CSE 4392 Special Topics
Natural Language Processing

Transformer and Large Language Model

2024 Spring

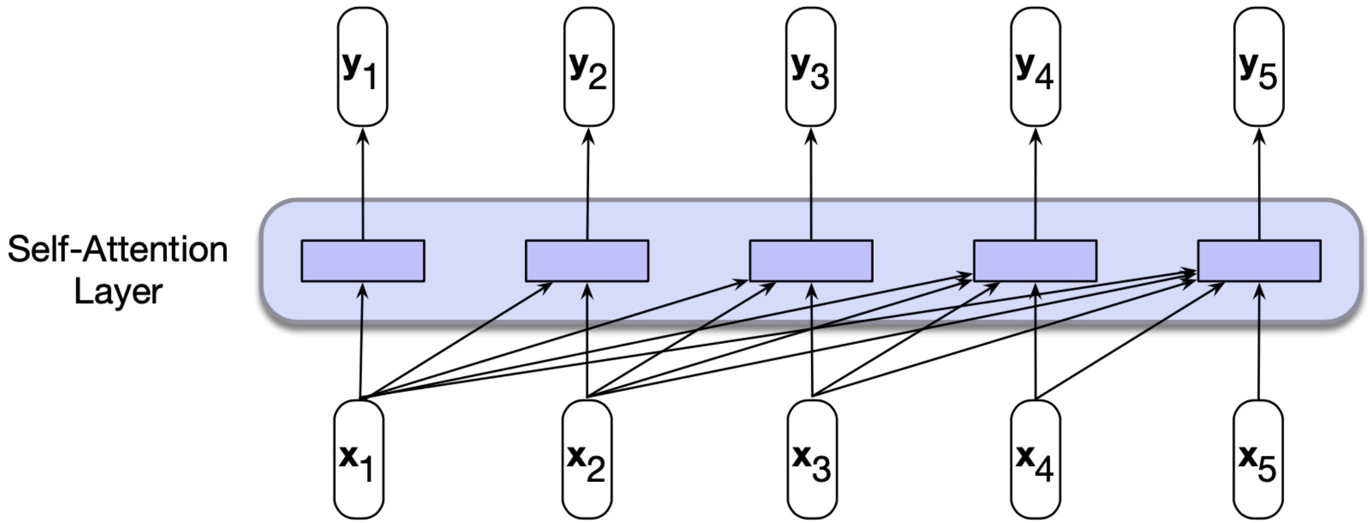
PRETRAINING

- Knowledge of vocabulary is acquired by "reading".
- **Distributional hypothesis**:
  - Meaning of a word can be determined by its context
  - Context can be representated by word distribution
  - Knowledge acquired can be useful in language processing *long after* its initial acquisition
- **Pretraining:**
  - the process of learning some sort of representation of meaning for words or sentences by processing very large amounts of text.
  - RNN and even Feedforward NN can be pretrained to learn language models
  - *Transformer* is a better choice

TRANSFORMER

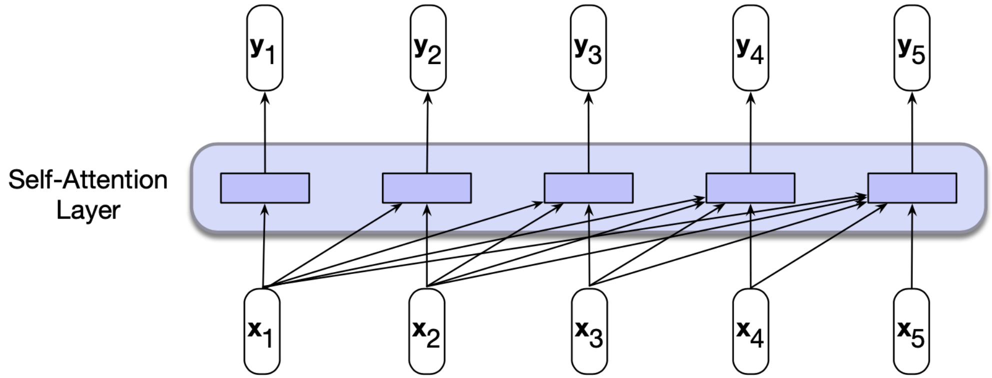
- Like LSTM, transformers can handle long-range dependencies
- But it doesn't use recurrent connections
  - recurrent architectures are hard to parallelize
  - transformers can be parallelized and are more efficient
- Two main ideas in transformers:
  - **Self-attention**
  - **Positional embeddings**

SELF ATTENTION NETWORK



- "**Causal**" self-attention model
- Each layer maps inputs $x_1, \dots, x_n$ to outputs $y_1, \dots, y_n$ (equal length) → *language model* (auto-regressive generation)
- y_i depends on $x_1, \dots, x_i$, can be computed independently from other y_j. → *parallelism*

A SIMPLE SELF-ATTENTION



- The computation of $\boldsymbol{y}_i$ depends on the comparison tween $\boldsymbol{x}_i$ with $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, up to $\boldsymbol{x}_i$ itself.
- Simple form: $score(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{x}_i \cdot \boldsymbol{x}_j$ (dot product)
- The larger the score, the the more similar they are.
- Attention weight vector:

$$\alpha_{ij} = \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \ \forall j \leq i$$
$$= \frac{\exp(\text{score}(\mathbf{x}_i, \mathbf{x}_j))}{\sum_{k=1}^{i} \exp(\text{score}(\mathbf{x}_i, \mathbf{x}_k))} \ \forall j \leq i$$

$$\mathbf{y}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{x}_j$$

The self-attention in transformers

- Each input $\boldsymbol{x}_i$ plays three roles:
- Query: *current focus of attention* when compared to all preceding input;
- Key: *preceding input* being compared to current focus of attention;
- Value: used to compute the output of current focus of attention;

$$\mathbf{q}_i = \mathbf{W}^{\mathbf{Q}}\mathbf{x}_i; \;\; \mathbf{k}_i = \mathbf{W}^{\mathbf{K}}\mathbf{x}_i; \;\; \mathbf{v}_i = \mathbf{W}^{\mathbf{V}}\mathbf{x}_i$$

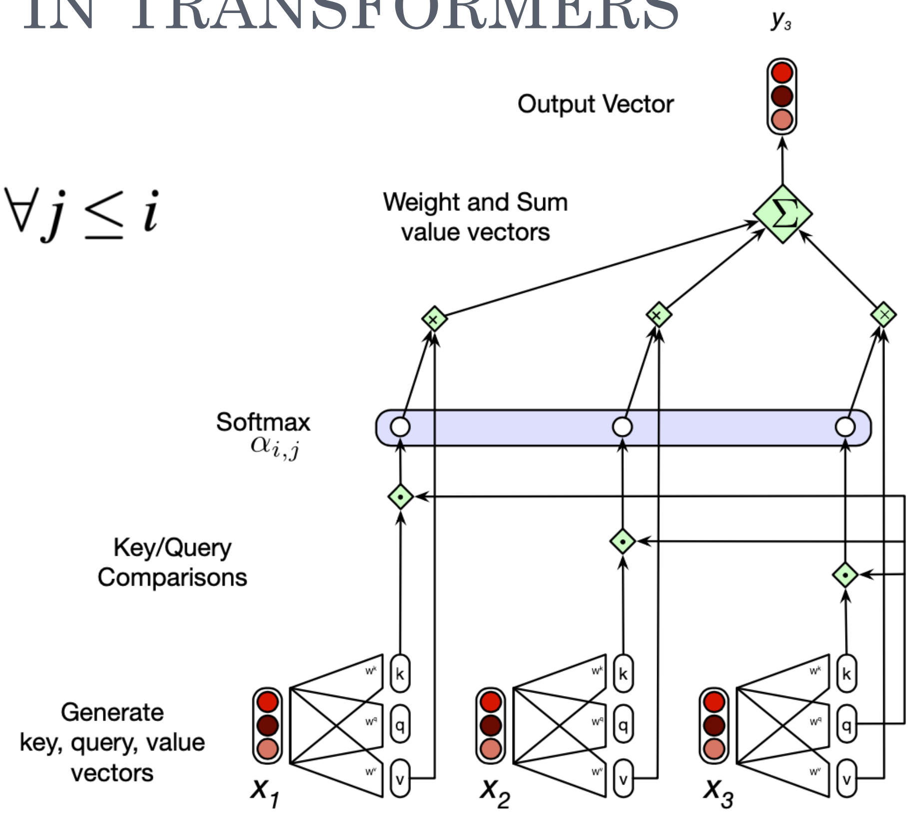
- $\boldsymbol{x}_i$ and $\boldsymbol{y}_i$ are vectors of d-dimension.
- $W^Q \in \mathbb{R}^{d\times d}, W^K \in \mathbb{R}^{d\times d}, W^V \in \mathbb{R}^{d\times d}$

The self-attention in transformers

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{q}_i \cdot \mathbf{k}_j$$

$$\alpha_{ij} = \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \; \forall j \leq i$$

$$\mathbf{y}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}_j$$



Scale the score down:

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$$

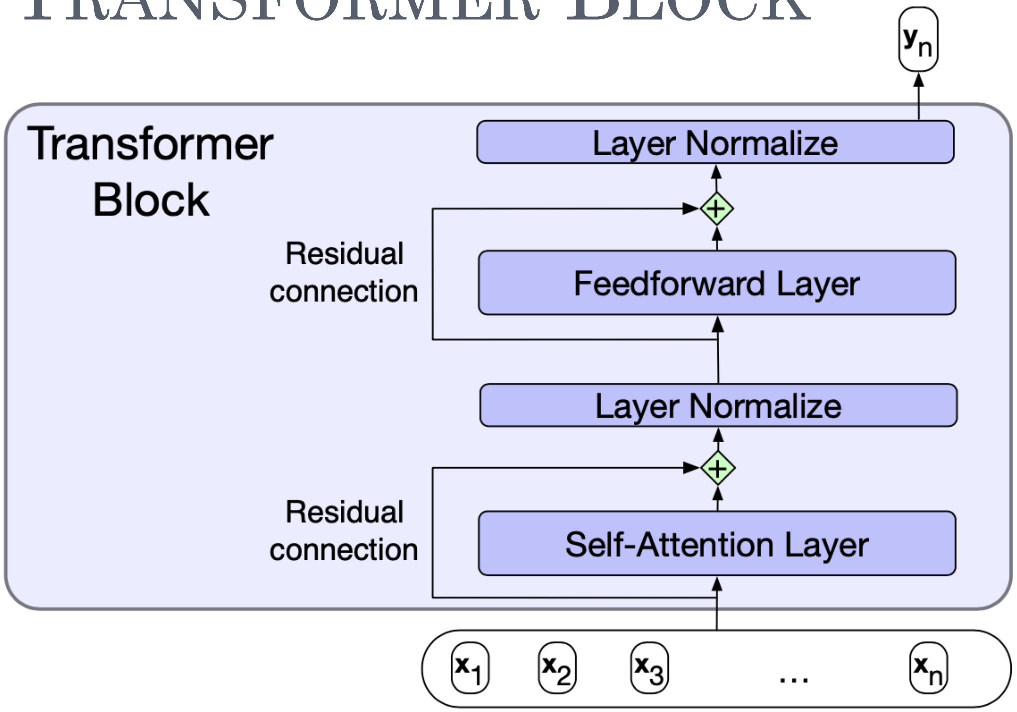
Computing all inputs together:

$$\mathbf{Q} = \mathbf{X}\mathbf{W}^{\mathbf{Q}}; \;\; \mathbf{K} = \mathbf{X}\mathbf{W}^{\mathbf{K}}; \;\; \mathbf{V} = \mathbf{X}\mathbf{W}^{\mathbf{V}}$$

Quiz: Complexity of Attention

- What is the time complexity of computing attention, in terms of the length of input N?

Transformer Block



$$\mathbf{z} = \text{LayerNorm}(\mathbf{x} + \text{SelfAttention}(\mathbf{x}))$$
$$\mathbf{y} = \text{LayerNorm}(\mathbf{z} + \text{FFN}(\mathbf{z}))$$

- Residual connection by-passes the information from lower layer to higher layer without going through the intermediate layer
- Residual info is summed with the output the intermediate layer.

Layer Norm

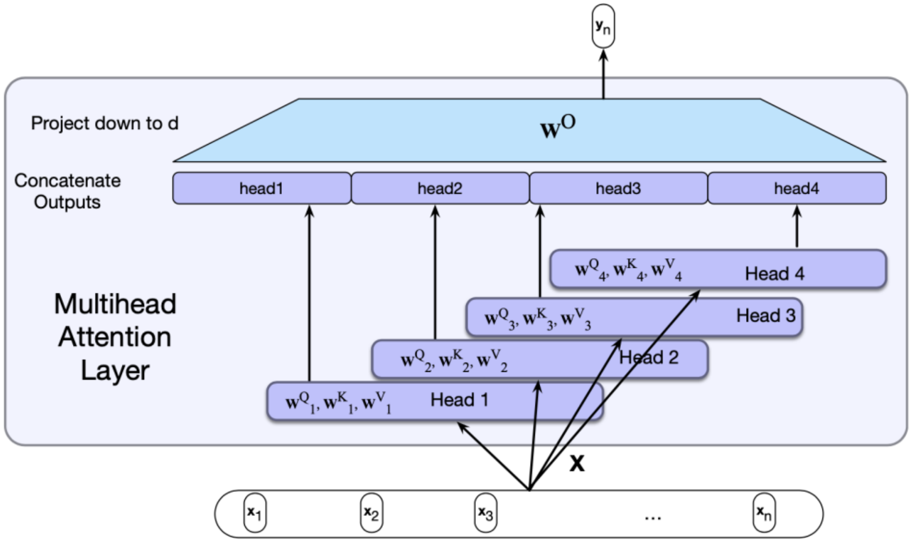
- Layer normalization can be any normalization that keeps the values of hidden layers in a range that is "gradient friendly."
- Mean: $$\mu = \frac{1}{d_h} \sum_{i=1}^{d_h} x_i$$
- Standard dev: $$\sigma = \sqrt{\frac{1}{d_h} \sum_{i=1}^{d_h} (x_i - \mu)^2}$$
- normalized: $$\hat{\mathbf{x}} = \frac{(\mathbf{x} - \mu)}{\sigma}$$

$$\text{LayerNorm} = \gamma \hat{\mathbf{x}} + \beta$$

trainable params

Multi-head Attention

- Different words in a sentence can related to each other in different ways:
  - syntactic
  - semantic
  - discourse
  - …



- Instead of one self-attention layer, multiple self-attention layers (called **heads**) in parallel (concatenated):

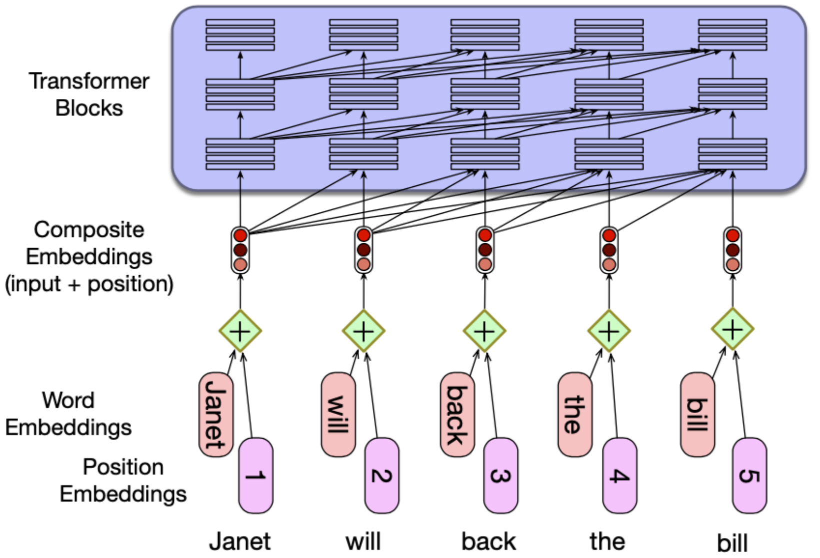
$$\text{MultiHeadAttention}(\mathbf{X}) = (\mathbf{head}_1 \oplus \mathbf{head}_2 \ldots \oplus \mathbf{head}_h)\mathbf{W}^O$$

$$\mathbf{Q} = \mathbf{X}\mathbf{W}_i^Q \,;\, \mathbf{K} = \mathbf{X}\mathbf{W}_i^K \,;\, \mathbf{V} = \mathbf{X}\mathbf{W}_i^V$$

$$\mathbf{head}_i = \text{SelfAttention}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$$

Positional Embedding

- In a transformer, input tokens are in parallel.
- There's no notion of order at all!
- Idea: add a positional embedding to word embedding to get the new input embedding
- Positional embeddings are learned just like word embedding:
  - randomly initialized
  - one vector for each position such as 1, 2, 3
  - Problem: far positions such as 100, 200 are poorly trained



Quiz: Multi-head vs Positional Embedding

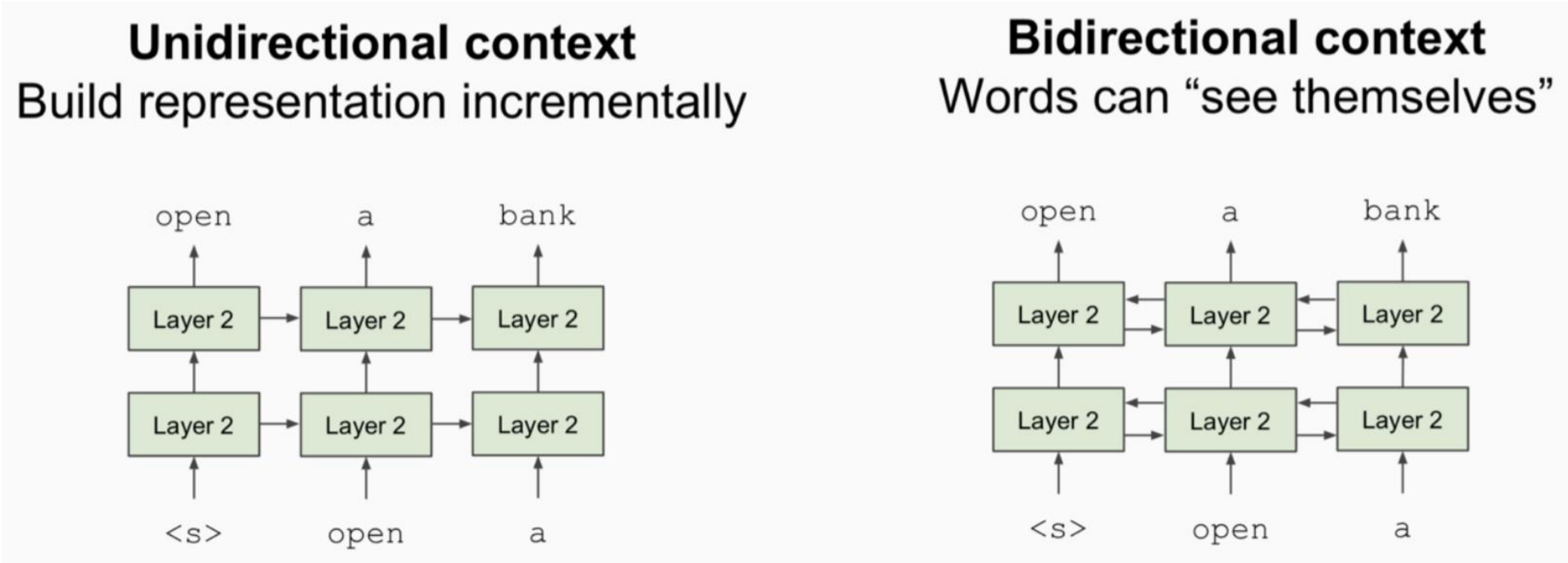
- Why do we concatenate the multipile head vectors together to get the overall attention, but simply add (element-wise) the word vector and positional vector to create the new input vector?

BERT

- “Bidirectional Encoder Representations from Transformers”
- First released in Oct 2018.
- NAACL’19: BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding
- BERT provides contextualized word embedding
- An improvement from ELMo:
  - bidirectional context vs unidirectional context
  - Transformers vs LSTMs
  - The weights are not frozen, called *fine-tuning*

Bidirectional Encoders

- Language models only use left context or right context (although ELMo used two independent LMs from each direction).
- Language understanding is bidirectional



Masked Language Models

- How to pretrain the language model?
- Solution: Mask out 15% of the input words, and then predict the masked words

- Too little masking: too expensive to train
- Too much masking: not enough context

Masked Language Models

- Because BERT will never see [MASK] in real-world data, training data is a little more complicated:

  - Rather than *always* replacing the chosen words with `[MASK]`, the data generator will do the following:
  - 80% of the time: Replace the word with the `[MASK]` token, e.g., `my dog is hairy` → `my dog is [MASK]`
  - 10% of the time: Replace the word with a random word, e.g., `my dog is hairy` → `my dog is apple`
  - 10% of the time: Keep the word unchanged, e.g., `my dog is hairy` → `my dog is hairy`. The purpose of this is to bias the representation towards the actual observed word.

Next Sentence Prediction (NSP)

- Always sample two sentences, predict whether the second sentence is followed after the first one.

Input = `[CLS] the man went to [MASK] store [SEP]`

`he bought a gallon [MASK] milk [SEP]`

Label = `IsNext`

Input = `[CLS] the man [MASK] to the store [SEP]`

`penguin [MASK] are flight ##less birds [SEP]`

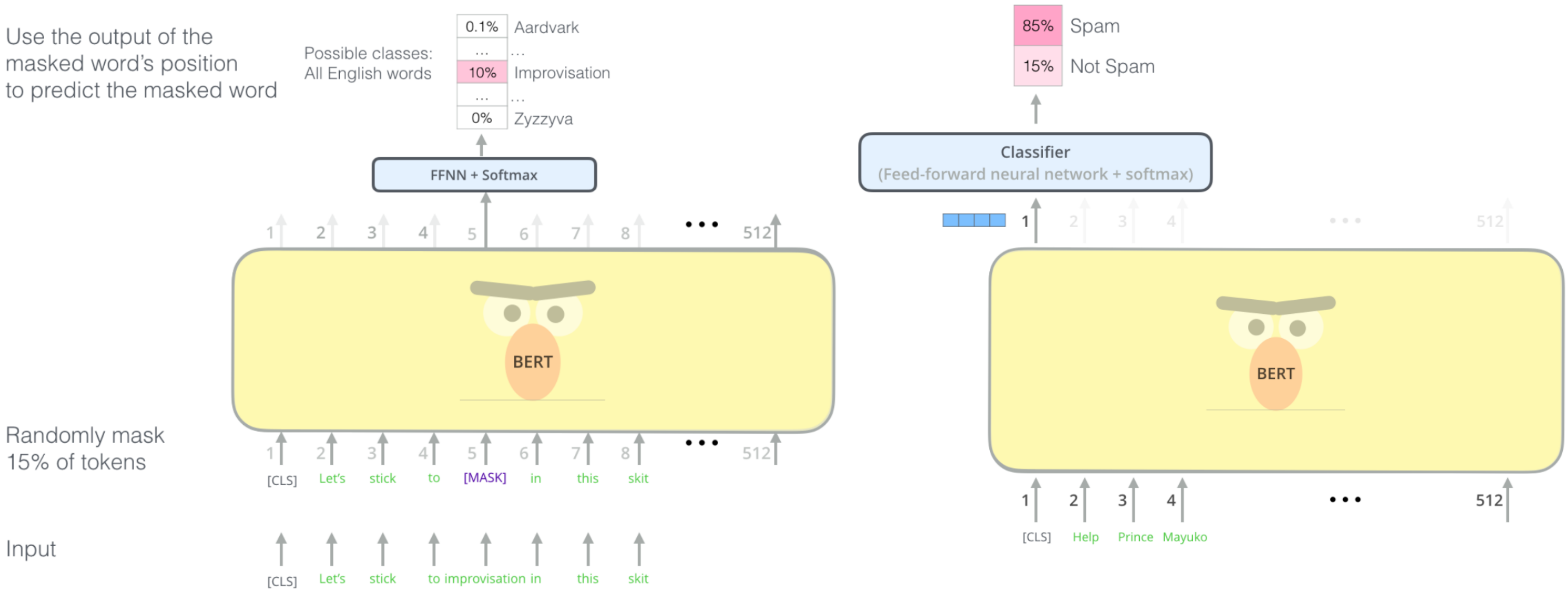
Label = `NotNext`

- Recent paper shows that NSP is not necessary…

(Joshi*, Chen* et al, 2019) :SpanBERT: Improving Pre-training by Representing and Predicting Spans
(Liu et al, 2019): RoBERTa: A Robustly Optimized BERT Pretraining Approach

Pretraining and Fine-tuning

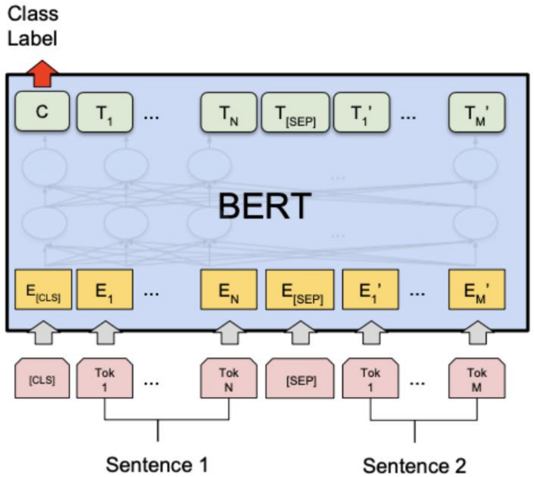
- Key idea: all the weights are fine-tuned on downstream tasks



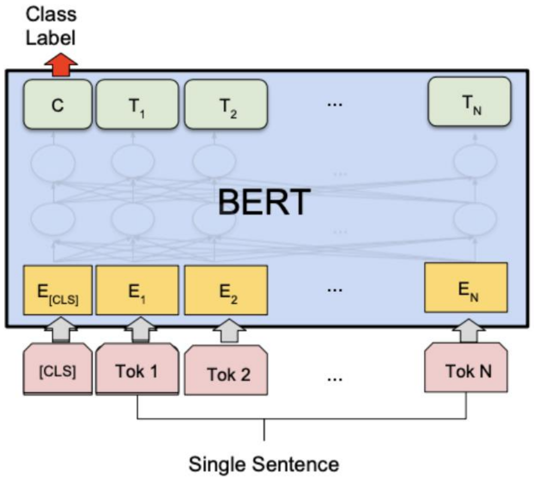
Pretrain

Fine-tune

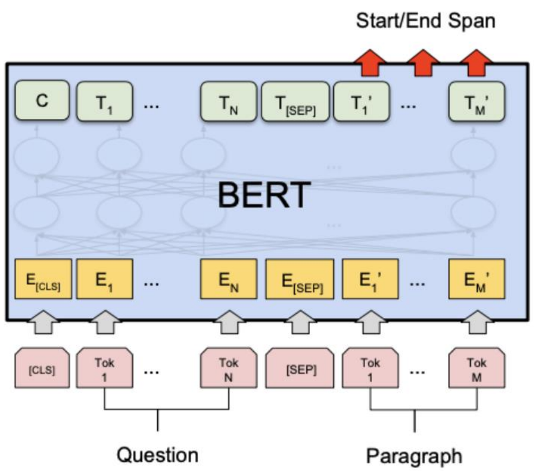
BERT Applications



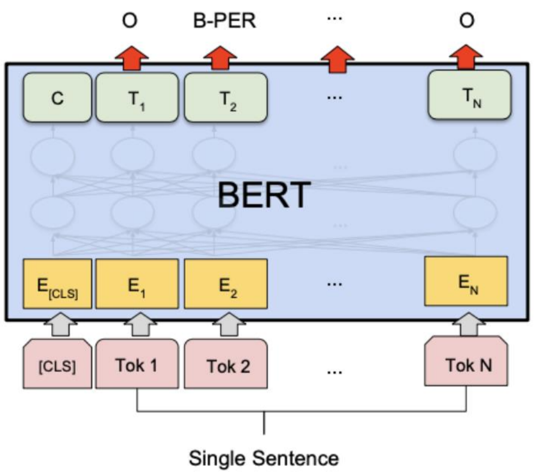
(a) Sentence Pair Classification Tasks:
MNLI, QQP, QNLI, STS-B, MRPC,
RTE, SWAG



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



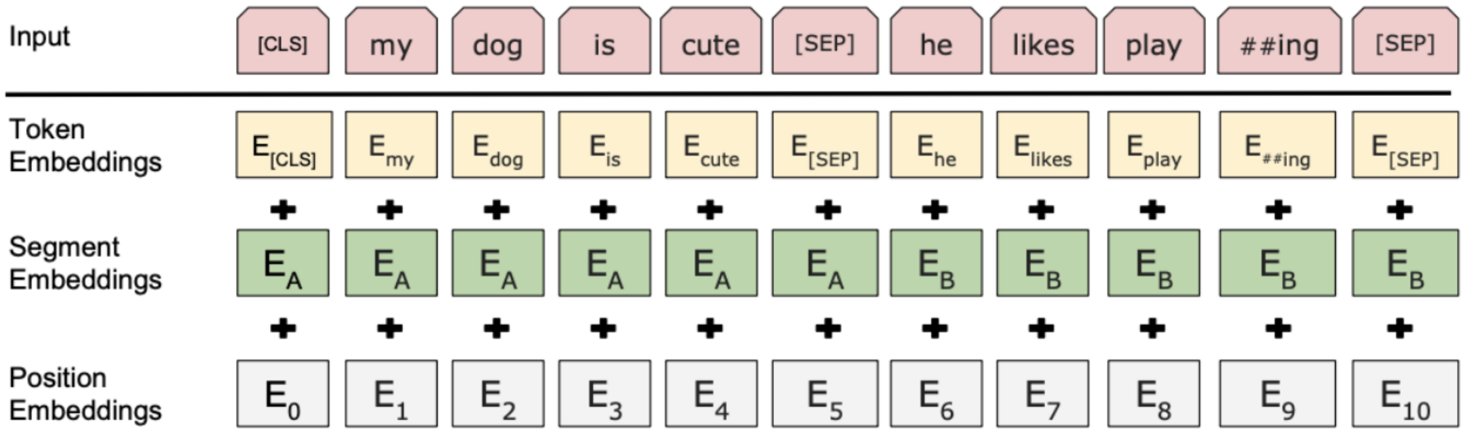
(c) Question Answering Tasks:
SQuAD v1.1



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

BERT More Details

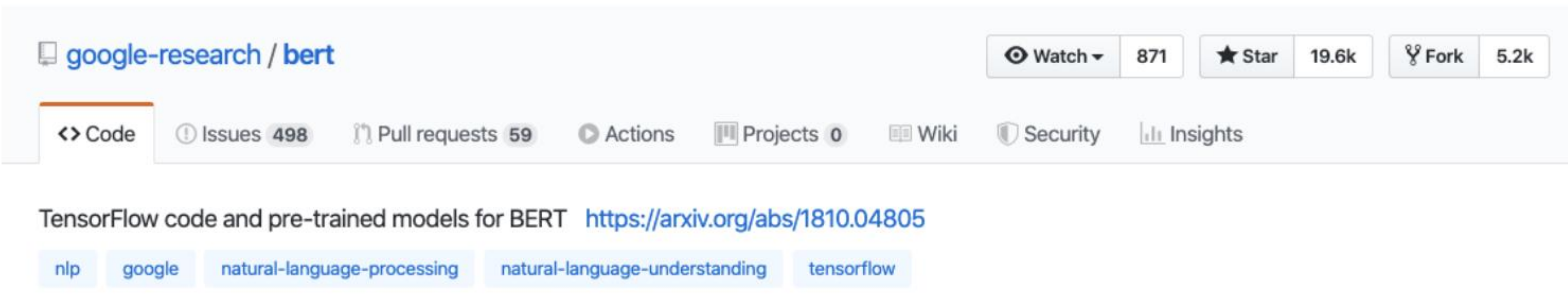
- Input representations:



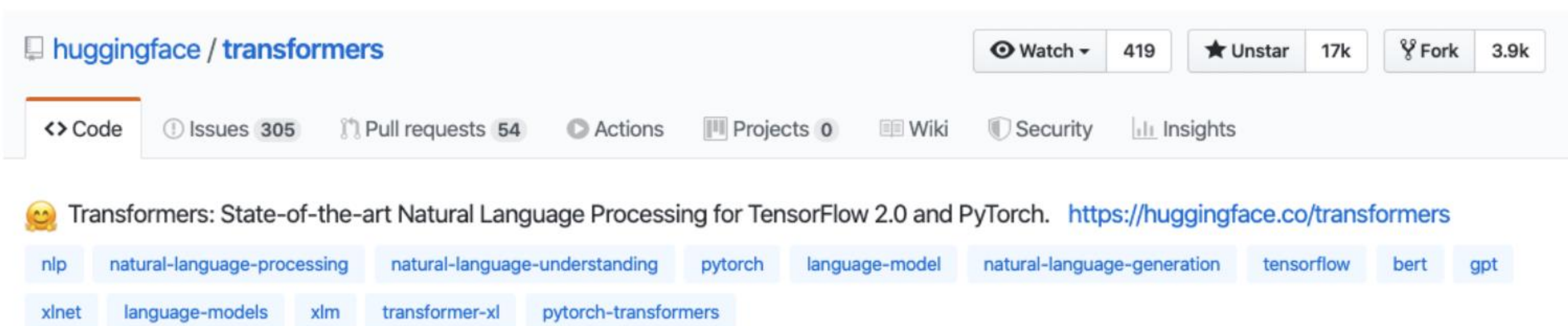
- Use sub-word embedding instead of words
  - playing → play, ##ing
- Trained 40 epoches on Wikipedia (2.5B tokens) + BookCorpus (0.8B tokens)
- Two releases: BERT-base, BERT-large

USE BERT IN PRACTICE

- **TensorFlow**: https://github.com/google-research/bert



- **PyTorch**: https://github.com/huggingface/transformers



BERT is very strong for many tasks

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BiLSTM: 63.9

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.9	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	88.1	91.3	45.4	80.0	82.3	56.0	75.2
$BERT_{BASE}$	84.6/83.4	71.2	90.1	93.5	52.1	85.8	88.9	66.4	79.6
$BERT_{LARGE}$	**86.7/85.9**	**72.1**	**91.1**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**81.9**

Model	**data**	**bsz**	**steps**	**SQuAD** (v1.1/2.0)	**MNLI-m**	**SST-2**
RoBERTa						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	**94.6/89.4**	**90.2**	**96.4**
$BERT_{LARGE}$						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7
$XLNet_{LARGE}$						
with BOOKS + WIKI	13GB	256	1M	94.0/87.8	88.4	94.4
+ additional data	126GB	2K	500K	94.5/88.8	89.8	95.6

RoBERTa and XLNet are optimized versions of BERT with different pretraining approach. Archi is the same!

Original Transformer

- Encoder-decoder archi.