



# Transformers and Attention

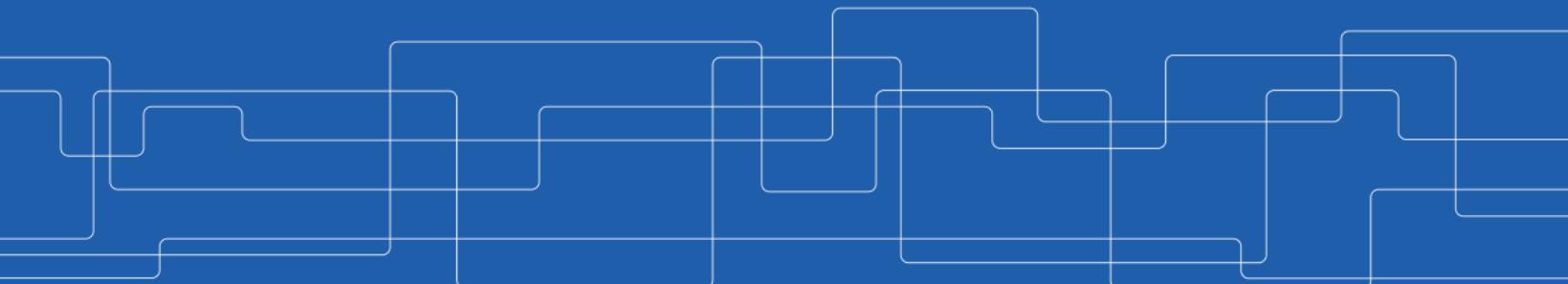
## ID2223 Scalable Machine Learning and Deep Learning

**Francisco J. Peña**

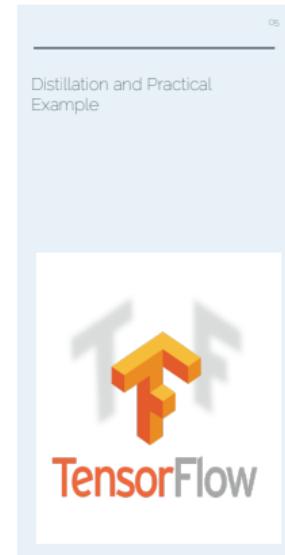
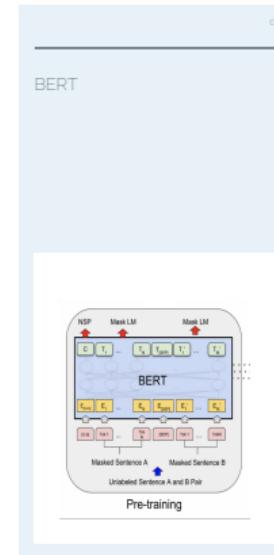
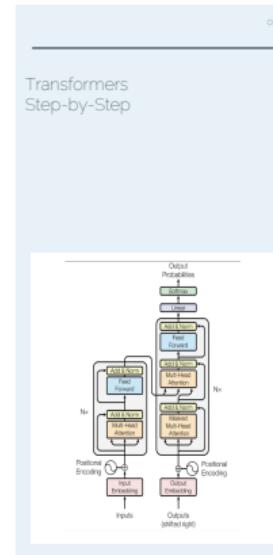
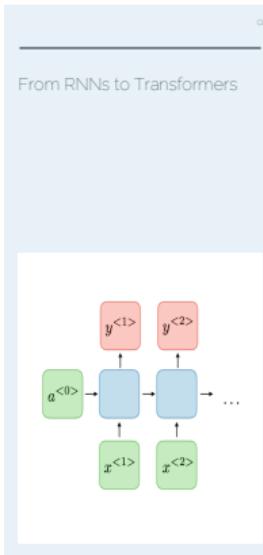
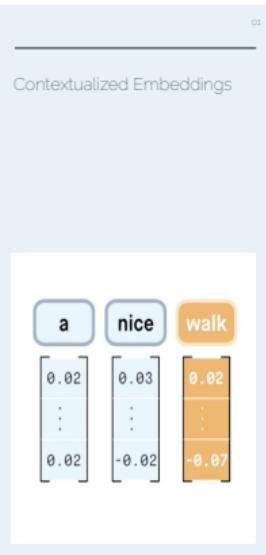
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2021-12-02



# Roadmap





# Acknowledgements

Material based on:

- ▶ Christoffer Manning's [NLP Lectures at Stanford](#)
- ▶ [The Illustrated Transformer](#) by Jay Alammar
- ▶ [Slides](#) from Jacob
- ▶ [Self-attention Video](#) from Peltarion
- ▶ Slides from Karl Erliksson



# Contextualized Embeddings

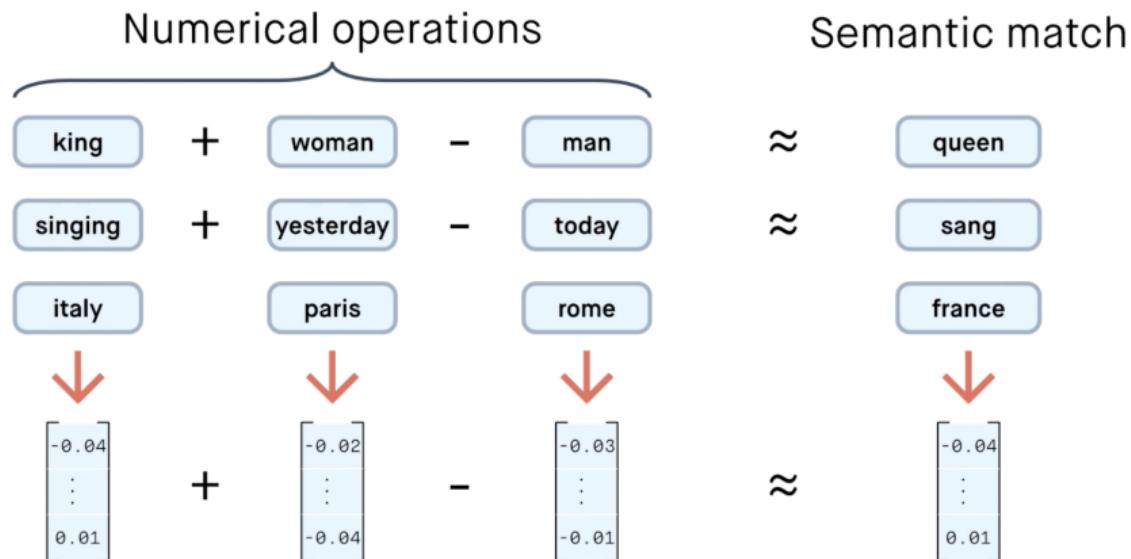
# Background to Natural Language Processing (NLP)

- ▶ Word embeddings are the basis of NLP
- ▶ Popular embeddings like GloVe and Word2Vec are pre-trained on large text corpuses based on co-occurrence statistics
- ▶ “A word is characterized by the company it keeps” [Firth, 1957]

best	-	selling	music	artists
-0.11	0.01	-0.01	0.06	-0.02
0.01	0.07	-0.03	0.11	0.00
-0.17	-0.04	0.15	0.05	-0.05
:	:	:	:	:
0.13	-0.05	0.00	0.14	0.05
-0.13	-0.11	-0.07	-0.12	-0.12
-0.09	-0.25	0.05	-0.04	0.02

[Peltarion, 2020]

# Word Embeddings



[Peltarion, 2020]

# Word Embeddings

**Problem:** Word embeddings are **context-free**

a	nice	walk	by	the	river	bank
0.02	0.03	0.02	-0.00	-0.04	-0.01	-0.02
:	:	:	:	:	:	:
0.02	-0.02	-0.07	0.03	-0.03	-0.04	-0.03

walk	to	the	bank	and	get	cash
0.02	0.01	-0.04	-0.02	-0.02	-0.06	0.01
:	:	:	:	:	:	:
-0.07	0.02	-0.03	-0.03	0.02	0.04	-0.01

[Peltarion, 2020]

# Word Embeddings

**Problem:** Word embeddings are **context-free**

a	nice	walk	by	the	river	bank
0.02	0.03	0.02	-0.00	-0.04	-0.01	-0.02
:	:	:	:	:	:	:
0.02	-0.02	-0.07	0.03	-0.03	-0.04	-0.03

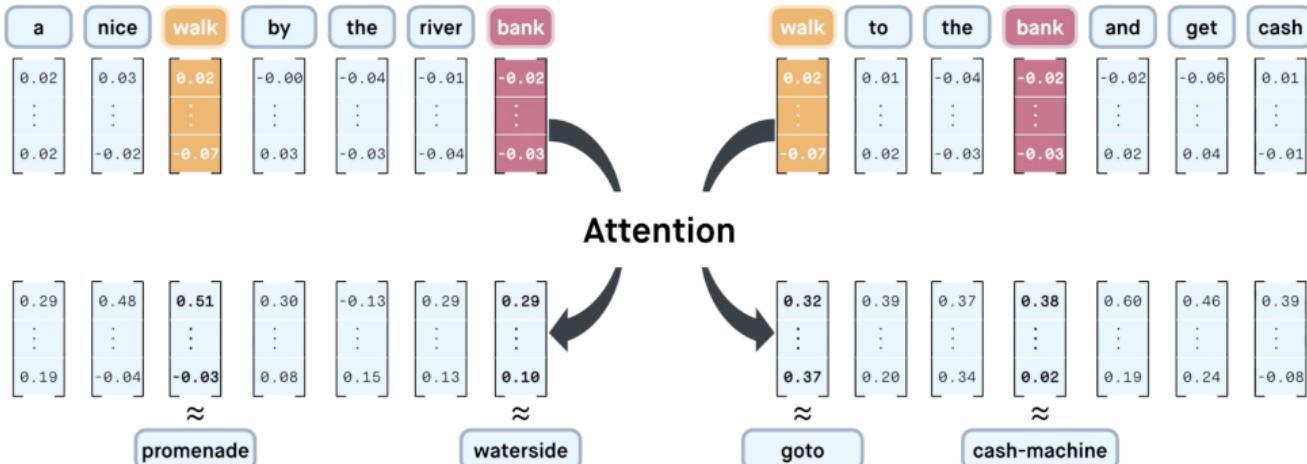
walk	to	the	bank	and	get	cash
0.02	0.01	-0.04	-0.02	-0.02	-0.06	0.01
:	:	:	:	:	:	:
-0.07	0.02	-0.03	-0.03	0.02	0.04	-0.01

[Peltarion, 2020]

# Word Embeddings

**Problem:** Word embeddings are **context-free**

**Solution:** Create **contextualized** representation



[Peltarion, 2020]



# From RNNs to Transformers

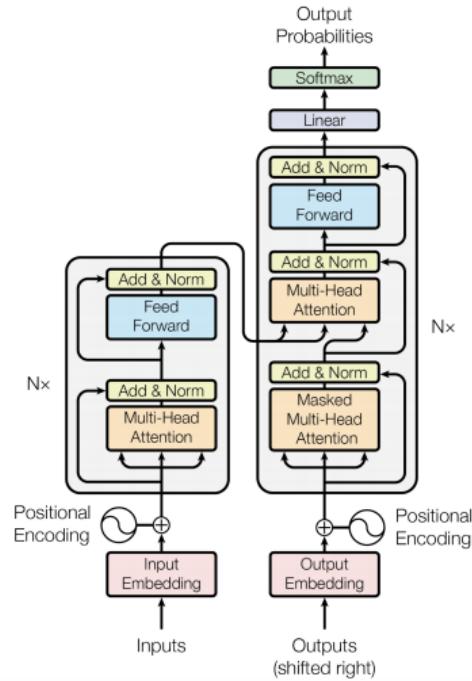


## Problems with RNNs - Motivation for Transformers

- ▶ Sequential computations **prevents parallelization**
- ▶ Despite GRUs and LSTMs, RNNs still need attention mechanisms to deal with **long range dependencies**
- ▶ Attention gives us access to any state... Maybe we don't need the costly recursion?
- ▶ Then NLP can have deep models, solves our computer vision envy!

# Attention is all you need! [Vaswani, 2017]

- ▶ Sequence-to-sequence model for Machine Translation
- ▶ Encoder-decoder architecture
- ▶ Multi-headed **self-attention**
  - Models context and no locality bias



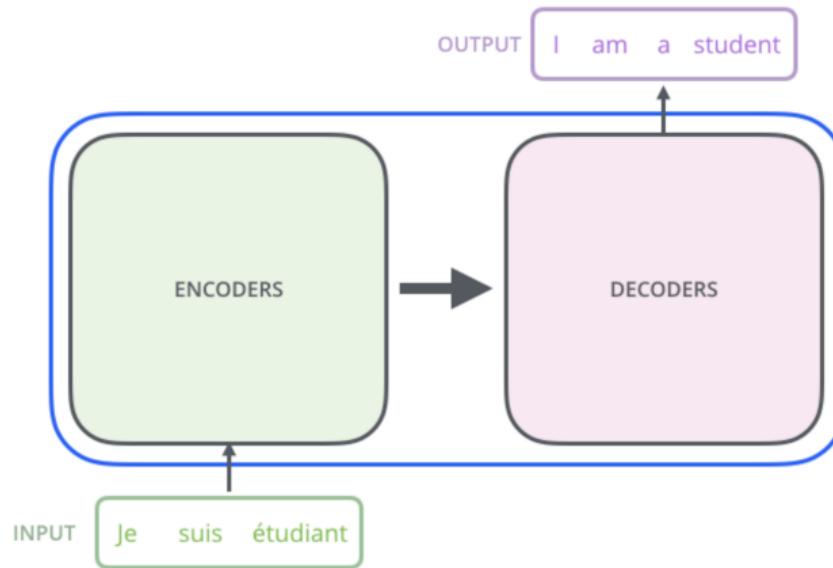
[Vaswani et al., 2017]



# Transformers Step-by-Step



# Understanding the Transformer: Step-by-Step

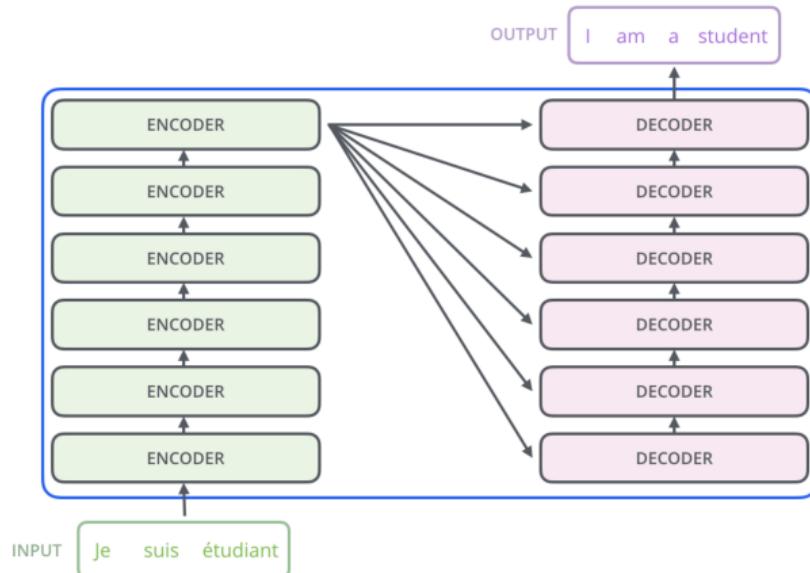


[Alammar, 2018]

# Understanding the Transformer: Step-by-Step

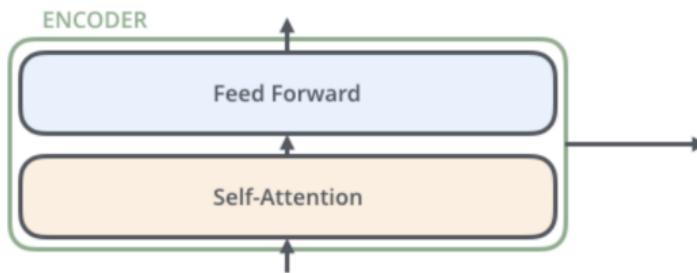
No recursion, instead  
stacking encoder and  
decoder blocks

- ▶ Originally: 6 layers
- ▶ BERT base: 12 layers
- ▶ BERT large: 24 layers
- ▶ GPT2-XL: 48 layers
- ▶ GPT3: 96 layers



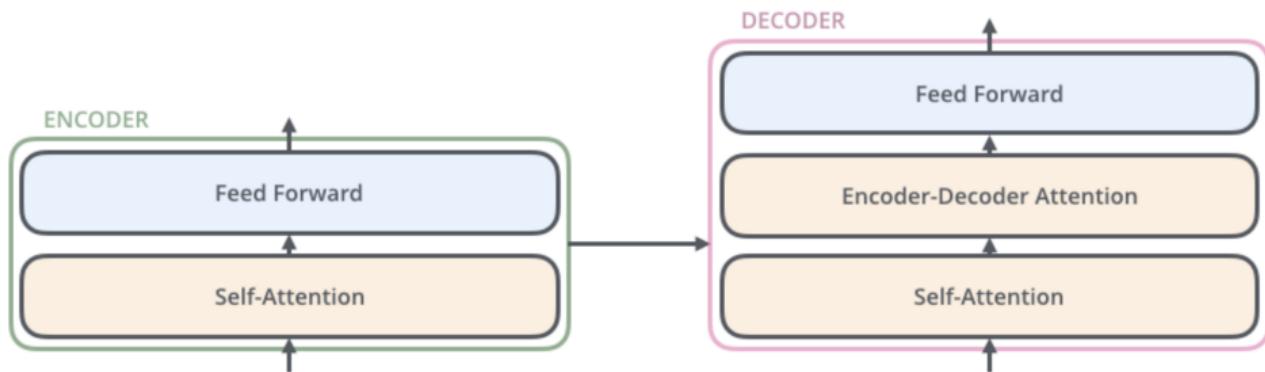
[Alammar, 2018]

# The Encoder and Decoder Blocks



[Alammar, 2018]

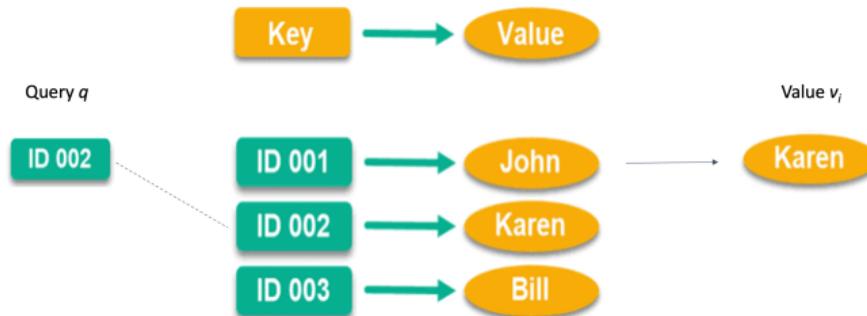
# The Encoder Block



[Alammar, 2018]

# Attention Preliminaries

Mimics the retrieval of a value  $v_i$  for a query  $q$  based on a key  $k_i$  in a database, but in a probabilistic fashion





# Dot-Product Attention

- ▶ Queries, keys and values are vectors
- ▶ Output is a **weighted sum** of the values
- ▶ Weights are computed as the **scaled dot-product** (similarity) between the query and the keys

$$\text{Attention}(q, K, V) = \sum_i \text{Similarity}(q, k_i) \cdot v_i = \sum_i \frac{e^{q \cdot k_i / \sqrt{d_k}}}{\sum_j e^{q \cdot k_j / \sqrt{d_k}}} v_i$$

Output is a  
row-vector

- ▶ Can stack multiple queries into a matrix  $Q$

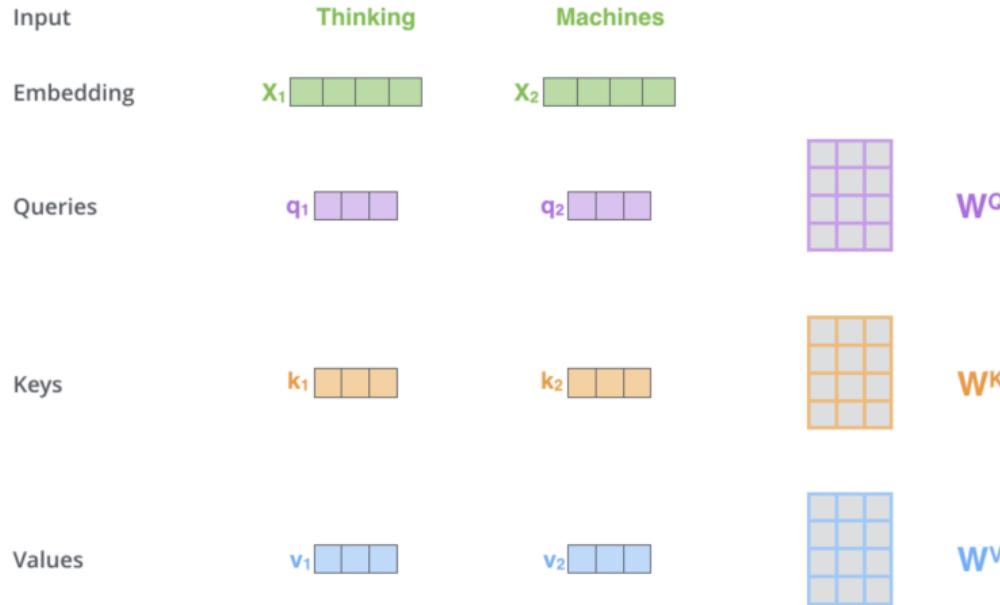
$$\text{Attention}(Q, K, V) = \text{softmax} \left( \frac{QK^\top}{\sqrt{d_k}} \right) V$$

Output is again  
a matrix

- ▶ Self-attention: Let the word embeddings be the queries, keys and values, i.e. **let the words select each other**

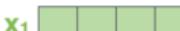
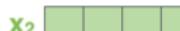
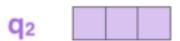
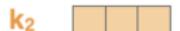


# Self-Attention Mechanism



[Alammar, 2018]

# Self-Attention Mechanism

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

[Alammar, 2018]

# Self-Attention Mechanism in Matrix Notation

$$X \times W^Q = Q$$

Diagram showing matrix multiplication: A green 3x3 input matrix  $X$  is multiplied by a purple 3x3 weight matrix  $W^Q$ , resulting in a purple 3x3 output matrix  $Q$ .

$$X \times W^K = K$$

Diagram showing matrix multiplication: A green 3x3 input matrix  $X$  is multiplied by an orange 3x3 weight matrix  $W^K$ , resulting in an orange 3x3 output matrix  $K$ .

$$X \times W^V = V$$

Diagram showing matrix multiplication: A green 3x3 input matrix  $X$  is multiplied by a blue 3x3 weight matrix  $W^V$ , resulting in a blue 3x3 output matrix  $V$ .

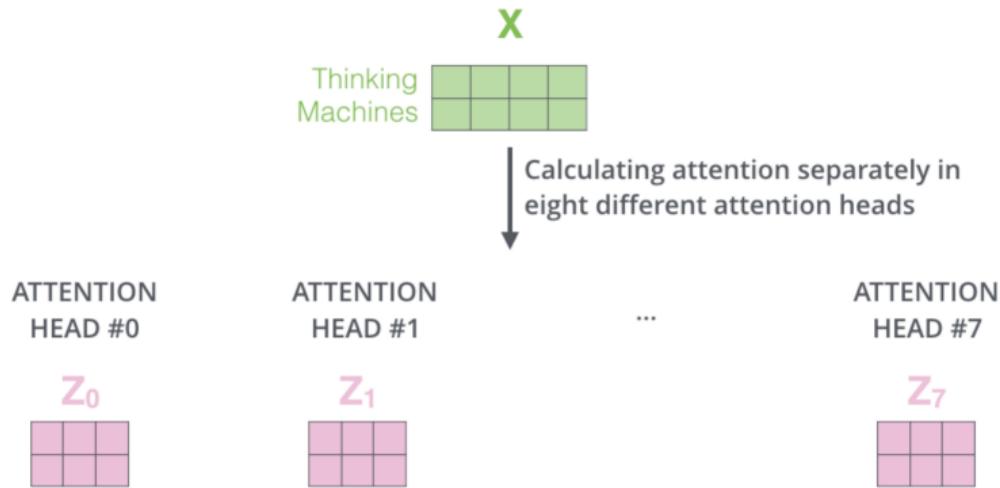
$$\text{softmax}\left(\frac{Q \times K^T}{\sqrt{d_k}}\right) = Z$$

Diagram illustrating the final computation: The matrices  $Q$  and  $K^T$  are multiplied together, and the result is divided by  $\sqrt{d_k}$ . This result is passed through a softmax function to produce the output matrix  $Z$ .

[Alammar, 2018]

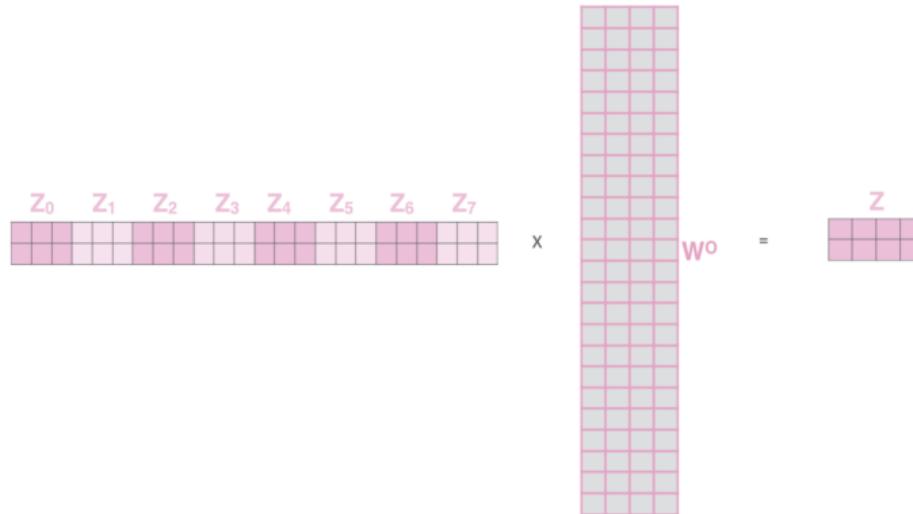


# Multi-Headed Self-Attention



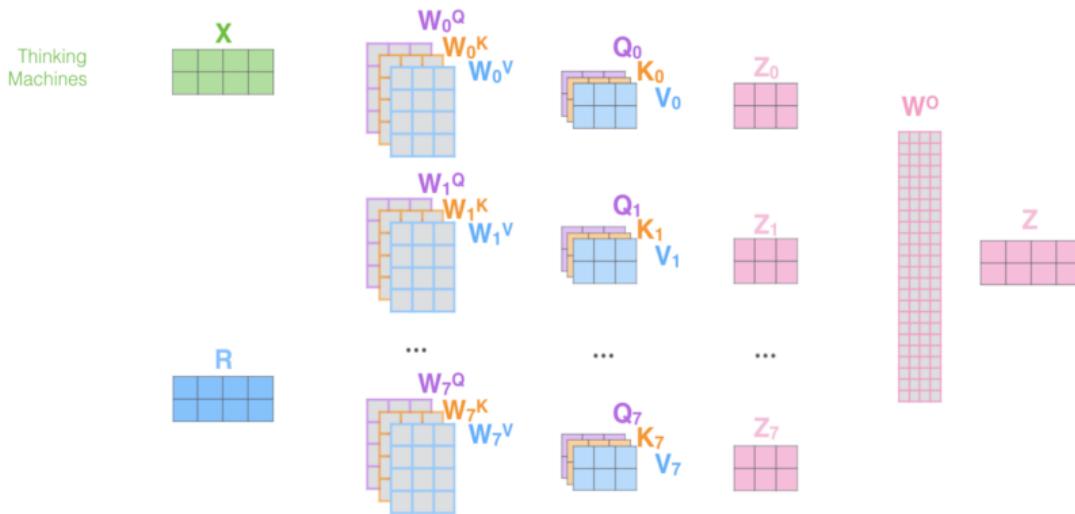
[Alammar, 2018]

# Multi-Headed Self-Attention



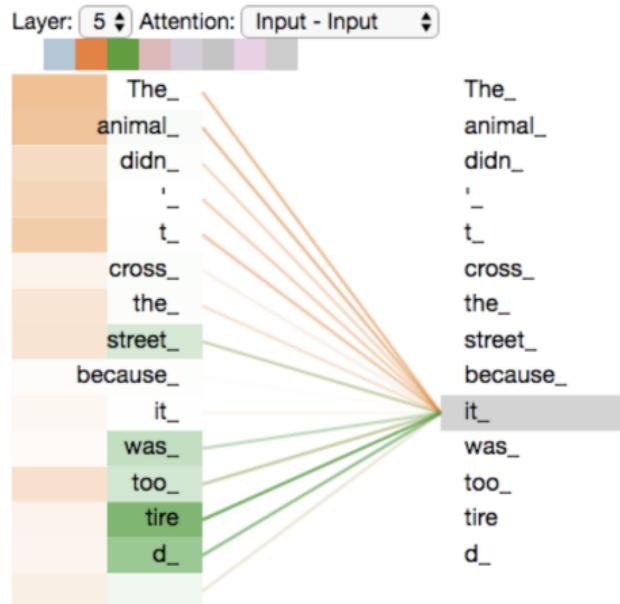
[Alammar, 2018]

# Self-Attention: Putting It All Together



[Alammar, 2018]

# Attention Visualized

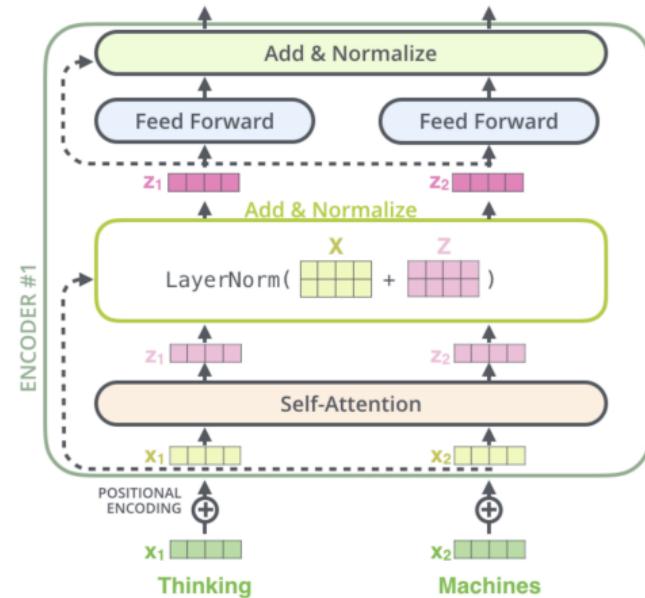


[Alammar, 2018]

# The Full Encoder Block

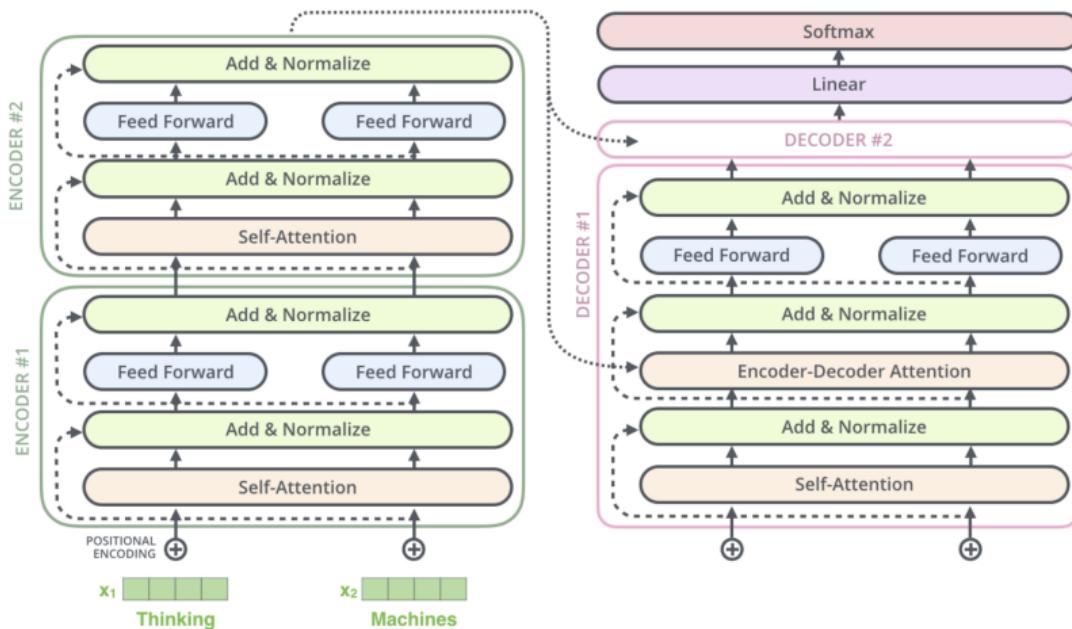
Encoder block consisting of:

- ▶ Multi-headed self-attention
- ▶ Feedforward NN (FC 2 layers)
- ▶ Skip connections
- ▶ Layer normalization - Similar to batch normalization but computed over features (words/tokens) for a single sample



[Alammar, 2018]

# Encoder-Decoder Architecture - Small Example



[Alammar, 2018]

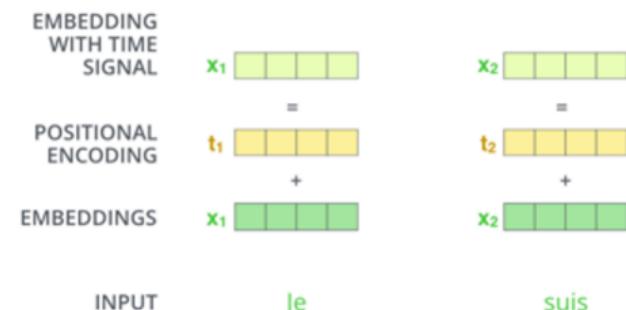
# Positional Encodings

Encoder block consisting of:

- ▶ Attention mechanism has no locality bias - **no notion of word order**
- ▶ **Add positional encodings** to input embeddings to let model learn relative positioning

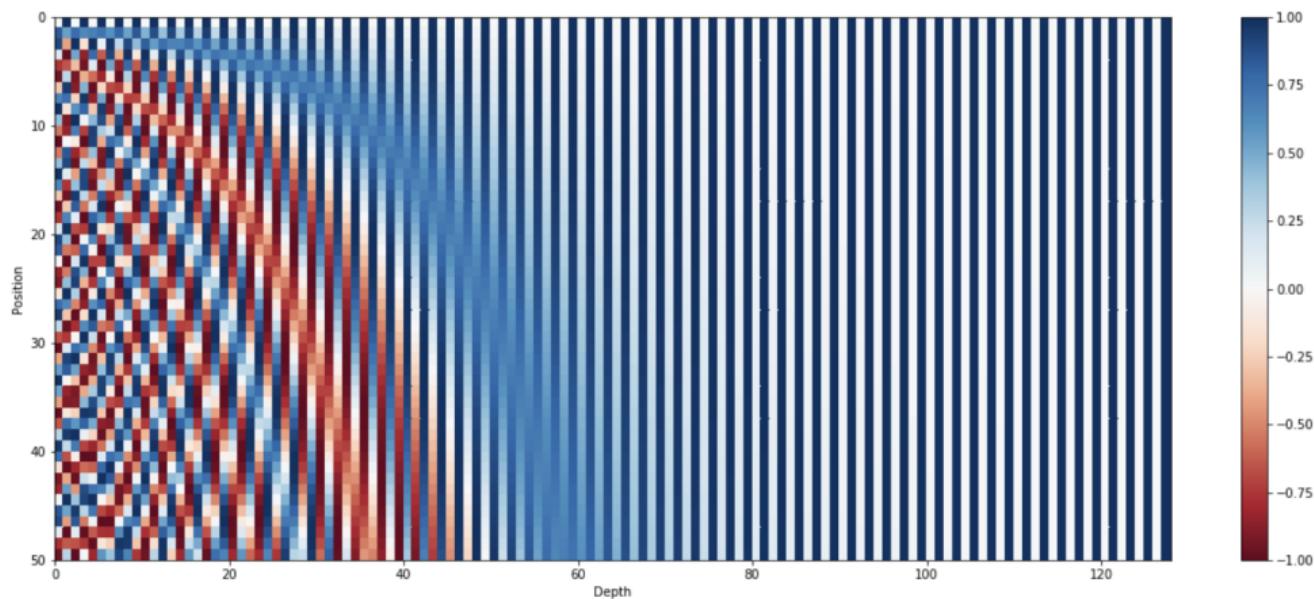
$$\text{PE}(\text{pos}, 2i) = \sin\left(\frac{\text{pos}}{10000^{2i/d_{\text{model}}}}\right)$$

$$\text{PE}(\text{pos}, 2i + 1) = \cos\left(\frac{\text{pos}}{10000^{2i/d_{\text{model}}}}\right)$$



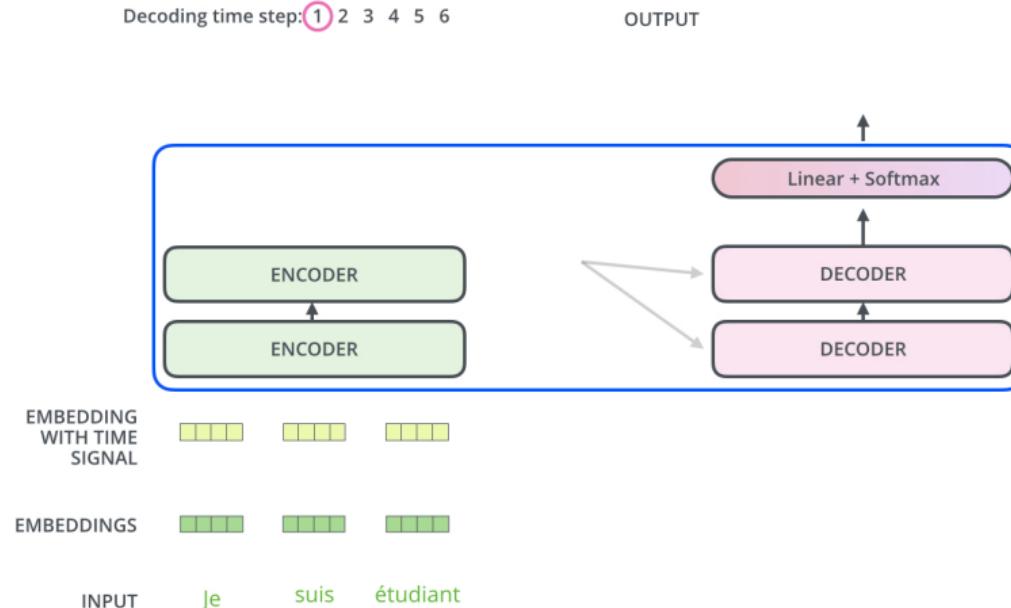
[Alammar, 2018]

# Positional Encodings



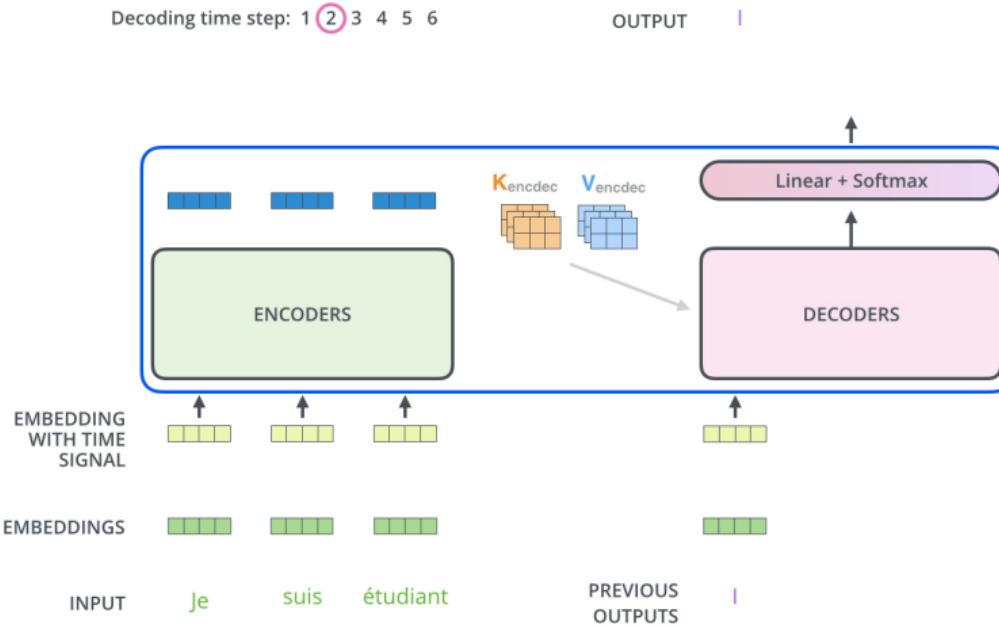
[Kazemnejad, 2019]

# Let's start the encoding!



[Alammar, 2018]

# Decoding procedure

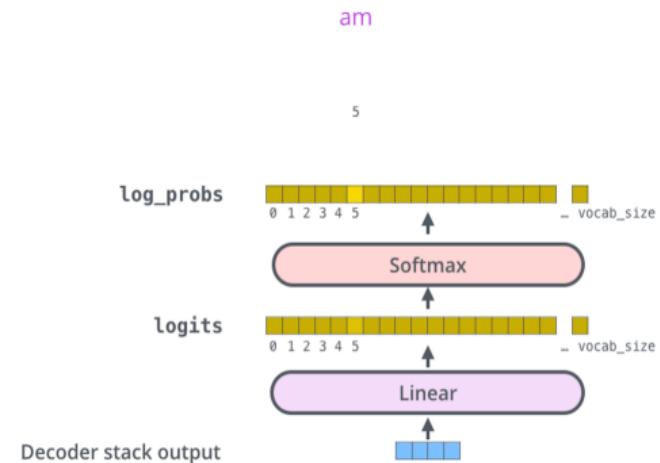


[Alammar, 2018]

# Producing the output text

Encoder block consisting of:

- ▶ The output from the decoder is passed through a final fully connected **linear layer** with a **softmax** activation function
- ▶ Produces a probability distribution over the pre-defined vocabulary of output words (tokens)
- ▶ **Greedy decoding** picks the word with the highest probability at each time step



[Alammar, 2018]

# Training Objective

## Target Model Outputs

Output Vocabulary: a am I thanks student <eos>

position #1	0.0	0.0	<b>1.0</b>	0.0	0.0	0.0
-------------	-----	-----	------------	-----	-----	-----

position #2	0.0	<b>1.0</b>	0.0	0.0	0.0	0.0
-------------	-----	------------	-----	-----	-----	-----

position #3	<b>1.0</b>	0.0	0.0	0.0	0.0	0.0
-------------	------------	-----	-----	-----	-----	-----

position #4	0.0	0.0	0.0	0.0	<b>1.0</b>	0.0
-------------	-----	-----	-----	-----	------------	-----

position #5	0.0	0.0	0.0	0.0	0.0	<b>1.0</b>
-------------	-----	-----	-----	-----	-----	------------

a am I thanks student <eos>

## Trained Model Outputs

Output Vocabulary: a am I thanks student <eos>

position #1	0.01	0.02	<b>0.93</b>	0.01	0.03	0.01
-------------	------	------	-------------	------	------	------

position #2	0.01	<b>0.8</b>	0.1	0.05	0.01	0.03
-------------	------	------------	-----	------	------	------

position #3	<b>0.99</b>	0.001	0.001	0.001	0.002	0.001
-------------	-------------	-------	-------	-------	-------	-------

position #4	0.001	0.002	0.001	0.02	<b>0.94</b>	0.01
-------------	-------	-------	-------	------	-------------	------

position #5	0.01	0.01	0.001	0.001	0.001	<b>0.98</b>
-------------	------	------	-------	-------	-------	-------------

a am I thanks student <eos>



[Alammar, 2018]

# Complexity Comparison

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(\log_k(n))$

[Vaswani et al., 2017]

# Results

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [31]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [8]	26.36	<b>41.29</b>	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1		<b><math>3.3 \cdot 10^{18}</math></b>
Transformer (big)	<b>28.4</b>	<b>41.0</b>		$2.3 \cdot 10^{19}$

[Vaswani et al., 2017]



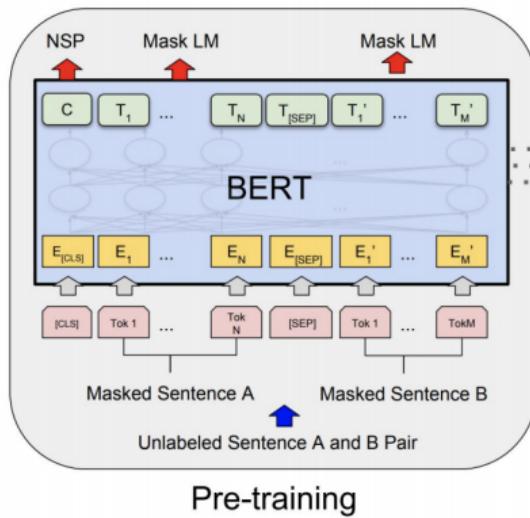
# BERT

## Bidirectional Encoder Representations from Transformers

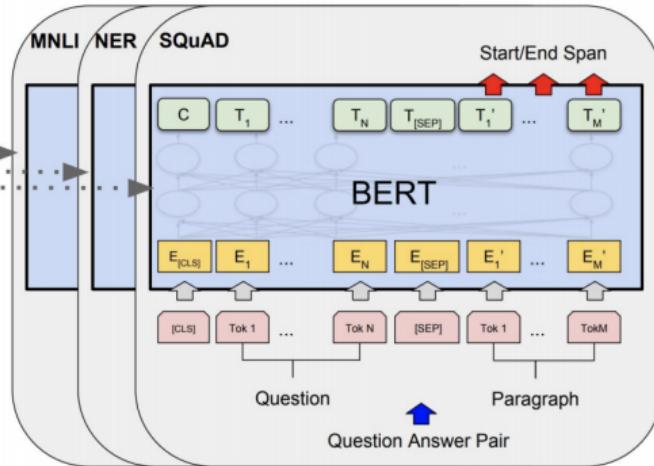
- ▶ Self-supervised pre-training of Transformers encoder for language understanding
- ▶ Fine-tuning for specific downstream task



# BERT Training Procedure



Pre-training



Fine-Tuning

[Devlin et al., 2018]



# BERT Training Objectives

## Masked Language Modelling

the man went to the [MASK] to buy a [MASK] of milk

↑                              ↑  
store                          gallon

## Next Sentence prediction

**Sentence A** = The man went to the store.

**Sentence B** = He bought a gallon of milk.

**Label** = IsNextSentence

**Sentence A** = The man went to the store.

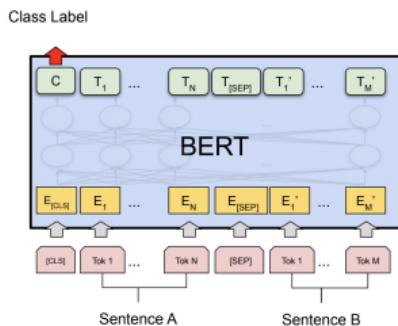
**Sentence B** = Penguins are flightless.

**Label** = NotNextSentence

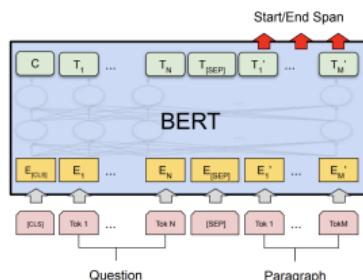
[Devlin et al., 2018]

# BERT Fine-Tuning Examples

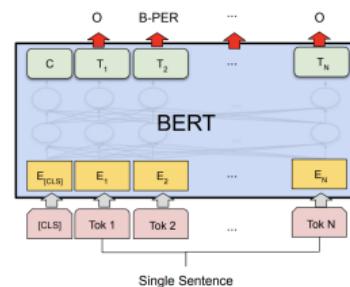
## Sentence Classification



## Question Answering



## Named Entity Recognition



[Devlin et al., 2018]



# How good are transformers?

- ▶ Scaling up **models size** and amount of **training data** helps a lot
- ▶ Best model is 10B (!!!) parameters
- ▶ Two models have already surpassed human performance!!!
- ▶ Exact **pre-training objective** (MLM, NSP, corruption) doesn't matter too much
- ▶ SuperGLUE benchmark:

Rank	Name	Model	URL	Score	BoolQ	CB	COPA	MultIRC	ReCoRD	RTE	WiC	WSC	AX-g	AX-b	
1	ERNIE Team - Baidu	ERNIE 3.0		90.6	91.0	98.6/99.2	97.4	88.6/63.2	94.7/94.2	92.6	77.4	97.3	92.7/94.7	68.6	
+	2	Zirui Wang	T5 + UDG, Single Model (Google Brain)		90.4	91.4	95.8/97.6	98.0	88.3/63.0	94.2/93.5	93.0	77.9	96.6	92.7/91.9	69.1
+	3	DeBERTa Team - Microsoft	DeBERTa / TuringNLv4		90.3	90.4	95.7/97.6	98.4	88.2/63.7	94.5/94.1	93.2	77.5	95.9	93.3/93.8	66.7
	4	SuperGLUE Human Baselines	SuperGLUE Human Baselines		89.8	89.0	95.8/98.9	100.0	81.8/51.9	91.7/91.3	93.6	80.0	100.0	99.3/99.7	76.6
+	5	T5 Team - Google	T5		89.3	91.2	93.9/96.8	94.8	88.1/63.3	94.1/93.4	92.5	76.9	93.8	92.7/91.9	65.6
+	6	Huawei Noah's Ark Lab	NEZHA-Plus		86.7	87.8	94.4/96.0	93.6	84.6/55.1	90.1/89.6	89.1	74.6	93.2	87.1/74.4	58.0

[Raffel et al., 2019]



# Practical Examples



# BERT in low-latency production settings

GOOGLE \ TECH \ ARTIFICIAL INTELLIGENCE

## Google is improving 10 percent of searches by understanding language context

Say hello to BERT

By Dieter Bohn | @backlon | Oct 25, 2019, 3:01am EDT

## Bing says it has been applying BERT since April

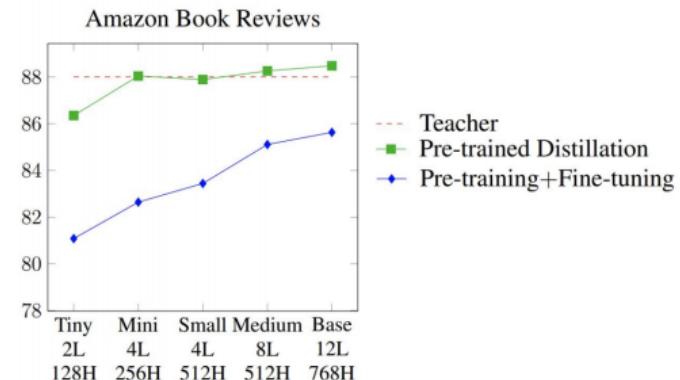
The natural language processing capabilities are now applied to all Bing queries globally.

[George Nguyen](#) on November 19, 2019 at 1:38 pm

[Devlin, 2020]

# Distillation

- ▶ Modern pre-trained language models are **huge** and very **computationally expensive**
- ▶ How are these companies applying them to low-latency applications?
- ▶ Distillation!
  - Train SOTA **teacher model** (pre-training + fine-tuning)
  - Train smaller **student model** that **mimics** the teacher's output on a large dataset on unlabeled data
- ▶ Distillation works *much* better than pre-training + fine-tuning with smaller model



[Devlin, 2020] [Turc, 2020]



# Transformers in TensorFlow using HuggingFace 😊

- ▶ The [HuggingFace Library](#) contains a majority of the recent pre-trained State-of-the-art NLP models, as well as over 4 000 community uploaded models
- ▶ Works with both [TensorFlow](#) and [PyTorch](#)



HUGGING FACE

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<a href="#">cl-tohoku/bert-base-japanese-whole-word-masking</a>		
<a href="#">distilroberta-base</a> ★		
<a href="#">bert-base-cased</a> ★		
<a href="#">xlm-roberta-base</a> ★		



# Transformers in TensorFlow using HuggingFace 😊

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from transformers import BertTokenizerFast, TFBertForSequenceClassification
from datasets import load_dataset
import tensorflow as tf

dataset = load_dataset("imdb").shuffle()
tokenizer = BertTokenizerFast.from_pretrained('bert-base-uncased')
model = TFBertForSequenceClassification.from_pretrained('bert-base-uncased', num_labels=2)

train_encodings = tokenizer(dataset['train']['text'], truncation=True, padding=True)
train_dataset = tf.data.Dataset.from_tensor_slices((dict(train_encodings), dataset['train']['label']))
val_dataset = ... // Analogously

optimizer = tf.keras.optimizers.Adam(learning_rate=5e-5)
model.compile(optimizer=optimizer, loss=model.compute_loss)
model.fit(train_dataset.batch(16), epochs=3, batch_size=16)

model.evaluate(val_dataset.batch(16), verbose=0)
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# Wrap Up

# Summary

- ▶ Transformers have blown other architectures out of the water for NLP
- ▶ Get rid of recurrence and rely on **self-attention**
- ▶ NLP pre-training using **Masked Language Modelling**
- ▶ Most recent improvements using **larger models** and **more data**
- ▶ **Distillation** can make model serving and inference more tractable





Thanks!  
Questions?

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