Applied Machine Learning for Business Analytics

Lecture 3: Transformers

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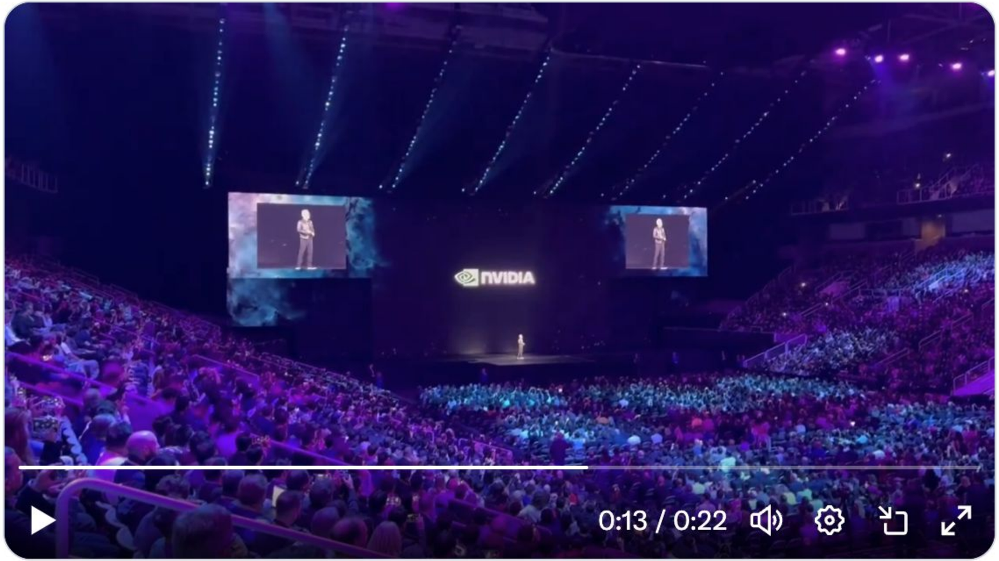
Jensen Huang is the new Taylor Swift



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Transforming AI Panel at GTC 2024

Jensen Huang will host a panel with the authors of "*Attention Is All You Need*", a seminal research paper that introduced the Transformer neural network architecture (NeurIPS, 2017)

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Founder and CEO
NVIDIA

Ashish Vaswani
Co-Founder & CEO
Essential AI

Noam Shazeer
CEO and Co-Founder
Character.AI

Niki Parmar
Co-Founder
Essential AI

Jakob Uskoreit
CEO
Inceptive

Llion Jones
Co-Founder and CTO
Sakana AI

Aidan Gomez
Co-Founder and CEO
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Lukasz Kaiser
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Attention Is All You Need

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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 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.

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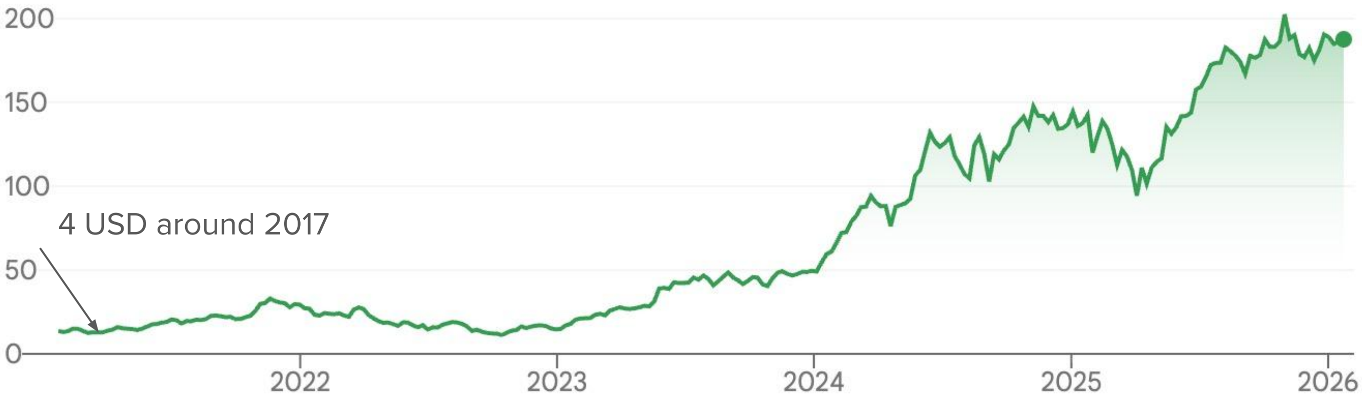

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High	189.60	P/E ratio	46.48	Qtrly div amt	0.010
Low	186.82	52-wk high	212.19	52-wk low	86.63

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DeepSeek is still on top of Transformer

performance comparable to OpenAI's o1 series models.

In this paper, we take the first step toward improving language model reasoning capabilities using pure reinforcement learning (RL). Our goal is to explore the potential of LLMs to develop reasoning capabilities without any supervised data, focusing on their self-evolution through a pure RL process. Specifically, we use DeepSeek-V3-Base as the base model and employ GRPO (Shao et al., 2024) as the RL framework to improve model performance in reasoning. During training, DeepSeek-R1-Zero naturally emerged with numerous powerful and interesting reasoning behaviors. After thousands of RL steps, DeepSeek-R1-Zero exhibits super performance on reasoning benchmarks. For instance, the pass@1 score on AIME 2024 increases from 15.6% to 71.0%, and with majority voting, the score further improves to 86.7%, matching the performance of OpenAI-o1-0912.

DeepSeekR1: https://arxiv.org/abs/2501.12948

2.1 Basic Architecture

The basic architecture of DeepSeek-V3 is still within the Transformer (Vaswani et al., 2017) framework. For efficient inference and economical training, DeepSeek-V3 also adopts MLA and DeepSeekMoE, which have been thoroughly validated by DeepSeek-V2. Compared with DeepSeek-V2, an exception is that we additionally introduce an auxiliary-loss-free load balancing strategy (Wang et al., 2024a) for DeepSeekMoE to mitigate the performance degradation induced by the effort to ensure load balance. Figure 2 illustrates the basic architecture of DeepSeek-V3, and we will briefly review the details of MLA and DeepSeekMoE in this section.

DeepSeekv3: https://arxiv.org/html/2412.19437v1

Agenda

1. Transformers
2. **Attention** is all you need
    a. Self-Attention
    b. Positional Embeddings
3. Summary
4. Appendix
    a. Masked Self-Attention
    b. Encoder-Decoder Attention

1. Transformers

What is Transformer

Transformer is a sequence to sequence model (Encoder and Decoder)

Attention Is All You Need

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Abstract

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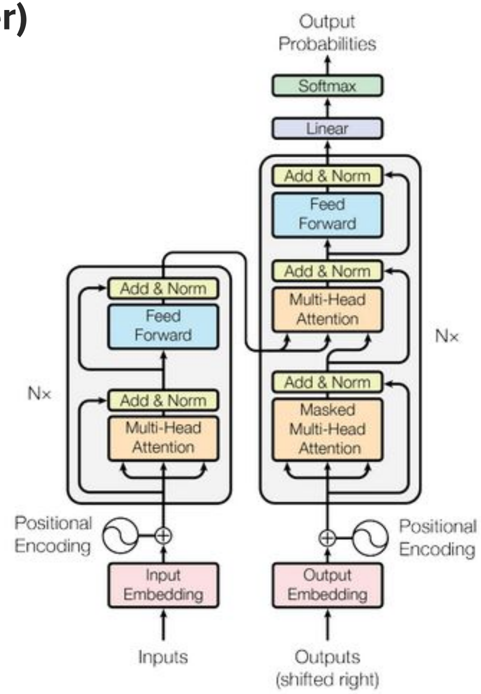
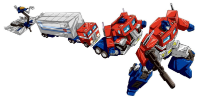


https://proceedings.neurips.cc/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

All LLMs so far use transformer architecture

- BERT and GPT are the most representative ones



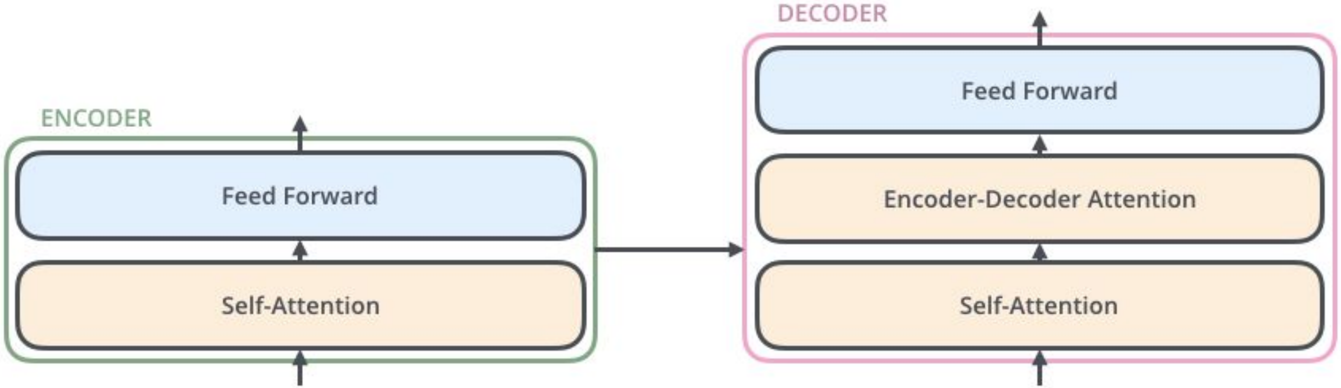
Bi-directional Encoder Representations from Transformers

OpenAI
GPT-3

Generative Pre-trained Transformers

Transformer is solving Seq2Seq

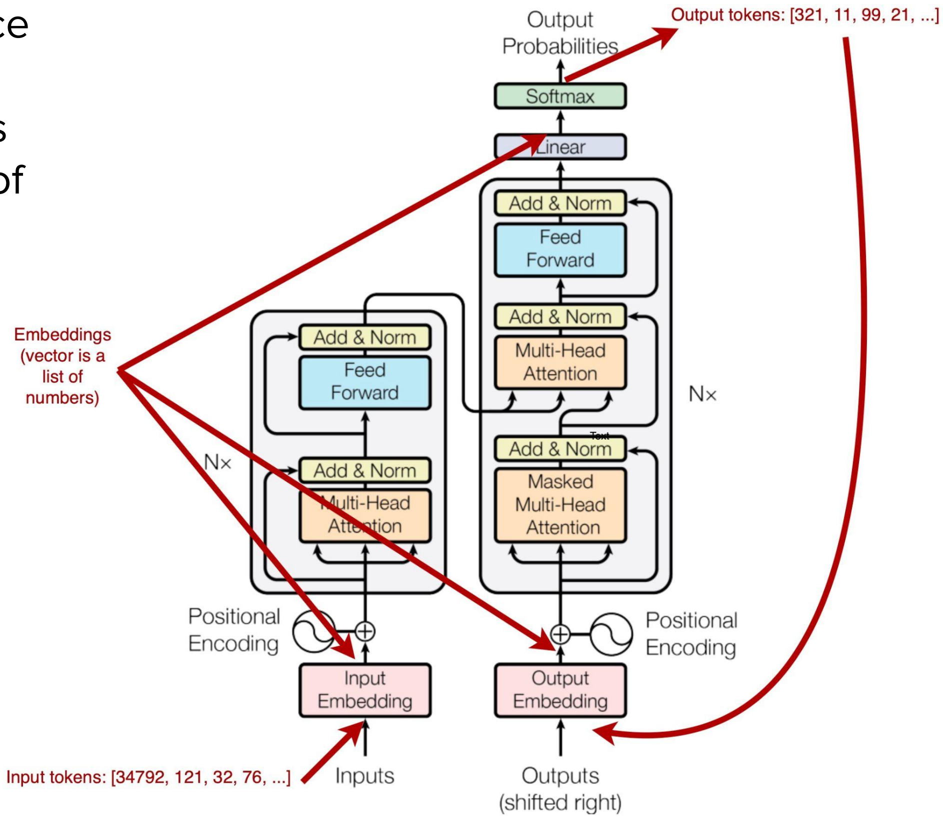
Next word



Input Sequence

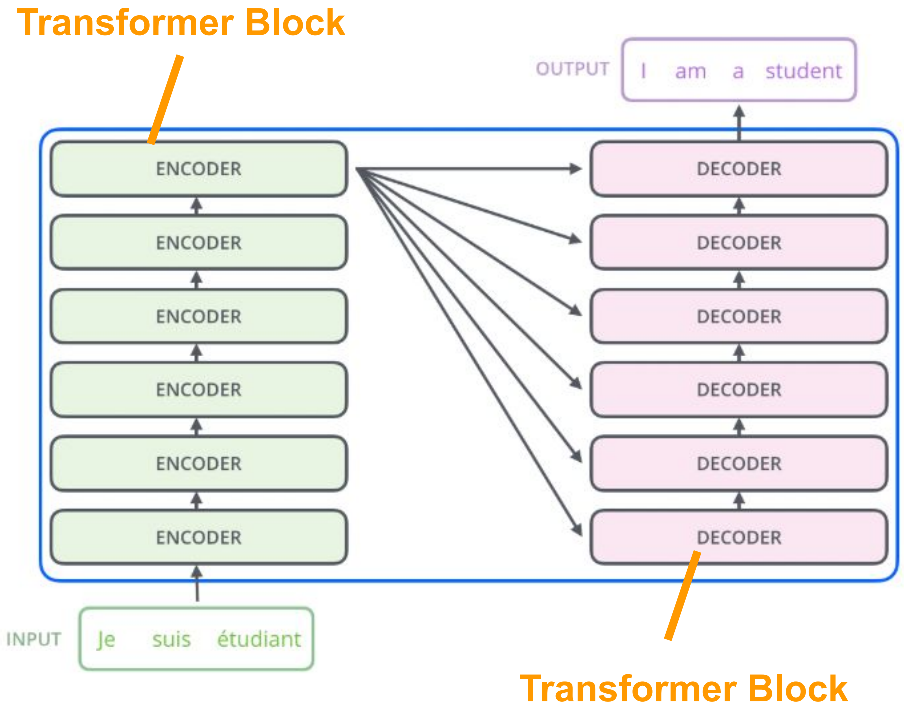
Sampled word in the output sequence

- Input text is encoded with tokenizers to sequence of integers
- Input tokens are mapped to sequence of vectors
- Output vectors can be classified to a sequence of tokens
- Output tokens can then be decoded back to the text

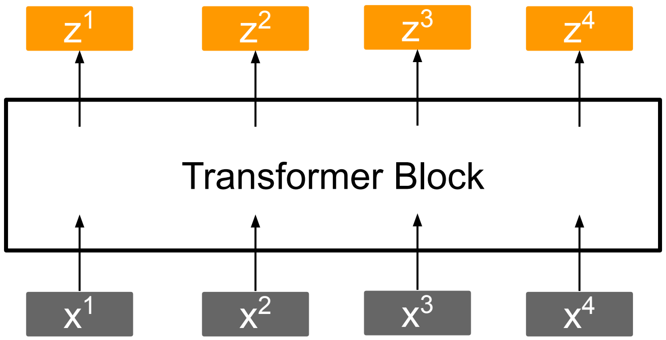


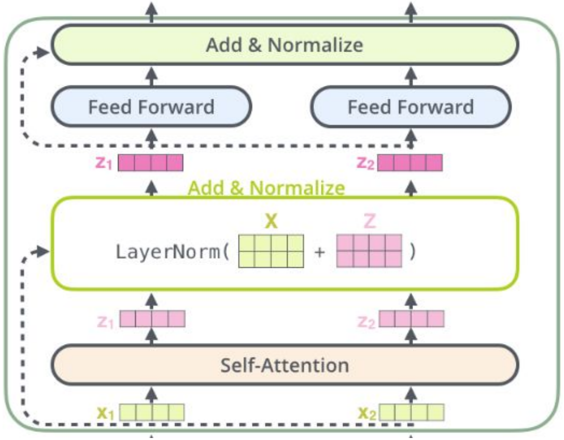
Transformer

1. Transformer block: operation unit
   a. Consists of multiple computations
   b. A sequence of embeddings in
   c. A sequence of embeddings out
2. Encoder:
   a. Stack 6 transformer blocks
   b. Learn representations for the input sequence
3. Decoder:
   a. Stack another 6 transformer blocks.
   b. Generate output sequences conditioned on the learned representations from encoder.



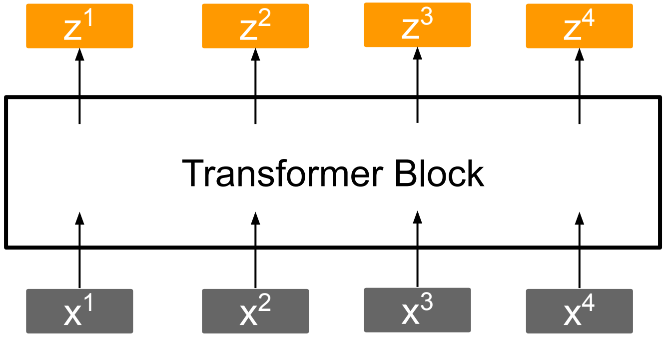
Transformer block in Encoder

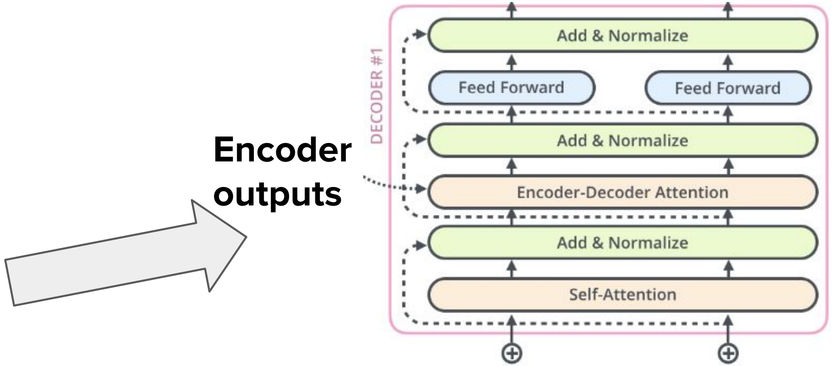




1. Input: A sequence of vectors
2. Output: A sequence of vectors
3. Key Components:
   a. **Self-attention Layer**
   b. **Positional Embeddings**
   c. Residual and Normalization Layer
   d. Fully-connected Layer

Transformer block in Decoder



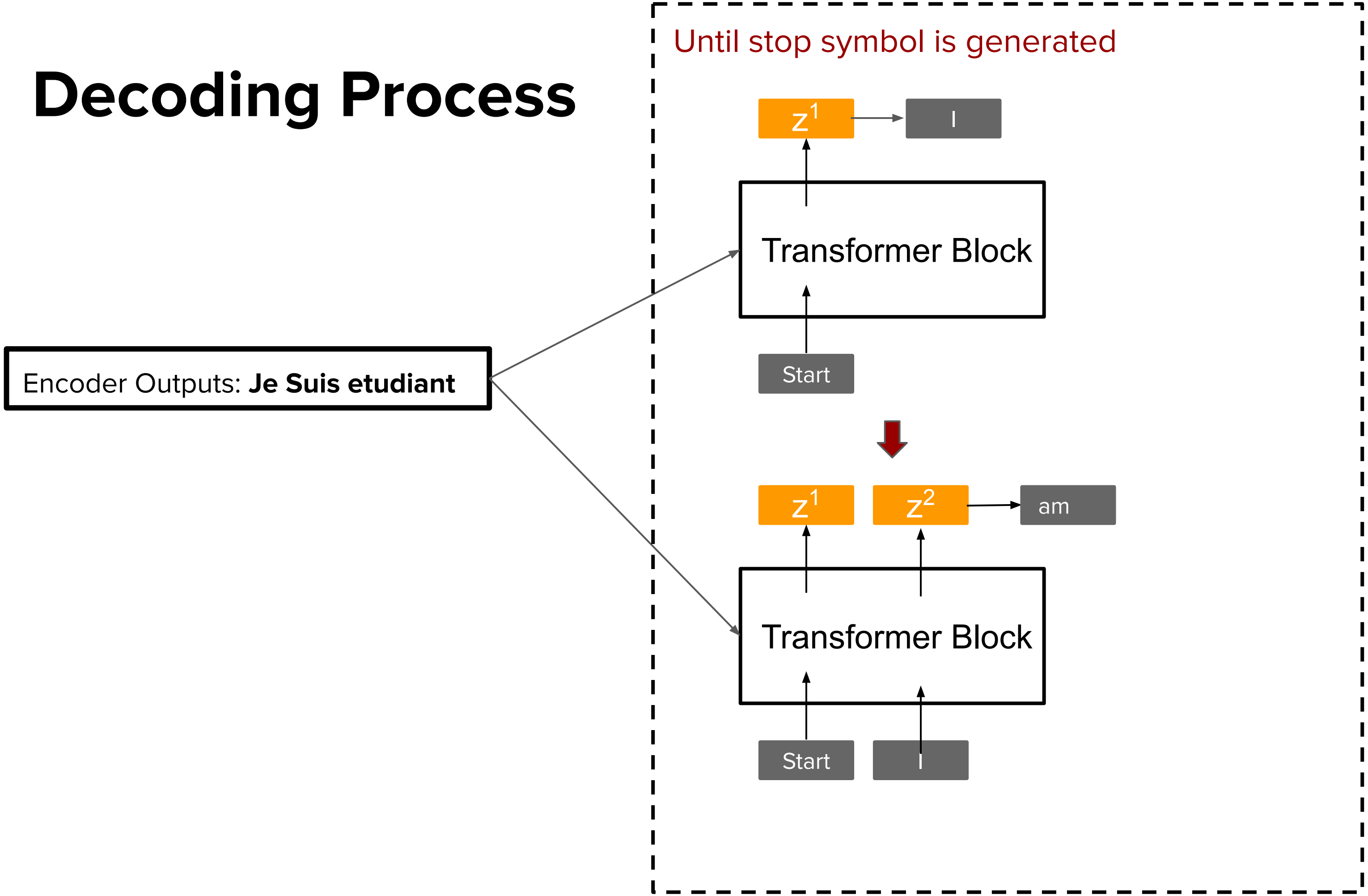


1. Input: A sequence of vectors
2. Output: A sequence of vectors
3. Key Components:
   a. **Masked Self-attention Layer**
   b. Positional Embeddings
   c. **Encoder-Decoder Attention**
   d. Residual and Normalization Layer
   e. Fully-connected Layer

Decoding Process

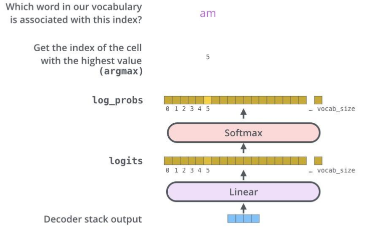
- The decoder is **autoregressive**
    - Begins with a start token
    - Before the stop token is generated, repeat
        - Take the list of previous outputs with the encoder outputs that contain the attention information from the input
        - Generate the current output

Decoding Process



Decoding Process

- Linear Classifier with Final softmax for output probabilities
  - The output of the classifier would be the size of vocabulary
  - After softmax, probability scores between 0 and 1 will be generated
  - Decoding Strategies:
    - Greedy search: alway select the most likely token
    - Random Sampling: sample from the probability distribution
    - Beam search: takes into account the N most likely tokens
      - Keeps top k sequences in parallel at each step
    - Other advanced sampling: https://deci.ai/blog/from-top-k-to-beam-search-llm-decoding-strategies/



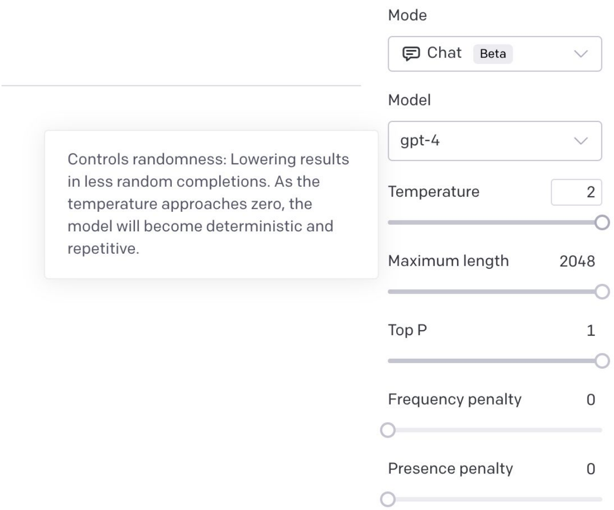
This figure starts from the bottom with the vector produced as the output of the decoder stack. It is then turned into an output word.

Temperature Sampling

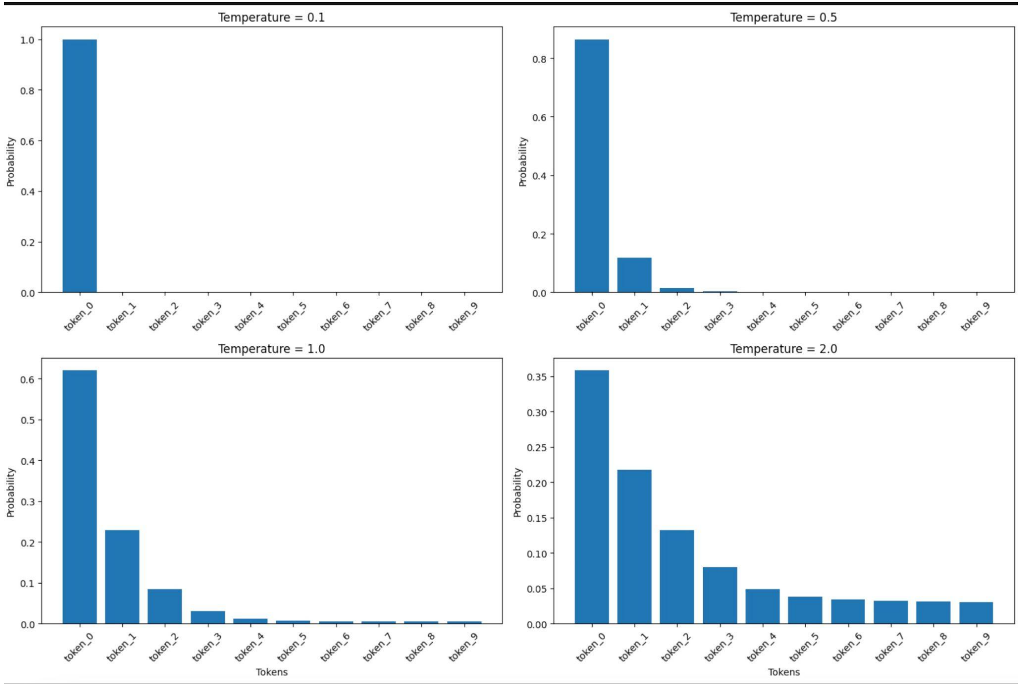
$$p_i = \mathrm{Softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{n} \exp(z_j)}$$

$$p_i(T) = \mathrm{Softmax}(z_i/T) = \frac{\exp(z_i/T)}{\sum_{j=1}^{n} \exp(z_j/T)}$$

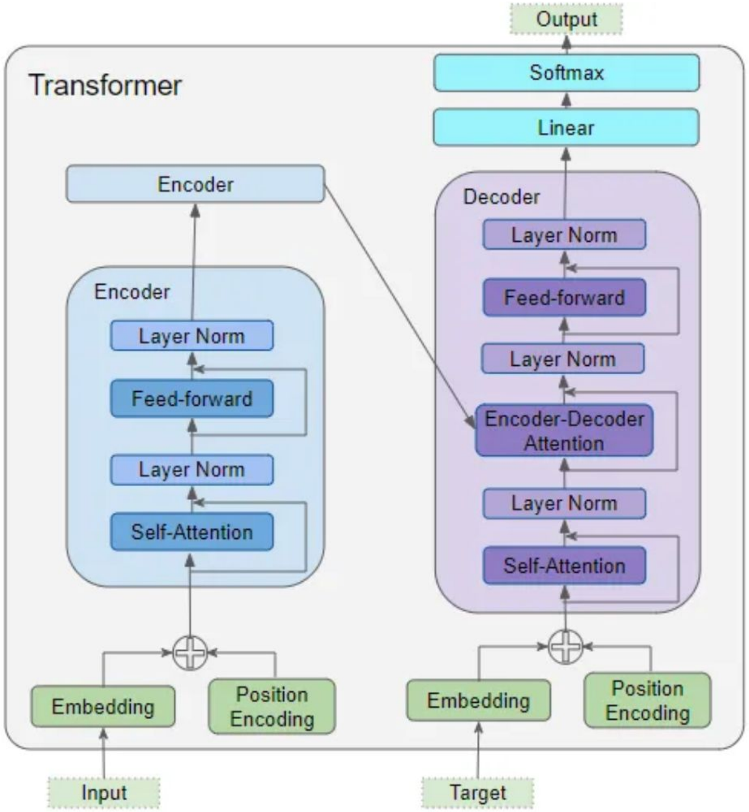
Temperature is a scaling function applied to softmax inputs



Temperature Sampling



Encoder-Decoder



Three kinds of attention in transformers:

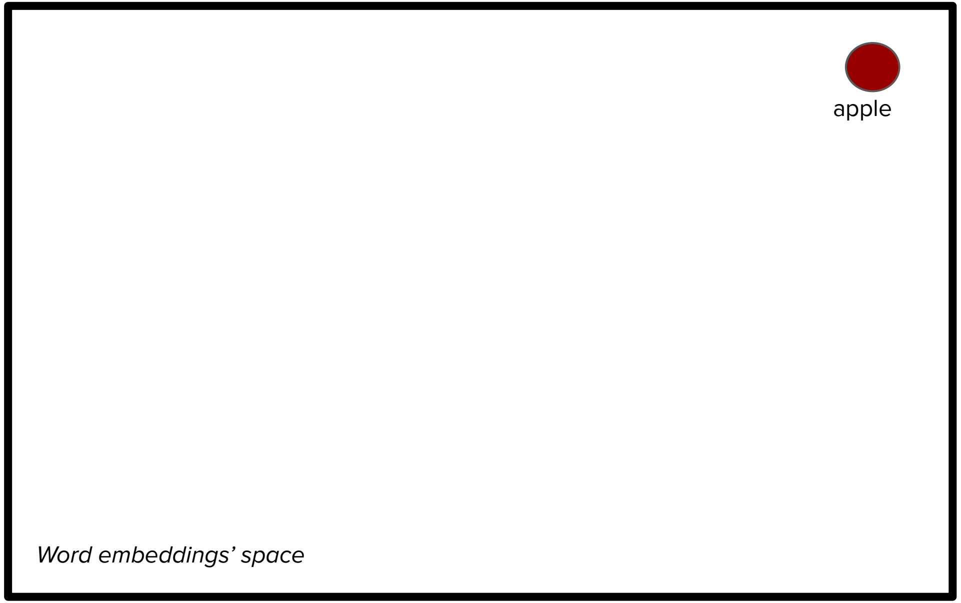
- Self-attention
  - Input sequence <> Input sequence
- Masked self-attention
  - Previous steps in output sequence <> current steps in output sequence
- Encoder-Decoder attention
  - Input sequence <> Output sequence

Source: https://towardsdatascience.com/transformers-explained-visually-part-2-how-it-works-step-by-step-b49fa4a64f34

2. Attention

Word Embeddings

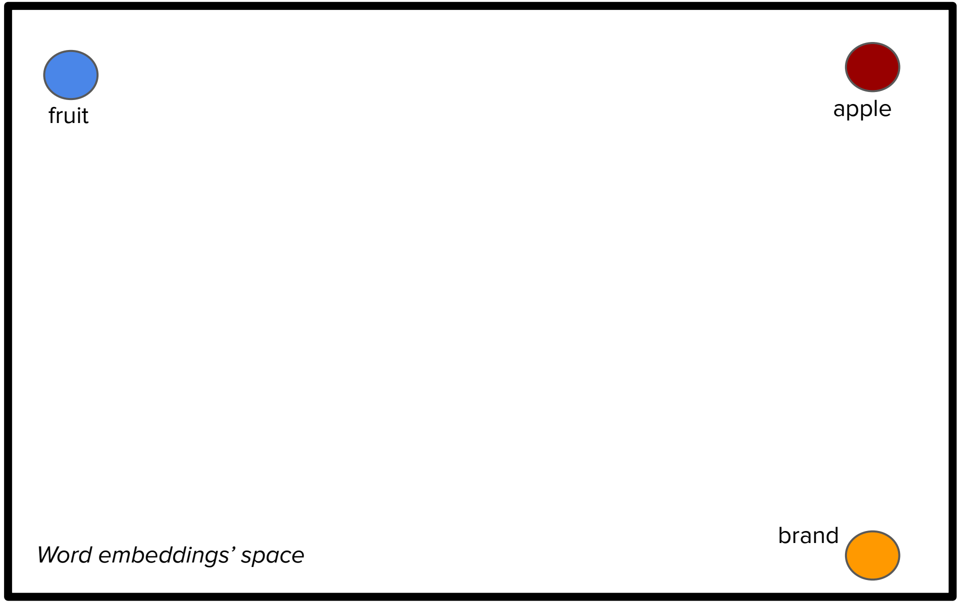
- **Apple** in two sentences:
  - Sentence 1: My favorite fruit is **apple**
  - Sentence 2: Solution: My favorite brand is **apple**



One embedding has multiple senses

Contextualized Word Embeddings

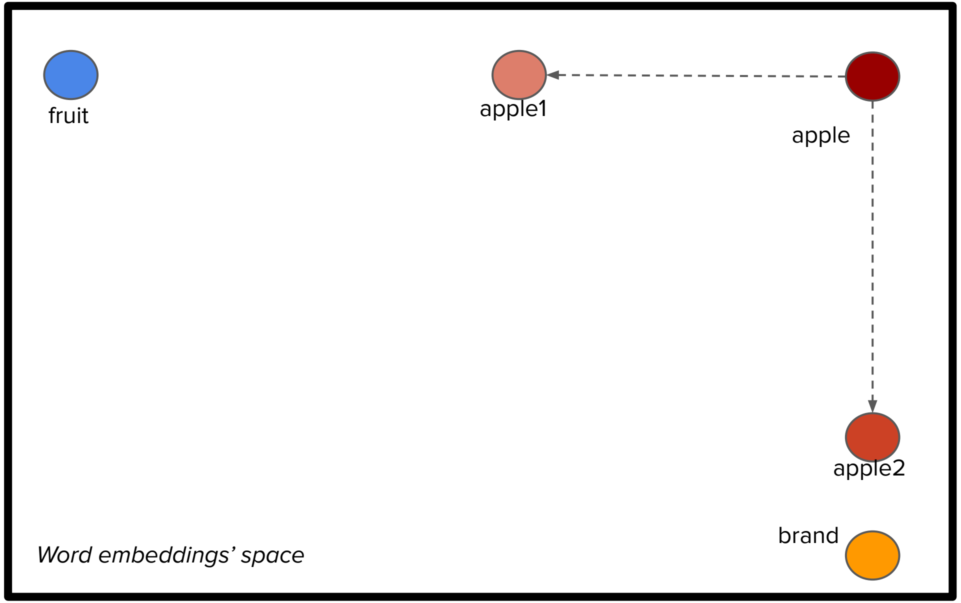
- Telling context in words
  - Sentence 1: My favorite fruit is **apple1**
  - Sentence 2: Solution: My favorite brand is **apple2**



From nearby words, we can guess two different meanings of this word (i.e., food and brand)

Contextualized Word Embeddings

- Telling context in words
  - Sentence 1: My favorite fruit is **apple1**
  - Sentence 2: Solution: My favorite brand is **apple2**



1. In sentence 1, move the word embedding of apple towards the word "fruit"
2. In sentence 2, move the word embedding of apple toward the word "brand"

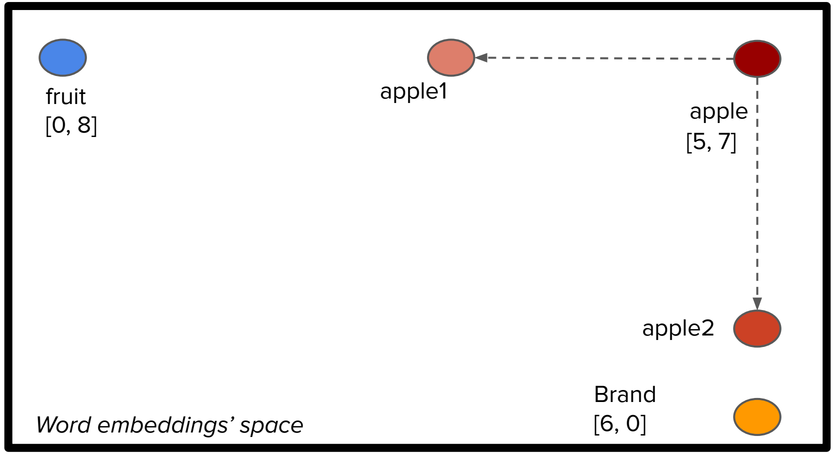
This is how attention will work

How to move one word closer to another one

- Average two words
  - apple1 = 0.8*apple + 0.2*fruit = 0.8*[5,7] + 0.2*[0,8]= [4.0, 7.2]
  - apple2 = 0.9*apple + 0.1*brand = 0.9*[5,7] + 0.1*[6,0]= [5.1, 6.3]

Similarity/Attention

Embeddings



Attention mechanism is able to learn multiple embeddings for the same word in multiple sentences

How to derive similarity

- **Apple** in two sentences:
  - Sentence 1: My favorite fruit is **apple**
  - Sentence 2: My favorite brand is **apple**
- Why we move apple to fruit in sentence 1? Instead of other words as “my” and “is”
- It is based on the similarity!
- Assume every word has its own base vector (as word2vec), the contextualized word embedding of **apple** in the sentence: my favorite fruit is apple

= Attention(apple, my)*base_vec(my) + Attention(apple, favorite)*base_vec(favorite) + Attention(apple, fruit)*base_vec(fruit) + Attention(apple, is)*base_vec(is) + Attention(apple, apple)*base_vec(apple)

Target word **Context word**

How to derive similarity

- Via embeddings, the similarity between two irrelevant words would be zero, while the similarity between the related pair would be high

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

	my	favourite	brand	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
brand	0	0	1	0	0.11
is	0	0	0	1	0
apple	0	0	0.11	0	1

How to derive similarity

- The diagonal entries are all 1
- The similarity between any irrelevant words is 0 (for simplicity)
- The similarity between apple and fruit is 0.25 while the one between apple and brand is 0.11 considering apple is used more often in the same context as fruit

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

	my	favourite	brand	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
brand	0	0	1	0	0.11
is	0	0	0	1	0
apple	0	0	0.11	0	1

How to derive similarity

- Contextualized Target Word = The sum of a product between the similarity between target word and context word * context word embeddings
- We should also normalize the similarity along the sentence (**softmax**)
- Therefore
  - my (in the sentence 1) = my
  - apple (in the sentence 1) = 0.2 * fruit + 0.8 * apple
  - apple (in the sentence 2) = ?

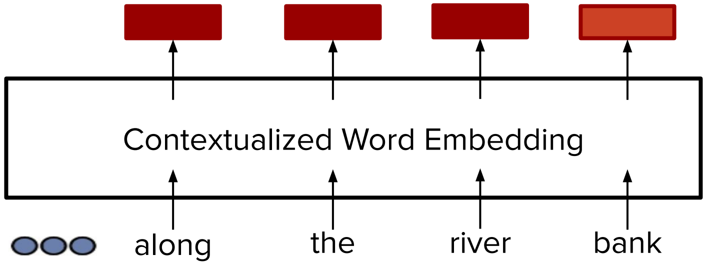
	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	0.8	0	0.2
is	0	0	0	1	0
apple	0	0	0.2	0	0.8

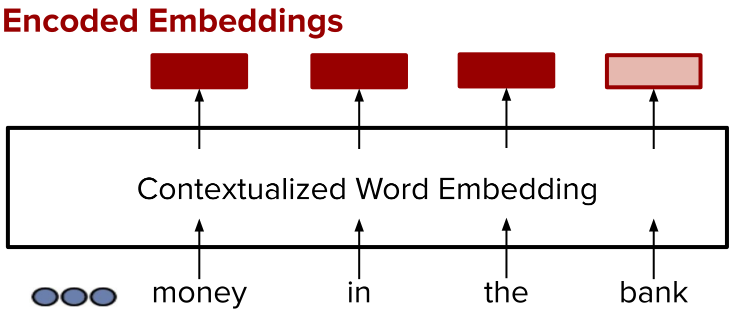
Normalized

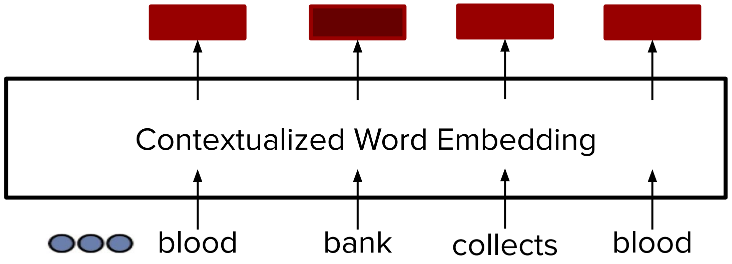
	my	favourite	brand	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
brand	0	0	0.9	0	0.1
is	0	0	0	1	0
apple	0	0	0.1	0	0.9

Contextualized Word Embeddings

- Transformers is proposed to learn better feature for NLP data
- The core layer is self-attention layer which can map a sequence of word embeddings to another sequence of word embeddings which is contextualized





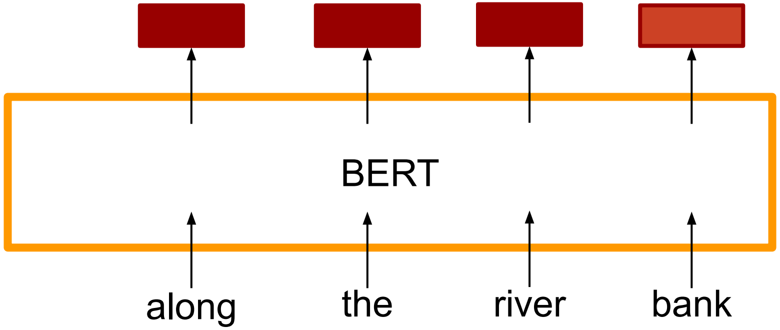


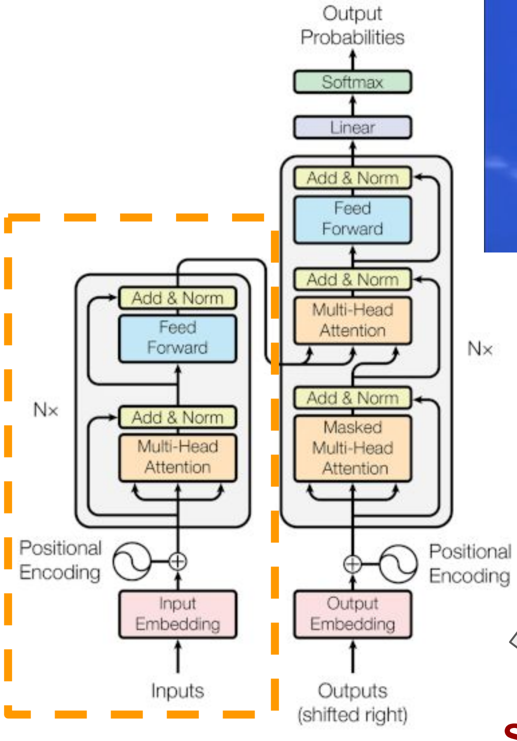
Different Contexts,
Different Encoded Embeddings for bank.

What is BERT

- **B**idirectional **E**ncoder **R**epresentations from **T**ransformers (**BERT**)
- BERT: Encoder of Transformer,

Transformer



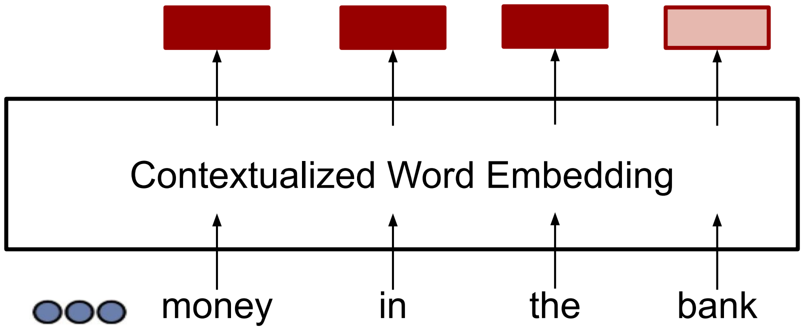


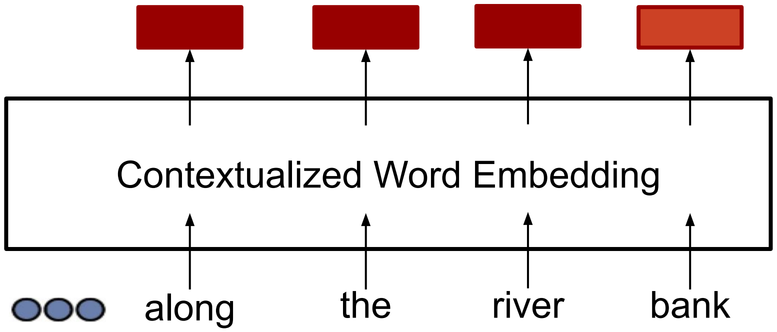
Given a sequence of words, generate a sequence of vectors and then can be used for various NLP tasks

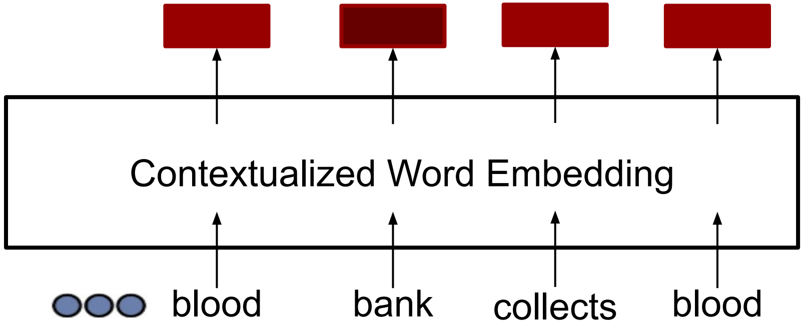
Solve Seq2Seq Task

Contextualized Word Embeddings

Encoded Embeddings





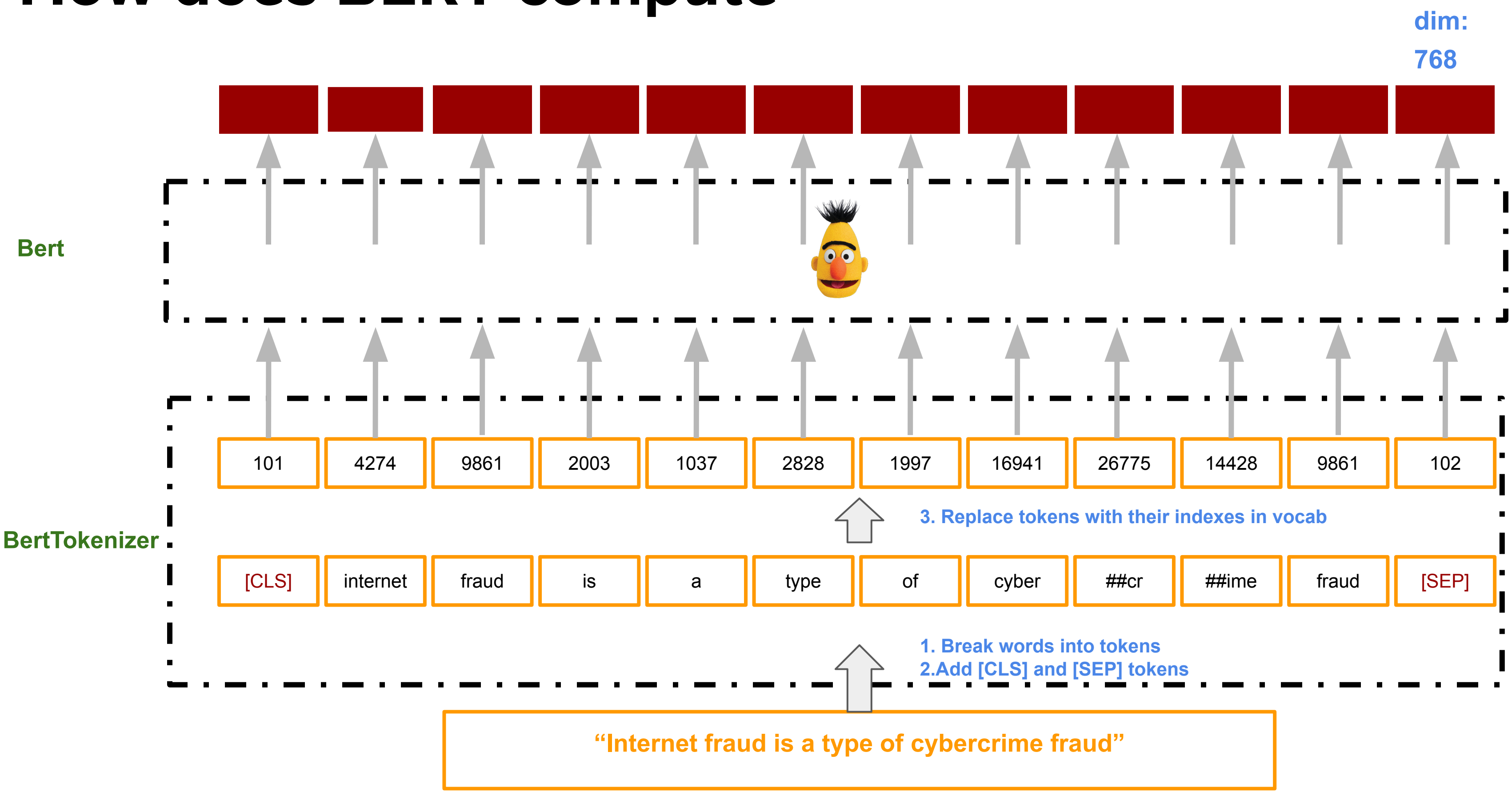


Different Contexts,
Different Encoded Embeddings for bank.

Embeddings generated from BERT

Cos-similarities among vectors of “apple” in different context

How does BERT compute



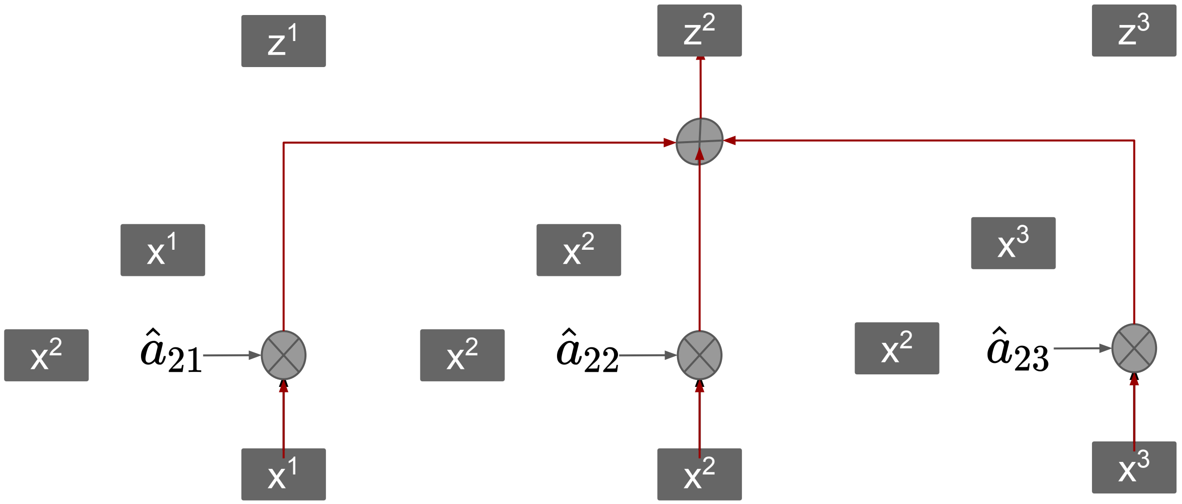
In the case of ChatGPT the generated numbers are probabilities. ChatGPT has a limited vocabulary, and the probabilities indicate how likely each vocabulary word is based on the input word sequence. ChatGPT has a limited reading range, and the input sequence has a maximum length of about 3000 words, broken into 4000 sub-word tokens. Once ChatGPT generates a word, it adds that word to the input sequence, and generates a new word. This process continues until it produces a special word called a “stop” token, or it hits a preset word limit.

Why is the reading range limited?

2.1 Self-Attention

Basic Self-Attention

- A sequence-to-sequence operation taking a sequence of vectors in and generate a sequence of vectors out
    - [x1, x2, x3] -> [z1, z2, z3]
- Relating different positions of the input sequence in order to compute the representation



$$z^i = \sum_j \hat{a}_{ij} x^j$$

$$a_{ij} = (x^i)^T (x^j)$$

$$\hat{a}_{ij} = \frac{e^{a_{ij}}}{\sum_j e^{a_{ij}}}$$

Basic Self-Attention

Sentence i: My favourite fruit is apple

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

New Word Index	Attention Step
my_i	my
favourite_i	favourite
fruit_i	0.8*fruit+0.2*apple
is_i	is
apple_i	0.2*fruit+0.8*apple

Basic Self-Attention

- There are no model parameters. It is totally determined by the embedding layer
  - Solution: introduce model parameters -> using three sets of embeddings to get contextualized embeddings
- Self attention is permutation equivariant. It ignores the order information.
  - Solution: add positional embeddings

Self-Attention layer

Step 1: Generate **query**, **key**, and **value** vector for the **input** vector at each time step.

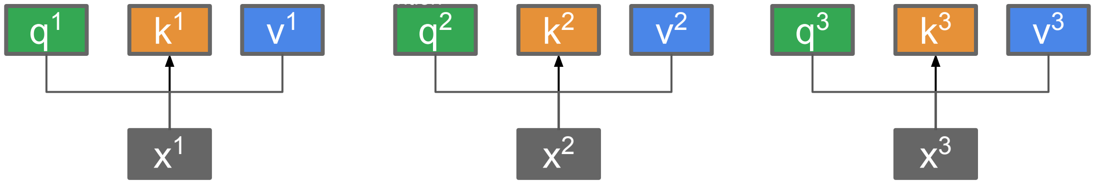
Query (to match others): $q^i = W^q x^i$

Key (to be matched): $k^i = W^k x^i$

Value (representation): $v^i = W^v x^i$

Model parameters are introduced here.

In practice, bias vectors may be added to the product of matrix multiplication



Word embeddings

264

+50

The key/value/query formulation of attention is from the paper Attention Is All You Need.

> How should one understand the queries, keys, and values

The key/value/query concept is analogous to retrieval systems. For example, when you search for videos on Youtube, the search engine will map your **query** (text in the search bar) against a set of **keys** (video title, description, etc.) associated with candidate videos in their database, then present you the best matched videos (**values**).

The attention operation can be thought of as a retrieval process as well.

As mentioned in the paper you referenced (Neural Machine Translation by Jointly Learning to Align and Translate), attention by definition is just a weighted average of values,

$$c = \sum_j \alpha_j h_j$$

where $\sum \alpha_j = 1$.

Self-Attention layer

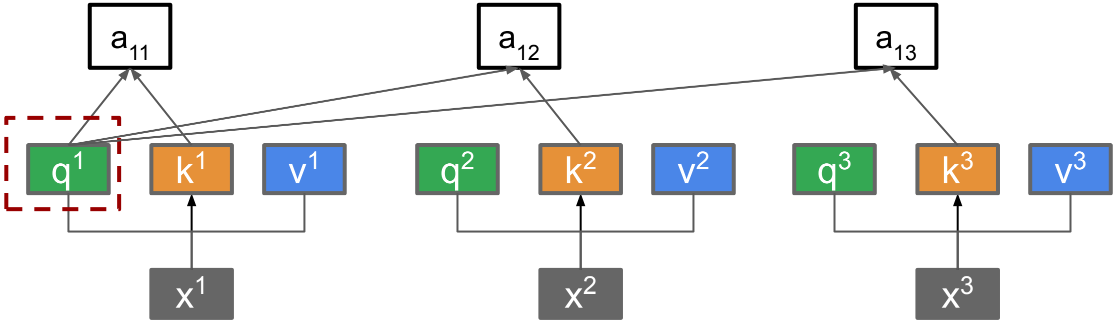
Step 2: Compute attention scores using query vectors and key vectors

To encode the i-th word in the sequence, we need to compute the attention scores between this i-th word and all the words in the sequence.

1. Pick the query vector from the i-th word: q^i
2. Attention score computation between q^i and all key vectors of the nearby words (including the target word itself)

$$a_{i,j} = \frac{q^i \cdot {k^j}^T}{\sqrt{d_k}}$$

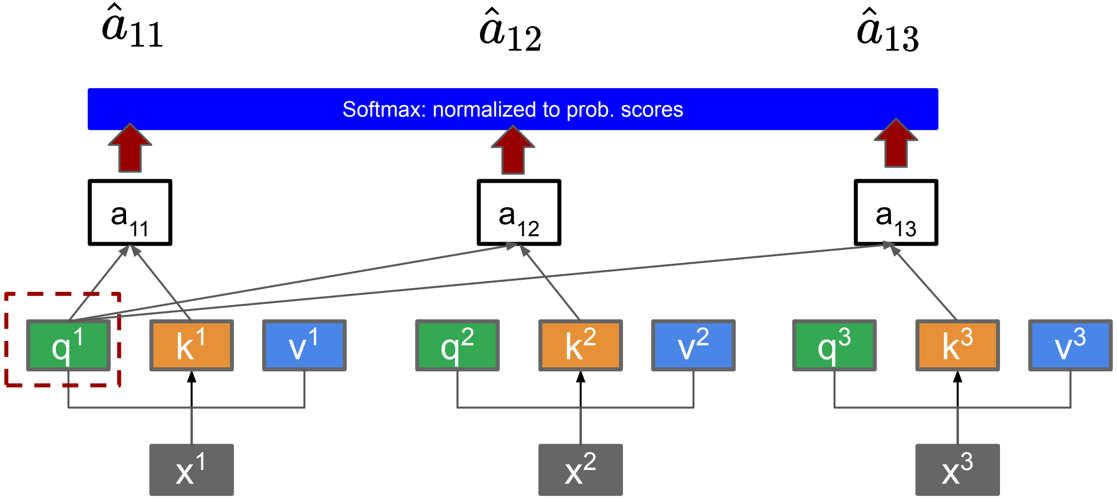
Dim of key vectors



Word vectors

Self-Attention layer

Step 3: Fed unscaled attention scores into softmax layers $\hat{a}_{1i} = \frac{e^{a_{1i}}}{\sum_j e^{a_{1j}}}$



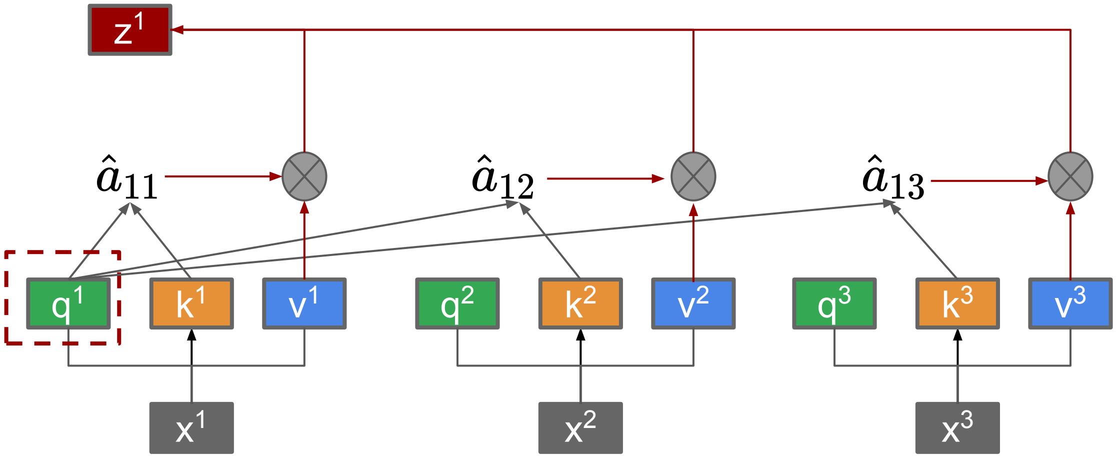
Word vectors

Self-Attention layer

Step 4: Take the sum of all the value vectors weighted by the attention scores.

Encoded vector for the first element

$$z^1 = \sum_i \hat{a}_{1i} v^i$$



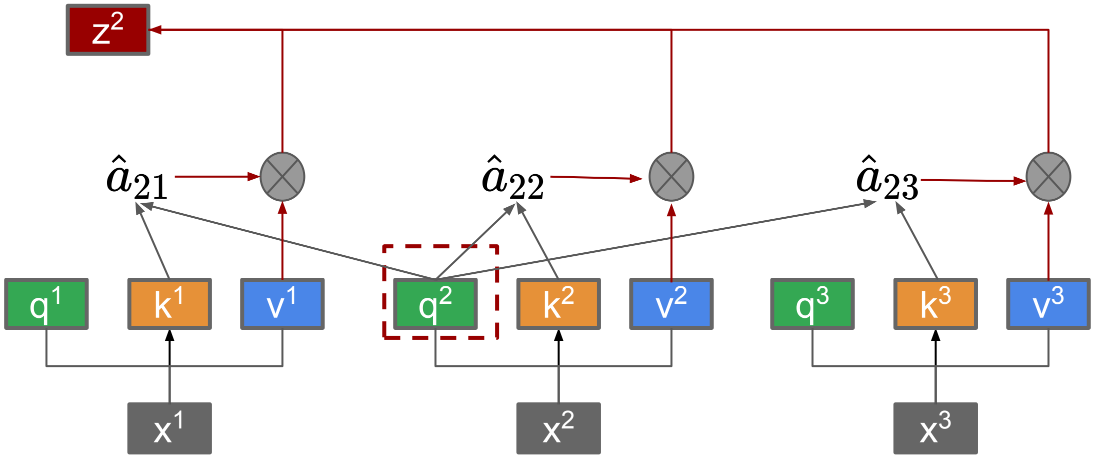
Word vectors

Self-Attention layer

Step 5: All elements in input sequence x^i will be encoded into new vectors z^i

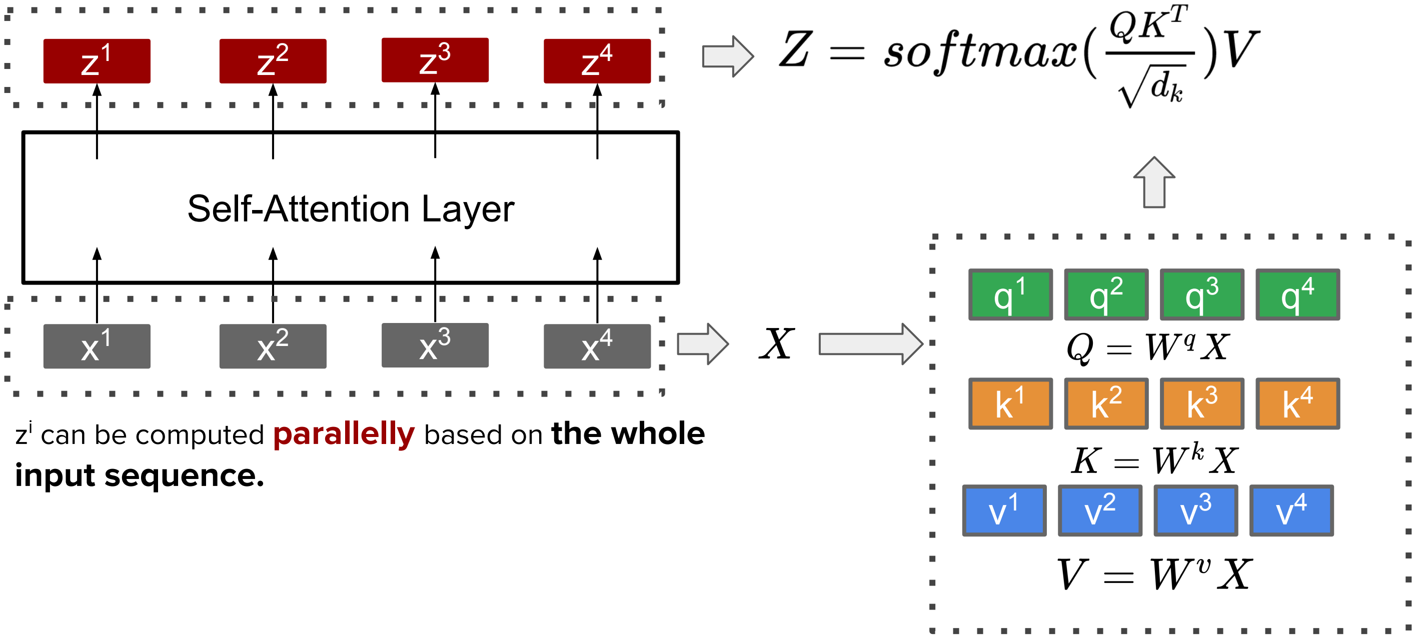
Encoded vector for the second element

$$z^2 = \sum_i \hat{a}_{2i} v^i$$



Word vectors

Matrix formulation



Matrix Multiplication

z^i can be computed **parallelly** based on **the whole input sequence.**

Which token should have high attention from “it”?

The animal didn’t cross the street because **it** was too tired.

Multi-head Self-Attention

- Model parameters: W^k, W^q, W^v specific one kind of attention
- We can have multiple set of W^k, W^q, W^v

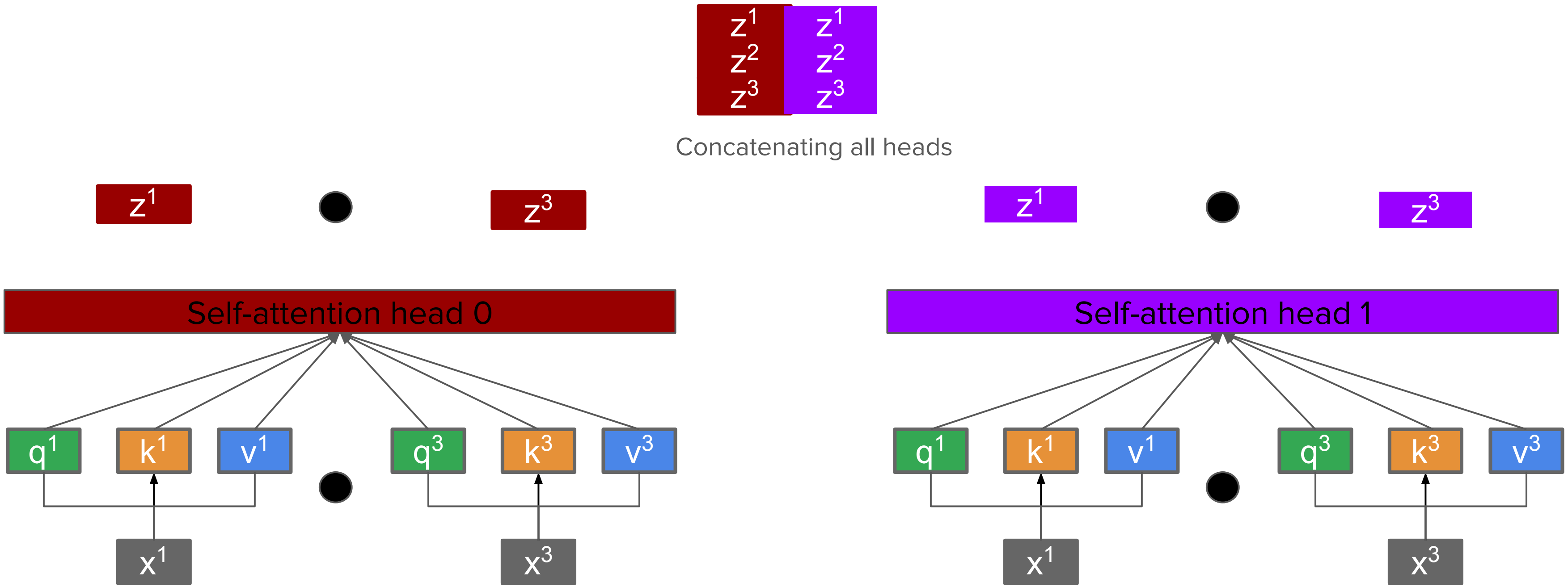
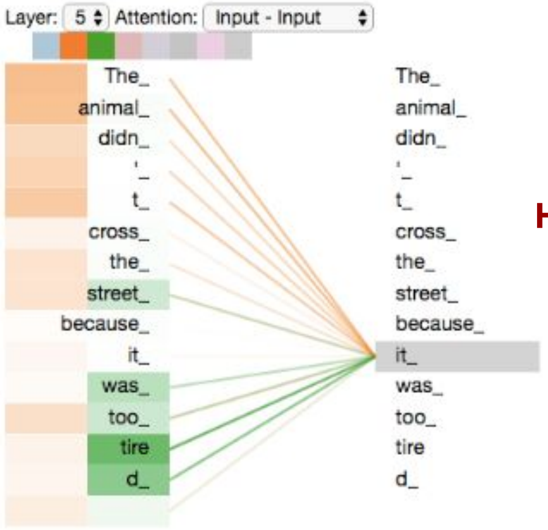


Illustration of Self-Attention

- Multi-head means separate W^k, W^q, W^v matrices
  - Expands the model's ability to focus on different positions
  - Gives the attention layer multiple "representation subspaces"
  - For example, two-head self-attention

High attention from one head



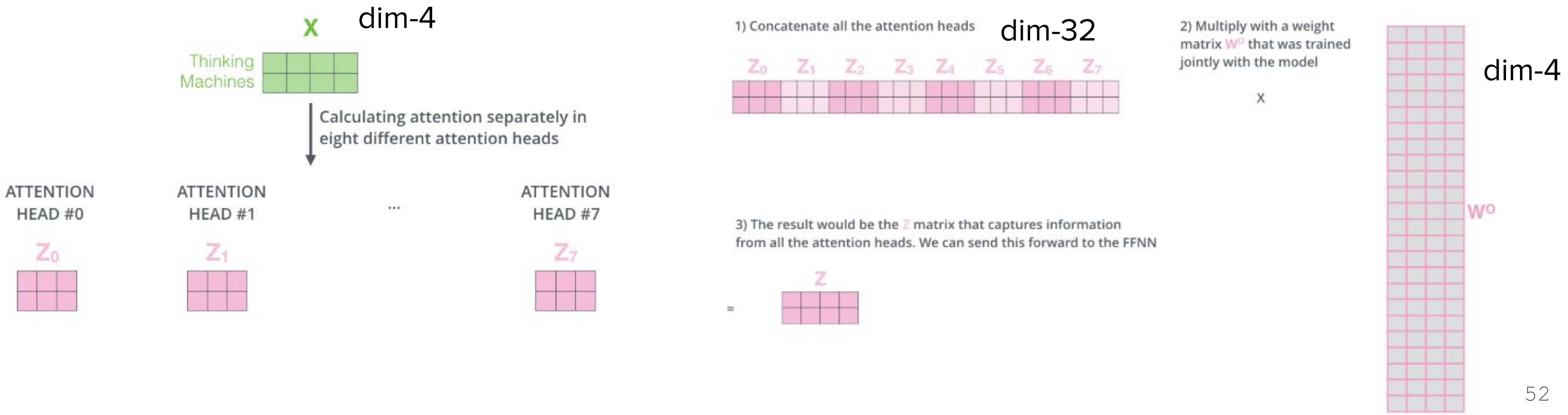
High attention from another head

Head here is similar to

1. **the filter in convolutional layer**
2. **the neuron in fully-connected layer**

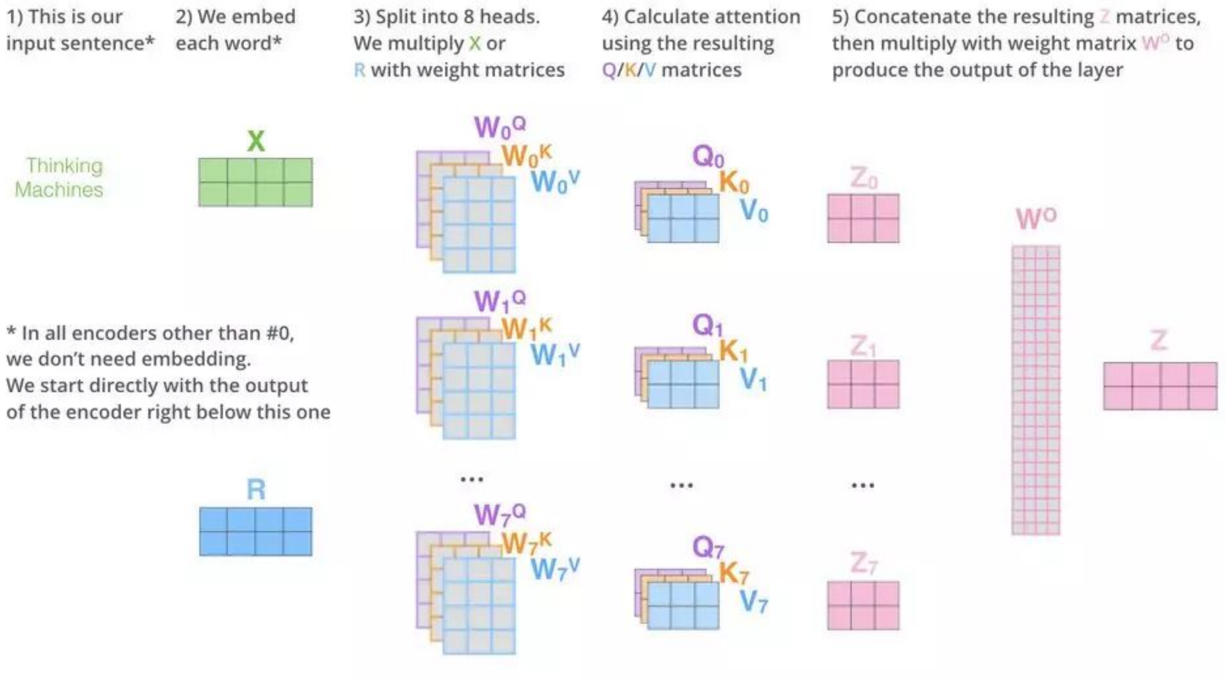
Multi-head Self-Attention

- If the layer has k heads, the output would be k sets of embeddings
  - ML models do not like high-dimensionality!
- We need to reduce the dimensionality by concatenating and projection into the low dimensional
  - One more projection matrix is introduced here
  - For example, as below: 4->32->4



Self-attention layer

That's pretty much all there is to multi-headed self-attention. It's quite a handful of matrices, I realize. Let me try to put them all in one visual so we can look at them in one place



What are model parameters?

MultiHeadAttention in Keras

```
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.layers import MultiHeadAttention
```

```
target = tf.keras.Input(shape=[6, 16])

# assume it is a sentence of 6 words. Then, each word has a
```

```
layer = MultiHeadAttention(num_heads=1, key_dim=2)
output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
print(output_tensor.shape)
print(attention_scores.shape)
```

```
(None, 6, 16)
(None, 1, 6, 6)
```

```
for matrix in layer.weights:
    print(matrix.shape)
```

```
(16, 1, 2)
(1, 2)
(16, 1, 2)
(1, 2)
(16, 1, 2)
(1, 2)
(1, 2, 16)
(16,)
```

MultiHeadAttention in Keras

```
layer = MultiHeadAttention(num_heads=3, key_dim=2)
target = tf.keras.Input(shape=[6, 16])
output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
print(output_tensor.shape)
print(attention_scores.shape)
```

```
(None, 6, 16)
(None, 3, 6, 6)
```

```
for matrix in layer.weights:
    print(matrix.shape)
```

```
(16, 3, 2)
(3, 2)
(16, 3, 2)
(3, 2)
(16, 3, 2)
(3, 2)
(3, 2, 16)
(16,)
```

MultiHeadAttention in Keras

If we change the key_dim from 2 to 5?

```
layer = MultiHeadAttention(num_heads=3, key_dim=2)
target = tf.keras.Input(shape=[6, 16])
output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
print(output_tensor.shape)
print(attention_scores.shape)
```

```
(None, 6, 16)
(None, 3, 6, 6)
```

```
for matrix in layer.weights:
    print(matrix.shape)
```

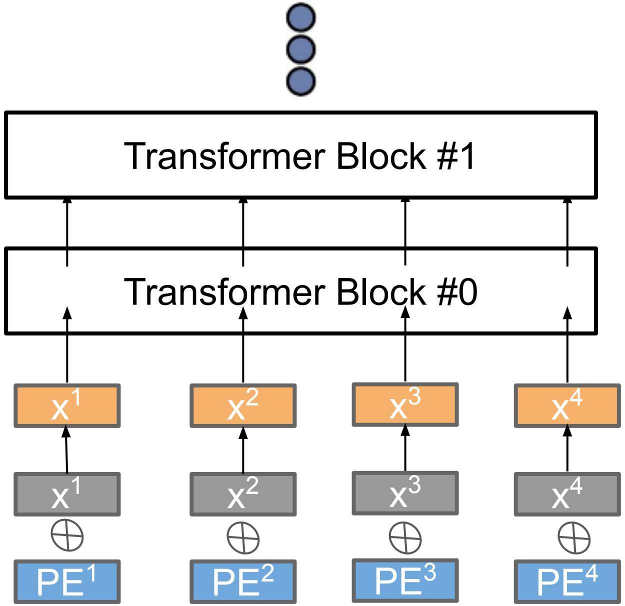
```
(16, 3, 2)
(3, 2)
(16, 3, 2)
(3, 2)
(16, 3, 2)
(3, 2)
(3, 2, 16)
(16,)
```

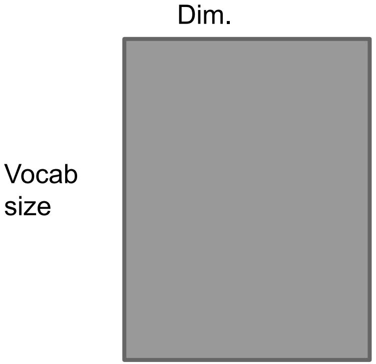
Source:
https://github.com/rz0718/BT5153_2025/blob/main/codes/lab_lecture03/Attention_Layer_in_Keras.ipynb

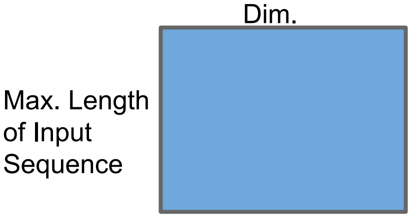
2.2 Position Embedding

Positional embeddings

- No position information in self-attention
- Positional Embeddings: each position has a unique positional vector PE(pos)
  - Add this vector to each input embeddings
  - Expands the model’s ability to focus on different positions.







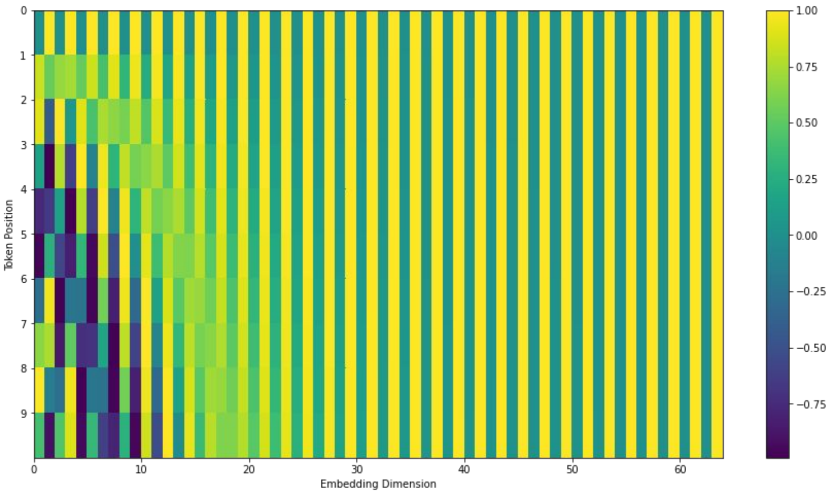
Input Embedding Matrix (Learned from the data)

Positional Embedding Matrix (Pre-defined and Fixed)

Positional embeddings

- The equation in the original paper:

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

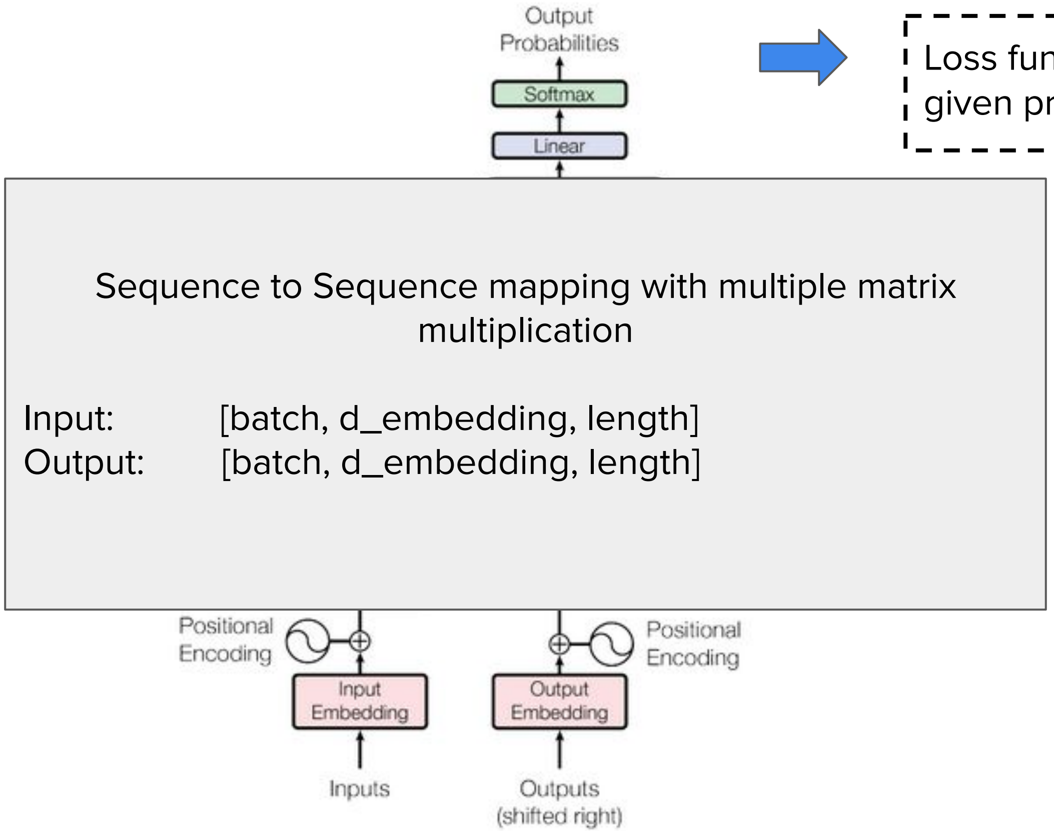


Core idea: using fixed weights which encode information related to a specific position of a token in a sentence

More details: https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

3. Summary

A “functional” viewpoint on Transformer



Loss function (predict next token given previous context)

Function parameters are updated via backpropagation.

Transformers is replacing RNN and CNN

BLOG ›

Transformer: A Novel Neural Network Architecture for Language Understanding

THURSDAY, AUGUST 31, 2017

Posted by Jakob Uszkoreit, Software Engineer, Natural Language Understanding

Source: https://blog.research.google/2017/08/transformer-novel-neural-network.html

- Compared to Transformers, RNN
  - can not be trained in parallel
  - suffers from long dependency issues
- Compared to Transformers, CNN
  - is unable to capture all possible combinations of words (filter size is predefined)
- Compared to the previous NN, Transformers
  - **Non sequential**: the input sequence are processed as a whole
  - **Self Attention**: contextualized word embeddings
  - **Positional embeddings**: a better way than recurrence to capture order information
- Podcast about transformers
  - https://www.youtube.com/watch?v=9uw3F6rndnA

Must Read !!

The illustrated transformer (the source of the awesome visualizations)

Implementations of Transformers

- Build Transformer from Scratch
- We can import it from huggingface

Next Class: LLM Fundamentals

Appendix

Masked Self-Attention

Masked Self-Attention

- This is the attention layer used to compute the dependency among the target words
- Since the sequence is generated word by word, we need to prevent it from conditioning to the future tokens
- For example:
    - to generate “a”, we should not have access to “student”

Target Self Attention Score

	I	am	a	student
I	0.7	0.1	0.1	0.1
am	0.1	0.6	0.2	0.1
a	0.1	0.3	0.6	0.1
student	0.1	0.3	0.3	0.3

+

Look-ahead Bias

	I	am	a	student
I	0	-inf	-inf	-inf
am	0	0	-inf	-inf
a	0	0	0	-inf
student	0	0	0	0

=

Masked Self Attention Score

	I	am	a	student
I	0.7	-inf	-inf	-inf
am	0.1	0.6	-inf	-inf
a	0.1	0.3	0.6	-inf
student	0.1	0.3	0.3	0.3

Masked Self-Attention

- Add look-ahead mask matrix
- Apply softmax to get the probabilistic scores
  - The negative infinities would become zero after softmax
  - For example, the attention score for “a”
    - has values for itself and all words before it
    - Zero for the word “student”

Masked Self Attention Score

	I	am	a	student
I	0.7	-inf	-inf	-inf
am	0.1	0.6	-inf	-inf
a	0.1	0.3	0.6	-inf
student	0.1	0.3	0.3	0.3

softmax

Normalized Masked Self-Attention Scores

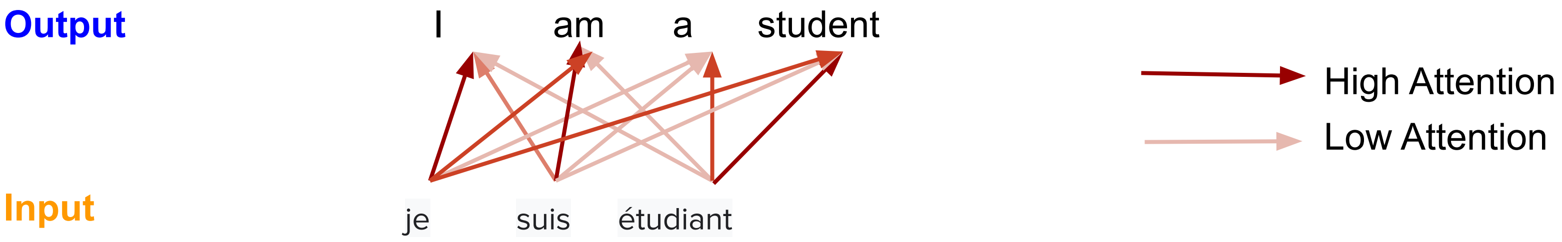
	I	am	a	student
I	1	0	0	0
am	0.37	0.62	0	0
a	0.26	0.3	0.43	0
student	0.21	0.26	0.26	0.26

Encoder-decoder Attention

Encoder-decoder attention

Attention in decoder layer:

1. Attention vectors: a vector of importance weights (measure the interaction between each target word with each input word)



2. The target is approximated by the sum of their input values weighted by the attention scores.

$$Vec_{student}=0.15*Vec_{je} + 0.05*Vec_{suis} + 0.8*Vec_{etudiant}$$

Encoder-Decoder attention layer

Different from Self attention layer

1. Generate **query** vector for the generated output sequence (from itself: Decoder)
2. Generate **key** and **value** vector for the **input** sequence at each time step (from Encoder)

Self Attention Score n

	je	suis	eludient
je			
suis			
eludient			

Encoder-decoder Attention Score

	I	am	a	student
je				
suis				
eludient				

Matrix formulation