Natural Language Processing with Deep Learning

Lecture 7 — BERT as encoder-only transformer

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Motivation

1 Motivation

2 BERT — Encoder architecture in detail

3 Input and pre-training

4 Pre-training

5 Downstream tasks and fine-tuning

Motivation

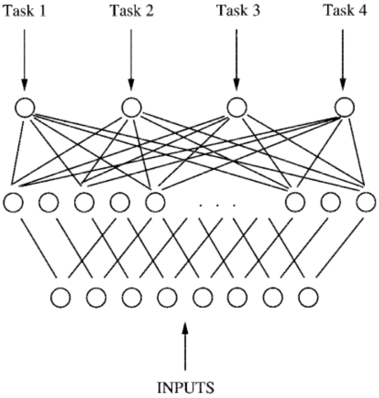
Multi-task learning

Multi-task Learning

R. Caruana (1997). **"Multi-task Learning".** In: *Machine Learning* 28.1, pp. 41–75

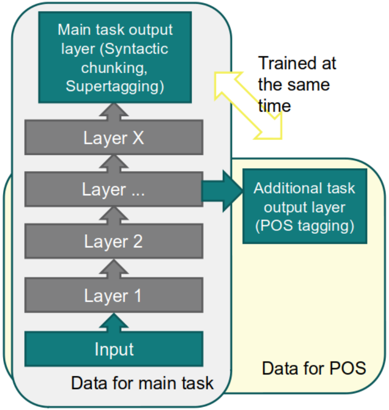
Approach to inductive transfer that improves generalization

By learning tasks in parallel while using a shared representation



Multi-task learning in NLP

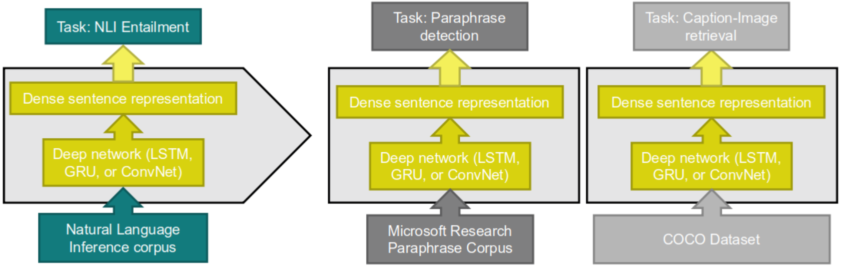
"In case we suspect the existence of a hierarchy between the different tasks, we show that it is worth-while to incorporate this knowledge in the MTL architecture's design, by making lower level tasks affect the lower levels of the representation."



Main task output layer (Syntactic chunking, Supertagging)
Layer X
Layer ...
Layer 2
Layer 1
Input
Data for main task
Trained at the same time
Additional task output layer (POS tagging)
Data for POS

A. Søgaard and Y. Goldberg (2016). **"Deep multi-task learning with low level tasks supervised at lower layers".** In: *Proceedings of ACL*. Berlin, Germany: Association for Computational Linguistics, pp. 231–235

Learn a sentence representation on a different task


Task: NLI Entailment
Dense sentence representation
Deep network (LSTM, GRU, or ConvNet)
Natural Language Inference corpus
Task: Paraphrase detection
Dense sentence representation
Deep network (LSTM, GRU, or ConvNet)
Microsoft Research Paraphrase Corpus
Task: Caption-Image retrieval
Dense sentence representation
Deep network (LSTM, GRU, or ConvNet)
COCO Dataset

A. Conneau, D. Kiela, H. Schwenk, L. Barrault, and A. Bordes (2017). **“Supervised Learning of Universal Sentence Representations from Natural Language Inference Data”.** In: *Proceedings of EMNLP*. Copenhagen, Denmark, pp. 670–680

"Models learned on NLI can perform better than models trained in unsupervised conditions or on other supervised tasks."

Bottlenecks of RNN for representation learning

Inherently **sequential** nature

- No parallelization
- Long-range dependencies modeling: Distance plays a role!

...but when the goal is to learn a good representation of the input sequence, we might have better/faster architectures

Also recall disadvantages of **static word embeddings**

Today: Transformers and the BERT architecture

Bidirectional **E**ncoder **R**epresentations from **T**ransformers

BERT was a game-changer in NLP:

“BERT is conceptually simple and empirically powerful. It obtains new **state-of-the-art results on eleven natural language processing tasks**, including pushing the GLUE score to 80.5% (**7.7% point absolute improvement**), MultiNLI accuracy to 86.7% (**4.6% absolute improvement**), SQuAD v1.1 question answering Test F1 to 93.2 (1.5 point absolute improvement) and SQuAD v2.0 Test F1 to 83.1 (**5.1 point absolute improvement**).”

After this lecture you should be able to build BERT

J. Devlin, M.-W. Chang, K. Lee, and K. Toutanova (2019). **“BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding”.** In: *Proceedings of NAACL*. Minneapolis, Minnesota: Association for Computational Linguistics, pp. 4171–4186

BERT — Encoder architecture in detail

1 Motivation

2 BERT — Encoder architecture in detail

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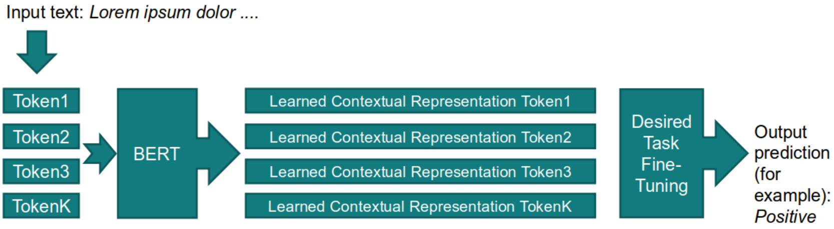
4 Pre-training

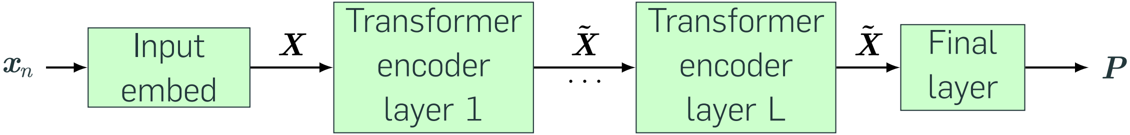
5 Downstream tasks and fine-tuning

BERT: Very abstract view


Input text: *Lorem ipsum dolor ....*
Token1
Token2
Token3
TokenK
BERT
Learned Contextual Representation Token1
Learned Contextual Representation Token2
Learned Contextual Representation Token3
Learned Contextual Representation TokenK
Desired Task Fine-Tuning
Output prediction (for example): *Positive*

- BERT produces contextualized token embeddings
- BERT can learn them in a ‘clever’ way
- BERT can be applied to many downstream tasks

Transformer encoder (BERT)



As usual, green boxes are functions with trainable parameters

$\tilde{\boldsymbol{X}}$ is just a placeholder for **updated** token embeddings matrix $\boldsymbol{X}$

Some details (Notation)

Notation and formal description of algorithms adopted from M. Phuong and M. Hutter (2022). **Formal Algorithms for Transformers.** arXiv: `2207.09238` Note that they use column-vector notation while here (and in all lectures) we use row-vector notation.

Simplify the set notation

$\{1, 2, \ldots, N\}$ is a set of integers $1, 2, \ldots, N-1, N$

simplify to $[N]$

For example $t \in [N] \equiv t \in \{1, 2, \ldots, N\}$

BERT (encoding-only transformer, forward pass)

```
function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    . . .
```

Input:

$\boldsymbol{x}$ — $\boldsymbol{x} \in V^*$, a sequence of token IDs

$\boldsymbol{\mathcal{W}}$ — all trainable parameters

Output:

Typically an embedding vector for each input token

Or: $\boldsymbol{P} \in (0,1)^{\ell_\mathsf{x} \times N_\mathsf{V}}$, where each row of $\boldsymbol{P}$ is a distribution over the vocabulary

Input embeddings

The cat sat $\boldsymbol{x}_n = \begin{pmatrix} 21 & 11987 & 5438 \end{pmatrix}$

$$\begin{bmatrix} 21 & 11987 & 5438 \end{bmatrix} \xrightarrow{\boldsymbol{x}_n} \boxed{\text{Input embeddings}} \xrightarrow{\boldsymbol{X}} \begin{bmatrix} \cdots & \boldsymbol{e}_1 & \cdots \\ \cdots & \boldsymbol{e}_2 & \cdots \\ \cdots & \boldsymbol{e}_3 & \cdots \end{bmatrix}$$

Positional embeddings

For each input position t, we learn (train) an embedding vector $\boldsymbol{W_p}[t]$, for example

$$\boldsymbol{W_p} = \begin{pmatrix} \boldsymbol{W_p}[1] \\ \boldsymbol{W_p}[2] \\ \vdots \\ \boldsymbol{W_p}[\ell] \end{pmatrix} = \begin{pmatrix} 1.12 & -78.6 & \cdots \\ \vdots & & \vdots \\ \vdots & & \vdots \\ -0.1 & 799.7 & \cdots \end{pmatrix}$$

The model knows with which part of the input/output is dealing with

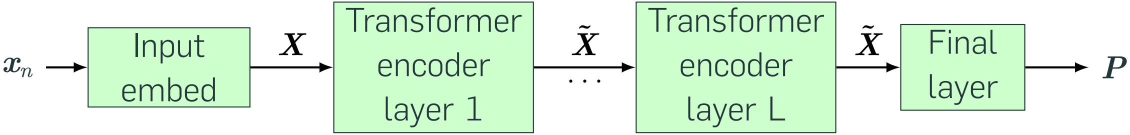
Originally proposed for CNNs for MT, state-of-the-art results and **9.3–21.3× faster** than LSTMs on GPU

J. Gehring, M. Auli, D. Grangier, D. Yarats, and Y. N. Dauphin (2017). **"Convolutional Sequence to Sequence Learning".** In: *Proceedings of the 34th International Conference on Machine Learning*. Ed. by D. Precup and Y. W. Teh. Sydney, Australia: PMLR, pp. 1243–1252

BERT (encoding-only transformer, forward pass)

```
function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    $\ell \leftarrow$ length($\boldsymbol{x}$)
    for $t \in [\ell]$ : $\boldsymbol{e}_t \leftarrow \boldsymbol{W}_{\boldsymbol{e}}[x[t], :] + \boldsymbol{W}_{\boldsymbol{p}}[t, :]$        ▷ Token emb. + positional emb.
    $\boldsymbol{X} \leftarrow$ Stack row-wise$[\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots \boldsymbol{e}_\ell]$
    $\ldots$
```

Transformer encoder (BERT)

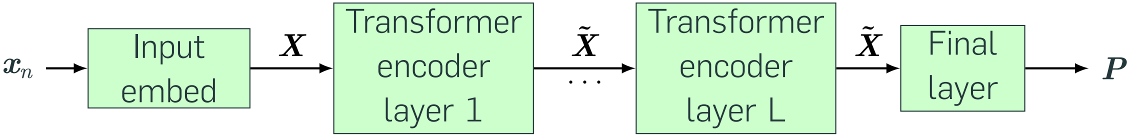


The transformer encoder layer is repeated L-times (each with **different** parameters)

BERT (encoding-only transformer, forward pass)

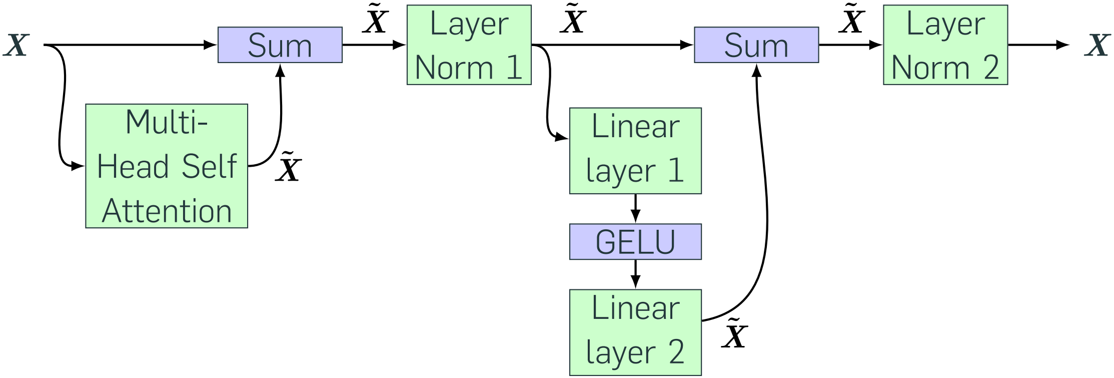
```
function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    $\ell \leftarrow$ length($\boldsymbol{x}$)
    for $t \in [\ell] : \boldsymbol{e}_t \leftarrow \boldsymbol{W}_{\boldsymbol{e}}[x[t], :] + \boldsymbol{W}_{\boldsymbol{p}}[t, :]$        ▷ Token emb. + positional emb.
    $\boldsymbol{X} \leftarrow$ Stack row-wise$[\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots \boldsymbol{e}_\ell]$
    for $l = 1, 2, \ldots, L$ do
        $\ldots$
```

Transformer encoder (BERT)



Let’s look at a single transformer encoder layer

Transformer encoder layer (BERT)

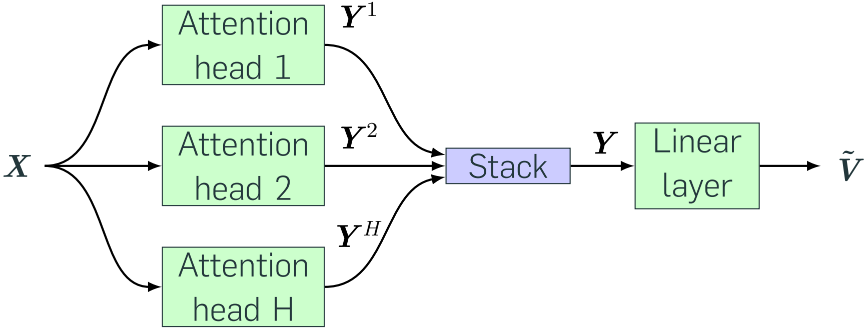


Let's focus on Multi-Head Self Attention

BERT (encoding-only transformer, forward pass)

```
function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    $\ell \leftarrow \text{length}(\boldsymbol{x})$
    for $t \in [\ell] : \boldsymbol{e}_t \leftarrow \boldsymbol{W_e}[x[t], :] + \boldsymbol{W_p}[t, :]$    ▷ Token emb. + positional emb.
    $\boldsymbol{X} \leftarrow \text{Stack row-wise}[\boldsymbol{e}_1, \boldsymbol{e}_2, \dots \boldsymbol{e}_\ell]$
    for $l = 1, 2, \dots, L$ do
        $\boldsymbol{X} \leftarrow \boldsymbol{X} + \text{MHAttention}(\boldsymbol{X} | \boldsymbol{\mathcal{W}}_l)$    ▷ Multi-head att., residual conn
        $\dots$
```

Multi-head unmasked self-attention



Some notation details

Concatenate matrices of the same dimensions along rows

$$\boldsymbol{Y} = [\boldsymbol{X}^1; \boldsymbol{X}^2; \ldots; \boldsymbol{X}^H] \qquad \boldsymbol{X}^i \in \mathbb{R}^{m \times n} \qquad \boldsymbol{Y} \in \mathbb{R}^{m \times H \cdot n}$$

Example

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}, \boldsymbol{B} = \begin{pmatrix} 11 & 12 \\ 13 & 14 \\ 15 & 16 \end{pmatrix} \qquad \boldsymbol{Y} = [\boldsymbol{A}; \boldsymbol{B}] = \begin{pmatrix} 1 & 2 & 11 & 12 \\ 3 & 4 & 13 & 14 \\ 5 & 6 & 15 & 16 \end{pmatrix}$$

Multi-head bidirectional unmasked self-attention

Input: $\boldsymbol{X} \in \mathbb{R}^{\ell_{\mathsf{x}} \times d_{\mathsf{x}}}$, vector representations of the sequence of length ℓ_{x}

Output: $\tilde{\boldsymbol{V}} \in \mathbb{R}^{\ell_{\mathsf{x}} \times d_{\mathsf{out}}}$, updated vector representations of tokens in $\boldsymbol{X}$

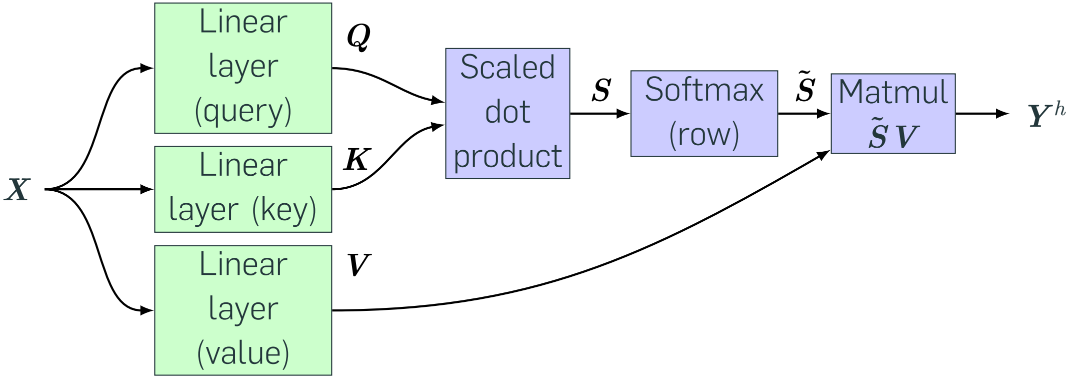
Hyper-param: H, number of attention heads

Params for each $h \in [H] : \boldsymbol{\mathcal{W}}^h_{\boldsymbol{qkv}}$:

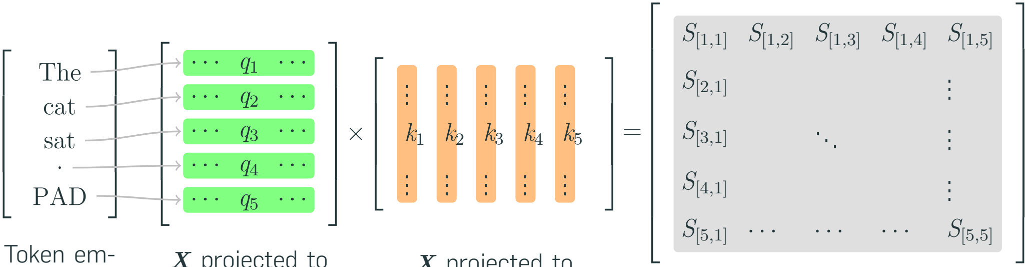
- $\boldsymbol{W}^h_{\boldsymbol{q}}, \boldsymbol{W}^h_{\boldsymbol{k}} \in \mathbb{R}^{d_{\mathsf{x}} \times d_{\mathsf{attn}}}$, $\boldsymbol{b}^h_{\boldsymbol{q}}, \boldsymbol{b}^h_{\boldsymbol{k}} \in \mathbb{R}^{d_{\mathsf{attn}}}$, $\boldsymbol{W}_{\boldsymbol{v}} \in \mathbb{R}^{d_{\mathsf{x}} \times d_{\mathsf{mid}}}$, $\boldsymbol{b}_{\boldsymbol{v}} \in \mathbb{R}^{d_{\mathsf{mid}}}$
- $\boldsymbol{W}_{\boldsymbol{o}} \in \mathbb{R}^{H \cdot d_{\mathsf{mid}} \times d_{\mathsf{out}}}$, $\boldsymbol{b}_{\boldsymbol{o}} \in \mathbb{R}^{d_{\mathsf{out}}}$

```
function MHAttention($\boldsymbol{X}; \boldsymbol{\mathcal{W}}$)
    for $h \in [H]$ do
        $\boldsymbol{Y}^h \leftarrow$ Attention($\boldsymbol{X}; \boldsymbol{\mathcal{W}}^h_{\boldsymbol{qkv}}$)        ▷ $\boldsymbol{Y}^h \in \mathbb{R}^{\ell_{\mathsf{x}} \times d_{\mathsf{mid}}}$
    $\boldsymbol{Y} \leftarrow [\boldsymbol{Y}^1; \boldsymbol{Y}^2; \ldots; \boldsymbol{Y}^H]$        ▷ $\boldsymbol{Y} \in \mathbb{R}^{\ell_{\mathsf{x}} \times H \cdot d_{\mathsf{mid}}}$
    return $\tilde{\boldsymbol{V}} = \boldsymbol{Y}\boldsymbol{W}_{\boldsymbol{o}} + \boldsymbol{b}_{\boldsymbol{o}}$
```

Single unmasked self-attention head



Self-attention in detail — query, key, scaled dot product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=
$S_{[1,1]}$ $S_{[1,2]}$ $S_{[1,3]}$ $S_{[1,4]}$ $S_{[1,5]}$
$S_{[2,1]}$ $\vdots$
$S_{[3,1]}$ $\ddots$ $\vdots$
$S_{[4,1]}$ $\vdots$
$S_{[5,1]}$ $\cdots$ $\cdots$ $\cdots$ $S_{[5,5]}$

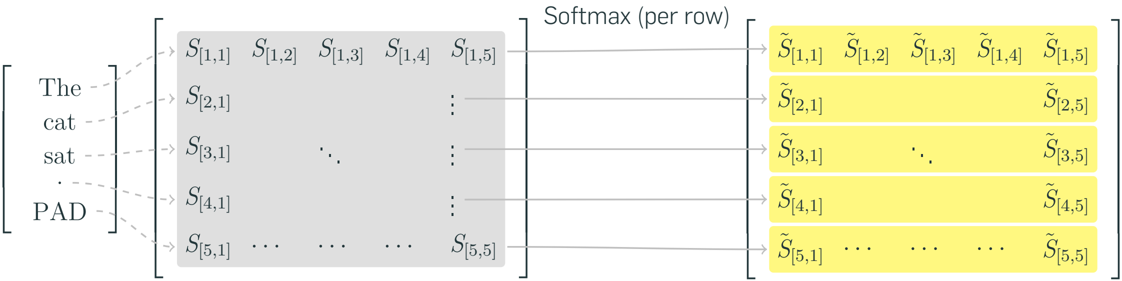
Token embeddings $\boldsymbol{X}$ (input or previous transformer layer)

$\boldsymbol{X}$ projected to query matrix $\boldsymbol{Q}$

$\boldsymbol{X}$ projected to key matrix $\boldsymbol{K}$ and transposed

Scaled dot product $\boldsymbol{S}$ (raw associations) (each entry divided by $\sqrt{d_{\text{attn}}}$)

Self-attention in detail — softmax over scaled dot product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$S_{[3,1]}$ $\ddots$ $\vdots$
$S_{[4,1]}$ $\vdots$
$S_{[5,1]}$ $\cdots$ $\cdots$ $\cdots$ $S_{[5,5]}$
$\tilde{S}_{[1,1]}$ $\tilde{S}_{[1,2]}$ $\tilde{S}_{[1,3]}$ $\tilde{S}_{[1,4]}$ $\tilde{S}_{[1,5]}$
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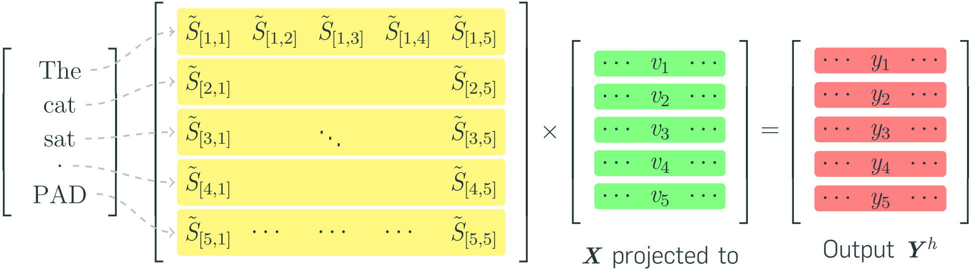
$\tilde{S}_{[3,1]}$ $\ddots$ $\tilde{S}_{[3,5]}$
$\tilde{S}_{[4,1]}$ $\tilde{S}_{[4,5]}$
$\tilde{S}_{[5,1]}$ $\cdots$ $\cdots$ $\cdots$ $\tilde{S}_{[5,5]}$

Softmax (per row)

Scaled dot product
(raw associations)
(each entry divided by $\sqrt{d_{\text{attn}}}$)

Normalized
associations

Self-Attention in detail — head output by weighting the value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$\cdots\ y_4\ \cdots$
$\cdots\ y_5\ \cdots$

Normalized associations

$\boldsymbol{X}$ projected to value matrix $\boldsymbol{V}$

Output $\boldsymbol{Y}^h$ of y-th self-attention head

Some notation details

How to add a single vector $\boldsymbol{b}$ to each row in a matrix $\boldsymbol{W}$ ($\boldsymbol{W} \in \mathbb{R}^{m \times n}, \boldsymbol{b} \in \mathbb{R}^{n}$)

We want $\boldsymbol{Z} = \boldsymbol{X} +_{\text{(rows)}} \boldsymbol{b}$

Let $\mathbf{1}^m = (1, 1, \ldots, 1_m)$, then $\boldsymbol{Z} = \boldsymbol{X} +_{\text{(rows)}} \boldsymbol{b} = \boldsymbol{X} + (\boldsymbol{b}^\top \mathbf{1}^m)^\top$

Example

$$\boldsymbol{X} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}, \boldsymbol{b} = \begin{pmatrix} 10 & 20 \end{pmatrix}$$

$$\boldsymbol{b}^\top \mathbf{1}^m = \begin{pmatrix} 10 \\ 20 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 10 & 10 & 10 \\ 20 & 20 & 20 \end{pmatrix} \qquad (\boldsymbol{b}^\top \mathbf{1}^m)^\top = \begin{pmatrix} 10 & 20 \\ 10 & 20 \\ 10 & 20 \end{pmatrix}$$

Some notation details

Soft-max for matrices row-wise, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$

$$\underset{\text{row}}{\operatorname{softmax}} : \mathbb{R}^{m \times n} \mapsto \mathbb{R}^{m \times n}$$

$$\underset{\text{row}}{\operatorname{softmax}}(\boldsymbol{A})[i, j] = \frac{\exp(\boldsymbol{A}[i, j])}{\sum_{k=1}^{n} \exp(\boldsymbol{A}[i, k])}$$

Bidirectional unmasked self-attention precisely

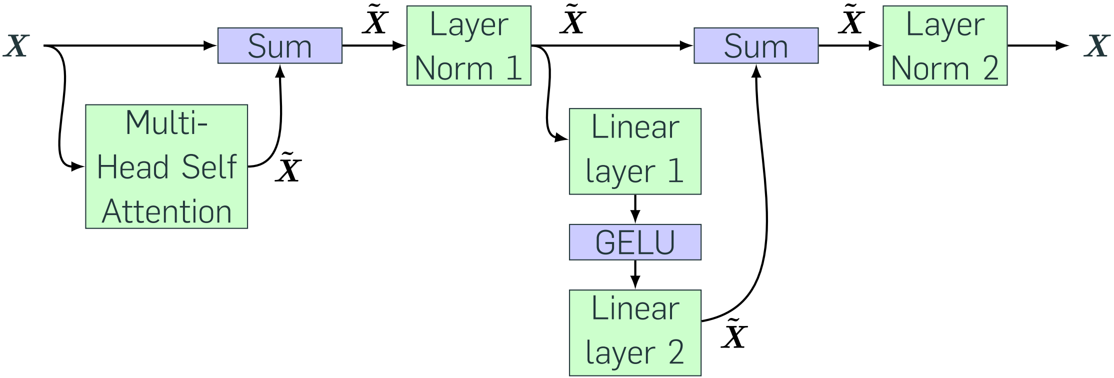
Input: $\boldsymbol{X} \in \mathbb{R}^{\ell_\mathsf{x} \times d_\mathsf{x}}$, vector representations of the sequence of length ℓ_x

Output: $\tilde{\boldsymbol{V}} \in \mathbb{R}^{\ell_\mathsf{x} \times d_\mathsf{out}}$, updated vector representations of tokens in $\boldsymbol{X}$

Params $\boldsymbol{\mathcal{W}}_{\boldsymbol{qkv}}$: $\boldsymbol{W_q}, \boldsymbol{W_k} \in \mathbb{R}^{d_\mathsf{x} \times d_\mathsf{attn}}$, $\boldsymbol{b_q}, \boldsymbol{b_k} \in \mathbb{R}^{d_\mathsf{attn}}$, $\boldsymbol{W_v} \in \mathbb{R}^{d_\mathsf{x} \times d_\mathsf{out}}$, $\boldsymbol{b_v} \in \mathbb{R}^{d_\mathsf{out}}$

```
function Attention($\boldsymbol{X}; \boldsymbol{\mathcal{W}}_{\boldsymbol{qkv}}$)
    $\boldsymbol{Q} \leftarrow \boldsymbol{X}\boldsymbol{W_q} +_{\mathsf{(rows)}} \boldsymbol{b_q}$        ▷ Query $\in \mathbb{R}^{\ell_\mathsf{x} \times d_\mathsf{attn}}$
    $\boldsymbol{K} \leftarrow \boldsymbol{X}\boldsymbol{W_k} +_{\mathsf{(rows)}} \boldsymbol{b_k}$        ▷ Key $\in \mathbb{R}^{\ell_\mathsf{x} \times d_\mathsf{attn}}$
    $\boldsymbol{V} \leftarrow \boldsymbol{X}\boldsymbol{W_v} +_{\mathsf{(rows)}} \boldsymbol{b_v}$        ▷ Value $\in \mathbb{R}^{\ell_\mathsf{x} \times d_\mathsf{out}}$
    $\boldsymbol{S} \leftarrow \frac{1}{\sqrt{d_\mathsf{attn}}}(\boldsymbol{Q}\boldsymbol{K}^\top)$        ▷ Scaled score $\in \mathbb{R}^{\ell_\mathsf{x} \times \ell_\mathsf{x}}$
    return $\tilde{\boldsymbol{V}} = \mathrm{softmax}_\mathsf{row}(\boldsymbol{S})\,\boldsymbol{V}$
```

Transformer encoder layer (BERT)



Let's look at Layer Normalization and GELU

Layer normalization

Input: $\boldsymbol{e} \in \mathbb{R}^d$, output of a layer

Input: $\hat{\boldsymbol{e}} \in \mathbb{R}^d$, normalized output of a layer

Parameters: $\boldsymbol{\gamma}, \boldsymbol{\beta} \in \mathbb{R}^d$, element-wise scale and offset

```
function LayerNorm($\boldsymbol{e}; \boldsymbol{\gamma}, \boldsymbol{\beta}$)
    $m \leftarrow \frac{1}{d} \sum_{i=1}^{d} \boldsymbol{e}[i]$                              ▷ ‘Sample mean’ of $\boldsymbol{e}$
    $v \leftarrow \frac{1}{d} \sum_{i=1}^{d} (\boldsymbol{e}[i] - m)^2$                 ▷ ‘Sample variance’ of $\boldsymbol{e}$
    return $\hat{\boldsymbol{e}} = \frac{\boldsymbol{e} - m}{\sqrt{v}} \odot \boldsymbol{\gamma} + \boldsymbol{\beta}$    ▷ $\odot$ element-wise product
```

(some transformers use $m = \beta = 0$)

Simplifying notation: Perform LayerNorm on each row

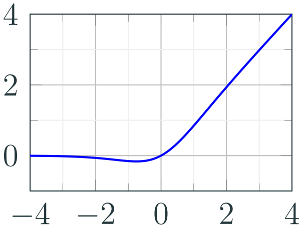
```
function LayerNormEachRow($\boldsymbol{X} \in \mathbb{R}^{m \times n} | \boldsymbol{\gamma}, \boldsymbol{\beta}$)
    for $t \in [m]$ do
        $\boldsymbol{X}[t, :] \leftarrow \text{LayerNorm}(\boldsymbol{X}[t, :] | \boldsymbol{\gamma}, \boldsymbol{\beta})$
    return $\boldsymbol{X}$
```

GELU — Gaussian Error Linear Units

Recall: CDF $\Phi(x)$ of standard normal $X \sim \mathcal{N}(0;1)$

$$\Phi(x) = \Pr(X \leq x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp\left(\frac{-t^2}{2}\right) \mathrm{d}t$$

$$\begin{aligned} \text{GELU}(x) &= x \cdot \Phi(x) \\ &\approx x \cdot \sigma(1.702x) \qquad \text{(if speed > exactness)} \end{aligned}$$



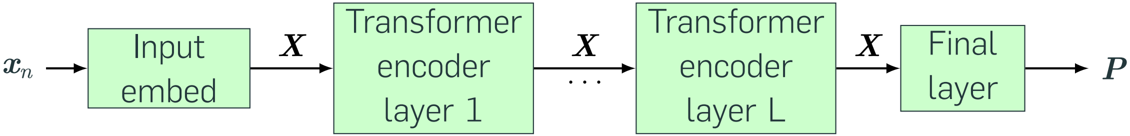
D. Hendrycks and K. Gimpel (2016). **Gaussian Error Linear Units (GELUs).** arXiv: `1606.08415`

For vectors $\boldsymbol{x} \in \mathbb{R}^n$, GELU($\boldsymbol{x}$) is applied element-wise

BERT (encoding-only transformer, forward pass)

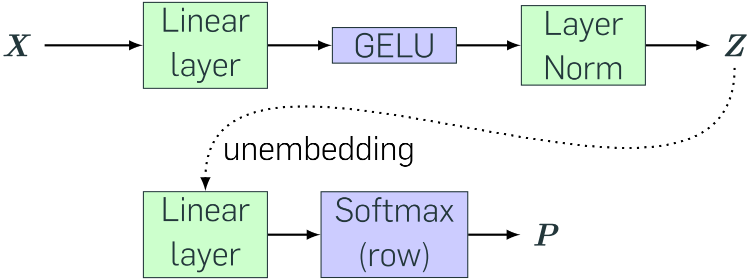
```
function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    $\ell \leftarrow$ length($\boldsymbol{x}$)
    for $t \in [\ell]$ : $\boldsymbol{e}_t \leftarrow \boldsymbol{W}_{\boldsymbol{e}}[x[t], :] + \boldsymbol{W}_{\boldsymbol{p}}[t, :]$        ▷ Token emb. + positional emb.
    $\boldsymbol{X} \leftarrow$ Stack row-wise$[\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots \boldsymbol{e}_\ell]$
    for $l = 1, 2, \ldots, L$ do
        $\boldsymbol{X} \leftarrow \boldsymbol{X} +$ MHAttention($\boldsymbol{X} | \boldsymbol{\mathcal{W}}_l$)        ▷ Multi-head att., residual conn
        $\boldsymbol{X} \leftarrow$ LayerNormPerRow($\boldsymbol{X} | \boldsymbol{\gamma}_l^{\mathbf{1}}, \boldsymbol{\beta}_l^{\mathbf{1}}$)
        $\boldsymbol{X} \leftarrow \boldsymbol{X} + \left(\text{GELU}(\boldsymbol{X}\boldsymbol{W}_l^{\text{mlp1}} +_{\text{(row)}} \boldsymbol{b}_l^{\text{mlp1}})\boldsymbol{W}_l^{\text{mlp2}} +_{\text{(row)}} \boldsymbol{b}_l^{\text{mlp2}}\right)$        ▷ MLP
        $\boldsymbol{X} \leftarrow$ LayerNormPerRow($\boldsymbol{X} | \boldsymbol{\gamma}_l^{\mathbf{2}}, \boldsymbol{\beta}_l^{\mathbf{2}}$)
    $\ldots$
```

Transformer encoder (BERT)



Let’s look at the final layers

Final layer (BERT)



BERT (encoding-only transformer, forward pass)

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function ETransformer($\boldsymbol{x}; \boldsymbol{\mathcal{W}}$)
    $\ell \leftarrow \text{length}(\boldsymbol{x})$
    for $t \in [\ell]$ : $\boldsymbol{e}_t \leftarrow \boldsymbol{W_e}[x[t], :] + \boldsymbol{W_p}[t, :]$          ▷ Token emb. + positional emb.
    $\boldsymbol{X} \leftarrow \text{Stack row-wise}[\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots \boldsymbol{e}_\ell]$
    for $l = 1, 2, \ldots, L$ do
        $\boldsymbol{X} \leftarrow \boldsymbol{X} + \text{MHAttention}(\boldsymbol{X} | \boldsymbol{\mathcal{W}}_l)$          ▷ Multi-head att., residual conn
        $\boldsymbol{X} \leftarrow \text{LayerNormPerRow}(\boldsymbol{X} | \boldsymbol{\gamma}_l^{\boldsymbol{1}}, \boldsymbol{\beta}_l^{\boldsymbol{1}})$
        $\boldsymbol{X} \leftarrow \boldsymbol{X} + \left(\text{GELU}(\boldsymbol{X}\boldsymbol{W}_l^{\text{mlp1}} +_{\text{(row)}} \boldsymbol{b}_l^{\text{mlp1}})\boldsymbol{W}_l^{\text{mlp2}} +_{\text{(row)}} \boldsymbol{b}_l^{\text{mlp2}}\right)$          ▷ MLP
        $\boldsymbol{X} \leftarrow \text{LayerNormPerRow}(\boldsymbol{X} | \boldsymbol{\gamma}_l^{\boldsymbol{2}}, \boldsymbol{\beta}_l^{\boldsymbol{2}})$
    $\boldsymbol{X} \leftarrow \text{GELU}(\boldsymbol{X}\boldsymbol{W_f} +_{\text{(row)}} \boldsymbol{b_f})$
    $\boldsymbol{X} \leftarrow \text{LayerNormPerRow}(\boldsymbol{X} | \boldsymbol{\gamma}_l, \boldsymbol{\beta}_l)$
    return $\boldsymbol{P} = \mathrm{softmax}(\boldsymbol{X}\boldsymbol{W_u})$          ▷ Project to vocab., probabilities
```

BERT parameters and hyperparameters

Hyperparameters: $\ell_{\mathsf{max}}, L, H, d_{\mathsf{e}}, d_{\mathsf{mlp}}, d_{\mathsf{f}} \in \mathbb{N}$

Parameters:

$\boldsymbol{W_e} \in \mathbb{R}^{N_{\mathsf{V}} \times d_{\mathsf{e}}}$, $\boldsymbol{W_p} \in \mathbb{R}^{\ell_{\mathsf{max}} \times d_{\mathsf{e}}}$, the token and positional embedding matrices

For $l \in [L]$: $\boldsymbol{\mathcal{W}}_l$, multi-head attention parameters for layer l:

- $\boldsymbol{\gamma}_l^{\mathbf{1}}, \boldsymbol{\beta}_l^{\mathbf{1}}, \boldsymbol{\gamma}_l^{\mathbf{2}}, \boldsymbol{\beta}_l^{\mathbf{2}}$, two sets of layer-norm parameters
- $\boldsymbol{W}_l^{\mathsf{mlp1}} \in \mathbb{R}^{d_{\mathsf{e}} \times d_{\mathsf{mlp}}}$, $\boldsymbol{b}_l^{\mathsf{mlp1}} \in \mathbb{R}^{d_{\mathsf{mlp}}}$
- $\boldsymbol{W}_l^{\mathsf{mlp2}} \in \mathbb{R}^{d_{\mathsf{mlp}} \times d_{\mathsf{e}}}$, $\boldsymbol{b}_l^{\mathsf{mlp2}} \in \mathbb{R}^{d_{\mathsf{e}}}$

$\boldsymbol{W_f} \in \mathbb{R}^{d_{\mathsf{e}} \times d_{\mathsf{f}}}$, $\boldsymbol{b_f} \in \mathbb{R}^{d_{\mathsf{f}}}$, $\boldsymbol{\gamma}, \boldsymbol{\beta} \in \mathbb{R}^{d_{\mathsf{f}}}$, the final linear projection and layer-norm parameters.

$\boldsymbol{W_u} \in \mathbb{R}^{d_{\mathsf{e}} \times N_{\mathsf{V}}}$, the unembedding matrix

Input and pre-training

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BERT: Tokenization

Tokenizing into a multilingual WordPiece inventory

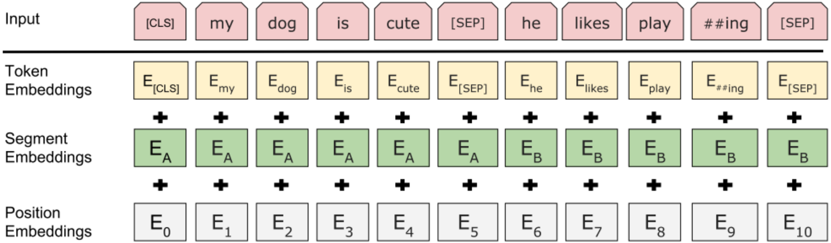
- Recall that WordPiece units are sub-word units
- 30,000 WordPiece units (newer models 110k units, 100 languages)

Implications: BERT can ”consume” any language

BERT: Input representation

- Each WordPiece token from the input is represented by a **WordPiece embedding** (randomly initialized)
- Each position from the input is associated with a **positional embedding** (also randomly initialized)
- Input length limited to **512** WordPiece tokens, using `<PAD>`ding
- Special tokens
  - The fist token is always a special token **[CLS]**
  - If the task involves two sentences (e.g., NLI), these two sentences are separated by a special token **[SEP]**; also special two **segment position embeddings**

BERT: Input representation summary



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}

Pre-training

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BERT: Self-supervised multi-task pre-training

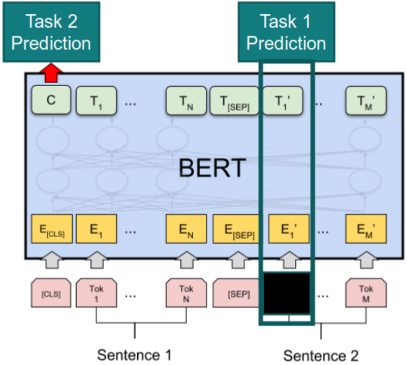
Prepare two auxiliary tasks that need no labeled data

Task 1: Cloze-test task

- Predict the masked WordPiece unit (multi-class, 30k classes)

Task 2: Consecutive segment prediction

- Did the second text segment appeared after the first segment? (binary)



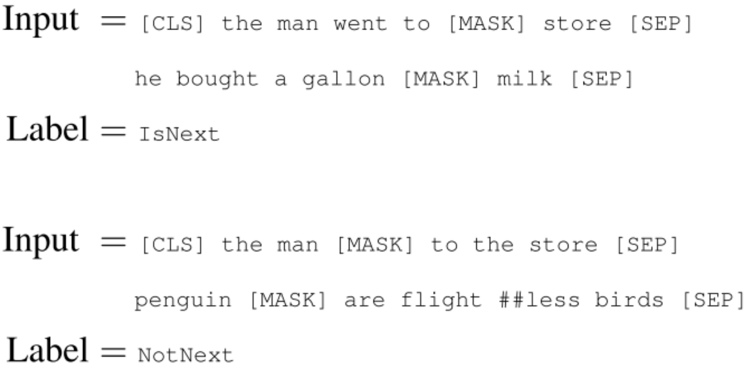
BERT: Pre-training data generation

Take the entire Wikipedia (in 100 languages; 2,5 billion words)

To generate a single training instance, sample two segments (max combined length 512 WordPiece tokens)

- For Task 2, replace the second segment randomly in 50% (negative samples)
- For Task 1, choose random 15% of the tokens, and in 80% replace with a [MASK]

BERT: Pre-training data – Simplified example



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

- <PAD>ding is missing
- The actual segments are longer and not necessarily sentences (just spans)
- The WordPiece tokens match full words here

BERT: pre-training by masked language modeling

```
function ETraining($\{\boldsymbol{x}_n\}_{n=1}^{N_\text{data}}$ seqs, $\boldsymbol{\theta}$ init. params; $p_\text{mask} \in (0, 1)$, $N_\text{epochs}$, $\eta$)
    for $i \in [N_\text{epochs}]$ do
        for $n \in [N_\text{data}]$ do
            $\ell \leftarrow \text{length}(\boldsymbol{x}_n)$
            for $t \in [\ell]$ do
                $\tilde{\boldsymbol{x}}_n[t] \leftarrow$ <mask_token> with prob. $p_\text{mask}$, otherwise $\boldsymbol{x}_n[t]$
            $\tilde{T} \leftarrow \{t \in [\ell] : \tilde{\boldsymbol{x}}_n[t] = \texttt{<mask\_token>}\}$        ▷ Indices of masked tokens
            $\boldsymbol{P}_{\boldsymbol{\theta}} \leftarrow \text{ETransformer}(\tilde{\boldsymbol{x}}_n | \boldsymbol{\theta})$
            $\text{loss}_{\boldsymbol{\theta}} \leftarrow -\sum_{t \in \tilde{T}} \log \boldsymbol{P}_{\boldsymbol{\theta}}[t, \boldsymbol{x}_n[t]]$
            $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \cdot \nabla \text{loss}_{\boldsymbol{\theta}}$
    return $\boldsymbol{\theta}$
```

Simple example explaining lines 6–7 (masking)

$$\begin{pmatrix}\text{The} & \text{cat} & \text{sat}\end{pmatrix} \to \boldsymbol{x}_n =$$

$$\begin{pmatrix}21 & 11987 & 5438\end{pmatrix} \quad \text{(Indices in } V\text{)}$$

Random masking (index of `<mask_token>` = 50001):

1. For $t = 1$, the random outcome is "mask"
2. For $t = 2$, the random outcome is "keep"
3. For $t = 3$, the random outcome is "mask"

$$\tilde{\boldsymbol{x}}_n = \begin{pmatrix}50001 & 11987 & 50001\end{pmatrix}, \tilde{T} = \{1, 3\}$$

Explaining line 9 (negative log likelihood)

$\begin{pmatrix}\text{The} & \text{cat} & \text{sat}\end{pmatrix} \to \boldsymbol{x}_n = \begin{pmatrix}21 & 11987 & 5438\end{pmatrix}, \tilde{\boldsymbol{x}}_n = \begin{pmatrix}50001 & 11987 & 50001\end{pmatrix}, \tilde{T} = \{1, 3\}$

$\boldsymbol{P_\theta} \leftarrow \text{ETransformer}(\tilde{\boldsymbol{x}}_n | \boldsymbol{\theta})$

$$\boldsymbol{P_\theta} = \begin{pmatrix} 0.001 & 0.0007 & \dots & 0.0003 \\ 0.0013 & 0.0065 & \dots & 0.0001 \\ 0.079 & 0.015 & \dots & 0.0001 \end{pmatrix}$$

$\boldsymbol{P_\theta} \in (0, 1)^{\ell_{\mathsf{x}} \times N_{\mathsf{V}}}$, where each row of $\boldsymbol{P}$ is a distribution over the vocabulary

Explaining line 9 (negative log likelihood), $t = 1$

$\boldsymbol{x}_n = (21, 11987, 5438), \tilde{\boldsymbol{x}}_n = (50001, 11987, 50001), \tilde{T} = \{1, 3\}$

$$\boldsymbol{P_\theta} = \begin{pmatrix} 0.001 & \dots & 0.0041_{21} & \dots 0.0003 \\ \vdots & & & \end{pmatrix}$$

For $t = 1$, the model should learn to predict "The" (index 21)

Gold: $\boldsymbol{y} = (0, 0, \dots, 1_{21}, \dots, 0) \in \mathbb{R}^{N_\mathrm{V}}$

Pred: $\hat{\boldsymbol{y}} = \boldsymbol{P_\theta}[1, :] = (0.001, \dots, 0.0041_{21}, \dots 0.0003) \in \mathbb{R}^{N_\mathrm{V}}$

Recall: Categorical cross entropy loss

$$L(\hat{\boldsymbol{y}}, \boldsymbol{y}) := -\sum_{k=1}^{K} \boldsymbol{y}_{[k]} \log\left(\hat{\boldsymbol{y}}_{[k]}\right)$$
$$= -1 \cdot \log(\hat{\boldsymbol{y}}[21]) = -\log(\boldsymbol{P_\theta}[1, 21])$$
$$= -\log(\boldsymbol{P_\theta}[1, \boldsymbol{x}_n[1]]) = -\log(\boldsymbol{P_\theta}[t, \boldsymbol{x}_n[t]])$$

Explaining line 9 (negative log likelihood), $t = 3$

$\boldsymbol{x}_n = (21, 11987, 5438), \tilde{\boldsymbol{x}}_n = (50001, 11987, 50001), \tilde{T} = \{1, 3\}$

$$\boldsymbol{P_\theta} = \begin{pmatrix} \vdots & \dots & \dots & \end{pmatrix}$$

For $t = 3$, the model should learn to predict "sat" (id 5438)

Categorical cross entropy loss

$L(\hat{\boldsymbol{y}}, \boldsymbol{y}) := -\sum_{k=1}^{K} \boldsymbol{y}_{[k]} \log \left(\hat{\boldsymbol{y}}_{[k]} \right)$
$= -1 \cdot \log(\hat{\boldsymbol{y}}[5438]) = -\log(\boldsymbol{P_\theta}[3, 5438]) = -\log(\boldsymbol{P_\theta}[t, \boldsymbol{x}_n[t]])$

Sum over all masked token positions in $\tilde{T}$ gives us line 9:

$$\text{loss}_{\boldsymbol{\theta}} \leftarrow -\sum_{t \in \tilde{T}} \log \boldsymbol{P_\theta}[t, \boldsymbol{x}_n[t]]$$

Downstream tasks and fine-tuning

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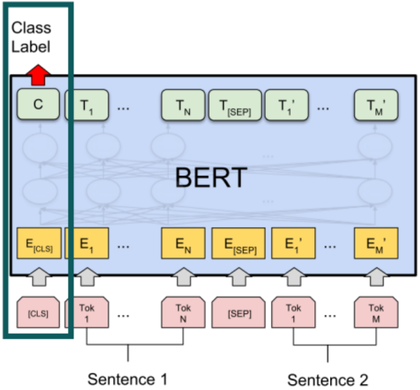
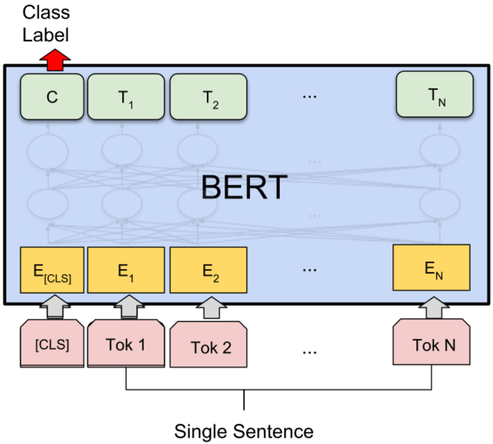
BERT: Representing various NLP tasks



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

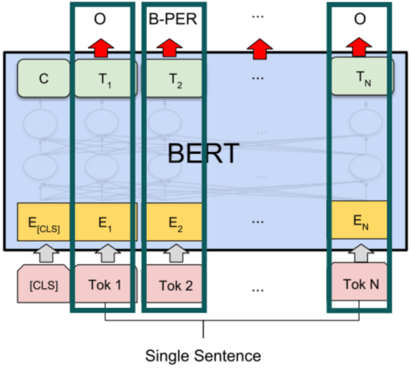
That explains the special [CLS] token at sequence start

BERT: Representing various NLP tasks



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

BERT: Representing various NLP tasks



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

Not conditioned on surrounding predictions

BERT pre-training time

Pretraining BERT took originally 4 days on 64 TPUs[1]

Once pre-trained, transfer and "fine-tune" on your small-data task and get competitive results

P. Izsak, M. Berchansky, and O. Levy (2021). **"How to Train BERT with an Academic Budget".** In: *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing.* Online and Punta Cana, Dominican Republic: Association for Computational Linguistics, pp. 10644–10652

[1] Can be done more efficiently, see, e.g., Izsak, Berchansky, and Levy (2021)

Recap

A. Rogers, O. Kovaleva, and A. Rumshisky (2020). **"A Primer in BERTology: What We Know About How BERT Works".** In: *Transactions of the Association for Computational Linguistics* 8, pp. 842–866

BERT stays on the shoulders of many clever concepts and techniques, mastered into a single model

What do we know about how BERT works?

"BERTology has clearly come a long way, but it is fair to say we still have more questions than answers about how BERT works." — Rogers, Kovaleva, and Rumshisky (2020)[2]

[2] Highly recommended reading!

License and credits

Credits

Ivan Habernal

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