Deep learning

Attention models

Hamid Beigy

Sharif University of Technology

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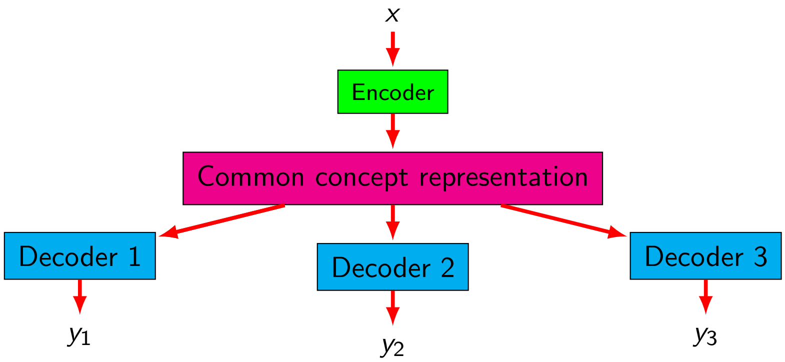
Introduction

Common concept representation

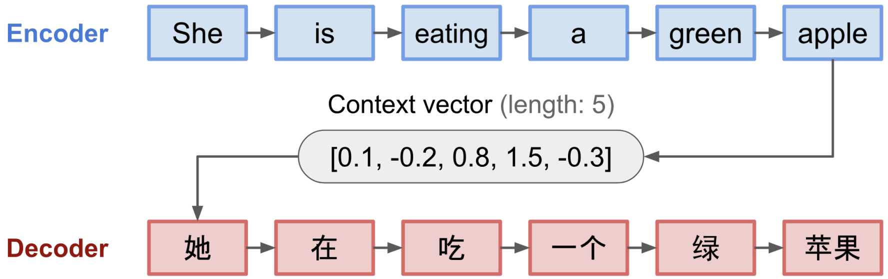
1. Consider the task of transferring a concept from a source domain to different target domains.



2. For example, consider the following tasks
   - A translation from Persian language to English language
   - A translation from Persian language to German language
   - A translation from Persian language to French language

Sequence to sequence models

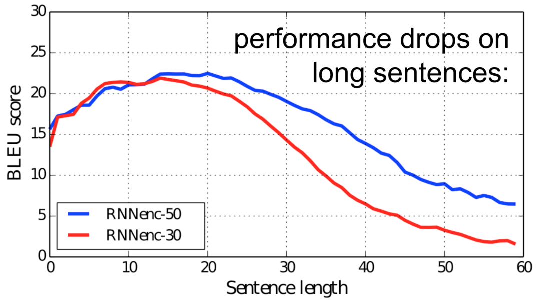
1. In seq2seq, the idea is to have two recurrent neural networks (RNNs) with an encoder-decoder architecture:
   - read the input words one by one to obtain a vector representation of a fixed dimensionality (encoder), and
   - conditioned on these inputs, extract the output words one by one using another RNN (decoder).
2. Both the encoder and decoder are recurrent neural networks such as LSTM or GRU units.



3. A critical disadvantage of this fixed-length context vector design is incapability of remembering long sentences.

Attention models

1. RNNs cannot remember longer sentences and sequences due to the vanishing/exploding gradient problem.
2. The performance of the encoder-decoder network degrades rapidly as the length of the input sentence increases.



3. In psychology, attention is the cognitive process of selectively concentrating on one or a few things while ignoring others.

Example (Counting the number of people in a photo)

Counting the number of heads and ignoring the rest.

Attention models (examples)

1. Consider two different tasks : neural machine translation and image captioning.

neural machine translation (heatmap)

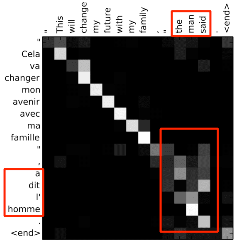
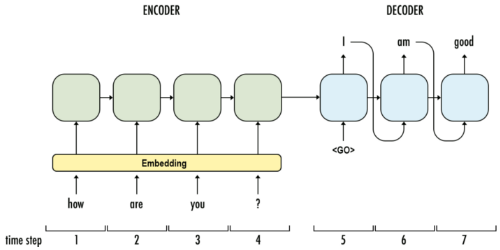


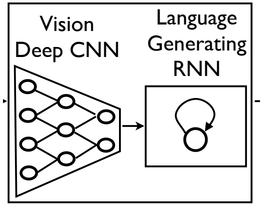
Image captioning

a red double decker bus driving down a street.

Neural network model



Neural network model



Attention models

Attention models

1. The attention mechanism was born to help memorize long source sentences in neural machine translation (NMT) (Bahdanau, Cho, and Bengio 2015).
2. Instead of building a single context vector out of the encoder's last hidden state, the goal of attention is to create shortcuts between the context vector and the entire source input.
3. The weights of these shortcut connections are customizable for each output element.
4. The alignment between the source and target is learned and controlled by the context vector.
5. Essentially the context vector consumes three pieces of information:
    - Encoder hidden states
    - Decoder hidden states
    - Alignment between source and target

Attention models

1. Assume that we have a source sequence x of length n and try to output a target sequence y of length m

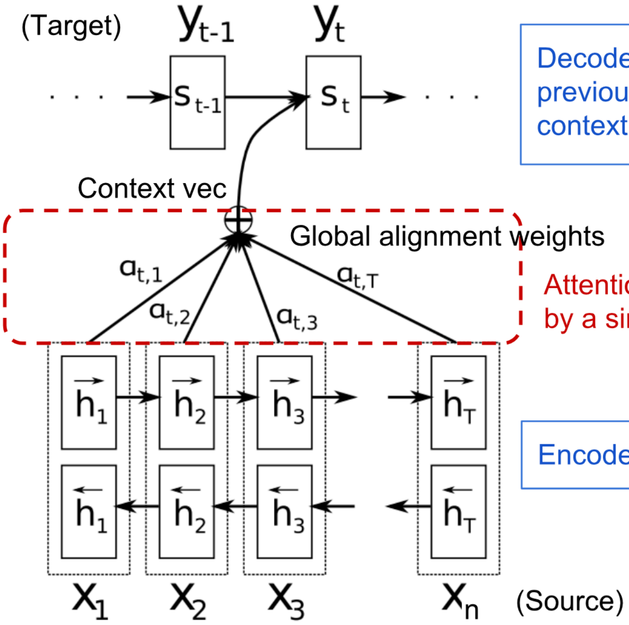
$$x = [x_1, x_2, \ldots, x_n]$$
$$y = [y_1, y_2, \ldots, y_m]$$

2. The encoder is a bidirectional RNN with a forward hidden state $\overrightarrow{h}_i$ and a backward one $\overleftarrow{h}_i$.
3. A simple concatenation of these two hidden states represents the encoder state.
4. The motivation is to include both the preceding and following words in the annotation of one word.

$$\boldsymbol{h}_i = \left[\overrightarrow{\boldsymbol{h}}_i^\top ; \overleftarrow{\boldsymbol{h}}_i^\top\right]^\top \quad i = 1, 2, \ldots, n$$

Attention models

1. Model of attention


(Target)
y_{t-1}
y_t
s_{t-1}
s_t
Context vec
Global alignment weights
$a_{t,1}$
$a_{t,2}$
$a_{t,3}$
$a_{t,T}$
$\overrightarrow{h}_1$ $\overrightarrow{h}_2$ $\overrightarrow{h}_3$ $\overrightarrow{h}_T$
$\overleftarrow{h}_1$ $\overleftarrow{h}_2$ $\overleftarrow{h}_3$ $\overleftarrow{h}_T$
X_1 X_2 X_3 X_n
(Source)

Decoder: RNN with input from previous state + dynamic context vector.

Attention layer: parameterized by a simple feed-forward network

Encoder: bidirectional RNN

Attention models

1. The decoder network has hidden state $\boldsymbol{s}_t = f(\boldsymbol{s}_{t-1}, y_{t-1}, \mathbf{c}_t)$ at position $t = 1, 2, \ldots, m$.
2. The context vector $\mathbf{c}_t$ is a sum of hidden states of the input sequence, weighted by alignment scores:

$$\mathbf{c}_t = \sum_{i=1}^{n} \alpha_{t,i} \boldsymbol{h}_i \qquad \text{Context vector for output } y_t$$

$$\alpha_{t,i} = \text{align}(y_t, x_i) \qquad \text{How well two words } y_t \text{ and } x_i \text{ are aligned.}$$

$$= \frac{exp\left(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_i)\right)}{\sum_{j=1}^{n} \exp\left(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_j)\right)} \qquad \text{Softmax of predefined alignment score.}$$

3. The alignment model assigns a score $\alpha_{t,i}$ to the pair of (y_t, x_i) based on how well they match.
4. The set of $\{\alpha_{t,i}\}$ are weights defining how much of each source hidden state should be considered for each output.

Attention models

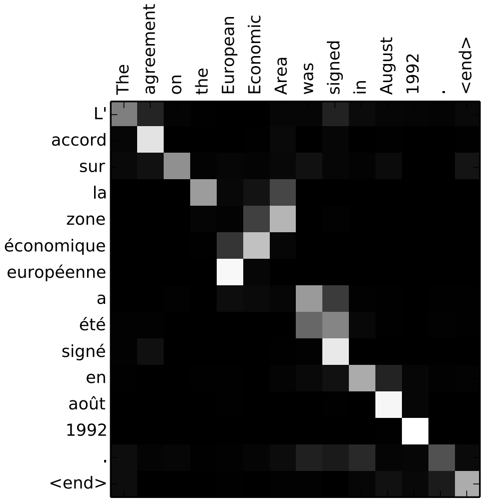
1. The alignment score α is parametrized by a feed-forward network with a single hidden layer (Bahdanau, Cho, and Bengio 2015).
2. This network is jointly trained with other parts of the model.
3. The score function is in the following form.

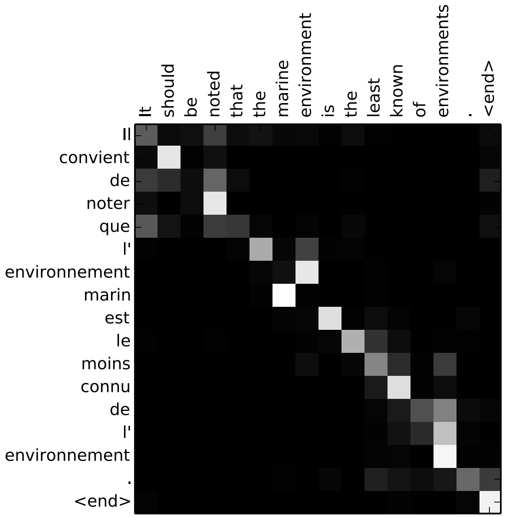
$$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \mathbf{v}_a^\top \tanh(\mathbf{W}_a[\boldsymbol{s}_t; \boldsymbol{h}_i])$$

where both $\mathbf{V}_a$ and $\mathbf{W}_a$ are weight matrices to be learned in the alignment model.

Alignment scores

1. The matrix of alignment scores explicitly show the correlation between source and target words.





Alignment scores

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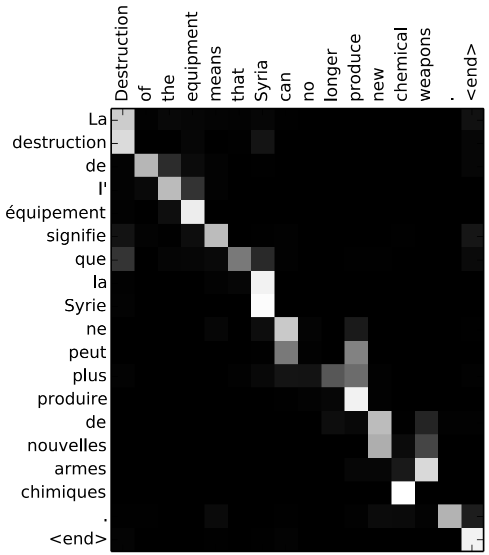
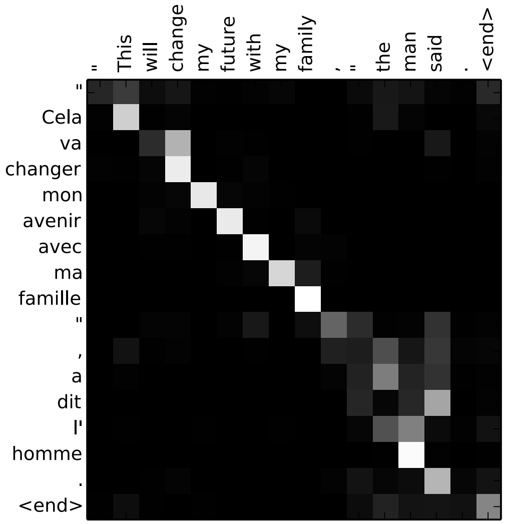
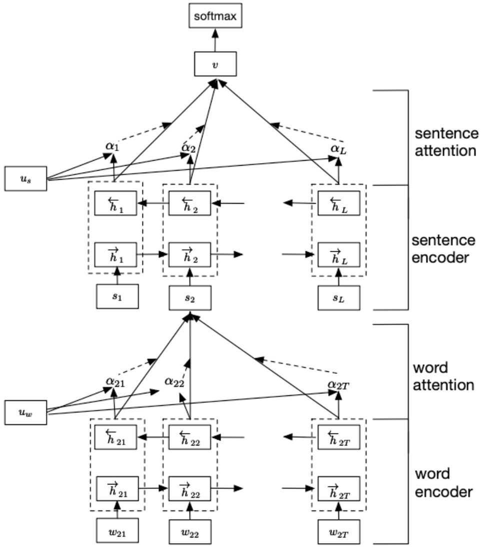




hierarchical attention network (HAN)

1. Attention can be effectively used on various levels (Yang et al. 2016).
2. HAN applicable to classification problem, not sequence generation.
3. HAN has two encoders: word and sentence.
   - Word encoder processes each word and aligns them a sentence of interest.
   - Then, sentence encoder aligns each sentence with final output.
4. HAN enables hierarchical interpretation of
   - which sentence is crucial in classifying document,
   - which part of a sentence (which words) are salient in that sentence.



Self-Attention

1. Consider the following example

Example (Self-Attention)

- Consider the following sentence

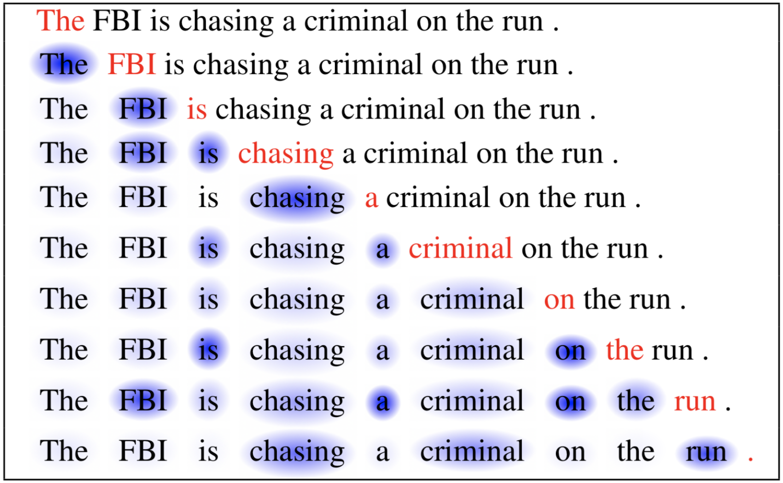
  The animal didn't cross the street because it was too tired.

- What does **it** in this sentence refer to?
- Is it referring to **the street** or to **the animal**?

2. Self-attention (intra-attention) is an attention mechanism relating different positions of a single sequence in order to compute a representation of the same sequence (Cheng, Dong, and Lapata 2016).
3. It is very useful in
   - Machine reading (the automatic, unsupervised understanding of text)
   - Abstractive summarization
   - Image description generation

Self Attention

1. The self-attention mechanism enables us to learn the correlation between the current words and the previous part of the sentence.


The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .
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The FBI is chasing a criminal on the run .
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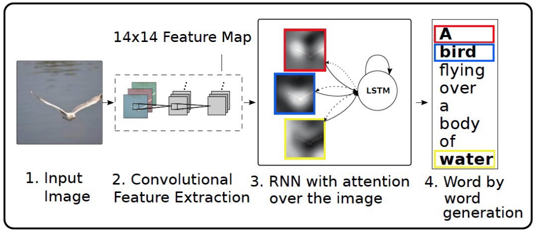
2. The current word is in red and the size of the blue shade indicates the activation level.

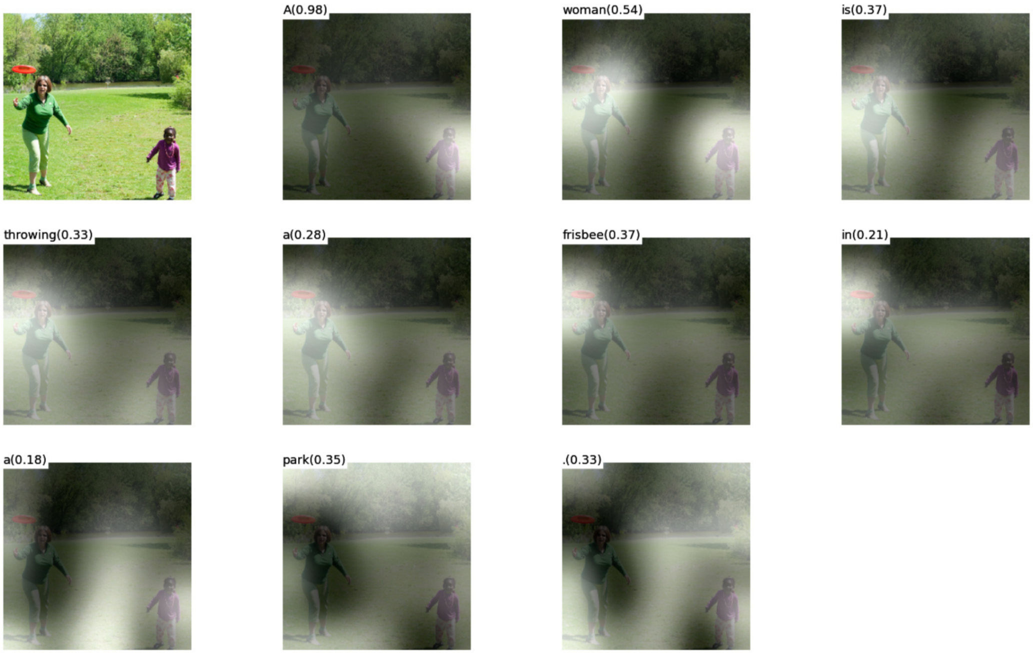
Self Attention

1. Self-attention is applied to the image to generate descriptions (Xu et al. 2015).


14x14 Feature Map
LSTM
A
bird
flying
over
a
body
of
water
1. Input Image
2. Convolutional Feature Extraction
3. RNN with attention over the image
4. Word by word generation

2. Image is encoded by a CNN and a RNN with self-attention consumes the CNN feature maps to generate the descriptive words one by one.
3. The visualization of the attention weights clearly demonstrates which regions of the image, the model pays attention to output a certain word.

Self Attention



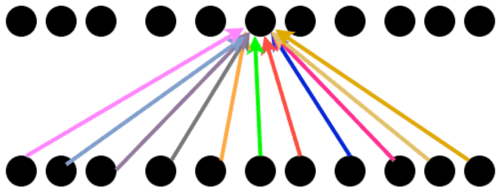
Soft vs Hard Attention

1. The soft vs hard attention is another way to categorize how attention is defined based on whether the attention has access to the entire image or only a patch.
   - Soft Attention: the alignment weights are learned and placed “softly” over all patches in the source image (same idea as in (Bahdanau, Cho, and Bengio 2015)).
     - Soft attention, in its simplest variant, is no different for images than for vector-valued features and is implemented exactly.
     - Pro: the model is smooth and differentiable.
     - Con: expensive when the source input is large.
   - Hard Attention: only selects one patch of the image to attend to at a time.
     - Hard attention for images has been known for a very long time: **image cropping**.
     - Pro: less calculation at the inference time.
     - Con: the model is non-differentiable and requires more complicated techniques such as variance reduction or reinforcement learning to train.

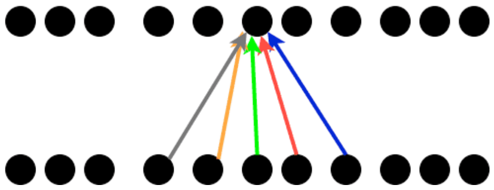
Global vs Local Attention

1. Global and local attention are proposed in (Luong, Pham, and Manning 2015).
2. The idea of a global attentional model is to consider all the hidden states of the encoder when deriving the context vector.

Global attention



Local attention



Global vs Local Attention

1. The global attention has a drawback that it has to attend to all words on the source side for each target word, which is expensive and can potentially render it impractical to translate longer sequences,
2. The local attentional mechanism chooses to focus only on a small subset of the source positions per target word.
3. Local one is an interesting blend between hard and soft, an improvement over the hard attention to make it differentiable:
4. The model first predicts a single aligned position for the current target word and a window centered around the source position is then used to compute a context vector.

$$\boldsymbol{p}_t = n \times \mathit{sigmoid}\left(\mathbf{v}_p^\top \tanh(\mathbf{W}_p \boldsymbol{h}_t)\right)$$

n is length of source sequence. Hence, $\boldsymbol{p}_t \in [0, n]$.

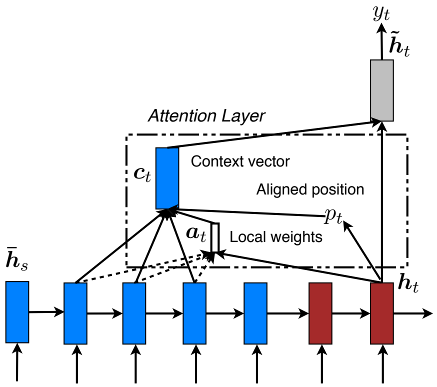
Global vs Local Attention

1. To favor alignment points near $\boldsymbol{p}_t$, they placed a Gaussian distribution centered around $\boldsymbol{p}_t$. Specifically, the alignment weights are defined as

$$a_{st} = align(h_t, \bar{h}_s) \exp\left(-\frac{(s - p_t)^2}{2\sigma^2}\right)$$

and

$$\boldsymbol{p}_t = n \times sigmoid\left(\mathbf{v}_p^\top \tanh(\mathbf{W}_p \boldsymbol{h}_t)\right)$$



Generalized model of attention

Retrieving a record from a relational database

1. Consider the following table, called PERSONS, in a relational database.

ID	Name	Family
005123174812	Ali	Ahmadi
015843268901	Mohammad Reza	Ali Mohammadi
005123174823	Ashkan	Mohammadi

2. Now consider the following queries.
    - SELECT ID, Name, Family FROM PERSONS WHERE ID='015843268901'
    - SELECT ID, Name, Family FROM PERSONS WHERE ID like '00512317%'
3. Here, concepts of query,key, and value become and the result is retrieved using the following similarity function.

$$\mathit{Similarity}(\mathbf{q},\mathbf{k},\mathbf{v}) = \sum_i \mathit{Similarity}(\mathbf{q},\mathbf{k}_i) \times \mathbf{v}_i$$

Retrieving a value from neural Turing machine memory

1. Consider the following memory in the neural Turing machine.

Key	Value
key 1	Value 1
key 2	Value 2
key 3	Value 3

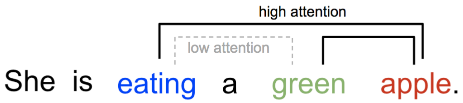
2. When reading from the memory at time t, an attention vector of size p, $\mathbf{w}_t$ controls how much attention to assign to different memory locations.
3. The read vector $\mathbf{r}_t$ is a sum weighted by attention intensity:

$$\mathbf{r}_t = \sum_{i=1}^{p} w_t(i)\mathbf{M}_t(i)$$

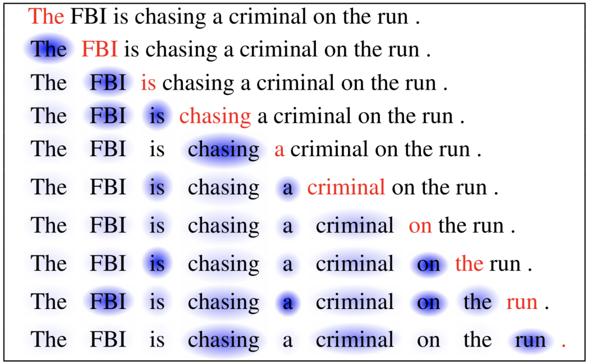
$$\sum_{i=1}^{p} w_t(i) = 1, \forall i : 0 \leq w_t(i) \leq 1$$

Generalized model of attention

1. Consider the following sentence.



2. For calculating the attention of a target word with respect to the input word,
   - we first use the query of the target word and the key of the input word,
   - next calculate a matching score, and
   - finally calculate the weighted sum of value vectors using the matching scores.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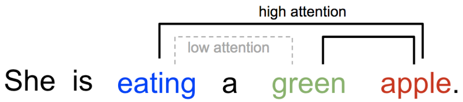
The FBI is chasing a criminal on the run .
The FBI is chasing a criminal on the run .

Generalized model of attention

1. Each word is key, query and value.
2. Each word w is represented by a vector $\mathbf{x} \in \mathbb{R}^d$ by using an embedding method.
3. Calculate query ($\mathbf{q} \in \mathbb{R}^p$) for $\mathbf{x} \in \mathbb{R}^d$, which is projection of $\mathbf{x}$ to a new space.
$$\mathbf{q} = \mathbf{w}_q^\top \mathbf{x}.$$
4. Calculate key ($\mathbf{k} \in \mathbb{R}^p$) for $\mathbf{x} \in \mathbb{R}^d$, which is projection of $\mathbf{x}$ to a new space.
$$\mathbf{k} = \mathbf{w}_k^\top \mathbf{x}.$$
5. Calculate value ($\mathbf{w} \in \mathbb{R}^p$) for $\mathbf{x} \in \mathbb{R}^d$, which is projection of $\mathbf{x}$ to a new space.
$$\mathbf{v} = \mathbf{w}_v^\top \mathbf{x}.$$
6. A single word $\mathbf{x}$ has three different representations. Sometimes, we look at this word as query, sometimes as key, and sometimes as value.
7. The self-attention means that looking a word as query and compute the similarity of the query with all of the words seen as key.
8. Then use the softmax for computing the weights and compute the weighted average all of the words seen as value.
9. This computes the attention vector.

Generalized model of attention

1. Consider the following sentence.



2. Calculating the attention for word apple.
3. Taking the inner product of the query vector of apple to the key vector of the previous words.

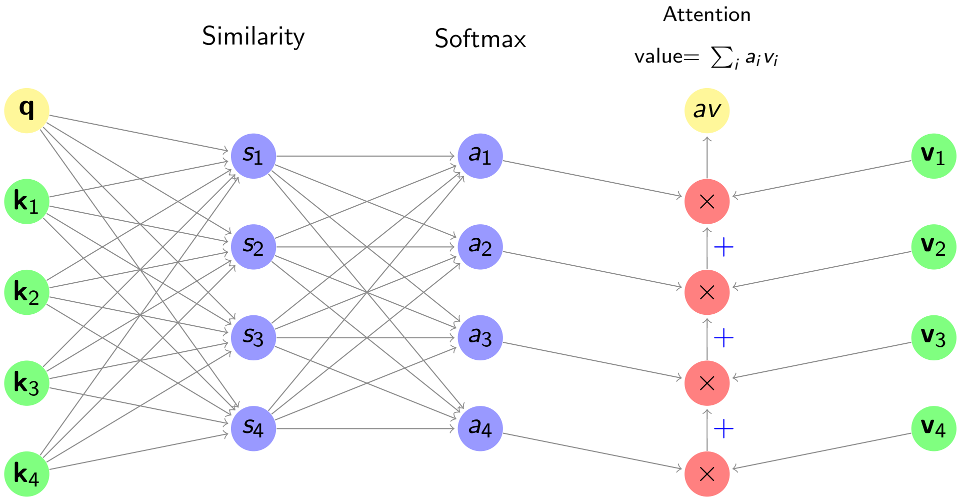
$$\mathbf{a} = softmax\left(\mathbf{q}_{apple}^\top \mathbf{k}_{she}, \mathbf{q}_{apple}^\top \mathbf{k}_{is}, \mathbf{q}_{apple}^\top \mathbf{k}_{eating}, \mathbf{q}_{apple}^\top \mathbf{k}_{a}, \mathbf{q}_{apple}^\top \mathbf{k}_{green}\right)$$

4. Suppose that we obtain $\mathbf{a} = (0.1, 0.1, 0.5, 0.1, 0.2)$. Then we obtain

$$\mathbf{v}_{apple} = 0.1\mathbf{v}_{she} + 0.1\mathbf{v}_{is} + 0.5\mathbf{v}_{eating} + 0.1\mathbf{v}_{a} + 0.2\mathbf{v}_{green}$$

Generalized model of attention

1. Self-attention uses the following neural network architecture.



Generalized model of attention

1. By defining three different vectors corresponding to each word.
   - Key $\mathbf{k} \in \mathbb{R}^p$ and $\mathbf{k} = \mathbf{W}_k^\top \mathbf{x}$, where $\mathbf{W}_k \in \mathbb{R}^{d \times p}$ and $\mathbf{x} \in \mathbb{R}^d$.
   - Query $\mathbf{q} \in \mathbb{R}^p$ and $\mathbf{q} = \mathbf{W}_q^\top \mathbf{x}$, where $\mathbf{W}_q \in \mathbb{R}^{d \times p}$ and $\mathbf{x} \in \mathbb{R}^d$.
   - Value $\mathbf{v} \in \mathbb{R}^p$ and $\mathbf{v} = \mathbf{W}_v^\top \mathbf{x}$, where $\mathbf{W}_v \in \mathbb{R}^{d \times p}$ and $\mathbf{x} \in \mathbb{R}^d$.
2. By defining the following matrices
   - $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]$, where $\mathbf{X} \in \mathbb{R}^{d \times n}$.
   - $\mathbf{K} = [\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_n]$, where $\mathbf{K} \in \mathbb{R}^{p \times n}$.
   - $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n]$, where $\mathbf{Q} \in \mathbb{R}^{p \times n}$.
   - $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n]$, where $\mathbf{V} \in \mathbb{R}^{p \times n}$.
3. Then, the new value $\mathbf{Z} \in \mathbb{R}^{p \times n}$ equals to $\mathbf{Z} = \mathbf{V}\ \mathit{Softmax}\left(\frac{\mathbf{Q}^\top \mathbf{K}}{\sqrt{p}}\right)$.

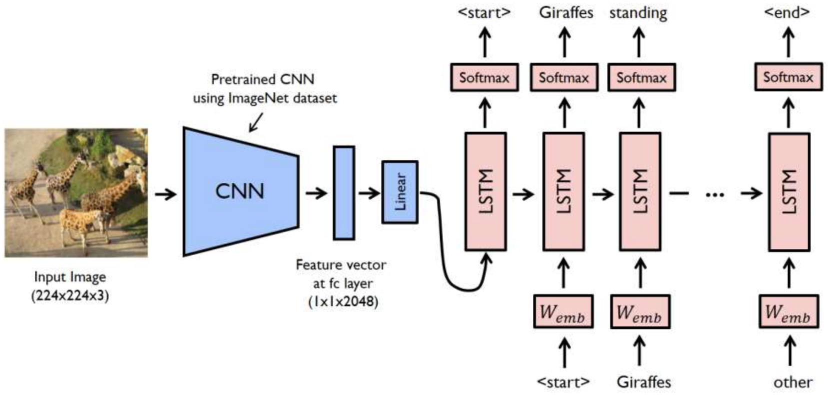
Alignment scores

Name	Alignment score function	Paper (https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html)
Content-base attention	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \text{cosine}[\boldsymbol{s}_t, \boldsymbol{h}_i]$	A. Graves, et al. "Neural Turing machines", arXiv, 2014.
Additive	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \mathbf{v}_a^\top \tanh(\mathbf{W}_a[\boldsymbol{s}_t; \boldsymbol{h}_i])$	D. Bahdanau, et al."Neural machine translation by jointly learning to align and translate", ICLR 2015.
Location-Base	$\alpha_{t,i} = \text{softmax}(\mathbf{W}_a \boldsymbol{s}_t)$	T. Luong, , et al. "Effective Approaches to Attention-based Neural Machine Translation", EMNLP 2015.
General	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \mathbf{W}_a \boldsymbol{h}_i$	Same as the above
Dot-Product	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \boldsymbol{h}_i$	Same as the above
Scaled Dot-Product	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \frac{\boldsymbol{s}_t^\top \boldsymbol{h}_i}{\sqrt{n}}$	A. Vaswani, et al. "Attention is all you need", NIPS 2017.

Attention in computer vision

Image captioning

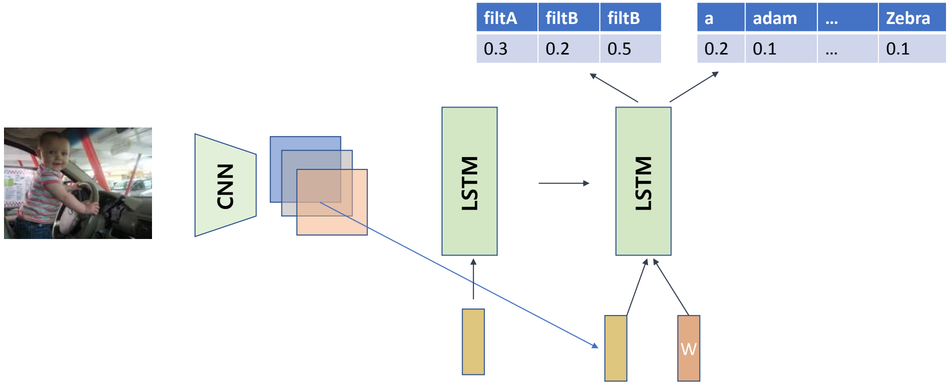
1. The natural image caption generator was proposed in (Xu et al. 2015).



2. This network is a combination of CNN and LSTM networks.

Image captioning

1. The outputs of lower layers of CNN are used as representation of values.

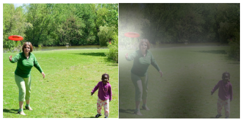


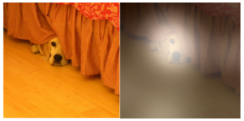
filtA	filtB	filtB
0.3	0.2	0.5

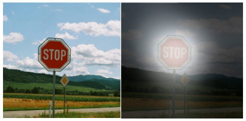
a	adam	...	Zebra
0.2	0.1	...	0.1

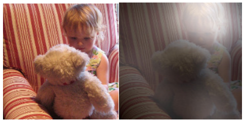
Image captioning results

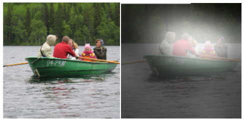
1. Examples of attending to the correct object

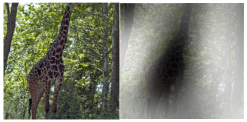

A woman is throwing a frisbee in a park.


A dog is standing on a hardwood floor.

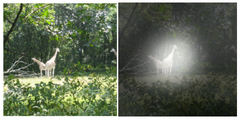

A stop sign is on a road with a mountain in the background.

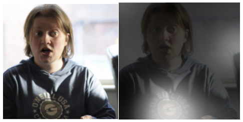

A little girl sitting on a bed with a teddy bear.

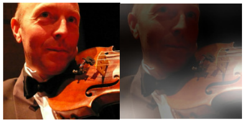

A group of people sitting on a boat in the water.

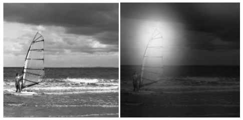

A giraffe standing in a forest with trees in the background.

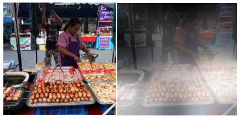
2. Examples of mistakes


A large white bird standing in a forest.


A woman holding a clock in her hand.


A man wearing a hat and a hat on a skateboard.


A person is standing on a beach with a surfboard.


A woman is sitting at a table with a large pizza.

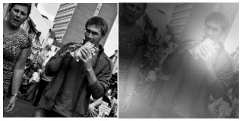
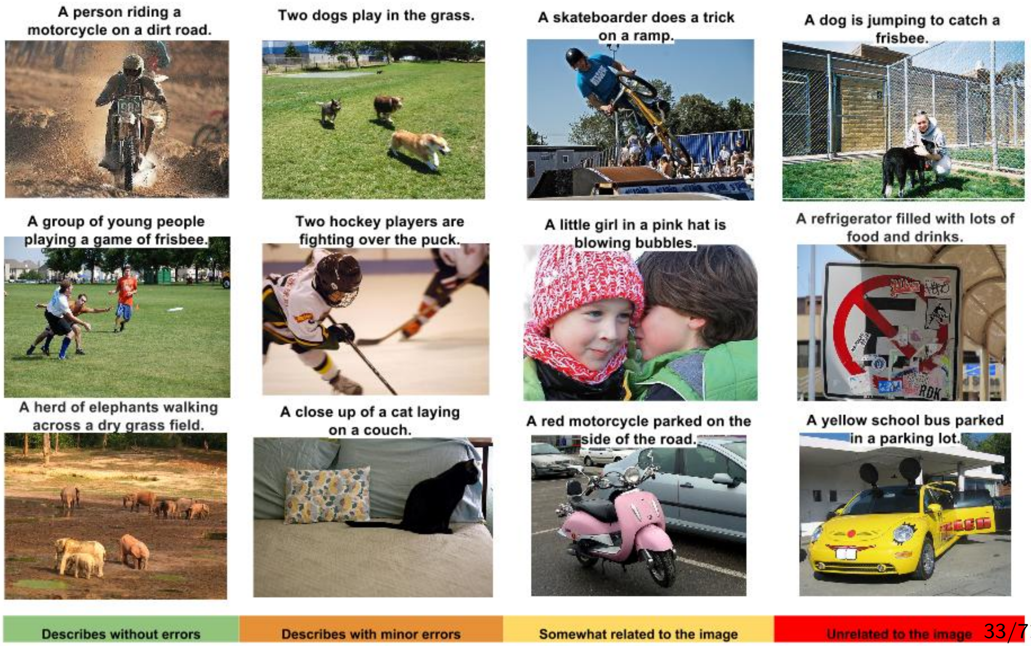

A man is talking on his cell phone while another man watches.

Image captioning results

1. There is also a method given in (Vinyals et al. 2015).


A person riding a motorcycle on a dirt road.
Two dogs play in the grass.
A skateboarder does a trick on a ramp.
A dog is jumping to catch a frisbee.
A group of young people playing a game of frisbee.
Two hockey players are fighting over the puck.
A little girl in a pink hat is blowing bubbles.
A refrigerator filled with lots of food and drinks.
A herd of elephants walking across a dry grass field.
A close up of a cat laying on a couch.
A red motorcycle parked on the side of the road.
A yellow school bus parked in a parking lot.
Describes without errors
Describes with minor errors
Somewhat related to the image
Unrelated to the image

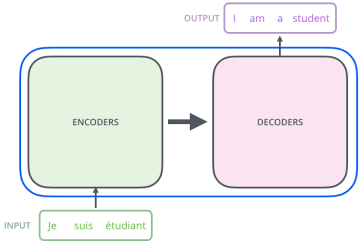
Transformers family

Transformers family

Transformers model

Transformers model

1. The soft attention make it possible to do sequence to sequence modeling without recurrent network units (Vaswani et al. 2017).
2. The transformer model is entirely built on the self-attention mechanisms without using sequence-aligned recurrent architecture.



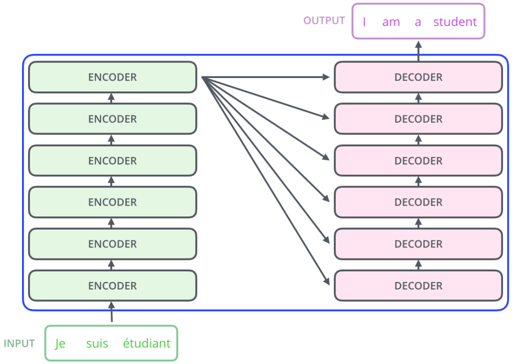


Figure: Jay Alammar

3. The encoding component is a stack of six encoders.
4. The decoding component is a stack of decoders of the same number.

Transformers training

1. The Transformers works slightly differently during training and inference.
2. Input sequence: You are welcome in English.
3. Target sequence: De nada in Spanish

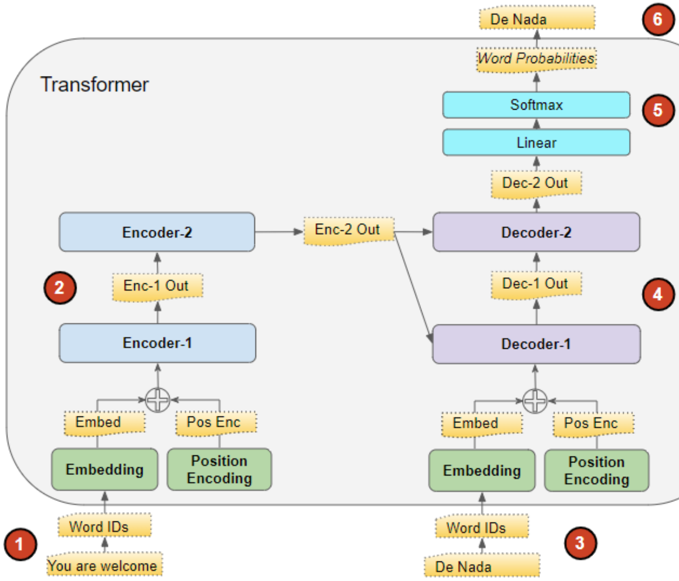


Figure:Ketan Doshi

Transformers inference

1. During Inference, we have only the input sequence and don't have the target sequence to pass as input to the Decoder.
2. The goal is to produce the target sequence from the input sequence alone.

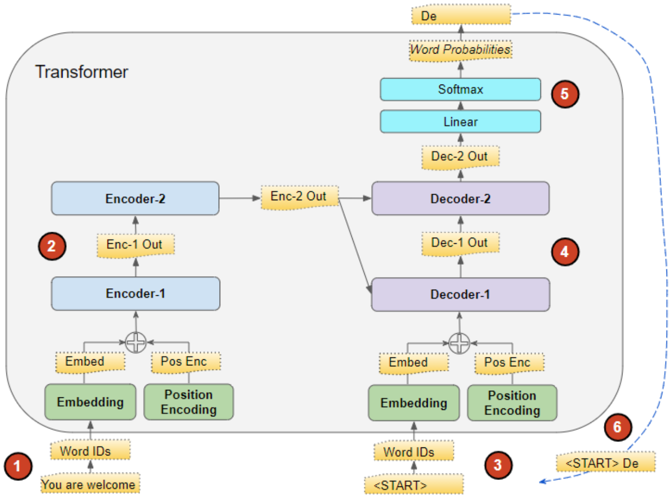
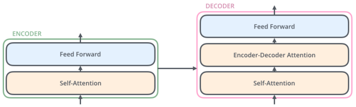
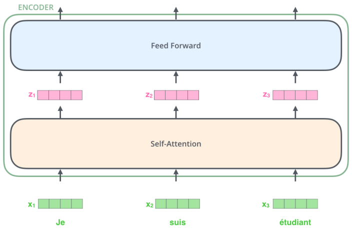


Figure:Ketan Doshi

Transformers encoder

1. Each encoder has two sub-layers and each decoder has three sub-layers
2. Each sublayer has residual connection.
3. All encoders receive a list of vectors each of the size 512.
4. The size of this list is hyper-parameter we can set (it would be the length of the longest sentence in our training dataset).





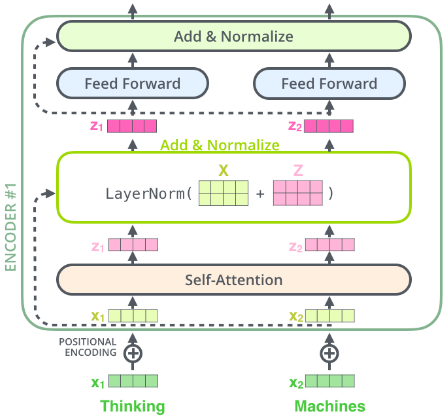


Figure: Jay Alammar

Transformers

1. A transformer of two stacked encoders and decoders

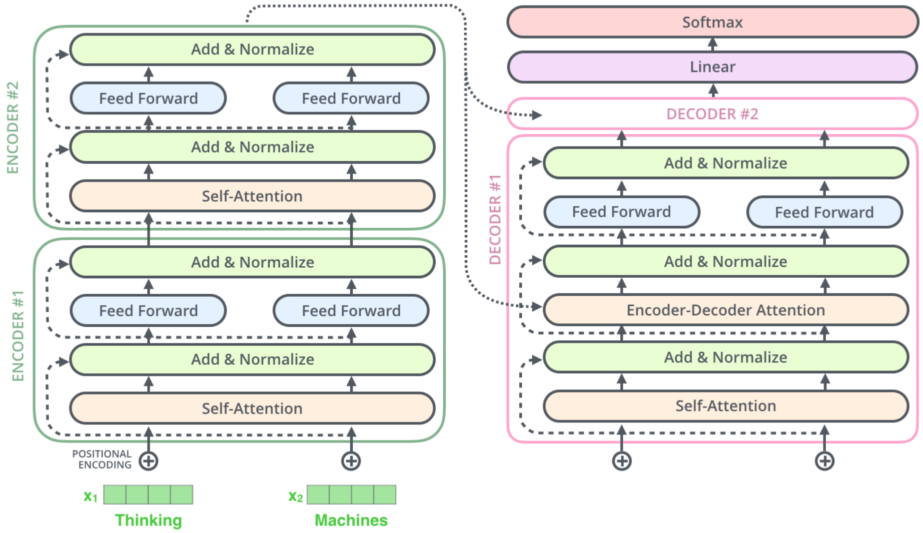
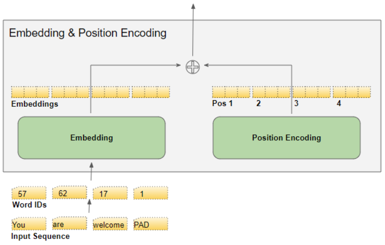


Figure: Jay Alammar

Transformers embedding and position encoding

1. Transformers needs two things for a word:
   - its meaning
   - its position in sequence



2. Transformers have two Embedding layers.
   - Input sequence is fed to the first embedding layer (Input Embedding).
   - Target sequence is fed to the second embedding layer after shifting the targets right by one position and inserting a START token in the first position.

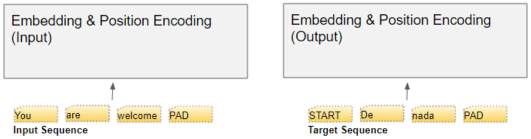

Embedding & Position Encoding (Input)
You
are
welcome
PAD
Input Sequence
Embedding & Position Encoding (Output)
START
De
nada
PAD
Target Sequence

Figure:Ketan Doshi

Transformers position encoding

1. There are two position encoding layers for: input sequence and output sequence.
2. Let d be size of embedding for each word and L be length of input sequence.
3. Transformers consider an array of $d \times L$ to encode positions of input sequence.

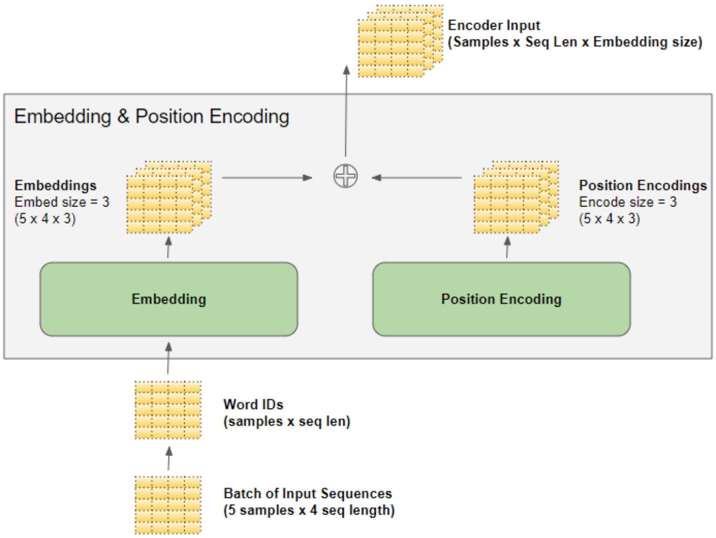


Figure:Ketan Doshi

Transformers position encoding

1. All words in input sentence simultaneously flow through Transformer's encoder/decoder stack and model doesn't have any sense of position/order of each word.
2. Hence, we need for a way to incorporate the order of words into our model.
3. The first solution is to assign a number to each time-step within interval $[0, 1]$ range in which 0 means the first word and 1 is the last time-step.
   Problem: can't figure out how many words are present within a specific range, i.e, time-step delta doesn't have consistent meaning across different sentences.
4. The second solution is to assign a number to each time-step linearly.
   Problem: not only the values could get quite large, but also our model can face sentences longer than the ones in training.
5. Ideally, the following criteria should be satisfied for positional embedding
   - It should output a unique encoding for each time-step (word's position in a sentence)
   - Distance between any two time-steps should be consistent across sentences with different lengths.
   - The model should generalize to longer sentences without any efforts. Its values should be bounded.
   - It must be deterministic.

Transformers position encoding

1. The encoding of Transformers is simple and satisfies all of those criteria.
   - It is d-dimensional vector containing information about a specific position in a sentence.
   - This encoding is not integrated into the model itself. this vector is used to equip each word with information about its position in a sentence.
2. Let pos be the position of word in sequence.
3. Let $i \in \{1, 2, \dots, d\}$ be the index value in positional encoding.
4. Then, PE is computed using

$$PE(pos, i) = \begin{cases} \sin\left(\frac{pos}{10000^{i/d}}\right) & \text{if } i = 2k \\ \cos\left(\frac{pos}{10000^{i/d}}\right) & \text{if } i = 2k+1 \end{cases}$$

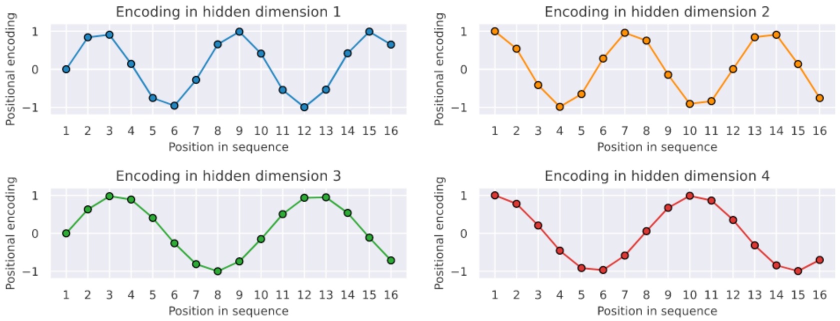
5. Let $d = 512$ and $pos = 0$, then $PE(0)$ and $PE(1)$equal to

$$PE(0) = (0, 1, 0, \dots, 0, 1)$$
$$PE(1) = (0.8414, 0.5403, 0.8218, \dots, 0.0001, 0.9999)$$

Transformers position encoding

1. For word w at position $pos \in [0, L-1]$ in the input sequence $w = (w_0, \dots, w_{L-1})$, with 4-dimensional embedding e_w, and $d = 4$, the operation would be

$$
\begin{aligned}
e'_w &= e_w + \left[sin\left(\frac{pos}{10000^0}\right), cos\left(\frac{pos}{10000^0}\right), sin\left(\frac{pos}{10000^{2/4}}\right), cos\left(\frac{pos}{10000^{2/4}}\right) \right] \\
&= e_w + \left[sin\left(pos\right), cos\left(pos\right), sin\left(\frac{pos}{100}\right), cos\left(\frac{pos}{100}\right) \right]
\end{aligned}
$$



Transformers position encoding

1. Position encoding interleaves a *sine* curve and a *cos* curve, with sine values for all even indexes and cos values for all odd indexes.
2. This results the following position encoding and the corresponding curves.

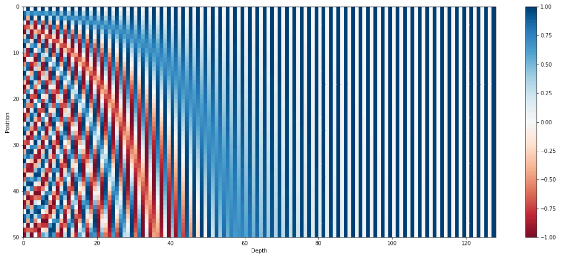


Figure: Amirhossein Kazemnejad

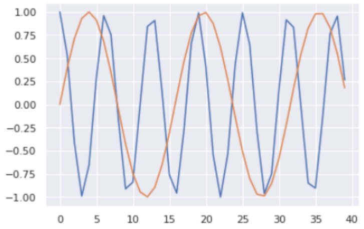
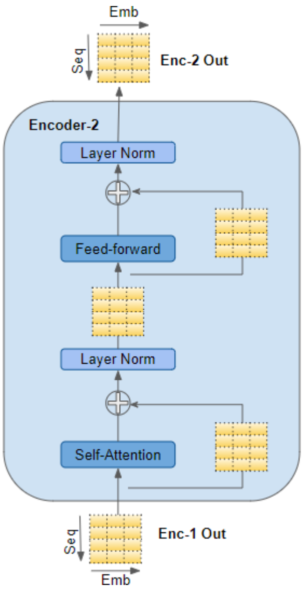


Figure: Ketan Doshi

Transformers encoder

1. The Encoder passes its input into a Multi-head Self-attention layer.
2. The Self-attention output is passed into a Feed-forward layer, which then sends its output upwards to the next Encoder.



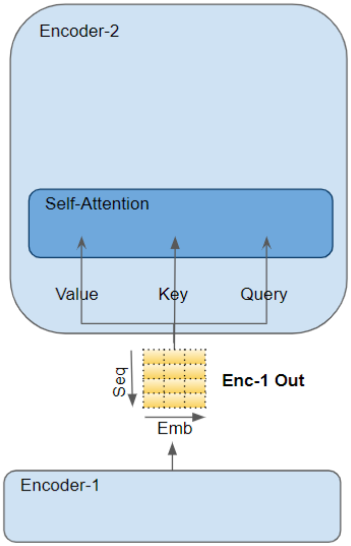


Figure: Ketan Doshi

Transformers decoder

1. The Decoder passes its input into a Multi-head Self-attention layer.
2. This operates in a slightly different way than the one in the Encoder.
3. It is only allowed to attend to earlier positions in the sequence. This is done by masking future positions.

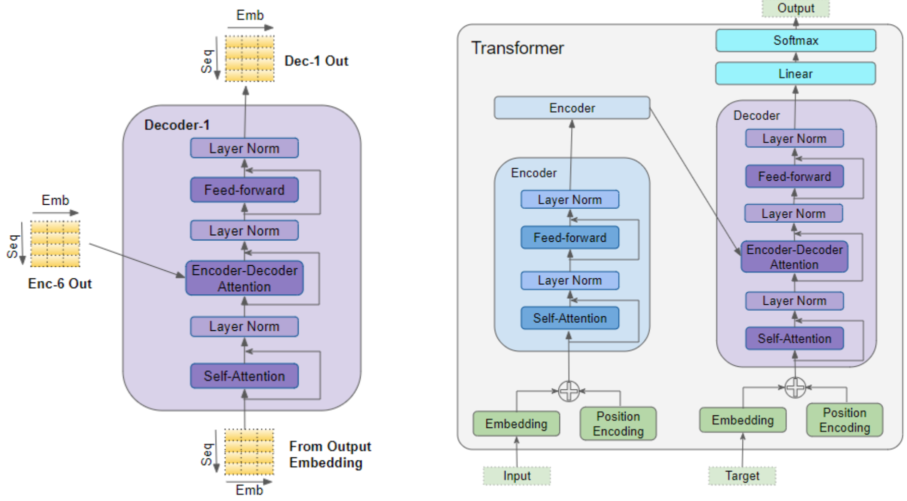
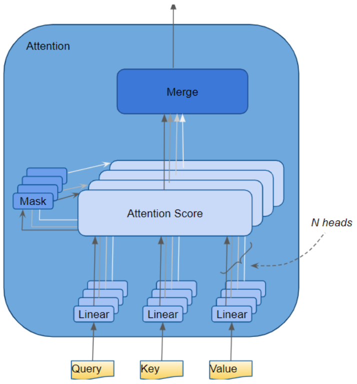


Figure: Ketan Doshi

Transformers multi-head attention

1. The Transformers calls each Attention processor an Attention Head and repeats it several times in parallel.
2. This is known as Multi-head attention.
3. It gives its Attention greater power of discrimination, by combining several similar Attention calculations.



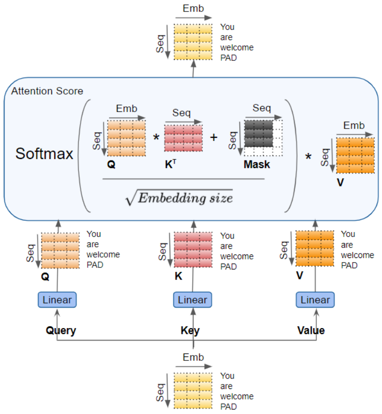


Figure: Ketan Doshi

Transformers multi-head attention

1. There are three separate Linear layers for the Query, Key, and Value.
2. Each Linear layer has its own weights.
3. The input is passed through these Linear layers to produce the **Q**, **K**, and **V** matrices.

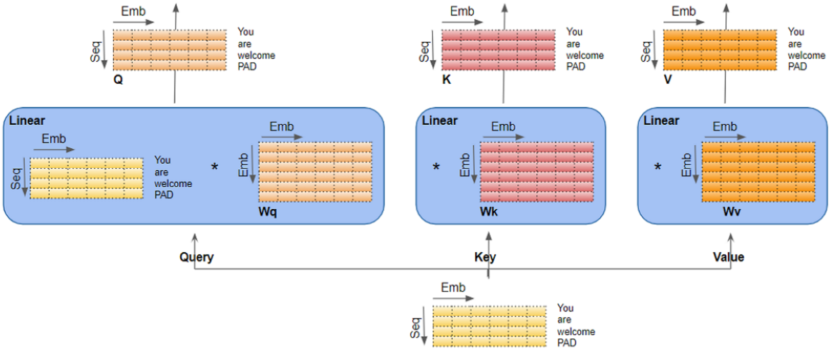
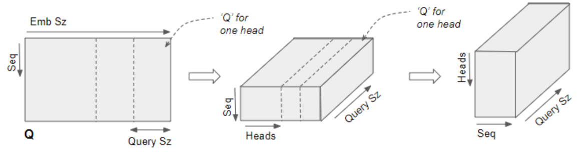


Figure: Ketan Doshi

Transformers multi-head attention

1. The data are split across the multiple Attention heads so that each can process it independently.
2. This is a logical split only. The Query, Key, and Value are not physically split into separate matrices, one for each Attention head.
3. A single data matrix is used for the Query, Key, and Value, respectively, with logically separate sections of the matrix for each Attention head.



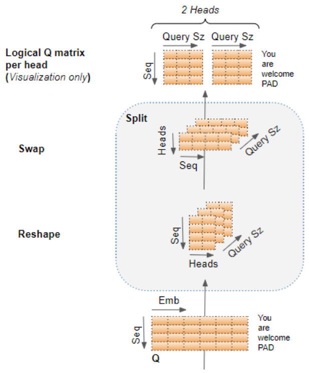


Figure: Ketan Doshi

Transformers multi-head attention

1. We now have separate Attention Scores for each head.
2. They need to be combined together into a single score.
3. This Merge operation is essentially the reverse of the Split operation.
4. It is done by simply reshaping the result matrix to eliminate the Head dimension.
    - Reshape the Attention Score matrix by swapping the Head and Sequence dimensions.
    - Collapse the Head dimension by reshaping .

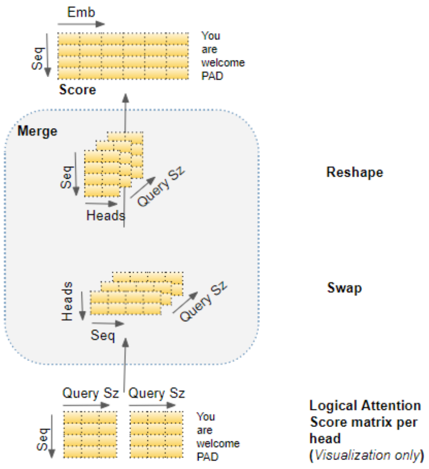


Figure: Ketan Doshi

Transformers multi-head attention

1. The end-to-end flow of the Multi-head Attention is

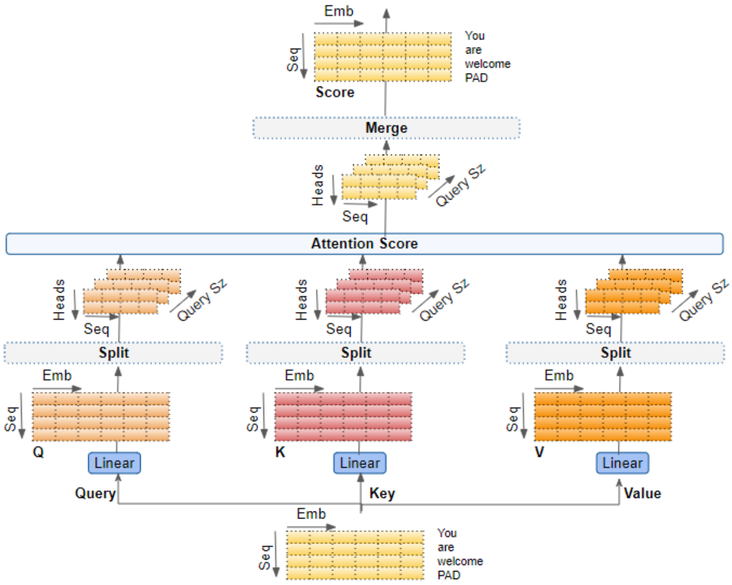
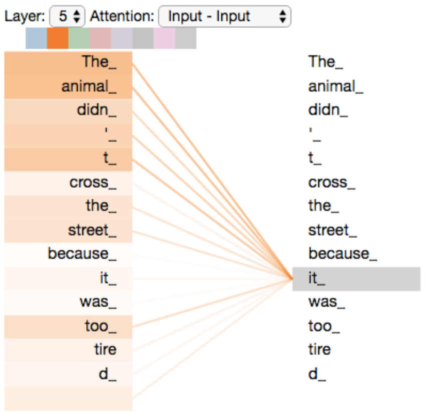


Figure: Ketan Doshi

Transformers multi-head attention

1. The different attention heads are focusing on different words as we encode the word it.



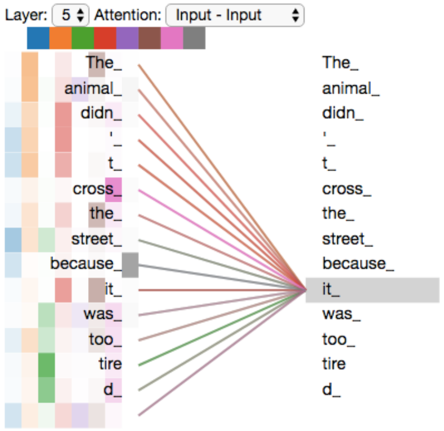


Figure: Jay Alammar

Transformers decoder attention layers

1. The attention layers of Transformers decoder are

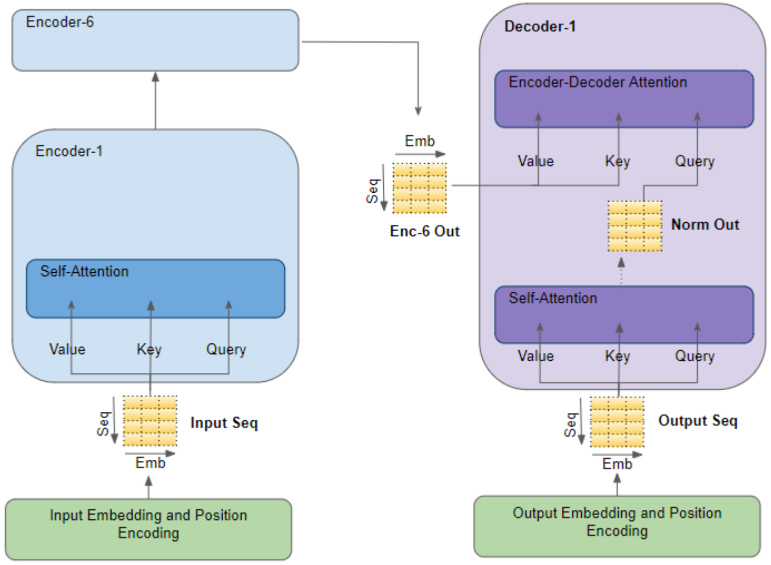


Figure: Ketan Doshi

Transformers decoder self-attention and masking

1. The Decoder Self-Attention works just like the Encoder Self-Attention, except that it operates on each word of the target sequence.

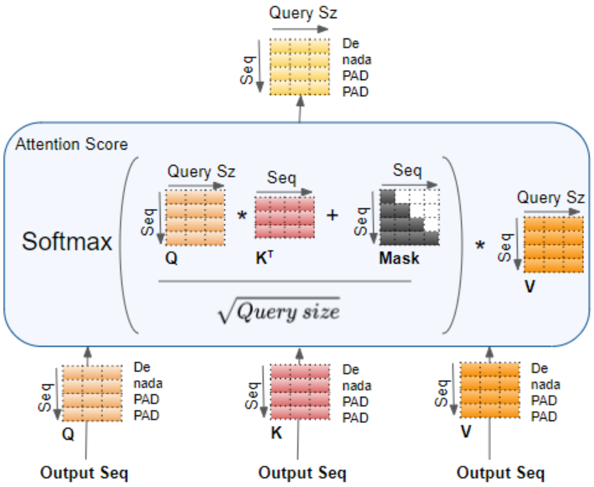


Figure: Ketan Doshi

Transformers decoder encoder-decoder attention and masking

1. The Encoder-Decoder Attention takes its input from two sources.
2. The Encoder-Decoder Attention computes the interaction between each target word with each input word.
3. The Masking masks out the Padding words in the target sequence.

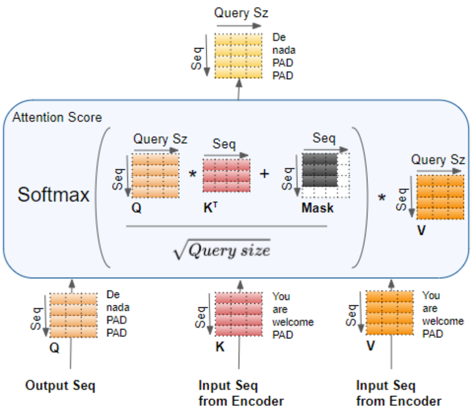


Figure: Ketan Doshi

Simple Neural Attention Meta-Learner (SNAIL)

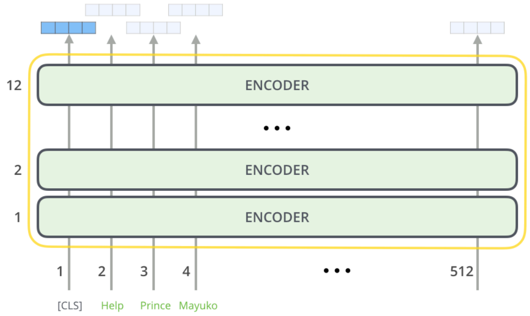
1. The SNAIL was developed partially to resolve the problem with positioning in the transformer model by combining the self-attention mechanism in transformer with convolutions (Mishra et al. 2018).
2. It has been demonstrated to be good at both supervised learning and reinforcement learning tasks.

Transformers family

BERT model

BERT model

1. BERT (Pre-training of Deep Bidirectional Transformers for Language Understanding) is basically a trained Transformers Encoder stack (Devlin et al. 2019).
2. Each position outputs a vector. For the sentence classification, we focus on the output of only the first position ([CLS]).
3. That vector can now be used as the input for a classifier. The paper achieves great results by just using a single-layer neural network as the classifier.



4. BERT makes use of a novel technique called Masked LM (MLM): it randomly masks words in the sentence and then it tries to predict them.

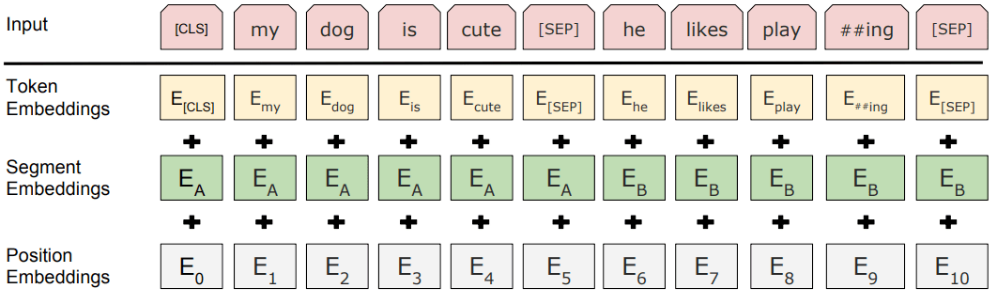
BERT model

1. BERT needs the input to be massaged and decorated with some extra meta data:

   Token embeddings A [CLS] token is added to the input word tokens at the beginning of the first sentence and a [SEP] token is inserted at the end of each sentence.

   Segment embeddings A marker indicating Sentence A or Sentence B is added to each token. This allows the encoder to distinguish between sentences.

   Positional embeddings A positional embedding is added to each token to indicate its position in the sentence.



Input
[CLS] my dog is cute [SEP] he likes play ##ing [SEP]
Token Embeddings
$E_{[CLS]}$ E_{my} E_{dog} E_{is} E_{cute} $E_{[SEP]}$ E_{he} E_{likes} E_{play} $E_{\#\#ing}$ $E_{[SEP]}$
Segment Embeddings
E_A E_A E_A E_A E_A E_A E_B E_B E_B E_B E_B
Position Embeddings
E_0 E_1 E_2 E_3 E_4 E_5 E_6 E_7 E_8 E_9 E_{10}

BERT sentence classification

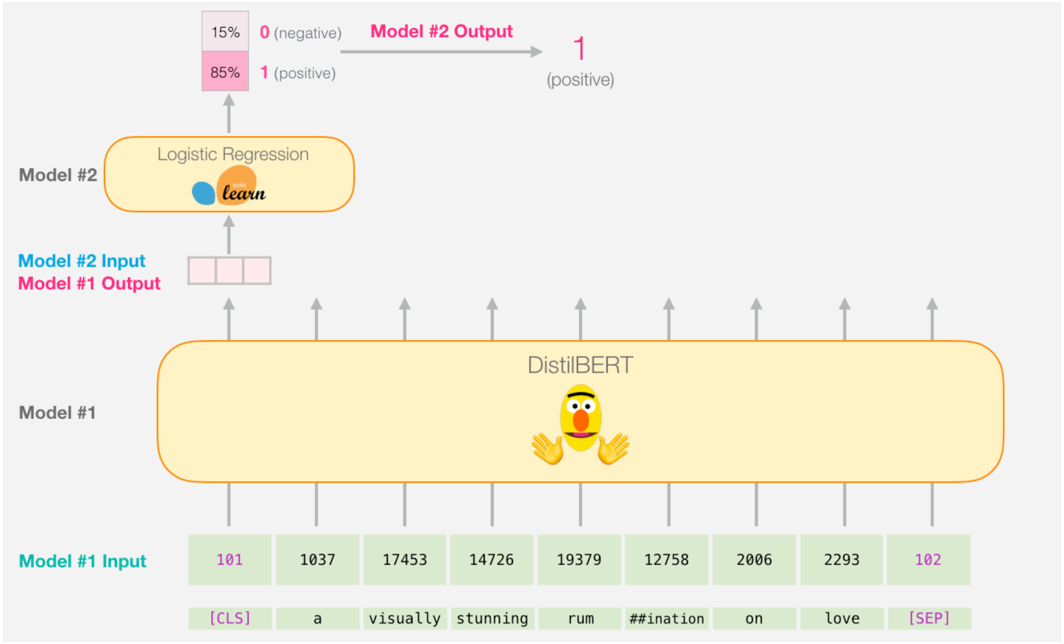


Figure: Jay Alammar

Training BERT using masked language model

1. Randomly mask out 15% of the words in the input (replacing them with a [MASK] token) .
2. Then run the entire sequence through the BERT attention based encoder and predict only the masked words, based on the context provided by the other non-masked words in the sequence.
3. The problem here is : the model only tries to predict when the [MASK] token is present in the input, while we want the model to try to predict the correct tokens regardless of what token is present in the input.
4. To deal with this issue, out of the 15% of the tokens selected for masking:
   - 80% of the tokens are actually replaced with the token [MASK].
   - 10% of the time tokens are replaced with a random token.
   - 10% of the time tokens are left unchanged.

Training BERT using next Sentence prediction model

1. To understand relationship between two sentences, BERT training process also uses next sentence prediction.
2. A pre-trained model with this kind of understanding is relevant for tasks like question answering.
3. During training the model gets as input pairs of sentences and it learns to predict if the second sentence is the next sentence in the original text as well.
4. BERT separates sentences with a special [SEP] token.
5. During training the model is fed with two input sentences at a time such that
   - 50% of the time the second sentence comes after the first one.
   - 50% of the time it is a a random sentence from the full corpus.
6. BERT is then required to predict whether the second sentence is random or not.
7. To predict if the second sentence is connected to the first one or not, the output of the [CLS] token is given to a classifier.

BERT pre-trained architecture

1. There are two types of pre-trained versions of BERT depending on the scale of the model architecture

   BERT-Base 12-layer, 768-hidden-nodes, 12-attention-heads, 110M parameters.

   BERT-Large 24-layer, 1024-hidden-nodes, 16-attention-heads, 340M parameters.

Transformers family

GPT-2 model

GPT-2 model

1. The GPT-2 is built using transformer decoder blocks (Radford et al. 2019).
2. BERT uses transformer encoder blocks.
3. A key difference between the two is that GPT2 outputs one token at a time.

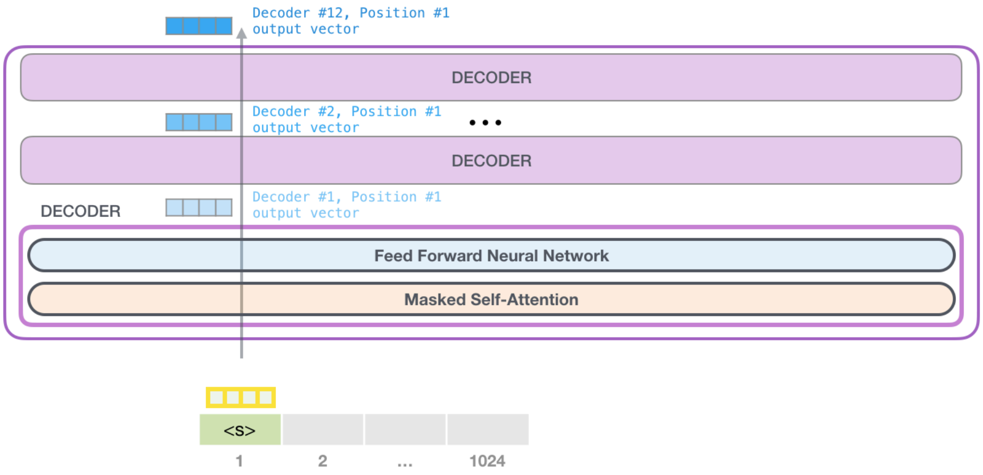


Figure: Jay Alammar

GPT-2 pre-trained architecture

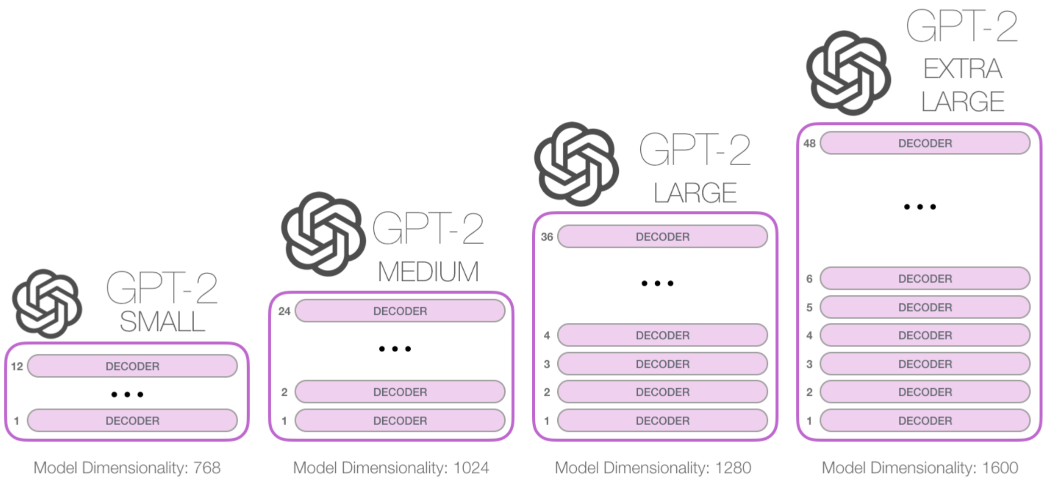
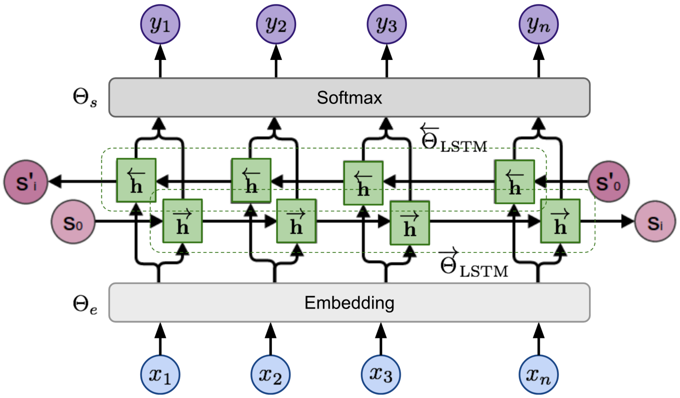


Figure: Jay Alammar

ELMo model

Embeddings from Language Model (ELMo)

1. ELMo learns contextualized word representation by pre-training a language model in an unsupervised way (Peters et al. 2018).



y_1
y_2
y_3
y_n
Θ_s
Softmax
$\overleftarrow{\Theta}_{\text{LSTM}}$
S'i
S'0
S0
Si
$\overleftarrow{\mathbf{h}}$
$\overrightarrow{\mathbf{h}}$
$\overrightarrow{\Theta}_{\text{LSTM}}$
Θ_e
Embedding
x_1
x_2
x_3
x_n

Embeddings from Language Model (ELMo)

1. The bidirectional Language Model (biLM) is the foundation for ELMo.
2. While the input is a sequence of n tokens, $(x_1, \ldots, x_n)$, the language model learns to predict the probability of next token given the history.
3. In the forward pass, the history contains words before the target token,

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_1, \ldots, x_{i-1})$$

4. In the backward pass, the history contains words after the target token,

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i \mid x_{i+1}, \ldots, x_n)$$

5. The predictions in both directions are modeled by multi-layer LSTMs with hidden states.

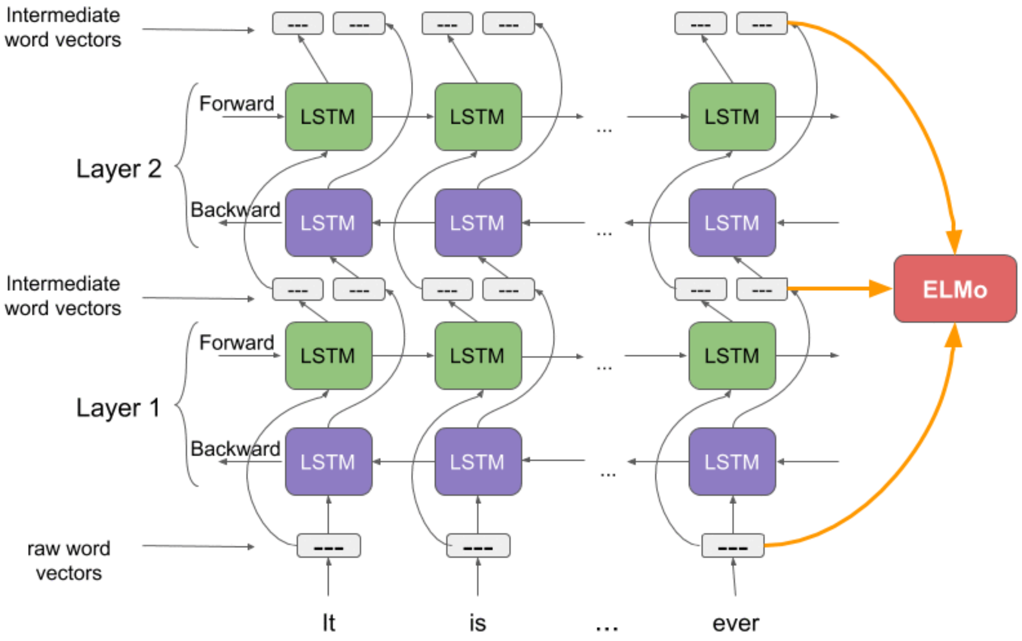
Embeddings from Language Model (ELMo)

1. The model is trained to minimize the negative log likelihood (= maximize the log likelihood for true words) in both directions:

$$\mathcal{L} = -\sum_{i=1}^{n} \Big(\log p(x_i \mid x_1, \ldots, x_{i-1}; \Theta_e, \overrightarrow{\Theta}_{\text{LSTM}}, \Theta_s) + \log p(x_i \mid x_{i+1}, \ldots, x_n; \Theta_e, \overleftarrow{\Theta}_{\text{LSTM}}, \Theta_s) \Big)$$

2. ELMo word representations are functions of the entire input sentence.
3. A linear combination of the vectors stacked above each input word is learned as the representation of each token.

Embeddings from Language Model (ELMo)



Reading

References i

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Questions?