# Advanced Prediction Models

## Today's Outline

- Recap of Attention in Sequence to Sequence Models
- Transformer Architecture and Self-Attention
- Transfer Learning using a pre-trained NLP model
- BERT and related architectures

#### What does attention mean?

- Attend to certain steps/parts of the input sequence while deciding/predicting the current output (of the output sequence)
- By 'attend', we just mean that the prediction of the current output depends on **specific** parts of the input sequence.

• Next, we will revisit the attention mechanism in a neural machine translation sequence to sequence modelling setting.

#### **Neural Machine Translation**

SEQUENCE TO SEQUENCE MODEL WITH ATTENTION





#### **Neural Machine Translation** SEQUENCE TO SEQUENCE MODEL WITH ATTENTION



#### **Neural Machine Translation**

SEQUENCE TO SEQUENCE MODEL WITH ATTENTION



Collect the hidden layer outputs from all RNN steps

#### Neural Machine Translation SEQUENCE TO SEQUENCE MODEL WITH ATTENTION

Encoder RNN Encode

#### **Neural Machine Translation** SEQUENCE TO SEQUENCE MODEL WITH ATTENTION







While decoding happens sequentially, each RNN step involves attention!



A combination of encoder vectors is concatenated with the decoder hidden vector



#### **Neural Machine Translation** SEQUENCE TO SEQUENCE MODEL WITH ATTENTION



Because the attention mechanism spans across encoder and decoder, we will refer to it as encoder-decoder attention

#### Neural Machine Translation SEQUENCE TO SEQUENCE MODEL WITH ATTENTION



An example illustrating the attention scores: in this example, the attention scores seem quite natural



<sup>1</sup>Reference: https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-modelswith-attention/. Also see https://github.com/tensorflow/nmt

An example illustrating the attention scores: in this example, the attention scores for 'European Economic Area' capture the non-triviality

Attention visualization – example of the alignments between source and target sentences



<sup>1</sup>Reference: Bahdanau et al., 2015

## Questions?

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# Transformer Architecture and Self-Attention

Is a new model/architecture (from 2017) that we will look at that can also be used for sequence to sequence modelling

Attention (same idea as before, but a slightly different take) is a core component of this model

Lets start again with neural machine translation as the running application.



#### Transformer



#### Transformer

Lets now see the insides of both the encoder and the decoder in order.



In particular, lets focus on one encoder unit.

The number of such units is fixed and does not depend on the input sequence length (thanks to parallel treatment of all input elements/words, as we will see later).



The encoder units don't share weights.

Have two sub-layers: self-attention followed by a fully connected/feed forward (FF) layer.

All words will be input at the same time. So the FF layer's weights are reused across words

(Decoder has self-attention as well as the classical encoder-decoder attention)



Self-attention helps 'transform' inputs taking other inputs into consideration <sup>1</sup>Reference: https://jalammar.github.io/illustrated-transformer/

Lets start with vector embeddings of words (fix some max length say 20) at the lowest/starting layer. Say the embedding size is 512. In other layers, its not embeddings but vector outputs of previous encoder units



Transformation of each word depends on transformations of other words in each encoding unit E.g.:  $z_1$  depends on  $x_1$  and  $x_2$ 



Self-attention: while processing the word 'it' below, attend to words related to it



Self-attention: helps better encode the word 'it'. Analogous to cell state changes in LSTMs. <sup>1</sup>Reference: https://jalammar.github.io/illustrated-transformer/

Create three vectors for each input: q, k and v using three matrices (that need to be learned)



After create the three vectors, a set of scores per input word are calculated.



These scores are then normalized. They determine how much attention is needed on itself and other words (e.g., Machines below).



A score weighted sum of 'value' vectors is the output encoding of the input in this encoder unit



The computation of queries, keys and values actually happens via matrix multiplication.



Similarly, the scores are also computed using matrix-matrix multiplications.



Exercise: This should seem similar to the encoder-decoder attention we saw in seq2seq models

## **Transformer : Multi-Headed Attention**

Multi-headed attention: doing multiple attention computations in parallel.

Empirically validated.

How it might help: (a) model can better focus on multiple inputs, (b) get 'different' representations (basically we can get different 'output embeddings' due to random initializations)



## **Transformer : Multi-Headed Attention**


Need to merge these vectors before passing onto the FF layer: concatenate and transform.

## 1) Concatenate all the attention heads

<b>~</b> 0		<b>~</b> 1		<b>~</b> 2		<b>~</b> 3		- 1	<b>4</b>		<b>4</b> 5		<b>4</b> 0		<b>~</b> /					

2) Multiply with a weight matrix W<sup>o</sup> that was trained jointly with the model

Х

**W**o

3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN



=



Two heads are focusing on two different related words. The orange head focuses on animal, the green head focusses on tired.





We need to account for word ordering. We can do that by adding a 'disambiguating vector' to each embedding.





Each row below is an example positional encoding vector (512 dimensional, from Transformer2Transformer).



Each row below is an example positional encoding vector (64 dimensional).







#### Layer Normalization

Jimmy Lei Ba, Jamie Ryan Kiros, Geoffrey E. Hinton

#### **Download PDF**

Training state-of-the-art, deep neural networks is computationally expensive. One way to reduce the training time is to normalize the activities of the neurons. A recently introduced technique called batch normalization uses the distribution of the summed input to a neuron over a mini-batch of training cases to compute a mean and variance which are then used to normalize the summed input to that neuron on each training case. This significantly reduces the training time in feed-forward neural networks. However, the effect of batch normalization is dependent on the mini-batch size and it is not obvious how to apply it to recurrent neural networks. In this paper, we transpose batch normalization into layer normalization by computing the mean and variance used for normalization from all of the summed inputs to the neurons in a layer on a single training case. Like batch normalization, we also give each neuron its own adaptive bias and gain which are applied after the normalization but before the non-linearity. Unlike batch normalization, layer normalization performs exactly the same computation statistics separately at each time step. Layer normalization is very effective at stabilizing the hidden state dynamics in recurrent networks. Empirically, we show that layer normalization can substantially reduce the training time compared with previously published techniques.

#### <sup>1</sup>Reference: https://arxiv.org/abs/1607.06450

A 2-layer transfer example is below. Layer-normalization is part of the decoder unit as well.



The outputs of the top encoder unit are transformed to keys and values. These will be used in **all** encoder-decoder attention sub-layers.



Decoder self-attention: can only attend to previous words. Achieved by masking Decoding time step: 1 (2) 3 4 5 6 am OUTPUT Linear + Softmax Vencdec Kencdec **ENCODERS** DECODERS EMBEDDING WITH TIME SIGNAL EMBEDDINGS PREVIOUS étudiant suis le INPUT

OUTPUTS

Decoder's encoder-decoder attention: queries are generated from below (sub)-layers.





Decoding time step: 1 2 3 4(5)6

**OUTPUT** I am a student <end of sentence>



#### **Transformer : Final Layer**



The output is compared to ground truth translation after the forward pass. E.g.: Consider a 6 word vocabulary as shown below.

Output Voca	Output Vocabulary									
WORD	a	am	I	thanks	student	<eos></eos>				
INDEX	0	1	2	3	4	5				

	Output Vocabul	ary								
WORD	а	am	I	thanks	student	<eos></eos>				
INDEX	0	1	2	3	4	5				
One-hot encoding of the word "am"										
	0.0	1.0	0.0	0.0	0.0	0.0				

#### Use cross-entropy loss, summed across all outputs.





After training, output probabilities at each position should reflect the translated sentence's word. Do beam-search decoding, probabilistic decoding or greedy decoding as needed.



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# **Transfer Learning in NLP**

#### Bidirectional Encoder Representations from Transformers

- Key idea: transfer learning
- Similar to how we can use pre-trained models in vision, we can use pre-trained models for language
- We have seen this idea before:
  - Word2Vec
  - Glove
- Since 2018, embeddings generated using transformer based pre-trained models have further improved the state of the art for multiple NLP tasks.
- Lets first see how to use such a model (distillBERT) in a classification task.
  - BERT stands for **B**idirectional **E**ncoder **R**epresentations from **T**ransformers

<sup>1</sup>Reference: <u>https://github.com/google-research/bert</u> and <u>https://arxiv.org/abs/1910.01108</u> 63

- BERT has been used in versatile products such as Google Search.
  - "... the biggest leap forward in the past five years, and one of the biggest leaps forward in the history of Search."
- For us, we want to use BERT (or distillBERT) in a specific NLP task.
  - Lets pick a movie review classification task



sentence	label
a stirring , funny and finally transporting re imagining of beauty and the beast and 1930s horror films	1
apparently reassembled from the cutting room floor of any given daytime soap	0
they presume their audience won't sit still for a sociology lesson	0
this is a visually stunning rumination on love , memory , history and the war between art and commerce	1
jonathan parker 's bartleby should have been the be all end all of the modern office anomie films	1

<sup>1</sup>Reference: <u>https://jalammar.github.io/a-visual-guide-to-using-bert-for-the-first-time/</u> and <u>https://colab.research.google.com/github/jalammar/jalammar.github.io/blob/master/notebooks/bert%A Visual Notebook to Using BERT for the First Time.ipynb</u>

The 'review embedding' that will be passed on the logistic regression model will be of size 768.



The embedding vector is the output of the first position (associated with the so called [CLS] token) among multiple positions (recall transformer encoder) DistillBERT has been pretrained on English using a suitable learning task and a large dataset





Step #3: Train the logistic regression model using the training set



Lets focus on a single prediction with a trained model. We need to 'tokenize' our input sentence and add [CLS] and [SEP] at the start and the end. visually stunning [CLS] [SEP] ##ination love а rum on **Tokenization** DistilBertTokenizer 2) Add [CLS] and [SEP] tokens visually stunning ##ination а rum on love 1) Break words into tokens **Tokenize** "a visually stunning rumination on love"



tokenizer.encode("a visually stunning rumination on love", add\_special\_ tokens=True)


This sequence is passed through DistillBERT (again, think of this as a transformer encoder. We will look at key details later).



As mentioned before, we only use the vector corresponding to the first dimension.



The rest of the process is standard ML workflow: cross-validated training or training after a traintest split.



The code is as follows:

```
import numpy as np
import pandas as pd
import torch
import transformers as ppb # pytorch transformers
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import train_test_split
model_class, tokenizer_class, pretrained_weights = (ppb.DistilBertModel, ppb.Distil
BertTokenizer, 'distilbert-base-uncased')
```

```
## Want BERT instead of distilBERT? Uncomment the following line:
#model_class, tokenizer_class, pretrained_weights = (ppb.BertModel, ppb.BertTokeniz
er, 'bert-base-uncased')
```

#### # Load pretrained model/tokenizer

tokenizer = tokenizer\_class.from\_pretrained(pretrained\_weights)
model = model\_class.from\_pretrained(pretrained\_weights)

df = pd.read\_csv('https://github.com/clairett/pytorch-sentiment-classification/raw/
master/data/SST2/train.tsv', delimiter='\t', header=None)

#### 0 1

0 a st	tirring , funny	and finally	transporting re	1
--------	-----------------	-------------	-----------------	---

- 1 apparently reassembled from the cutting room f... 0
- 2 they presume their audience wo n't sit still f... 0
- 3 this is a visually stunning rumination on love... 1
- 4 jonathan parker 's bartleby should have been t... 1

<sup>1</sup>Reference: <u>https://jalammar.github.io/a-visual-guide-to-using-bert-for-the-first-time/</u> and <u>https://github.com/clairett/pytorch-sentiment-classification/</u>

We are applying tokenization over all training data.

tokenized = df[0].apply((lambda x: tokenizer.encode(x, add\_special\_tokens=True)))



We will pad short sentences with token 0. The largest sentence length is 66.

# BERT/DistilBERT Input Tensor



	_	0	1	 66
Input sequences (reviews)	0	101	1037	 0
	1	101	2027	 0
	1,999	101	1996	 0



The output variable has a shape (#examples, max no of tokens, number of hidden units) So, 2000 \* 66 \* 768.



Here is an illustration for a single example (the first one).



We only need the output vector corresponding to the first position/token. That part of the output tensor is highlighted.



*# Slice the output for the first position for all the sequences, take all hidden unit outputs* 

```
features = last_hidden_states[0][:,0,:].numpy()
```



See <u>https://huggingface.co/transformers/examples.html</u> for more example that not only use pre-trained models as feature extractors, but also fine-tune them.

Its standard ML from this point out for our running example (movie review classification).







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# **BERT and Friends**

BERT, or Bidirectional Encoder Representations from Transformers, is a new method of pre-training language representations which obtains state-of-the-art results on a wide array of Natural Language Processing (NLP) tasks.

There are many models out there.





<sup>1</sup>Reference: <u>https://medium.com/huggingface/distilbert-8cf3380435b5</u> and <u>https://en.wikipedia.org/wiki/GPT-3</u>

Here are the ExactMatch (EM) and F1 scores evaluated on the test set of SQuAD v1.1.

Rank	Model	EM	F1
	Human Performance Stanford University (Rajpurkar et al. '16)	82.304	91.221
12 Oct 05, 2018	BERT (single model) Google AI Language https://arxiv.org/abs/1810.04805	85.083	91.835

 Stanford Question Answering Dataset (SQuAD) is a reading comprehension dataset, consisting of questions posed by crowdworkers on a set of Wikipedia articles, where the answer to every question is a segment of text, or span, from the corresponding reading passage, or the question might be unanswerable.

<sup>1</sup>Reference: <u>https://rajpurkar.github.io/SQuAD-explorer/</u>

SQuAD v1.1 Leaderboard (Oct 8th 2018)	Test EM	Test F1
1st Place Ensemble - BERT	87.4	93.2
2nd Place Ensemble - nInet	86.0	91.7
1st Place Single Model - BERT	85.1	91.8
2nd Place Single Model - nlnet	83.5	90.1

And several natural language inference tasks:

System	MultiNLI	Question NLI	SWAG
BERT	86.7	91.1	86.3
OpenAl GPT (Prev. SOTA)	82.2	88.1	75.0

Plus many other tasks.

Moreover, these results were all obtained with almost no task-specific neural network architecture design.

#### <sup>1</sup>Reference: <u>https://github.com/google-research/bert</u>

- A general-purpose "language understanding" model on a large text corpus (like Wikipedia)
- Use the model for downstream NLP tasks that we care about (like question answering)
- BERT outperforms previous methods because it is the first unsupervised, deeply bidirectional system for pre-training NLP
  - Unsupervised: trained only on plain text (no metadata)

- Pre-trained representations can also either be context-free or contextual, and contextual representations can further be unidirectional or bidirectional.
- Context-free models such as <u>word2vec</u> or <u>GloVe</u> generate a single "word embedding" representation
- Contextual models instead generate a representation of each word that is based on the other words in the sentence.
- Bidirectionality: BERT represents words using both its left and right context

#### Two step process

### 1 - Semi-supervised training on large amounts of text (books, wikipedia..etc).

The model is trained on a certain task that enables it to grasp patterns in language. By the end of the training process, BERT has language-processing abilities capable of empowering many models we later need to build and train in a supervised way.



#### Semi-supervised Learning Step

<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

The second step is problem specific

2 - Supervised training on a specific task with a labeled dataset.



<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

For instance, BERT can be used for classification (we saw this in detail earlier) If the BERT parameters are also changed, this would be considered fine-tuning (we saw this for vision)



There are two pre-trained versions for BERT (just like resnet18 vs resnet50 or vgg16 vs vgg19)



<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

The encoder units/layers (also called transformer blocks) is 12 or 24. FF networks have 768 or 1024 hidden units. The number of attention heads is 12 or 16. (vs 6 units, 512 units, 8 heads before)



First input is a special symbol (cls means classification). Architecture same as Transformer so far.



Each position outputs a 768 dim vector in BERT base.



For classification, as we saw earlier, we use only the first vector.



<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

Similar to a CNN classificer (CNN layers followed by a fully connected layer)





- A word can have different meaning depending on its context
- This was not captured in word2vec and Glove for instance.
- ELMo (2018) produces contextualized word embeddings.

<sup>1</sup>Reference: <u>https://jalammar.github.io/illustrated-bert/</u> and <u>https://arxiv.org/pdf/1802.05365.pdf</u>

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### ELMo

Look at the entire sentence before embedding each word in the sentence. Based on LSTMs. Trained as a language model.



<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

### **ELMo**



<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

#### ELMo

The hidden vectors computed in the forward pass are used for generating embeddings.

Embedding of "stick" in "Let's stick to" - Step #1



Backward Language Model


### ELMo

ELMo is actually a bidirectional LSTM. The hidden vectors are aggregated to get the embedding.



ELMo embedding of "stick" for this task in this context

In addition to embeddings, the model parameters can also be changed later on (ULM-FiT)

Transformers are able to capture long-term dependencies better than LSTMs (empirical)

Use just the decoder for language modelling. Can predict the next word and masks future tokens.



Has 12 decoder units (the encoder-decoder attention is removed).



Can then be used for downstream NLP tasks.



Suitably processing the input can allow the OpenAl Transformer to be used for various tasks



- ELMo was bi-directional but OpenAl Transformer was not
- The next natural idea (that lead to BERT) is whether a transformer-based model can look both forward and backward while predicting the next word.

The key idea is to use **masks and encoders.** We need to prevent word from seeing itself. **We will skip much of the details here about masking.** 



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In addition to language modelling, BERT also pre-trains on sentence sequencing task.



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Pre-trained BERT can be used for other tasks (beyond classification) as well:



(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG



(b) Single Sentence Classification Tasks: SST-2, CoLA



SQuAD v1.1



(d) Single Sentence Tagging Tasks: CoNLL-2003 NER

<sup>1</sup>Reference: https://jalammar.github.io/illustrated-bert/

BERT can be used as a word embedding model like ELMo. The embeddings are contextual.



#### The choice of which hidden vector to use as the word-embedding can be data driven.

What is the best contextualized embedding for "Help" in that context?

For named-entity recognition task CoNLL-2003 NER



# Questions?

# Summary

- Self-attention is the key building block of transformer variants
- Transformer based encoders can be used for contextualized embeddings of words
- BERT and related architectures can be used to improve many NLP tasks. This is similar to using pre-trained vision models (e.g., resnet50). Finetuning can also be done.
- Readily available pre-trained models alleviate the need for compute heavy resources in application specific ML projects
- Exercise: BERT finetuning tutorial on Google Colab
  - <u>https://colab.research.google.com/github/tensorflow/tpu/blob/master/tools/colab/bert\_finetuning\_with\_cloud\_tpus.ipynb</u>