Multilingual NLP

4. Attention & Transformer

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Image: Alexander Mikhalchyk

After this lecture, you'll...

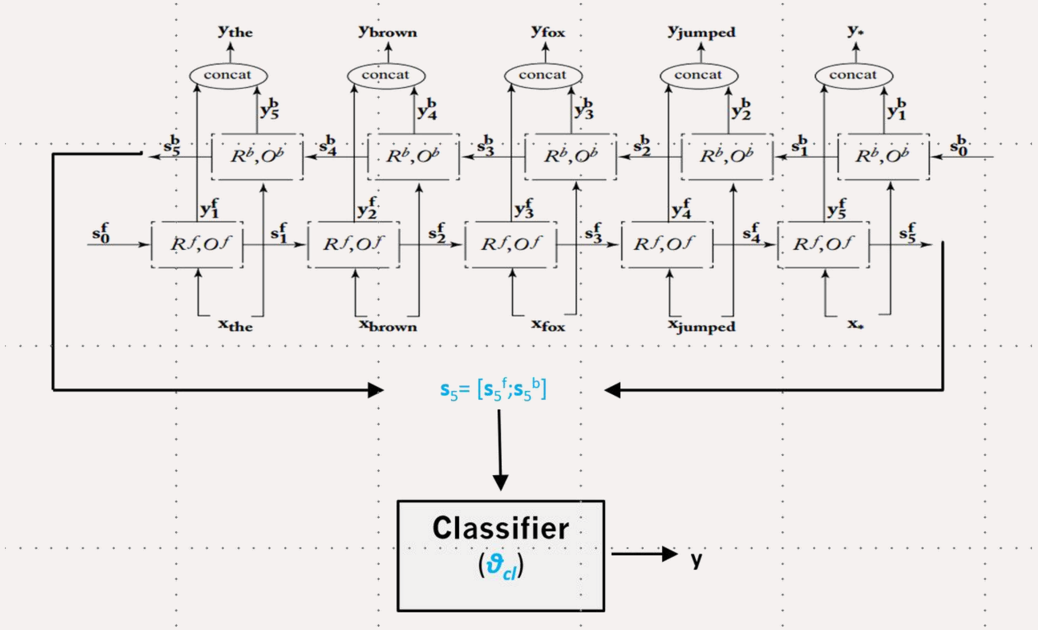
- Understand the concept of attention in NNs
- Know the exact building blocks of the Transformer architecture
- Understand the pre-training–fine-tuning paradigm

Content

- **Attention mechanism**
- Transformer – dissected
  - Positional Embeddings
  - Multi-Head Self-Attention
- Pretraining + fine-tuning

Origins of Attention

- Before the Transformer was introduced (in 2017, 2018), recurrent nets were SotA for language understanding and generation
  - E.g., a bidirectional LSTM for sequence classification tasks



Origins of Attention

- Before the Transformer was introduced (in 2017, 2018), recurrent nets were SotA for language understanding and generation
    - E.g., RNN-based sequence-to-sequence models

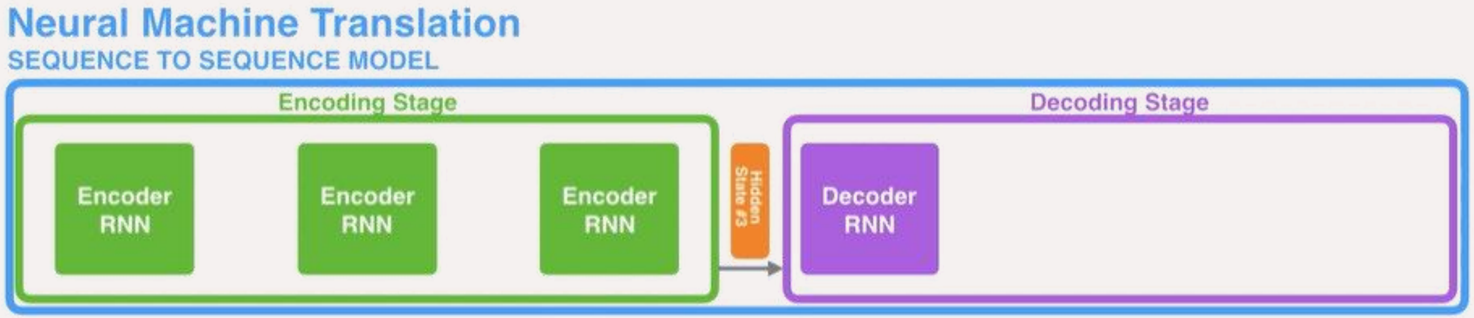
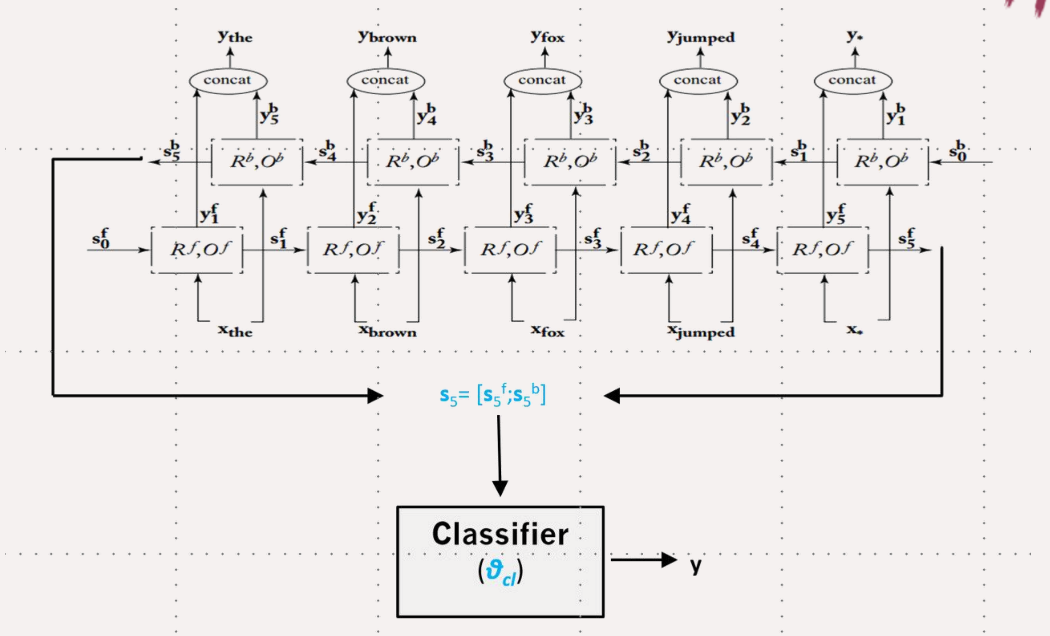
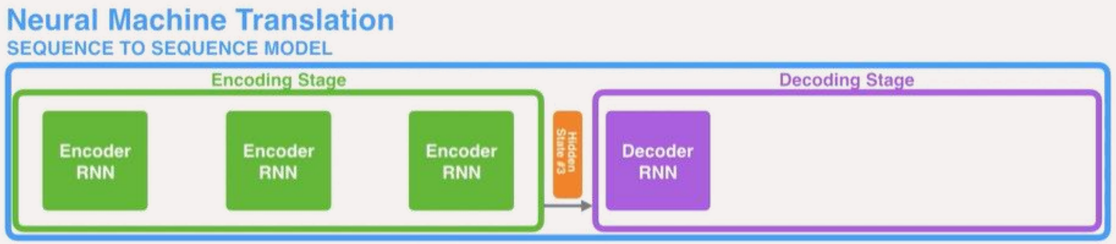


Image from: https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/

Origins of Attention

- Problems with RNNs stem from their sequential nature
- Tokens last processed contribute more to the final representation
- Difficult to combine representations of distant tokens (aka long dependencies)
- Tokens not given equal chance to contribute to the sequence representation





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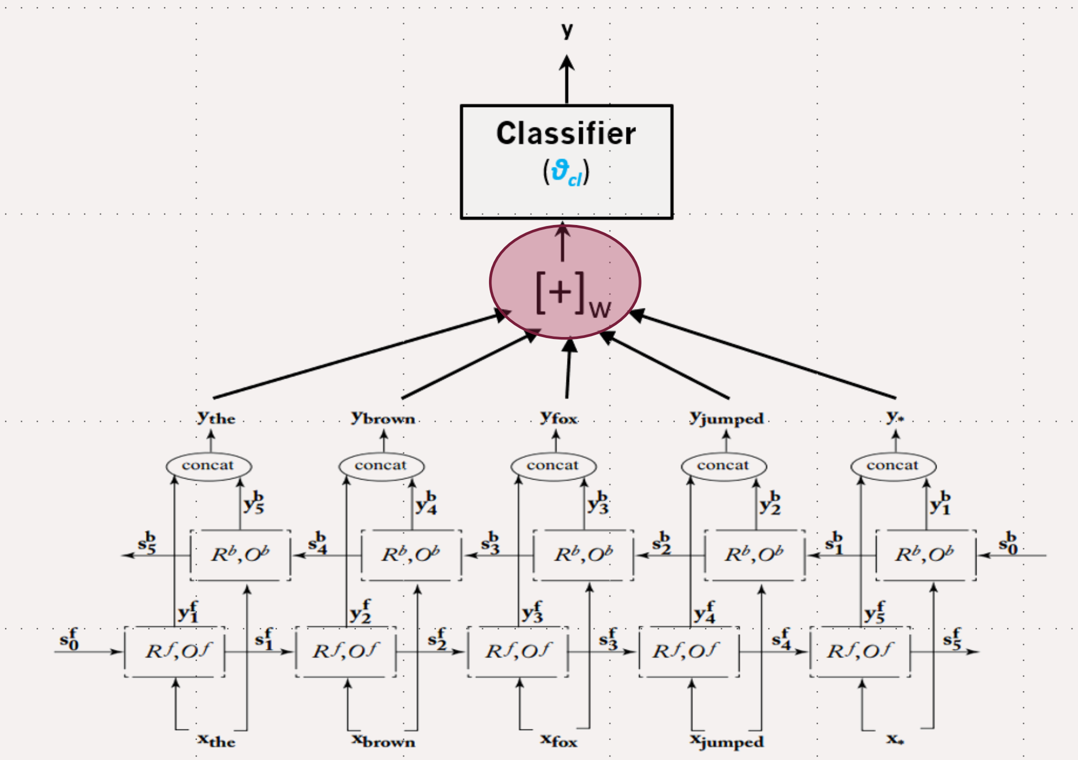
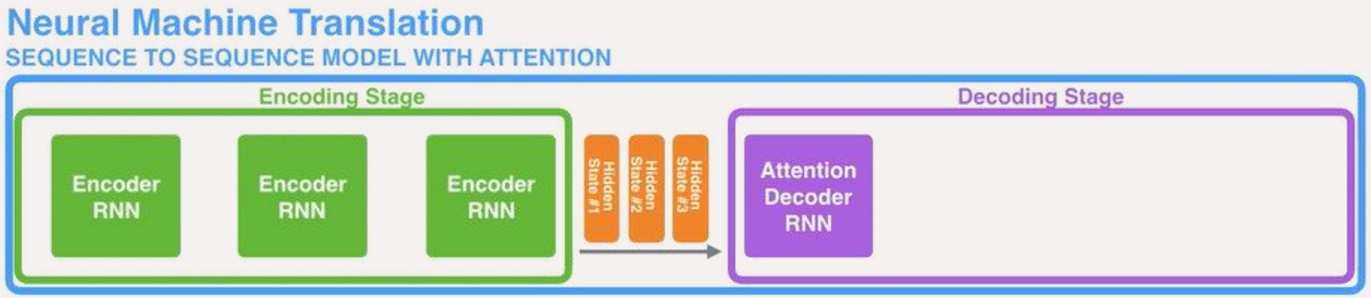
Origins of Attention

- Enter **attention**: representation of the sequence as a weighted average of token representations
  - Weights are produced by a parametrized (i.e., trainable) attention function
  - With RNNs, token representations are the hidden state of the RNN after processing of the token



Origins of Attention

- Enter **attention**: representation of the sequence as a weighted average of token representations
- In sequence-to-sequence (encoder-decoder) for generative tasks
  - At each decoding step, we re-compute the average of the encoded tokens
  - The hidden representation of the decoder is the „query" for the attention mechanism over encoded tokens



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Attention Mechanism

- Given a set of objects (e.g., tokens in text), the **attention mechanism** computes a weighted average of value vectors
- The weights are based on the similarity between the respective key vectors of those same objects with the query
- Query vector represent the context with respect to which we want to aggregate object representations

Attention Mechanism

- Let $t_1, t_2, \ldots, t_N$ be a set of tokens over which we're „attending"
- Let $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_N \in \mathbb{R}^k$ and $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N \in \mathbb{R}^v$ be the key and value vectors of those tokens, respectively
  - k is the length of key vectors
  - v is the length of value vectors
- Let $\mathbf{q} \in \mathbb{R}^q$ be the query vector
  - In most cases, the query vector must be of same length as key vectors of tokens, $q = k$

Attention Mechanism

- The **attention mechanism** is then defined with by:
  - The scoring function $s(\mathbf{q}, \mathbf{k})$, which produces a (single scalar) score that indicates the compatibility of a key $\mathbf{k}$ with the query $\mathbf{q}$
  - The output of the attention mechanism is the weighted sum of value vectors, with corresponding scores as weights:

$$\sum_{i=1}^{N} s(\mathbf{q}, \mathbf{k}_i) * \mathbf{v}_i$$

Attention Mechanism

$$\sum_{i=1}^{N} s(\mathbf{q}, \mathbf{k}_{\mathrm{i}}) \; * \; \mathbf{v}_{\mathrm{i}}$$

- Commonly used attention types (before Transformer):

1. Additive attention (parametrized scoring function):

$$s(\mathbf{q}, \mathbf{k}) = \mathbf{v}_{\mathbf{a}}\, tanh(\mathbf{W}_{\mathbf{a}} (\mathbf{k} \oplus \mathbf{q}))$$

   - **k** and **q** may be of different length, $\oplus$ denotes concatenation
   - $\mathbf{W}_{\mathbf{a}} \in \mathbb{R}^{h \times (K+Q)}$ and $\mathbf{v}_{\mathbf{a}} \in \mathbb{R}^{h}$: trainable params of the „attention layer”

Attention Mechanism

$$\sum_{i=1}^{N} s(\mathbf{q}, \mathbf{k}_i) \ * \ \mathbf{v}_i$$

- Commonly used attention types used (before Transformer):

2. Dot-product attention (non-parametrized scoring function)

$$s(\mathbf{q}, \mathbf{k}) = \mathbf{k}^{T}\mathbf{q}$$

- Raw (unnormalized) score for a key is a simple dot-product with the query
- Raw scores across keys are normalized with softmax:

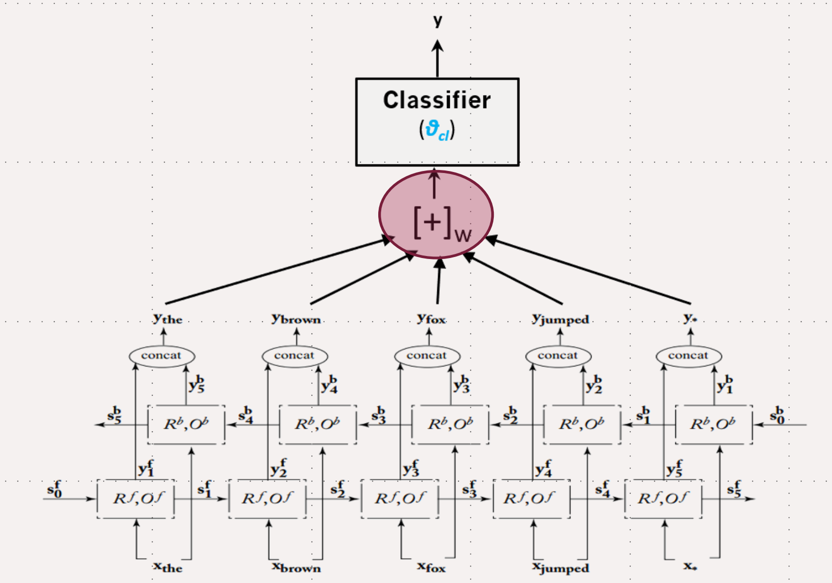
$$s(\mathbf{q}, \mathbf{k}) \rightarrow \frac{e^{s(\mathbf{q}, \mathbf{k}_i)}}{\sum_{j=1}^{N} e^{s(\mathbf{q}, \mathbf{k}_j)}}$$

Attention Mechanism

- Q: But where are keys, values, and queries coming from?
  - For each token we typically have only one vector
  - Token's embedding or RNN's state after processing that token
- Attention is a general mechanism, can be applied in various settings
  - We decide how to obtain keys, values, and queries in concrete use cases
- Use case #1: sequence classification with RNNs
  - Keys and values same vectors, one for hidden state of the RNN at each time step

$$\mathbf{k}_i = \mathbf{v}_i = \mathbf{s}_i^{RNN}$$

  - No context: $\mathbf{q}$ can be any fixed vector (e.g., a vector of 1s), or a trainable vector;

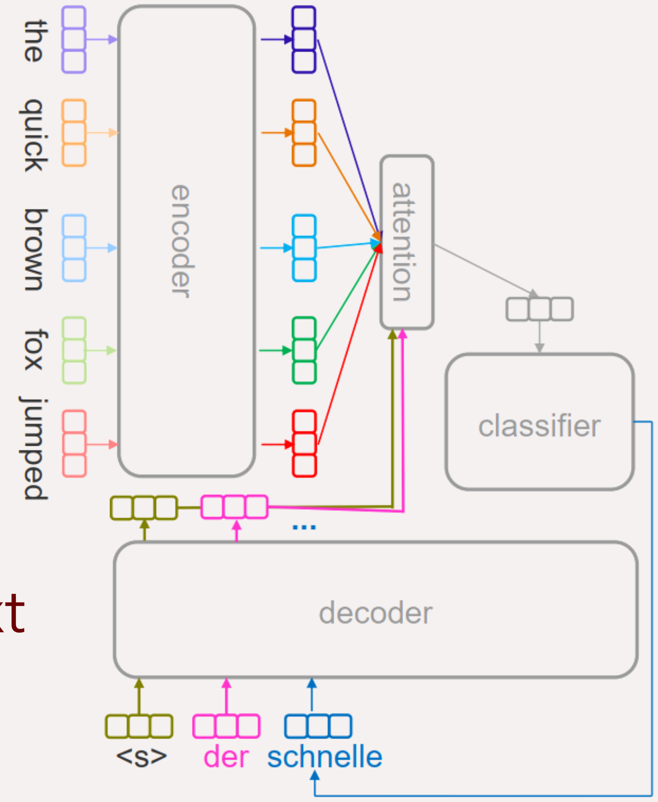


Attention Mechanism

- Attention is a general mechanism, can be applied in various settings
  - We decide how to obtain keys, values, and queries in concrete use cases and scenarios
- Use case #2: seq-to-seq generation (with RNNs)
  - Keys and values the same vectors, one for hidden state of encoder RNN at each time step

$$\mathbf{k}_i = \mathbf{v}_i = \mathbf{s}_i^{\text{Encoder}}$$

  - Query **q**: hidden state of the decoder
    - I.e., context is the representation of the text generated so far



Content

- Attention mechanism
- **Transformer – dissected**
  - Positional Embeddings
  - Multi-Head Self-Attention
- Pretraining + fine-tuning

Is Attention All We Need?

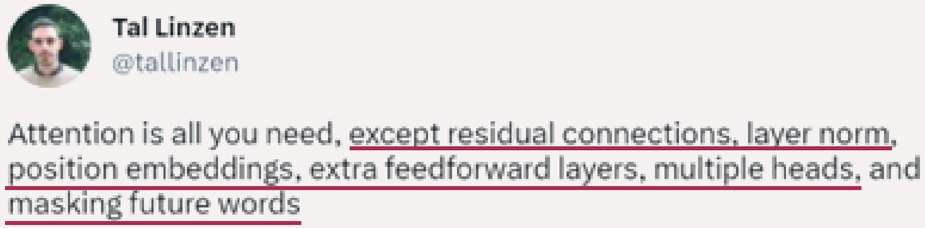
Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. Advances in neural information processing systems (NeurIPS).

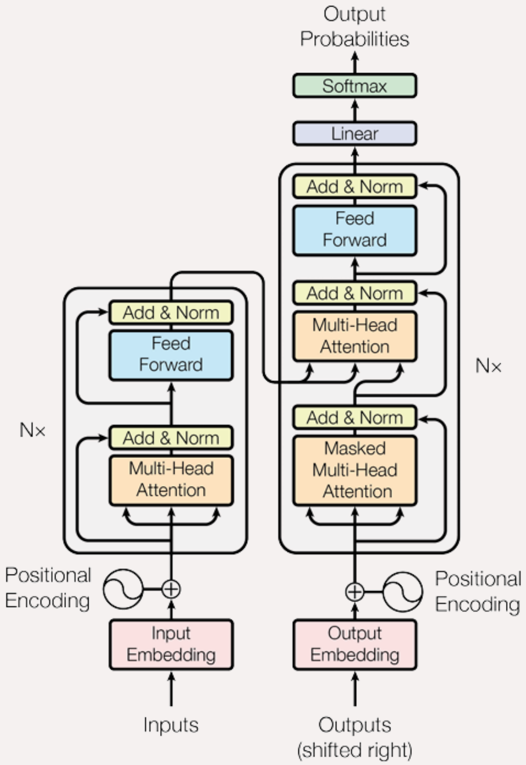
- So far, we applied attention over keys/values that come from a recurrent encoder
- RNNs are slow to train
    - „Backpropagation through time"
    - Computation over tokens sequential
- Research question that changed NLP and enabled LLMs:
    - Is recurrence actually necessary?
    - What happens if we just apply attention on top of token embeddings?

Transformer (Encoder-Decoder)

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. Advances in neural information processing systems (NeurIPS).

- Enter **Transformer**: a sequence-to-sequence architecture without recurrence, based **„only"** on the attention mechanism
- Is attention is all we need?





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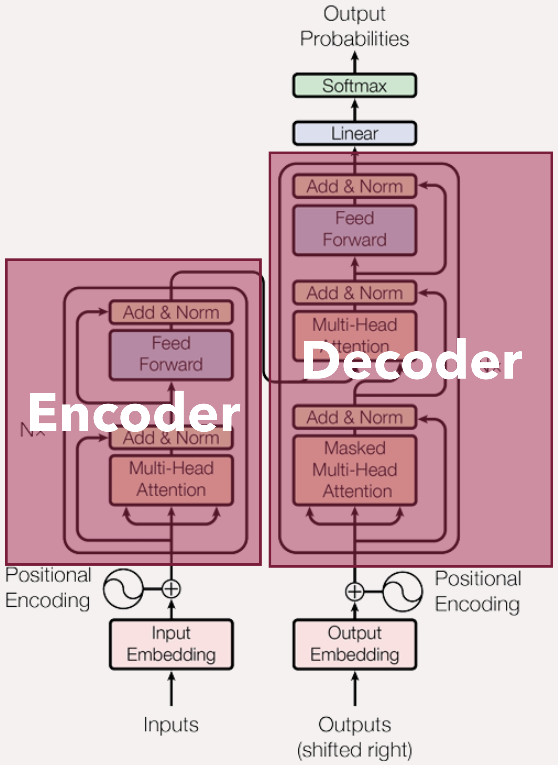
- **Transformer** as proposed by Vaswani et al. is an encoder-decoder model
  - Introduced for machine translation
- Two types of attention
  1. **Self-attention**: only in encoder
     - Keys, Values, and Queries all derived from token representations in encoder layers
  2. Cross-attention: keys and values from encoder representations + previous tokens in decoder
     - **q**: from representations of decoder tokens



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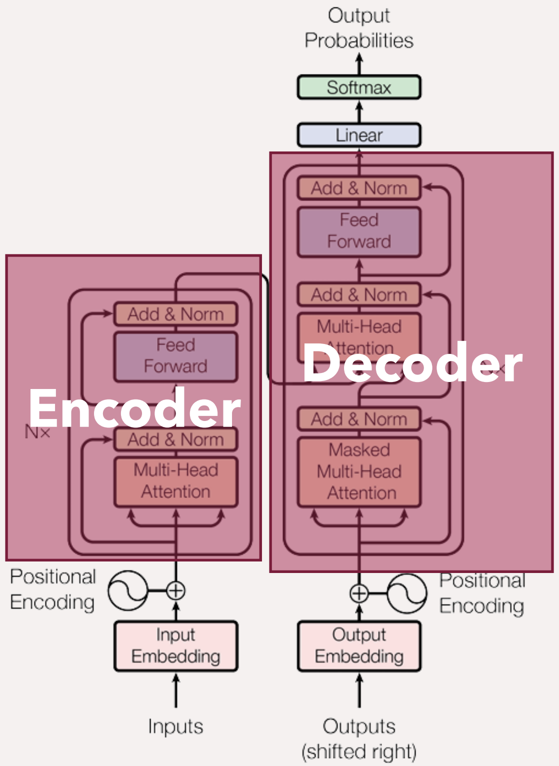
- **Transformer** as proposed by Vaswani et al. is an encoder-decoder model
  - Introduced for machine translation
- Two types of attention

Today

1. **Self-attention**: only in encoder
   - Keys, Values, and Queries all derived from token representations in encoder layers

L9: NMT

2. Cross-attention: keys & values from enc. representations + previous tokens in decoder
   - **q**: from representations of decoder tokens



Transformer

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019). BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. In Proceedings of NAACL-HLT (pp. 4171-4186).

- **Transformer** as proposed by Vaswani et al. is an encoder-decoder model
- Most NLP tasks are not generation tasks*

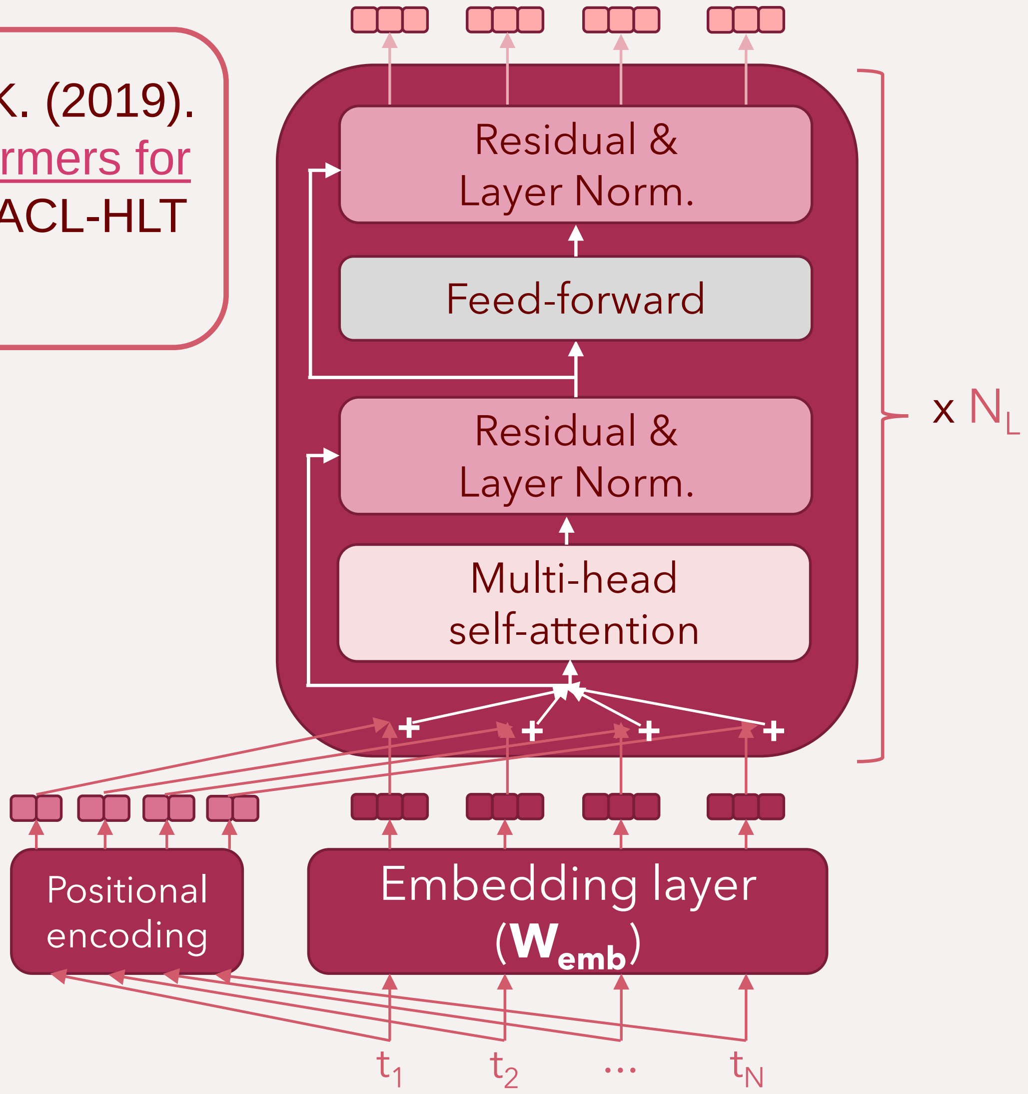
  * Most recently, with LLMs, many non-generation tasks have been successfully re-cast as generation tasks (**L11**: Prompting & LLMs)

- Most models used today are single-stack transformers
  - Encoder models (trained with masked LM-ing)
  - Decoder models (trained with autoregressive LM-ing)
- Devlin et al.'s **BERT** uses the encoder-only Transformer
  - This is the Transformer we'll primarily dissect in this lecture

Transformer

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019). BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. In Proceedings of NAACL-HLT (pp. 4171-4186).

- **Transformer** as **encoder**
  - Embedding layer
    - (sub)word embeddings
    - Positional embeddings
  - N_L identical Transformer layers
    - Multi-head self-attention sublayer
    - Residual connection
    - Layer normalization
    - Feed-forward sublayer



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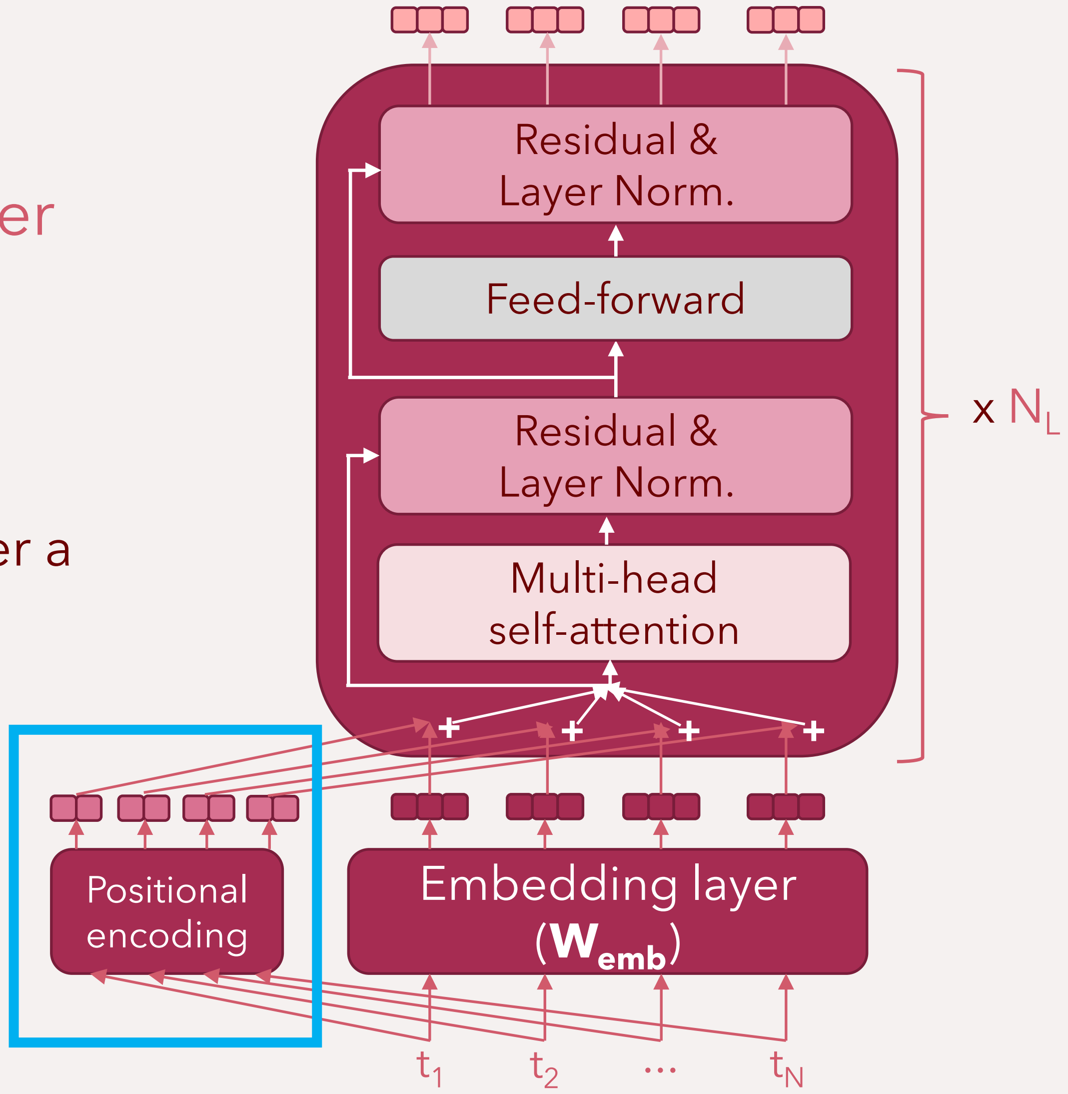
Positional Embeddings

- Recurrent networks implicitly retain the information about the word order
- At the core of the Transformer encoder is the so-called multi-head self-attention
  - But attention is just an aggregation over a set of vectors
  - Retains no order information
- Fix: **positional embeddings** that explicitly encode token positions in the sequence



Positional Embeddings

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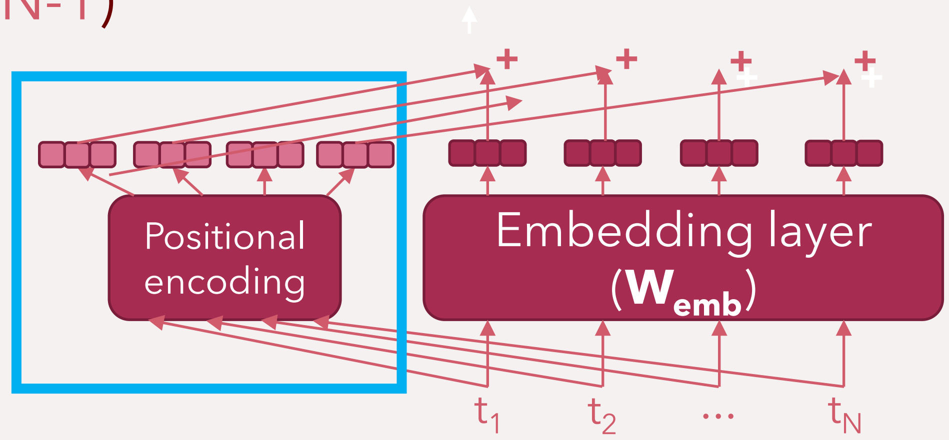
- Vaswani et al. propose fixed relative positional embeddings
- Positional embeddings added to (sub)word embeddings → same dim. *d*

- Maximal sequence length: N
- Position in the sequence: pos, in {0, 1, 2, ..., N-1)

- For each position/index in the pos. embedding, a different function generating the score
  - Indices: $2i$ (or $2i+1$) for $0 \leq i < d/2$



Positional Embeddings

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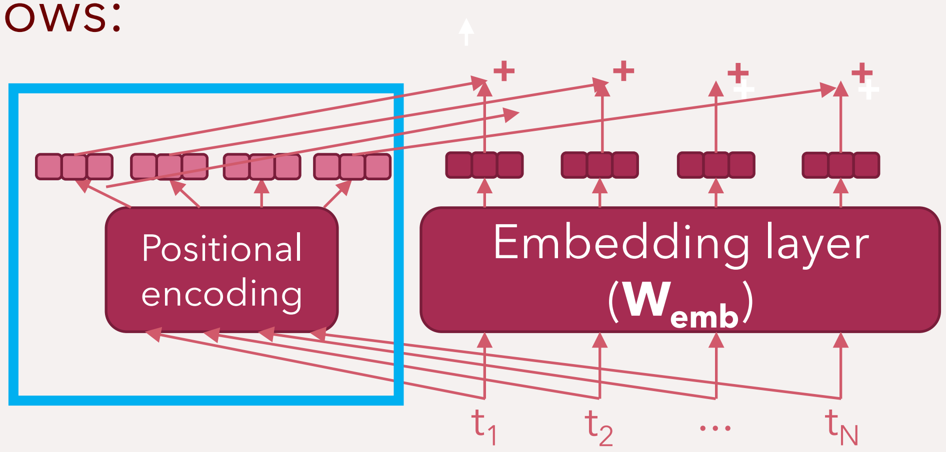
- Let n be an arbitrary scalar, a hyperparameter for positional embeddings
  - Vaswani et al. set n = 10000
- The value of the positional embedding for token position pos and embedding index 2i (or 2i+1) is given as follows:

$$PE(pos, 2i) = \sin\left(\frac{pos}{n^{2i/d}}\right)$$

$$PE(pos, 2i+1) = \cos\left(\frac{pos}{n^{2i/d}}\right)$$



Sines and Cosines?!

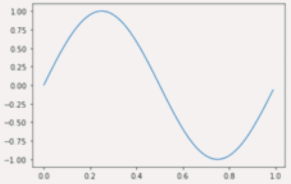
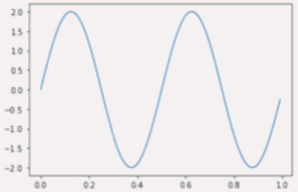
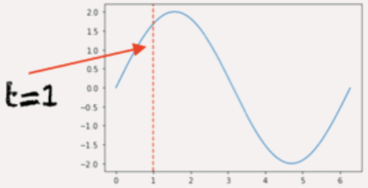
Equation	Graph	Frequency	Wavelength
$\sin(2\pi t)$		1	1
$\sin(2 * 2\pi t)$		2	1/2
$\sin(t)$		$1/2\pi$	2π
$\sin(ct)$	Depends on c	$c/2\pi$	$2\pi/c$

Image from: https://machinelearningmastery.com/a-gentle-introduction-to-positional-encoding-in-transformer-models-part-1/

Sines and Cosines?!

- Q: Why sines and cosines?!
  - Cyclical, encode well relative values in the argument range [0, 2π]
  - We can make the range of the repetition (wavelength) arbitrarily long
  - Values always in the [-1, 1] range

$$PE(pos, 2i) = \sin\left(\frac{pos}{n^{2i/d}}\right); \qquad PE(pos, 2i+1) = \cos\left(\frac{pos}{n^{2i/d}}\right)$$

- $c = 1/\,n^{2i/d}$; wavelength → $2\pi/c = 2\pi * n^{2i/d}$
  - The bigger the index i, the bigger the wavelength (wider cycle)

- For i = 0 (ind. 0 and 1) → $PE(pos, 0) = \sin(pos)$; $PE(pos, 1) = \cos(pos)$
- For i = 1 (ind. 2 and 3) → $PE(pos, 2) = \sin\left(\frac{pos}{n^{2/d}}\right)$; $PE(pos, 3) = \cos\left(\frac{pos}{n^{2/d}}\right)$

  …

- For i = d/2 (index d, assume d even) → $PE(pos, d) = \sin\left(\frac{pos}{n}\right)$

Sines and Cosines?!

- For different indices of the positional embedding vectors, position-dependent values are computed with sin/cos of different wavelengths
  - From wavelength of 2π (for $i = 0$) to wavelength of $n * 2\pi$ (for $i = d/2$)

- Store pos. embeddings in a matrix $\mathbf{W}_{PE} \in \mathbb{R}^{N \times d}$
  - Each row corresponds to one position (from 1 to N)
  - We can visualize $\mathbf{W}_{PE}$ – example with $d = 128$, $N = 50$, and $n = 10000$

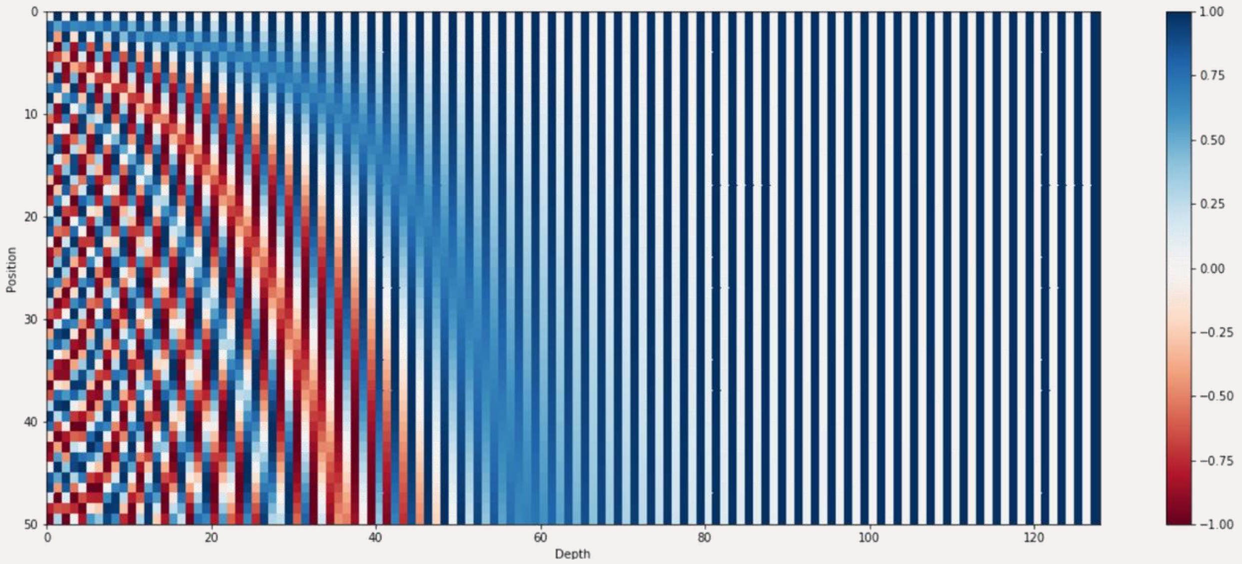
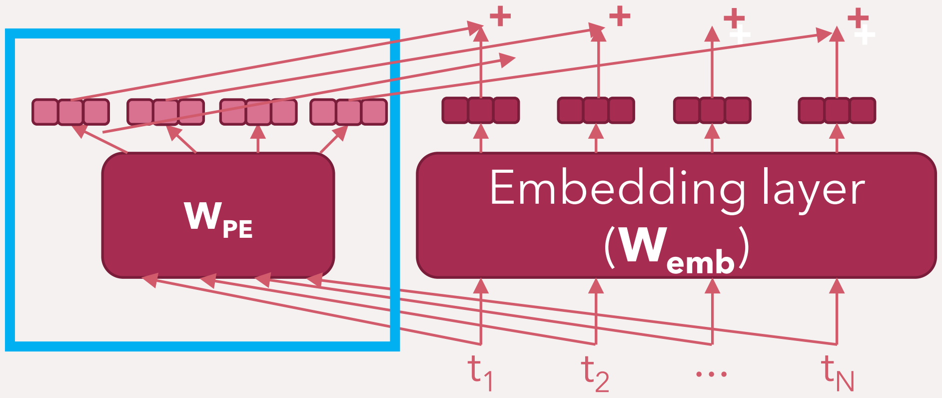


Image from: https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Positional Embeddings

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019). BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. In Proceedings of NAACL-HLT (pp. 4171-4186).

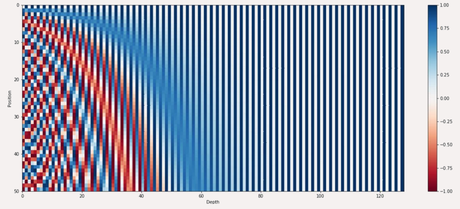
- In BERT, Devlin et al. resort to fully trainable positional embeddings
- I.e., $\mathbf{W}_{PE} \in \mathbb{R}^{N \times d}$ another parameter matrix, along with $\mathbf{W}_{emb} \in \mathbb{R}^{|V| \times d}$
- $\mathbf{W}_{PE}$ optimized with all other parameters of the whole neural LM



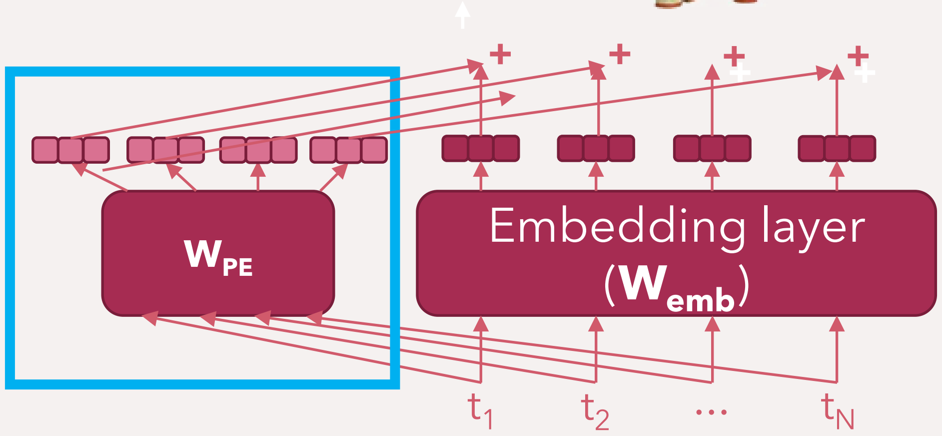
Positional Embeddings

Wang, B., Shang, L., Lioma, C., Jiang, X., Yang, H., Liu, Q., & Simonsen, J. G. (2021). On Position Embeddings in BERT. In International Conference on Learning Representations (ICLR).

- Which is better?
  - Fully trainable PEs or
  - Fixed relative PEs?
- The answer is not straightforward, seems to depend on the type of task
- Sequence classification: trainable PEs
- Token classification / span extraction: fixed relative PEs



vs.



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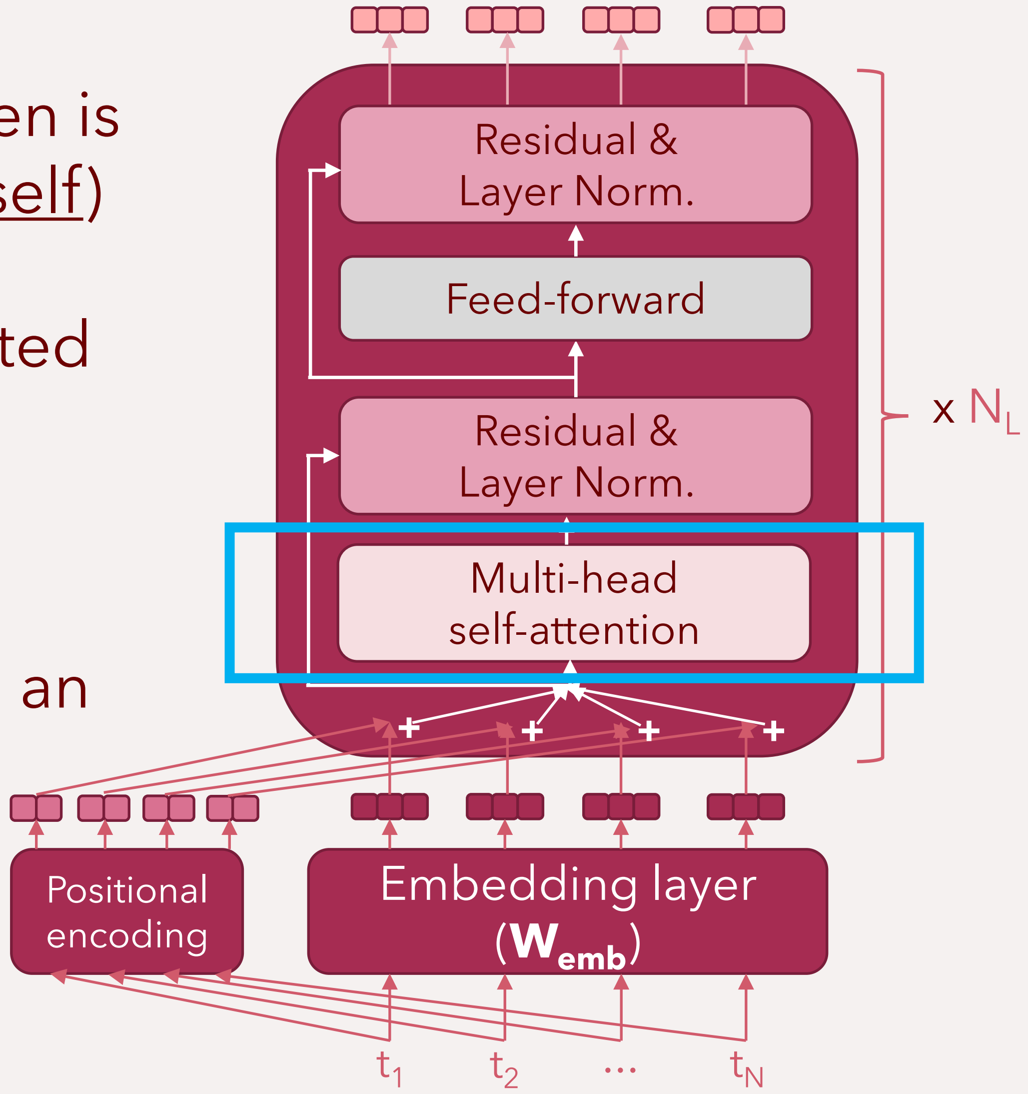
Multi-Head Attention

- **Self-attention** in Transformer: each token is „attending" over all tokens (including itself)

- Each token t_i (i = 1, ..., N) has an associated
  - Key vector $\mathbf{k}_i$
  - Value vector $\mathbf{v}_i$
  - Query vector $\mathbf{q}_i$

- One self-attention mechanism is called an attention head
  - Multi-head attention: multiple self-attention mechanisms



Self-Attention (Attention Head)

- **Self-attention**: each token is „attending" over <u>all</u> tokens

- Each token t_i ($i = 1, \ldots, N$) has an associated
  - Key vector $\mathbf{k}_i$, value vector $\mathbf{v}_i$, and query vector $\mathbf{q}_i$

- Let $\mathbf{x}_i$ be the embedding of t_i
  - I.e., sum of subword emb. and PE
  - Q: how do we obtain three different vectors ($\mathbf{k}_i$, $\mathbf{v}_i$, and $\mathbf{q}_i$) from $\mathbf{x}_i$?
  - Introduce <u>trainable parameters</u> that project $\mathbf{x}_i$ into different vectors

- Stack embeddings of tokens ($\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$) into a matrix $\mathbf{X} \in \mathbb{R}^{N \times d}$
  - In later transformer layers, $\mathbf{X}$ is not the matrix of embeddings from the embedding layer but is the the output of the previous layer

Self-Attention (Attention Head)

- **Self-attention**: Introduce trainable parameters that project $\mathbf{X}$ into matrices $\mathbf{K}$, $\mathbf{V}$, and $\mathbf{Q}$

- Query matrix: $\mathbf{Q} = \mathbf{X}\,\mathbf{W}^{\mathbf{Q}}$, $\mathbf{W}^{\mathbf{Q}} \in \mathbb{R}^{d \times k}$
- Key matrix: $\mathbf{K} = \mathbf{X}\,\mathbf{W}^{\mathbf{K}}$, $\mathbf{W}^{\mathbf{K}} \in \mathbb{R}^{d \times k}$
- Value matrix: $\mathbf{V} = \mathbf{X}\,\mathbf{W}^{\mathbf{V}}$, $\mathbf{W}^{\mathbf{V}} \in \mathbb{R}^{d \times v}$

- $\mathbf{Q} \in \mathbb{R}^{N \times k}$, $\mathbf{K} \in \mathbb{R}^{N \times k}$, and $\mathbf{V} \in \mathbb{R}^{N \times v}$
  - Query, key, and value vectors are not necessarily of same length d as input emb.
  - $\mathbf{Q}$ and $\mathbf{K}$ are of the same dimensionality

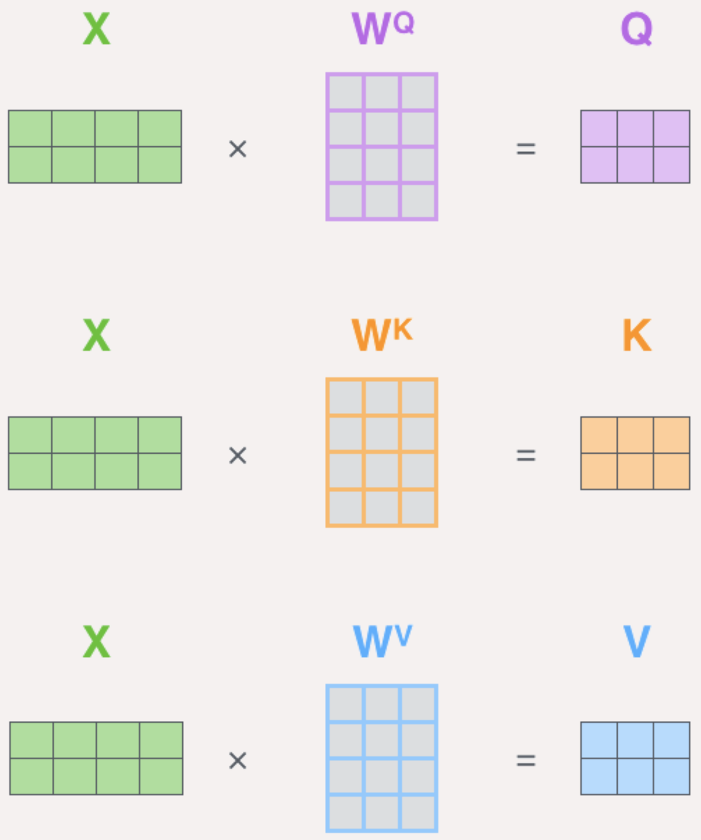


Image from: https://jalammar.github.io/illustrated-transformer/

Self-Attention (Attention Head)

- Query matrix: $\mathbf{Q} = \mathbf{X}\,\mathbf{W^Q}$, $\mathbf{W^Q} \in \mathbb{R}^{d \times k}$
- Key matrix: $\mathbf{K} = \mathbf{X}\,\mathbf{W^K}$, $\mathbf{W^K} \in \mathbb{R}^{d \times k}$
- Value matrix: $\mathbf{V} = \mathbf{X}\,\mathbf{W^V}$, $\mathbf{W^V} \in \mathbb{R}^{d \times v}$

- Output of the Transformer's self-attention is computed as:

$$\mathbf{Z} = \mathrm{softmax}\left(\frac{\mathbf{QK}^T}{\sqrt{k}}\right)\mathbf{V}\ ; \quad \mathbf{Z} \in \mathbb{R}^{N \times v}$$

- The matrix $\mathbf{QK}^T \in \mathbb{R}^{N \times N}$ is called an attention matrix
  - Often used for interpretability, how much each token attends over each other token

- softmax is applied row-wise on $\frac{\mathbf{QK}^T}{\sqrt{k}}$
- Q: Why normalization with $\sqrt{k}$?

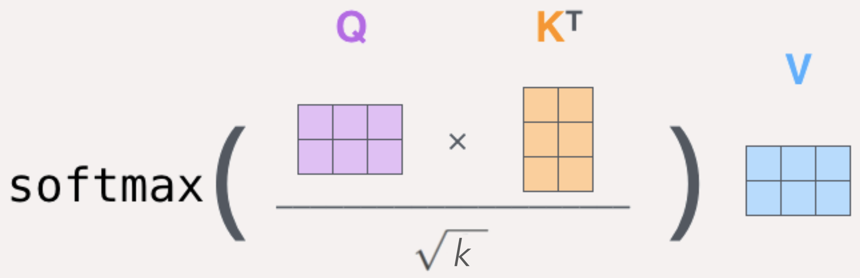


Image from: https://jalammar.github.io/illustrated-transformer/

Multi-Head Attention

- Simply multiple attention heads, independent of each other
  - Just operate on the same input **X**
  - H attention heads

1st attention head:

- $\mathbf{Q}_1 = \mathbf{X}\,\mathbf{W}_1^{\mathbf{Q}};\ \mathbf{K}_1 = \mathbf{X}\,\mathbf{W}_1^{\mathbf{K}};\ \mathbf{V}_1 = \mathbf{X}\,\mathbf{W}_1^{\mathbf{V}};$
- $\mathbf{Z}_1 = \mathrm{softmax}(\frac{\mathbf{Q}_1\mathbf{K}_1^T}{\sqrt{k}})\mathbf{V}_1$

…

H-th attention head

- $\mathbf{Q}_H = \mathbf{X}\,\mathbf{W}_H^{\mathbf{Q}};\ \mathbf{K}_i = \mathbf{X}\,\mathbf{W}_H^{\mathbf{K}};\ \mathbf{V}_i = \mathbf{X}\,\mathbf{W}_H^{\mathbf{V}};$
- $\mathbf{Z}_H = \mathrm{softmax}(\frac{\mathbf{Q}_H\mathbf{K}_H^T}{\sqrt{k}})\mathbf{V}_H$

Multi-Head Attention

- Simply multiple attention heads, independent of each other
  - Just operate on the same input $\mathbf{X}$
  - H attention heads
- Output of the multi-head attention layer is then a downprojection of the concatenation of the outputs of each head (i.e., each self-attention)

$$\text{mh-att}(\mathbf{X} \mid \boldsymbol{\theta}_{MHA}) = (\mathbf{Z}_1 \oplus \mathbf{Z}_2 \oplus \cdots \oplus \mathbf{Z}_{H-1} \oplus \mathbf{Z}_H)\, \mathbf{W}^{\mathbf{O}}$$

- Concatenation $(\mathbf{Z}_1 \oplus \mathbf{Z}_2 \oplus \cdots \oplus \mathbf{Z}_{H-1} \oplus \mathbf{Z}_H)$ has dimensions $N \times (v \cdot H)$
  - Desdiderata (because of multiple identical layers): output of multi-head attention has the same dimensionality as input: $\text{mh-att}(\mathbf{X}) \in \mathbb{R}^{N \times d}$
  - This mandates that the parameter matrix $\mathbf{W}^{\mathbf{O}}$ has dimensions $(v \cdot H) \times d$
- All parameters of one MHA (sub)layer: $\boldsymbol{\theta}_{MHA} = \{\mathbf{W}_1^{\mathbf{Q}}, \mathbf{W}_1^{\mathbf{K}}, \mathbf{W}_1^{\mathbf{V}}, \ldots, \mathbf{W}_H^{\mathbf{Q}}, \mathbf{W}_H^{\mathbf{K}}, \mathbf{W}_H^{\mathbf{V}}, \mathbf{W}^{\mathbf{O}}\}$

Multi-Head Attention – Visual Summary

- In the example below: **8** attention heads (indexed 0 to 7)

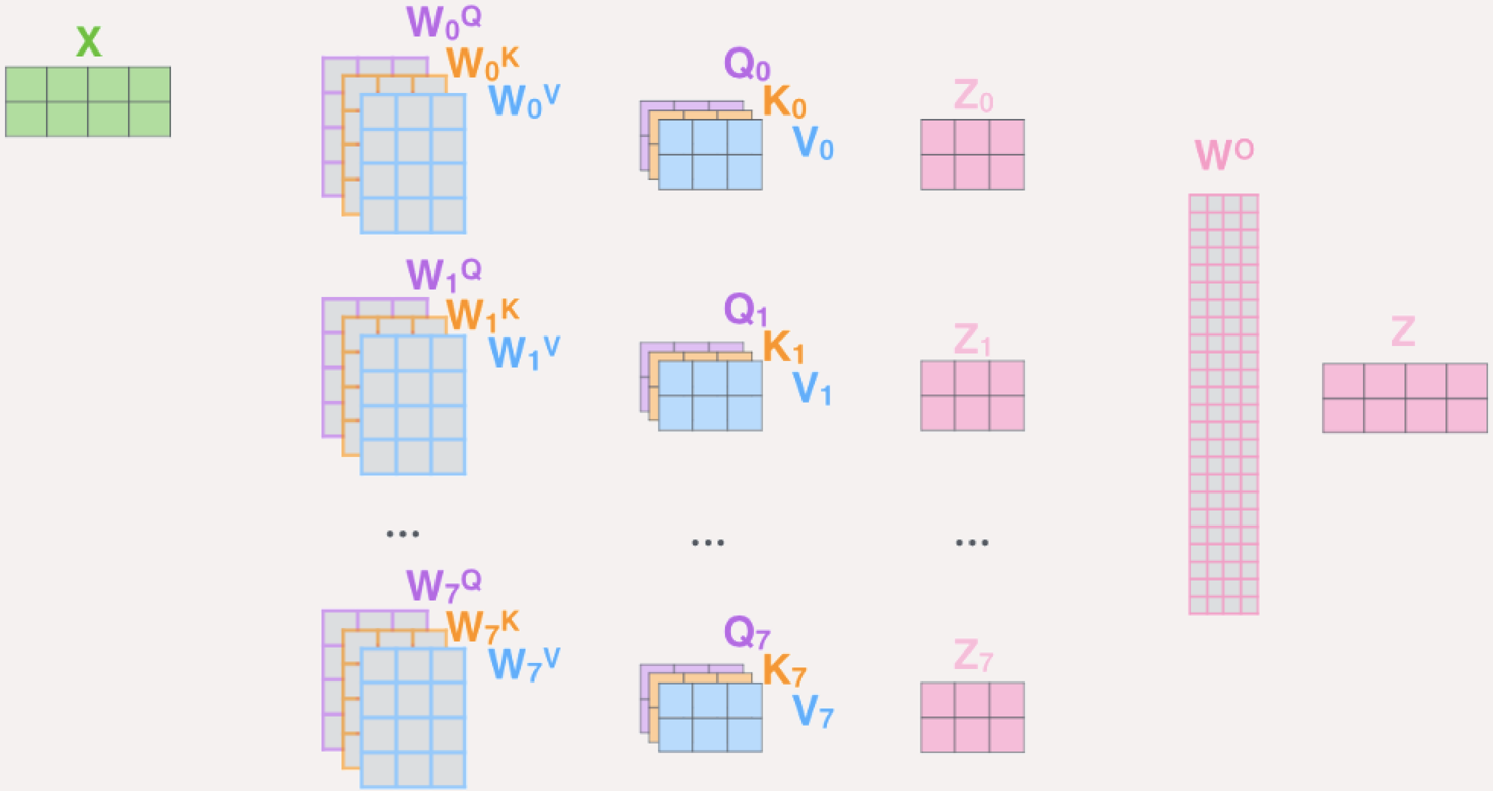


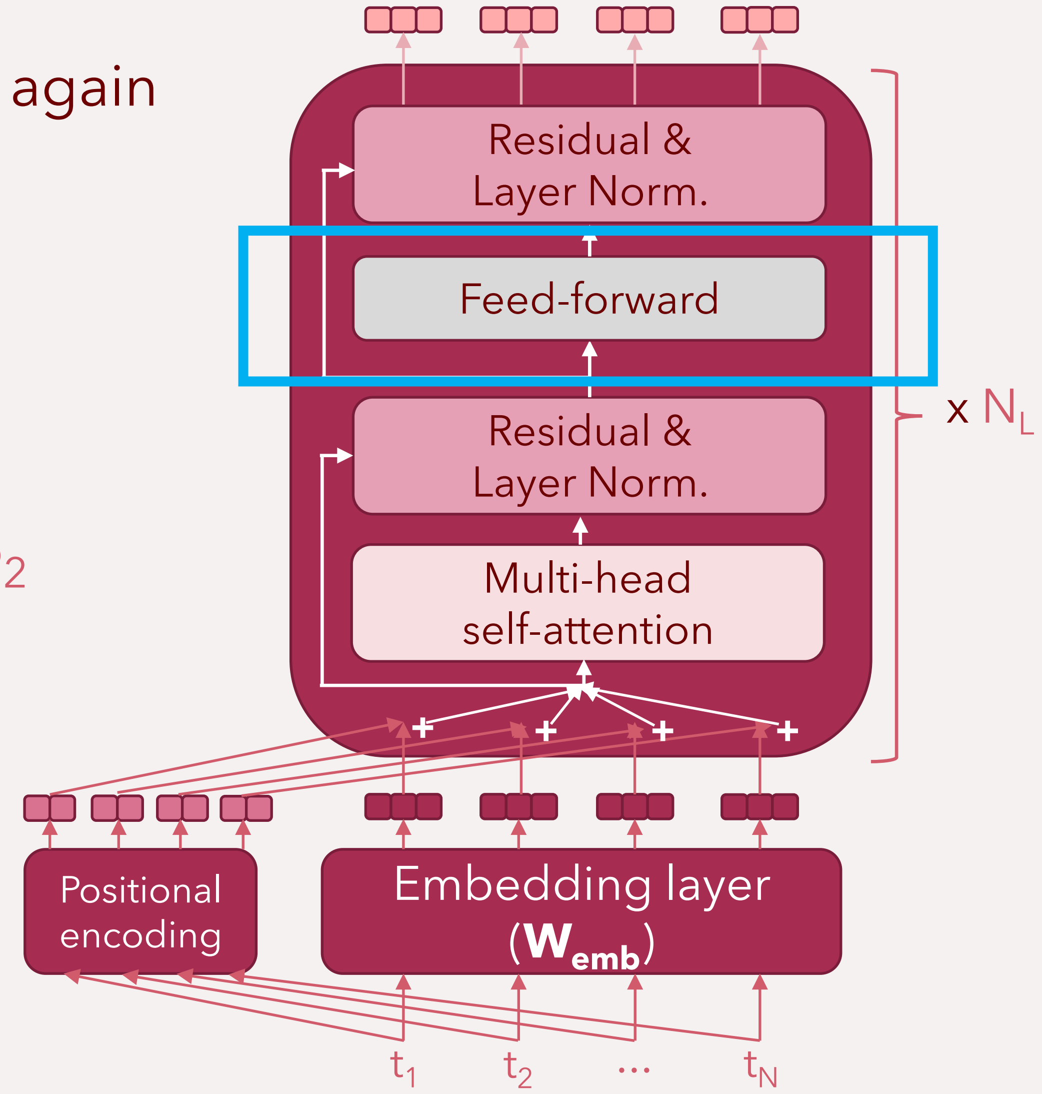
Image from: https://jalammar.github.io/illustrated-transformer/

Feed-Forward Layer

- Output of the multi-head attention layer is again a matrix of dimensions N x d
  - I.e., one d-dim. vector for each token
- Each token vector **x** is then independently transformed through the following FFN:

$$\mathrm{FFN}(\mathbf{x} \mid \boldsymbol{\theta}_{ffn}) = \mathrm{ReLU}(\mathbf{x}\mathbf{W}_1 + \mathbf{b}_1)\mathbf{W}_2 + \mathbf{b}_2$$

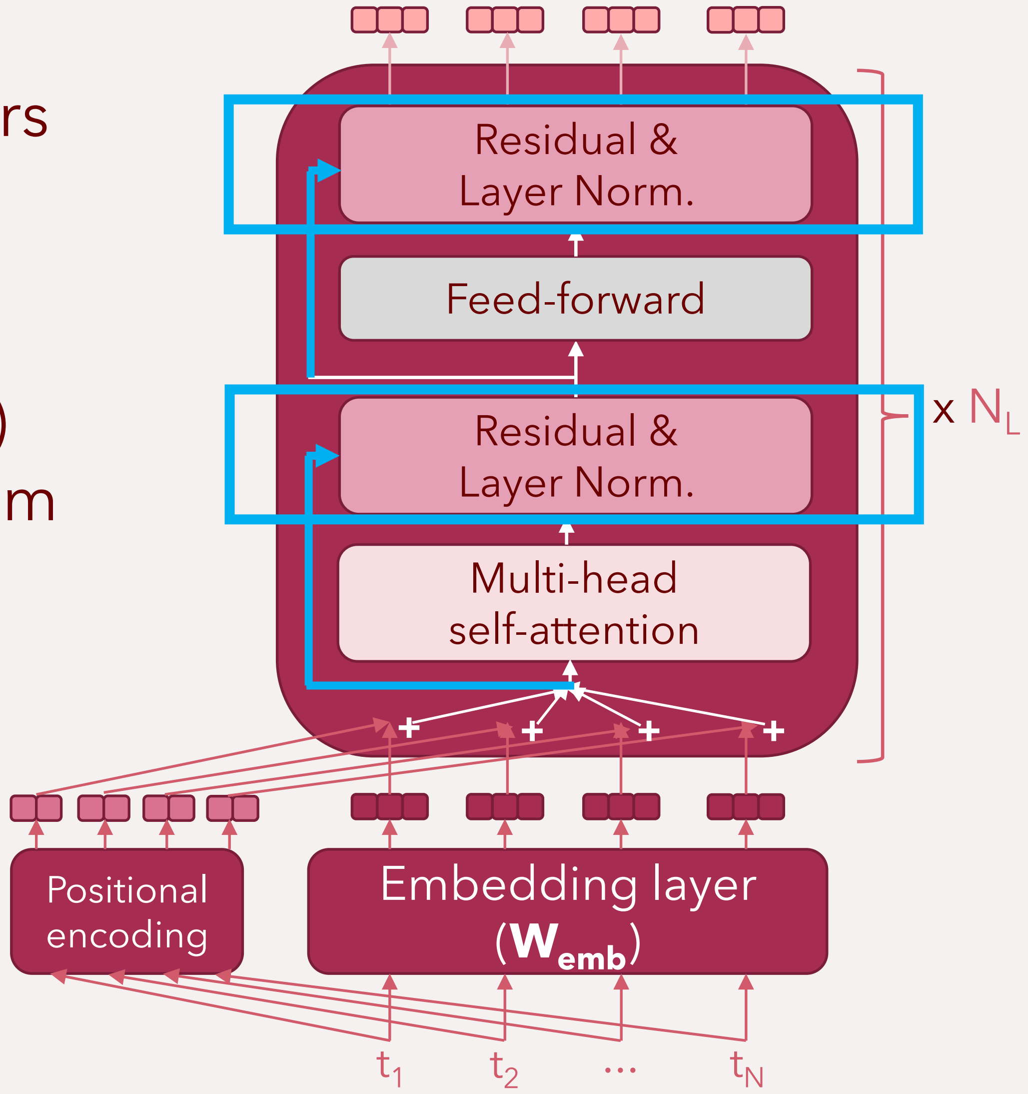
- $\mathrm{ReLU}(x) = \max(0, x)$
  - Common activation function
- Trainable parameters: $\boldsymbol{\theta}_{ffn} = \{\mathbf{W}_1, \mathbf{b}_1, \mathbf{W}_2, \mathbf{b}_2\}$
  - $\mathbf{W}_1 \in \mathbb{R}^{d \times f}$, $\mathbf{b}_1 \in \mathbb{R}^{f}$
  - $\mathbf{W}_2 \in \mathbb{R}^{f \times d}$, $\mathbf{b}_1 \in \mathbb{R}^{d}$
  - *Vaswani et al.* set f = 4d



Residuals

- Transformer layer has two main sublayers
  - Multi-head attention layer
  - Feed-forward layer
- Both those layers (i.e., param. functions) have a **residual connection** around them
- Residual (around a layer) – layer input added to its output

$$res(layer, \mathbf{X}) = \mathbf{X} + layer(\mathbf{X} \mid \boldsymbol{\theta}_{layer})$$

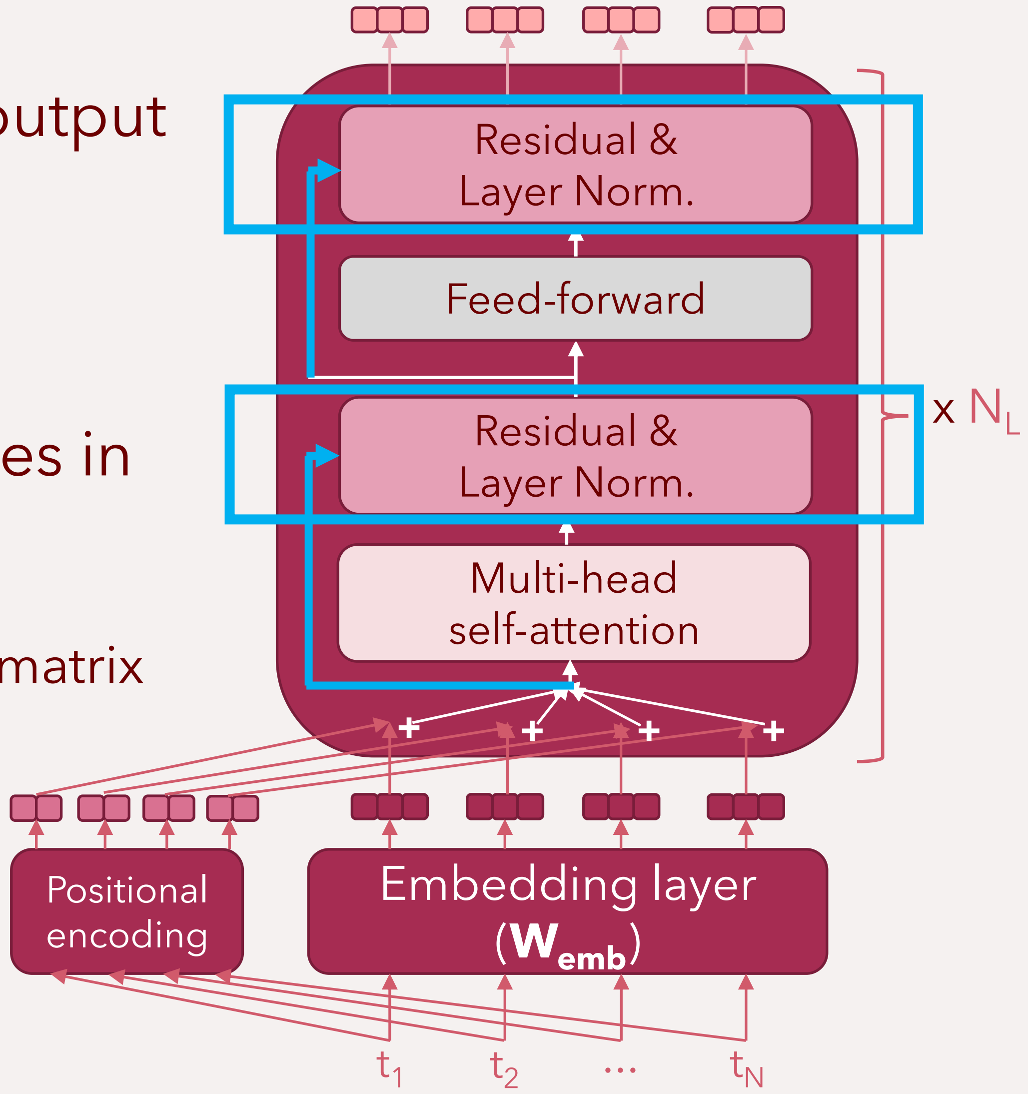


Layer Normalization

- After the residual summation, the final output is subdued to **layer normalization**

$$\textit{layer\_norm}(\mathbf{X'} = \mathbf{X} + \text{layer}(\mathbf{X} \mid \boldsymbol{\theta}_{\text{layer}}))$$

- Layer normalization normalizes the values in each of the row-vectors $\mathbf{x}$ in the input
  - Input is a matrix of dimensions $N \times d$
  - Let $\mathbf{x} \in \mathbb{R}^d$ be any of the row-vectors of that matrix
- We z-normalize values in $\mathbf{x} = [x_1, x_2, \ldots, x_d]$
  - $x_i \rightarrow \frac{x_i - \mu}{\sigma}$
  - μ as mean and σ as st. deviation on $\mathbf{x}$

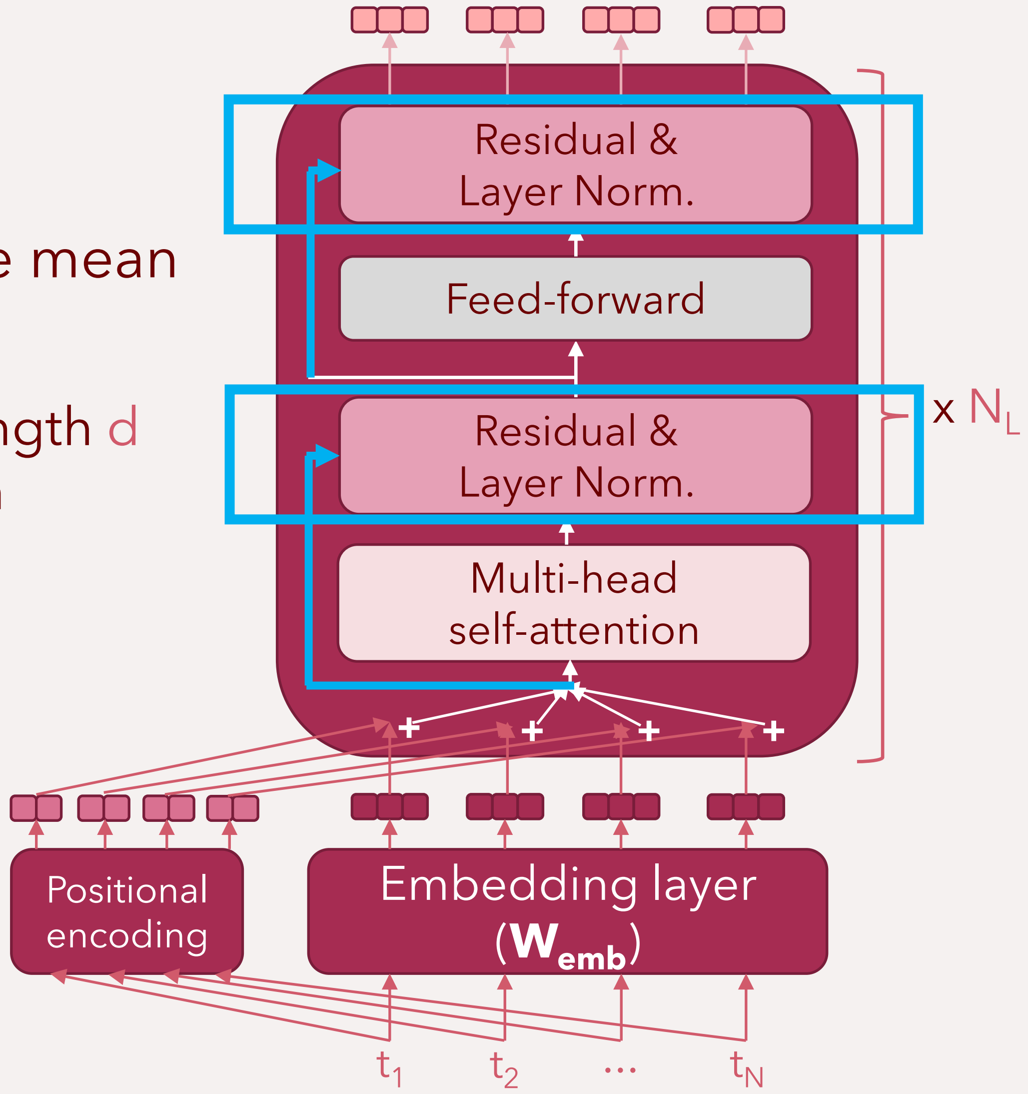


Layer Normalization

- We z-normalize (or standardize) values in **x**
  - $x_i \rightarrow \frac{x_i - \mu}{\sigma}$
  - This centers the values in **x** around the mean of 0, with the st. deviation of 1
- **X''** = matrix with N z-normalized vectors of length d
- The final layer normalized output is given with

$$\boldsymbol{\gamma} * \mathbf{X}'' + \boldsymbol{\beta}$$

- Where $\boldsymbol{\gamma}$ and $\boldsymbol{\beta} \in \mathbb{R}^d$ are trainable parameters of layer attention
  - $\boldsymbol{\gamma}$ element-wise multiplies each row of **X''**
  - $\boldsymbol{\beta}$ is then added to each of the rows



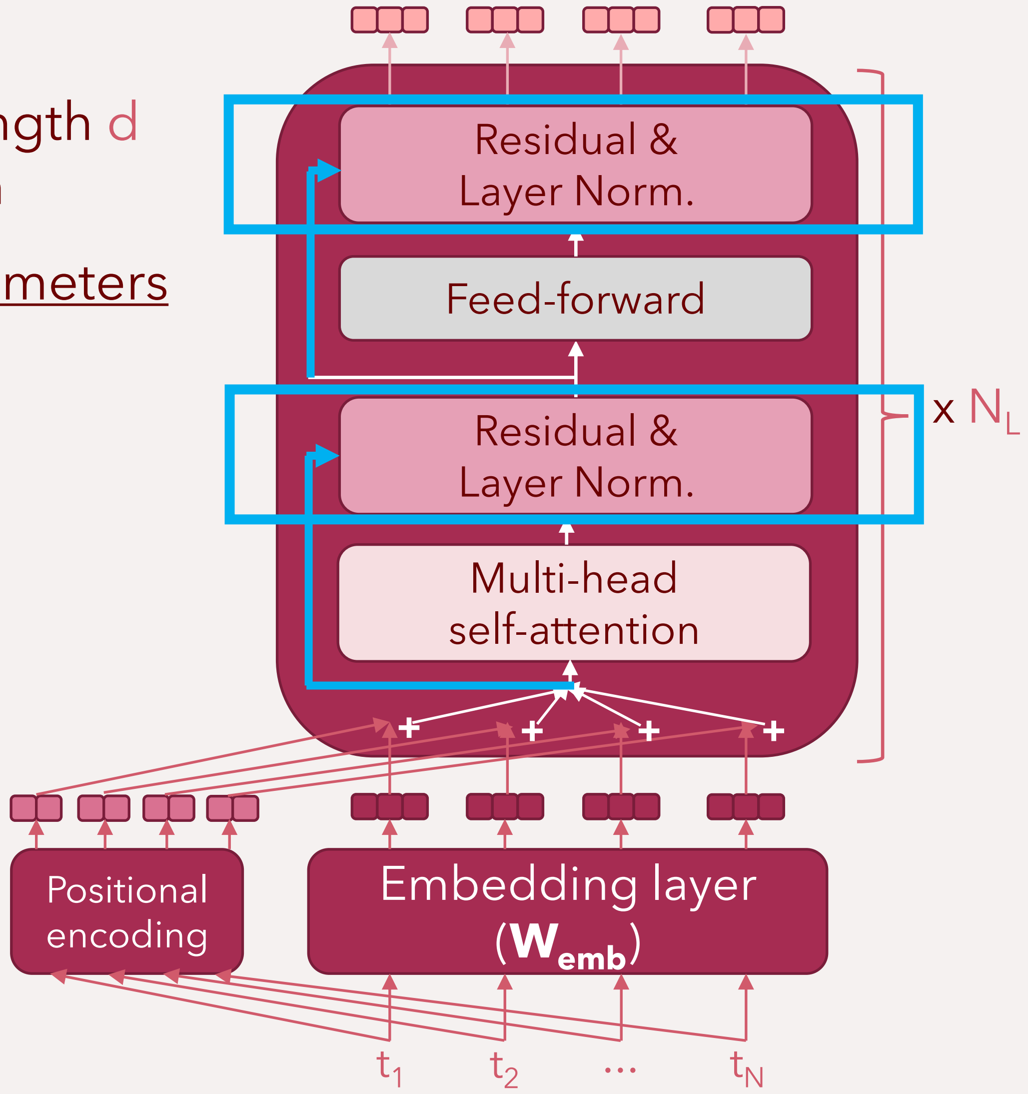
Layer Normalization

- **X''** = matrix with N z-normalized vectors of length d
- The final layer normalized output is given with

- γ * **X**'' + β, with γ and $\beta \in \mathbb{R}^d$ are trainable parameters of the layer normalization „layer"
  - γ element-wise multiplies each row of **X**''
  - β is then added to each of the rows

- Layer-normalization stabilizes training
  - All instances across all mini-batches normalized the same way

  - Q: But why do we need γ and β?
    - Normalization to *N(0, 1)* may be too restrictive, some layers may need „more expressive" distributions



Content

- Attention mechanism
- Transformer – dissected
  - Positional Embeddings
  - Multi-Head Self-Attention
- **Pretraining + fine-tuning**

Pretraining Transformers

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019). BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. In Proceedings of NAACL-HLT (pp. 4171-4186).

- **Pretrain – fine-tune paradigm**: the idea that we can
  (1) pretrain the parameters of the encoder θ_{ENC} via some self-supervised training objective on large corpus and then

  (2) further update (i.e., fine-tune) encoder's parameters θ_{ENC} while training for a concrete task – in this second step, we add task-specific classifier/regressor (head) on top of the encoder (body)

- **BERT**: pretraining–fine-tuning with a Transformer as the encoder
  - BERT not a first attempt at pretraining an encoder
    - But first where the encoder is a Transformer
  - ULMFit (Howard & Ruder, 2018), ELMo (Peters et al., 2018)

Pretraining Transformers

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- **Pretrain – fine-tune paradigm**
  (1) Pretrain (self-supervised objective)
  (2) Fine-tune (on annotated task data)

- Q: What is a suitable self-supervised objective for pretraining?

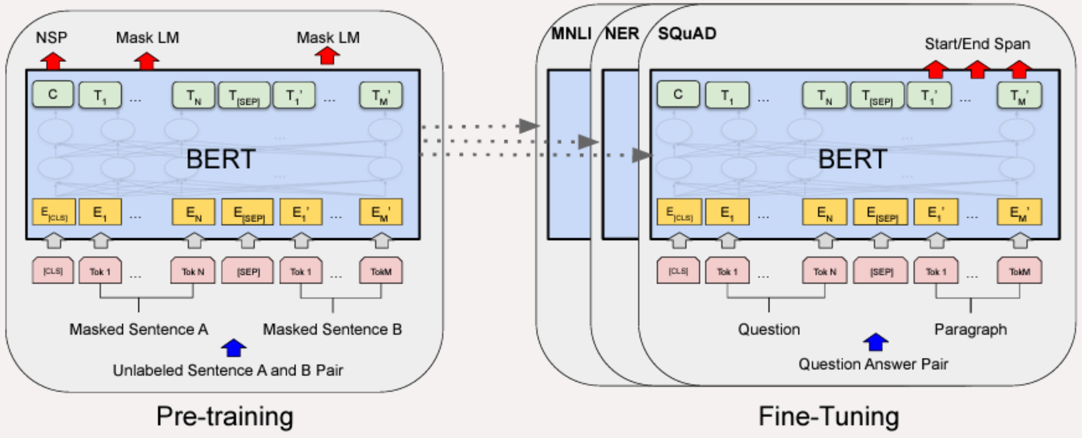

Image from Devlin et al.

Pretraining Transformers

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- Q: What is a suitable self-supervised objective for pretraining?

- Devlin et al. use two pretraining objectives
  1. Masked LM-ing (MLM)
  2. Next Sentence Prediction (NSP)

- Special input: pairs of sentences with special (artificial) tokens

[CLS] $t_1^1\ t_2^1 \ldots t_N^1$ [SEP] $t_1^2\ t_2^2 \ldots t_M^2$ [SEP]

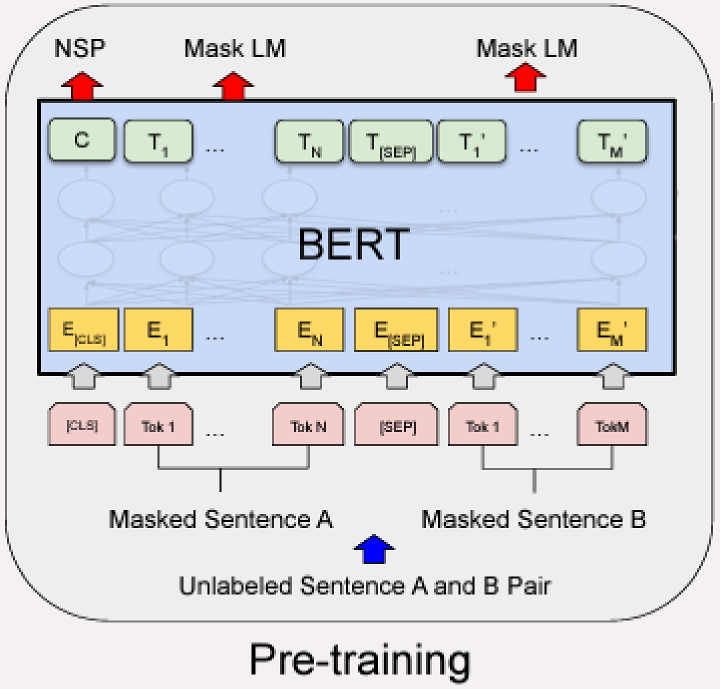

Image from Devlin et al.

Pretraining Transformers

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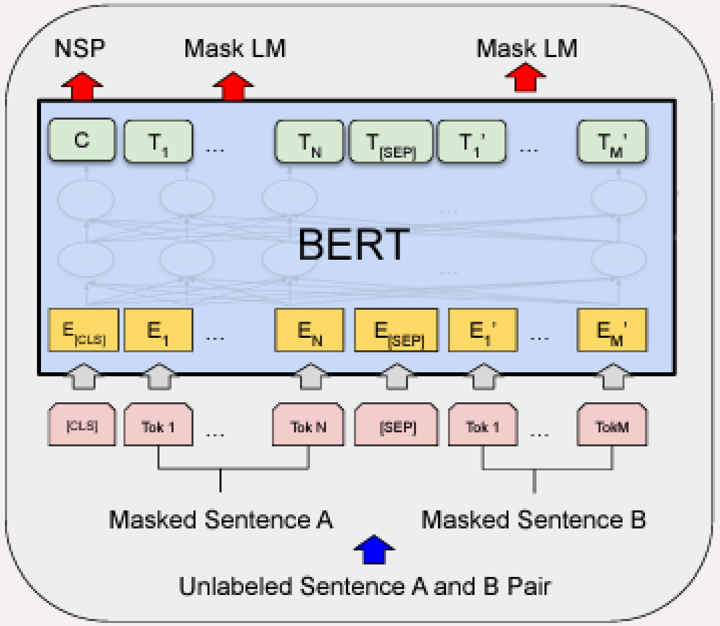
- Input: [CLS] $t_1^1\ t_2^1 \ldots t_N^1$ [SEP] $t_1^2\ t_2^2 \ldots t_M^2$ [SEP]
  - [CLS] – sequence start token
  - [SEP] – separator token

- The two sentences may or may not be adjacent in the training corpus

- Some percentage of (real) tokens masked out – replaced with the [MASK] token



Pre-training

Image from Devlin et al.

Pretraining Transformers

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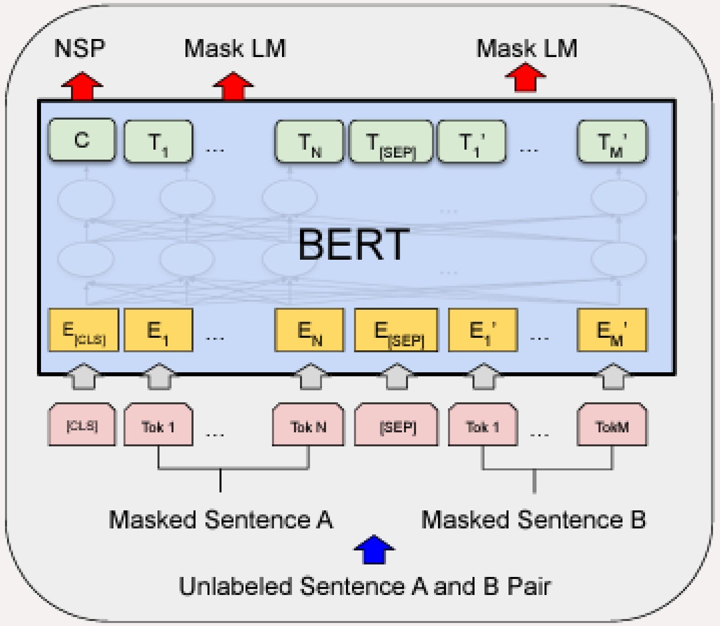
- BERT's pretraining objectives
  1. Masked LM-ing (MLM)
  2. Next Sentence Prediction (NSP)
- MLM: predict the original token for each masked position (in either sentence)
  - Standard LM-ing classification head + negative log-likelihood loss
- $\mathbf{x} \in \mathbb{R}^d$ = Transformer's output vector for some masked token [MASK]

$$\hat{\mathbf{y}} = \text{softmax}(\mathbf{x}\,\mathbf{W}_{lm}),\ \mathbf{W}_{lm} \in \mathbb{R}^{d \times |V|}$$

$$L(\mathbf{x}, \mathbf{y}\,|\theta_{enc}, \mathbf{W}_{lm}) = -\sum_{i=1}^{|V|} y_i \ln(\hat{y}_i)$$



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Pretraining Transformers

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- BERT's pretraining objectives
  1. Masked LM-ing (MLM)
  2. Next Sentence Prediction (NSP)

- NSP: Predict if the two sentences were adjacent in the corpus or not
  - Standard binary classification head + binary cross-entropy loss
  - Q: why NSP? For text-pair tasks (QA, NLI)

- RoBERTa: same Transformer pretrained on more data and only with MLM – better performance

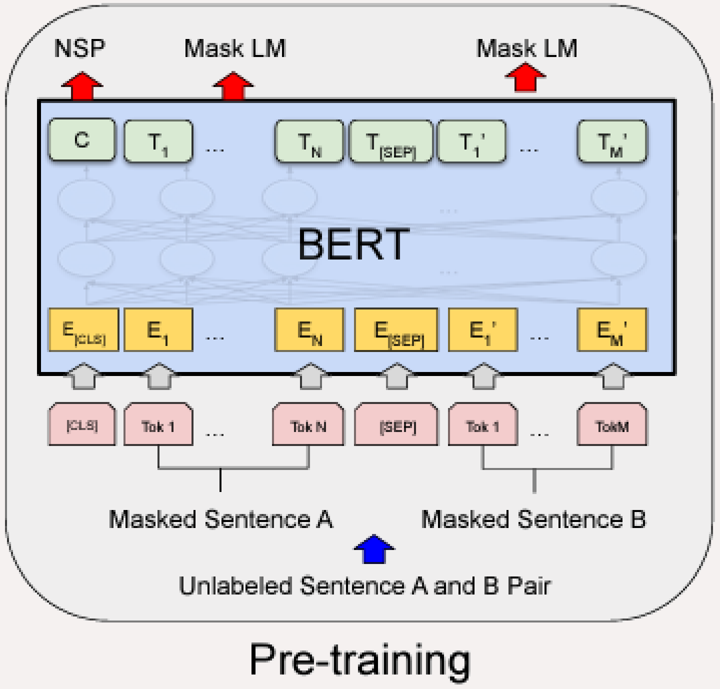

Image from Devlin et al.

Fine-Tuning Transformers

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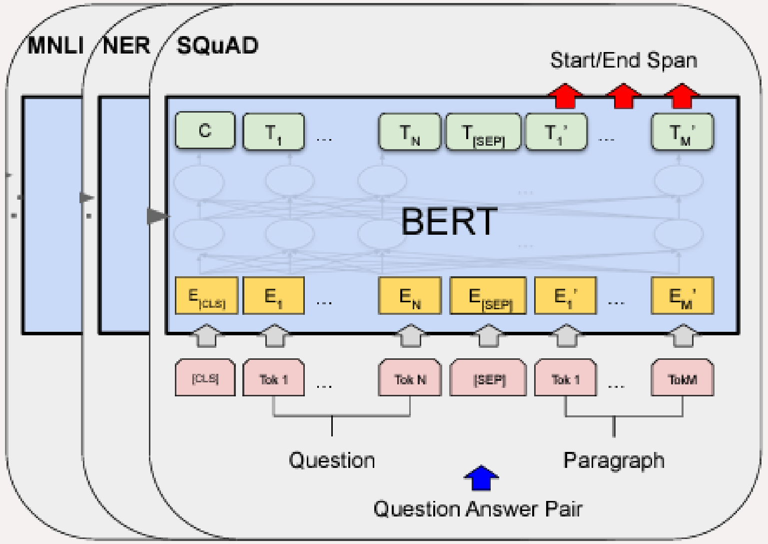
- **Pretrain – fine-tune paradigm**
  (1) Pretrain (self-supervised objective)
  (2) Fine-tune (on annotated task data)

- Q: How do we fine-tune BERT's Transformer for a concrete task?



Fine-Tuning

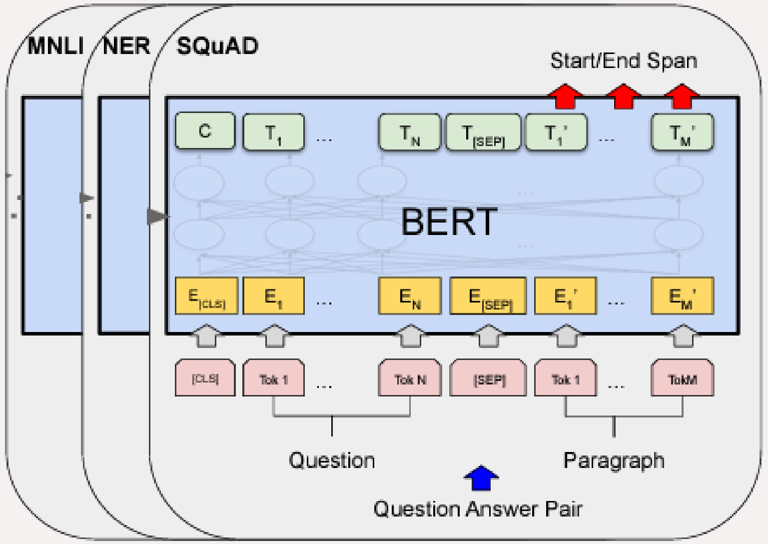
Image from Devlin et al.

Fine-Tuning Transformers

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019). [BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding](). In Proceedings of NAACL-HLT (pp. 4171-4186).

- **Sequence classification** (or regression) denotes tasks in which a label (class or score) is to be assigned to the whole input
  - $\mathbf{x}_{CLS} \in \mathbb{R}^d$ the representation of the sequence start token [CLS] output of the last Transformer layer
  - $\mathbf{x}_{CLS}$ represents the encoding of the whole sequence, and goes into the classifier

$$\hat{\mathbf{y}} = \mathit{classifier}(\mathbf{x}_{CLS}|\boldsymbol{\theta}_{cl})$$



Fine-Tuning

Image from Devlin et al.

Fine-Tuning Transformers

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- **Token classification** (or regression) denotes tasks in which a label (class or score) is to be assigned to the whole input
  - $\mathbf{x} \in \mathbb{R}^d$ the representation of a token (to be classified), output of the Transformer layer
  - $\mathbf{x}$ is the contextualized embedding of the token, and goes into the classifier

$$\hat{\mathbf{y}} = classifier(\mathbf{x}|\boldsymbol{\theta}_{cl})$$

  - Q: what if we're classifying word-level tokens (but have a subword tokenizer)?

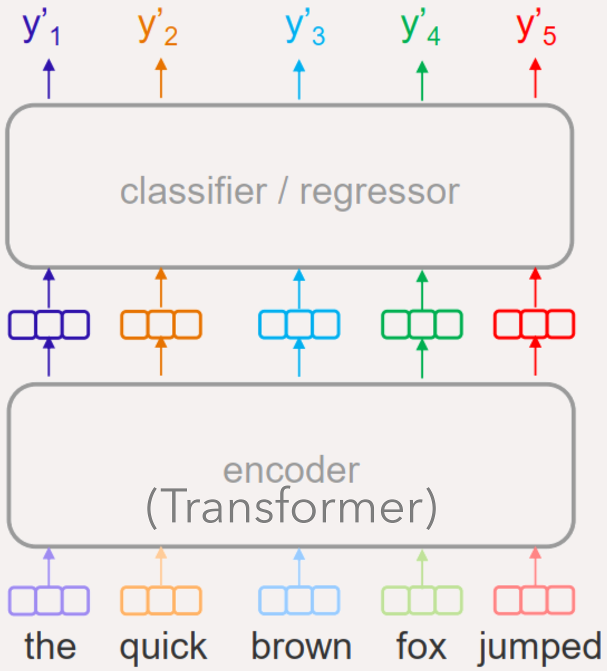

Image: Alexander Mikhalchyk