Lecture 2

CME 295: Transformers & Large Language Models

Afshine Amidi & Shervine Amidi

Stanford University

ICME

Recap of last episode…

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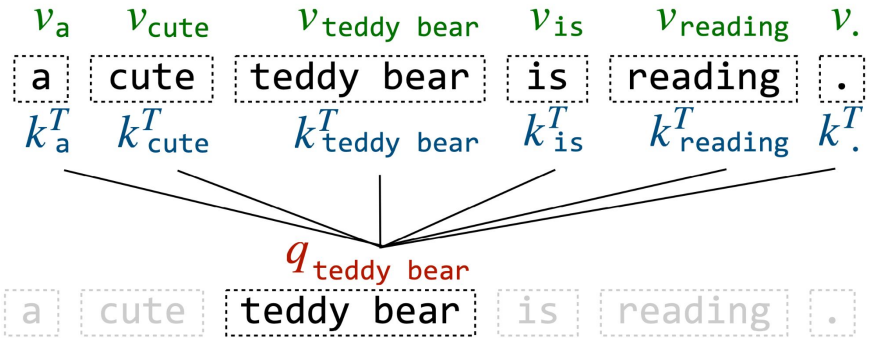

"*Attention Is All You Need*", Vaswani et al., 2017.

Recap of last episode...

$$\text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

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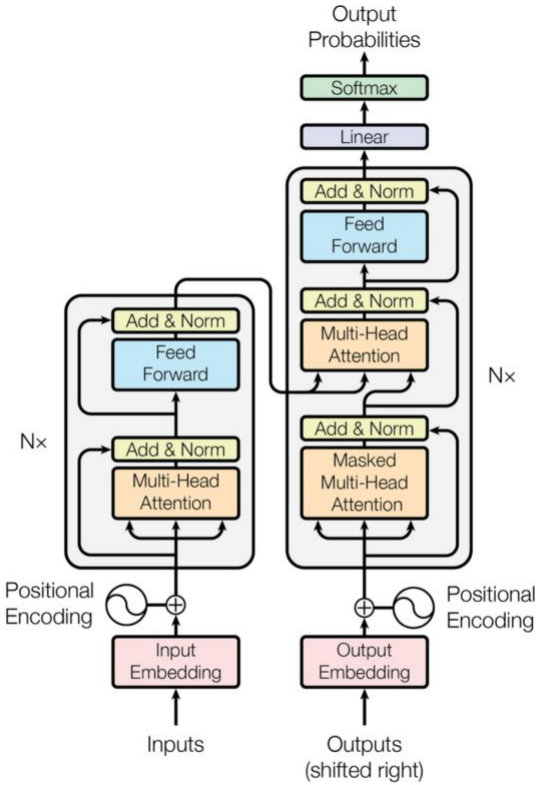

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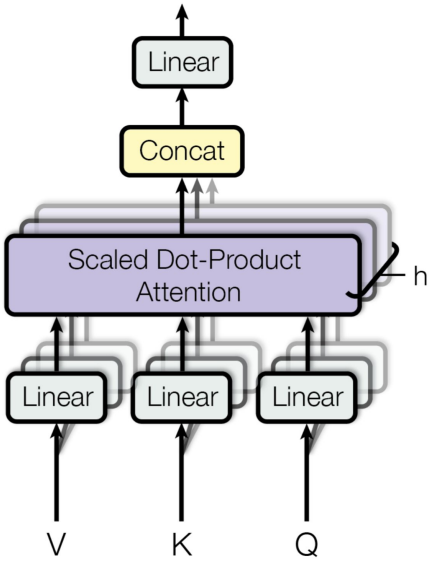

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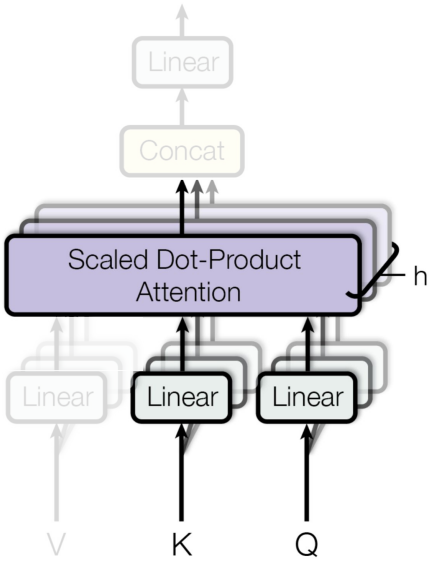

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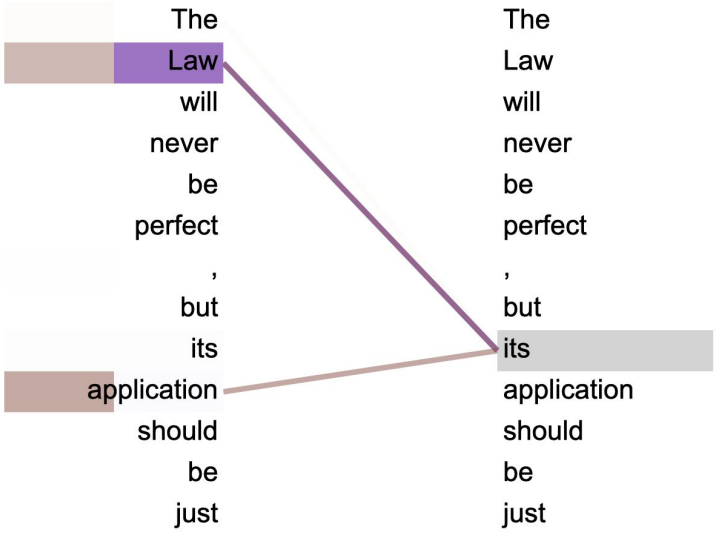
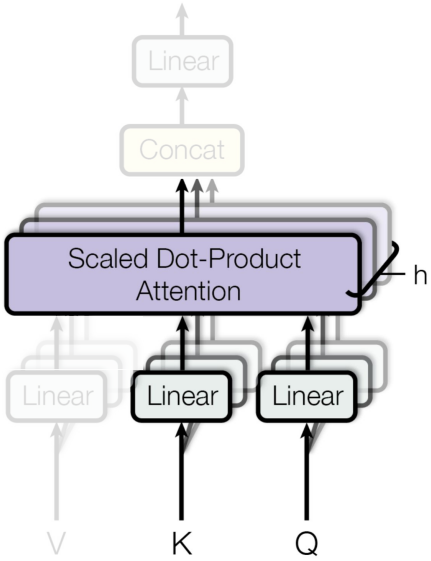
Recap of last episode...

Attention map



"Two attention heads, also in layer 5 of 6, apparently involved in anaphora resolution. [...] Isolated attentions from just the word 'its' for attention heads 5 and 6."

$$\text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



"Attention Is All You Need", Vaswani et al., 2017.

Suggested reading: original Transformer paper

Attention Is All You Need

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Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best

Transformers & Large Language Models

Position embeddings

Layer normalization

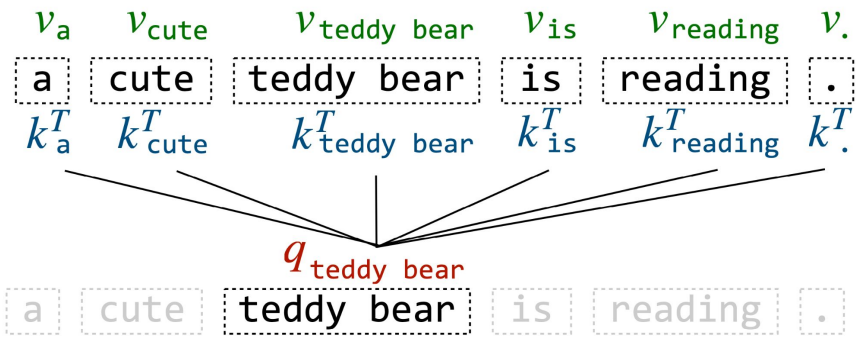
Attention approximation

Transformer-based models

BERT deep dive

Need for position information

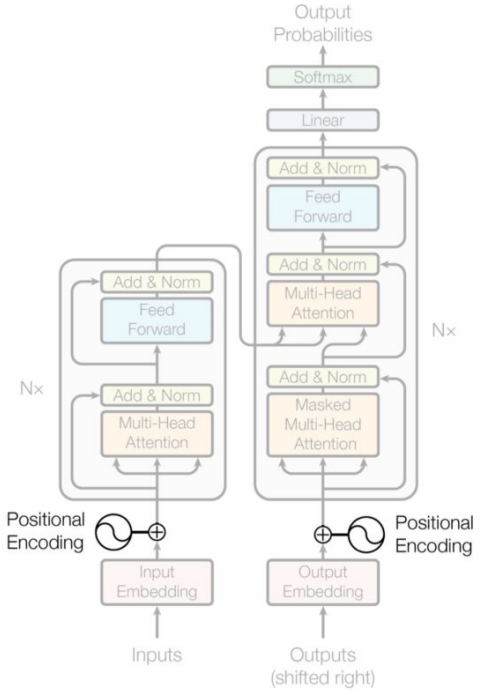
Motivation. Direct links "lose" position info



Need for position information

Motivation. Direct links "lose" position info

Idea. Add learned position-specific embedding to token vector



"Attention Is All You Need", Vaswani et al., 2017.

Need for position information

Motivation. Direct links "lose" position info

Idea. Add learned position-specific embedding to token vector

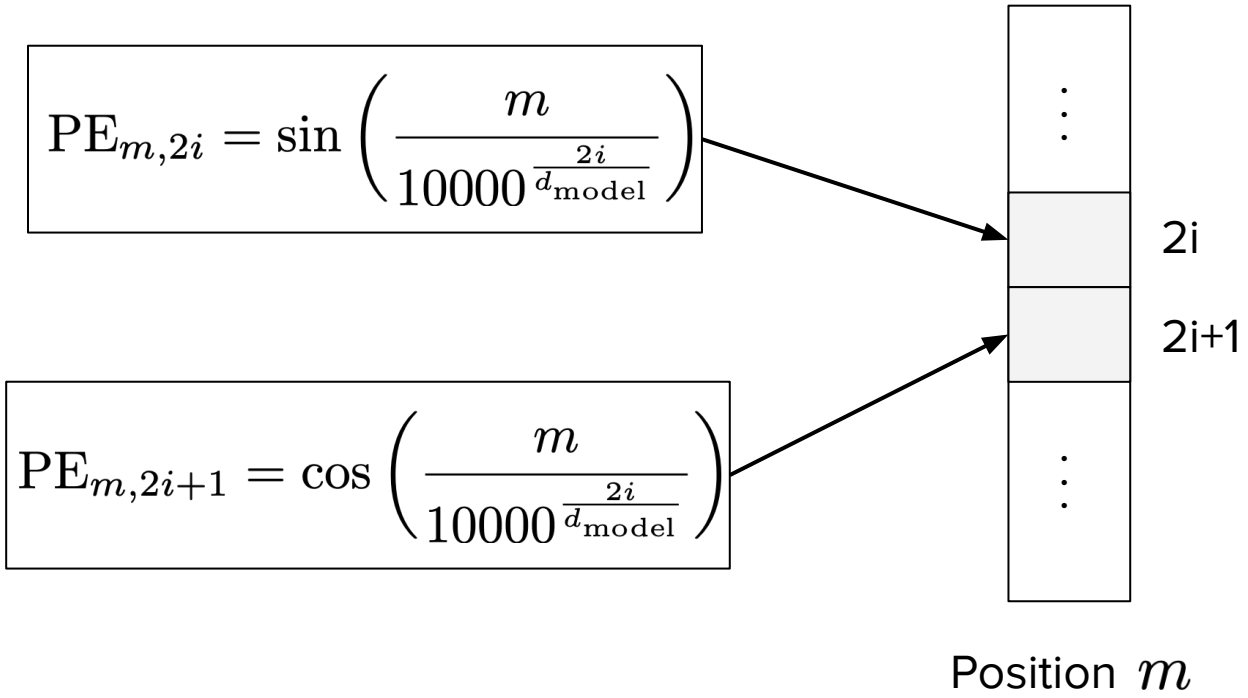
Limitations. Need to retrain for longer sequences

Hardcoded position embeddings

Idea. Hardcode values of position embedding

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

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



"Attention Is All You Need", Vaswani et al., 2017.

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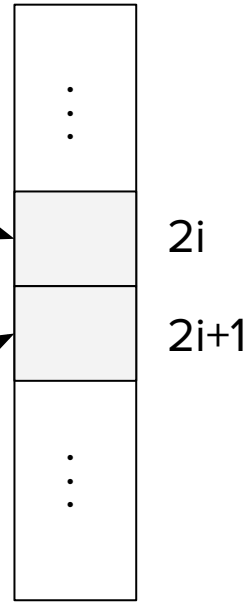
$$\mathrm{PE}_{m,2i} = \sin\left(\omega_i \times m\right)$$

with $\omega_i = 10000^{-\frac{2i}{d_{\text{model}}}}$

$$\mathrm{PE}_{m,2i+1} = \cos\left(\omega_i \times m\right)$$



Position m

"Attention Is All You Need", Vaswani et al., 2017.

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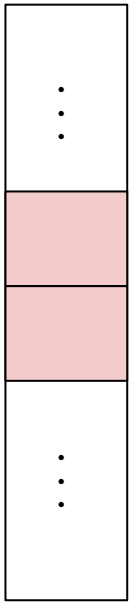

2i

2i+1

Position m

$$\mathrm{PE}_{n,2i} = \sin\left(\omega_i \times n\right)$$

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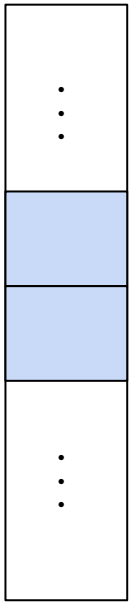

2i

2i+1

Position n

"Attention Is All You Need", Vaswani et al., 2017, "Transformer Architecture: The Positional Encoding", by Kazemnejad, 2019.

Hardcoded position embeddings

Idea. Hardcode values of position embedding

$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$

Hardcoded position embeddings

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$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$

$$\cos(\omega_i(m-n)) = \cos(\omega_i \times m)\cos(\omega_i \times n) + \sin(\omega_i \times m)\sin(\omega_i \times n)$$

Hardcoded position embeddings

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$$\cos(\omega_i(m-n)) = \cos(\omega_i \times m)\cos(\omega_i \times n) + \sin(\omega_i \times m)\sin(\omega_i \times n)$$

$$\langle \mathrm{PE}_m, \mathrm{PE}_n \rangle = \ldots + \cos(\omega_i(m-n)) + \ldots$$

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$$\langle \mathrm{PE}_m, \mathrm{PE}_n \rangle = \ldots + \cos(\omega_i(m-n)) + \ldots$$

$$\langle \mathrm{PE}_m, \mathrm{PE}_n \rangle = f(m-n)$$

Hardcoded position embeddings

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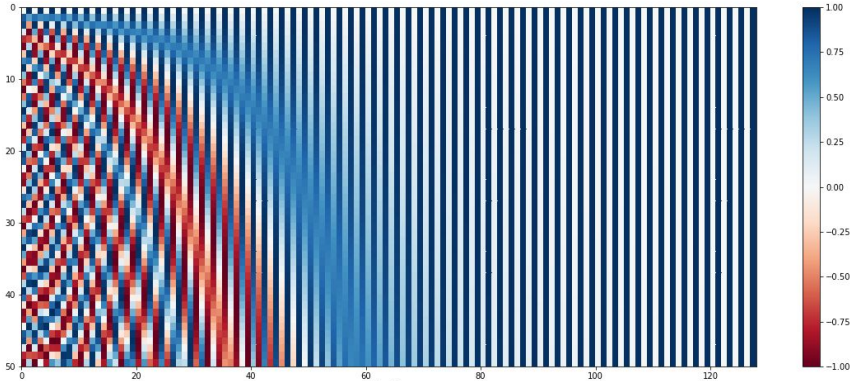
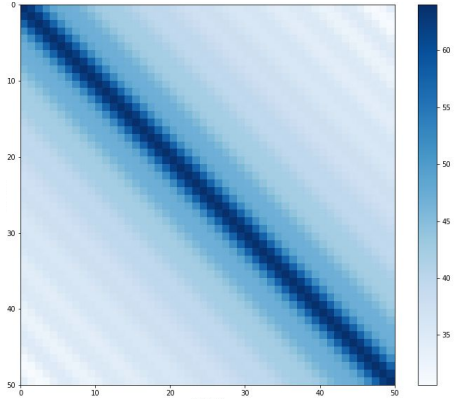


Value of embeddings



Similarity between positions

"Attention Is All You Need", Vaswani et al., 2017, "Transformer Architecture: The Positional Encoding", by Kazemnejad, 2019.

Hardcoded position embeddings

Idea. Hardcode values of position embedding

Value of embeddings

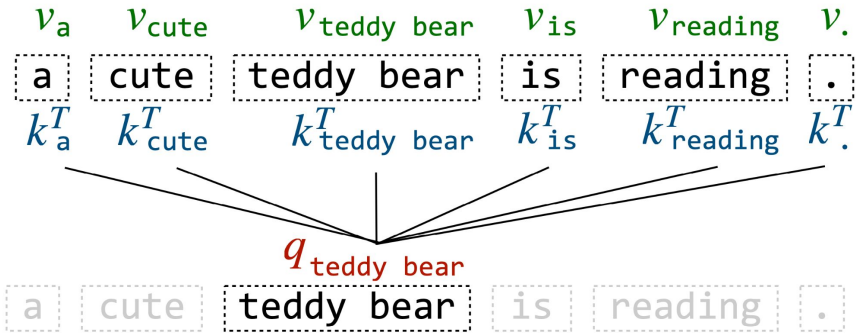
Similarity between positions

Benefits. Can extend to any sequence length

"Attention Is All You Need", Vaswani et al., 2017, "Transformer Architecture: The Positional Encoding", by Kazemnejad, 2019.

From absolute to relative position info

Motivation. Actually, we really care about relative position **with attention layer**



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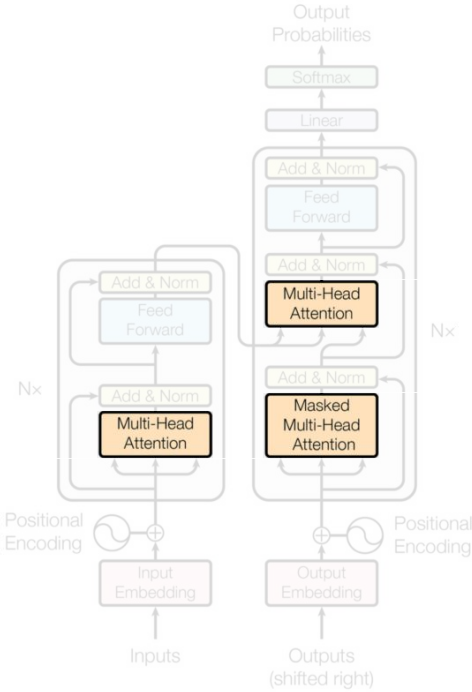
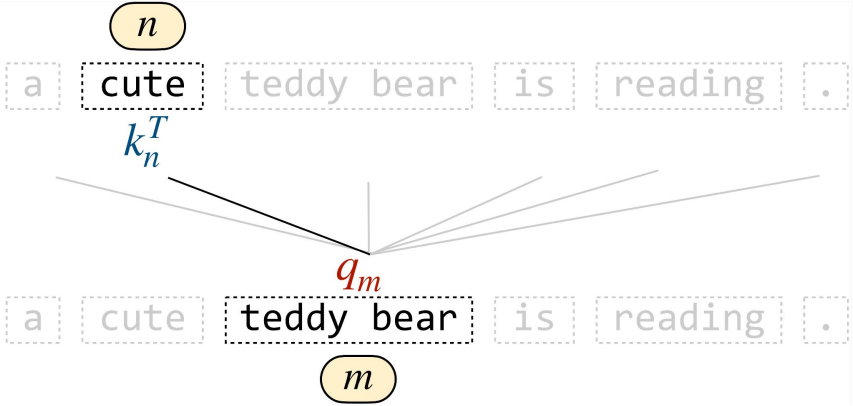


Idea. Let's change the attention layer instead

"*Attention Is All You Need*", Vaswani et al., 2017.

Linear bias in attention layer

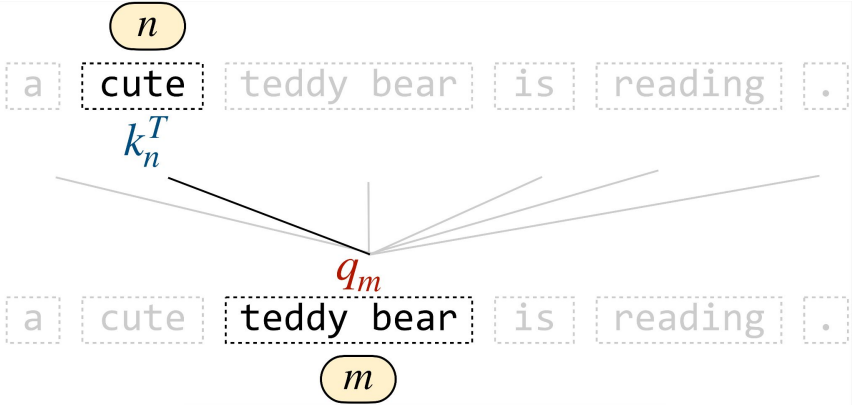
Idea. Add bias to query-key scores



$$\text{softmax}\left(\frac{\langle q_m, k_n \rangle}{\sqrt{d_k}} + \text{bias}(m, n)\right)$$

Linear bias in attention layer

Idea. Add bias to query-key scores



$$\text{softmax}\left(\frac{\langle q_m, k_n \rangle}{\sqrt{d_k}} + \text{bias}(m, n)\right)$$

T5 bias. Bias is **learned per head**

$$\text{bias}(m, n) = \beta_{\text{bucket}(m-n)}$$

"Super Study Guide: Transformers & Large Language Models", by Amidi, 2024.
"Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer", Raffel et al., 2023.

Linear bias in attention layer

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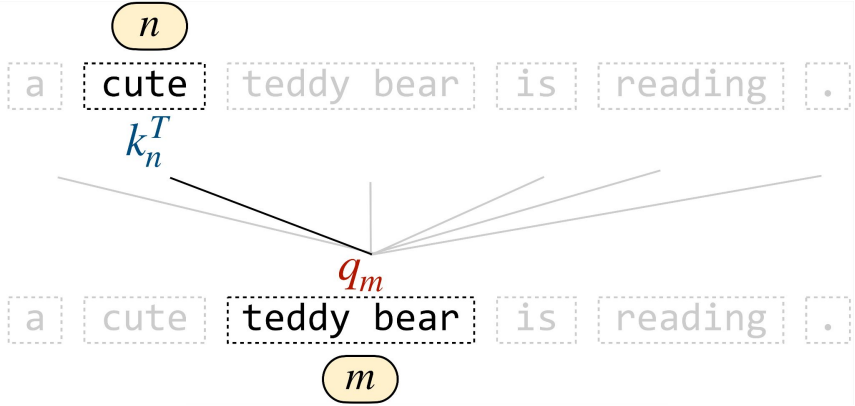

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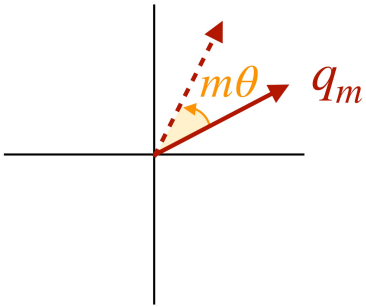
ALiBi. Bias is **linear**, **deterministic**, not bounded

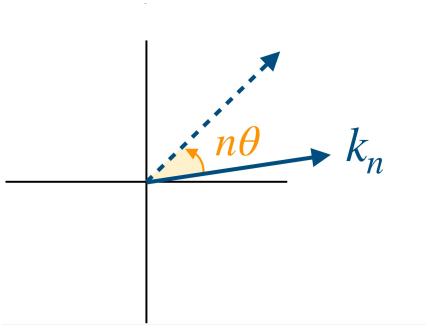
$$\text{bias}(m,n) = \mu \times (n-m)$$

"Super Study Guide: Transformers & Large Language Models", by Amidi, 2024.
"Train Short, Test Long: Attention with Linear Biases Enables Input Length Extrapolation", Press et al., 2021.

Default choice nowadays: rotations in attention layer

Idea. Rotate query and key vectors with rotation matrix





"RoFormer: Enhanced Transformer with Rotary Position Embeddings", Su et al., 2021.
Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Default choice nowadays: rotations in attention layer

Idea. Rotate query and key vectors with rotation matrix

Formula. Use rotation matrix: $R_{\theta,m} = \begin{pmatrix} \cos(m\theta) & -\sin(m\theta) \\ \sin(m\theta) & \cos(m\theta) \end{pmatrix}$

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Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Default choice nowadays: rotations in attention layer

RoPE = **Ro**tary **P**osition **E**mbeddings

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Extension to dimension d > 2. Rotate every block of dimension 2

$$R_{\theta,m} = \begin{pmatrix} \text{block}_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \text{block}_{\frac{d_k}{2}} \end{pmatrix} \qquad \text{block}_i = \begin{pmatrix} \cos(m\theta_i) & -\sin(m\theta_i) \\ \sin(m\theta_i) & \cos(m\theta_i) \end{pmatrix}$$

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Benefits. Relative distance nicely captured:

$$q_m k_n^T = x_m W_q R_{\theta,n-m} W_k^T x_n^T$$

Default choice nowadays: rotations in attention layer

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Attention weight has a long-term decay

Relative upper bound of $A(q_m k_n^T)$

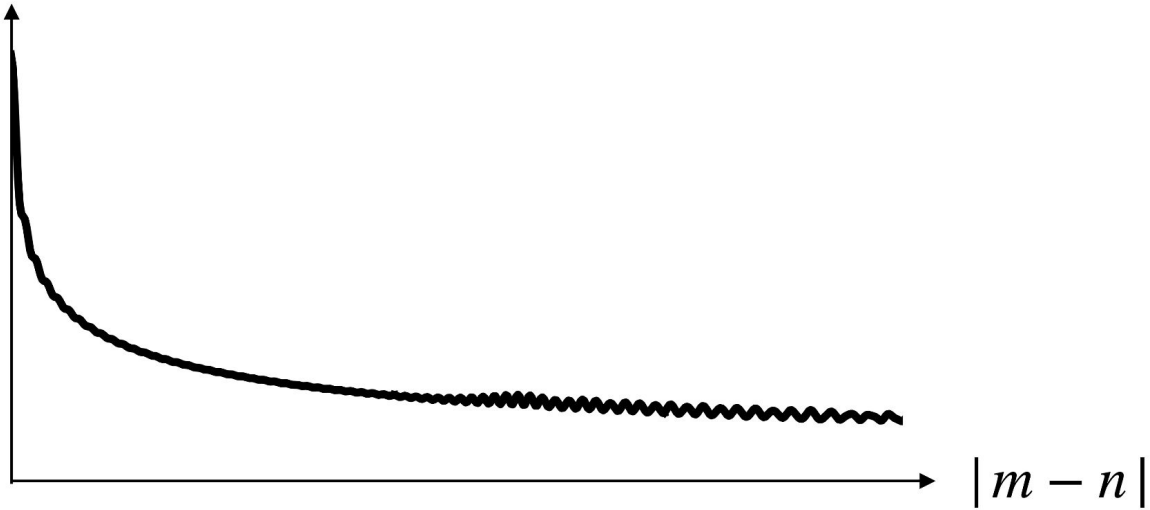


 Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Transformers & Large Language Models

Position embeddings

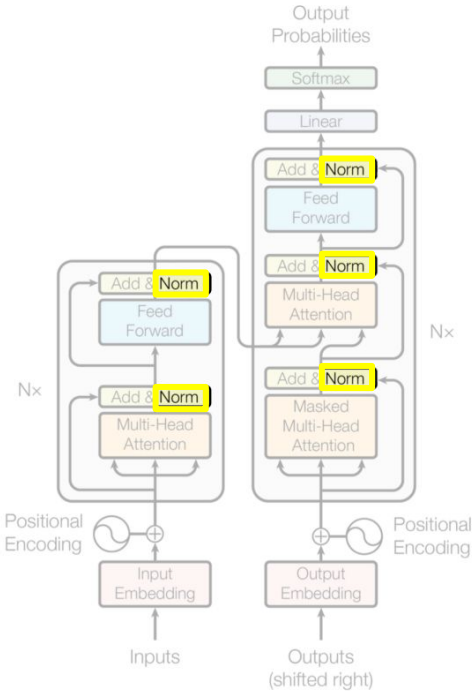
Layer normalization

Attention approximation

Transformer-based models

BERT deep dive

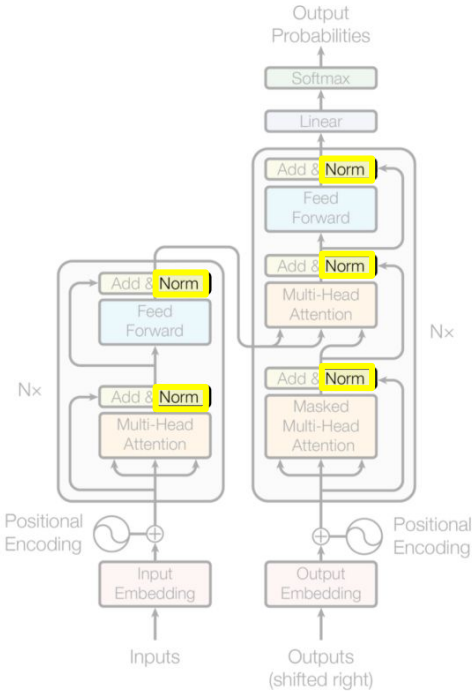
Layer normalization



"*Attention Is All You Need*", *Vaswani et al., 2017.*

Layer normalization

LN = **L**ayer **N**ormalization



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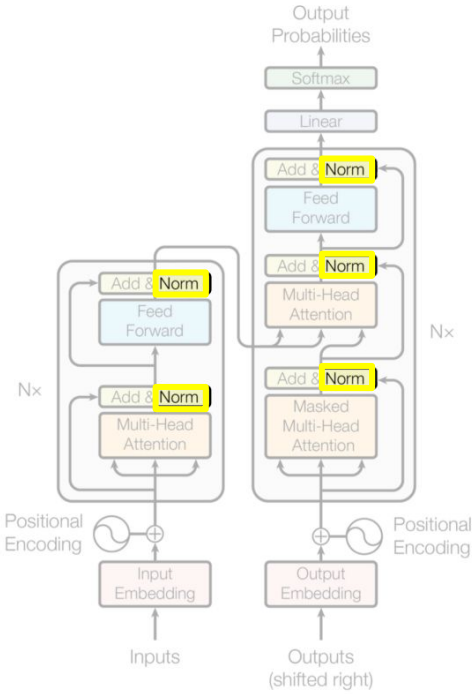

$$\boxed{\mathrm{LN}(x) = \gamma\hat{x} + \beta} \quad \text{with} \quad \hat{x} = \frac{x - \mu}{\sqrt{\sigma^2 + \epsilon}}$$

where $\mu = \frac{1}{d}\sum_{i=1}^{d} x_i$ and $\sigma^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \mu)^2$

"*Attention Is All You Need*", Vaswani et al., 2017.

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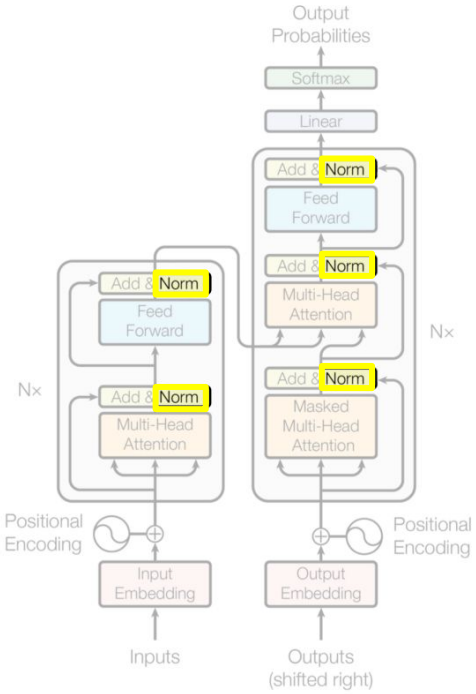

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where $\mu = \frac{1}{d}\sum_{i=1}^{d} x_i$ and $\sigma^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \mu)^2$

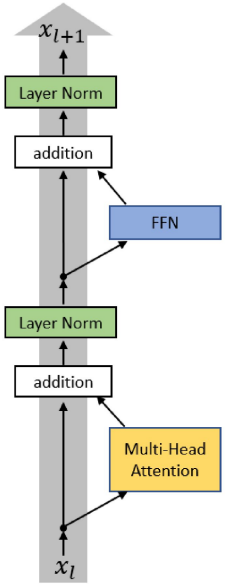
Benefits. Helps with training stability and convergence.

"Attention Is All You Need", Vaswani et al., 2017. "Layer Normalization", Ba et al., 2016.

Different kinds of layer normalization

Post-Norm

$$\text{Output} = \text{LayerNorm}(x + \text{SubLayer}(x))$$



After

residual connection

"On Layer Normalization in the Transformer Architecture", Xiong et al., 2020.

Different kinds of layer normalization

Post-Norm

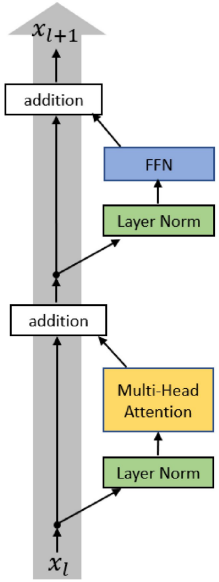
$$\text{Output} = \text{LayerNorm}(x + \text{SubLayer}(x))$$

After

residual connection

Pre-Norm

$$\text{Output} = x + \text{SubLayer}(\text{LayerNorm}(x))$$



Before

residual connection

"On Layer Normalization in the Transformer Architecture", Xiong et al., 2020.

Different kinds of layer normalization

Nowadays:

Pre-Norm

"On Layer Normalization in the Transformer Architecture", Xiong et al., 2020.

Different kinds of layer normalization

Nowadays:

Pre-Norm +

normalize to bring values in a range so that values are not too far off.

Text

RMSNorm

$$\gamma\hat{x} + \beta \longrightarrow \gamma \frac{x}{\text{RMS}(x)}$$

"On Layer Normalization in the Transformer Architecture", Xiong et al., 2020. "Root Mean Square Layer Normalization", Zhang et al., 2019.

Transformers & Large Language Models

Position embeddings

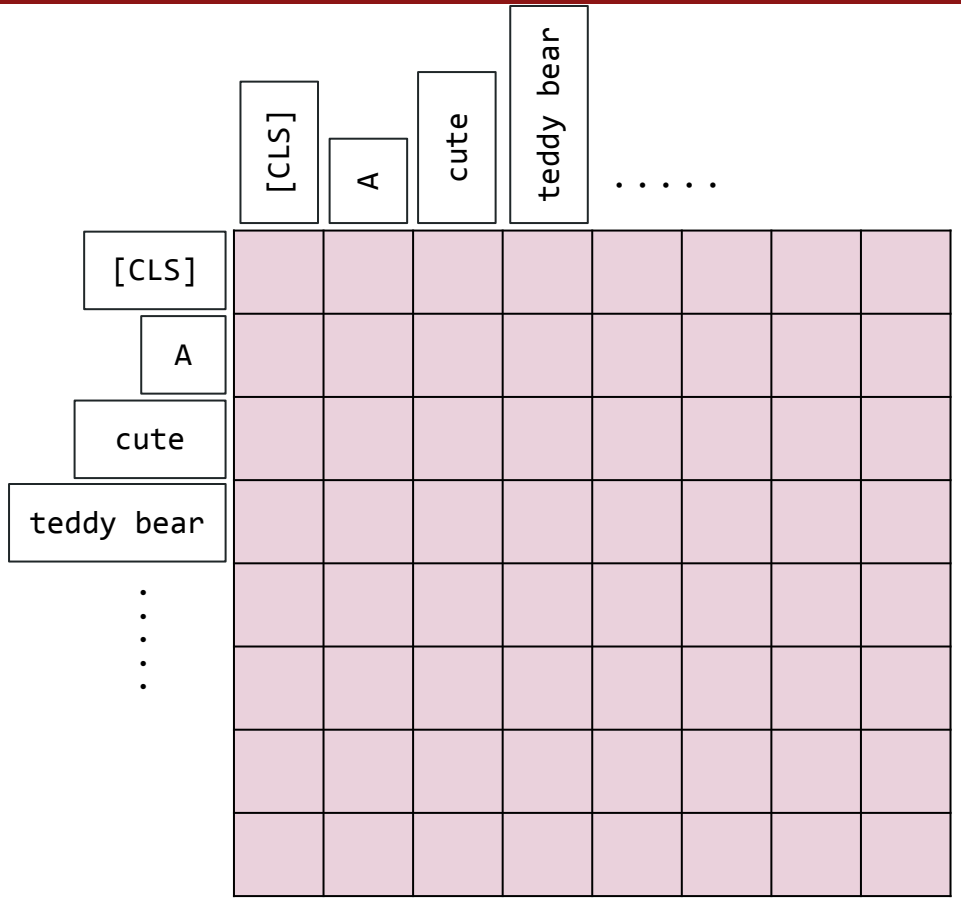
Layer normalization

Attention approximation

Transformer-based models

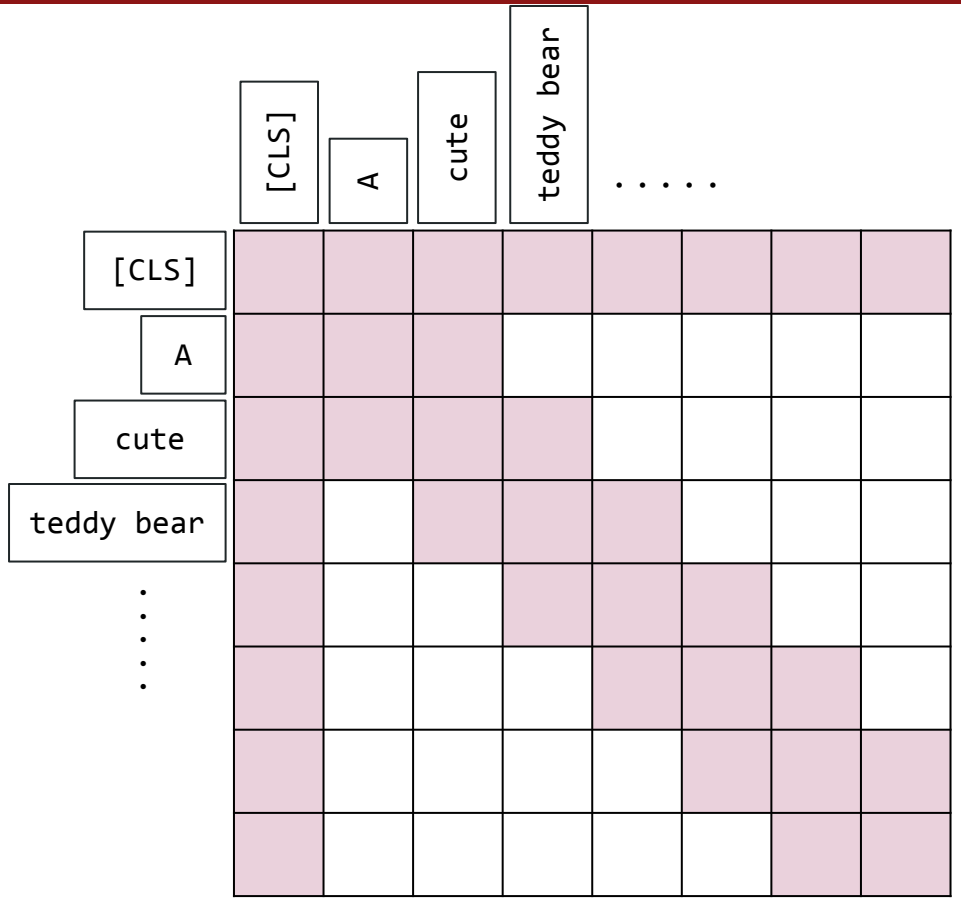
BERT deep dive

Sparse attention: Longformer



"Longformer: The Long-document Transformer", Beltagy et al., 2020.

Sparse attention: Longformer



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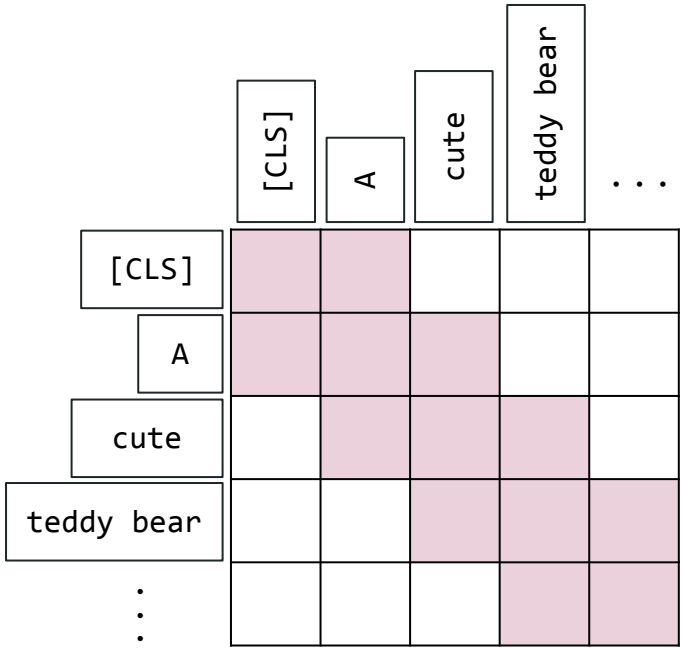
Leveraging local and global attention

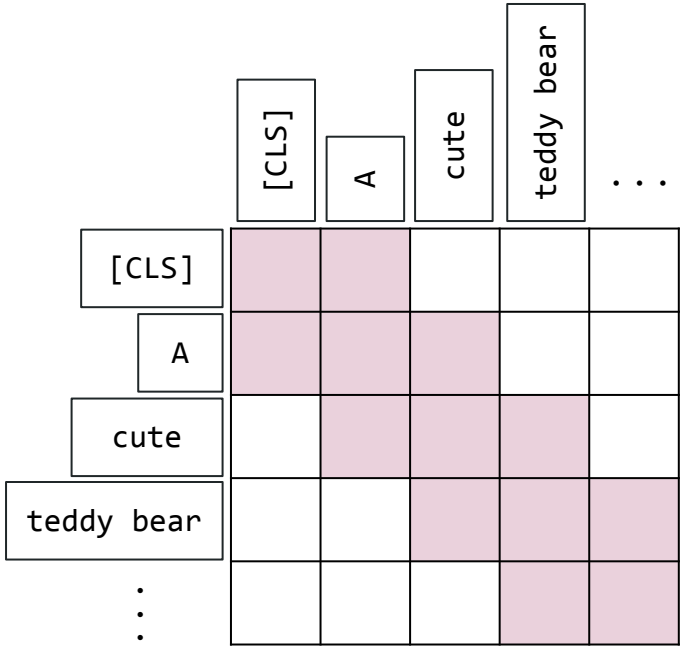
SWA = **S**liding **W**indow **A**ttention

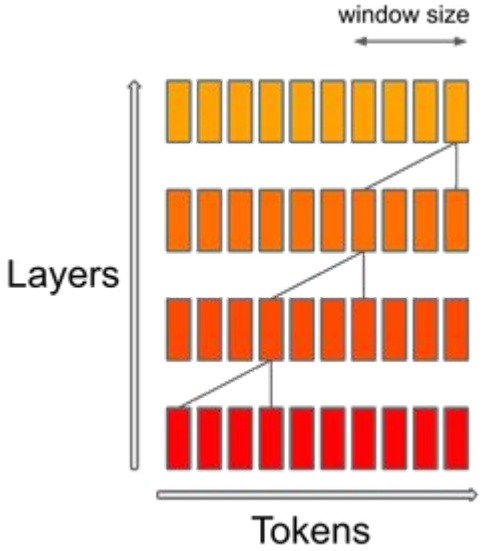


Variations include **interleaving local** and **global attention layers**

Leveraging local and global attention

SWA = **S**liding **W**indow **A**ttention



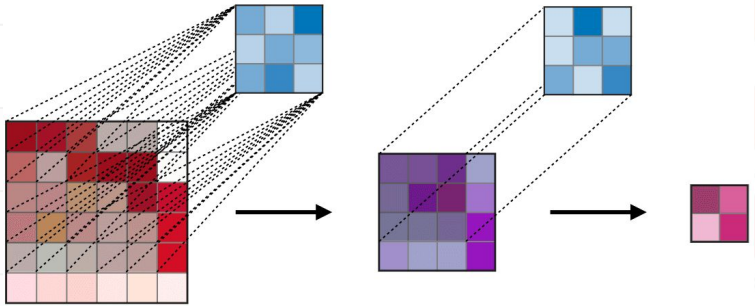


Mistral 7B

Right figure from Mistral 7B announcement, 2023.

Leveraging local and global attention

Similar to "**receptive field**" in computer vision



"*VIP Cheatsheet: Convolutional Neural Networks*", *Amidi, 2018.*

Sharing attention heads

Idea. Share key/value attention heads within groups of queries

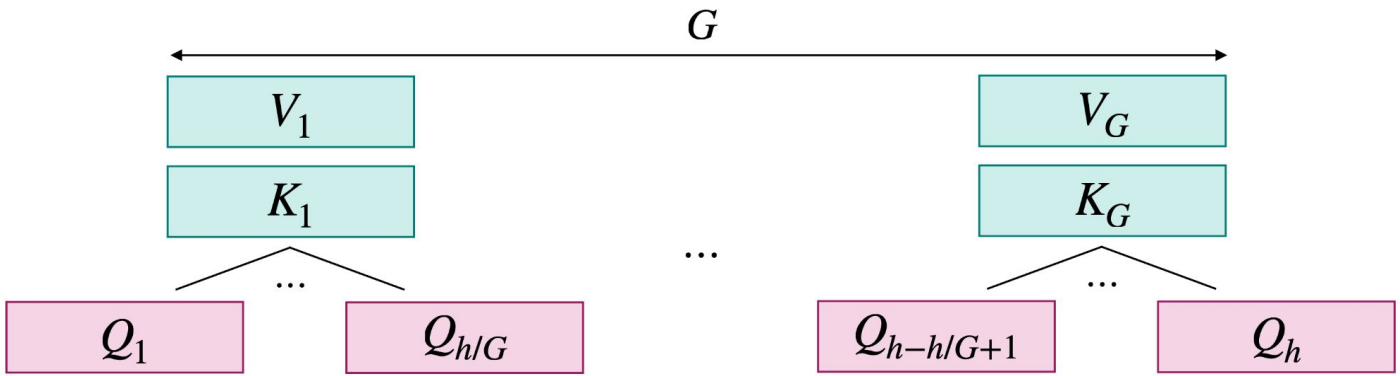


Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Sharing attention heads

$G = 1$

Multi-**Q**uery **A**ttention (MQA)

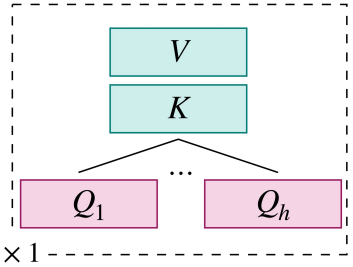


Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Sharing attention heads

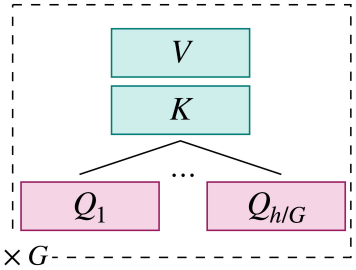
$G = 1$	**M**ulti-**Q**uery **A**ttention (MQA)	
$1 < G < h$	**G**roup-**Q**uery **A**ttention (GQA)	

Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Sharing attention heads

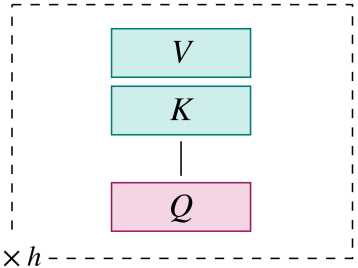
$G = 1$	**M**ulti-**Q**uery **A**ttention (MQA)	
$1 < G < h$	**G**roup-**Q**uery **A**ttention (GQA)	
$G = h$	**M**ulti-**H**ead **A**ttention (MHA)	

Figure from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Transformers & Large Language Models

Attention approximation

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Transformer-based models

BERT deep dive

Overview of Transformer-based models

3 categories of Transformer-based models:

T5 task - span corruption task. fill in the missing parts in sentence denoted by sentinel tokens

Encoder-decoder	Text to text	T5, mT5, ByT5

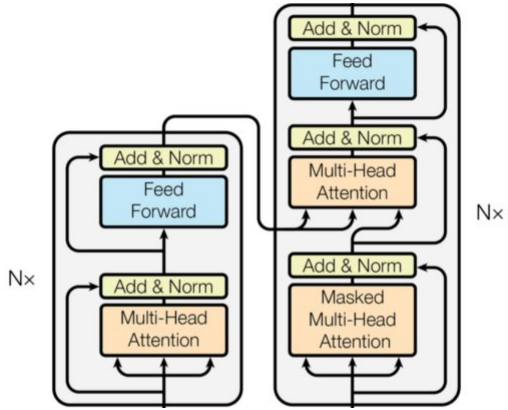

Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

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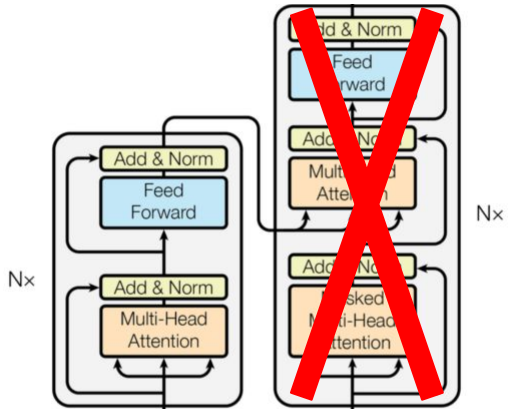
Encoder-only	Projection of embedding for class prediction (e.g. sentiment extraction)	BERT, DistilBERT, RoBERTa



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Decoder-only	Text to text	GPT series next word prediction

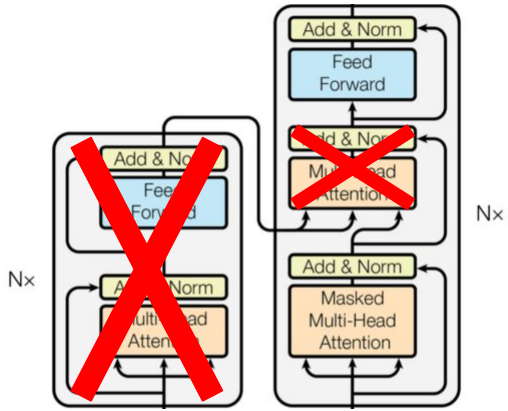

Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

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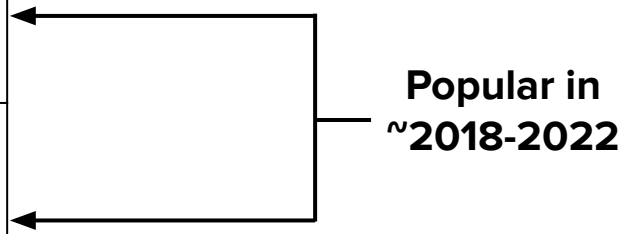

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Popular now!

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BERT deep dive

Why "BERT"?

BERT = **B**idirectional **E**ncoder **R**epresentations from **T**ransformers

"*BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding*", *Devlin et al., 2018.*

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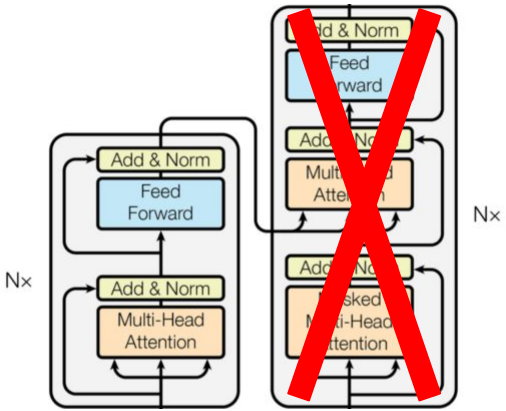

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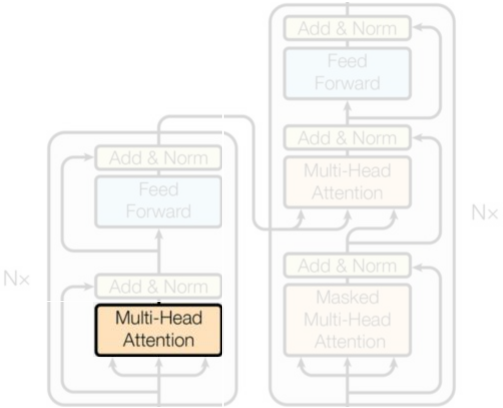
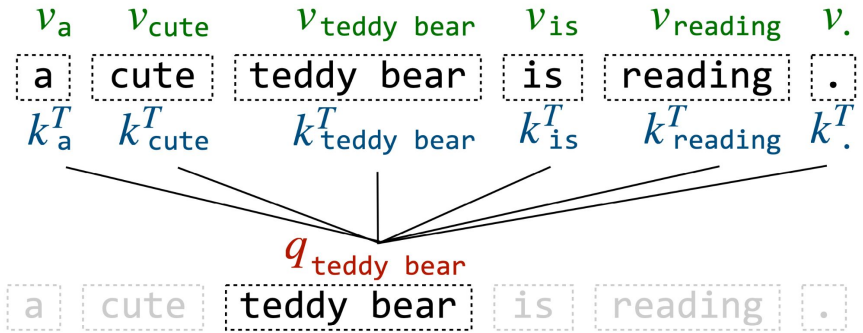


Bidirectional



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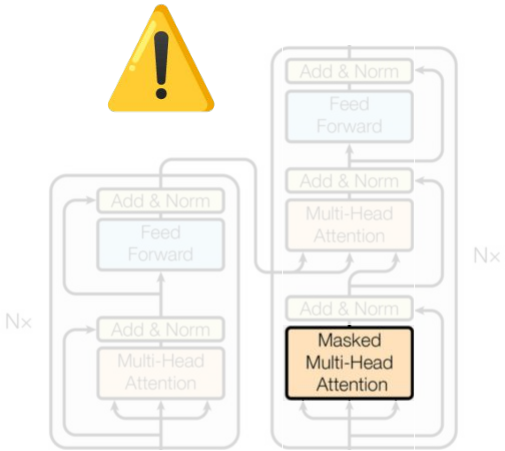
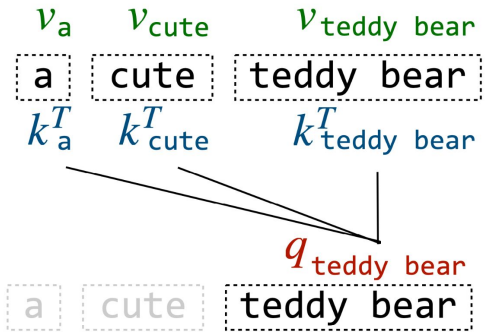
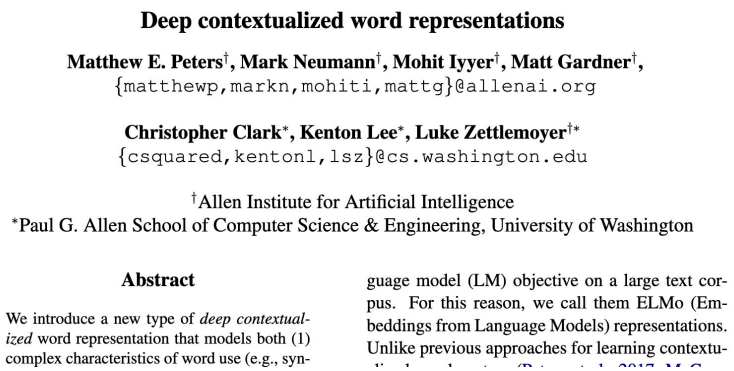




decoder only is **Not** bidirectional

Figure adapted from "Attention is All You Need", Vaswani et al., 2017.

Why "BERT"?



Deep contextualized word representations

Matthew E. Peters[†], **Mark Neumann**[†], **Mohit Iyyer**[†], **Matt Gardner**[†],
{matthewp,markn,mohiti,mattg}@allenai.org

Christopher Clark[*], **Kenton Lee**[*], **Luke Zettlemoyer**[†*]
{csquared,kentonl,lsz}@cs.washington.edu

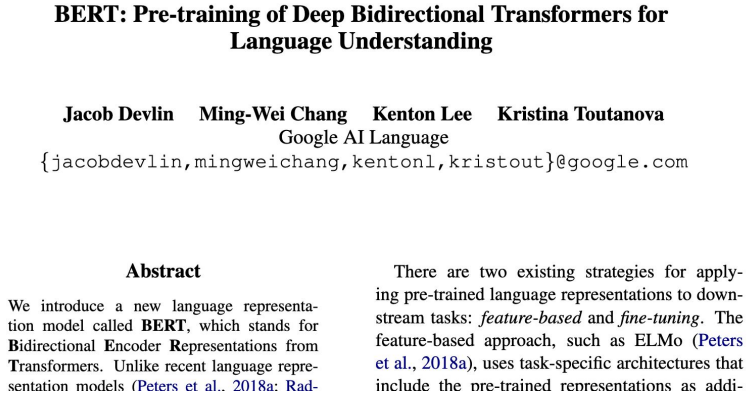
[†]Allen Institute for Artificial Intelligence
[*]Paul G. Allen School of Computer Science & Engineering, University of Washington

Abstract

We introduce a new type of *deep contextualized* word representation that models both (1) complex characteristics of word use (e.g., syn-

guage model (LM) objective on a large text corpus. For this reason, we call them ELMo (Embeddings from Language Models) representations. Unlike previous approaches for learning contextu-

ELMo paper
[submitted in Feb 2018]



BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

Jacob Devlin **Ming-Wei Chang** **Kenton Lee** **Kristina Toutanova**
Google AI Language
{jacobdevlin,mingweichang,kentonl,kristout}@google.com

Abstract

We introduce a new language representation model called **BERT**, which stands for **B**idirectional **E**ncoder **R**epresentations from **T**ransformers. Unlike recent language repre-sentation models (Peters et al., 2018a; Rad-

There are two existing strategies for applying pre-trained language representations to downstream tasks: *feature-based* and *fine-tuning*. The feature-based approach, such as ELMo (Peters et al., 2018a), uses task-specific architectures that include the pre-trained representations as addi-

BERT paper
[submitted in Oct 2018]

Why "BERT"?

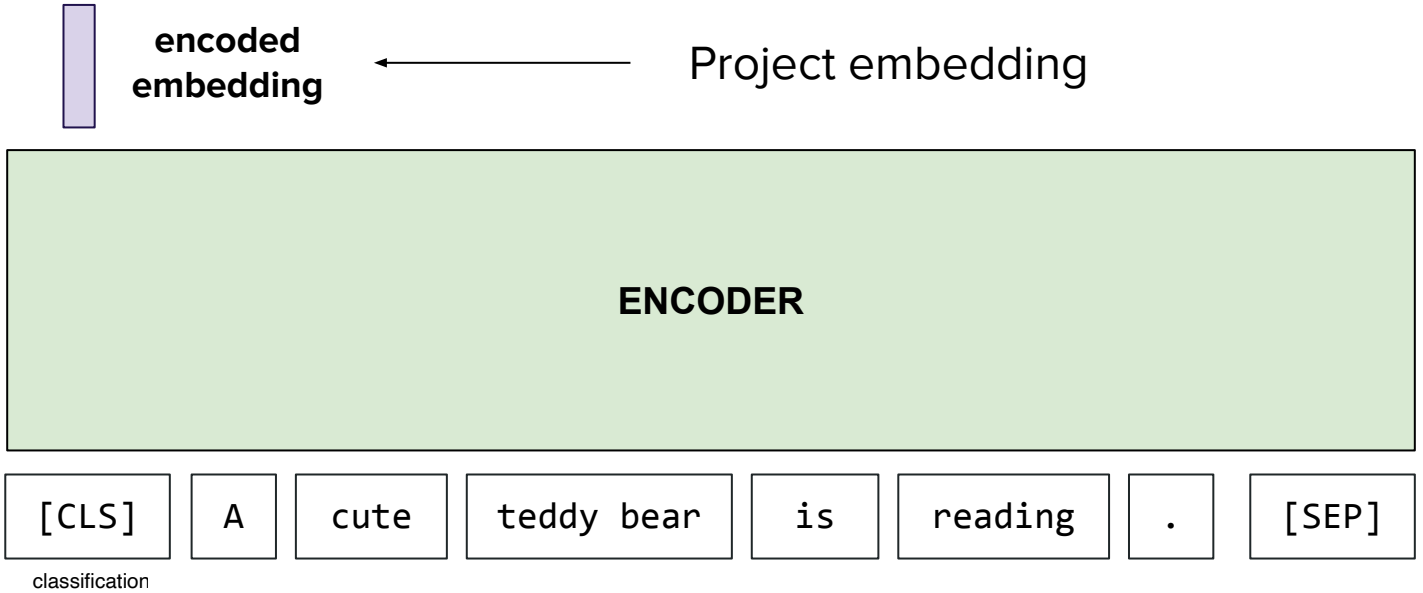
Elmo

Bert

For more background: Sesame Street, Wikipedia.

BERT and encoder-only models

Idea. Keep only **encoders** + leverage **encoded embeddings** to make predictions.



"BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", Devlin et al., 2018.

BERT and encoder-only models

Strategy.

masked language model ->learn internal structure of inputs

next sentence prediction -; if the ordering of sentences makes sence

- **Step 1**: Pretraining with proxy tasks (MLM and NSP)
- **Step 2**: Finetuning for given end task

BERT and encoder-only models

Strategy.

- **Step 1**: Pretraining with proxy tasks (MLM and NSP)
- **Step 2**: Finetuning for given end task

Discussion.

Pros	Cons
• Finetuning does not need a lot of data • Good performance	• Not suited for a range of tasks (e.g. text generation) • Finetuning is a required step

BERT and encoder-only models

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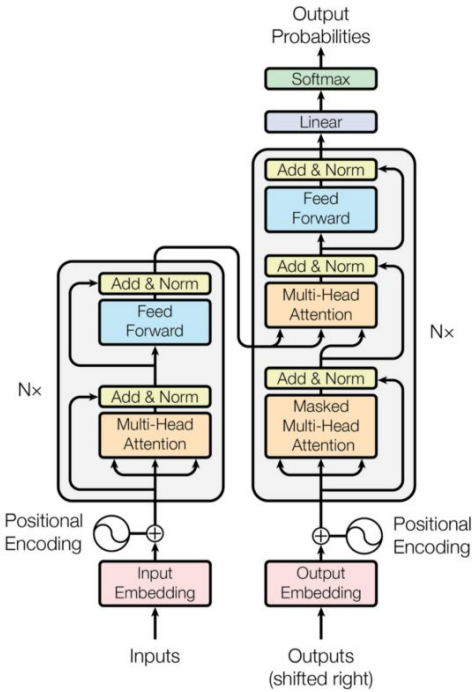
Pros	Cons
• Finetuning does not need a lot of data • Good performance	• Not suited for a range of tasks (e.g. text generation) • Finetuning is a required step

Variants. RoBERTa, DistilBERT, ALBERT

BERT architecture

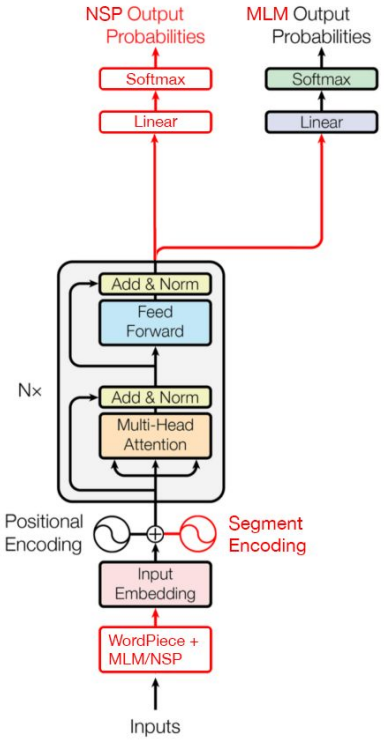


Original transformer (2017)

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

BERT architecture

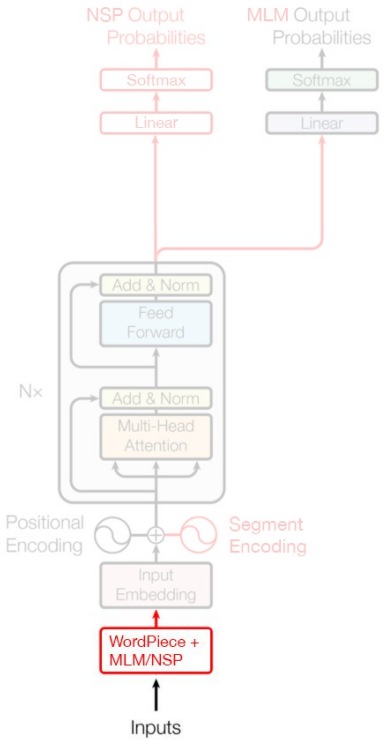
Original transformer (2017)



BERT (2018)

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Input processing



WordPiece algorithm

learns on training set based on merge rules that maximizes the likelihood
merges atomic tokens together to build target vocabulary

- Tokenizer trained on a training set beforehand
- Vocabulary size: ~30,000
- Great at detecting common particles

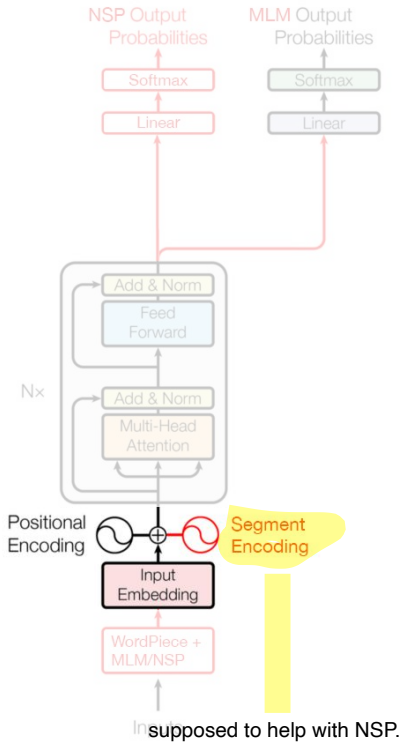
NSP / MLM task processing

- Add `[CLS]` token at the beginning of the input
- Separate consecutive segments with the `[SEP]` token and put another one at the end for NSP
- Use `[MASK]` to mask inputs

MLM task. mask some tokens

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Input embedding



supposed to help with NSP. to represent what could be the features that can helpfully represent a sentence that precedes another one

Input embeddings

- Gigantic lookup table
- Learns an embedding for each word of the vocabulary

Positional encoding

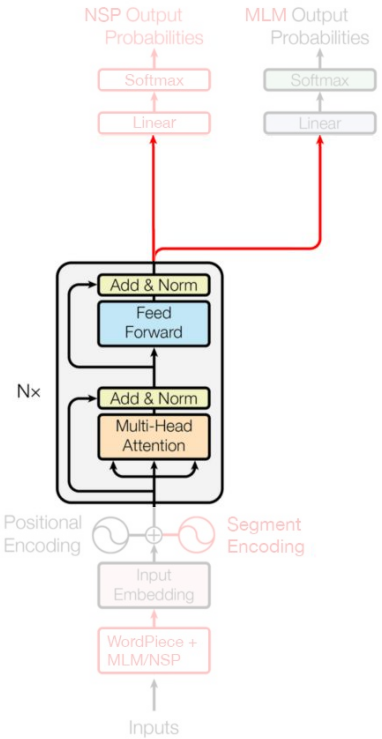
- Helps the network associate tokens with a position
- Encoding either learnt or fixed with cosines and sines

(new!) Segment encoding

- Shared embedding for a segment

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Encoder-only model



Model

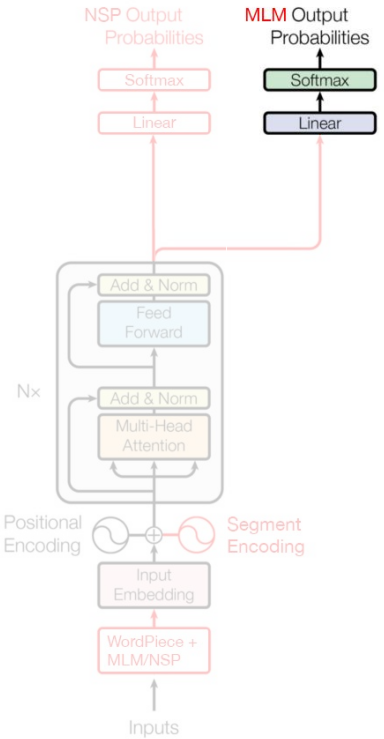
Encoder part of the original transformers paper

Goal

- Represent input data with features (hopefully) needed for NLP tasks
- Leverage the Transformer's self-attention mechanism
- Use learned embedding towards classification-oriented tasks

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Proxy task: Masked Language Modeling



Idea. 15% of input tokens are set up for prediction where:

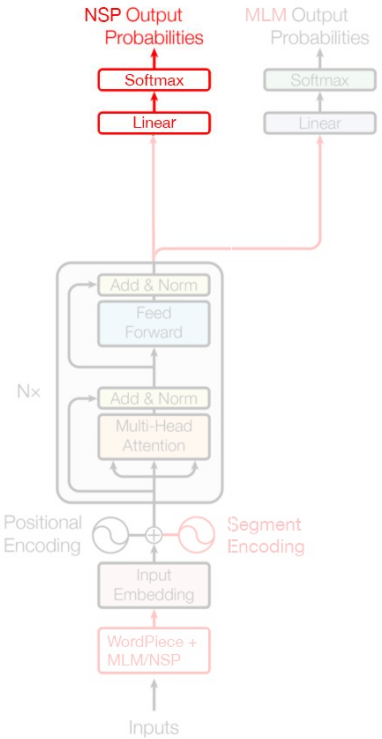
- 80% are masked
- 10% are changed to a random word
- 10% are unchanged

Benefits

- Network learns language modeling based on contextual information
- Regularization reflects probabilistic nature of language

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Proxy task: Next Sentence Prediction



Idea. Pick two sentences from the corpus, where:

- 50% of the time, they follow each other
- 50% of the time, they **do not** follow each other

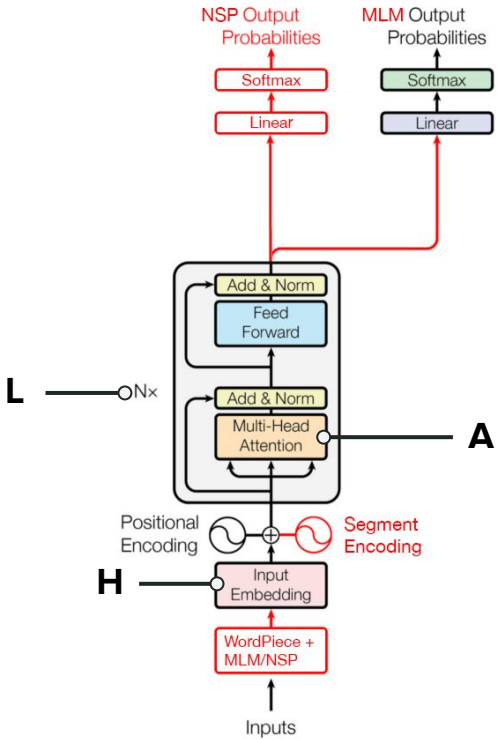
Task. Predict if they actually follow each other.

Benefits

- Network implicitly learns to detect useful contextual information
- Easy classification task that does not require any labels

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Hyperparameters



Model.

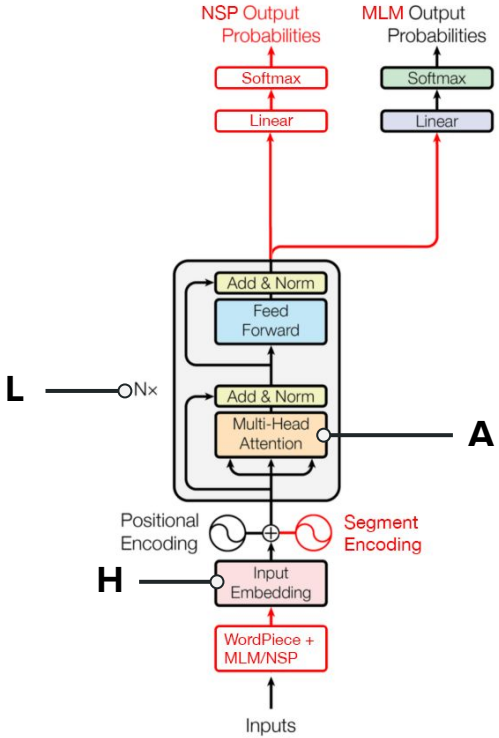
- **L** Layers.
- **H** Hidden layer size aka dimension of embeddings.
- **A** Attention heads operating in parallel.

Data.

- Language-specific / multilingual. Languages on which the model has been trained on.
- Cased / uncased. Whether inputs are converted to lowercase or not.

Figure adapted from "Attention Is All You Need", Vaswani et al., 2017.

Some numbers



	L	H	A	Parameters
BERT-Tiny	2	128	2	4M
BERT-Mini	4	256	4	11M
BERT-Small	4	512	8	30M
BERT-Medium	8	512	8	42M
BERT-Base	12	768	12	110M
BERT-Large	24	1024	16	340M

Left figure adapted from "Attention Is All You Need", Vaswani et al., 2017. Parameters in the right table were computed in this paper.

Overview of BERT finetuning

Goal. Leverage embeddings learned by BERT for a “sister” task

Overview of BERT finetuning

Goal. Leverage embeddings learned by BERT for a “sister” task

Tricks

- Use weights from **already massively pretrained** model
- **Freezing** early layers: sometimes better trade-off complexity/performance
- Great results possible with **minimal labeled data** (depending on complexity/proximity to pretrained data distribution + objectives)

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Use cases

- Sequence classification: e.g. sentiment extraction
- Token classification: e.g. question answering

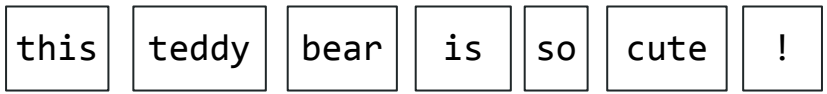
Finetuning: sentiment extraction

```
This teddy bear is SO CUTE!
```

Finetuning: sentiment extraction

this teddy bear is so cute!

Finetuning: sentiment extraction



Finetuning: sentiment extraction

Add [CLS] token as a placeholder for sentiment.

Finetuning: sentiment extraction

Finetuning: sentiment extraction

embedding

[CLS]	this	teddy	bear	is	so	cute	!	[SEP]	[PAD]	[PAD]	[PAD]	[PAD]	[PAD]	[PAD]

Finetuning: sentiment extraction

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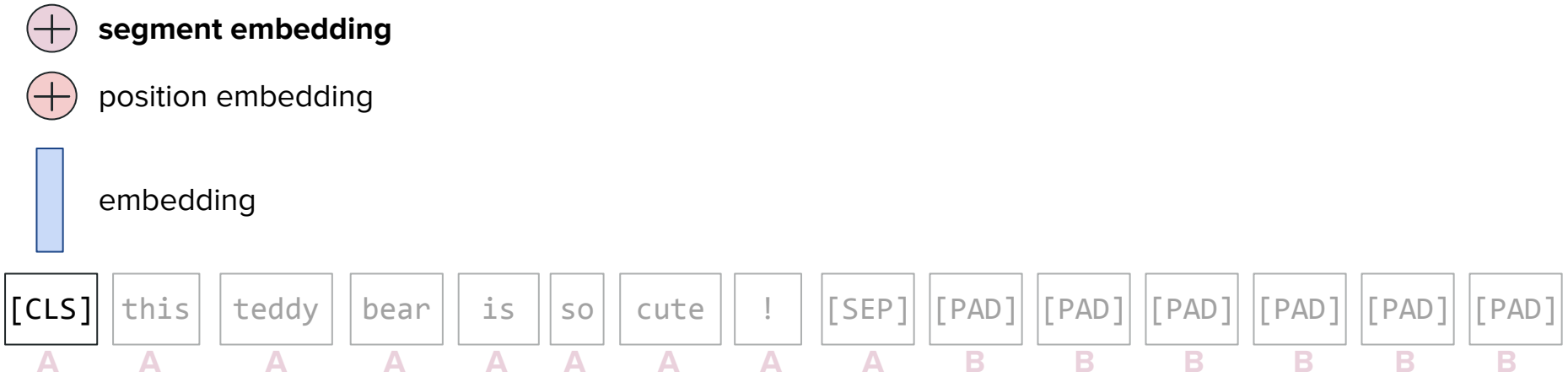
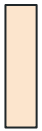


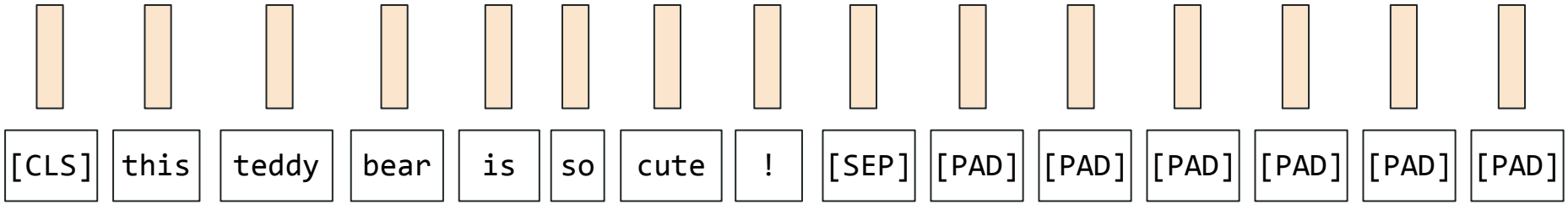
Finetuning: sentiment extraction



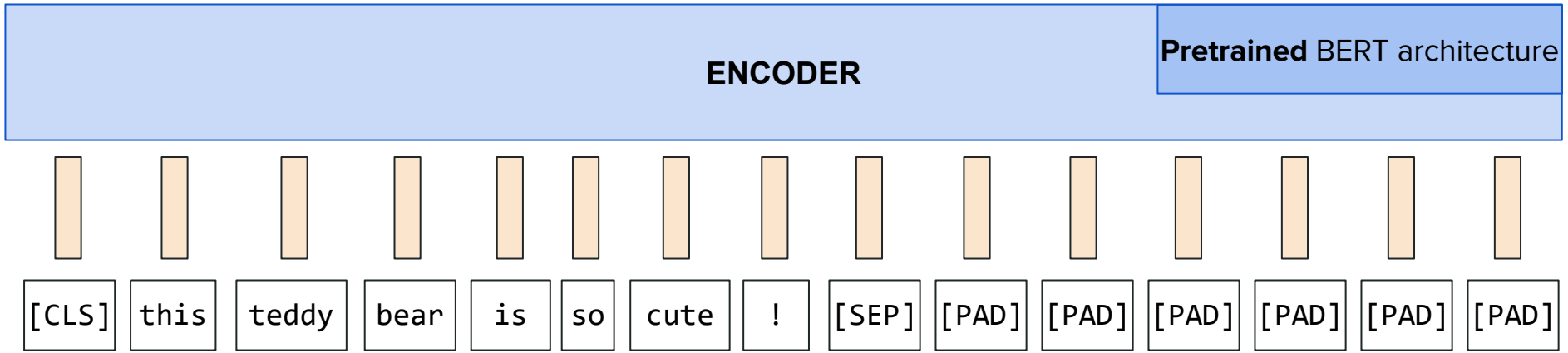
position- and segment-aware embedding

[CLS]	this	teddy	bear	is	so	cute	!	[SEP]	[PAD]	[PAD]	[PAD]	[PAD]	[PAD]	[PAD]

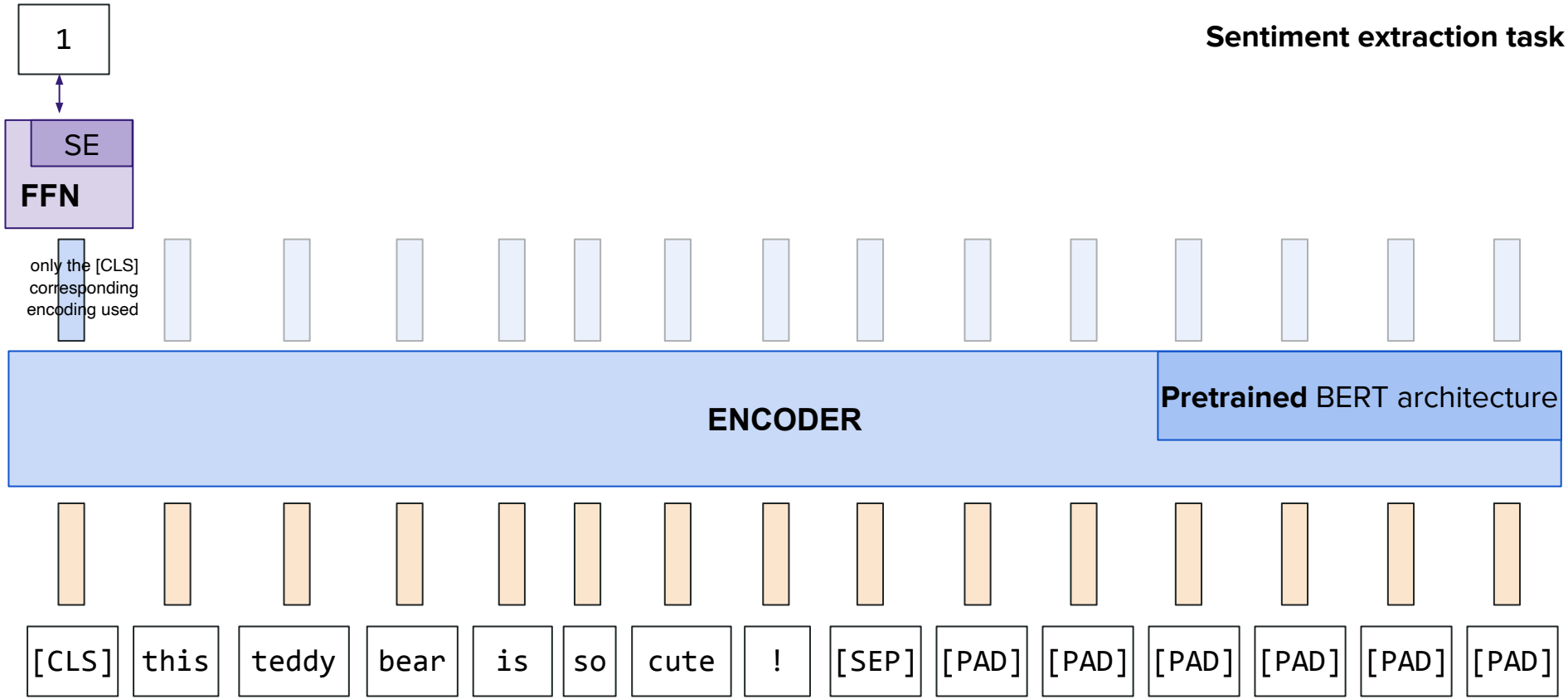
Finetuning: sentiment extraction



Finetuning: sentiment extraction



Finetuning: sentiment extraction



Takeaways and shortcomings

Benefits.

- State of the art results
- ~True contextual representation of words
- Adaptable to many classification tasks

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Applications. Widely used in the industry for anything related to encoding

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Limitations.

- Context window size is limited
- Computationally expensive: hard sell for low-latency/cost-sensitive applications
- Training paradigm is complex: MLM/NSP + finetuning

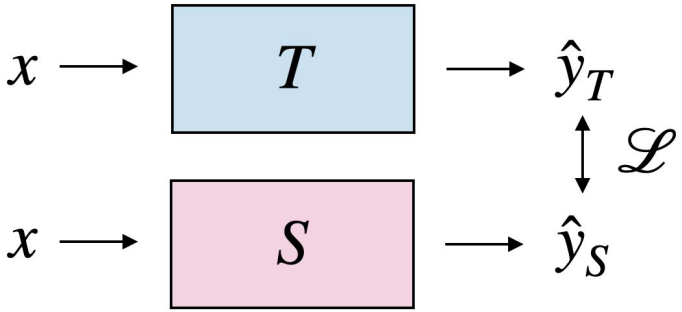
Trick: distillation

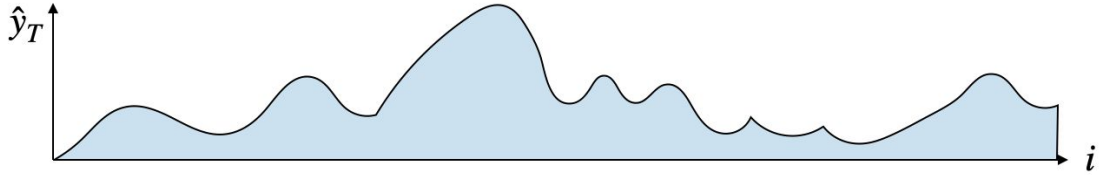
"The **soft targets** contain almost all the **knowledge**."

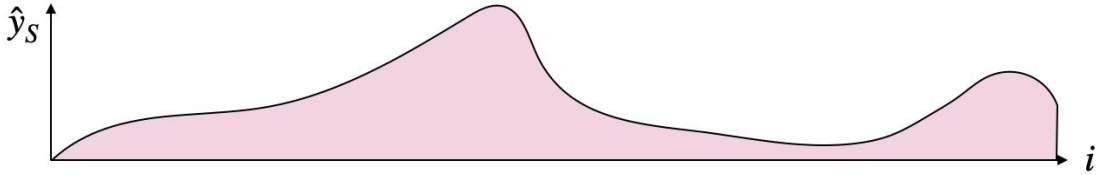
distribution output by. given model is super helpful to know what it has learned.
learning distribution is more helpful than learning the hard labels

"Dark knowledge", Hinton et al., 2014.

Trick: distillation

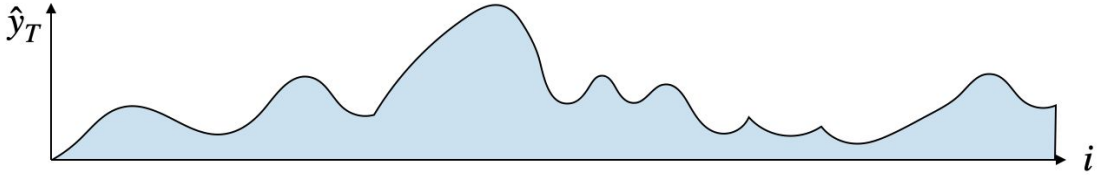




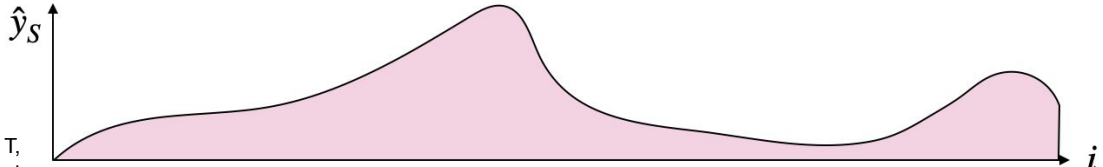


Figures from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Trick: distillation



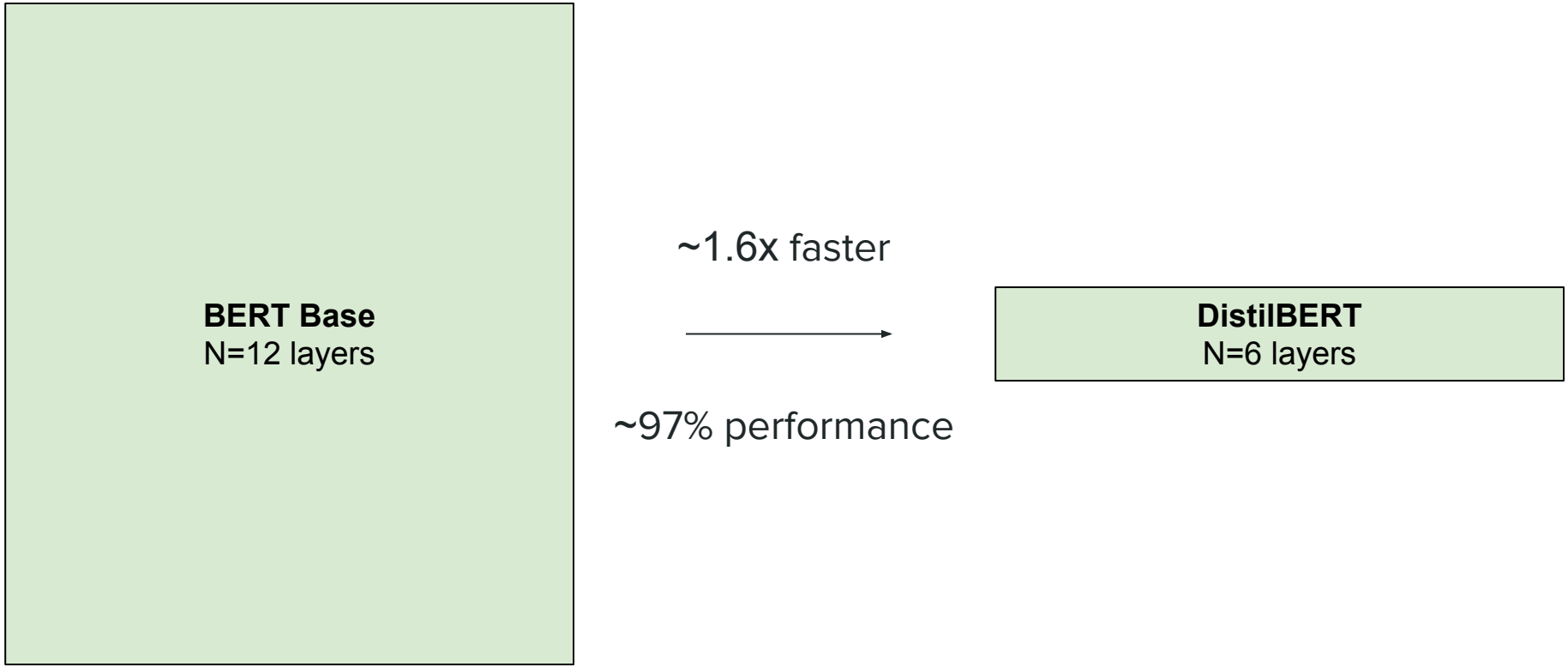
$$\mathrm{KL}(\widehat{y}_T||\widehat{y}_S) = \sum_i \widehat{y}_T^{(i)} \log\left(\frac{\widehat{y}_T^{(i)}}{\widehat{y}_S^{(i)}}\right)$$



in a world described by the teacher T,
how bad is it to model with the student
tries to ascess how close the students' distribution is going
to be to the world of T

Figures from "Super Study Guide: Transformers & Large Language Models", Amidi et al., 2024.

Variant for efficiency: DistilBERT



"DistilBERT, a distilled version of BERT: smaller, faster, cheaper and lighter", Sanh et al., 2019.

Variant for performance: RoBERTa

Goal. Thorough analysis of directions of optimization

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Goal. Thorough analysis of directions of optimization

Modeling

- Removing NSP/segment encodings: ~no effect!*
- Static ➜ dynamic masking across epochs

*DistilBERT had also removed it

Variant for performance: RoBERTa

Goal. Thorough analysis of directions of optimization

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Data

- Richer: 16 GB → 160 GB of pretraining corpus size
- For longer: 1M steps of batch size 256 vs. 500k of batch size 8k

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Result. +4% across benchmarks with same architecture

Thank you for your attention!