Recent Advances of Language Transformer Machine

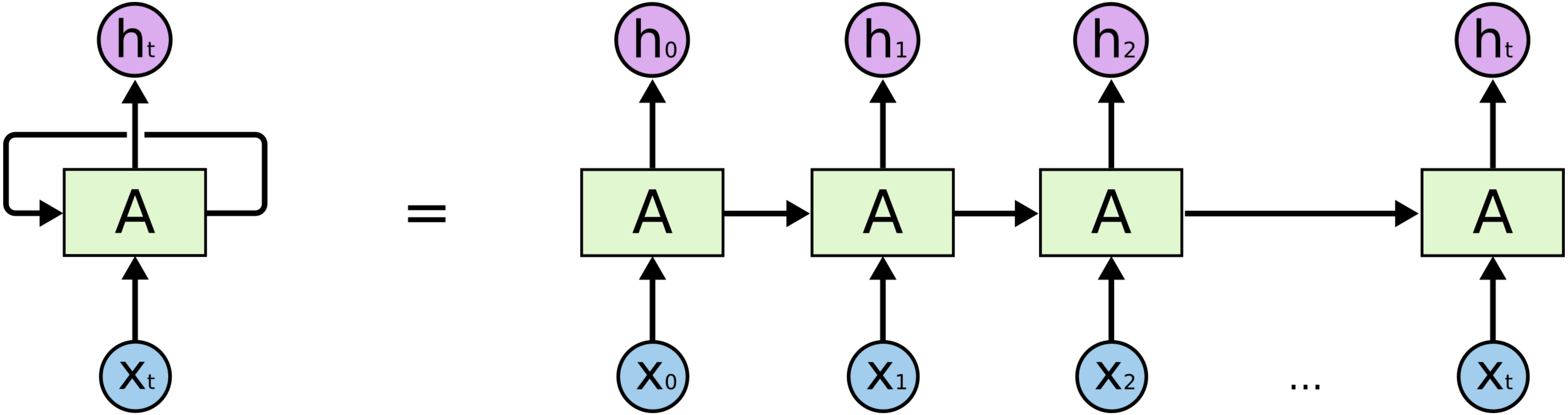
Presenters: Lecheng Zheng, Dawei Zhou

Outline

- Recurrent Neural Networks (RNN)
- Long-Short Term Memory (LSTM)
- Transformer
    - Encoder
    - Multi-head Attention
    - Decoder

Recurrent Neural Networks

- The Recurrent Neural Network $\boldsymbol{A}$ processes some input x_i and outputs h_i. A loop allows information to be passed from one state to the next.
- It aims to learn the dependencies of words.



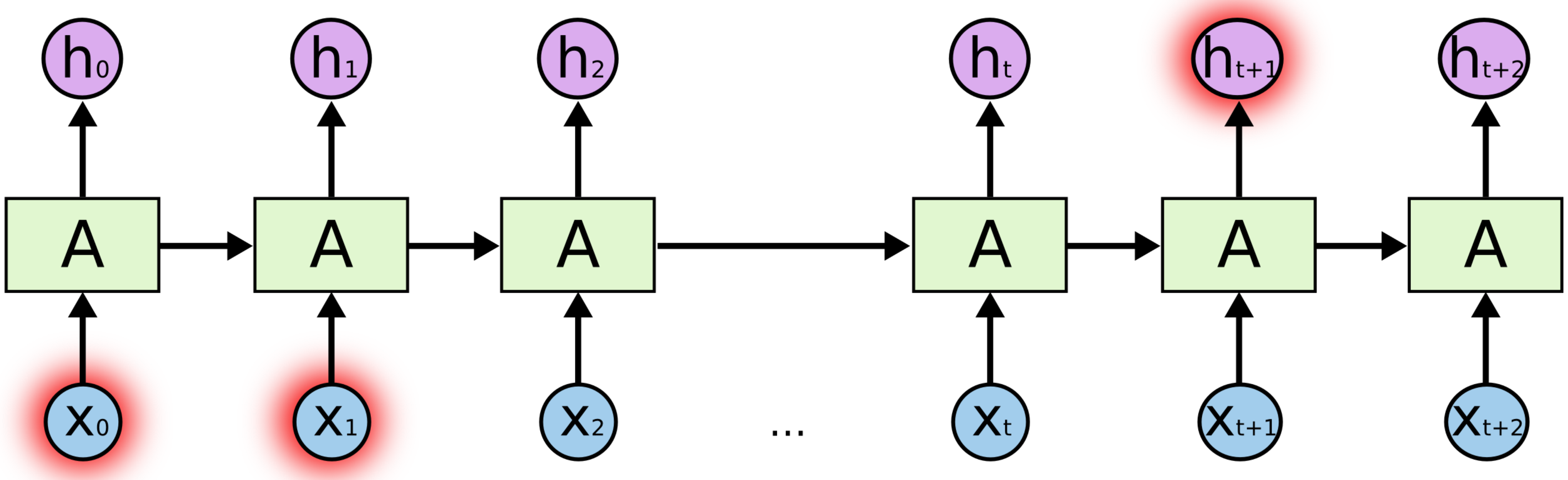
The problem of long-term dependencies

- If we are trying to predict the next word of the sentence **“the clouds in the __”**, we don’t need further context. It’s pretty obvious that the next word is going to be **sky.**

- However**,** you are trying to predict the last word of the text: “Tom grew up in France… Tom can speak fluent __?”**.**
  - Recent information suggests that the next word is probably a language.
  - If we want to narrow down which language, we need context of France, that is further back in the text.

The problem of long-term dependencies

- In theory, RNNs could learn this long-term dependencies.
- In practice, they don’t seem to learn them, as the model often forgets the content of distant positions in the sequence.



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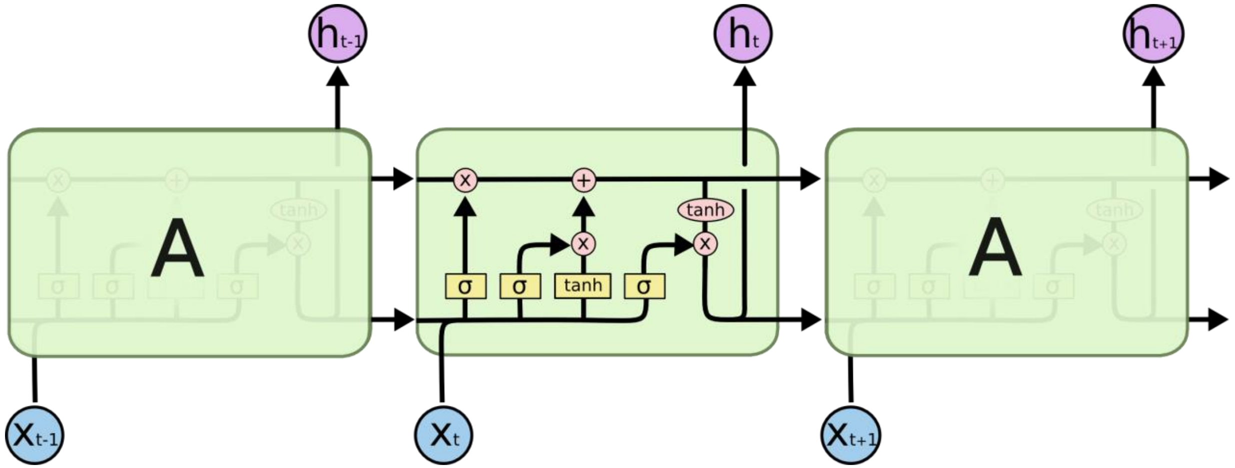
Long-Short Term Memory (LSTM)

- Each cell takes as inputs x_t, the previous cell state c_{t-1} and the output of the previous cell h_{t-1}.
- It generates a new cell state c_t, and an output h_t.
- The forget gate is responsible for removing irrelevant information and remember important information.



The problem with LSTMs

- The same problem that happens to RNNs generally, happen with LSTMs, i.e. when sentences are too long (maybe a paragraph) LSTMs still don’t do too well.

- The reason is that the probability of keeping the context from a word that is far away from the current word being processed decreases exponentially with the distance from it.

- That means that when sentences are too long, the model often forgets the content of distant positions in the sequence.

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What is a transformer?

- Transformer is a type of neural network architecture, which is developed to solve the problem of **neural machine translation.**
    - Speech recognition
    - Text-to-speech transformation
    - Language translation

Why transformer?

- **Efficiency is the key!**

- Feed forward layer of transformer could be computed in parallel.

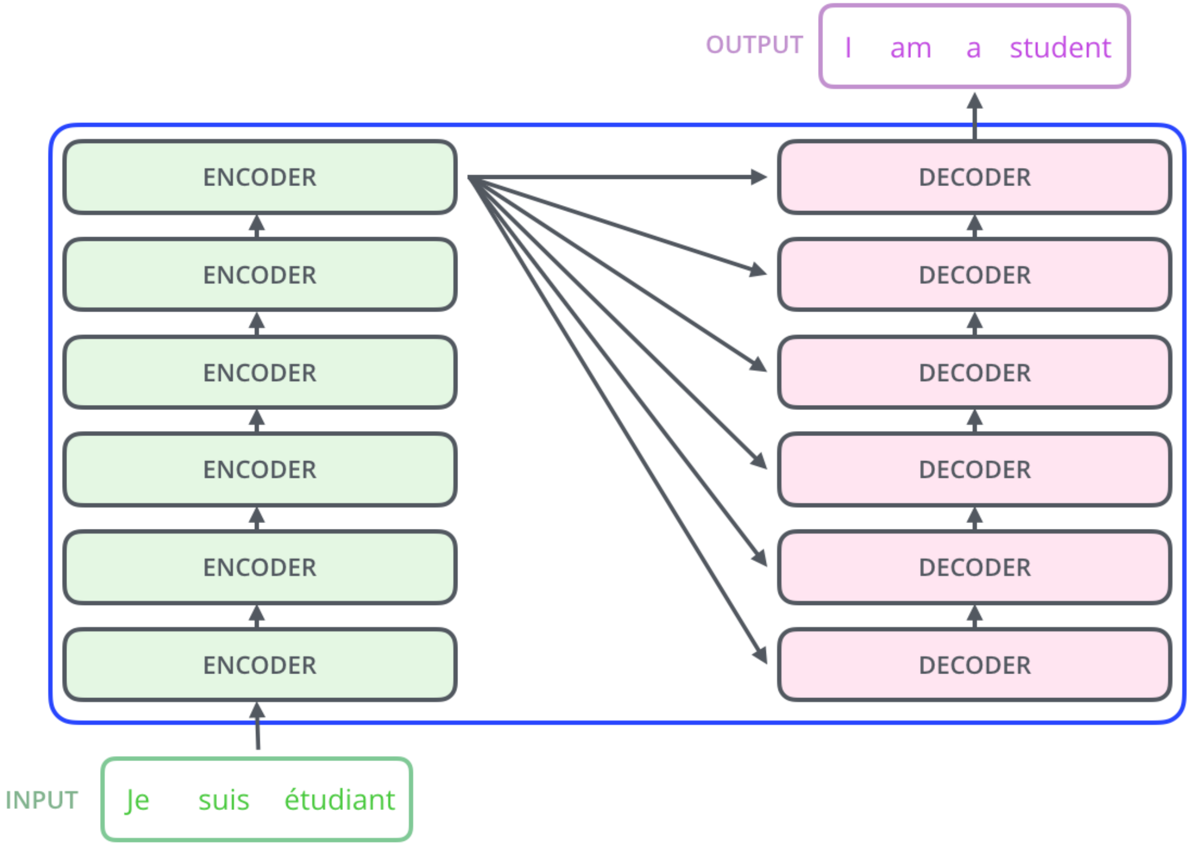
- Transformers try to solve the problem by using Convolutional Neural Networks together with attention models**.**

- Attention boosts the speed of how fast the model can translate from one sequence to another.

Structure of Transformer

- The transformer consists of encoders and decoders.

- The transformer shown in the figure on the right hand side stacks six encoders and six decoders.



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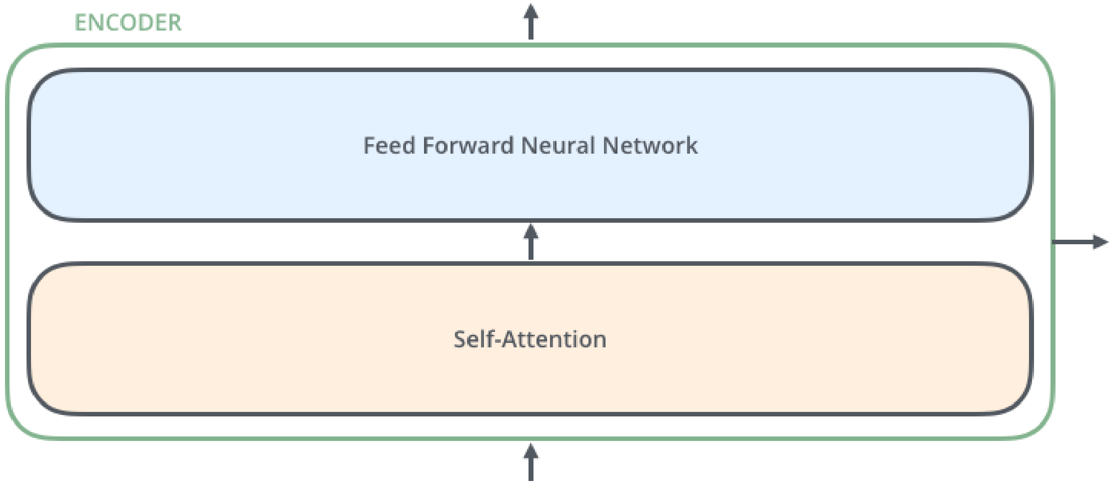
Encoder of a transformer

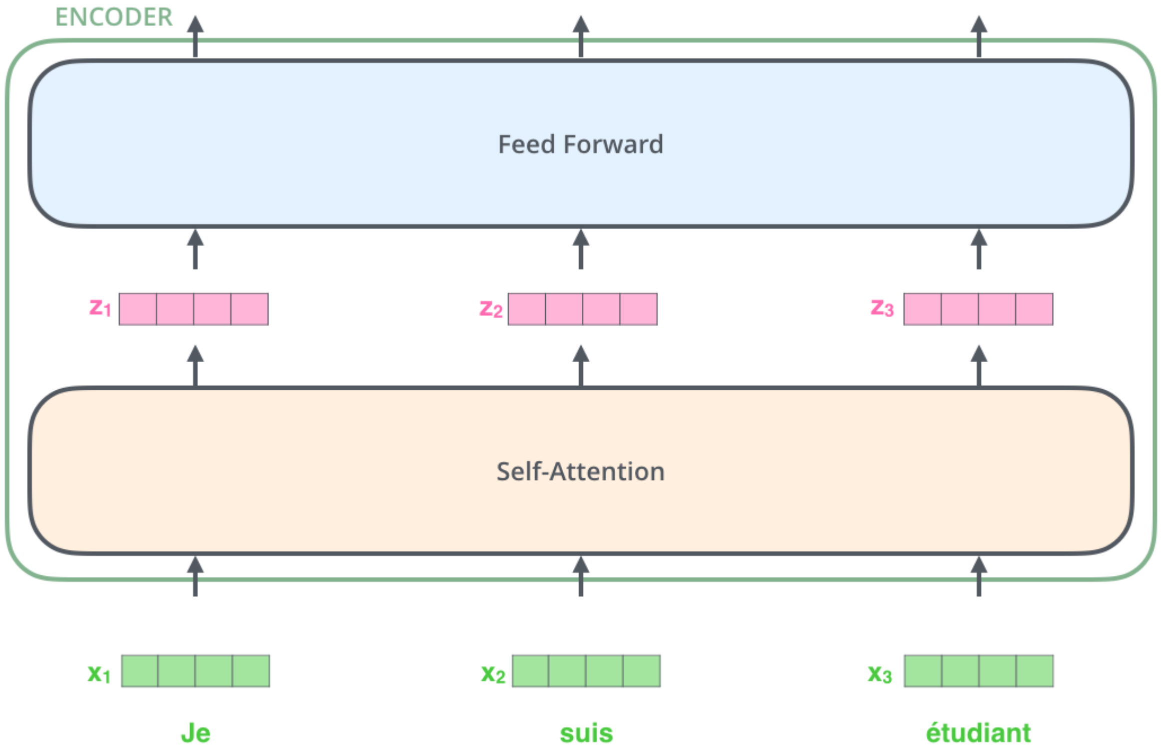
- Each encoder consists of two layers: Self-Attention Layer and Feed Forward Neural Network.

- The goals of self-attention layer
  - To learn the dependencies between the words in the sentence.
  - To use that information to capture the internal structure of the sentence.



Encoder

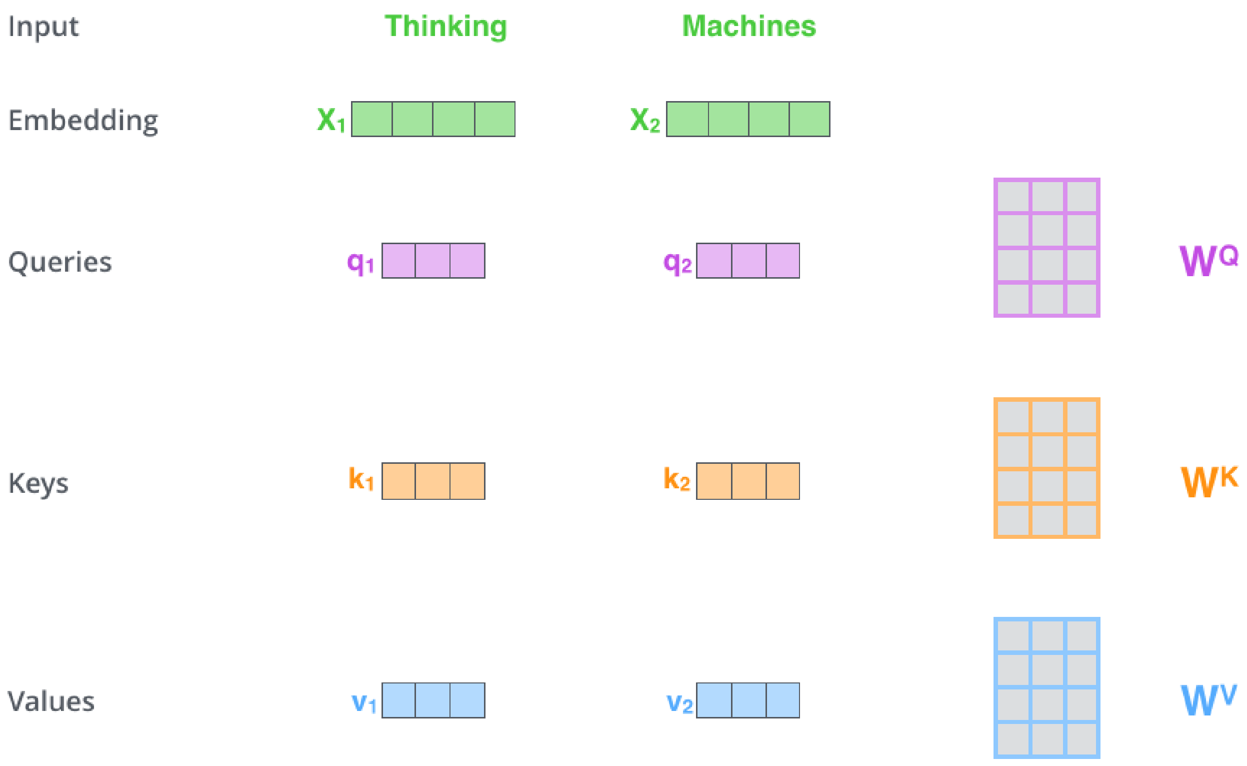
- The input of the encoder is the word embeddings.
- There are dependencies between words in the self-attention layer.
- The feed-forward layer does not have those dependencies, and thus the various paths can be executed in parallel.



Self-Attention Layer of Encoder

- The first step: for each word, we create a Query vector, a Key vector, and a Value vector, where $X_i \in R^{i \times d}$ is a word embedding, $W^Q \in R^{d \times p}$, $W^k \in R^{d \times p}$, $W^v \in R^{d \times p}$ are three weight matrices (hyperparameters), $q_i \in R^{1 \times p}$, $k_i \in R^{1 \times p}$, $v_i \in R^{1 \times p}$ are three vectors.

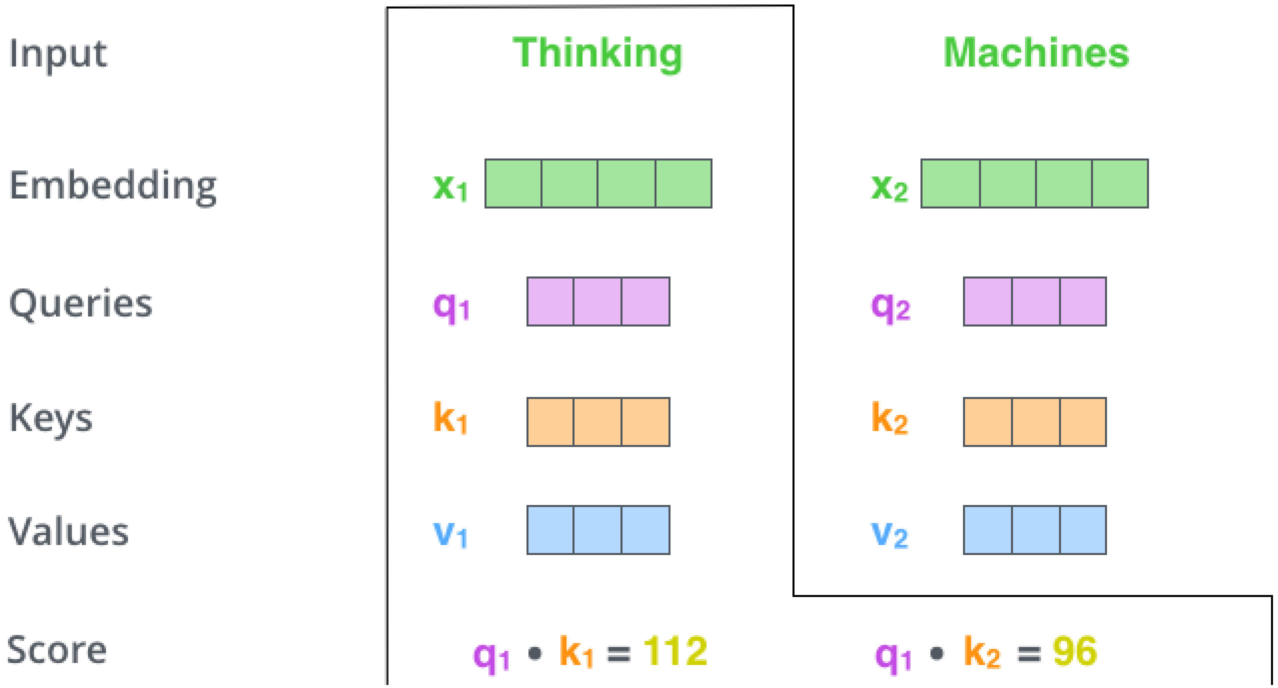
- Multiplying X_1 by the weight matrix W^Q produces q_1 (similar for v_1 and k_1).



Self-Attention Layer of Encoder

- The second step: we need to score each word of the input sentence against this word.

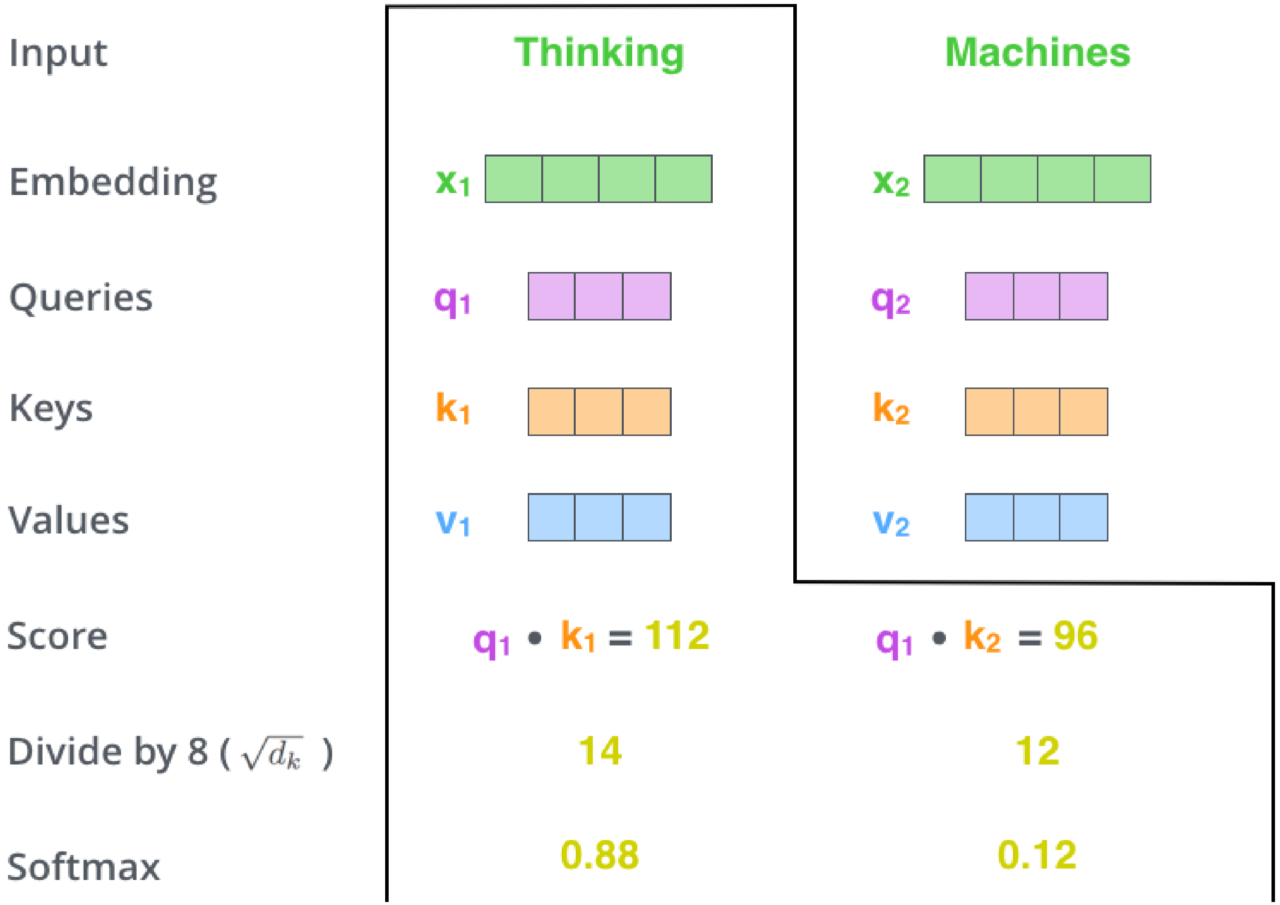
- The score determines how much focus to place on other words as we encode a word at a certain position.



Self-Attention Layer of Encoder

- The third step is to divide the scores by the square root of the dimension of the key vectors. This leads to having more stable gradients.

- The fourth step is to pass the result through a Softmax operation.

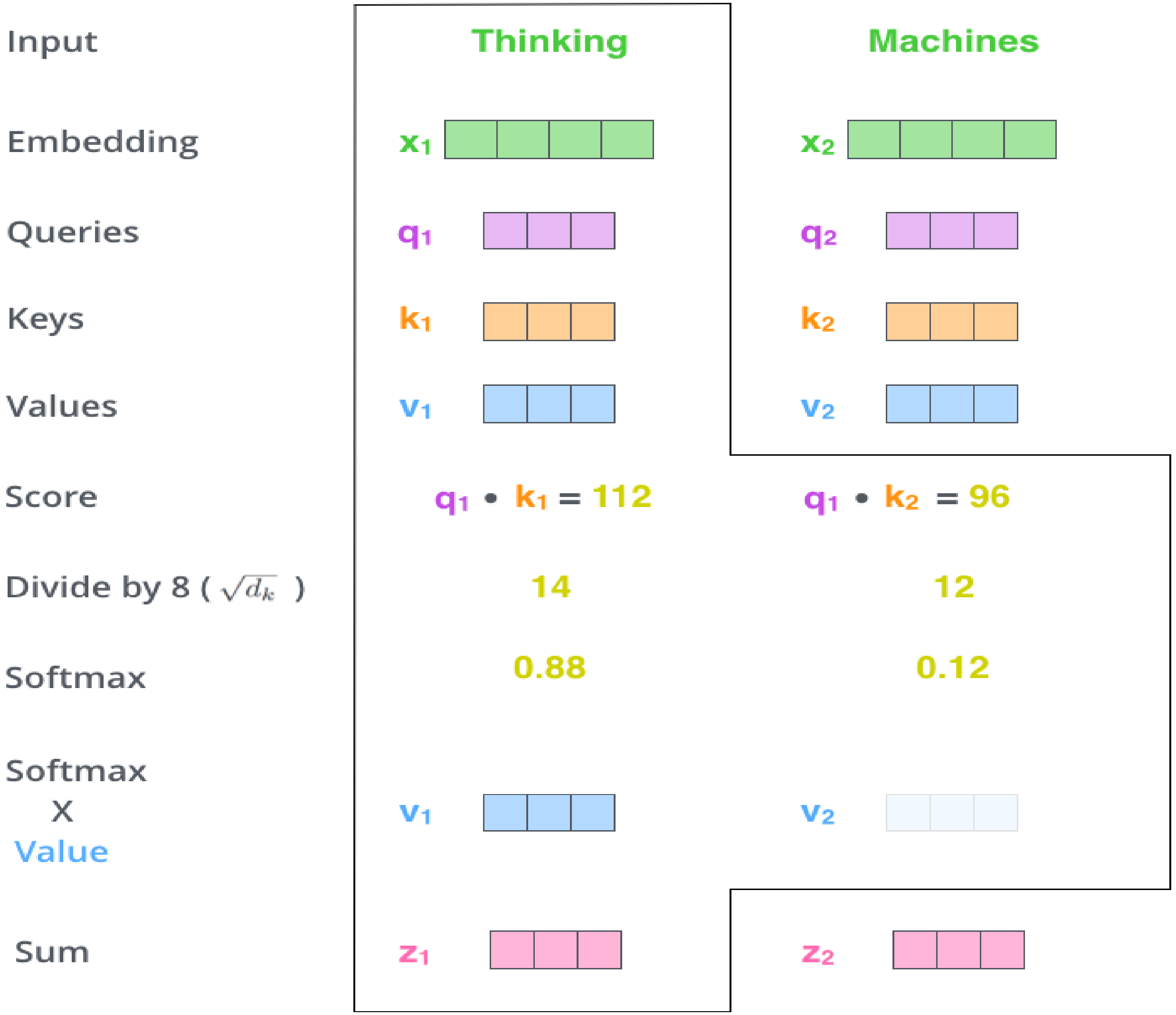


Self-Attention Layer of Encoder

- The fifth step is to multiply each value vector v_i by the Softmax score.

- The intuition here is to keep intact values of the word(s) we want to focus on, and dropout irrelevant words.

- The sixth step is to sum up the weighted value vectors.



Input: Thinking, Machines

Embedding: x_1, x_2

Queries: q_1, q_2

Keys: k_1, k_2

Values: v_1, v_2

Score: $q_1 \bullet k_1 = 112$, $q_1 \bullet k_2 = 96$

Divide by 8 ($\sqrt{d_k}$): 14, 12

Softmax: 0.88, 0.12

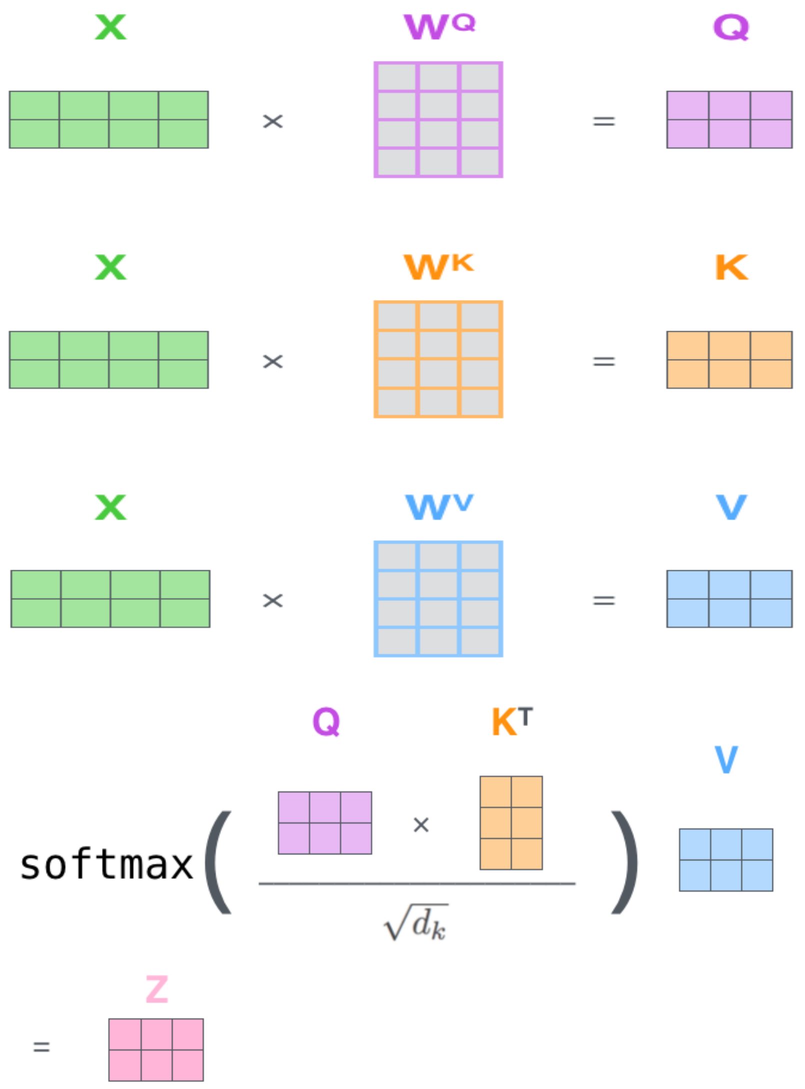
Softmax X Value: v_1, v_2

Sum: z_1, z_2

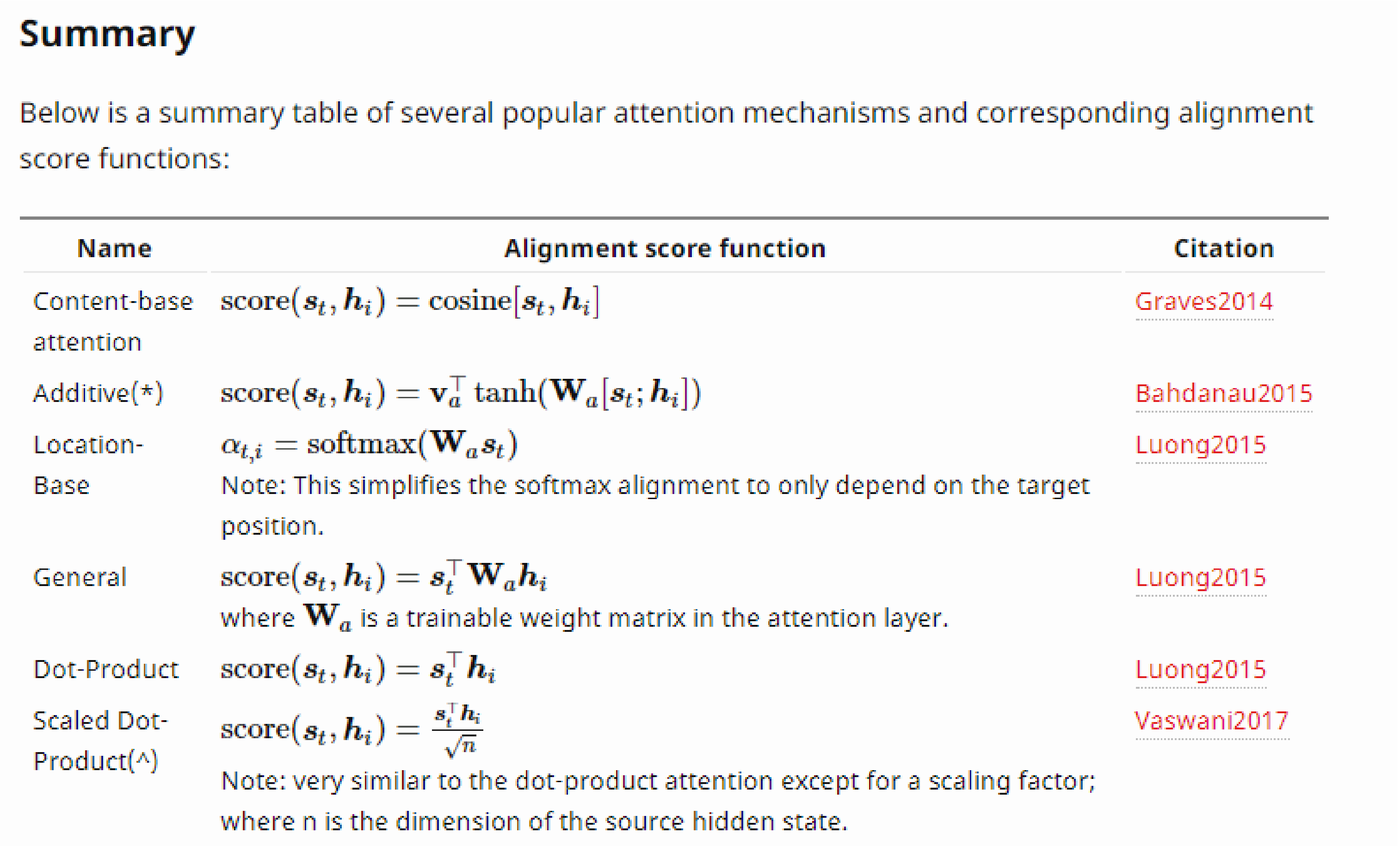
Recap: Self-Attention in Encoder

- The first step is to calculate the Query, Key, and Value matrices.

- Steps two through six, we calculate the outputs of the self-attention layer.



A Family of Attention Score Functions



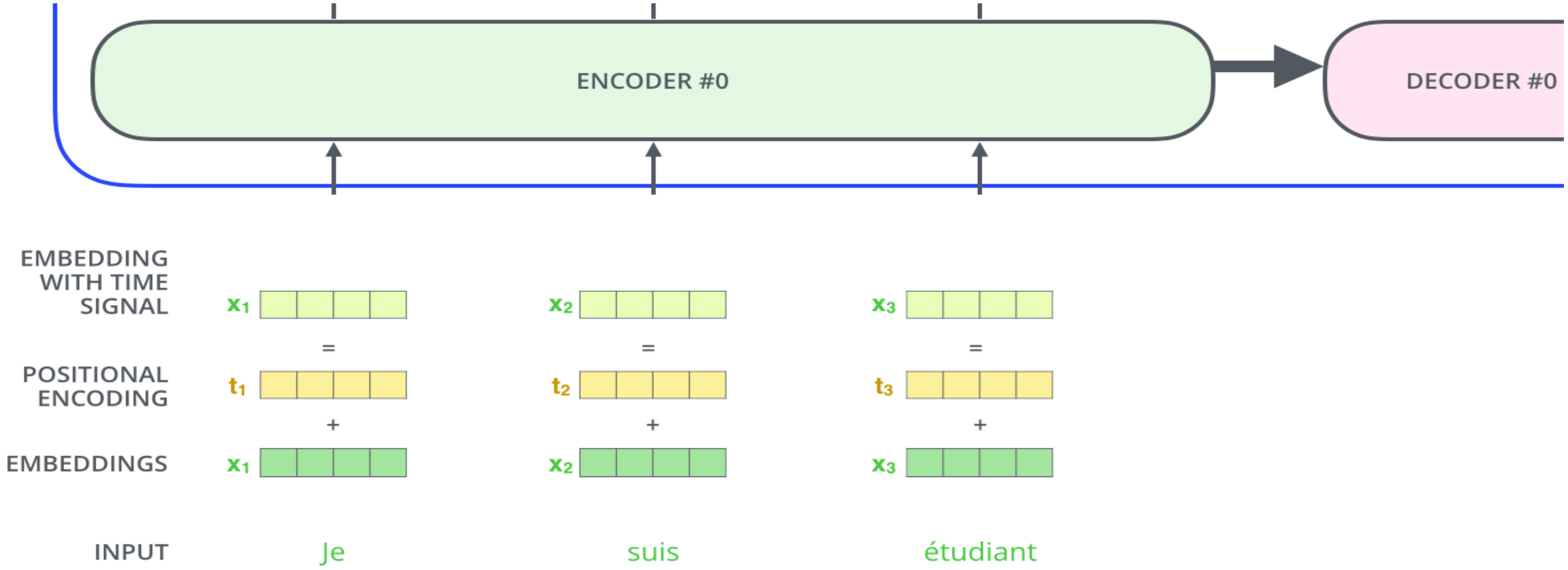
Summary

Below is a summary table of several popular attention mechanisms and corresponding alignment score functions:

Name	Alignment score function	Citation
Content-base attention	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \text{cosine}[\boldsymbol{s}_t, \boldsymbol{h}_i]$	Graves2014
Additive(*)	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \mathbf{v}_a^\top \tanh(\mathbf{W}_a[\boldsymbol{s}_t; \boldsymbol{h}_i])$	Bahdanau2015
Location-Base	$\alpha_{t,i} = \text{softmax}(\mathbf{W}_a \boldsymbol{s}_t)$ Note: This simplifies the softmax alignment to only depend on the target position.	Luong2015
General	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \mathbf{W}_a \boldsymbol{h}_i$ where $\mathbf{W}_a$ is a trainable weight matrix in the attention layer.	Luong2015
Dot-Product	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \boldsymbol{h}_i$	Luong2015
Scaled Dot-Product(^)	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \frac{\boldsymbol{s}_t^\top \boldsymbol{h}_i}{\sqrt{n}}$ Note: very similar to the dot-product attention except for a scaling factor; where n is the dimension of the source hidden state.	Vaswani2017

Positional Encoding

- To account for the order of the words in the input or output sequence, the transformer adds a vector to each input embedding to determine the position of each word.

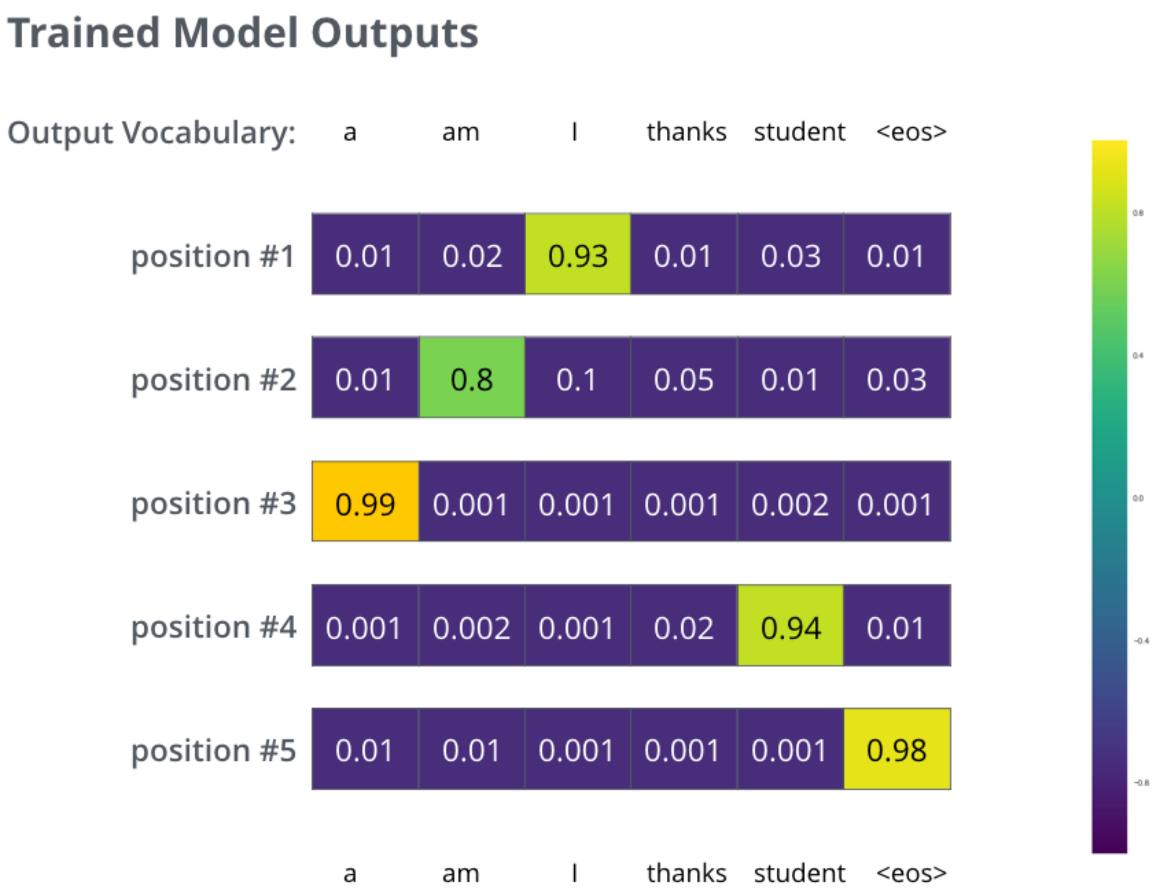


The intuition Behind Positional Encoding

- 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.

Positional Encoding

- In the positional encodings $U \in R^{L \times d}$, L is length of sequence and d is vocabulary size, and the i-th row U_i corresponds to the i-th word in the input/output sequence.
- Example of French to English translation:
  - input: “je suis étudiant”.
  - output: “I am a student”.
  - Token <eos> means the end of the sentence.



Trained Model Outputs

Output Vocabulary:	a	am	I	thanks	student	<eos>
position #1	0.01	0.02	0.93	0.01	0.03	0.01
position #2	0.01	0.8	0.1	0.05	0.01	0.03
position #3	0.99	0.001	0.001	0.001	0.002	0.001
position #4	0.001	0.002	0.001	0.02	0.94	0.01
position #5	0.01	0.01	0.001	0.001	0.001	0.98
	a	am	I	thanks	student	<eos>

0.8
0.4
0.0
−0.4
−0.8

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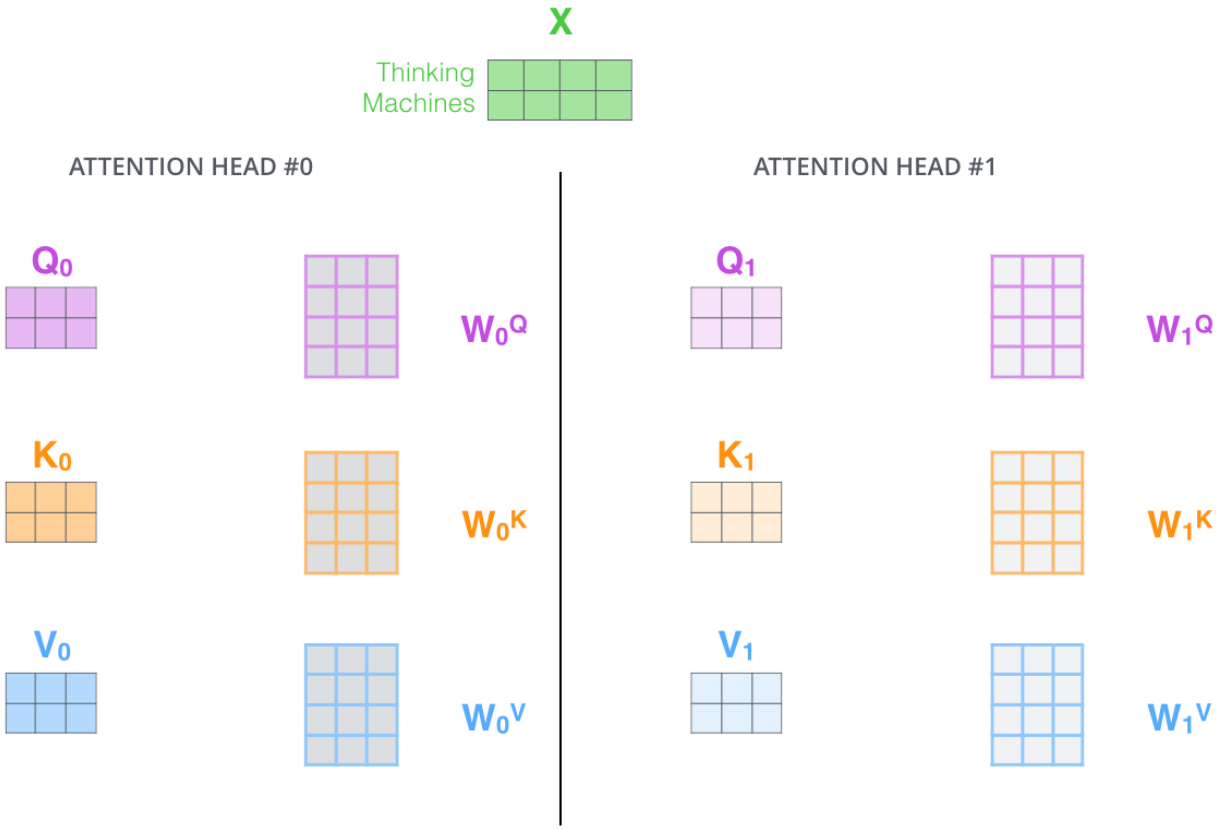
Benefits of Multi-head Attention

- It expands the model’s ability to focus on different positions.
  - In a single attention layer, output vector z contains a little bit of every other encoding, but it could be still dominated by the actual word itself.
  - If we’re translating a sentence like “The animal didn’t cross the street because it was too tired”, we would want to know which word “it” refers to.

- It gives the attention layer multiple “representation subspaces”.
  - With multi-headed attention we have multiple sets of Query/Key/Value weight matrices, and different representation subspace.

Multi-head Self Attention

- If we do the same self-attention calculation we outlined before, just eight different times with different weight matrices, we end up with eight different Z matrices or eight different representation subspace.



Multi-head Self Attention

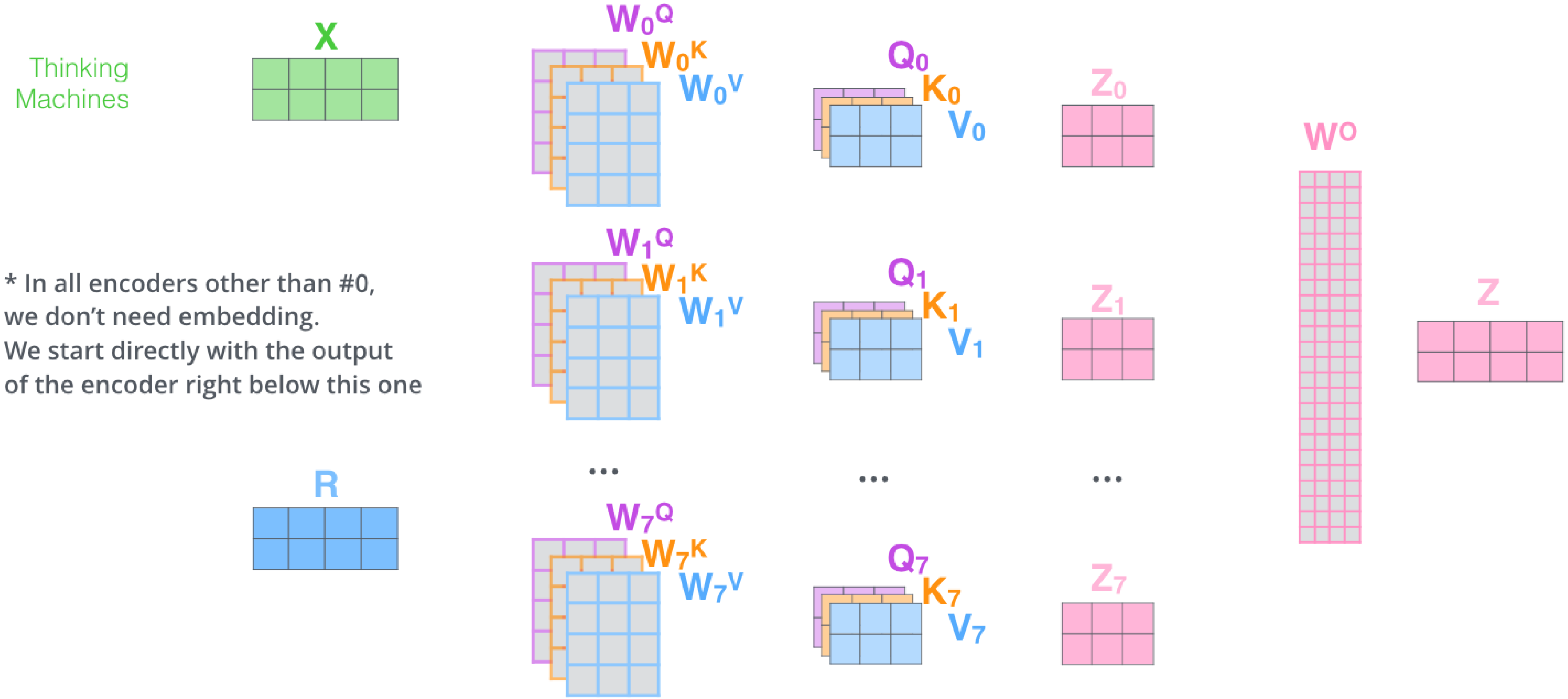
1) This is our input sentence*

2) We embed each word*

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



* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one

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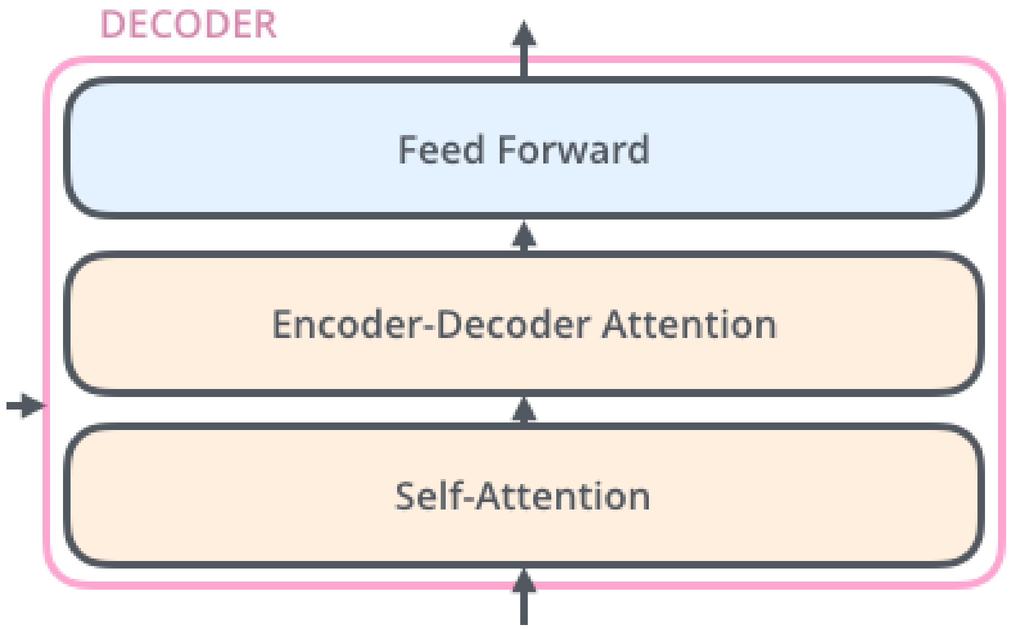
Decoder of a transformer

- The decoder has both those layers, but between them is an another attention layer (Encoder-Decoder Attention Layer) that helps the decoder focus on relevant parts of the input sentence.

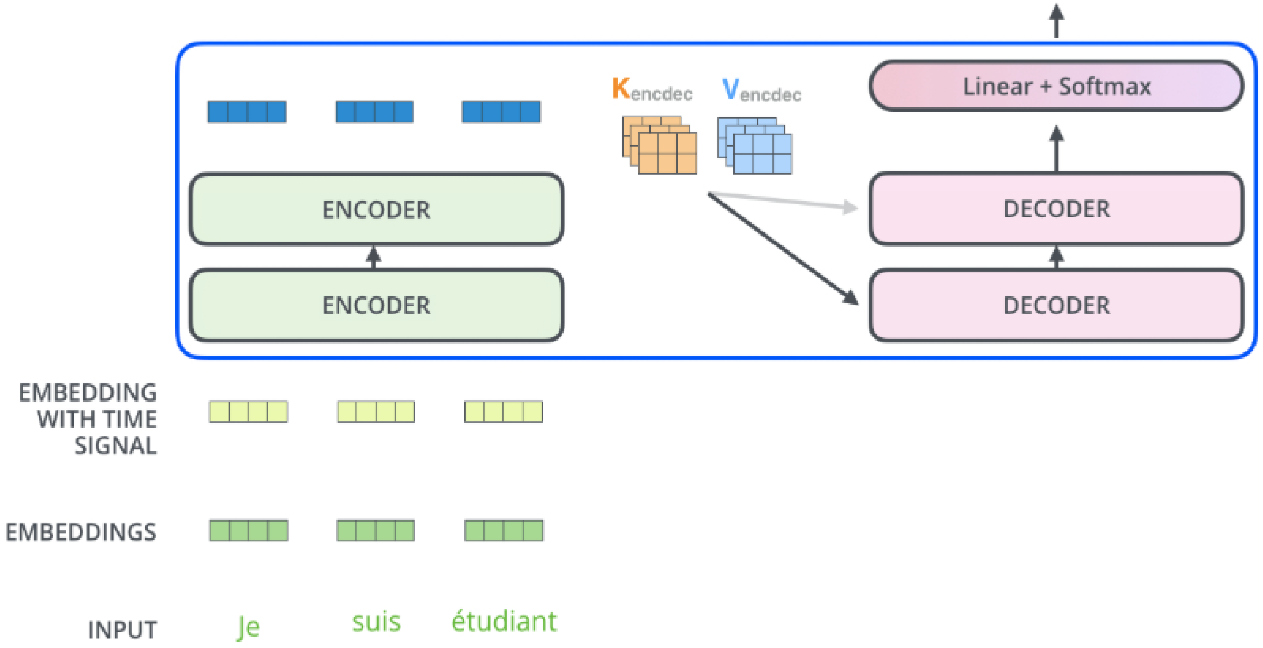
- The self-attention layer and feed forward network of a decoder work similarly to that of encoder.



Encoder-Decoder Attention Layer of Decoder

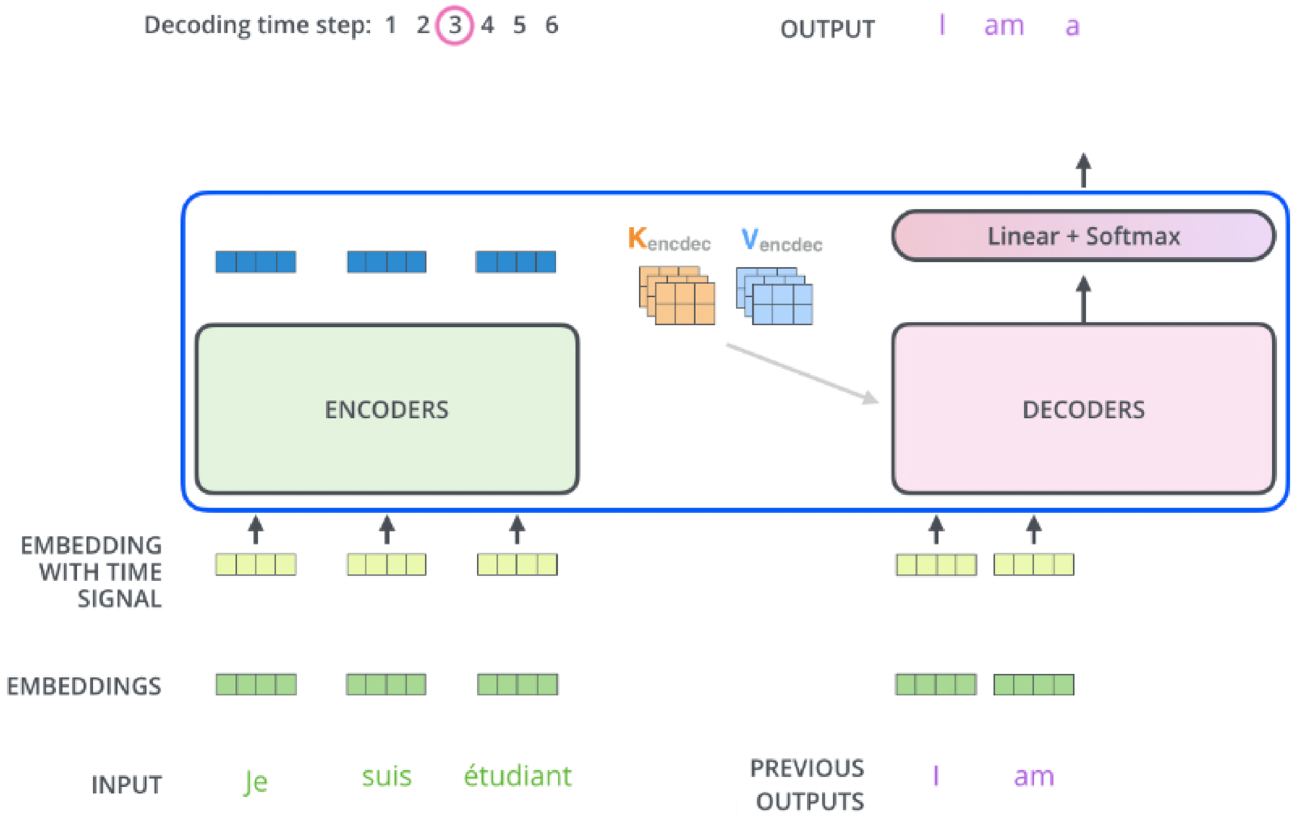
- The output of the top encoder is transformed into a set of attention vectors K and V.

- Just like we did with the encoder inputs, we embed and add positional encoding to those decoder inputs to indicate the position of each word.



Encoder-Decoder Attention Layer of Decoder

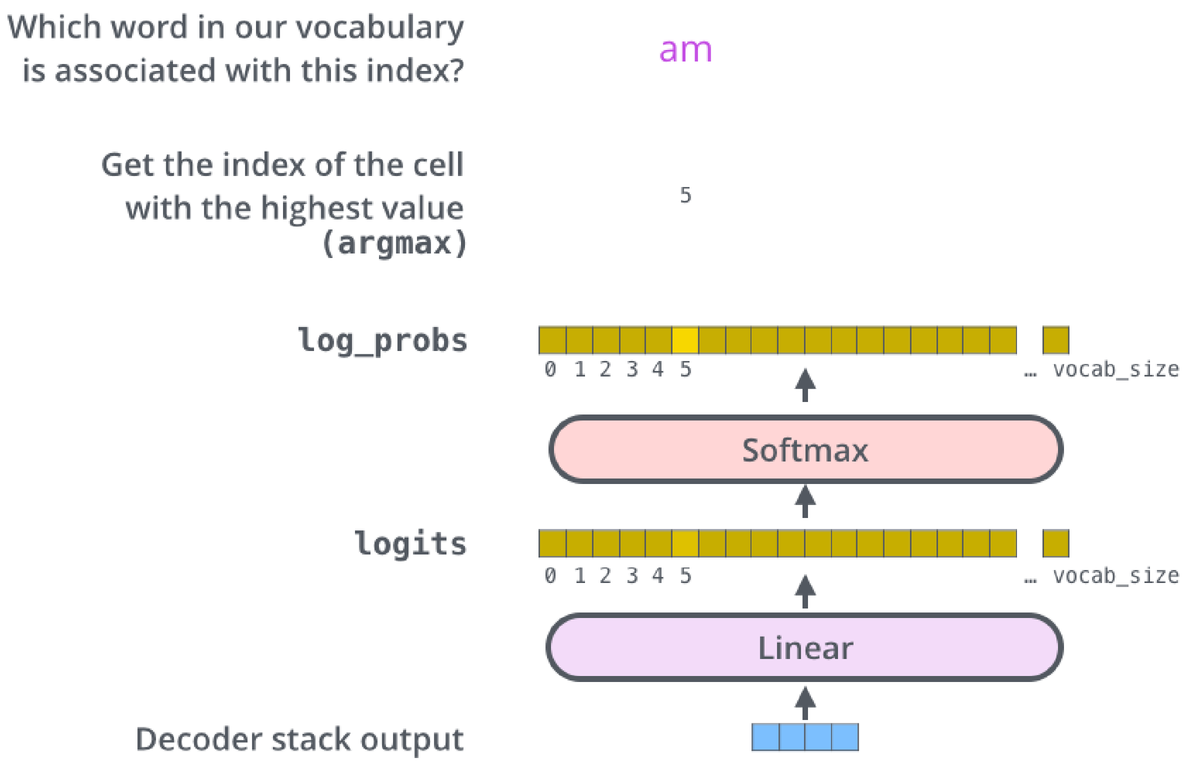
- These output vectors are used by each decoder in its encoder-decoder attention layer to help the decoder focus on appropriate places in the input sequence.



Linear and Softmax Layer of Decoder

- The Linear layer projects the output of decoders to a logits vector.

- The Softmax layer then turns those scores into probabilities.


Which word in our vocabulary is associated with this index?
am
Get the index of the cell with the highest value (argmax)
5
log_probs
0 1 2 3 4 5 … vocab_size
Softmax
logits
0 1 2 3 4 5 … vocab_size
Linear
Decoder stack output

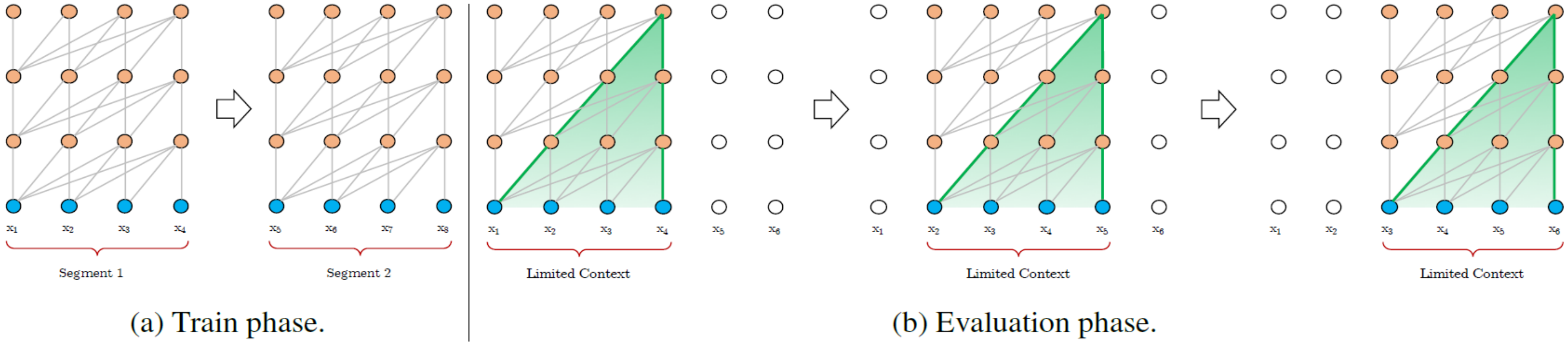
Useful Tutorial

- How Transformers Work
- http://jalammar.github.io/illustrated-transformer/
- Attention? Attention!
- http://nlp.seas.harvard.edu/2018/04/03/attention.html

Transformer XL: Attentive Language Models Beyond a Fixed-Length Context

Vanilla model

- The central problem is how to effectively encode an arbitrarily long context into a fixed size representation.
- Vanilla model splits the entire corpus into shorter segments of manageable sizes, and ignore all contextual information from previous segments.



(a) Train phase.

(b) Evaluation phase.

Figure 1: Illustration of the vanilla model with a segment length 4.

Major limitations of vanilla model

- The largest possible dependency length is upper bounded by the segment length.

- The model lacks necessary contextual information needed to well predict the first few symbols.

- Simply chunking a sequence into fixed-length segments lead to inefficient optimization and inferior performance.

Transformer-XL: Segment-Level Recurrence with State Reuse

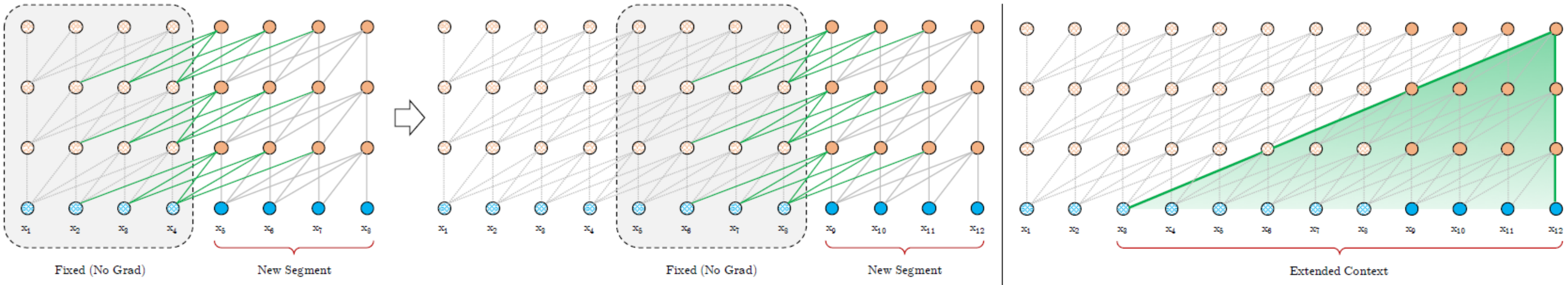
- To address these limitations, they take the advantage of the recurrence mechanism and apply it to the Transformer architecture.

- The goal of this mechanism is to enable long-term dependencies with the information from previous segments.

- Transformer-XL processes the first segment of tokens but keeps the output of the hidden layers. When the next segment is processed, each hidden layer receives two inputs.

Transformer-XL: Segment-Level Recurrence with State Reuse

- Two inputs:
  - The output of the previous hidden layer of that segment.
  - The output of the previous hidden layer from the previous segment.
- Advantages: Incorporate longer dependencies and speed up the evaluation.

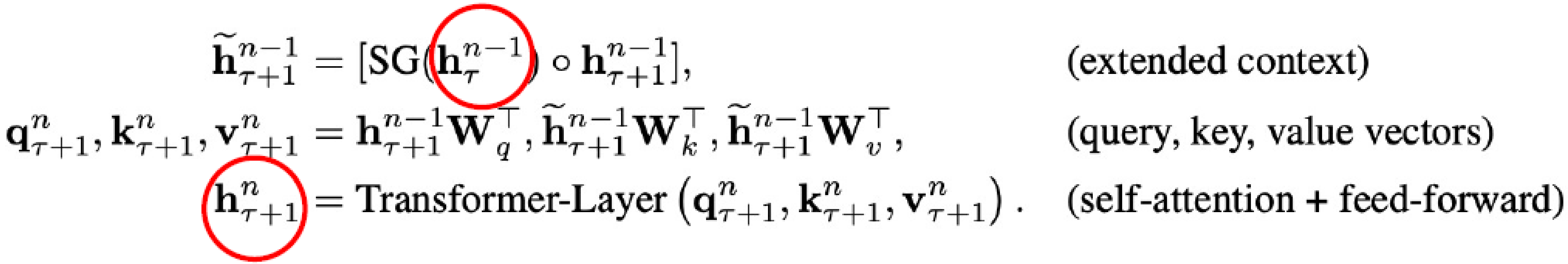

x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8
Fixed (No Grad)
New Segment
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10} x_{11} x_{12}
Fixed (No Grad)
New Segment
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10} x_{11} x_{12}
Extended Context

(a) Training phase.

(b) Evaluation phase.

Transformer-XL: Segment-Level Recurrence with State Reuse

- Let the two consecutive segments of length L be $s_\tau = [x_{\tau,1}, \ \dots, x_{\tau,L}]$ and $s_{\tau+1} = [x_{\tau+1,1}, \ \dots, x_{\tau+1,L}]$, respectively.
- Denote the n-th layer hidden state sequence produced for the τ -th segment s_τ as $h_\tau^n \in R^{L\times d}$, where d is the hidden dimension.
- The n-th layer hidden state for segment $s_{\tau+1}$ is produced as follows,



$$\widetilde{\mathbf{h}}_{\tau+1}^{n-1} = [\mathrm{SG}(\mathbf{h}_\tau^{n-1}) \circ \mathbf{h}_{\tau+1}^{n-1}], \qquad \text{(extended context)}$$

$$\mathbf{q}_{\tau+1}^n, \mathbf{k}_{\tau+1}^n, \mathbf{v}_{\tau+1}^n = \mathbf{h}_{\tau+1}^{n-1}\mathbf{W}_q^\top, \widetilde{\mathbf{h}}_{\tau+1}^{n-1}\mathbf{W}_k^\top, \widetilde{\mathbf{h}}_{\tau+1}^{n-1}\mathbf{W}_v^\top, \qquad \text{(query, key, value vectors)}$$

$$\mathbf{h}_{\tau+1}^n = \text{Transformer-Layer}\left(\mathbf{q}_{\tau+1}^n, \mathbf{k}_{\tau+1}^n, \mathbf{v}_{\tau+1}^n\right). \qquad \text{(self-attention + feed-forward)}$$

, where $\mathrm{SG}(\cdot)$ stands for stop-gradient.

Transformer-XL: Relative Positional Encodings

- Challenge to reuse the hidden states - keep the positional information coherent.
- In Transformer, the information of sequence order is provided by a set of positional encodings $U \in R^{L_{max} \times d}$, where the i-th row U_i corresponds to the i-th absolute position within a segment and L_{max} is the maximum possible length to be modeled.

$$\mathbf{h}_{\tau+1} = f(\mathbf{h}_{\tau}, \mathbf{E}_{\mathbf{s}_{\tau+1}} + \mathbf{U}_{1:L}) \quad \text{and} \quad \mathbf{h}_{\tau} = f(\mathbf{h}_{\tau-1}, \mathbf{E}_{\mathbf{s}_{\tau}} + \mathbf{U}_{1:L}),$$

- Notice that , both $E_{s_{\tau+1}}$ and E_{s_τ} are associated with the same positional encoding $U_{1:L}$.

Transformer-XL: Relative Positional Encodings

- To avoid this failure mode, they encode relative positional information in the hidden states.
  - Technically, it expands the simple multiplication of the Attention Head’s $Score(q_i \cdot k_j)$ to include the four parts mentioned previously.

$$\mathbf{A}^{\mathrm{abs}}_{i,j} = q_i^\top k_j = \underbrace{\mathbf{E}_{x_i}^\top \mathbf{W}_q^\top \mathbf{W}_k \mathbf{E}_{x_j}}_{(a)} + \underbrace{\mathbf{E}_{x_i}^\top \mathbf{W}_q^\top \mathbf{W}_k \mathbf{U}_j}_{(b)} + \underbrace{\mathbf{U}_i^\top \mathbf{W}_q^\top \mathbf{W}_k \mathbf{E}_{x_j}}_{(c)} + \underbrace{\mathbf{U}_i^\top \mathbf{W}_q^\top \mathbf{W}_k \mathbf{U}_j}_{(d)}.$$

$$\mathbf{A}^{\mathrm{rel}}_{i,j} = \underbrace{\mathbf{E}_{x_i}^\top \mathbf{W}_q^\top \mathbf{W}_{k,E} \mathbf{E}_{x_j}}_{(a)} + \underbrace{\mathbf{E}_{x_i}^\top \mathbf{W}_q^\top \mathbf{W}_{k,R} \mathbf{R}_{i-j}}_{(b)} + \underbrace{u^\top \mathbf{W}_{k,E} \mathbf{E}_{x_j}}_{(c)} + \underbrace{v^\top \mathbf{W}_{k,R} \mathbf{R}_{i-j}}_{(d)}.$$

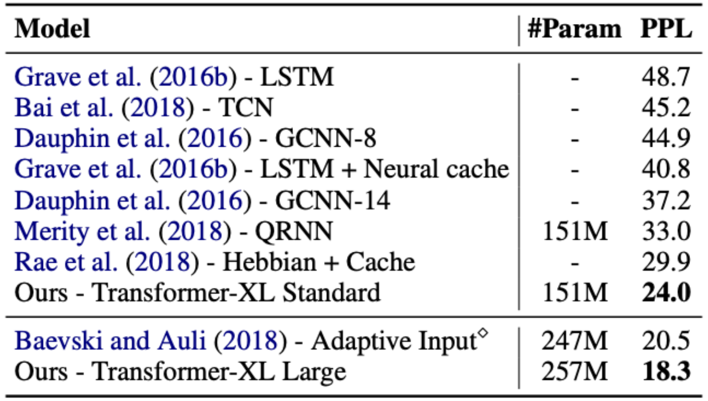
  - Relative positional encoding $R \in R^{L_{max} \times d}$ substitutes the positional encoding $U \in R^{L_{max} \times d}$, since we only need to know the relative distance of two words rather than the real order when calculating the self-attention.

Transformer-XL: Overall

- Equipping the recurrence mechanism with this relative positional embedding,

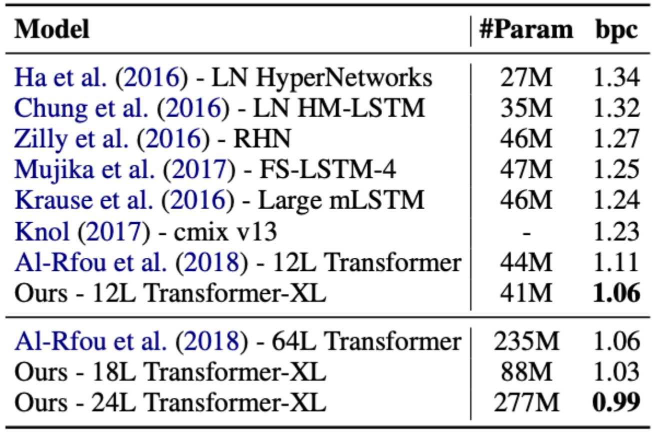
$$
\begin{aligned}
\text{For } n = 1, \ldots, N: \qquad \widetilde{\mathbf{h}}_{\tau}^{n-1} &= \left[\mathrm{SG}(\mathbf{m}_{\tau}^{n-1}) \circ \mathbf{h}_{\tau}^{n-1}\right] \\
\mathbf{q}_{\tau}^{n}, \mathbf{k}_{\tau}^{n}, \mathbf{v}_{\tau}^{n} &= \mathbf{h}_{\tau}^{n-1} {\mathbf{W}_{q}^{n}}^{\top}, \widetilde{\mathbf{h}}_{\tau}^{n-1} {\mathbf{W}_{k,E}^{n}}^{\top}, \widetilde{\mathbf{h}}_{\tau}^{n-1} {\mathbf{W}_{v}^{n}}^{\top} \\
\mathbf{A}_{\tau,i,j}^{n} &= {\mathbf{q}_{\tau,i}^{n}}^{\top} \mathbf{k}_{\tau,j}^{n} + {\mathbf{q}_{\tau,i}^{n}}^{\top} \mathbf{W}_{k,R}^{n} \mathbf{R}_{i-j} + u^{\top} \mathbf{k}_{\tau,j} + v^{\top} \mathbf{W}_{k,R}^{n} \mathbf{R}_{i-j} \\
\mathbf{a}_{\tau}^{n} &= \text{Masked-Softmax}(\mathbf{A}_{\tau}^{n}) \mathbf{v}_{\tau}^{n} \\
\mathbf{o}_{\tau}^{n} &= \text{LayerNorm}(\text{Linear}(\mathbf{a}_{\tau}^{n}) + \mathbf{h}_{\tau}^{n-1}) \\
\mathbf{h}_{\tau}^{n} &= \text{Positionwise-Feed-Forward}(\mathbf{o}_{\tau}^{n})
\end{aligned}
$$

Experimental Results



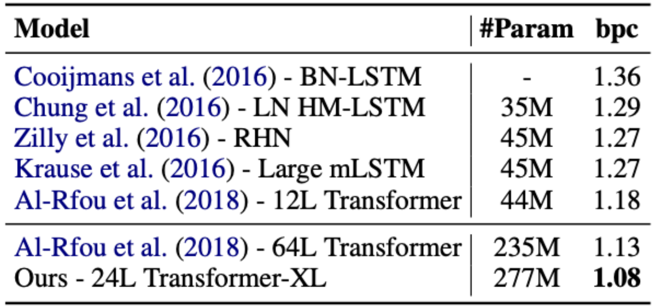
Model	#Param	PPL
Grave et al. (2016b) - LSTM	-	48.7
Bai et al. (2018) - TCN	-	45.2
Dauphin et al. (2016) - GCNN-8	-	44.9
Grave et al. (2016b) - LSTM + Neural cache	-	40.8
Dauphin et al. (2016) - GCNN-14	-	37.2
Merity et al. (2018) - QRNN	151M	33.0
Rae et al. (2018) - Hebbian + Cache	-	29.9
Ours - Transformer-XL Standard	151M	**24.0**
Baevski and Auli (2018) - Adaptive Input$^\diamond$	247M	20.5
Ours - Transformer-XL Large	257M	**18.3**

Table 1: Comparison with state-of-the-art results on WikiText-103. $^\diamond$ indicates contemporary work.



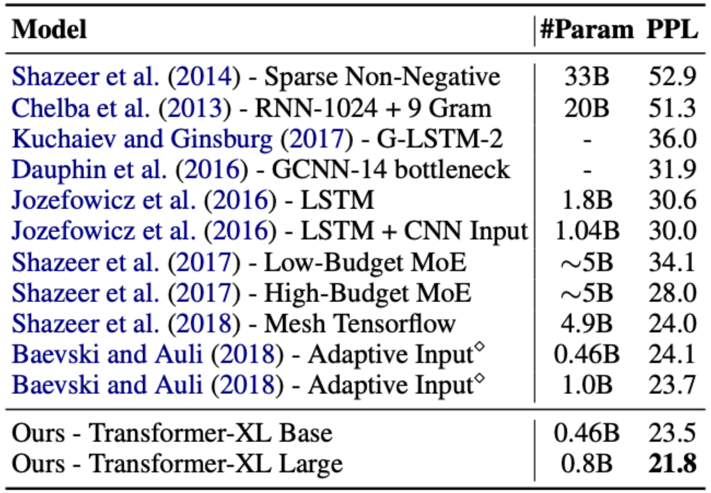
Model	#Param	bpc
Ha et al. (2016) - LN HyperNetworks	27M	1.34
Chung et al. (2016) - LN HM-LSTM	35M	1.32
Zilly et al. (2016) - RHN	46M	1.27
Mujika et al. (2017) - FS-LSTM-4	47M	1.25
Krause et al. (2016) - Large mLSTM	46M	1.24
Knol (2017) - cmix v13	-	1.23
Al-Rfou et al. (2018) - 12L Transformer	44M	1.11
Ours - 12L Transformer-XL	41M	**1.06**
Al-Rfou et al. (2018) - 64L Transformer	235M	1.06
Ours - 18L Transformer-XL	88M	1.03
Ours - 24L Transformer-XL	277M	**0.99**

Table 2: Comparison with state-of-the-art results on enwik8.



Model	#Param	bpc
Cooijmans et al. (2016) - BN-LSTM	-	1.36
Chung et al. (2016) - LN HM-LSTM	35M	1.29
Zilly et al. (2016) - RHN	45M	1.27
Krause et al. (2016) - Large mLSTM	45M	1.27
Al-Rfou et al. (2018) - 12L Transformer	44M	1.18
Al-Rfou et al. (2018) - 64L Transformer	235M	1.13
Ours - 24L Transformer-XL	277M	**1.08**

Table 3: Comparison with state-of-the-art results on text8.



Model	#Param	PPL
Shazeer et al. (2014) - Sparse Non-Negative	33B	52.9
Chelba et al. (2013) - RNN-1024 + 9 Gram	20B	51.3
Kuchaiev and Ginsburg (2017) - G-LSTM-2	-	36.0
Dauphin et al. (2016) - GCNN-14 bottleneck	-	31.9
Jozefowicz et al. (2016) - LSTM	1.8B	30.6
Jozefowicz et al. (2016) - LSTM + CNN Input	1.04B	30.0
Shazeer et al. (2017) - Low-Budget MoE	∼5B	34.1
Shazeer et al. (2017) - High-Budget MoE	∼5B	28.0
Shazeer et al. (2018) - Mesh Tensorflow	4.9B	24.0
Baevski and Auli (2018) - Adaptive Input$^\diamond$	0.46B	24.1
Baevski and Auli (2018) - Adaptive Input$^\diamond$	1.0B	23.7
Ours - Transformer-XL Base	0.46B	23.5
Ours - Transformer-XL Large	0.8B	**21.8**

Table 4: Comparison with state-of-the-art results on One Billion Word. $^\diamond$ indicates contemporary work.