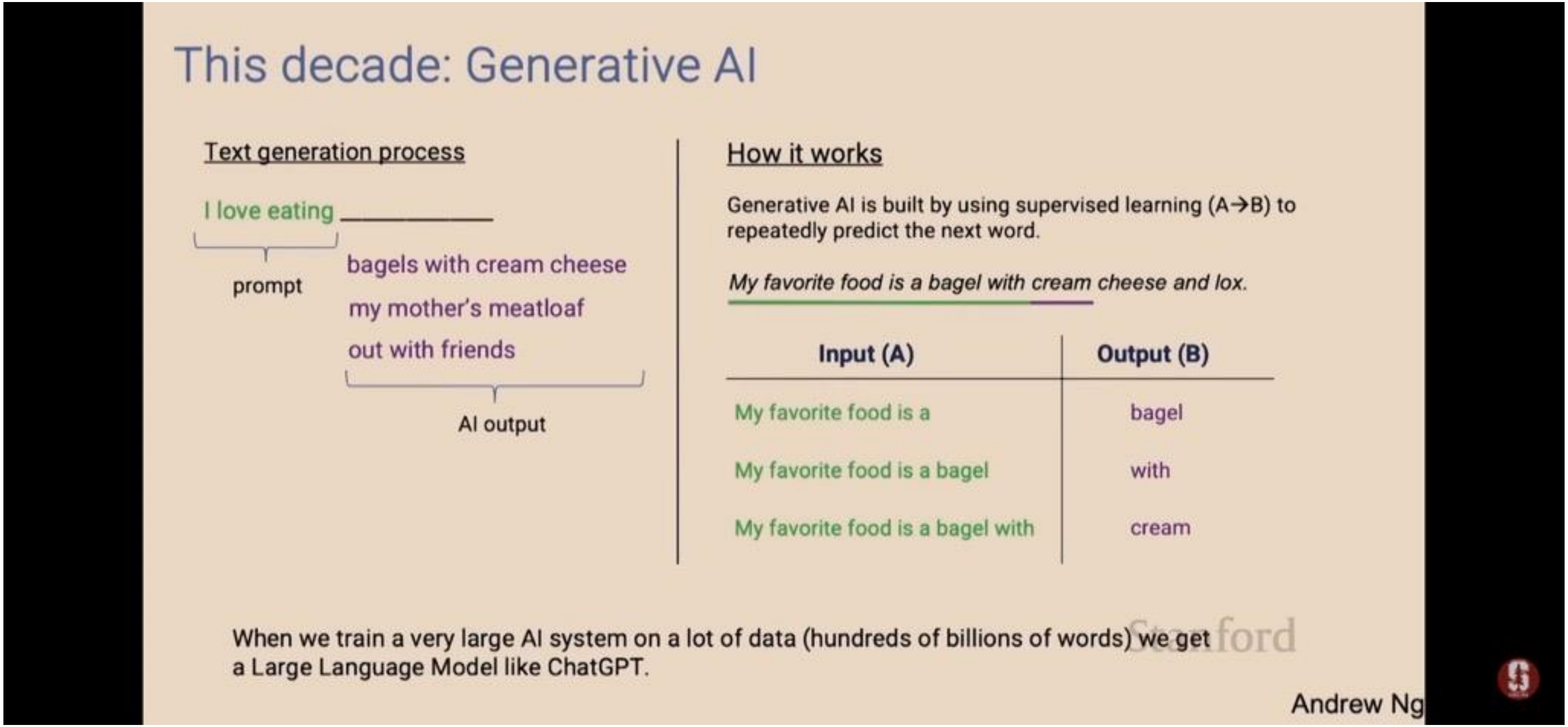
Transformer

Language Models



ML needs lots of training data

Unsupervised Learning

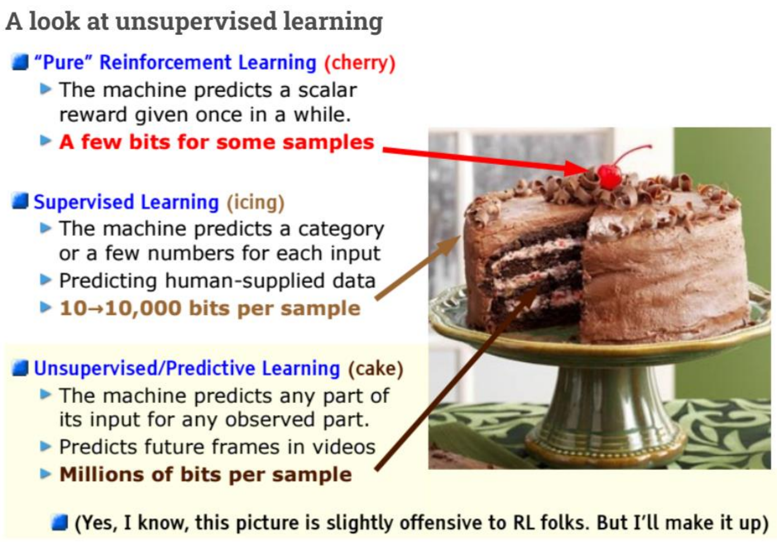
learning by observation

no target information → kind of "vague" pattern recognition (but plenty of data)

can be cast as **self-supervised learning**:

- input-output mapping like supervised learning
- but generating labels itself from input information

generative AI as unsupervised learning: generate variations of training data



Original LeCun cake analogy slide presented at NIPS 2016, the highlighted area has now been updated.

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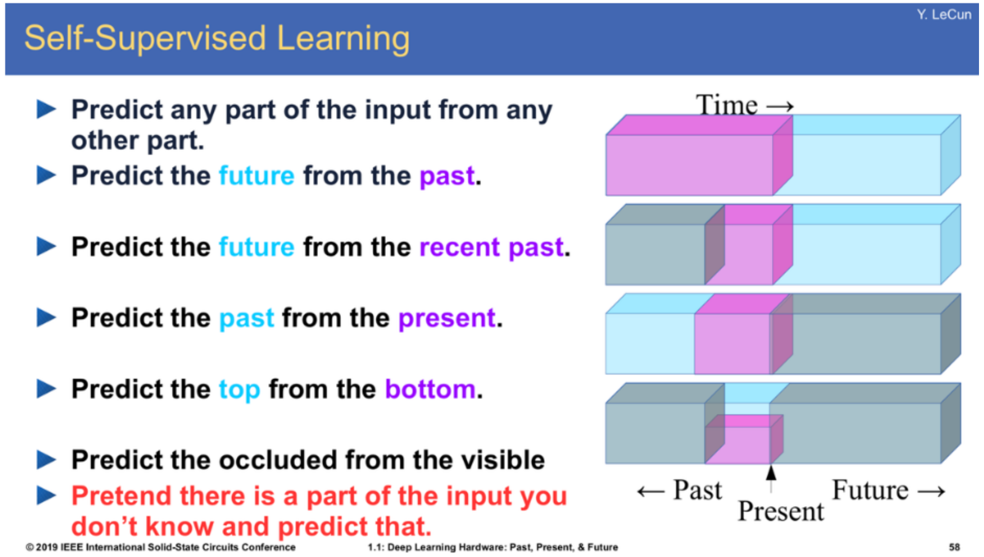


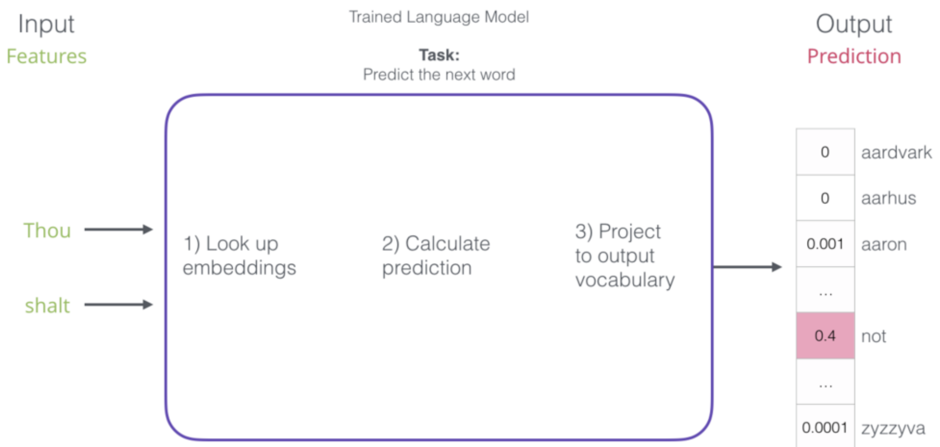
LeCun's self-supervised learning slide at ISSCC 2019

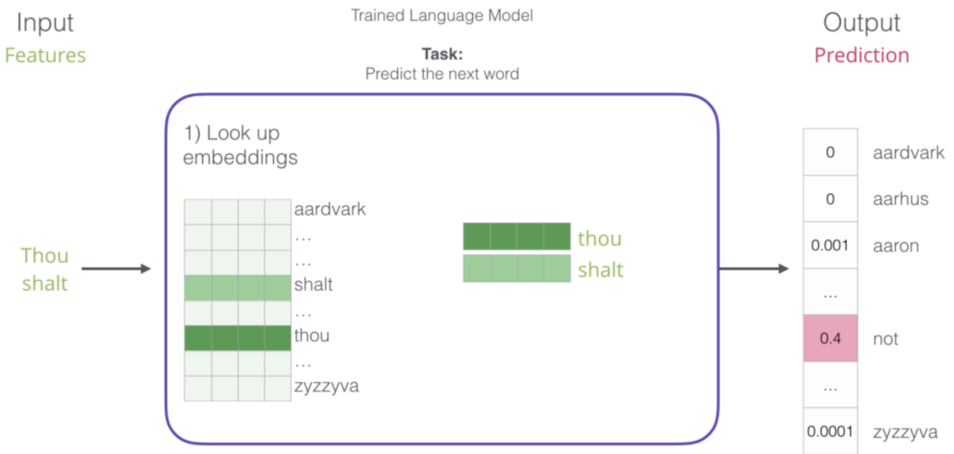
Word Embeddings as Part of Language Model

language models contain embedding matrix as part of learned parameters

- can be extracted and subsequently used as pre-trained embeddings for other task
- typically several hundred dimensions for word vectors
- trained on huge data sets (millions in vocabulary)

next-word prediction:





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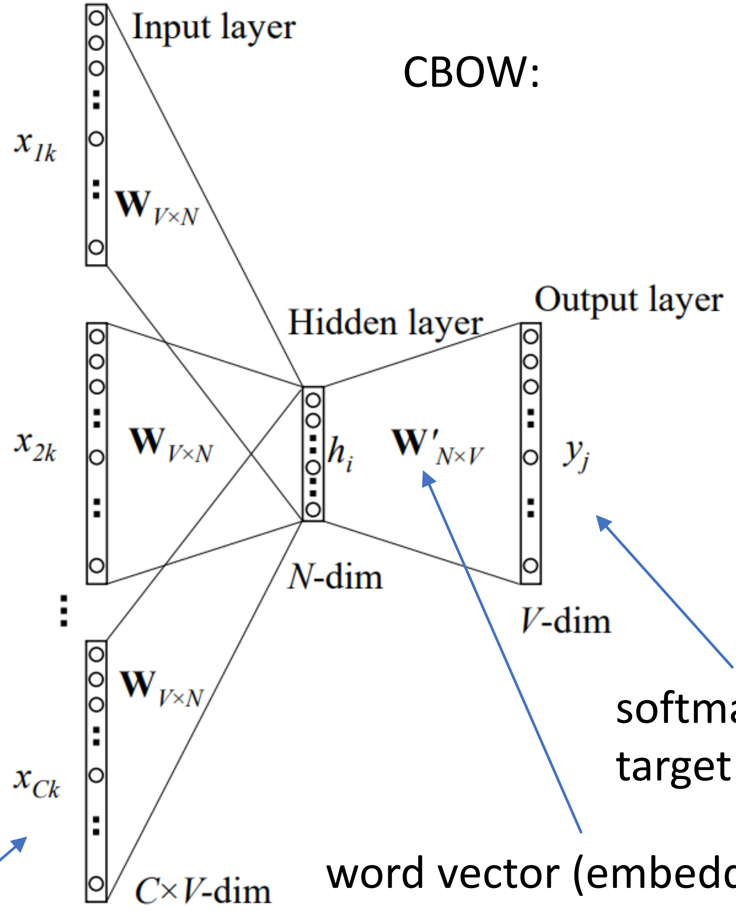
Some Thoughts on Word Embeddings

can be implemented as

- neural network with single hidden layer (linear activation)
- using, e.g., bag-of-words approach (predict masked word from its surroundings)

→ not context-aware (need for attention or RNN)

CBOW:



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softmax of target word

word vector (embedding) by multiplication with one-hot vector

one-hot vectors of context words

Context Awareness: Transformer

original transformer: sequence-to-sequence model (e.g., for machine translation)

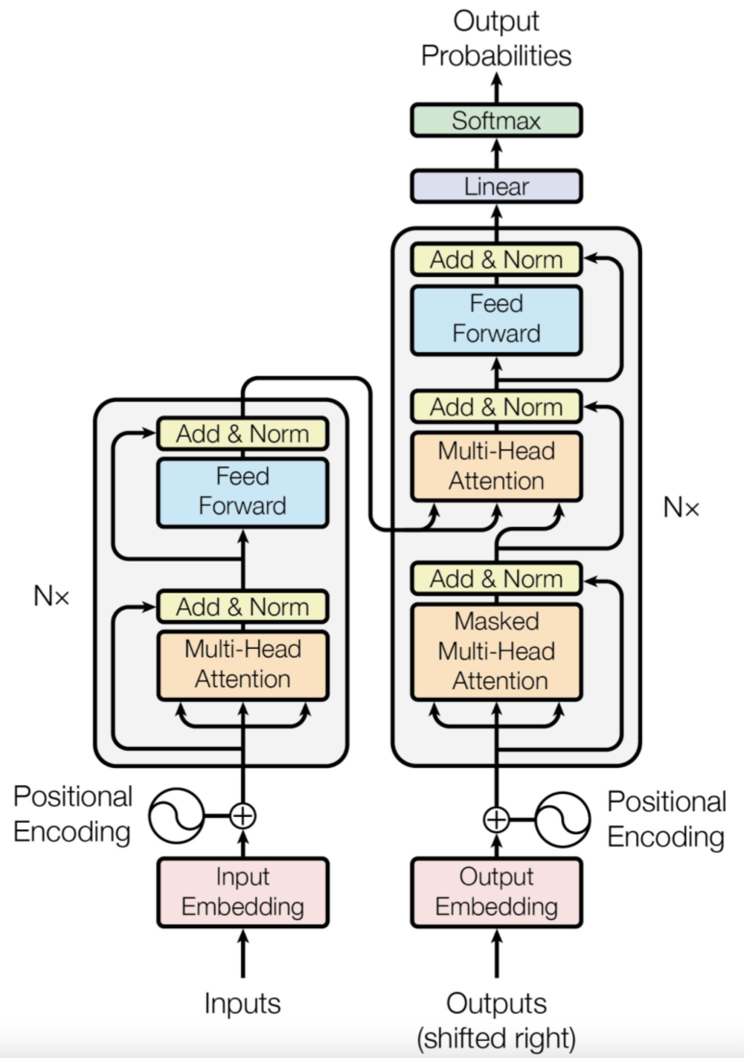
attention is all you need: RNNs replaced by multi-headed self-attention (implemented with matrix multiplications and feed-forward neural networks)

→ allowing for much more parallelization

→ allowing for bigger models (more parameters)

better long-range dependencies thanks to shorter path lengths in network (less sequential operations)

Let’s go through it step by step …



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Tokenization and Embeddings

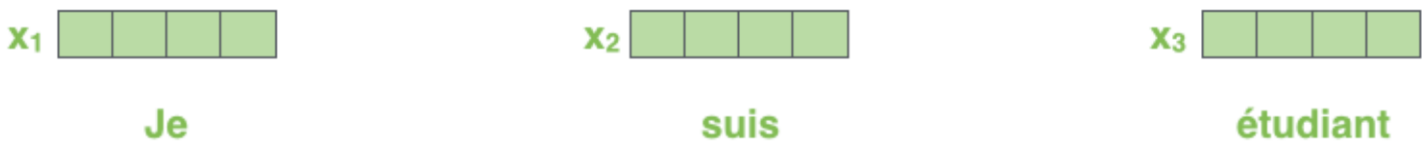
tokenization: *breaking text in chunks*

- word tokens: different forms, spellings, etc → undefined and vast vocabulary (need for stemming, lemmatization)
- character tokens: not enough semantic content (longer sequences)

→ byte-pair encoding as compromise for tokenization

one-hot encoding on tokens → token (word) embeddings:

only before bottom-most encoder/decoder



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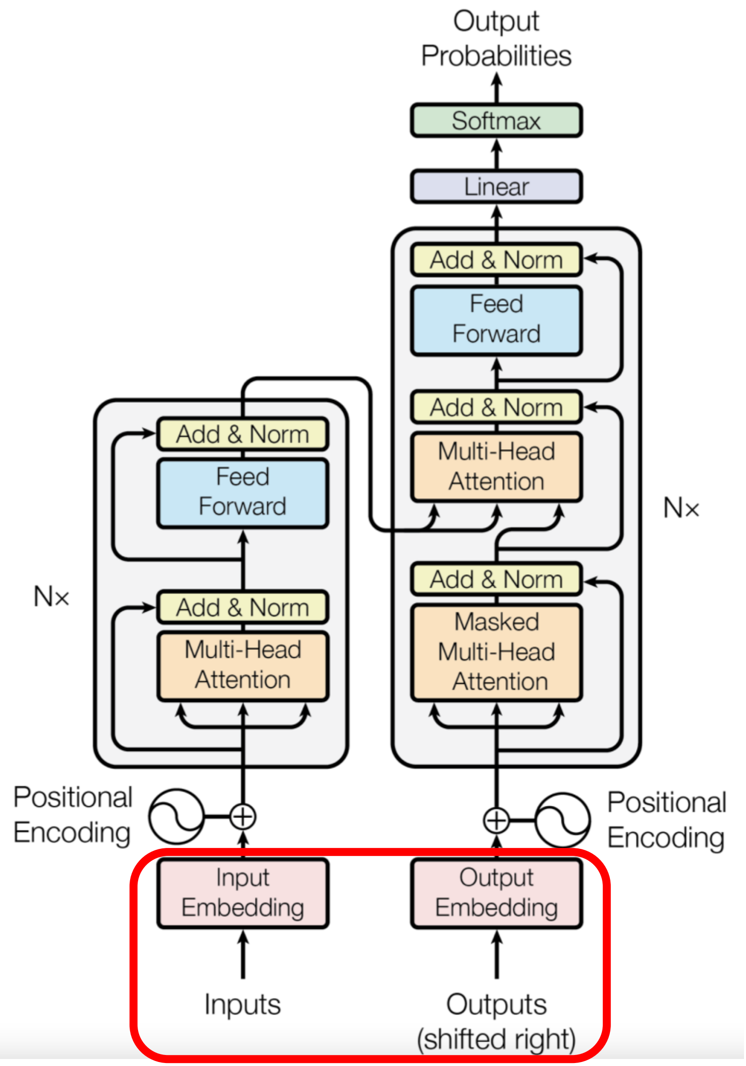

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Byte-Pair Encoding

data compression method used for encoding text as sequence of tokens

- merging token pairs (starting with characters) with maximum frequency
- continue merging until defined fixed vocabulary size (hyperparameter) is reached

→common words encoded as single token

→rare words encoded as sequence of tokens (representing word parts)

alternative: direct operation on bytes (e.g., [ByT5](ByT5))

aaabdaaabac

ZabdZabac
Z=aa

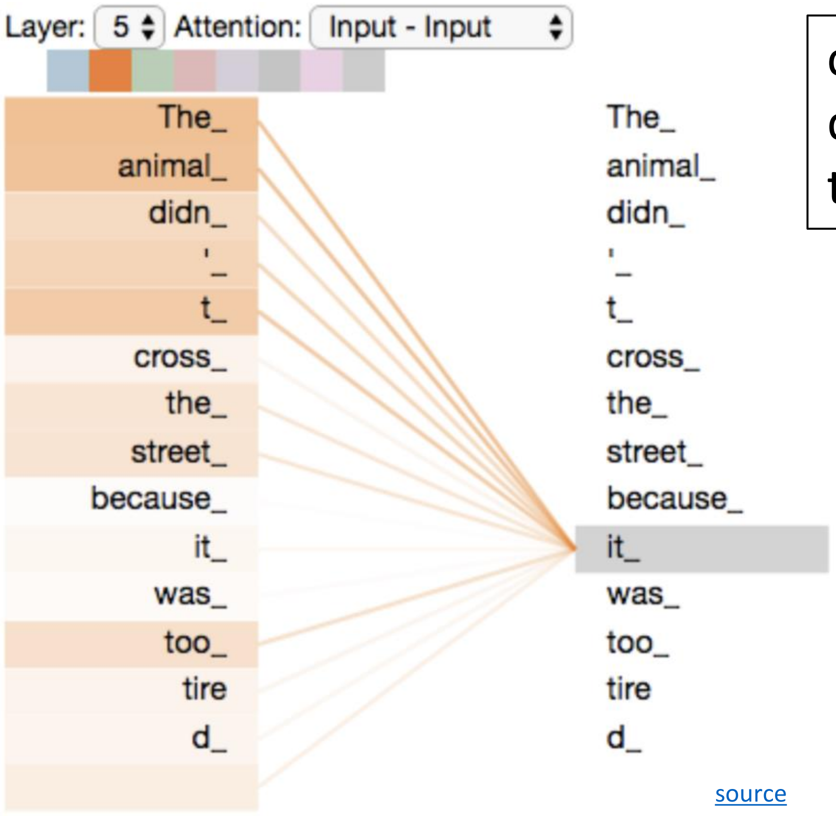
ZYdZYac
Y=ab
Z=aa

XdXac
X=ZY
Y=ab
Z=aa

example from wikipedia

Self-Attention

evaluating other input words in terms of relevance for encoding of given word



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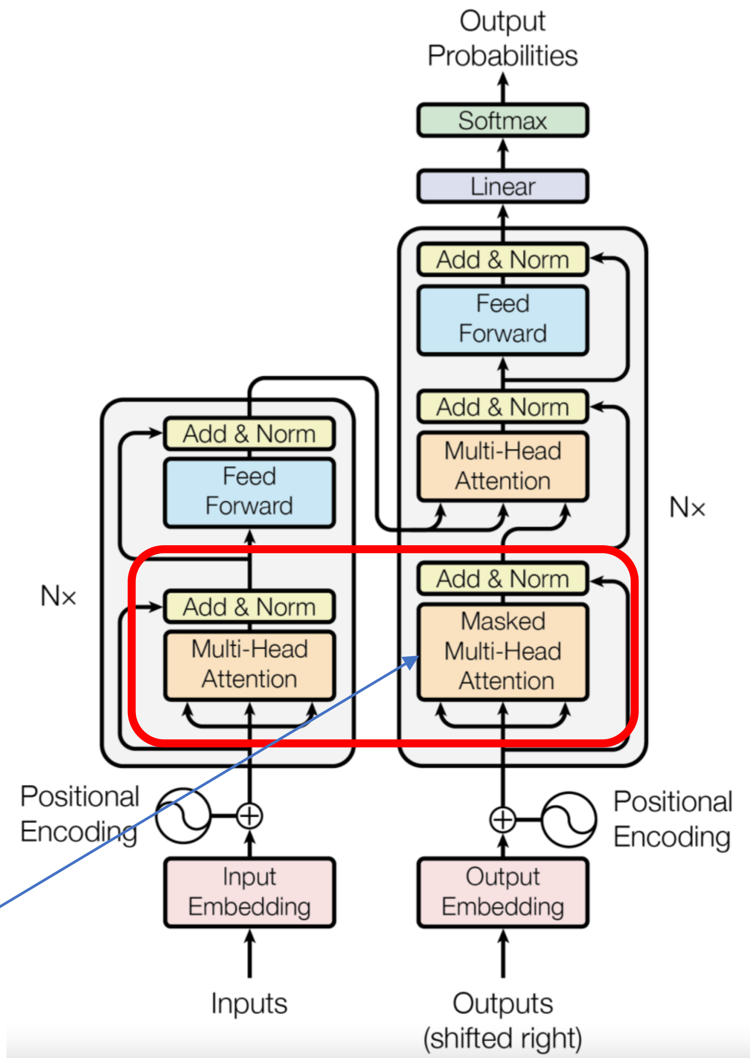
computational complexity quadratic in length of input (each token attends to each other token)

masked self-attention in decoder: only allowed to attend to earlier positions in output sequence (masking future positions by setting them to $-\infty$)



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Scaled Dot-Product Attention

softmax not scale invariant: largest inputs dominate output for large inputs (more embedding dimensions d_k)

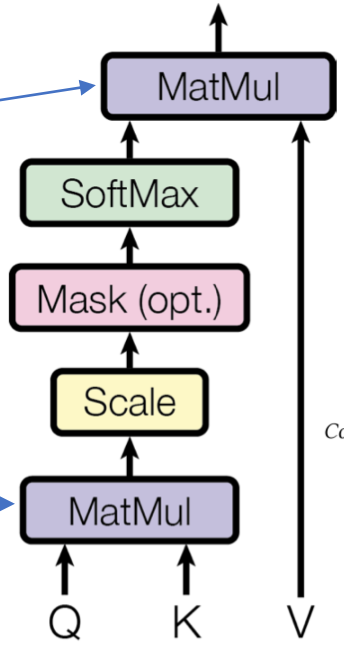
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

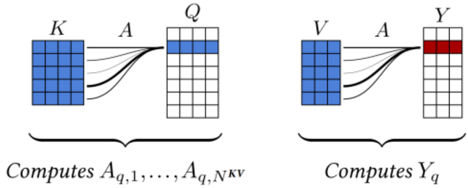
Scaled Dot-Product Attention

3 abstract matrices created from inputs (e.g., word embeddings) by multiplying inputs with 3 different weight matrices

- query Q
- key K
- value V

filtering: multiplication of attention probabilities with corresponding key word values





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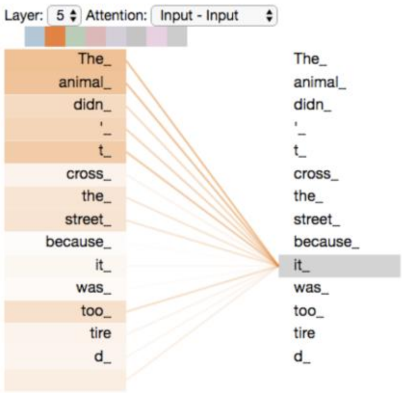
key-value pairs



query

scoring each of the key words (context) with respect to current query word: multiplication of inputs (in contrast to inputs times weights in neural networks)

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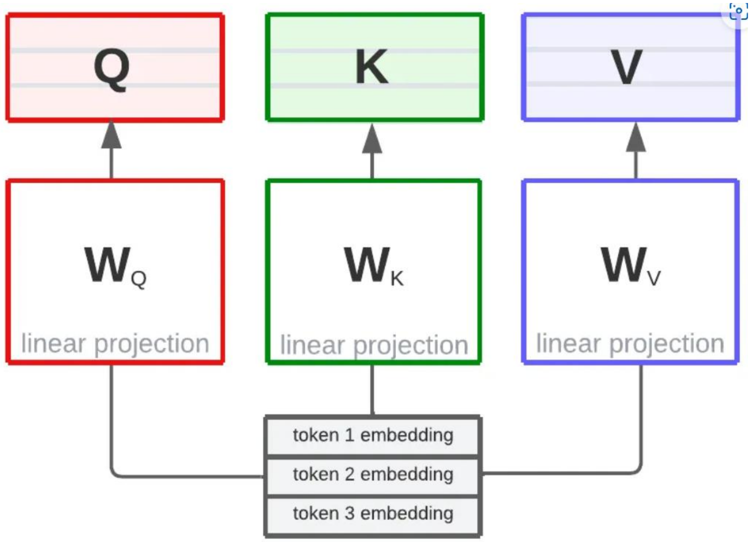
Self-Attention as Weighted Average

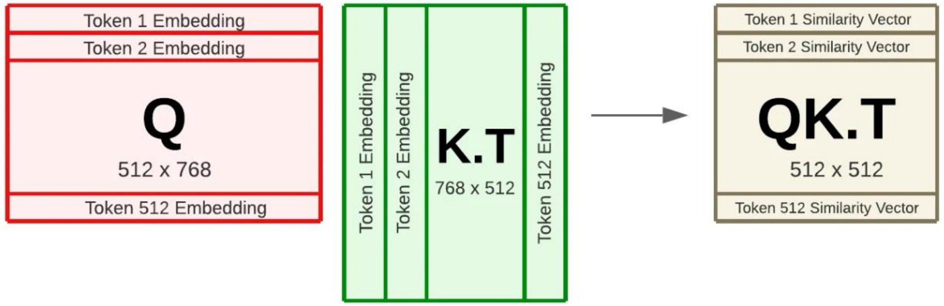
weighted average: reflecting to what degree a token is paying attention to the other tokens in the sequence

1



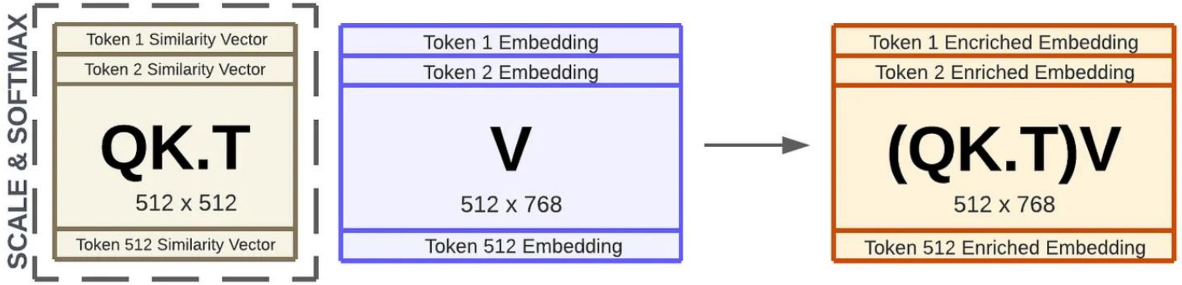
Projecting token embeddings into Query, Key, and Value vectors through matrix multiplication with their respective Weights (W).

2



The Query (Q) matrix multiplied with the Key (K.T) resulting in the matrix of similarity of scores (QK.T).

3



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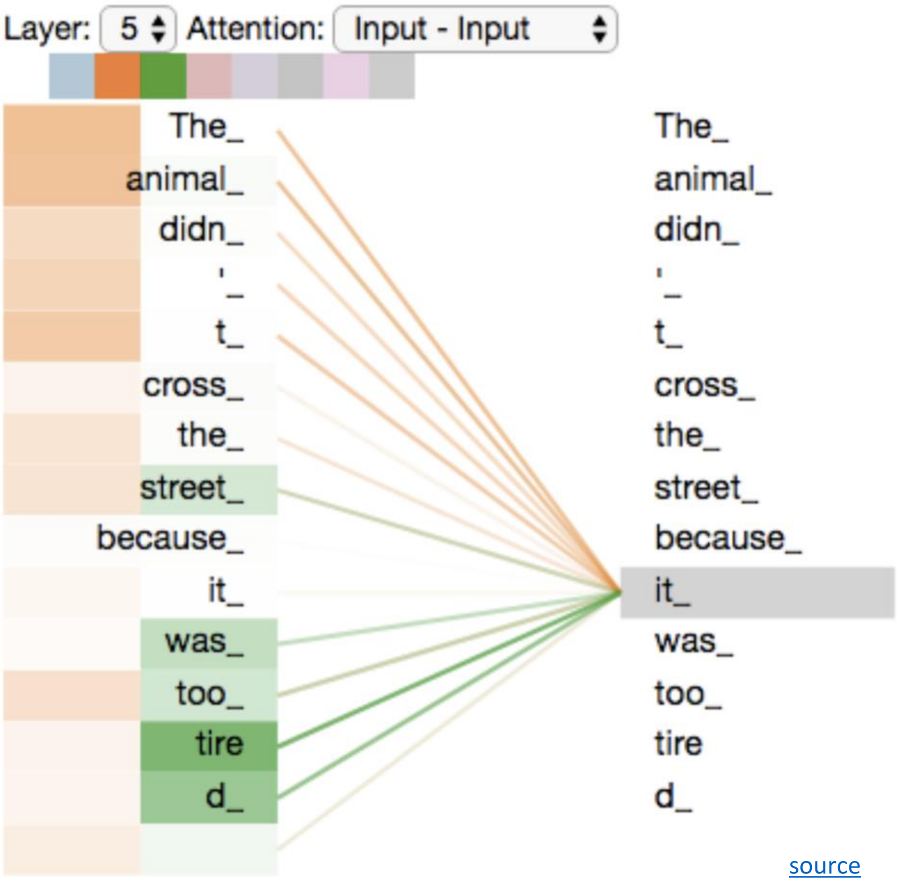
The scaled and soft similarity scores matrix multiplied with the values (V) resulting in enriched embeddings.

Multi-Head Attention

multiple heads: several attention layers running in parallel



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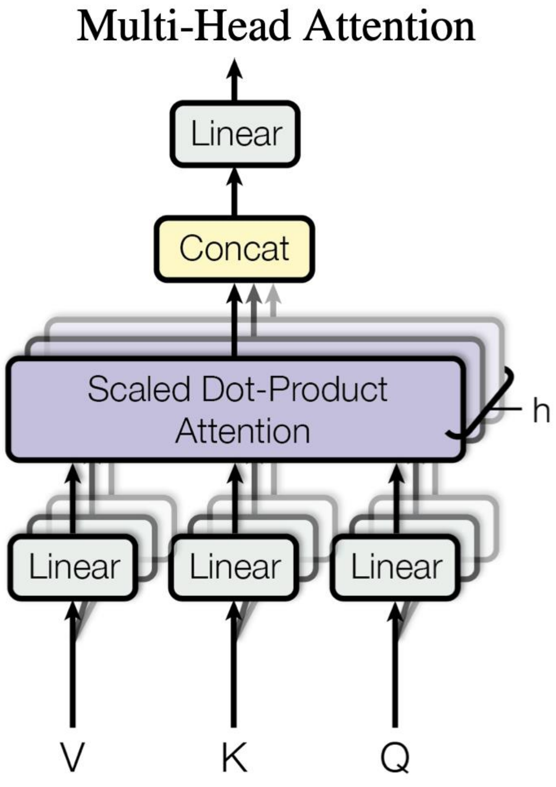
different heads can pay attention to different aspects of input (multiple representation sub-spaces)



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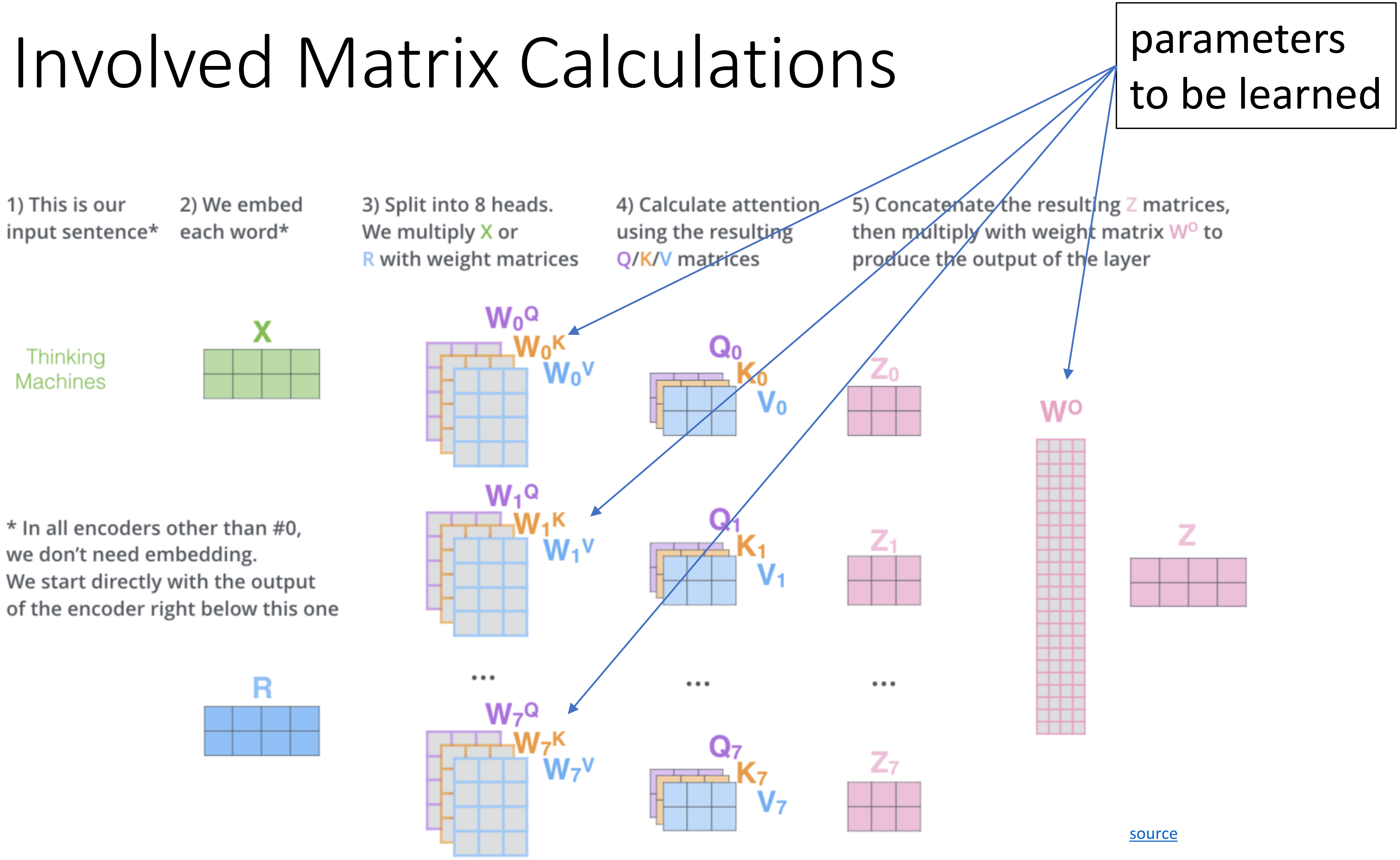
Involved Matrix Calculations



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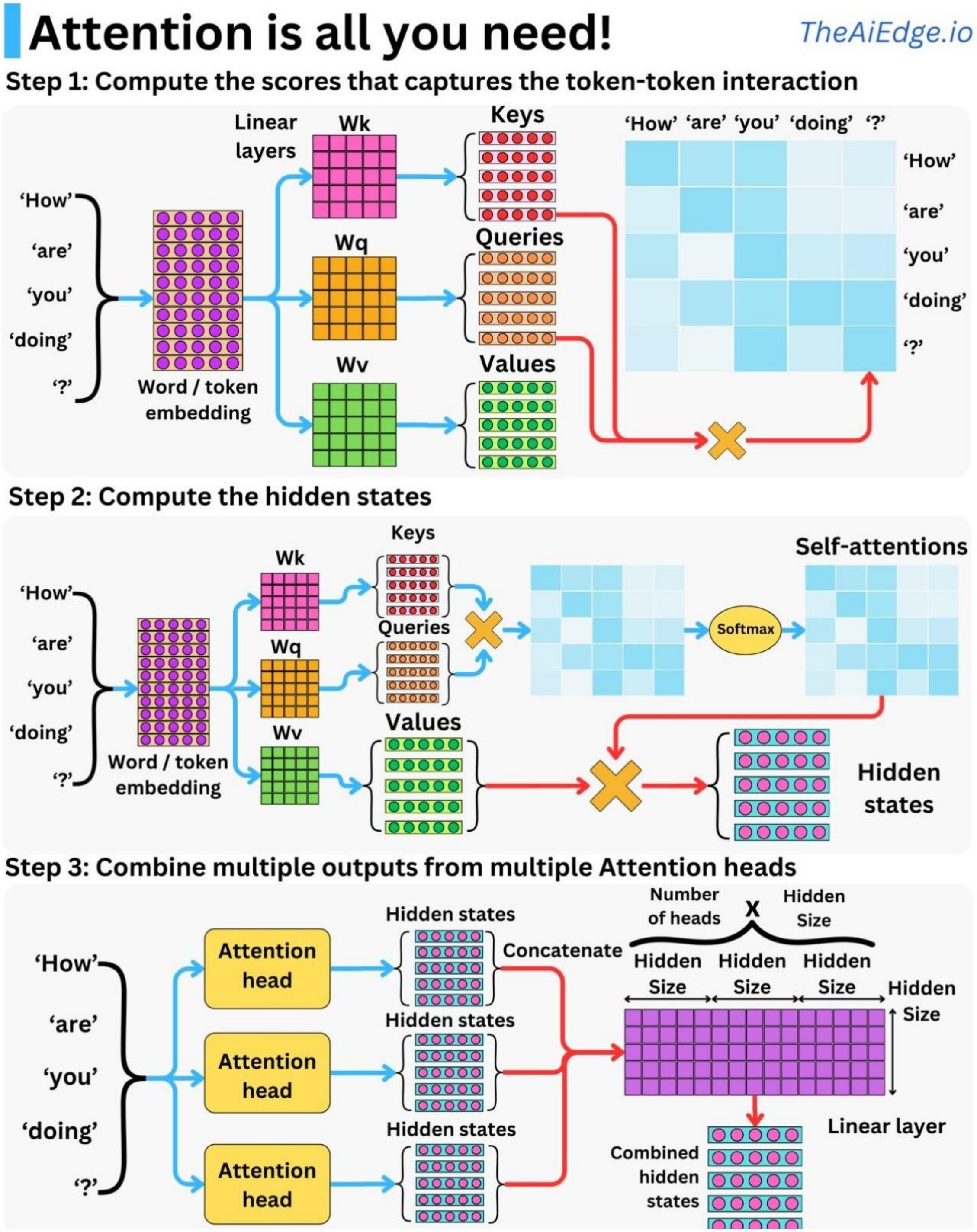

Attention is all you need!
TheAiEdge.io
Step 1: Compute the scores that captures the token-token interaction
Linear layers
Wk
Wq
Wv
Keys
Queries
Values
'How' 'are' 'you' 'doing' '?'
Word / token embedding
Step 2: Compute the hidden states
Self-attentions
Softmax
Hidden states
Step 3: Combine multiple outputs from multiple Attention heads
Attention head
Attention head
Attention head
Hidden states
Concatenate
Number of heads X Hidden Size
Hidden Size
Linear layer
Combined hidden states

Encoder-Decoder Attention

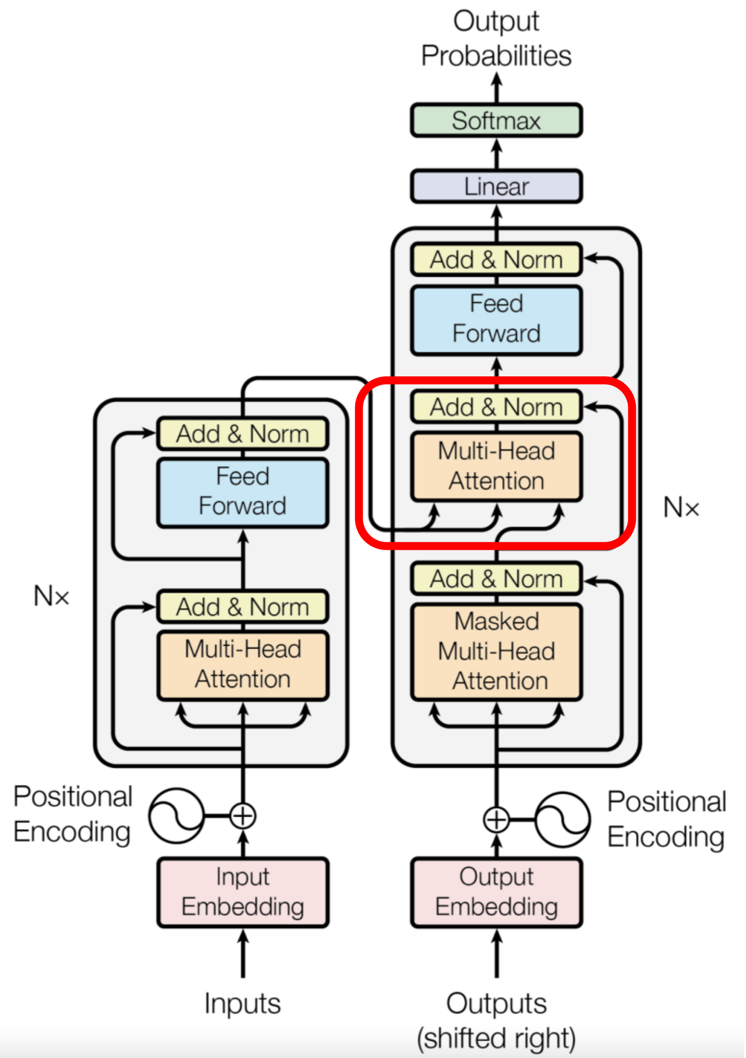
aka cross-attention

connection between encoders and decoders

attention layer helping decoder to focus on relevant parts of input sentence (similar to attention in seq2seq models)

output of last encoder transformed into set of attention matrices K and V → fed to each decoder's cross-attention layer (redundancy)

multiheaded self-attention with Q from decoder layer below and K, V from output of encoder stack



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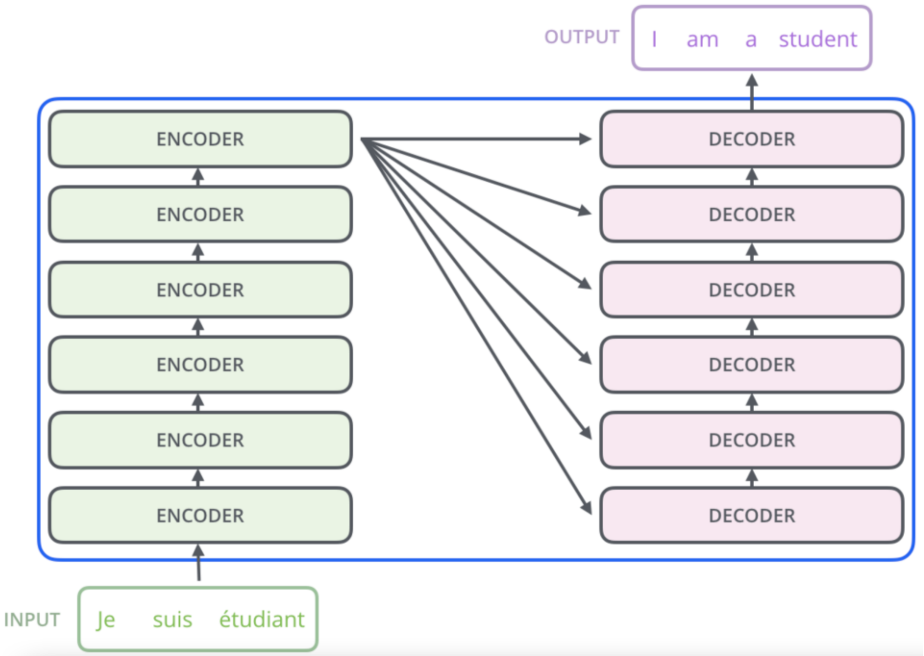
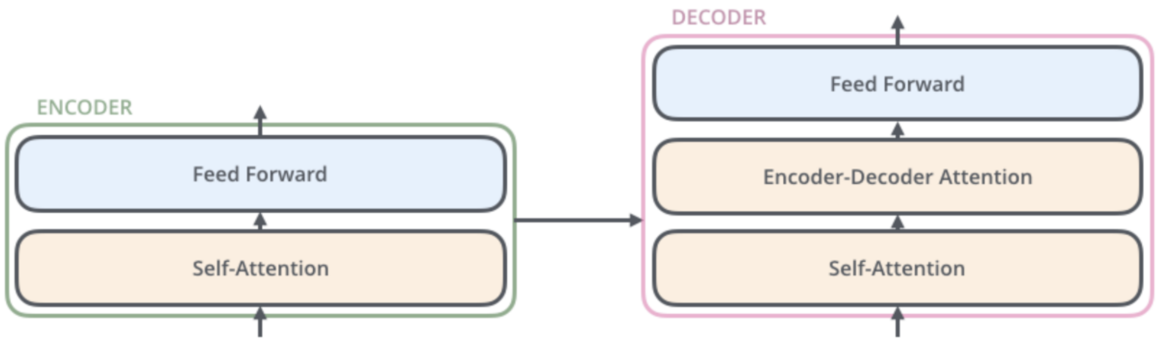
Encoder and Decoder Stacks



output of encoders/decoders fed as input to next ones



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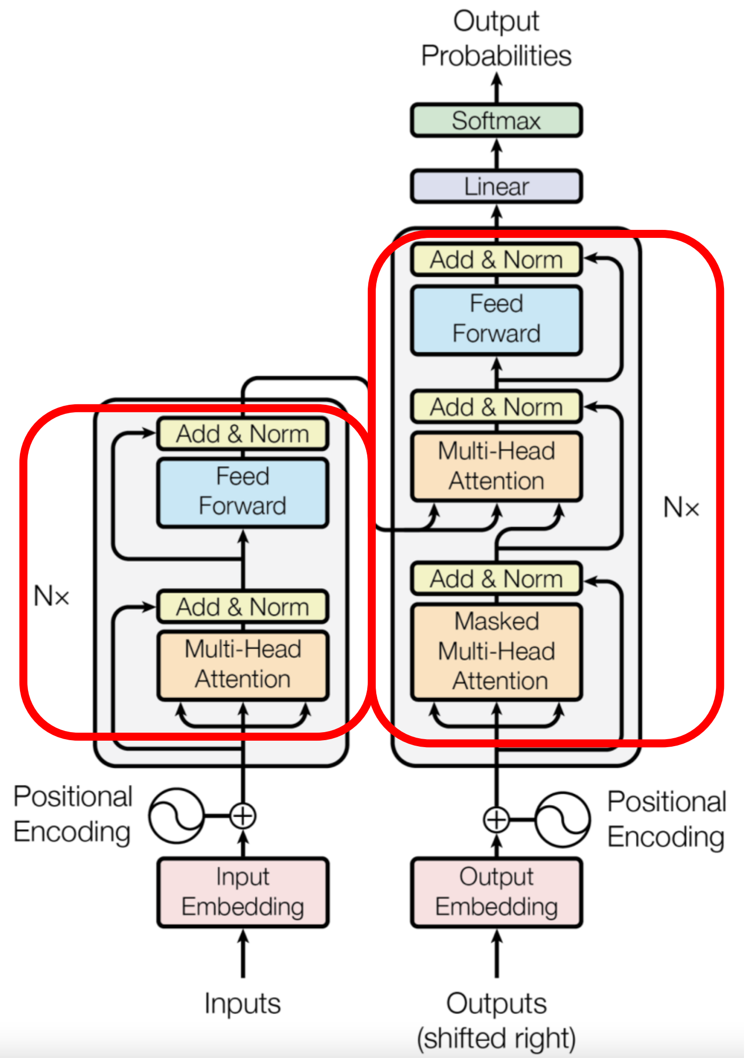

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Positional Encoding

attention permutation invariant → need for positional encoding to learn from order of sequence

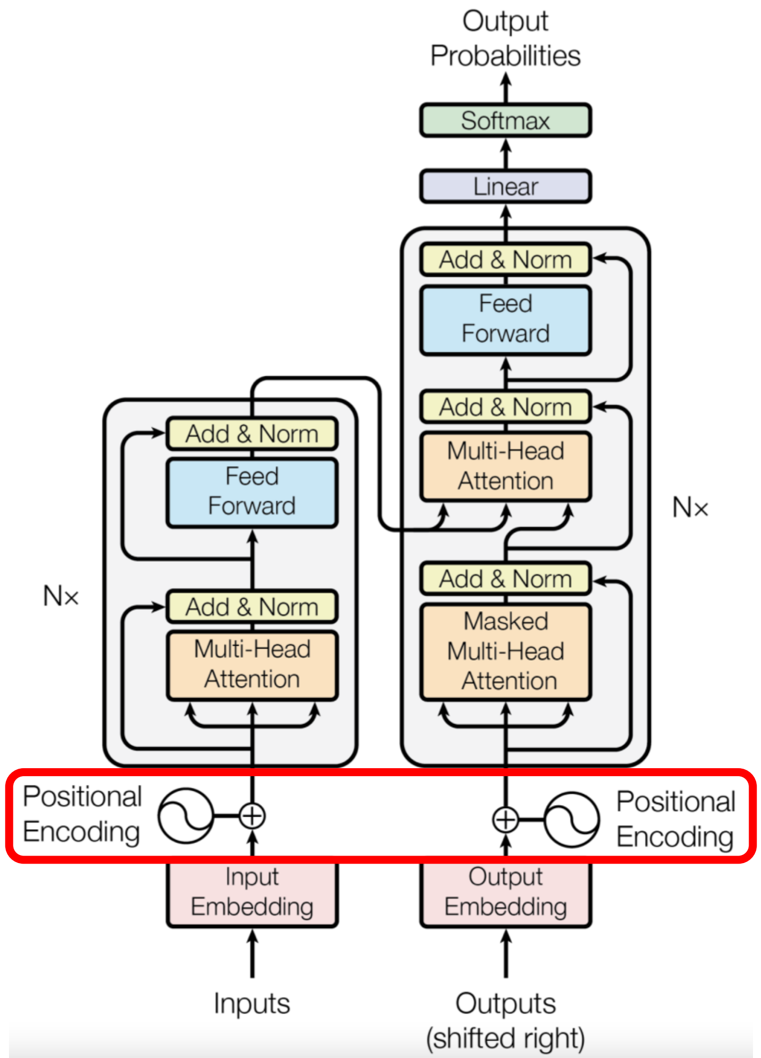
different choices:

- for each absolute position (from 1 to maximum sequence length), add a learned vector (of dimension d_{model}) to input embeddings → each positional embedding independent of others
- add fixed sinusoidal functions for each position and dimension i

$$PE_{pos,2i} = \sin\left(\frac{pos}{10000^{\frac{2i}{d_{\text{model}}}}}\right) \qquad PE_{pos,2i+1} = \cos\left(\frac{pos}{10000^{\frac{2i}{d_{\text{model}}}}}\right)$$

- rotate input embeddings by multiples (position) of a small angle (RoPE) → captures both absolute and relative positions

$$f_{\{q,k\}}(\boldsymbol{x}_m, m) = \begin{pmatrix} \cos m\theta & -\sin m\theta \\ \sin m\theta & \cos m\theta \end{pmatrix} \begin{pmatrix} W^{(11)}_{\{q,k\}} & W^{(12)}_{\{q,k\}} \\ W^{(21)}_{\{q,k\}} & W^{(22)}_{\{q,k\}} \end{pmatrix} \begin{pmatrix} x^{(1)}_m \\ x^{(2)}_m \end{pmatrix}$$



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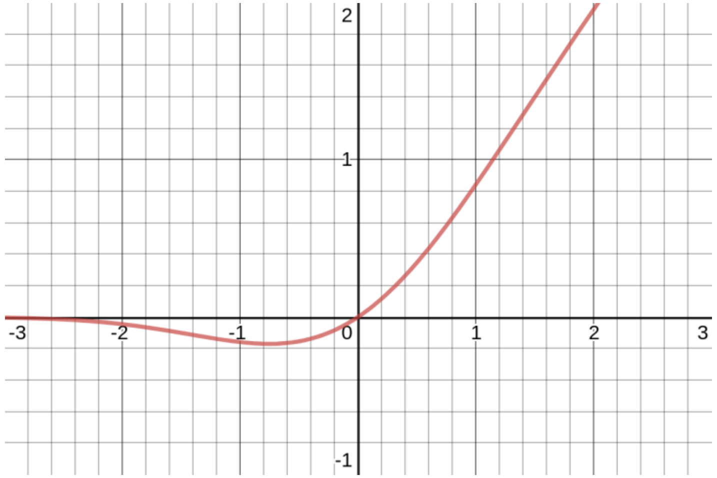
Position-Wise Feed-Forward Networks

for each encoder or decoder layer: identical feed-forward network independently applied to each position

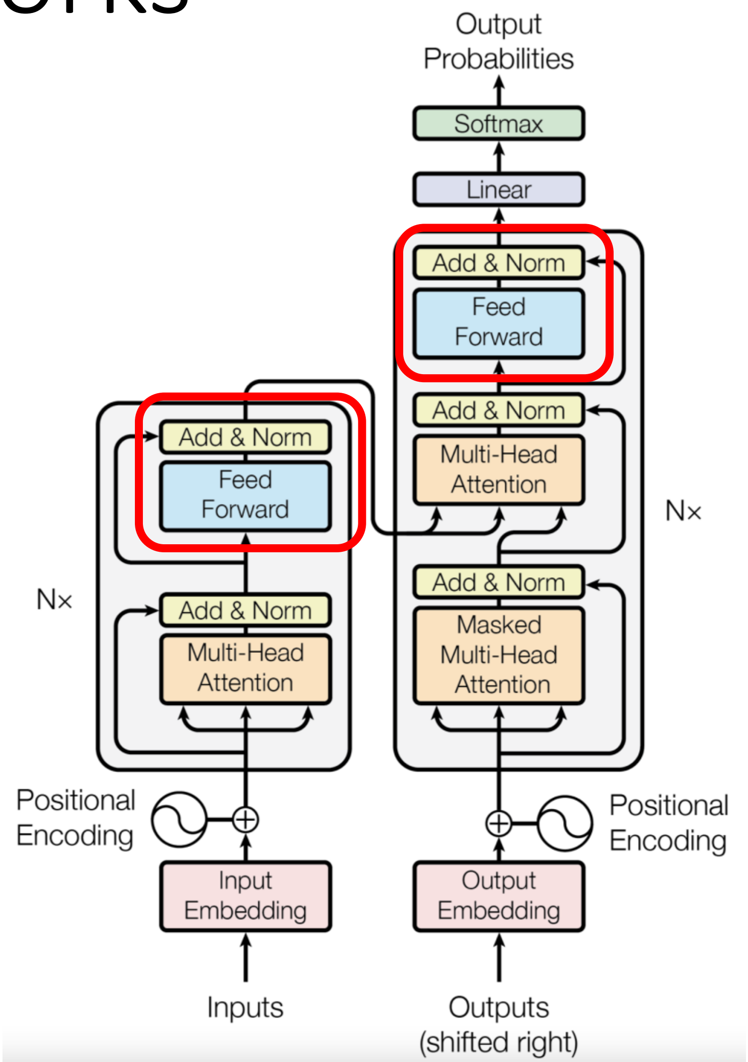
GeLU



from wikipedia

attention is just weighted averaging
→ need for non-linearities (often GeLU activations) to capture more complex patterns

typically expand-and-contract (two layers) network



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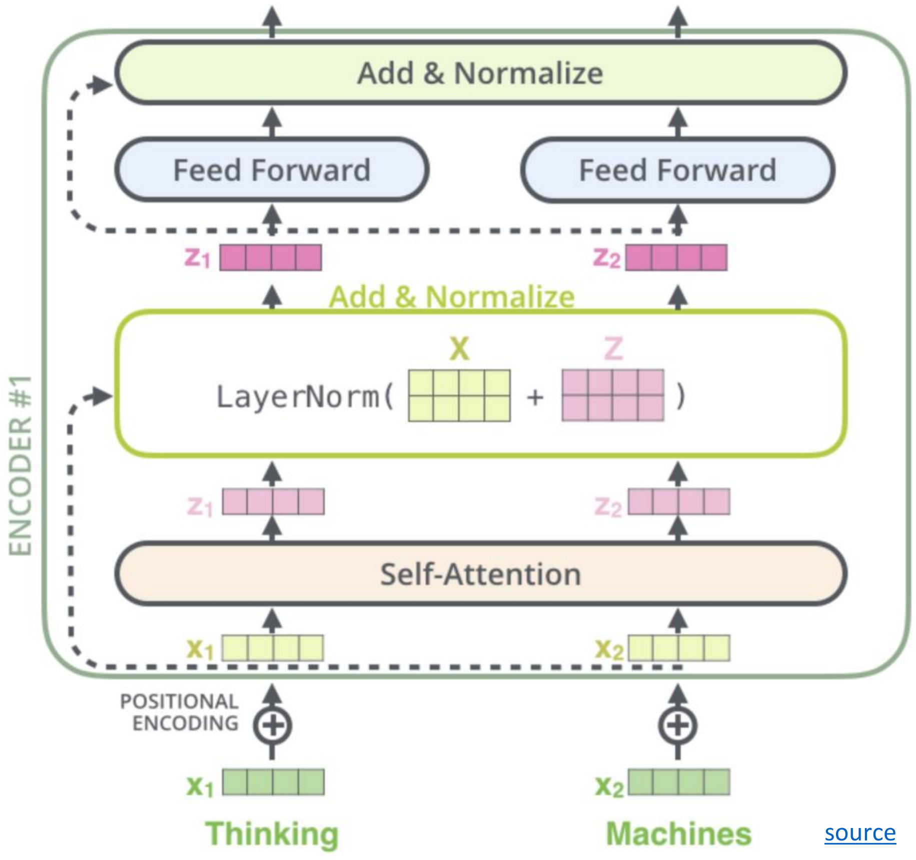
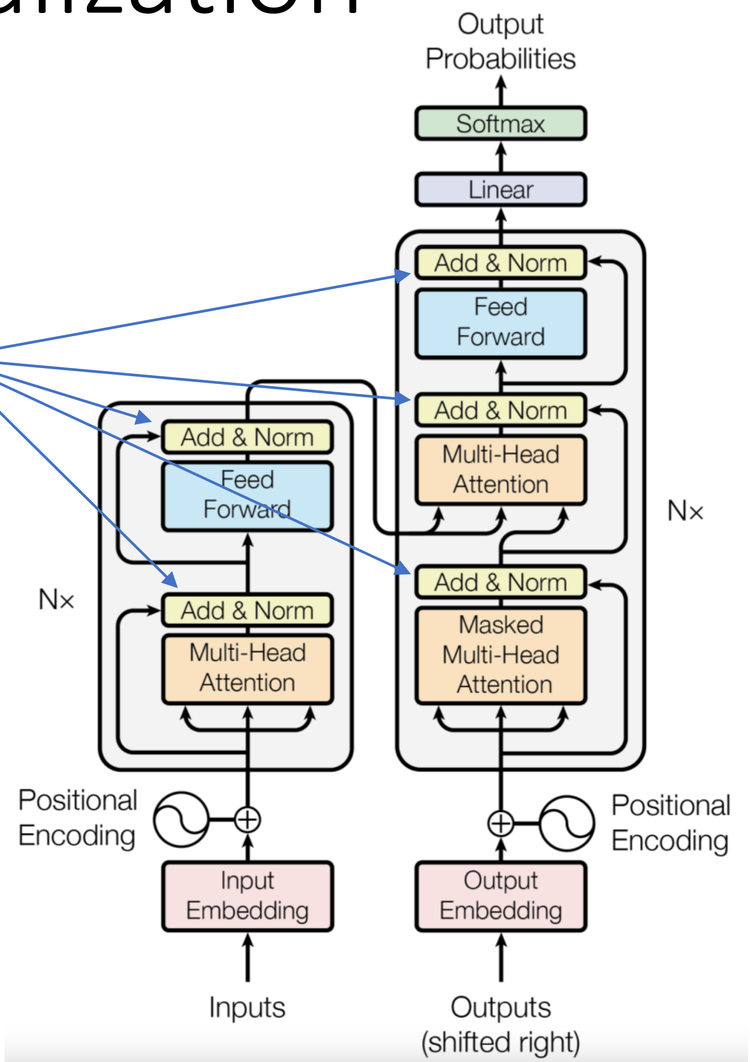
Skip Connections and Layer Normalization



source

skip connections and layer normalization for each sub-layer

skip connections improve robustness by
- preserving original input (attention layers as filters) as well as gradients (mitigate vanishing-gradient problem)
- easier learning of identity functions (useful for disregarding modules that do not improve model performance)



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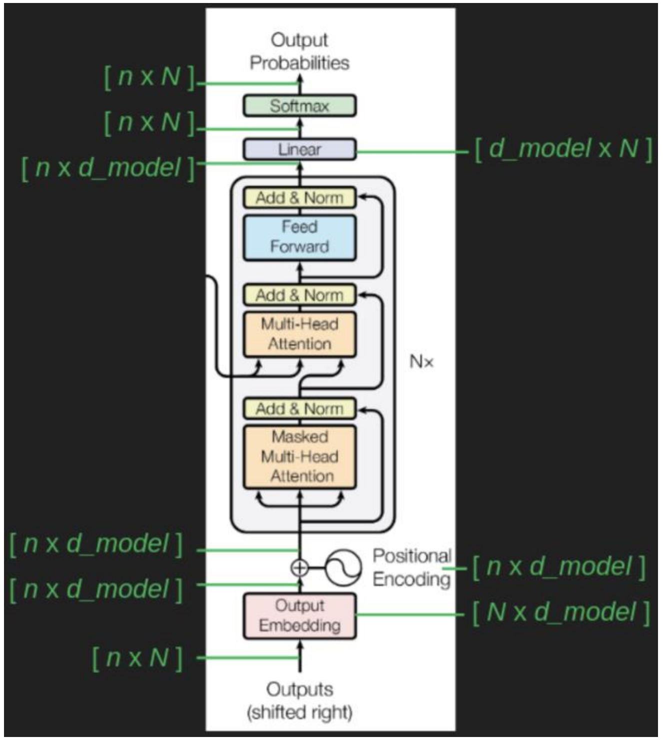
De-Embedding and Softmax

n: maximum sequence length
N: vocabulary size
d_model: embedding dimensions



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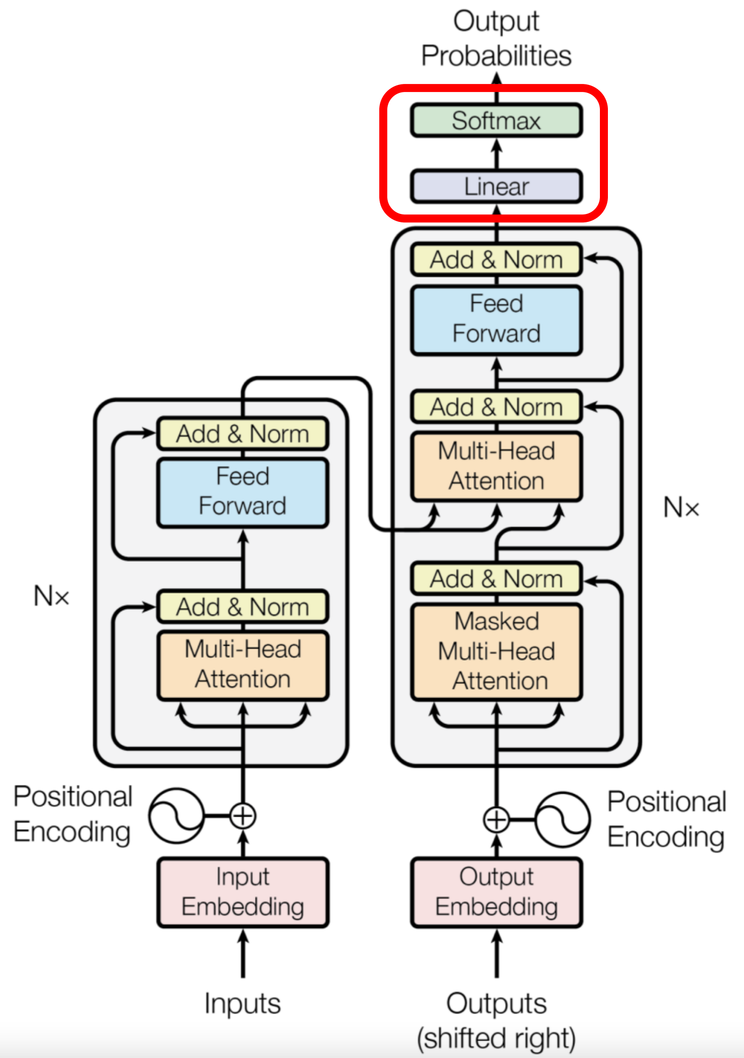
conversion of final decoder output to predicted next-token probabilities for output vocabulary

de-embedding: linear transformation (matrix multiplication / fully connected neural network layer)

softmax: transformation to probabilities ("softness" can be controlled by hyperparameter temperature)



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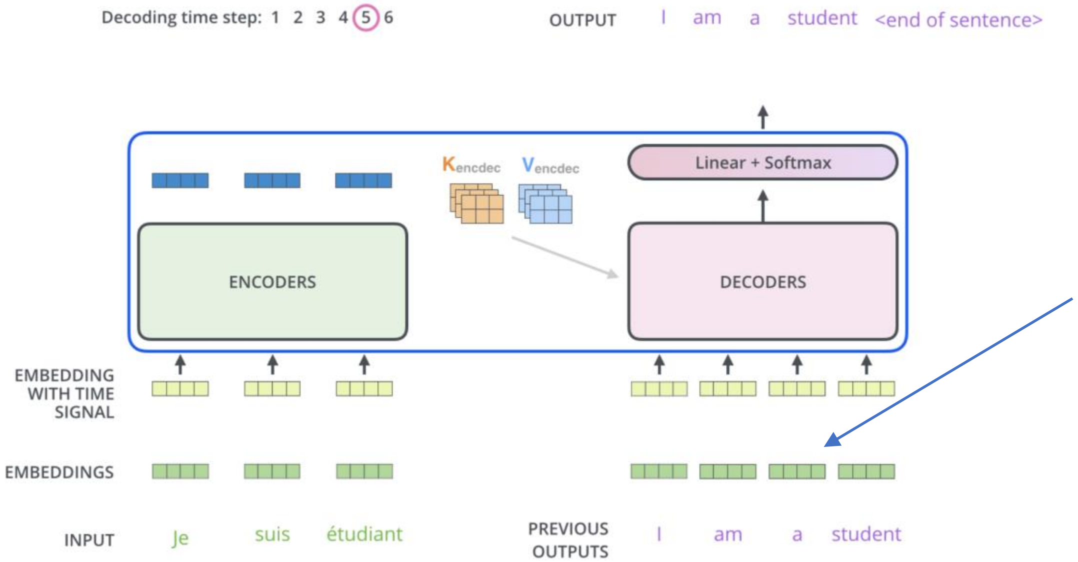
Sequence Completion

- greedily picking the one with highest probability
- pick according to probabilities (degree of randomness controlled by softmax temperature)
- beam search

for each step/token (iteratively), choose one output token to add to decoder input sequence → increasing uncertainty



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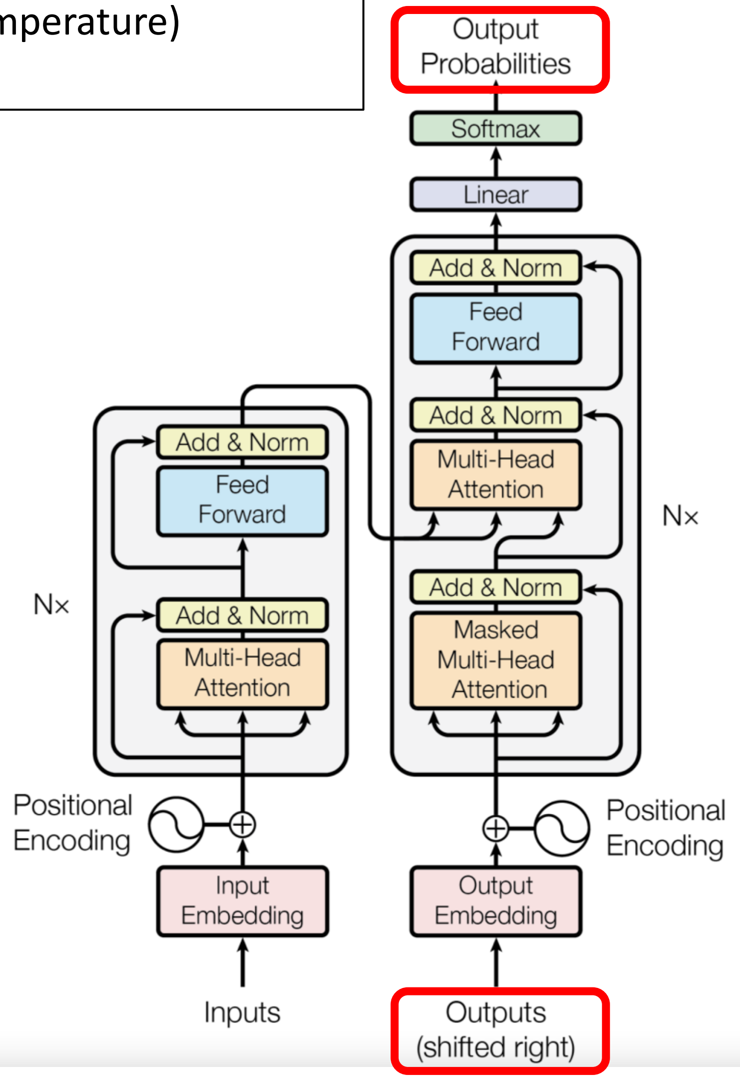
auto-regressive



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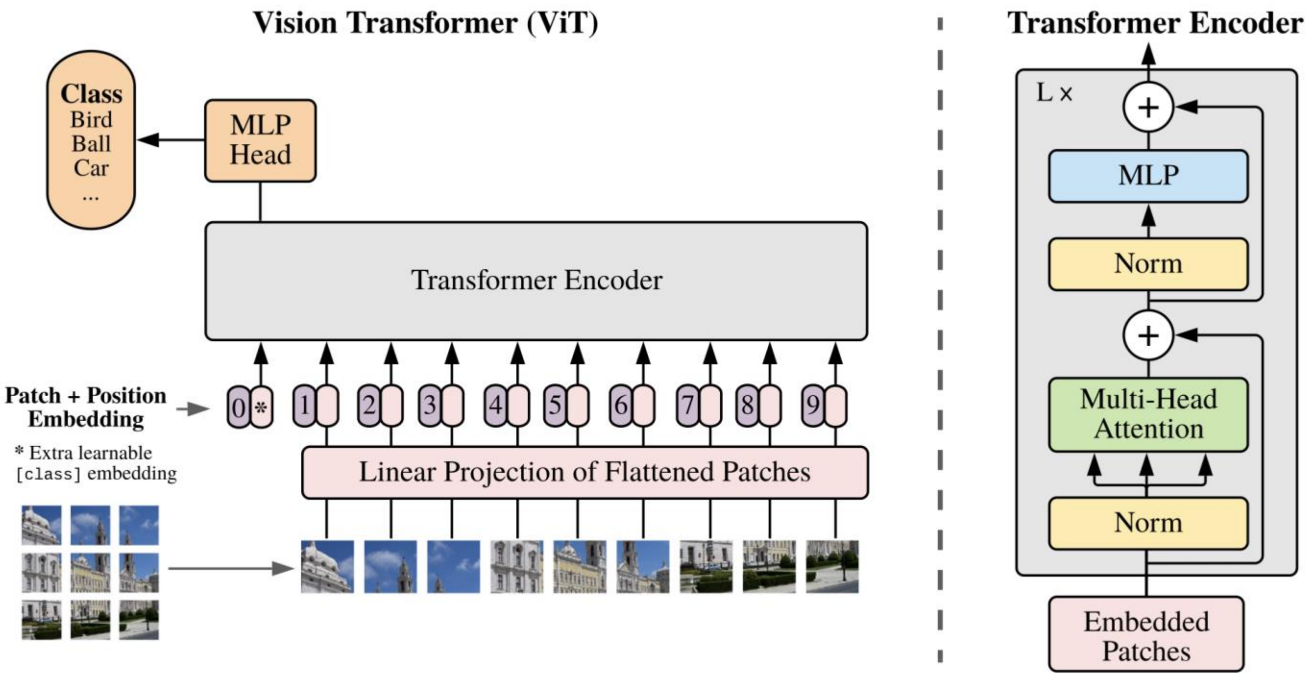
prompt: externally given initial sequence for running start and context on which to build rest of sequence ([prompt engineering]())

Image Classification with Vision Transformer



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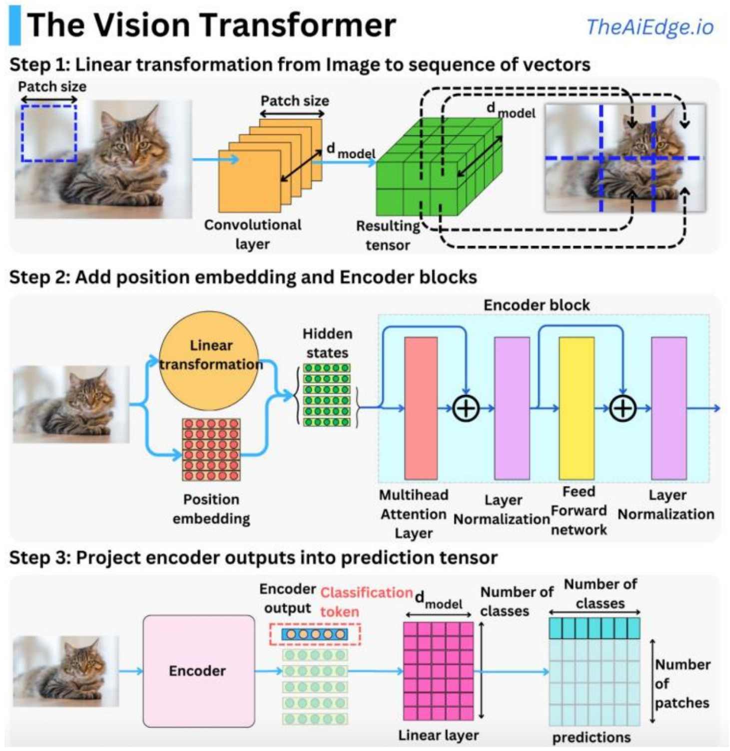
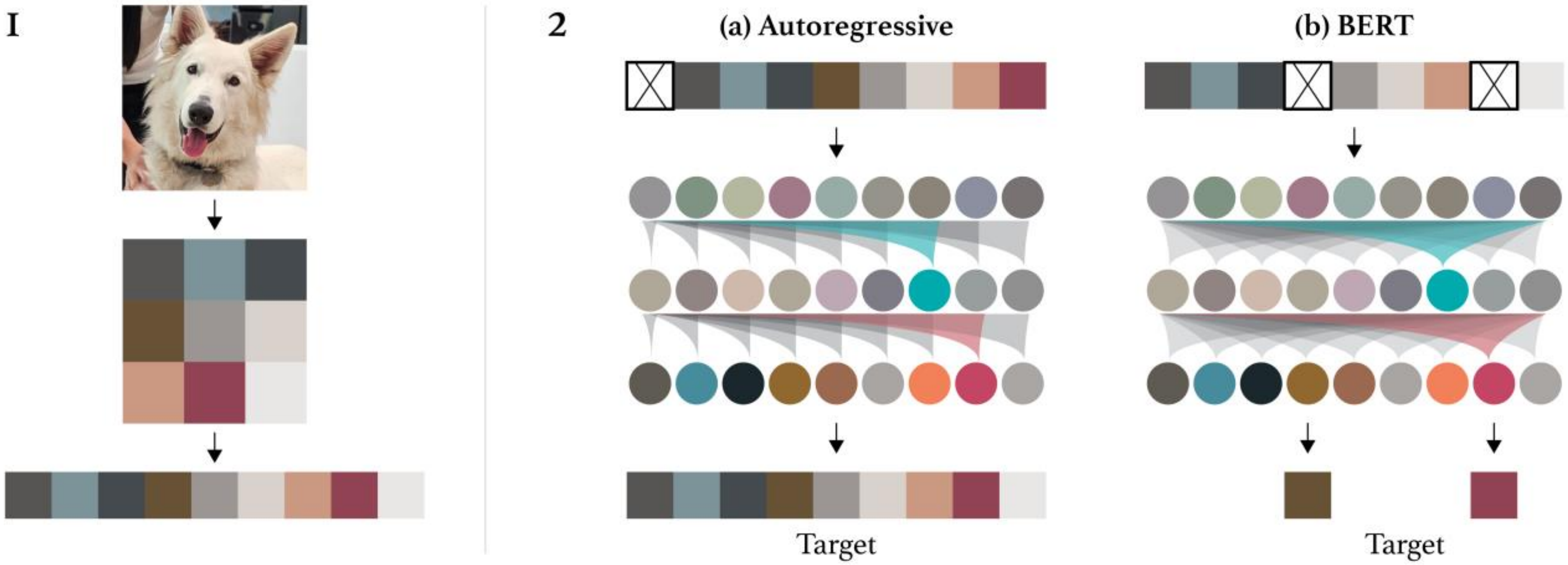


formulation as sequential problem:
split image into patches (tokens) and flatten,
add positional embeddings

processing by transformer encoder:
pre-train with image labels, fine-tune
on specific data set

Pixel Generation (iGPT)



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Open-Source Implementations

lightweight PyTorch re-implementation of GPT (decoder-only transformer):

minGPT

more powerful:

nanoGPT, LitGPT