Neural Sequence Modeling

He He

NEW YORK UNIVERSITY

Febuary 5, 2025

Table of Contents

Last Week

- What is the core principle underlying learning word vectors?

Last Week

- What is the core principle underlying learning word vectors?
  - **Distributional hypothesis**: a word's meaning can be represented by its context

Last Week

- What is the core principle underlying learning word vectors?
  - **Distributional hypothesis**: a word's meaning can be represented by its context
- **Count-based word embedding**: using SVD to discover latent features

Last Week

- What is the core principle underlying learning word vectors?
  - **Distributional hypothesis**: a word's meaning can be represented by its context
- **Count-based word embedding**: using SVD to discover latent features
- **Prediction-based word embedding**: directly learning word vectors to optimize "correlation" between a word and its context

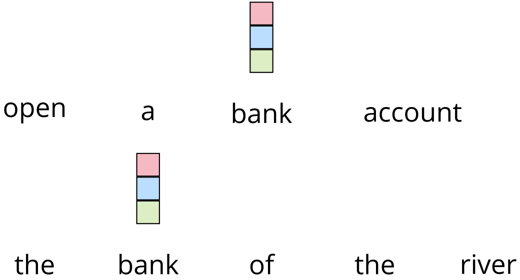
Last Week

- What is the core principle underlying learning word vectors?
  - **Distributional hypothesis**: a word's meaning can be represented by its context
- **Count-based word embedding**: using SVD to discover latent features
- **Prediction-based word embedding**: directly learning word vectors to optimize "correlation" between a word and its context
  - Use **negative sampling** to speed up training

Table of Contents

Limitation of word embeddings

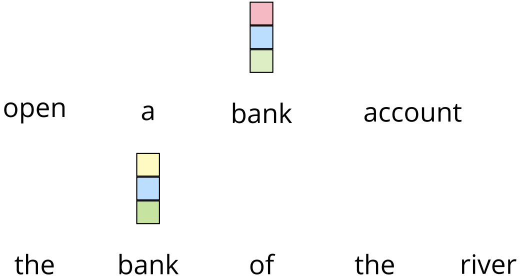
So far we have assumed tokens are (conditionally) independent to each other, and they have deterministic representations



Limitation of word embeddings

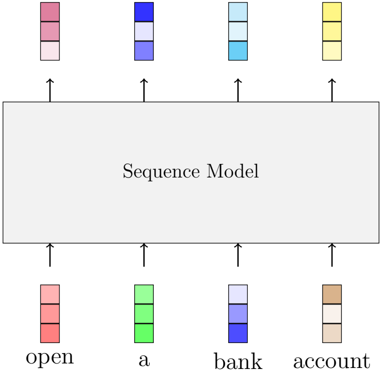
So far we have assumed tokens are (conditionally) independent to each other, and they have deterministic representations

Ideally we want the representation to depend on context



Modeling a sequence of tokens

Problem setup: given an input sequence of tokens (or their embeddings), outputs contextualized embeddings for each token, which can then be used for downstream tasks.



Modeling a sequence of tokens

Key challenge: how to model interaction among words?

Modeling a sequence of tokens

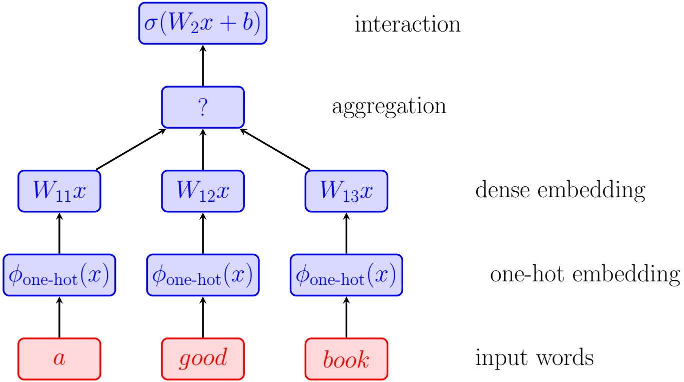
Key challenge: how to model interaction among words?

Approach:

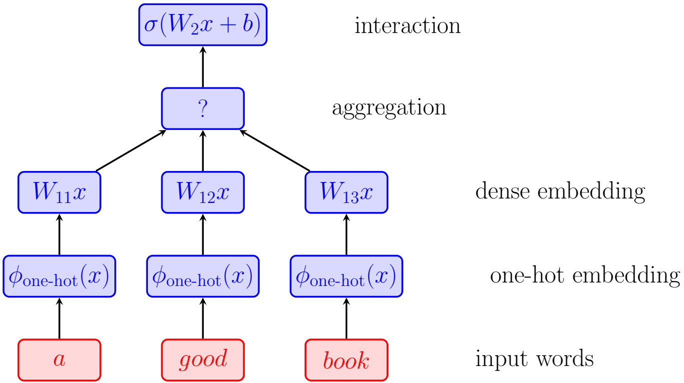
- Dense interaction
- Recurrence
- Self-attention

Table of Contents

Feed-forward neural network for sequence modeling

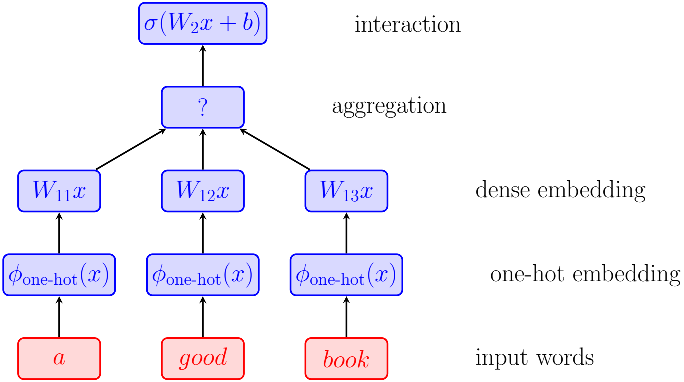


Feed-forward neural network for sequence modeling



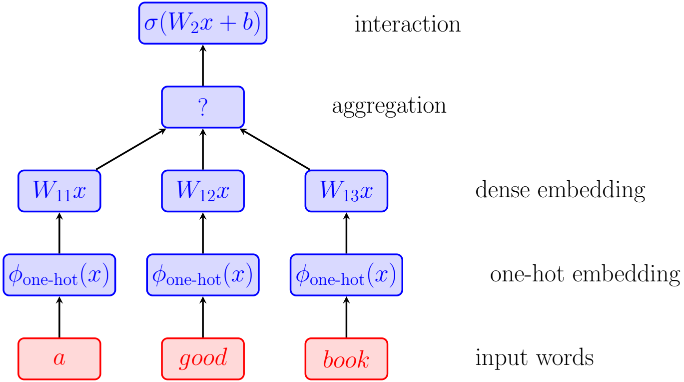
🤔 How to aggregate input word embeddings so that they can be interacted through a linear layer?

Feed-forward neural network for sequence modeling



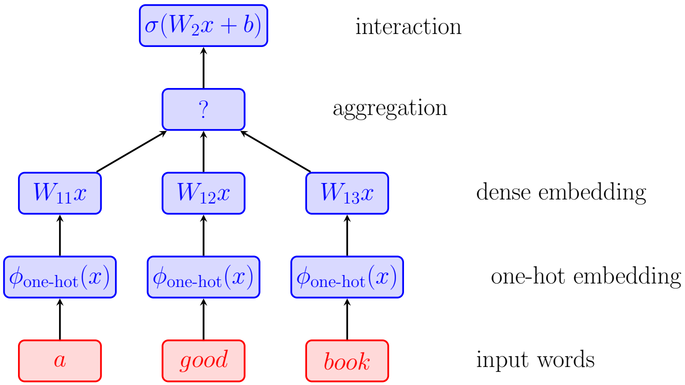
1. Concatenate along the feature dimension: $1 \times p \to 3p \times 1$

Feed-forward neural network for sequence modeling



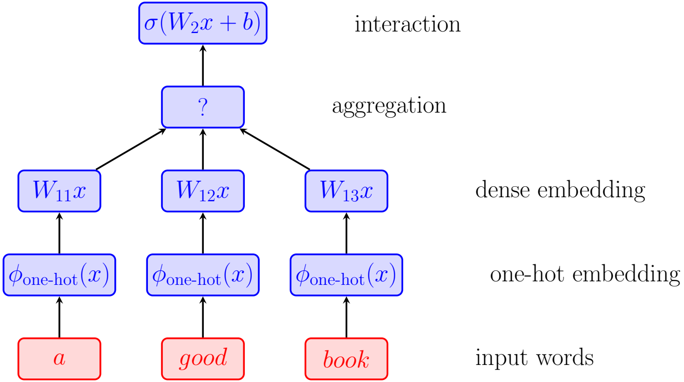
2. Concatenate along the token dimension: $1 \times p \to 3 \times p$

Feed-forward neural network for sequence modeling



3. Concatenate along the token dimension then transpose: $1 \times p \rightarrow p \times 3$

Feed-forward neural network for sequence modeling



Can it model sequences of arbitrary lengths?

Summary

- Different concatenation interacts different aspects of the input
  - Mixing all features in all tokens
  - Mixing a specific feature in all tokens
  - Mixing all features in a specific token
- Can use different mixing strategies in different MLP layers
- Design considerations: efficiency vs expressivity
- See more at MLP-Mixer: An all-MLP Architecture for Vision

Table of Contents

Recurrent neural networks

- **Idea**: combine new tokens with previous tokens recurrently

Recurrent neural networks

- **Idea**: combine new tokens with previous tokens recurrently
  - Update the representation, i.e. **hidden states** h_t, recurrently

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

    - Output from previous time step is the input to the current time step
    - Apply the same transformation f at each time step

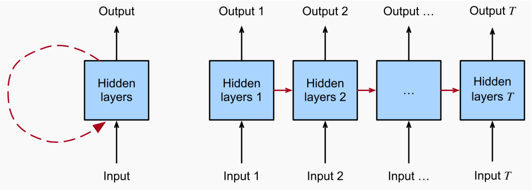
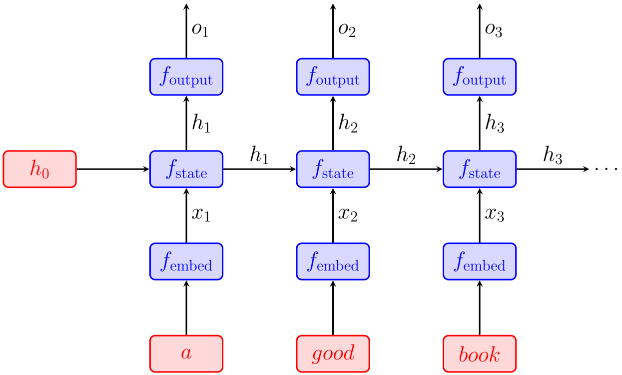


Figure: 9.1 from d2l.ai

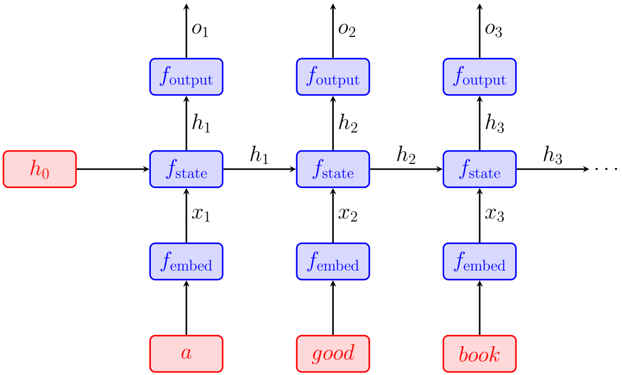
- Output the hidden states: the representation of the t-th token incorporates its left context

Forward pass



A deep neural network with shared weights in each layer

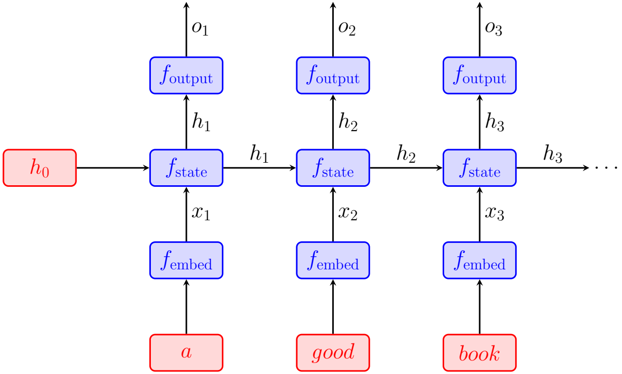
Forward pass



$$
\begin{aligned}
x_t &= f_{\text{embed}}(s_t) \\
&= W_e \phi_{\text{one-hot}}(s_t)
\end{aligned}
$$

A deep neural network with shared weights in each layer

Forward pass

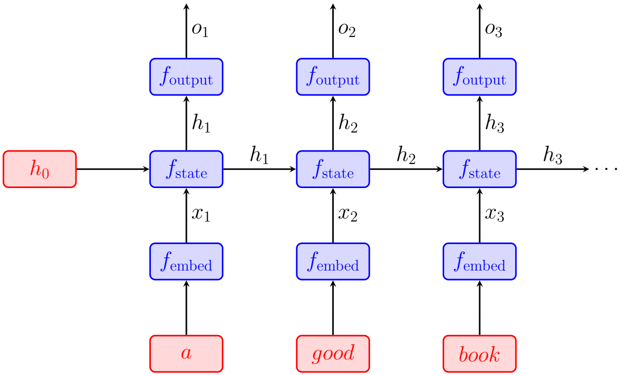


$$
\begin{aligned}
x_t &= f_{\text{embed}}(s_t) \\
&= W_e \phi_{\text{one-hot}}(s_t)
\end{aligned}
$$

$$
\begin{aligned}
h_t &= f_{\text{state}}(x_t, h_{t-1}) \\
&= \sigma(W_{hh} h_{t-1} + W_{ih} x_t + b_h)
\end{aligned}
$$

A deep neural network with shared weights in each layer

Forward pass



$$\begin{aligned} x_t &= f_{\text{embed}}(s_t) \\ &= W_e \phi_{\text{one-hot}}(s_t) \end{aligned}$$

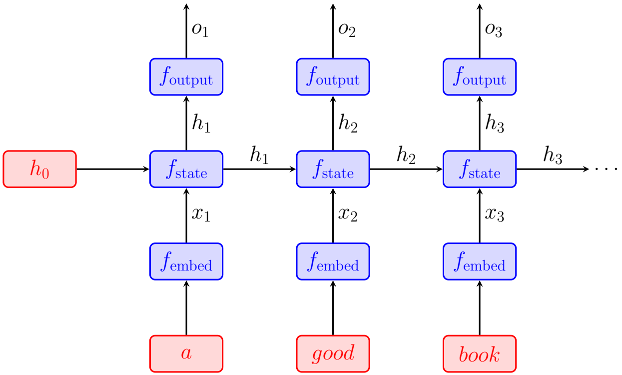
$$\begin{aligned} h_t &= f_{\text{state}}(x_t, h_{t-1}) \\ &= \sigma(W_{hh} h_{t-1} + W_{ih} x_t + b_h) \end{aligned}$$

$$\begin{aligned} o_t &= f_{\text{output}}(h_t) \\ &= \mathrm{softmax}(W_{ho} h_t + b_o) \end{aligned}$$

(a distribution over classes)

A deep neural network with shared weights in each layer

Forward pass



A deep neural network with shared weights in each layer

$$x_t = f_{\text{embed}}(s_t) = W_e \phi_{\text{one-hot}}(s_t)$$

$$h_t = f_{\text{state}}(x_t, h_{t-1}) = \sigma(W_{hh} h_{t-1} + W_{ih} x_t + b_h)$$

$$o_t = f_{\text{output}}(h_t) = \text{softmax}(W_{ho} h_t + b_o)$$

(a distribution over classes)

🤔 Which computation can be parallelized?

Using RNNs in downstream tasks

Sequence labeling and language modeling:

- Input: $x_1, \ldots, x_T$ (a sequence of tokens)
- Output: $y_1, \ldots, y_T$ (e.g., POS tags, next words)
- Loss function: $\sum_{i=1}^{T} \ell(y_t, o_t)$
  - NLL loss: $\sum_{i=1}^{T} - \log o_t[y_t]$

Using RNNs in downstream tasks

Sequence labeling and language modeling:

- Input: $x_1, \ldots, x_T$ (a sequence of tokens)
- Output: $y_1, \ldots, y_T$ (e.g., POS tags, next words)
- Loss function: $\sum_{i=1}^{T} \ell(y_t, o_t)$
  - NLL loss: $\sum_{i=1}^{T} -\log o_t[y_t]$

Text classification:

- Input: $x_1, \ldots, x_T$
- Output: $y \in \{1, \ldots, K\}$ (K classes)
- Loss function: $\ell(y, f_{\text{output}}(\mathrm{pool}(h_1, \ldots, h_T)))$
  - Can use last hidden state or mean of all hidden states

Backward pass

Given the loss $\ell(y_t, o_t)$, compute the gradient with respect to W_{hh}.

$$\frac{\partial \ell_t}{\partial W_{hh}} =$$

Backward pass

Given the loss $\ell(y_t, o_t)$, compute the gradient with respect to W_{hh}.

$$\frac{\partial \ell_t}{\partial W_{hh}} = \frac{\partial \ell_t}{\partial o_t} \frac{\partial o_t}{\partial h_t} \frac{\partial h_t}{\partial W_{hh}}$$

Backward pass

Given the loss $\ell(y_t, o_t)$, compute the gradient with respect to W_{hh}.

$$\frac{\partial \ell_t}{\partial W_{hh}} = \frac{\partial \ell_t}{\partial o_t} \frac{\partial o_t}{\partial h_t} \frac{\partial h_t}{\partial W_{hh}}$$

Computation graph of h_t: $h_t = \sigma(W_{hh} h_{t-1} + W_{hi} x_t + b)$

Backpropagation through time

Problem with standard backpropagation:

- Gradient involves repeated multiplication of W_{hh}
- Gradient will vanish / explode (depending on the eigenvalues of W_{hh})

Backpropagation through time

Problem with standard backpropagation:

- Gradient involves repeated multiplication of W_{hh}
- Gradient will vanish / explode (depending on the eigenvalues of W_{hh})

Quick fixes:

- **Truncated BPTT**: reduce the number of repeated multiplication by truncating after k steps (h_{t-k} has no influence on h_t)
- **gradient clipping**: limit the norm (or value) of the gradient in each step; can only mitigate explosion

Long-short term memory (LSTM)

Vanilla RNN: always update the hidden state

- Cannot handle long range dependency due to gradient vanishing

Long-short term memory (LSTM)

Vanilla RNN: always update the hidden state

- Cannot handle long range dependency due to gradient vanishing

LSTM: learn when to update the hidden state

- First successful solution to the gradient vanishing and explosion problem

Long-short term memory (LSTM)

Vanilla RNN: always update the hidden state

- Cannot handle long range dependency due to gradient vanishing

LSTM: learn when to update the hidden state

- First successful solution to the gradient vanishing and explosion problem

Key idea is to use a **gating mechanism**: multiplicative weights that modulate another variable

- How much should the new input affect the state?
- How much should the state affect the output?

Long-short term memory (LSTM) cell

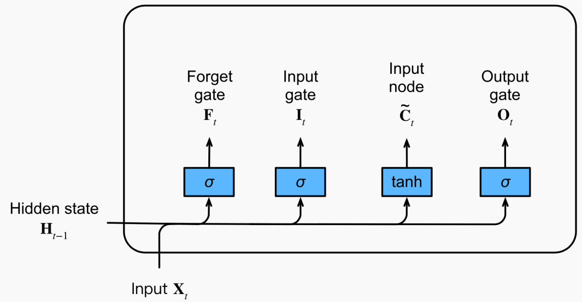


Figure: 10.1.2 from d2l.ai

Cell input: current state, new input
Cell output: updated state

Long-short term memory (LSTM) parametrization

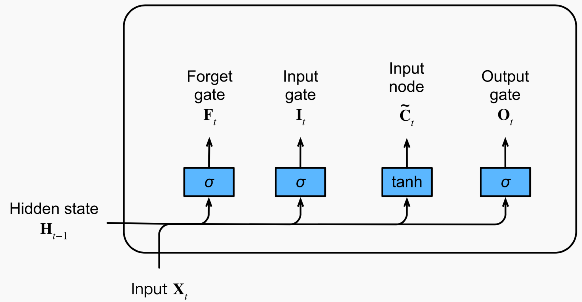


Figure: 10.1.2 from d2l.ai

Tentatively update with the new input x_t (same as in vanilla RNN)

$$\tilde{c}_t = \tanh(W_{xc}x_t + W_{hc}h_{t-1} + b_c) \quad \text{new cell content}$$

But don't commit to h_t yet.

Long-short term memory (LSTM) parametrization

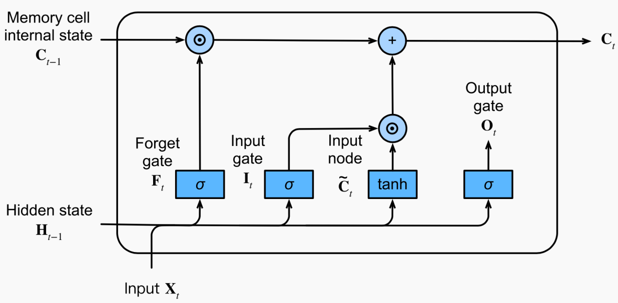


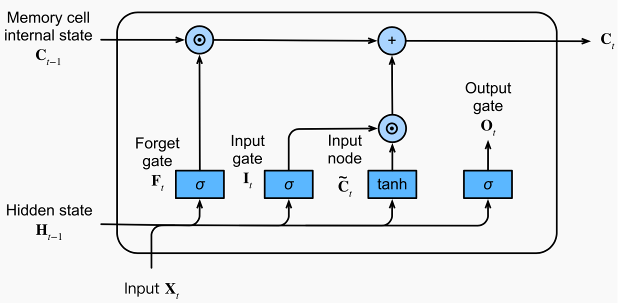
Figure: 10.1.3 from d2l.ai

Choose between $\tilde{c}_t$ (update) and c_{t-1} (no update): ($\odot$: elementwise product)

$$\textbf{memory cell} \quad c_t = i_t \odot \tilde{c}_t + f_t \odot c_{t-1}$$

- f_t: proportion of the old state (preserve $\uparrow$ or erase $\downarrow$ the old memory)
- i_t: proportion of the new state (write $\uparrow$ or ignore $\downarrow$ the new input)
- What is c_t if $f_t = 1$ and $i_t = 0$?

Long-short term memory (LSTM) parametrization



Input gate and forget gate depends on data:

$$
\begin{aligned}
i_t &= \text{sigmoid}(W_{xi}x_t + W_{hi}h_{t-1} + b_i)\ , \\
f_t &= \text{sigmoid}(W_{xf}x_t + W_{hf}h_{t-1} + b_f)\ .
\end{aligned}
$$

Each coordinate is between 0 and 1.

Long-short term memory (LSTM) parametrization

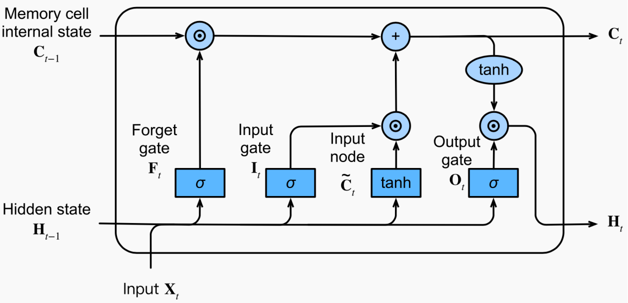


Figure: 10.1.4 from d2l.ai

How much should the memory cell state influence the rest of the network:

$$h_t = o_t \odot c_t$$
$$o_t = \text{sigmoid}(W_{xo}x_t + W_{ho}h_{t-1} + b_o)$$

c_t may accumulate information without impact the network if o_t is close to 0

How does LSTM mitigate gradient vanishing / explosion?

Intuition: gating allows the network to learn to control how much gradient should vanish.

- Vanilla RNN: gradient depends on repeated multiplication of the same weight matrix
- LSTM: gradient depends on repeated multiplication of some quantity that depends on the data (values of input and forget gates)
- So the network can learn to reset or update the gradient depending on whether there is long-range dependencies in the data.
- Gradient exploding can still happen if dependency is long!

Table of Contents

Improve the efficiency of RNN

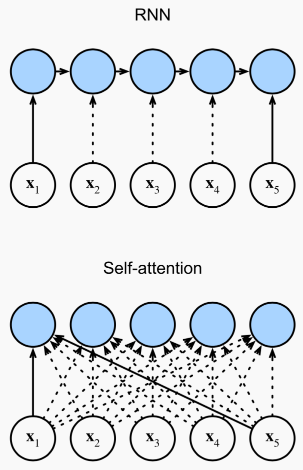


Figure: 11.6.1 from d2l.ai

Recall that our goal is to come up with a good respresentation of a sequence of words.

RNN:

- Past words influence the sentence representation through recurrent update
- Sequential computation O(sequence length), hard to scale

Improve the efficiency of RNN

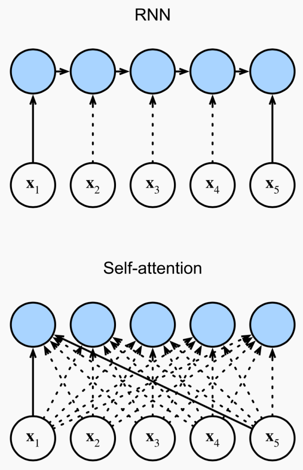


Figure: 11.6.1 from d2l.ai

Recall that our goal is to come up with a good respresentation of a sequence of words.

RNN:

- Past words influence the sentence representation through recurrent update
- Sequential computation O(sequence length), hard to scale

Can we handle dependency more efficiently?

- Interact pairs of tokens in the sequence
- Parallel computation

Motivating example

adapted from 3blue1brown

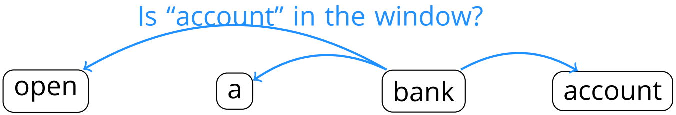
How do we figure out the meaning of ”bank”?

open a bank account

Motivating example

adapted from 3blue1brown

How do we figure out the meaning of ”bank”?

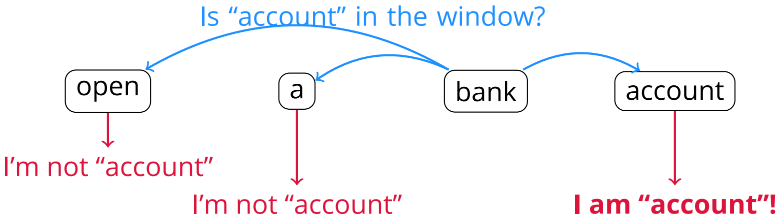


“bank” broadcasts a query

Motivating example

adapted from 3blue1brown

How do we figure out the meaning of ”bank”?

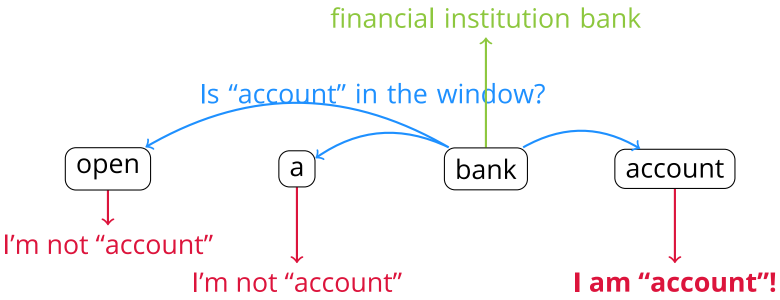


Every word sends a key corresponding to the query

Motivating example

adapted from 3blue1brown

How do we figure out the meaning of ”bank”?



The representation of “bank” is updated by words with **matched keys**

Model interaction between words

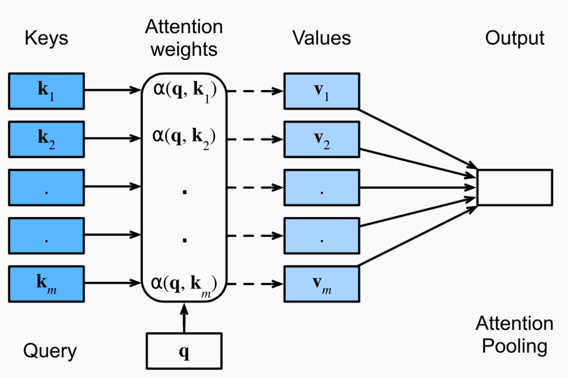


Figure: 11.1.1 from d2l.ai

- **Attention weights** $\alpha(q, k_i)$: how strong is q matched to k_i
- **Attention pooling**: combine v_i's according to their "relatedness" to the query
- Each word adds its "value" to the target word to modify its meaning

Model interaction between words

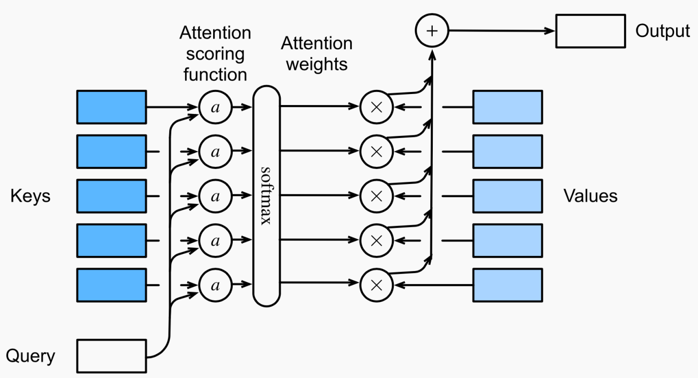
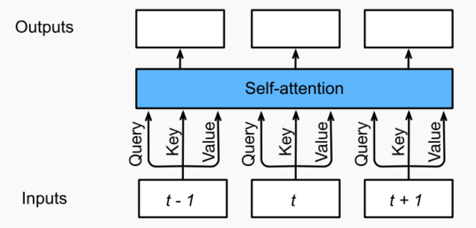


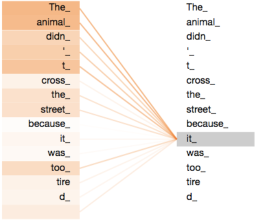
Figure: 11.3.1 from d2l.ai

- Model attention weights as a distribution: $\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m))$
- Output a weighted combination of values: $o_i = \sum_{i=1}^{m} \alpha(q, k_i) v_i$

Self-attention

Where do the key, query, and value come from?

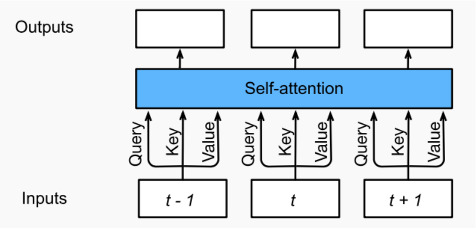


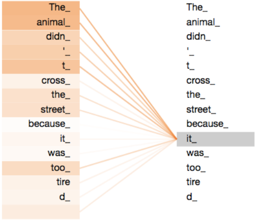


- Input: map each symbol to a query, a key, and a value (embeddings)

Self-attention

Where do the key, query, and value come from?

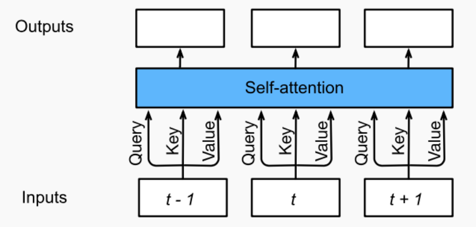


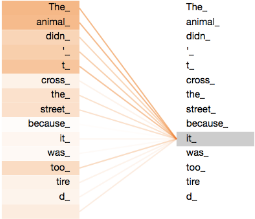


- Input: map each symbol to a query, a key, and a value (embeddings)
- Attend: each word (as a query) interacts with all words (keys)

Self-attention

Where do the key, query, and value come from?





- Input: map each symbol to a query, a key, and a value (embeddings)
- Attend: each word (as a query) interacts with all words (keys)
- Output: *contextualized* representation of each word (weighted sum of values)

Attention scoring functions

Design the function that measures relatedness between queries and keys:

$\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m)) \qquad a \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Attention scoring functions

Design the function that measures relatedness between queries and keys:

$\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m)) \qquad a \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Dot-product attention

$$a(q, k) = q \cdot k$$

Attention scoring functions

Design the function that measures relatedness between queries and keys:

$\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m)) \qquad a\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Dot-product attention

$$a(q, k) = q \cdot k$$

Scaled dot-product attention

$$a(q, k) = q \cdot k / \sqrt{d}$$

- $\sqrt{d}$: dimension of the key vector
- Avoids large attention weights that push the softmax function into regions of small gradients

Attention scoring functions

Design the function that measures relatedness between queries and keys:

$\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m)) \qquad a\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Dot-product attention

$$a(q, k) = q \cdot k$$

Scaled dot-product attention

$$a(q, k) = q \cdot k / \sqrt{d}$$

- $\sqrt{d}$: dimension of the key vector
- Avoids large attention weights that push the softmax function into regions of small gradients

MLP attention

$$a(q, k) = u^T \tanh(W[q; k])$$

Multi-head attention: motivation

Time flies like an arrow

- Each word attends to all other words in the sentence
- Which words should “like” attend to?

Multi-head attention: motivation

Time flies like an arrow

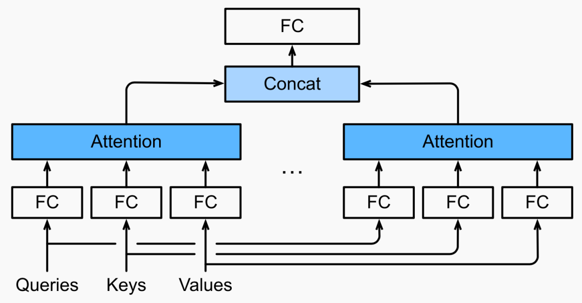
- Each word attends to all other words in the sentence
- Which words should “like” attend to?
  - Syntax: “flies”, “arrow” (a preposition)
  - Semantics: “time”, “arrow” (a metaphor)

Multi-head attention: motivation

Time flies like an arrow

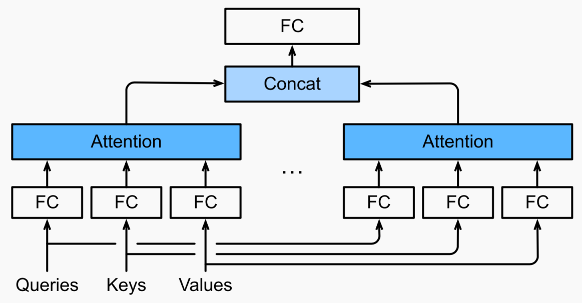
- Each word attends to all other words in the sentence
- Which words should "like" attend to?
  - Syntax: "flies", "arrow" (a preposition)
  - Semantics: "time", "arrow" (a metaphor)
- We want to represent different roles of a word in the sentence: need more than a single embedding
- Instantiation: multiple self-attention modules

Multi-head attention



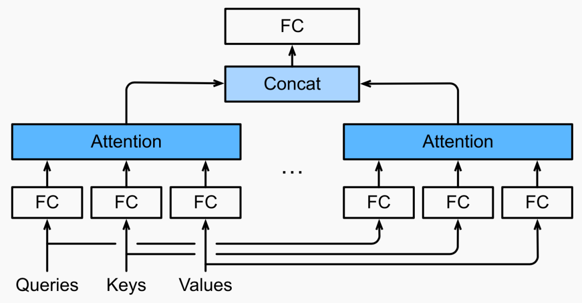
- Multiple attention modules: same architecture, different parameters

Multi-head attention



- Multiple attention modules: same architecture, different parameters
- A **head**: one set of attention outputs

Multi-head attention



- Multiple attention modules: same architecture, different parameters
- A **head**: one set of attention outputs
- Concatenate all heads (increased output dimension)
- Linear projection to produce the final output

Matrix representation: input mapping

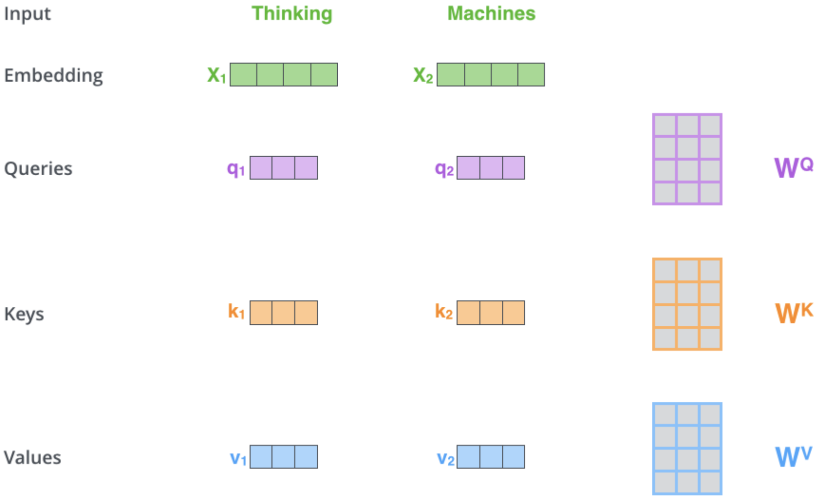


Figure: From The Illustrated Transformer

Matrix representation: attention weights

Scaled dot product attention

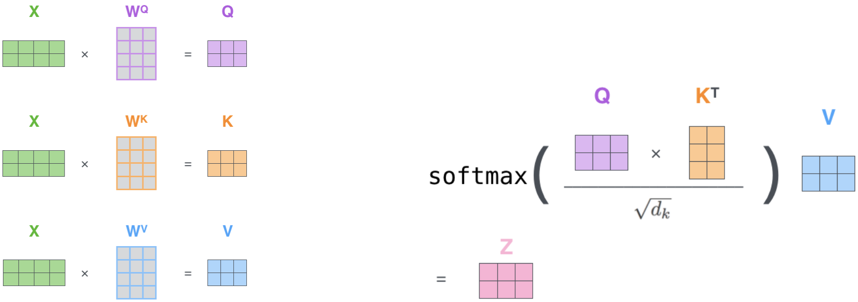


Figure: From The Illustrated Transformer

Multi-head attention

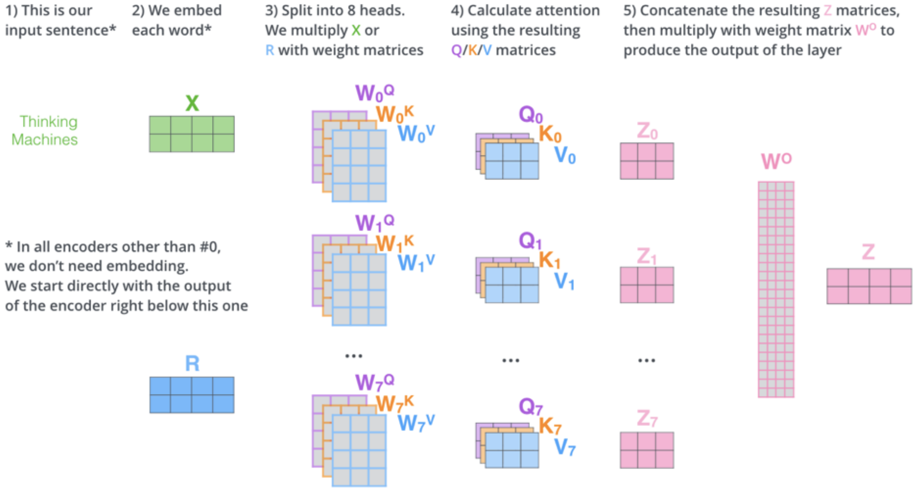


Figure: From The Illustrated Transformer

Summary so far

- Sequence modeling
  - Input: a sequence of words
  - Output: a sequence of contextualized embeddings for each word
  - Models interaction among words

Summary so far

- Sequence modeling
  - Input: a sequence of words
  - Output: a sequence of contextualized embeddings for each word
  - Models interaction among words
- Building blocks
  - Feed-forward / fully-connected neural network
  - Recurrent neural network
  - Self-attention

Summary so far

- Sequence modeling
  - Input: a sequence of words
  - Output: a sequence of contextualized embeddings for each word
  - Models interaction among words
- Building blocks
  - Feed-forward / fully-connected neural network
  - Recurrent neural network
  - Self-attention

🤔 Which of these can handle sequences of arbitrary length?

Table of Contents

Overview

- Use self-attention as the core building block
- Vastly increased scalability (model and data size) compared to recurrence-based models
- Initially designed for machine translation (next week)
  - *Attention is all you need*. Vaswani et al., 2017.
- The backbone of today's large-scale models
- Extended to non-sequential data (e.g., images and molecules)

Transformer block

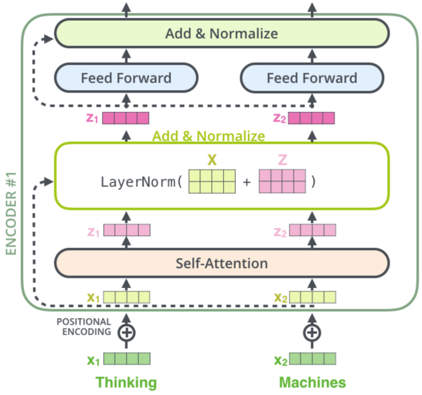


Figure: From The Illustrated Transformer

- Multi-head self-attention

Transformer block

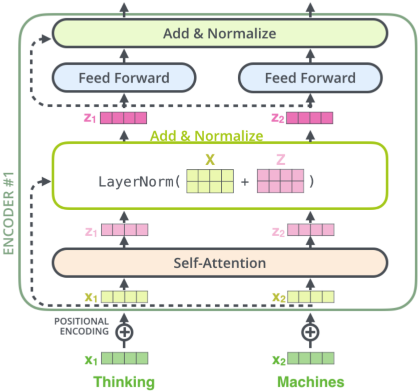


Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols

Transformer block

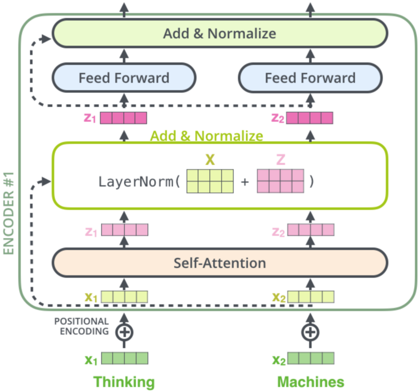


Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding

Transformer block

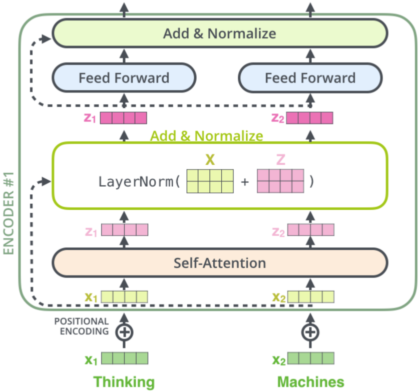


Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding
  - Capture the order of symbols

Transformer block

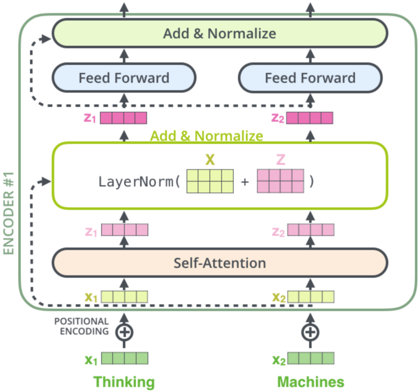


Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding
  - Capture the order of symbols
- Residual connection and layer normalization

Transformer block

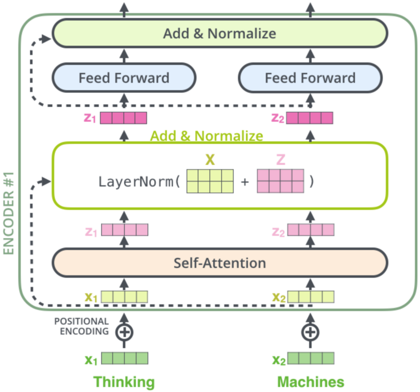
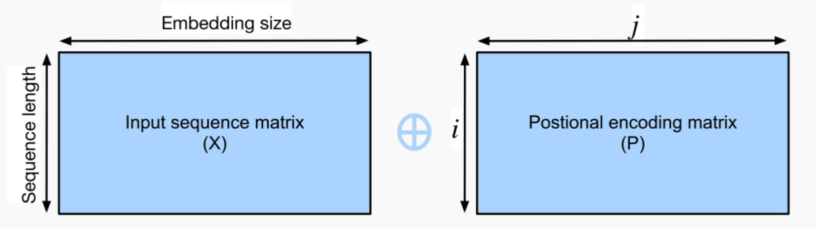


Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding
  - Capture the order of symbols
- Residual connection and layer normalization
  - More efficient and stable optimization

Position embedding

Motivation: model word order in the input sequence
Solution: add a position embedding to each word



Position embedding:

- Encode absolute and relative positions of a word
- Same dimension as word embeddings
- Learned or deterministic

Sinusoidal position embedding

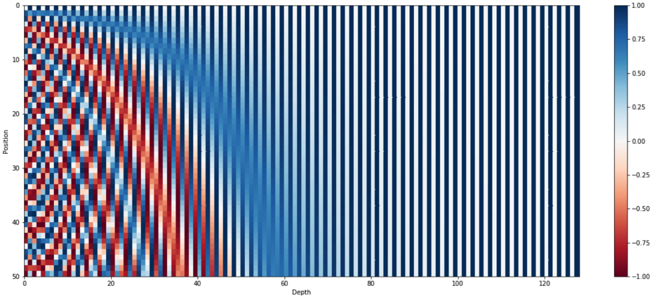
Intuition: continuous approximation of binary encoding of positions (integers)

0 :	0	0	0	0
1 :	0	0	0	1
2 :	0	0	1	0
3 :	0	0	1	1
4 :	0	1	0	0
5 :	0	1	0	1
6 :	0	1	1	0
7 :	0	1	1	1

Sinusoidal position embedding

Intuition: continuous approximation of binary encoding of positions (integers)

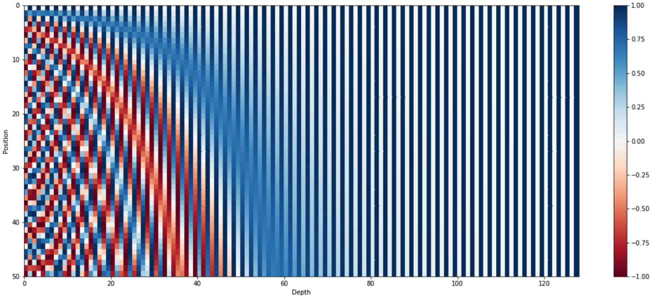
0 :	0	0	0	0
1 :	0	0	0	1
2 :	0	0	1	0
3 :	0	0	1	1
4 :	0	1	0	0
5 :	0	1	0	1
6 :	0	1	1	0
7 :	0	1	1	1



Sinusoidal position embedding

Intuition: continuous approximation of binary encoding of positions (integers)

0 :	0	0	0	0
1 :	0	0	0	1
2 :	0	0	1	0
3 :	0	0	1	1
4 :	0	1	0	0
5 :	0	1	0	1
6 :	0	1	1	0
7 :	0	1	1	1



$$\vec{p_t} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_{d \times 1}$$

Figure: From Amirhossein Kazemnejad's Blog

$$\omega_k = 1/10000^{\frac{2k}{d}}$$

Learned position embeddings

Sinusoidal position embedding:

- Not learnable
- Can extrapolate to longer sequences but doesn't work well

Learned position embeddings

Sinusoidal position embedding:

- Not learnable
- Can extrapolate to longer sequences but doesn't work well

Learned absolute position embeddings:

- Consider each position as a word. Map positions to dense vectors: $W_{d \times n} \phi_{\text{one-hot}}(\text{pos})$
- Column i of W is the embedding of position i

Learned position embeddings

Sinusoidal position embedding:

- Not learnable
- Can extrapolate to longer sequences but doesn't work well

Learned absolute position embeddings:

- Consider each position as a word. Map positions to dense vectors: $W_{d \times n} \phi_{\text{one-hot}}(\text{pos})$
- Column i of W is the embedding of position i
- Need to fix maximum position/length beforehand
- Cannot extrapolate to longer sequences

Residual connection

Motivation:

- Gradient explosion/vanishing is not RNN-specific!
- It happens to all very deep networks (which are hard to optimize).

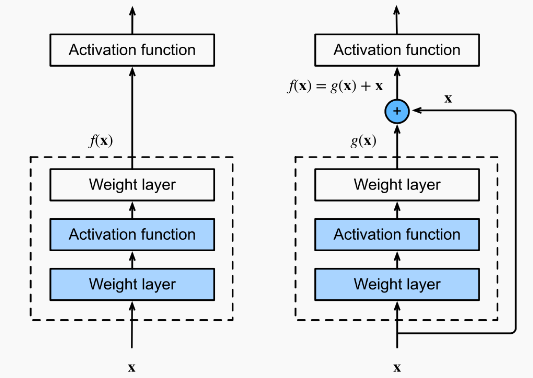
Residual connection

Motivation:

- Gradient explosion/vanishing is not RNN-specific!
- It happens to all very deep networks (which are hard to optimize).
- In principle, a deep network can always represent a shallow network (by setting higher layers to identity functions), thus it should be at least as good as the shallow network.
- For some reason, deep neural networks are bad at learning identity functions.
- How can we make it easier to recover the shallow solution?

Residual connection

Solution: Deep Residual Learning for Image Recognition [He et al., 2015]



Without residual connection: learn $f(x) = x$.

With residual connection: learn $g(x) = 0$ (easier).

Layer normalization

- **Problem**: inputs of a layer may shift during training
- **Solution**: normalize (zero mean, unit variance) across features [Ba et al., 2016]
- Let $x = (x_1, \dots, x_d)$ be the input vector (e.g., word embedding, previous layer output)

$$\mathrm{LayerNorm}(x) = \frac{x - \hat{\mu}}{\hat{\sigma}},$$

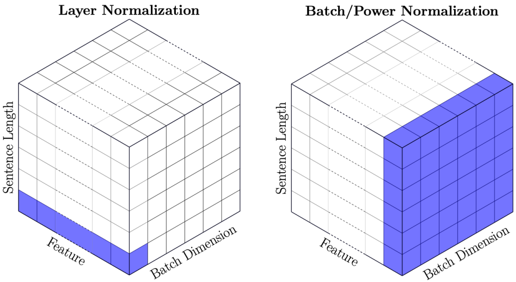
$$\text{where } \hat{\mu} = \frac{1}{d}\sum_{i=1}^{d} x_i, \quad \hat{\sigma}^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \hat{\mu})^2$$

Layer normalization

- **Problem**: inputs of a layer may shift during training
- **Solution**: normalize (zero mean, unit variance) across features [Ba et al., 2016]
- Let $x = (x_1, \ldots, x_d)$ be the input vector (e.g., word embedding, previous layer output)

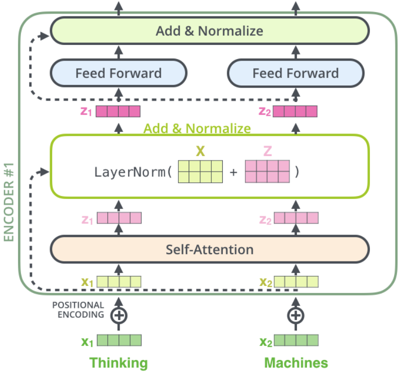
$$\mathrm{LayerNorm}(x) = \frac{x - \hat{\mu}}{\hat{\sigma}},$$

$$\text{where } \hat{\mu} = \frac{1}{d}\sum_{i=1}^{d} x_i, \quad \hat{\sigma}^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \hat{\mu})^2$$



- A deterministic transformation of the input
- Independent of train/inference and batch size

Residual connection and layer normalization in Transformer



- Add (residual connection) & Normalize (layer normalization) after each layer
- Position-wise feed-forward networks: same mapping for all positions

Summary

- We have seen two families of models for sequences modeling: **RNNs** and **Transformers**
- Both take a sequence of (discrete) symbols as input and output a sequence of embeddings
- They are often called **encoders** and are used to represent text
- Transformers are dominating today because of its scalability