

Master in Data Science

Mining Unstructured Data 12. RNN & LLM and LLM-based Assistants

Sequence-to-sequence Models

Attention

The Transformer



Outline

1 Sequence-to-sequence Models

- Introduction
- Neural Machine Translation
- Strengths and Limitations

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- Attention Types
- Advantages of Attention

3 The Transformer

- Issues with RNNs
- The Transformer Model
- Self-Attention
- Positional Encoding
- The attention block, Training Tricks
- Masked Attention
- Encoder-Decoder Attention

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Sequence-to-Sequence Tasks

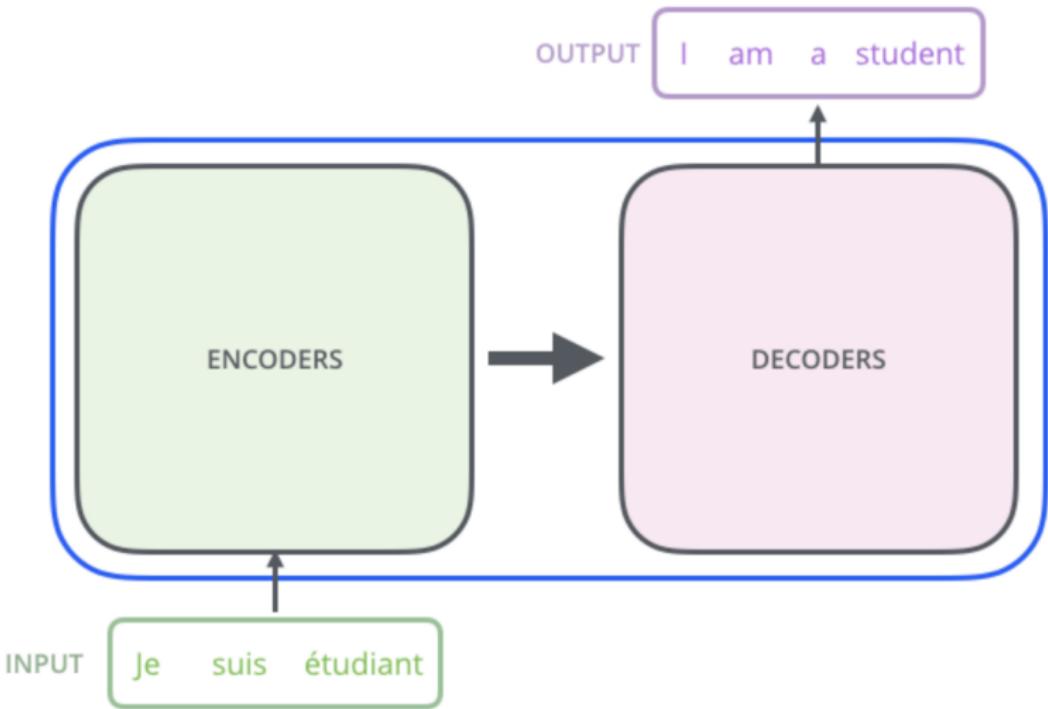
Many NLP tasks can be phrased as sequence-to-sequence:

- Summarization (long text → short text)
- Dialogue (previous utterances → next utterance)
- Parsing (input text → output parse as sequence)
- Code generation (Natural Language → Python Code)
- Translation (source sentence → translation)



se la summarizaton e' solo tieni o non
tieni questa frase potrebbe non essere
necessario usare seq-to-seq model

Sequence-to-Sequence Model



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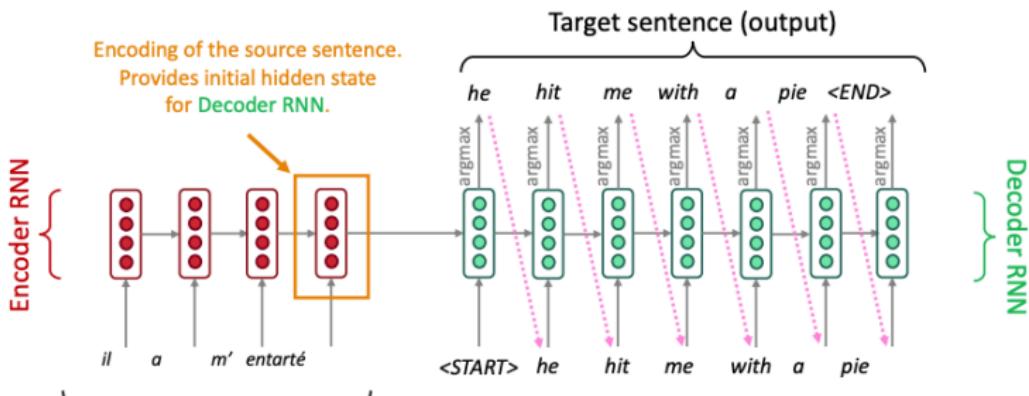
Sequence-to-Sequence Model

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Encoder RNN produces an **encoding** of the source sentence.

Decoder RNN is a Language Model that generates target sentence, *conditioned on encoding*.

Note: This diagram shows test time behavior: decoder output is fed in as next step's input

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Neural Machine Translation

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Neural Machine Translation

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- The sequence-to-sequence model is an example of a Conditional Language Model.
- Language Model because the decoder is predicting the next word of the target sentence y .
- Conditional because its predictions are also conditioned on the source sentence x .

$$p(y|x) = \prod_{t=1}^{T_y} p(y_t|y_{<t}, x)$$

- NMT computes the conditional probability distribution $p(y|x)$.
- We train these models with a parallel corpus.

Teacher Forcing

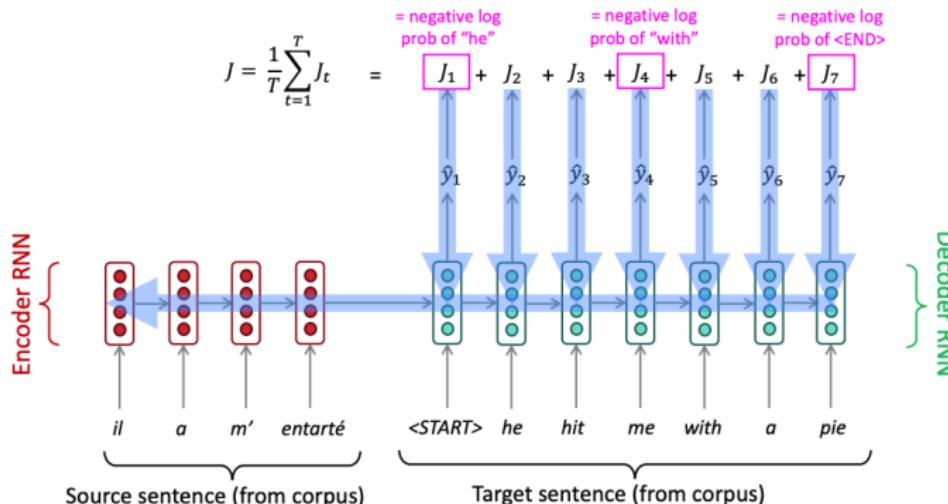
Sequence-to-sequence Models

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- During training, we use a technique called teacher forcing:
 - We feed the network the correct target sequence as input for each time step, rather than the predicted output from the previous time step
 - This helps to stabilize the training process and improve the quality of the final translation



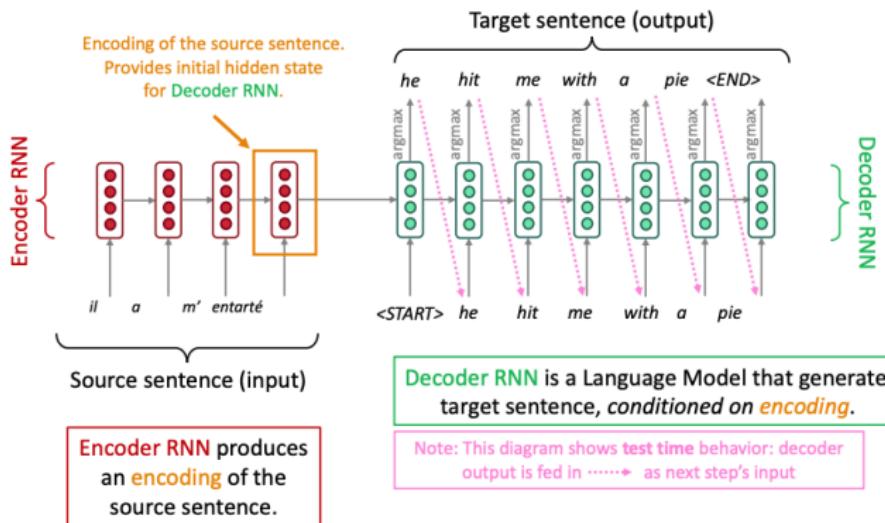
Greedy Decoding

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- During inference, we use a technique called greedy decoding:
 - At each time step, we choose the word with the highest probability as the next output word
 - This can lead to suboptimal translations, as the network may get stuck in local optima



Exhaustive Search Decoding

- To find the optimal translation, we could track all possible sequences
- This means that on each step t , we track possible partial translations, where V is the vocabulary size
- However, this complexity is too expensive

$$\arg \max_y P(y|x) = \arg \max_y \prod_{t=1}^{|y|} P(y_t|y_{<t}, x)$$

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Beam Search Decoding

- Beam search is a more efficient decoding algorithm than exhaustive search
- On each step of the decoder, we keep track of the k most probable partial translations (which we call hypotheses)
- Each hypothesis has a score, its log probability
- We search for high-scoring hypotheses, tracking top k on each step
- Beam search doesn't guarantee an optimal solution, but is more efficient than exhaustive search

$$\text{score}(y_{1:t}) = \sum_{i=1}^t \log P(y_i | y_{<i}, x)$$

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Beam Search Decoding (k=2)

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<START>

Calculate prob
dist of next word

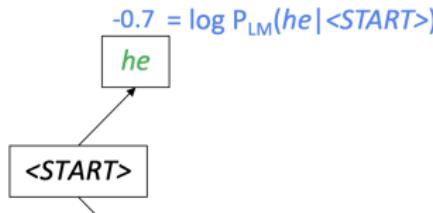
Beam Search Decoding (k=2)

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$$-0.7 = \log P_{LM}(he | <START>)$$

$$-0.9 = \log P_{LM}(I | <START>)$$

Take top k words
and compute scores

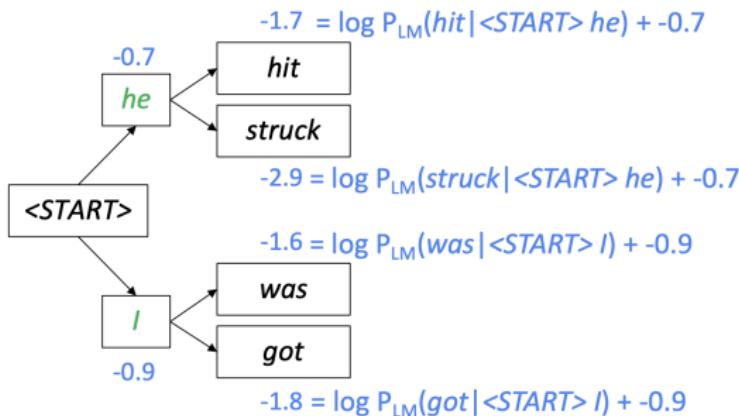
Beam Search Decoding (k=2)

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For each of the k hypotheses, find top k next words and calculate scores

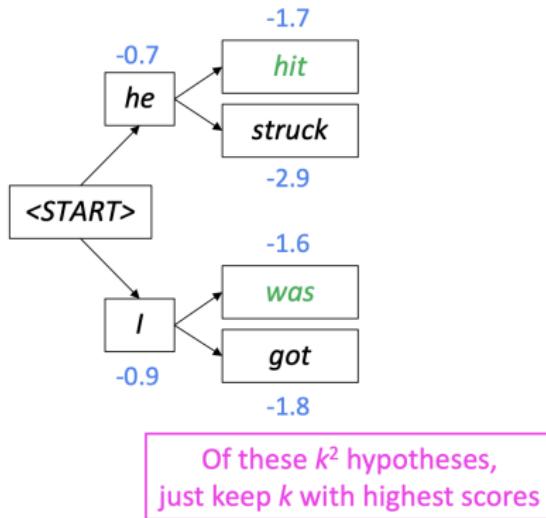
Beam Search Decoding (k=2)

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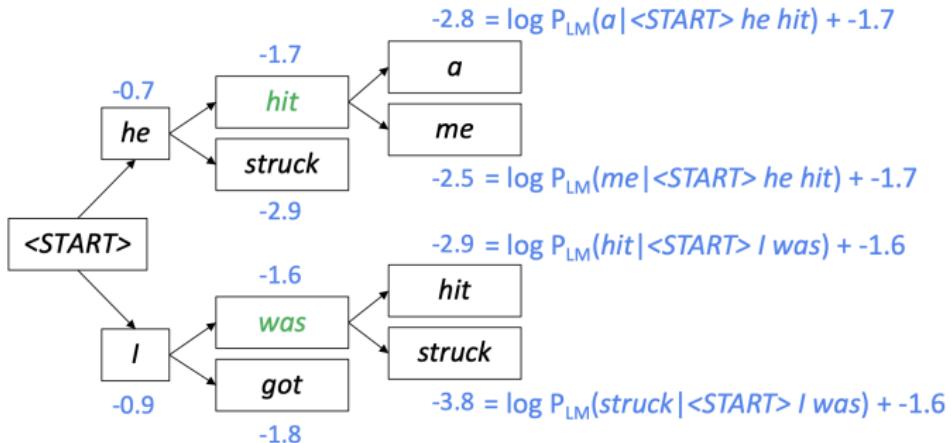
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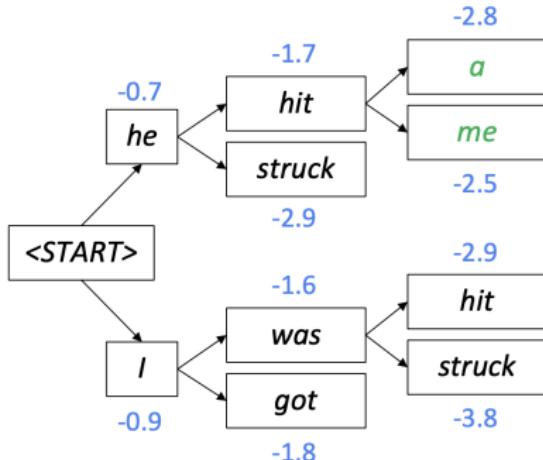
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For each of the k hypotheses, find
top k next words and calculate scores

Beam Search Decoding (k=2)

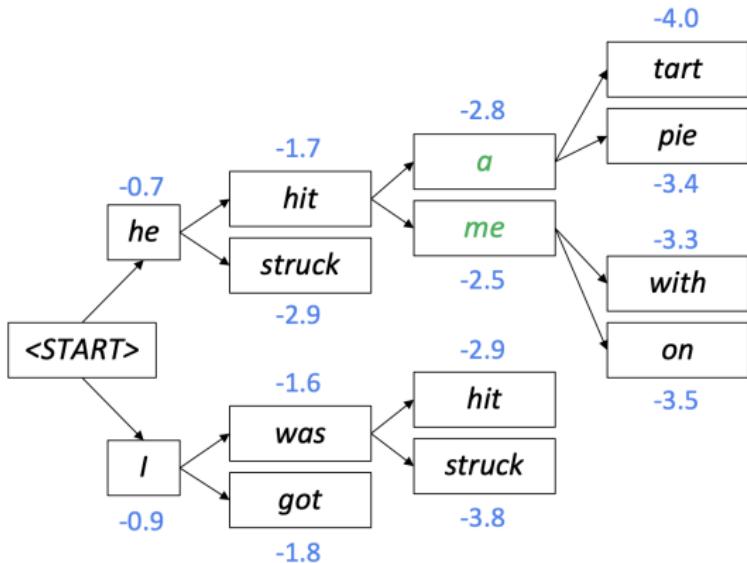
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Of these k^2 hypotheses,
just keep k with highest scores

Beam Search Decoding (k=2)

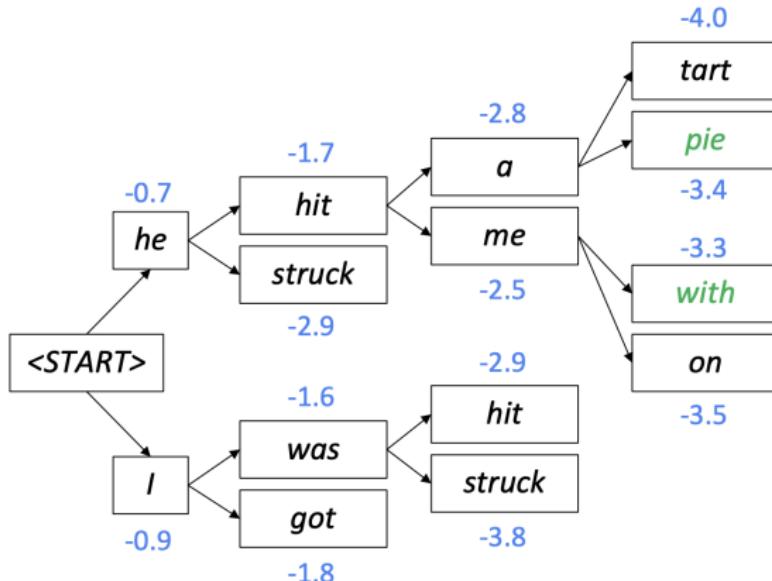
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For each of the k hypotheses, find top k next words and calculate scores

Beam Search Decoding (k=2)

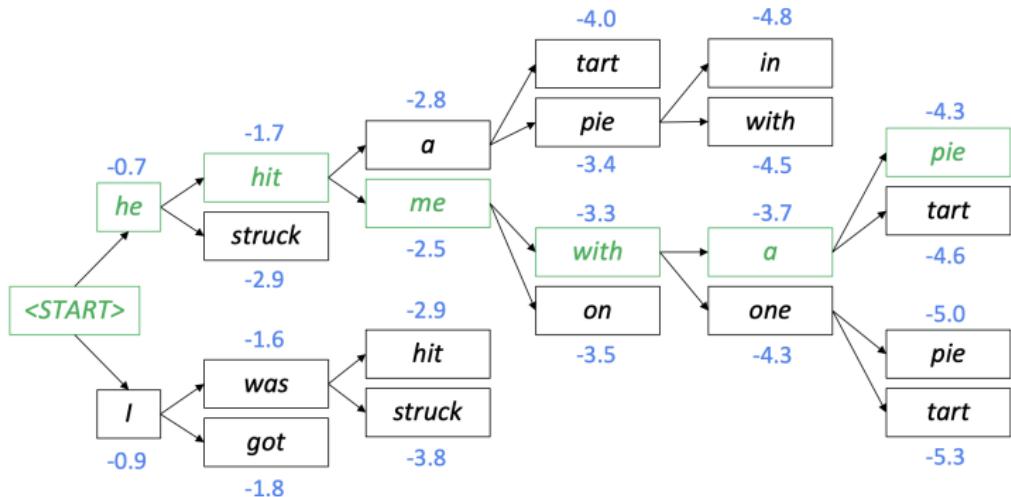
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Of these k^2 hypotheses,
just keep k with highest scores

Beam Search Decoding (k=2)

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Backtrack to obtain the full hypothesis

Beam Search Decoding - Stopping Criterion

- In greedy decoding, usually we decode until the model produces an **END** token:
 - **START** he hit me with a pie **END**
- In beam search decoding, different hypotheses may produce tokens on different timesteps.
- When a hypothesis produces **END**, that hypothesis is complete.
- Place it aside and continue exploring other hypotheses via beam search.
- Usually we continue beam search until:
 - We reach timestep T (where T is some pre-defined cutoff), or
 - We have at least n completed hypotheses (where n is pre-defined cutoff).

Beam Search Decoding - Selecting the Best Hypothesis

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- Each hypothesis in our list of hypotheses has a score.
- Problem with this: longer hypotheses have lower scores.
- Fix: Normalize by length. Use this to select top one instead:

$$\hat{y} = \arg \max_{y \in \mathcal{Y}} \frac{1}{|y|^\alpha} \log p(y|x) \quad (1)$$

- More negative terms are added for longer hypotheses.

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About the Success of NMT

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Neural Machine Translation went from a fringe research attempt in 2014 to the leading standard method in 2016.

- 2014: First seq2seq paper published.
- 2016: Google Translate switches from SMT to NMT
- 2018+: Transformers have become the dominant architecture for NMT. Examples include:
 - BART (Facebook AI Research) (2019)
 - T5 (Google AI) (2020)
 - UNILM (Microsoft Research Asia) (2020)

NMT is far from solved

NMT picks up biases in training data

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Malay - detected ▾

English ▾

Dia bekerja sebagai jururawat.

Dia bekerja sebagai pengaturcara. Edit

She works as a nurse.

He works as a programmer.

Didn't specify gender

NMT is far from solved (II)

Hard to interpret systems do strange things

Somali ▾
Translate from Irish

↔

English ▾

ag
ag ag ag ag ag ag ag ag ag ag ag ag ag ag
ag Edit

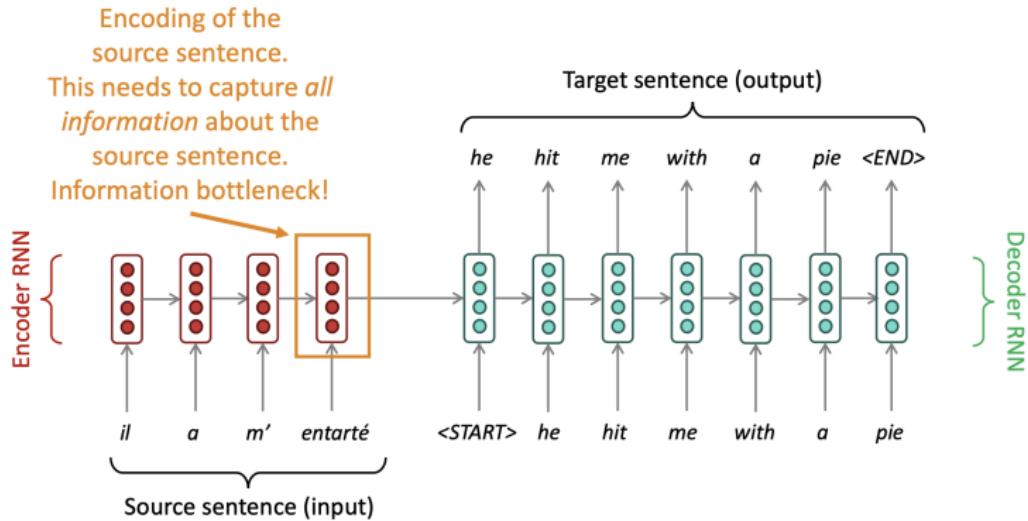
As the name of the LORD was written
in the Hebrew language, it was written
in the language of the Hebrew Nation

Open in Google Translate Feedback

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Sequence-to-sequence: the bottleneck problem

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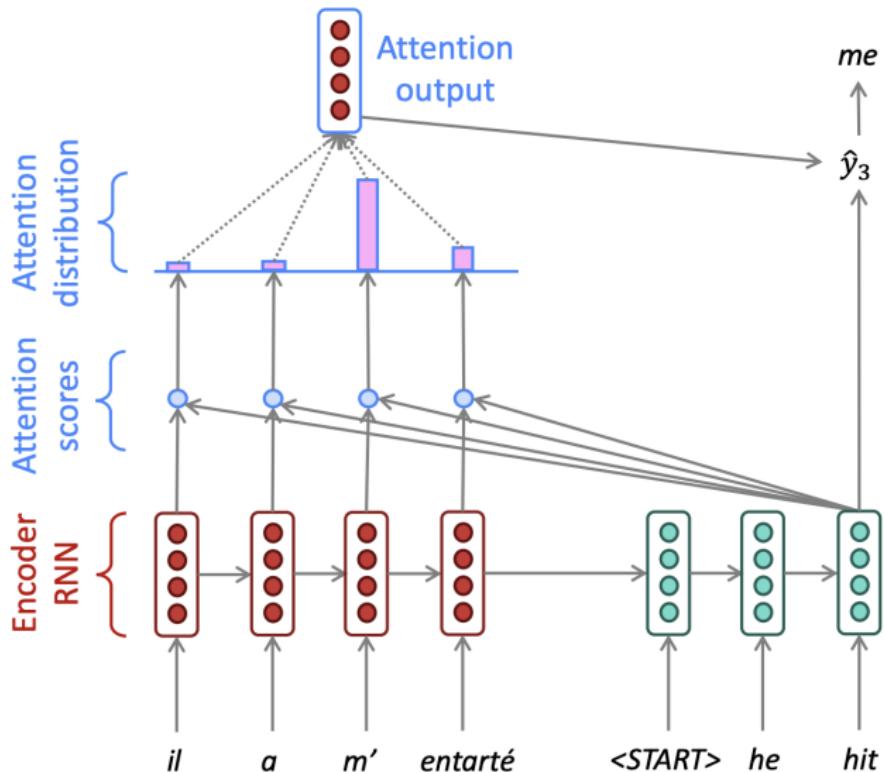
- Attention provides a solution to the bottleneck problem.
- **Core idea:** on each step of the decoder, use direct connection to the encoder to focus on a particular part of the source sequence

Attention (II)

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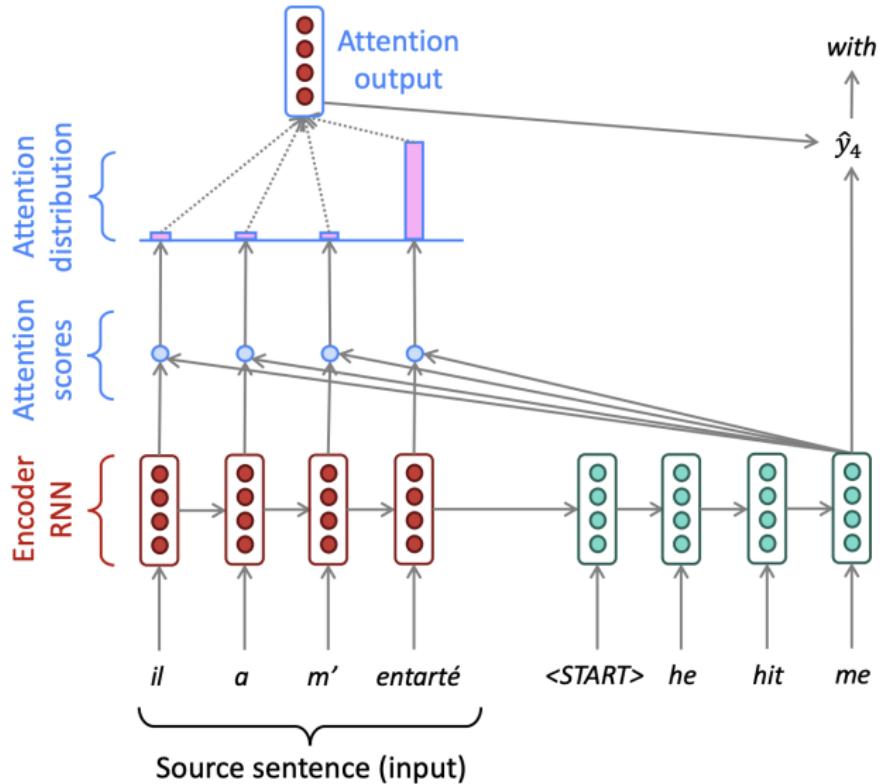


Attention (III)

Sequence-to-sequence Models

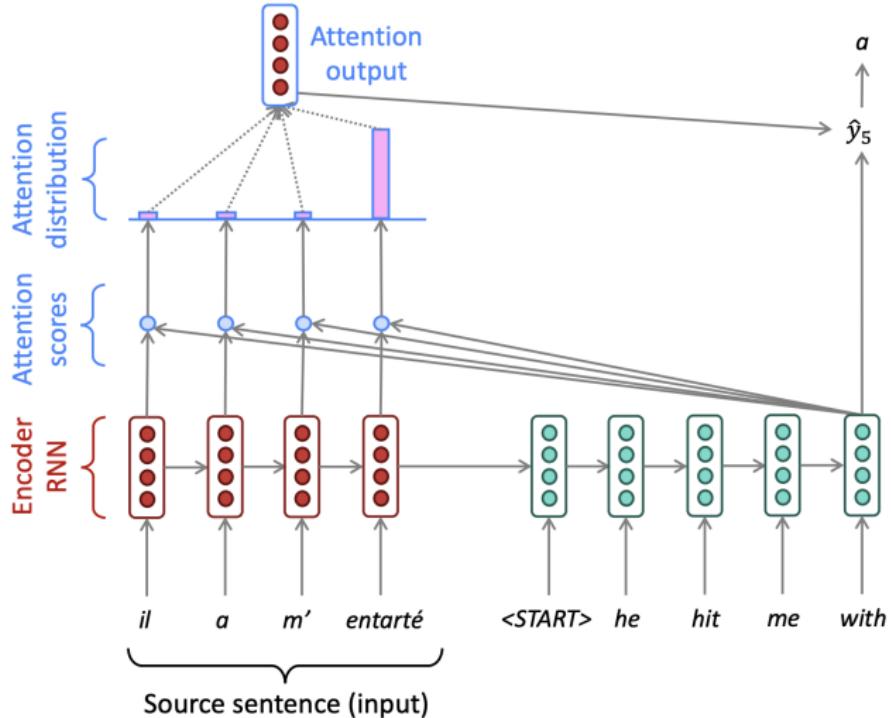
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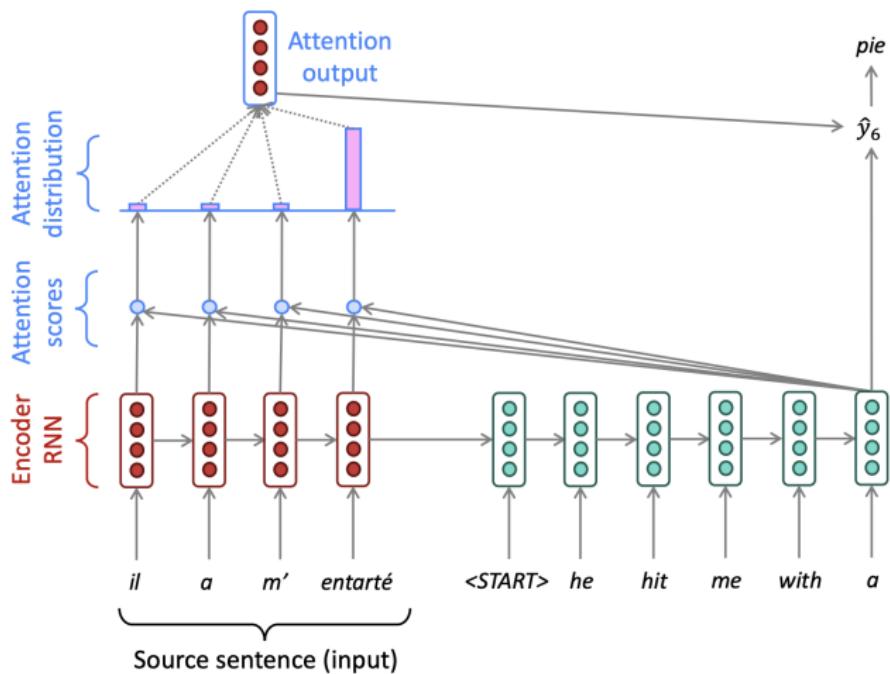
Attention (IV)

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Attention (V)

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Basic Attention (with no parameters)

Suppose we have a sequence of n items, represented as x_1, x_2, \dots, x_n , and we want to compute the attention weights for each item based on a query q .

$$s_i = x_i^T q$$

$$w_i = \frac{\exp(s_i)}{\sum_{j=1}^n \exp(s_j)}$$

$$\text{Attention}(q, x_1, x_2, \dots, x_n) = \sum_{i=1}^n w_i x_i$$

This gives us a weighted representation of the sequence based on the query. Note that the attention weights are computed based solely on the query and the representations of the items, with **no learned parameters**.

Generalization of Attention

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- We can use attention in many architectures (not just seq2seq) and many tasks (not just MT)
- General definition of attention:
 - Given a set of vector **values** and **keys**, and a vector **query**, attention is a technique to compute a weighted sum of the values, dependent on the query and keys.
- Intuition:
 - The weighted sum is a selective summary of the information contained in the values, where the query and keys determine which values to focus on.
 - Attention is a way to obtain a **fixed-size** representation of an arbitrary set of representations (the values), dependent on some other representation (the query).

Generalised Dot-Product Attention Formulas

In the dot-product attention mechanism, we compute the attention weights as follows:

$$\text{Attention}(Q, K, V) = \text{softmax} \left(\frac{QK^T}{\sqrt{d_k}} \right) V,$$

where Q , K , and V are the query, key, and value matrices, respectively, and d_k is the dimensionality of the key vectors.

- Q is of size (batch size $\times n_q \times d_k$)
- K is of size (batch size $\times n_k \times d_k$)
- V is of size (batch size $\times n_k \times d_v$)

Here, n_q and n_k denote the number of queries and keys, respectively, and d_v is the dimensionality of the value vectors.

Generalised Dot-Product Attention Formulas (II)

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We can also write the attention function as a weighted sum of the value vectors, where the attention weights are given by the dot product of the query and key vectors:

$$\text{Attention}(Q, K, V) = \sum_{i=1}^{n_k} \alpha_i v_i,$$

where $\alpha_i = \frac{\exp(qk_i/\sqrt{d_k})}{\sum_{j=1}^{n_k} \exp(qk_j/\sqrt{d_k})}$ is the attention weight for the i -th key, and v_i is the corresponding value vector.

Generalised Attention Formulas

- We can generalise to other attention models:

$$\alpha_i = \text{softmax}(\text{score}(q, h_i))$$

- score is a function that computes the similarity between the query vector and each input vector. Common choices for the score are:
 - Dot product: $\text{score}(q, h_i) = q^T h_i$
 - Scaled dot product: $\text{score}(q, h_i) = \frac{q^T h_i}{\sqrt{d}}$
 - General: $\text{score}(q, h_i) = q^T W h_i$
 - Concat: $\text{score}(q, h_i) = v^T \tanh(W[q; h_i])$
 - Additive: $\text{score}(q, h_i) = v^T \tanh(W_1 q + W_2 h_i)$
- Where d is the dimensionality of the query and input vectors, W and v are learned parameter matrices, and $[q; h_i]$ denotes the concatenation of the query and i -th input vector.

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Advantages of Attention

- Attention significantly improves NMT performance
- Attention provides more “human-like” model of the MT process
 - We look back at the source sentence while translating, rather than remembering it all
- **Attention solves the bottleneck problem**
 - Attention allows decoder to look directly at source; bypass bottleneck
- Attention helps with the **vanishing gradient** problem
 - Provides shortcut to faraway states
- Attention provides some interpretability
 - By inspecting attention distribution, we see what the decoder was focusing on
 - The network learns alignment by itself

Sequence-to-sequence Models

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Attention Solves the Bottleneck Problem

In a traditional seq2seq model, the decoder receives a **fixed-length vector** (the context vector) that summarizes the entire source sequence. This creates a bottleneck, as the decoder must use this one vector to generate the entire target sequence.

$$e_{i,j} = v_a^T \tanh(W_a s_{i-1} + U_a h_j)$$

$$\alpha_{i,j} = \frac{\exp(e_{i,j})}{\sum_{k=1}^n \exp(e_{i,k})}$$

$$c_i = \sum_{j=1}^n \alpha_{i,j} h_j$$

where s_{i-1} is the decoder hidden state at the previous time step, h_j is the j -th encoder hidden state, v_a , W_a , and U_a are learned parameters, and c_i is the context vector at time step i . The attention weights $\alpha_{i,j}$ determine which parts of the source sequence to focus on at each step.

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Attention Solves the Bottleneck Problem (II)

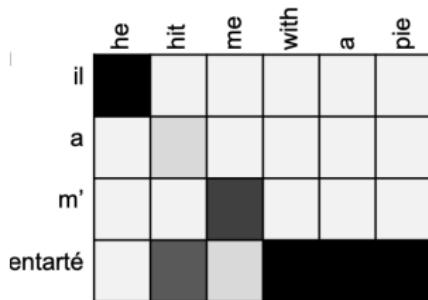
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This allows the decoder to attend to different parts of the source sequence at each step, and thus avoid the bottleneck problem.



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Issues with RNNs: Linear interaction distance

Linear locality

RNNs encode linear locality, which is useful since nearby words often affect each other's meaning.

Problem

However, RNNs take $O(\text{sequence length})$ steps for distant word pairs to interact, which makes it hard to learn long-distance dependencies due to vanishing gradients. Additionally, the meaning in sentences doesn't necessarily follow a *linear order*.

- This linear interaction distance limitation can be problematic for some NLP tasks, such as machine translation or sentiment analysis.
- This motivates the use of alternative models that can capture non-linear dependencies more effectively, such as transformers.

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Issues with RNNs

Issues with RNNs: Lack of parallelizability

Parallelizability

Forward and backward passes in RNNs have $O(\text{sequence length})$ unparallelizable operations.

- GPUs can perform a bunch of independent computations at once, which is great for speeding up training.
- However, future RNN hidden states can't be computed in full before past RNN hidden states have been computed.
- This lack of parallelizability inhibits training on very large datasets, which can be a major issue in modern NLP applications.

Solution

Transformers are highly parallelizable, allowing for much faster training on larger datasets.

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Source: <https://jalammar.github.io/illustrated-transformer/>

The Encoding and Decoding Components

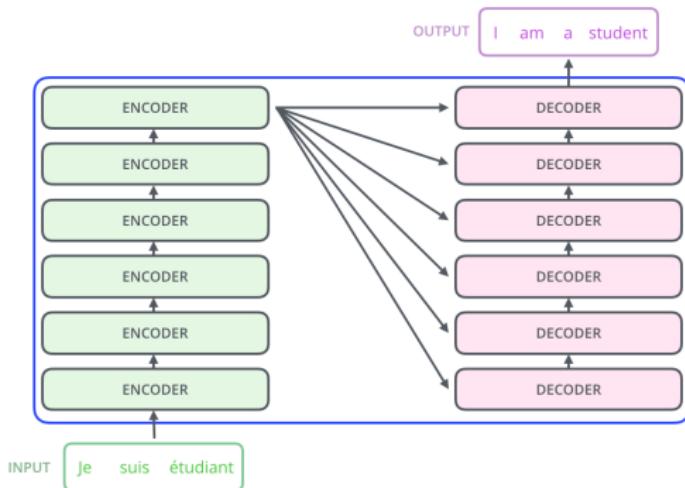
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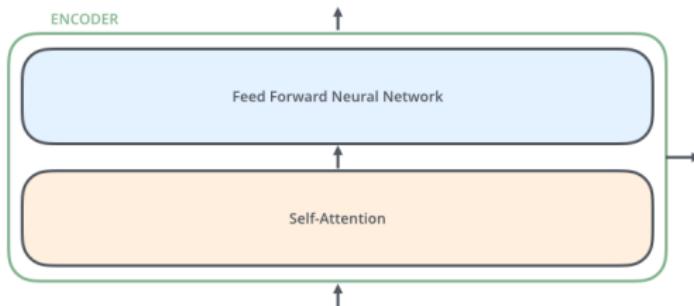
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- The Transformer consists of an encoding component, a decoding component, and connections between them.
- The encoding component is a stack of encoders, and the decoding component is a stack of decoders.
- The encoders and decoders are connected by attention layers.



The Encoder Sub-Layers

- Each encoder has two sub-layers: a self-attention layer and a feed-forward neural network.
- The self-attention layer helps the encoder look at other words in the input sentence as it encodes a specific word.
- The feed-forward network is applied independently to each position.
- The exact same structure is used for all encoders, but they do not share weights.



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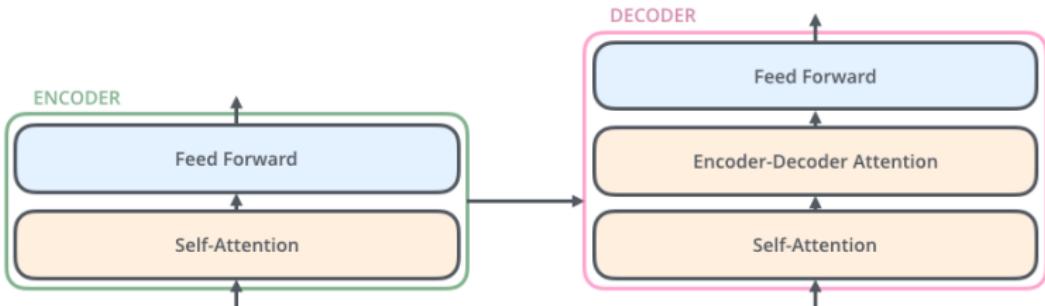
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The Decoder Sub-Layers

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- The decoder has both the self-attention and feed-forward layers, but between them is an attention layer that helps the decoder focus on relevant parts of the input sentence.
- The attention layer helps the decoder generate the output sequence.



The Input Embedding

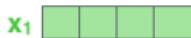
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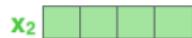
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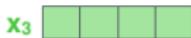
- Each input word is turned into a vector using an embedding algorithm.
- The embedding size is typically 512.
- The embedding only happens in the bottom-most encoder.
- Each encoder receives a list of vectors, the size of which is a hyperparameter we can set.



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Figure: Word embeddings for input sequence.

What is Byte Pair Encoding?

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The Transformer Model

- A simple and efficient compression algorithm that reduces the size of text data by replacing frequent pairs of bytes with a single byte.
- Originally proposed by Philip Gage in 1994 for compressing English text files.
- Later adapted for natural language processing tasks such as subword tokenization and neural machine translation.

How does Byte Pair Encoding work?

Sequence-to-sequence Models

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The Transformer Model

- 1 Initialize a vocabulary with all the unique bytes in the text data and a special end-of-word symbol (e.g. $\langle /w \rangle$).
- 2 Count the frequency of all the byte pairs in the text data.
- 3 Merge the most frequent byte pair into a new byte and add it to the vocabulary.
- 4 Repeat steps 2 and 3 until a desired vocabulary size or compression ratio is reached.
- 5 Encode the text data by replacing each byte pair with its corresponding merged byte.

Example of Byte Pair Encoding

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The Transformer Model

- Suppose we have a text data: “low lower newest widest”
- The initial vocabulary is: {"l", "o", "w", " ", "e", "r", "n", "s", "t", "i", "d", </w>}
- The most frequent byte pair is: ("e", "s")
- We merge ("e", "s") into a new byte: <es> and add it to the vocabulary.
- The new vocabulary is: {"l", "o", "w", " ", "e", "r", "n", "s", "t", "i", "d", </w>, <es>}
- The new text data is: “low lower new<es>t wid<es>t”
- We repeat this process until we get the final vocabulary and encoded text data.

The Encoding Process

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The Transformer Model

- Each word in the input sequence flows through its own path in the encoder.
- Dependencies between paths are captured in the self-attention layer.
- The same feed-forward layer weights are applied for all paths.

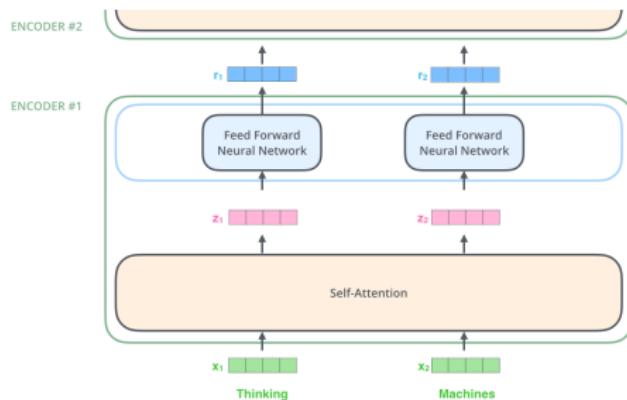


Figure: Encoding process in the Transformer.

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Self-Attention

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- Self-attention is a key component of the Transformer model that allows it to understand the context of a word in a sentence.
- It allows the model to associate a word with other relevant words in the sentence.
- For example, when processing the sentence "The animal didn't cross the street because it was too tired", self-attention helps the model understand that "it" refers to "animal".
- Self-attention works by looking at other positions in the input sequence for clues that can help lead to a better encoding for the current word.
- The Transformer uses self-attention to incorporate the representation of other relevant words into the one it is currently processing.

Self-Attention

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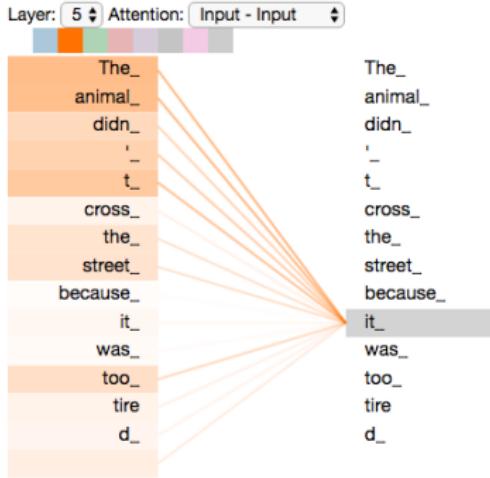


Figure: Example of self-attention in encoder #5 of the Transformer model. Part of the attention mechanism is focusing on “The Animal”, and this information is incorporated into the encoding of “it”.

Self-Attention in Detail

Sequence-to-sequence Models

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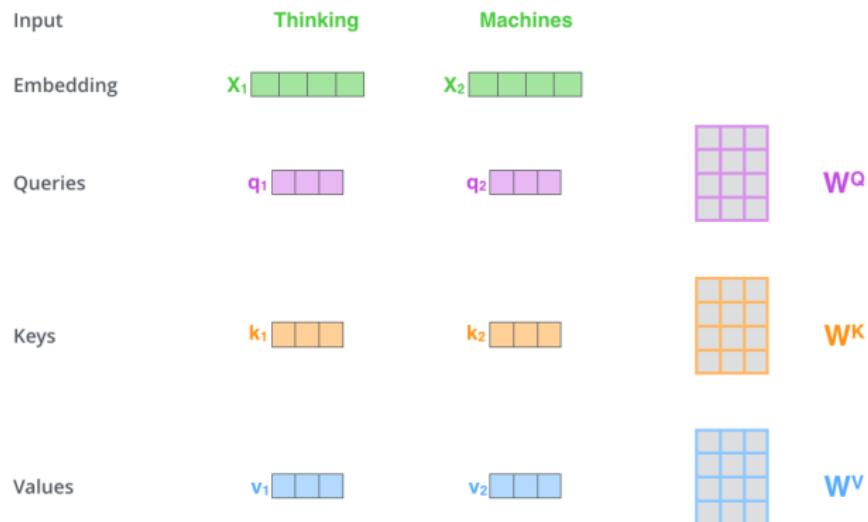
The Transformer

Self-Attention

- First step: create three vectors from each encoder's input vectors
 - Create Query, Key, and Value vectors by multiplying embedding by three matrices
 - Vectors are smaller in dimension than embedding vector (64 vs 512)

Self-Attention in Detail (I)

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Self-Attention in Detail (II)

Sequence-to-sequence Models

Attention

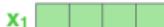
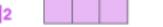
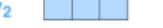
The Transformer

Self-Attention

- Second step: calculate a score for each word in the input sentence
 - Score is calculated by taking dot product of query vector with key vector of respective word
- Third step: divide scores by \sqrt{d} (scaled dot-product attention)
- Fourth step: pass through softmax operation
 - Softmax score determines how much each word will be expressed at this position

Self-Attention in Detail (II)

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| Input | Thinking | Machines |
|----------------------------|---|--|
| Embedding | x_1  | x_2  |
| Queries | q_1  | q_2  |
| Keys | k_1  | k_2  |
| Values | v_1  | v_2  |
| Score | $q_1 \cdot k_1 = 112$ | $q_1 \cdot k_2 = 96$ |
| Divide by $8 (\sqrt{d_k})$ | 14 | 12 |
| Softmax | 0.88 | 0.12 |

Self-Attention in Detail (III)

Sequence-to-sequence Models

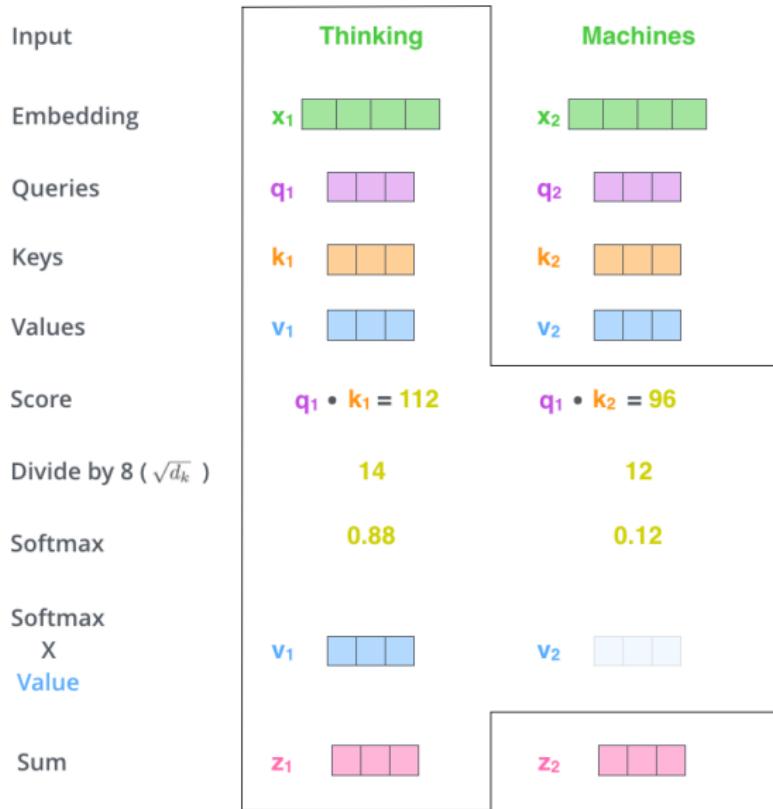
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- Fifth step: multiply each value vector by the softmax score
- Sixth step: sum up the weighted value vectors to produce output of self-attention layer
- Calculation is done in matrix form for faster processing in actual implementation

Self-Attention in Detail (III)

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Matrix Calculation of Self-Attention

Sequence-to-sequence Models
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- 1 Calculate Query, Key, and Value matrices by multiplying embedding matrix X with weight matrices WQ, WK, and WV respectively.
- 2 X matrix represents input sentence with each row representing a word and q/k/v vectors having a different size than embedding vector.
- 3 Outputs of the self-attention layer can be calculated using a single formula.

$$\begin{array}{ccc} \mathbf{X} & \times & \mathbf{W}^Q \\ \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} & \times & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ & = & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \end{array}$$
$$\begin{array}{ccc} \mathbf{X} & \times & \mathbf{W}^K \\ \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} & \times & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ & = & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \end{array}$$
$$\begin{array}{ccc} \mathbf{X} & \times & \mathbf{W}^V \\ \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} & \times & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ & = & \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \end{matrix} \end{array}$$

Multi-Head Self-Attention

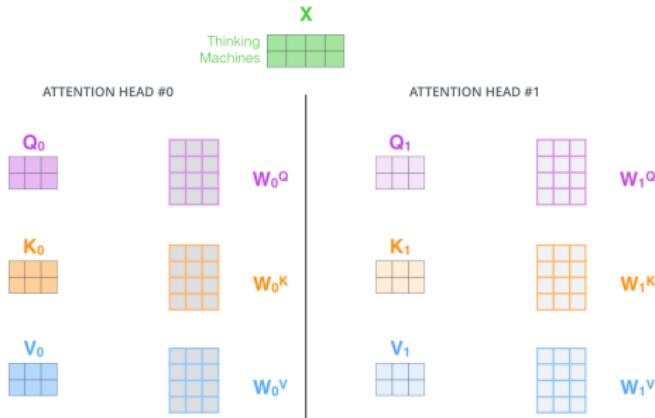
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Self-Attention

- 1 Multi-headed attention improves performance by expanding the model's ability to focus on different positions and **representation subspaces**
- 2 With multi-headed attention, we have multiple sets of Query/Key/Value weight matrices
- 3 We concatenate these matrices and multiply them by a weight matrix W_o to condense them into a single matrix



Multi-Head Self-Attention (II)

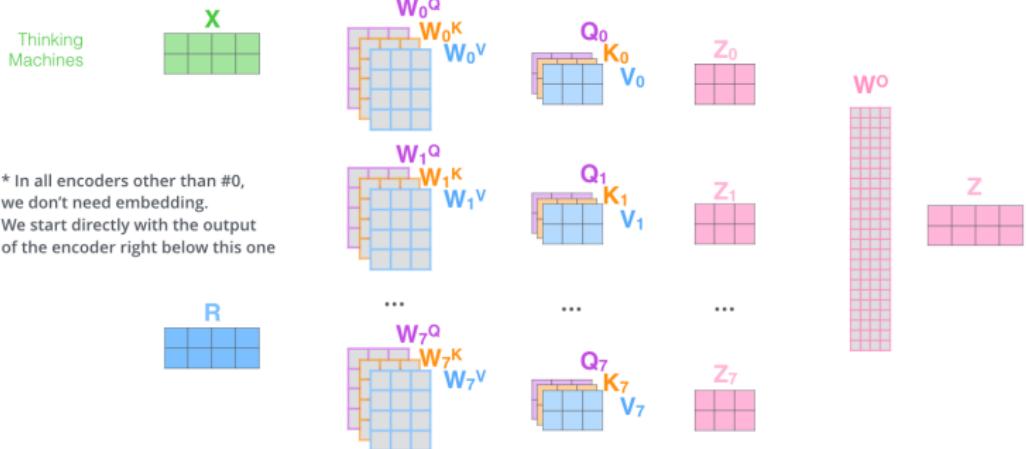
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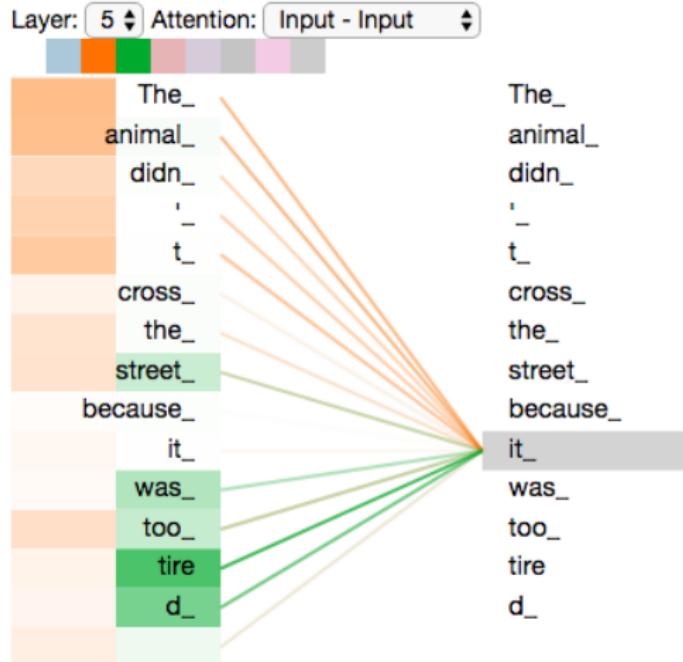
Self-Attention

- 1) This is our input sentence* each word*
- 2) We embed
- 3) Split into 8 heads. We multiply X or R with weight matrices
- 4) Calculate attention using the resulting $Q/K/V$ matrices
- 5) Concatenate the resulting Z matrices, then multiply with weight matrix W^o to produce the output of the layer



Attention Heads Example

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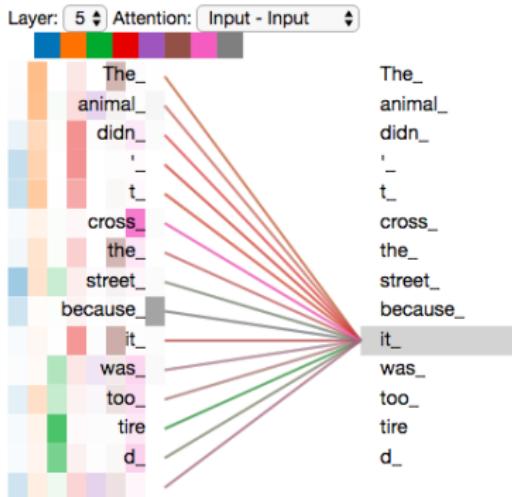
Attention Heads Example (II)

- Different heads focus on different parts of the input
- The model's representation of a word can include information from multiple heads.
- When all heads are combined, the output can be harder to interpret

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Representing The Order of The Sequence Using Positional Encoding

- In order to account for the order in the input sequence, the Transformer adds a vector to each input embedding.
- These vectors follow a specific pattern that the model learns, which helps it determine the position of each word or the distance between different words in the sequence
- The intuition is that adding these values to the embeddings provides meaningful distances between the embedding vectors once they're projected into $Q/K/V$ vectors and during dot-product attention.

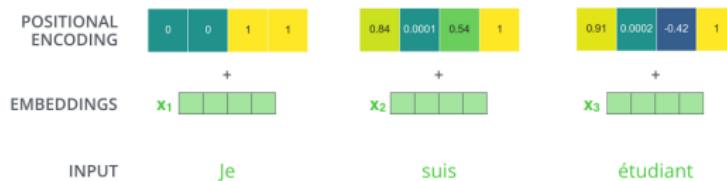


Figure: Example of positional encoding with a embedding size of 4

Real Example of Positional Encoding

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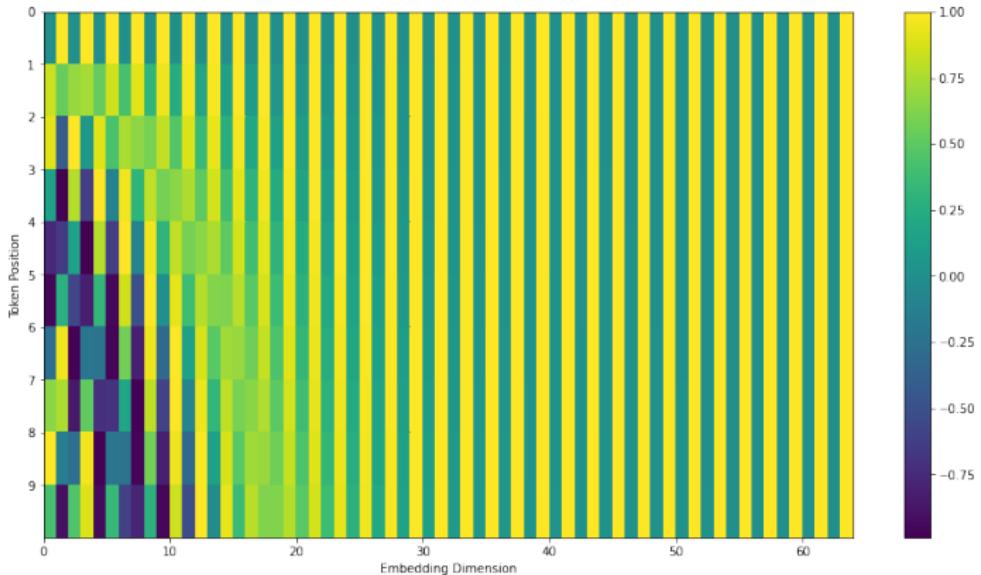


Figure: Real example of positional encoding for 10 words with an embedding size of 64.

Formula for Positional Encoding

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- The original “*Attention is all you need*” paper proposes a pre-defined formula for the positional encoding
- The encoding values are generated using a combination of sine and cosine functions, which are concatenated to form each of the positional encoding vectors.
- This method provides the advantage of being able to scale to unseen lengths of sequences, allowing the trained model to translate a sentence longer than any of those in the training set.

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

Positional Encoding Effect

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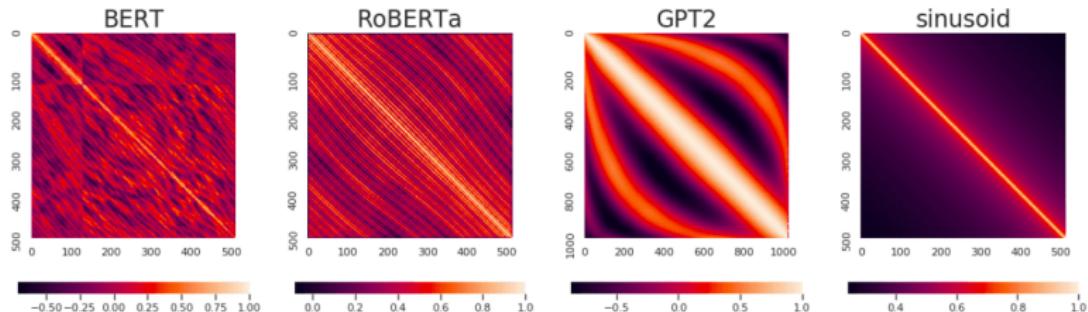


Figure: Position-wise similarity of multiple position embeddings. Note that larger models such as GPT2 process more tokens. Image from *Wang et Chen 2020*

for bert and roberta the pos embedding are learned
while for GPT2 and sinusoid its a formula

Example

For example, with $n = 5$ and $d = 4$, the positional encoding matrix is:

$$\begin{bmatrix} \sin(0/10000^{0/4}) & \cos(0/10000^{0/4}) & \sin(0/10000^{2/4}) & \cos(0/10000^{2/4}) \\ \sin(1/10000^{0/4}) & \cos(1/10000^{0/4}) & \sin(1/10000^{2/4}) & \cos(1/10000^{2/4}) \\ \sin(2/10000^{0/4}) & \cos(2/10000^{0/4}) & \sin(2/10000^{2/4}) & \cos(2/10000^{2/4}) \\ \sin(3/10000^{0/4}) & \cos(3/10000^{0/4}) & \sin(3/10000^{2/4}) & \cos(3/10000^{2/4}) \\ \sin(4/10000^{0/4}) & \cos(4/10000^{0/4}) & \sin(4/10000^{2/4}) & \cos(4/10000^{2/4}) \end{bmatrix}$$

$$\approx \begin{bmatrix} 0.0000 & 1.0000 & 0.0000 & 1.0000 \\ 0.8415 & 0.5403 & 0.0017 & 0.9999 \\ 0.9093 & -0.4161 & 0.0033 & 0.9999 \\ 0.1411 & -0.9900 & 0.0050 & 0.9999 \\ -0.7568 & -0.6536 & 0.0067 & 0.9999 \end{bmatrix}$$

Example (II)

$$\text{PE} \times \text{PE}^T =$$

$$\begin{bmatrix} 2.0000 & 1.3827 & 0.9126 & -0.8476 & -1.4104 \\ 1.3827 & 1.8325 & 0.8479 & -0.6605 & -1.1834 \\ 0.9126 & 0.8479 & 1.6806 & 0.6541 & -0.4506 \\ -0.8476 & -0.6605 & 0.6541 & 1.6989 & 1.2061 \\ -1.4104 & -1.1834 & -0.4506 & 1.2061 & 1.7998 \end{bmatrix}$$

We see that the elements in the diagonal have a much larger value. And the diagonal decreases the farther away from the diagonal. That is, closer positions have higher dot product values.

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Training trick 1: Residual Connections

Residual connections

Residual connections are a technique that helps models train better. Instead of only propagating information forward through a series of layers, residual connections also allow information to flow directly through the layers via a shortcut connection.

- Residual connections were first introduced in the ResNet architecture for image classification.
- They can help address the vanishing gradient problem and improve gradient flow through the network.
- Residual connections have been shown to be effective in a wide range of deep learning models.
- This technique can make the loss landscape considerably smoother and make the training process easier and more efficient.

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Training trick 2: Layer Normalization

Layer normalization

Layer normalization is a technique that helps models train faster by cutting down on uninformative variation in hidden vector values. This is achieved by normalizing the values to have a zero mean and unit standard deviation within each layer.

- Layer normalization is similar to batch normalization, but is applied at the layer level instead of the batch level.
- It has been shown to improve the performance of a wide range of deep learning models, including transformers.
- This technique can help address issues with internal covariate shift and the vanishing gradient problem.

also avoids exploding gradient

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Training trick 2: Layer Normalization (II)

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The equation for layer normalization is:

$$\text{LayerNorm}(x_i) = \frac{a_i}{\sqrt{\sigma^2 + \epsilon}}(x_i - \mu) + b_i$$

where x_i is the input to the i th layer, μ and σ are the mean and standard deviation of the input, a_i and b_i are learnable scaling and shifting parameters for each layer, and ϵ is a small value (usually 10^{-5}) added for numerical stability.

Training trick 3: Scaled Dot Product Attention

Dot product attention

The dot product in the attention mechanism tends to take on extreme values, as its variance scales with dimensionality d .

Solution

To mitigate this issue, we can use a scaling factor of $1/\sqrt{d}$ for the dot product, which is called scaled dot product attention.

- Scaled dot product attention is used in the self-attention mechanism in transformers.
- This technique ensures that the dot product stays within a reasonable range, which can help with the stability of the training process.
- Scaled dot product attention is also more computationally efficient than other attention mechanisms

The Attention Block

- Each sub-layer in each encoder has a residual connection around it and is followed by a layer-normalization step.

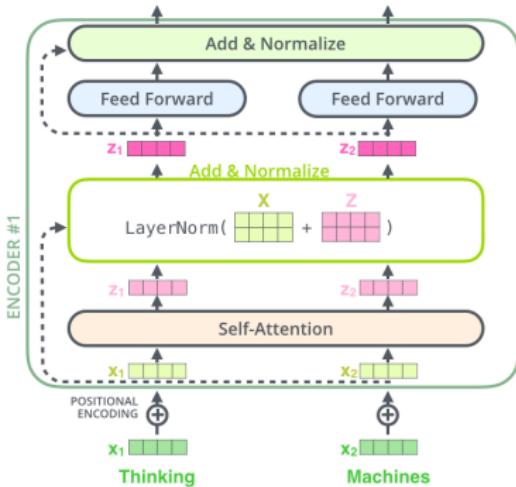


Figure: Visualization of the vectors and layer-norm operation associated with self-attention.

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The Attention Block (II)

the output of softmax
vocabulary is not words but
BPE tokens that will need to
be stitched to get the text

- This also applies to the decoder. A Transformer with 2 stacked encoders and decoders would look like this:

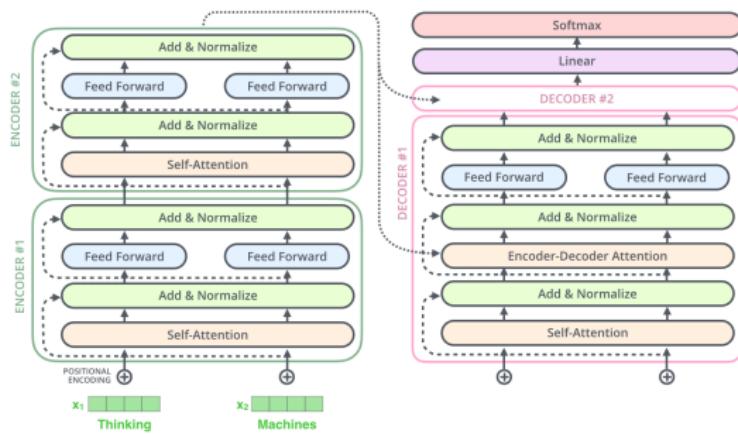


Figure: A Transformer with 2 stacked encoders and decoders.

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Fixing the decoder problem: Masked attention

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Problem

How do we prevent the decoder in a transformer network from “cheating” by looking ahead and “seeing” the answer when training on a language modeling objective?

Solution

Masked Multi-Head Attention: We mask (hide) information about future tokens from the model by setting attention scores to $-\infty$.

- To use self-attention in decoders, we need to ensure we can't peek at the future.
- At every timestep, we could change the set of keys and queries to include only past words, but this would be inefficient.

Fixing the decoder problem: Masked attention (II)

Masked attention

To enable parallelization, we mask out attention to future words by setting attention scores to $-\infty$.

- Masking is achieved by adding a mask matrix to the attention weights before the softmax operation.
- The mask matrix has the same shape as the attention weights, with $-\infty$ values in the positions where future words would be attended to.

Mask matrix

$$\text{mask}_{i,j} = \begin{cases} 0 & \text{if } j \leq i \\ -\infty & \text{otherwise} \end{cases}$$

- The masked attention scores are then passed through a softmax activation function to compute the weights

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Encoder-Decoder Attention

- The output of the top encoder is transformed into attention vectors K and V to be used in the “encoder-decoder attention” layer of each decoder.
- Each step in the decoding phase outputs an element from the output sequence and repeats until a special symbol is reached.
- The self-attention layer in the decoder can only attend to earlier positions in the output sequence, achieved by masking future positions.
- The “encoder-decoder attention” layer works like multiheaded self-attention, with the Queries matrix from the layer below and the Keys and Values matrix from the output of the encoder stack.

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The Decoder

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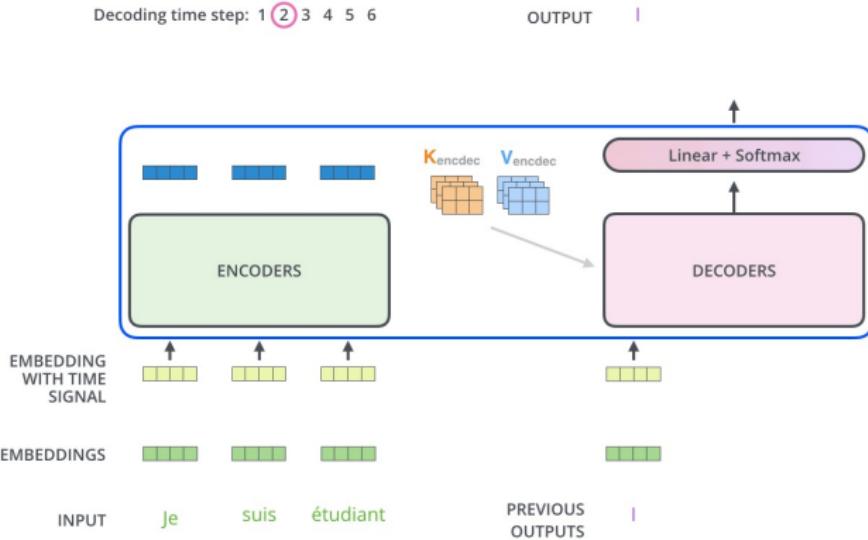


Figure: The decoder side of the Transformer architecture.

The Decoder (II)

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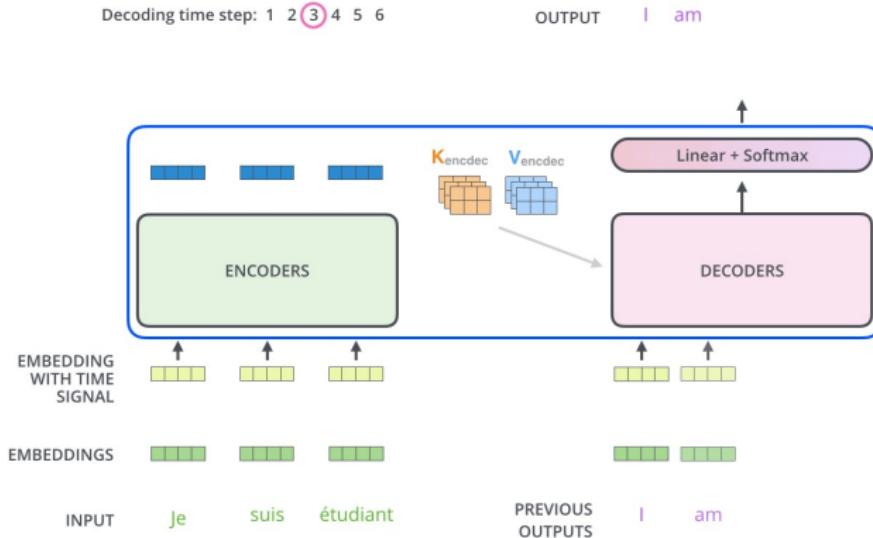


Figure: The decoder side of the Transformer architecture.

The Final Linear and Softmax Layer

- The final Linear layer projects the vector produced by the decoder to the vocabulary size
- The softmax layer turns those scores into probabilities

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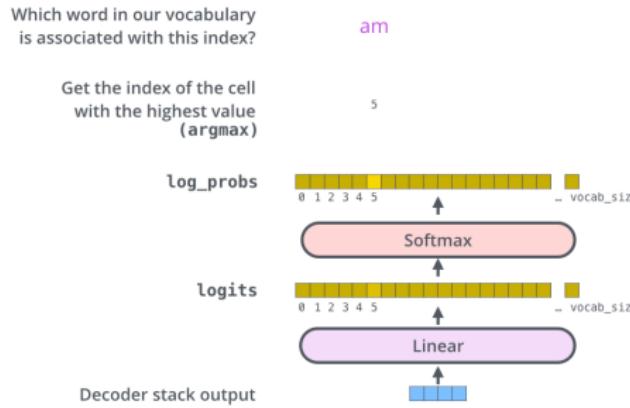


Figure: The final Linear and Softmax layers in the Transformer architecture.