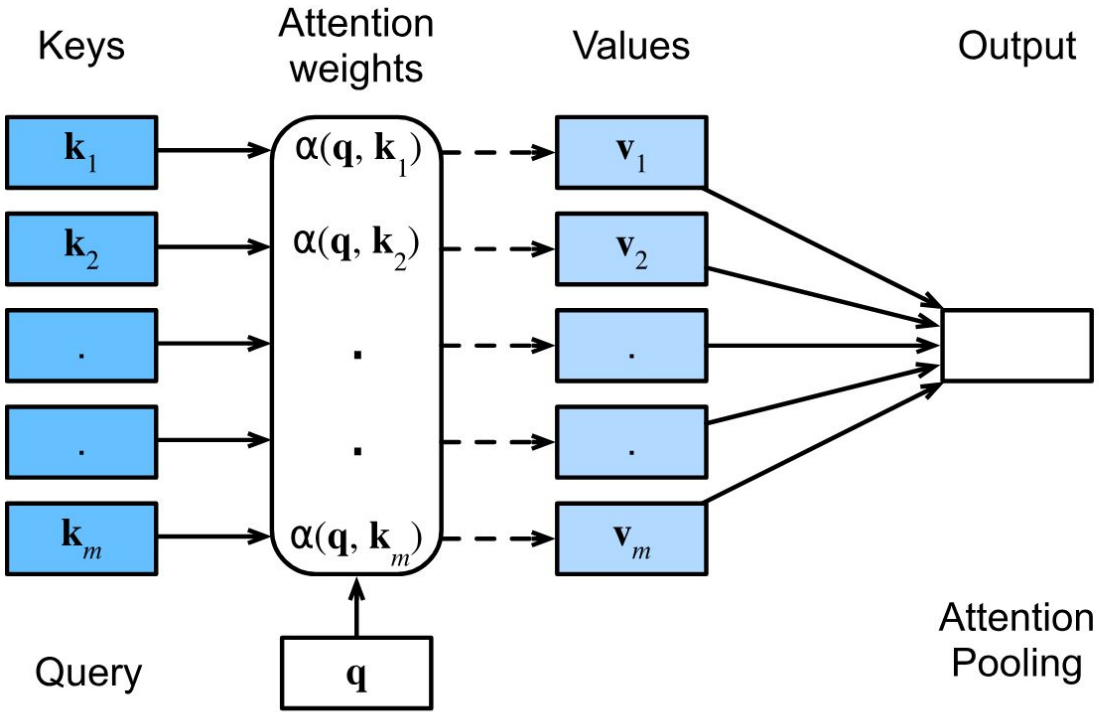
1. Encode **position** information
2. Extract **query, key, value** for search
3. Compute **attention weighting**
4. Extract **features with high attention**



$$softmax\left(\frac{Q \cdot K^T}{scaling}\right) \cdot V$$

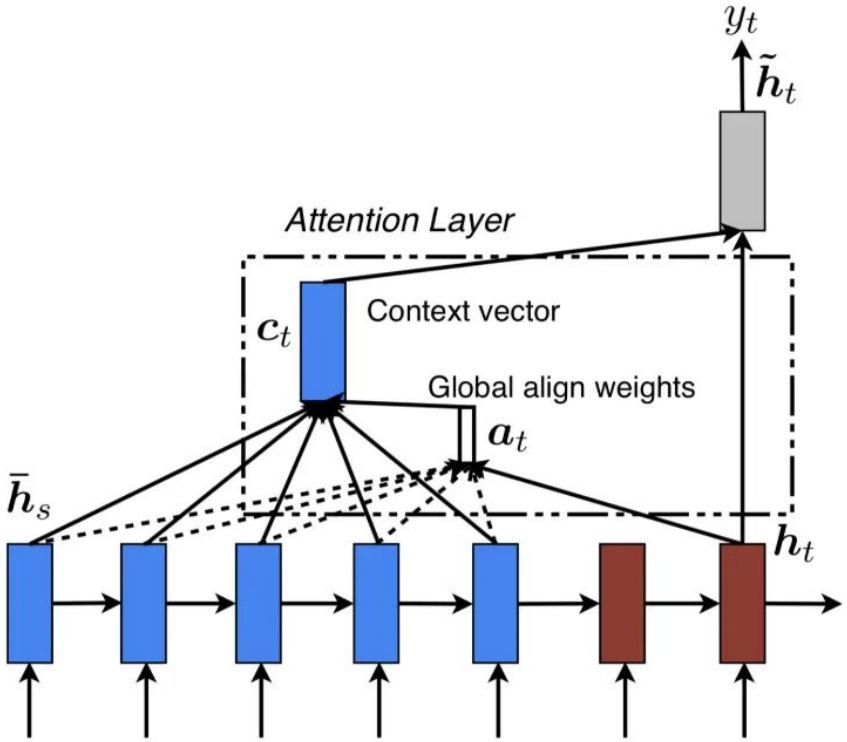
Queries, Keys, and Values

$$\text{Attention}(\mathbf{q}, \mathcal{D}) \stackrel{\text{def}}{=} \sum_{i=1}^{m} \alpha(\mathbf{q}, \mathbf{k}_i)\mathbf{v}_i$$

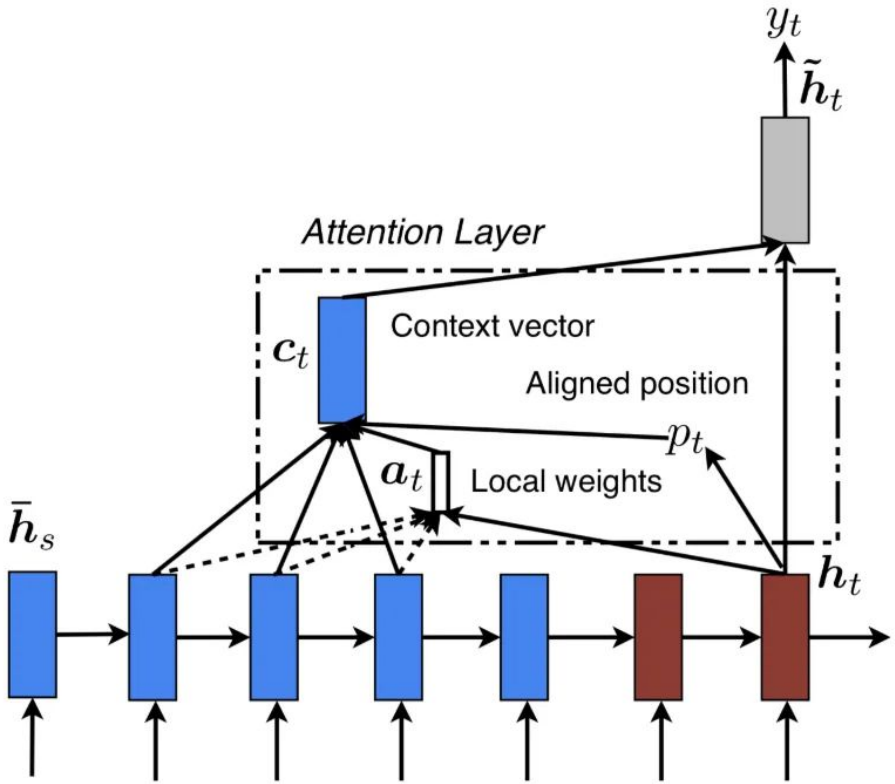


$$\alpha(\mathbf{q}, \mathbf{k}_i) = \frac{\exp(a(\mathbf{q}, \mathbf{k}_i))}{\sum_j \exp(a(\mathbf{q}, \mathbf{k}_j))}$$

Global vs local attention



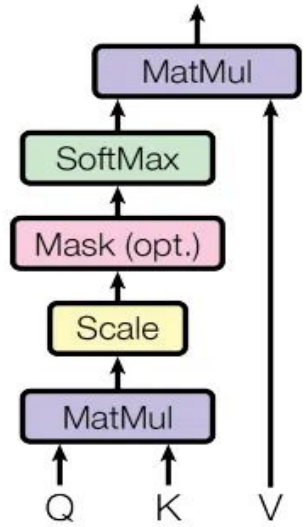
Global Attention Model



Local Attention Model

Self-Attention

Scaled Dot-Product Attention



Multi-Head Attention

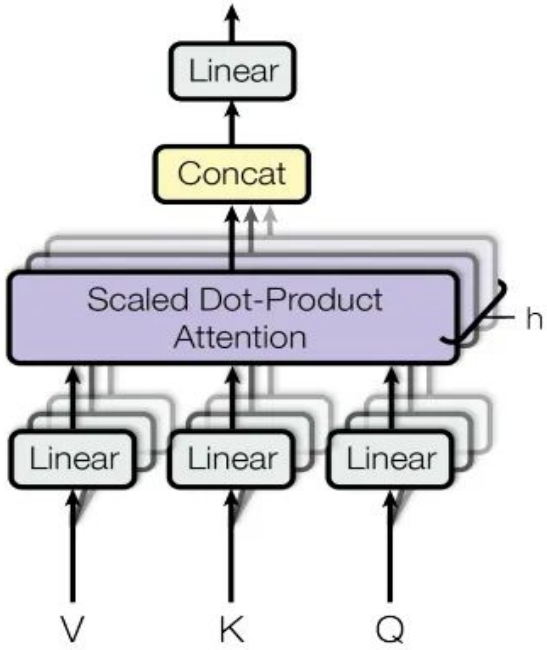


Figure source: Vaswani et al. 2017

Illustrated: Self-Attention

https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a

https://colab.research.google.com/drive/1rPk3ohrmVclqhH7uQ7qys4oznDdAhpzF

Encoder-Decoder Architecture

The Transformer model by Vaswani et al. 2017 stacks six encoder blocks followed by six decoder blocks.

Each encoder block has:

- a self-attention layer followed by a feedforward layer to capture non-linearities
- each of these is also followed by a layer norm
- there are residual connections between encoder blocks

Each decoder is similar to the encoder, except that it has a 3rd layer that performs multi-head attention on the output from the encoders and the previous layers of the decoder. Masking is used here to prevent positions from looking ahead during self-attention.

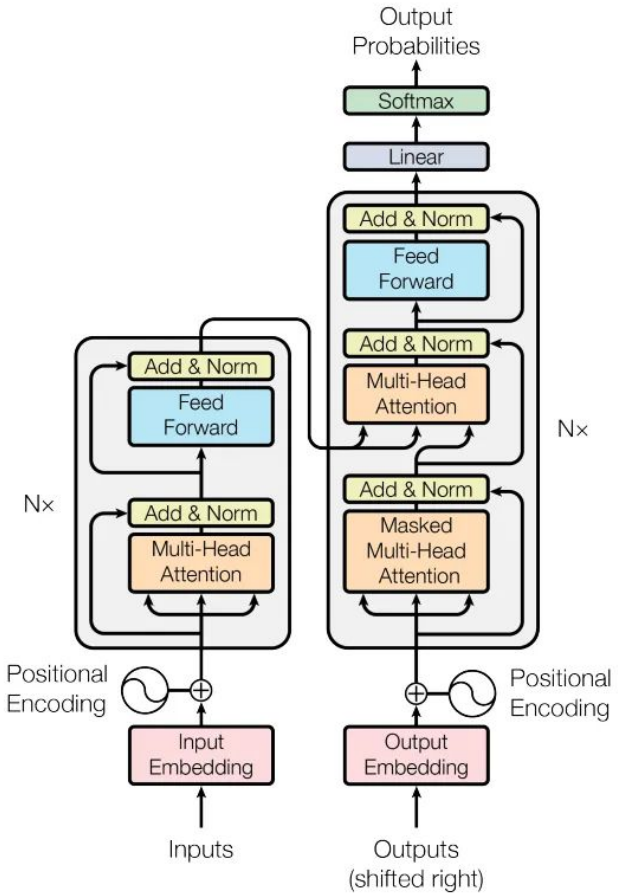
Encoder-Decoder Architecture

Advantages:

- constant path length between any two positions in the sequence (hence are better to model context in long sequences);
  - i.e., every token in the sequence is looking at every other token in the sequence; so now if you have a token that depends on another that is way far behind in the sequence, you don't have the issue of losing context.
- better parallelization because of how the computations are done; no sequential computation within a layer.

Drawbacks:

- Self-attention takes quadratic time and space (each token attends to all other tokens); scaling, which is now very popular and effective, has now become very

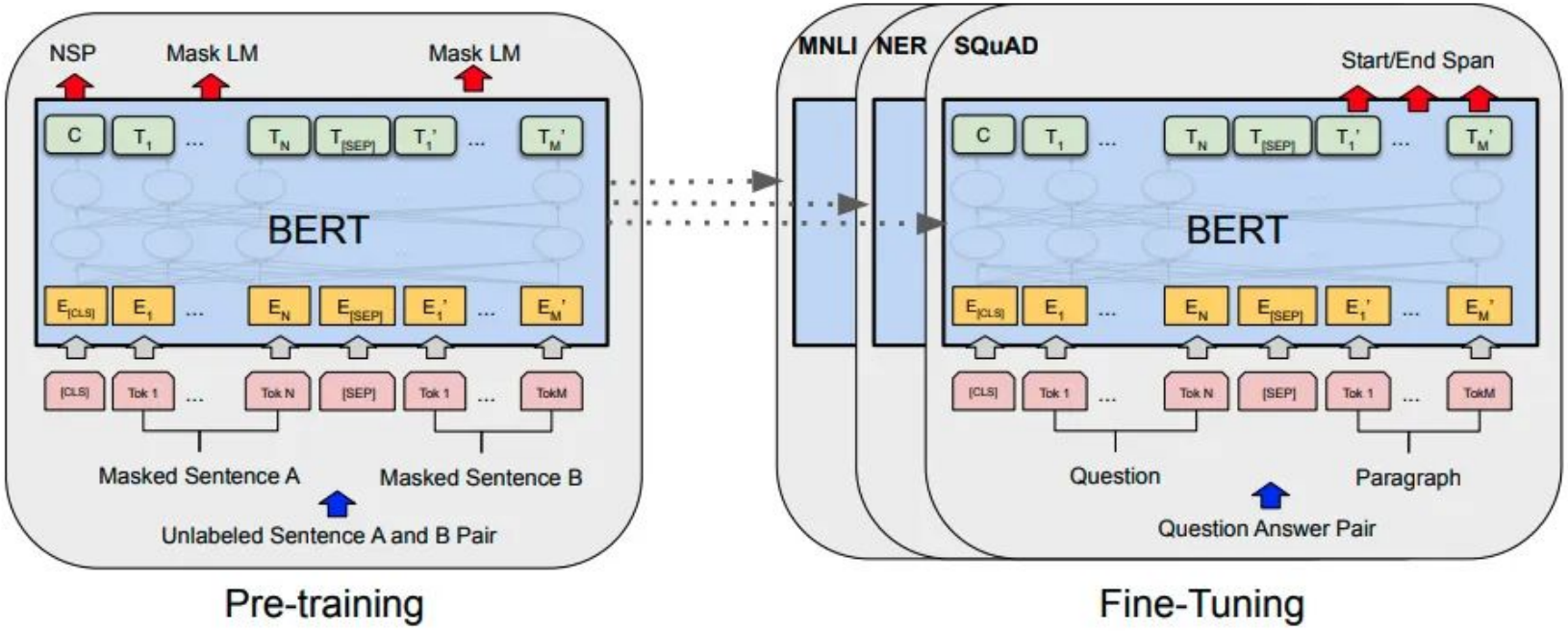


BERT

https://aclanthology.org/N19-1423/

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

- consists of only the encoder blocks from transformers.



Self-Attention Applied

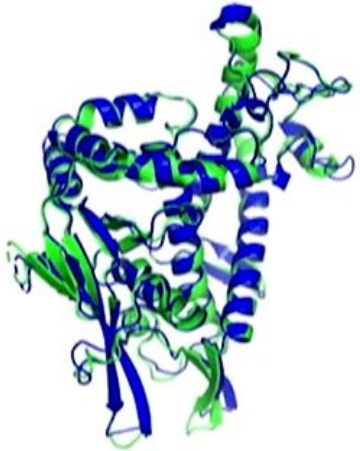
Language Processing

An armchair in the shape of an avocado

BERT, GPT-3

Devlin et al., *NAACL* 2019
Brown et al., *NeurIPS* 2020

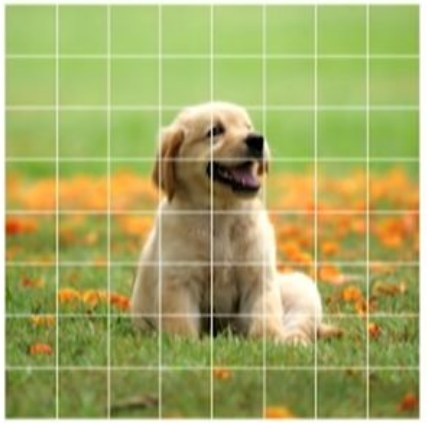
Biological Sequences



AlphaFold2

Jumper et al., *Nature* 2021

Computer Vision

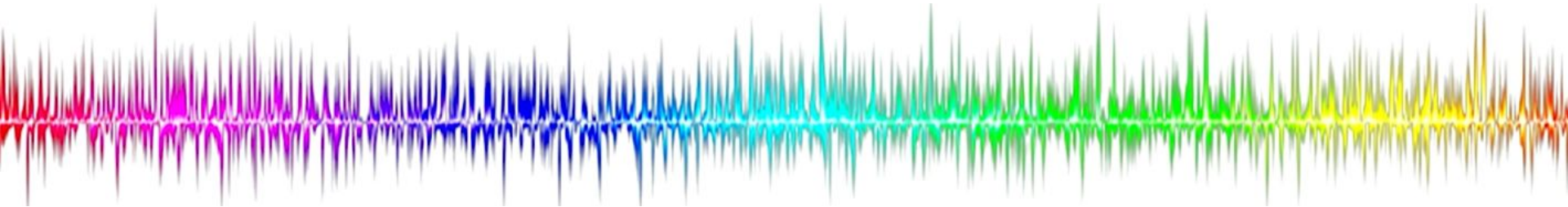


Vision Transformers

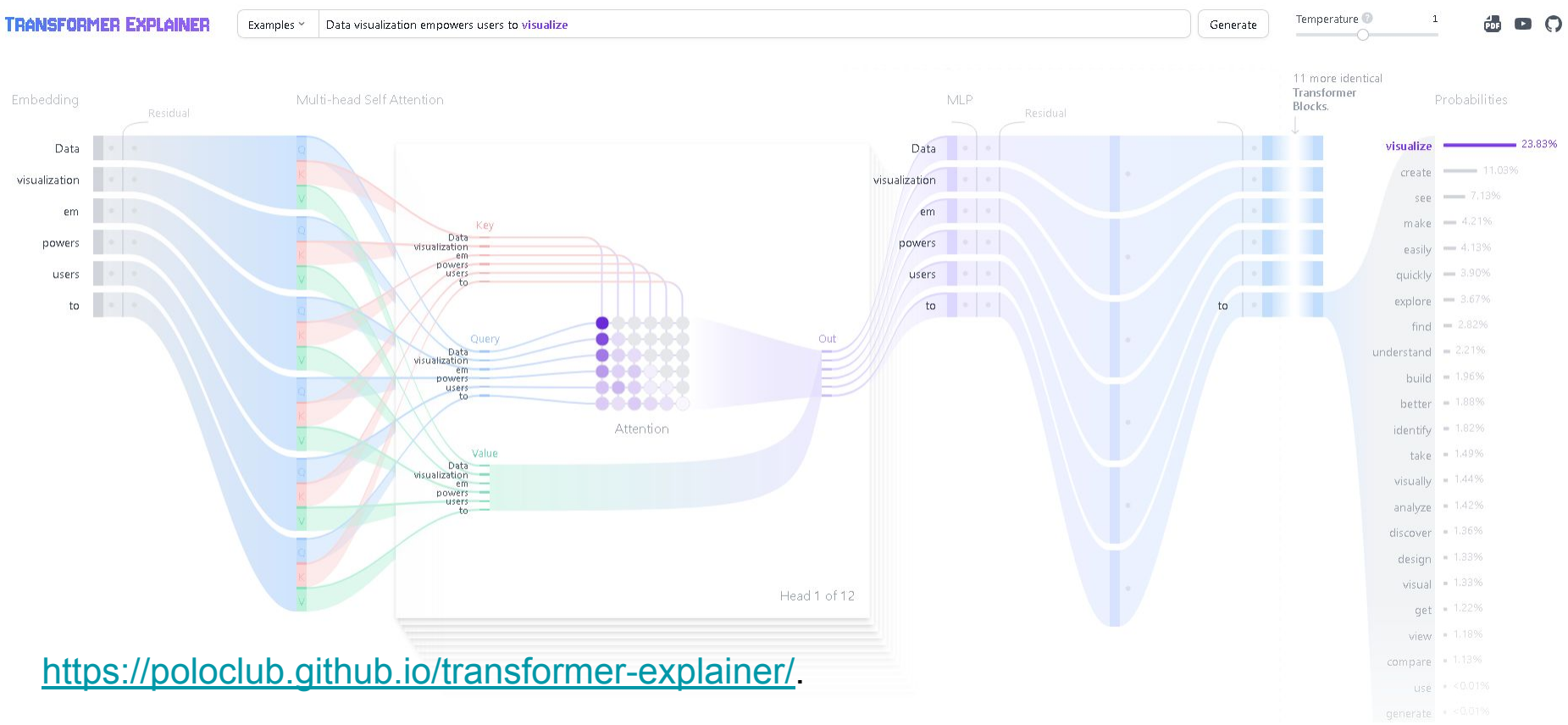
Dosovitskiy et al., *ICLR* 2020

Summary

1. RNNs are suited for sequence modeling
2. Model sequences via a recurrence relation
3. Backpropagtion through time
4. LSTM
5. Self-attention to model sequences without recurrence



References

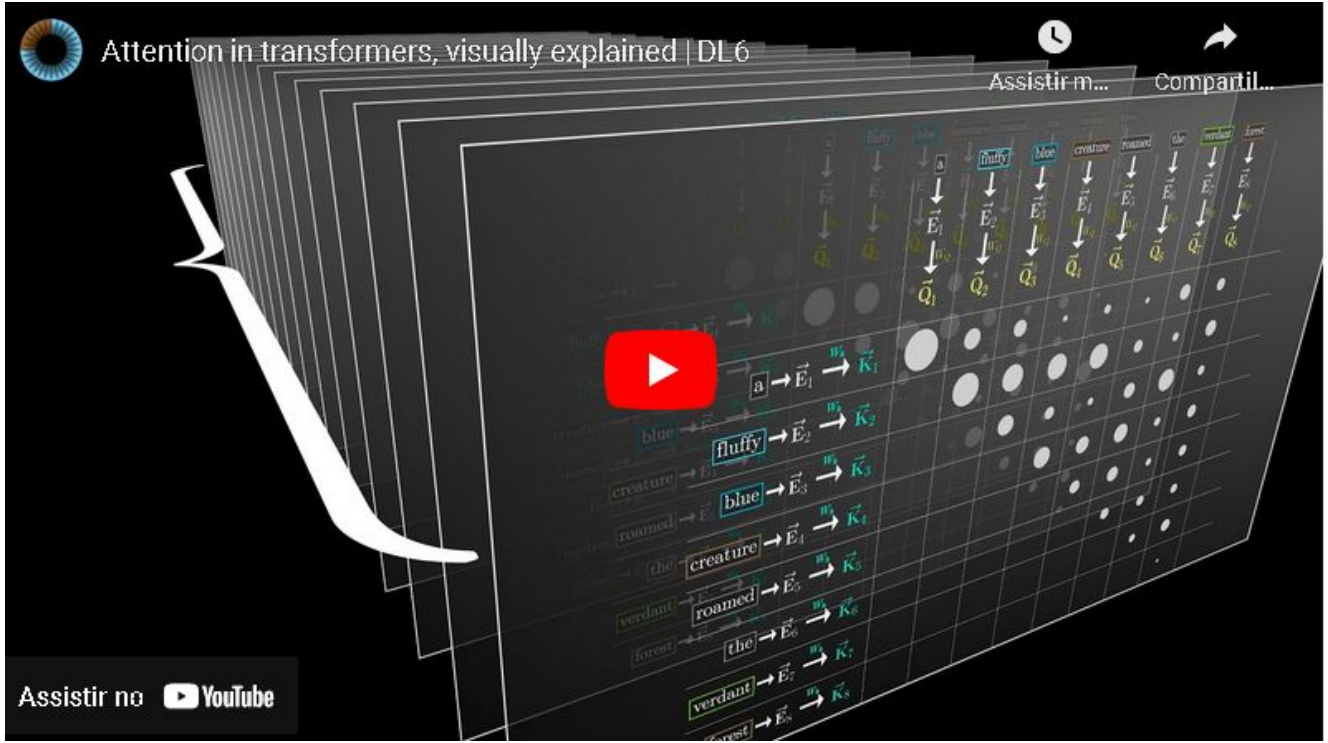


https://poloclub.github.io/transformer-explainer/.

The Illustrated Transformer

https://jalammar.github.io/illustrated-transformer/

References



https://www.youtube.com/watch?v=eMlx5fFNoYc

Transformers Notebooks

TensorFlow notebook

- https://colab.research.google.com/github/tensorflow/text/blob/master/docs/tutorials/transformer.ipynb

Hugging Face's notebooks 🤗

- https://huggingface.co/docs/transformers/en/notebooks

References

- https://d2l.ai/chapter_recurrent-neural-networks/index.html
  https://d2l.ai/chapter_recurrent-neural-networks/language-model.html
- https://d2l.ai/chapter_recurrent-modern/lstm.html
- https://dair-ai.notion.site/Lecture-2-RNNs-and-Transformers-71fb3ba2a24f4b6c8cc77281fc19cfab
- https://towardsdatascience.com/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21
- https://www.kaggle.com/code/hadeerismail/daily-climate-time-series-analysis-lstm/notebook
- https://www.kaggle.com/datasets/sumanthvrao/daily-climate-time-series-data/data

Prof. Dr. Patrick Terrematte

patrick.terrematte@ufrn.br

Discord patrickterrematte