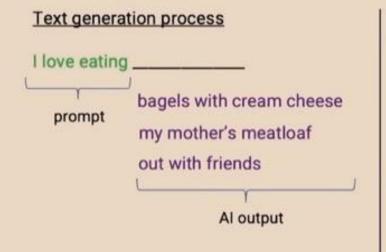
# Transformer

# Language Models

#### This decade: Generative Al



#### How it works

Generative AI is built by using supervised learning  $(A \rightarrow B)$  to repeatedly predict the next word.

My favorite food is a bagel with cream cheese and lox.

Input (A)	Output (B)
My favorite food is a	bagel
My favorite food is a bagel	with
My favorite food is a bagel with	cream

When we train a very large AI system on a lot of data (hundreds of billions of words) we get a Large Language Model like ChatGPT.



#### 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**:

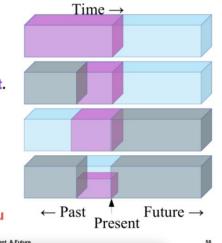
- input-output mapping like supervised learning
- but generating labels itself from input information

generative AI as unsupervised learning: generate variations of training data

# How Much Information is the Machine Given during Learning? > "Pure" Reinforcement Learning (cherry) > The machine predicts a scalar reward given once in a while. > A few bits for some samples > Supervised Learning (icing) > The machine predicts a category or a few numbers for each input > Predicting human-supplied data > 10→10,000 bits per sample > Self-Supervised Learning (cake génoise) > The machine predicts any part of its input for any observed part. > Predicts future frames in videos > Millions of bits per sample 2019 IEEE International Solid-State Circuits Conference 1.1: Deep Learning Hardware: Past, Present, & Future

#### Self-Supervised Learning

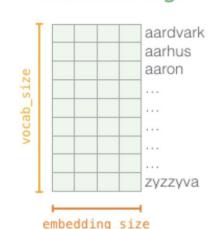
- Predict any part of the input from any other part.
- ▶ Predict the future from the past.
- Predict the future from the recent past.
- Predict the past from the present.
- ▶ Predict the top from the bottom.
- Predict the occluded from the visible
- Pretend there is a part of the input you don't know and predict that.



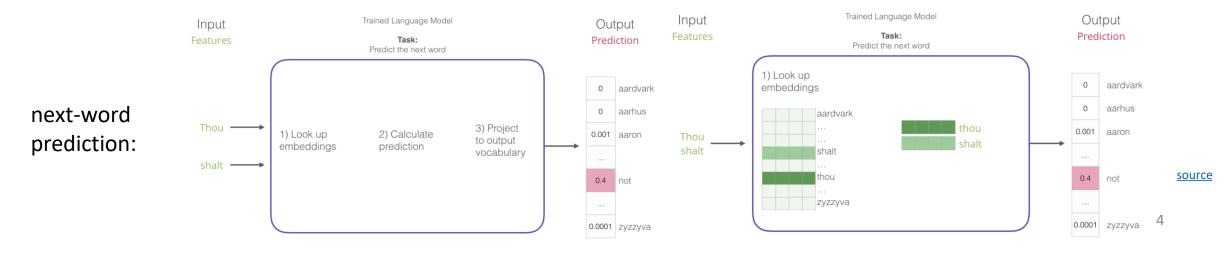
# Word Embeddings as Part of Language Model

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)



Embedding

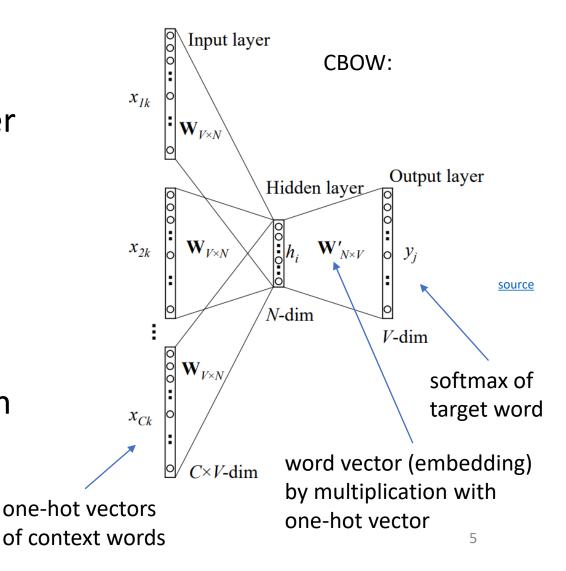


# Some Thoughts on Word Embeddings

#### 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)



## Context Awareness: Transformer

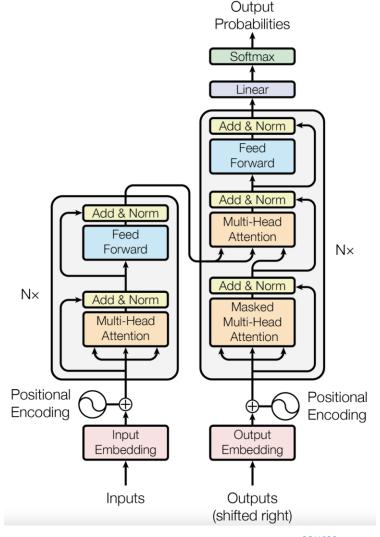
attention is all you need: RNNs replaced by multi-headed self-attention (implemented with matrix multiplications and feed-forward neural networks)

- → 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 ...

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

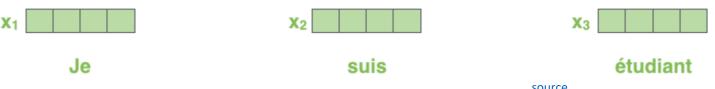


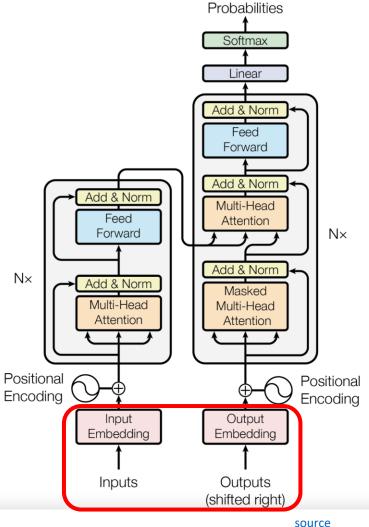
## Tokenization and Embeddings

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  $\rightarrow$  token (word) embeddings: only before bottom-most encoder/decoder





Output

source

# 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)

aaabdaaabac

ZabdZabac

Z=aa

ZYdZYac

Y=ab

Z=aa

XdXac

X=ZY

Y=ab

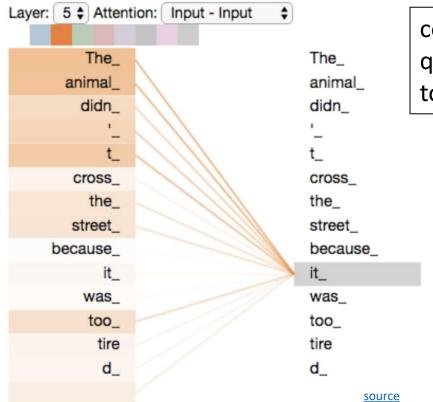
Z=aa

example from wikipedia

alternative: direct operation on bytes (e.g., <a href="ByT5">ByT5</a>)

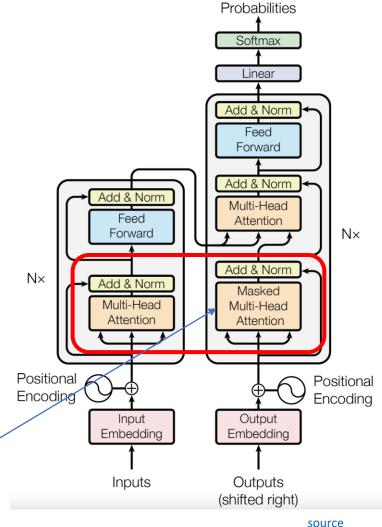
## Self-Attention

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



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  $-\infty$ )

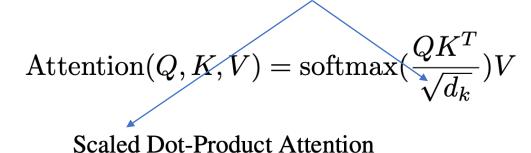


Output

## Scaled Dot-Product Attention

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

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

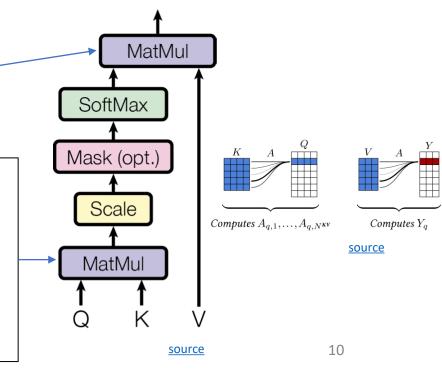


- query Q
- key K
- value V

the animal didn didn didn to cross the street because it was too tire d d

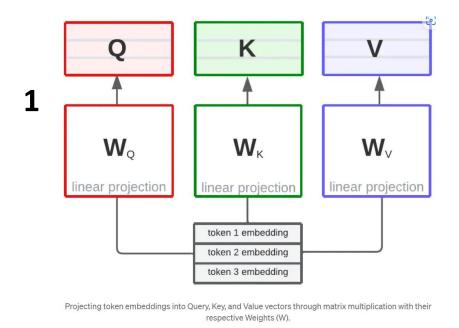
filtering: multiplication of attention probabilities with corresponding key word values

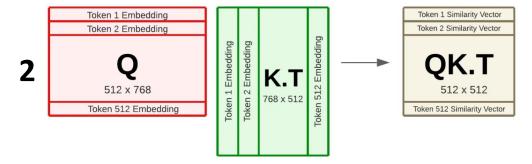
scoring each of the key words (context) with respect to current query word: multiplication of inputs (in contrast to inputs times weights in neural networks)



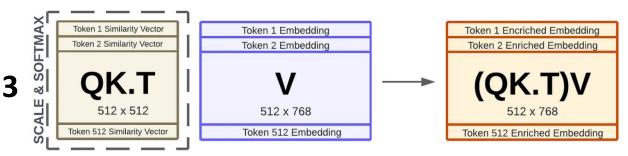
# Self-Attention as Weighted Average

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



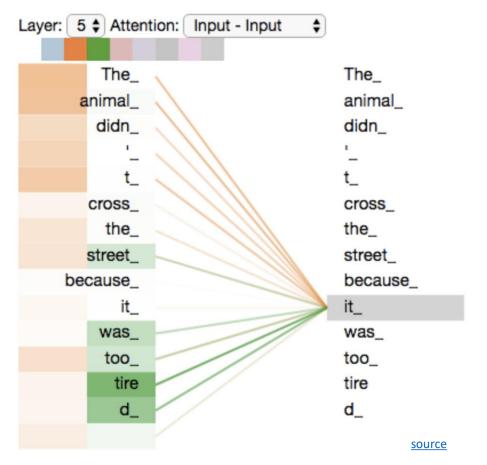


The Query (Q) matrix multiplied with the Key (K.T) resulting in the matrix of similarity of scores (QK.T).

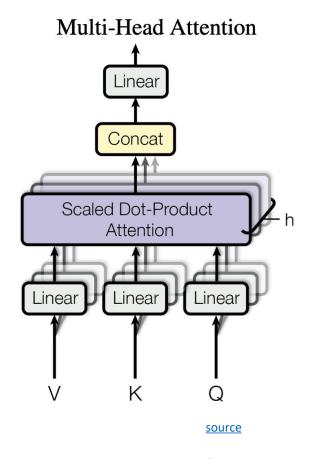


## Multi-Head Attention

multiple heads: several attention layers running in parallel



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



## Involved Matrix Calculations

#### parameters to be learned

1) This is our input sentence\*

2) We embed each word\*

3) Split into 8 heads. We multiply X or R with weight matrices

4) Calculate attention using the resulting Q/K/V matrices

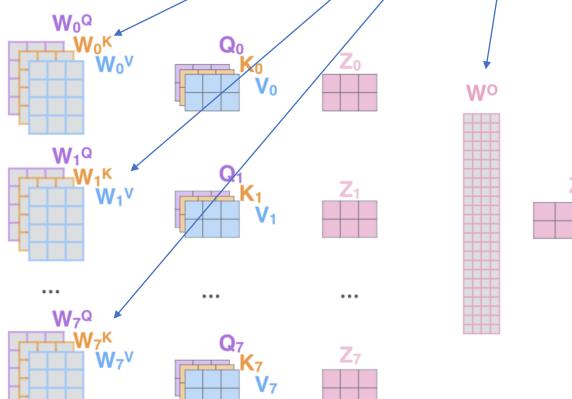
5) Concate nate the resulting Z matrices, then multiply with weight matrix Wo to produce the output of the layer

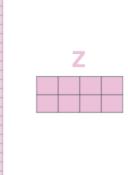
Thinking Machines



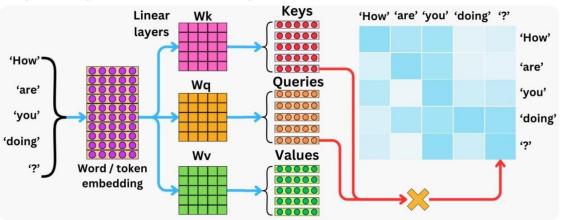
\* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one



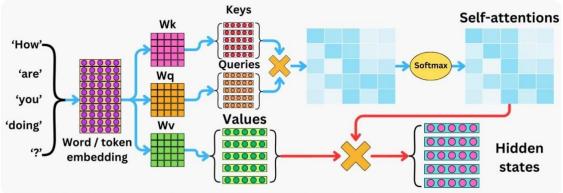




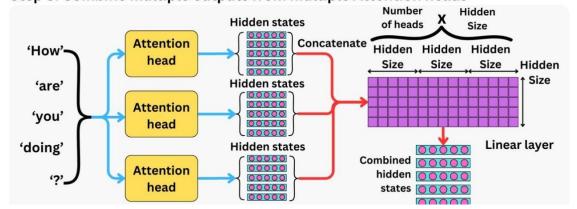
Step 1: Compute the scores that captures the token-token interaction



Step 2: Compute the hidden states



Step 3: Combine multiple outputs from multiple Attention heads



### **Encoder-Decoder Attention**

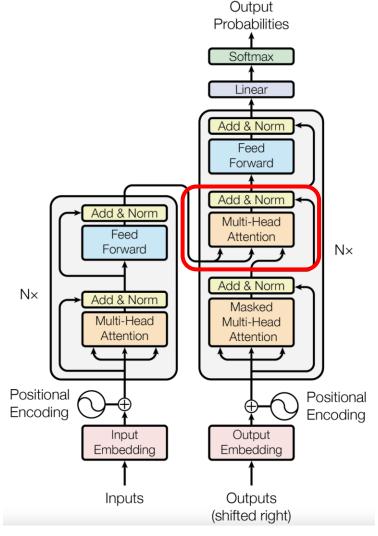
aka cross-attention

connection between encoders and decoders

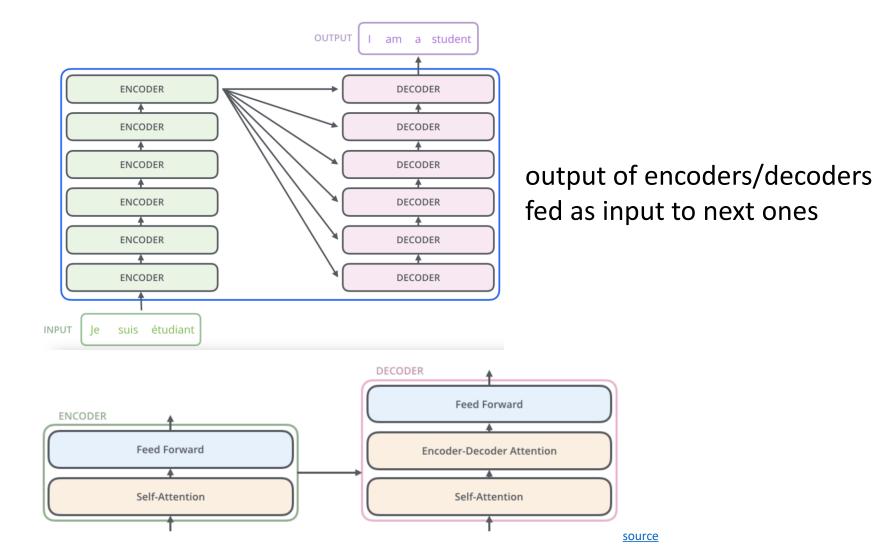
attention layer helping decoder to focus on relevant parts of input sentence (similar to attention in seq2seq models)

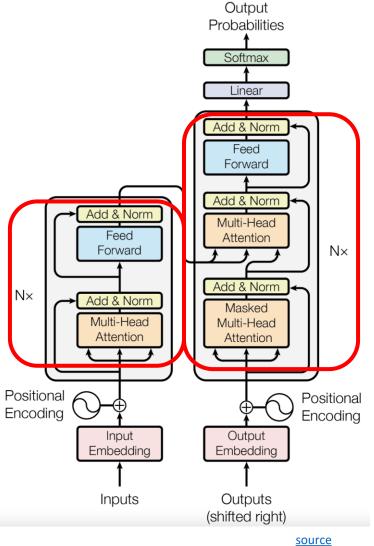
output of last encoder transformed into set of attention matrices K and V  $\rightarrow$  fed to each decoder's cross-attention layer (redundancy)

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



## Encoder and Decoder Stacks

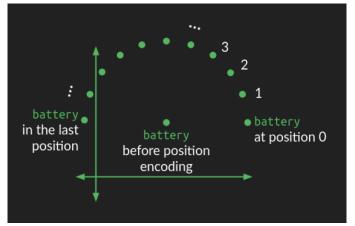




# Positional Encoding

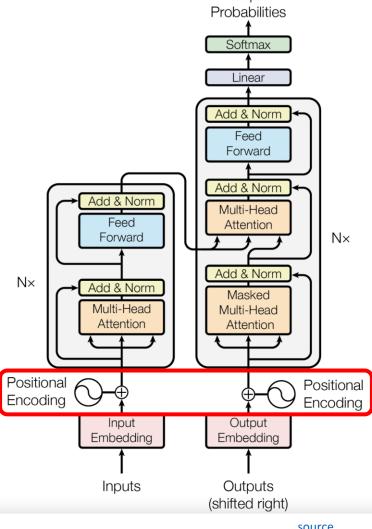
attention permutation invariant  $\rightarrow$  need for positional encoding to learn from order of sequence added to input embeddings (same dimension  $d_{\mathrm{model}}$ ) different choices for positional encoding:

- learned (by including absolute position in embedding)
- fixed, e.g., sine/cosine functions for each dimension i



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

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

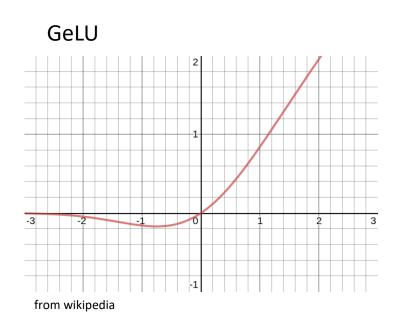


Output

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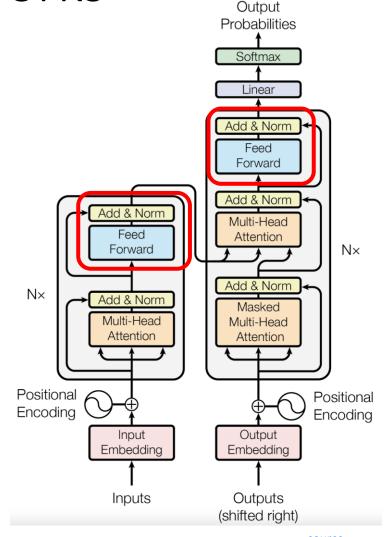
## Position-Wise Feed-Forward Networks

for each encoder or decoder layer: identical feedforward network independently applied to each position

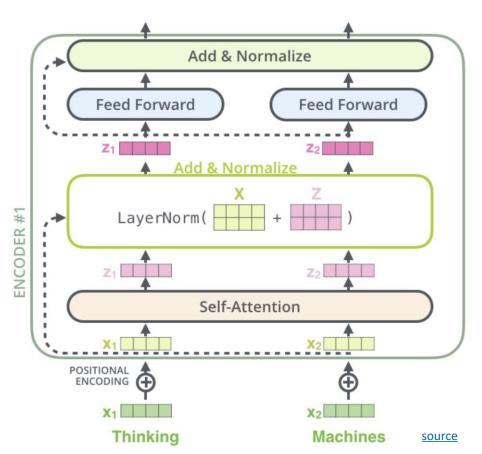


→ need for non-linearities (often
 GeLU activations) to capture more complex patterns

typically expand-and-contract (two layers) network



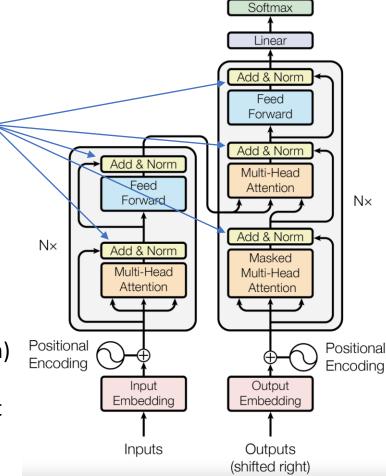
# Skip Connections and Layer Normalization



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)



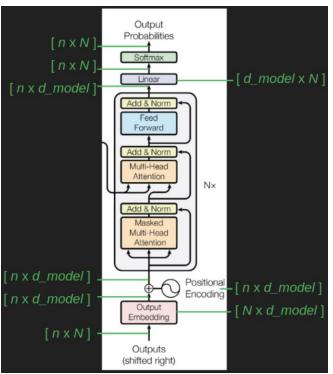
Output Probabilities

# De-Embedding and Softmax

n: maximum sequence length

N: vocabulary size

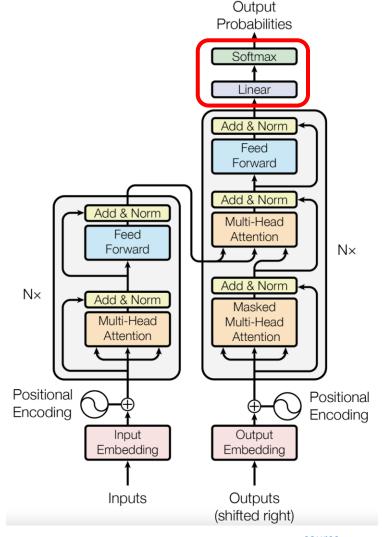
*d\_model*: embedding dimensions



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)

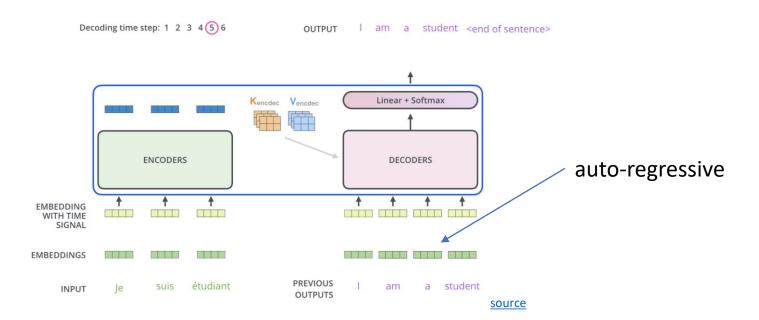


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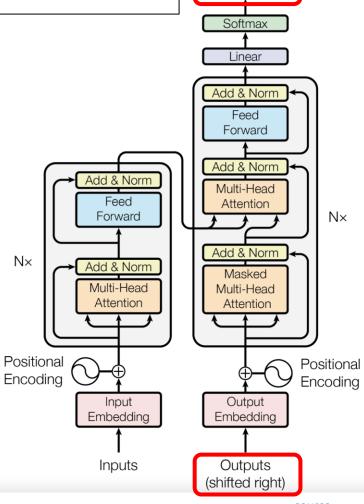
# Sequence Completion

- 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  $\rightarrow$  increasing uncertainty

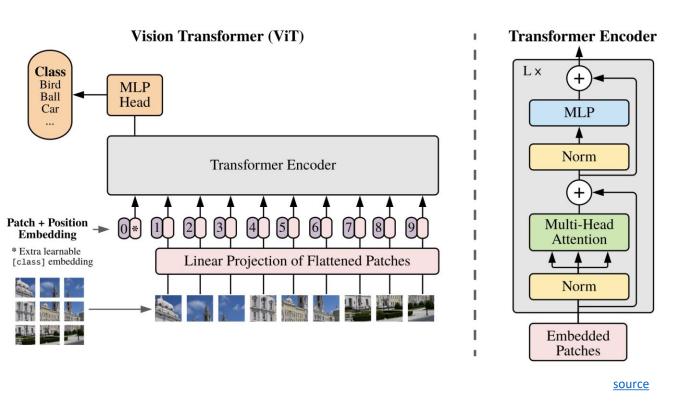


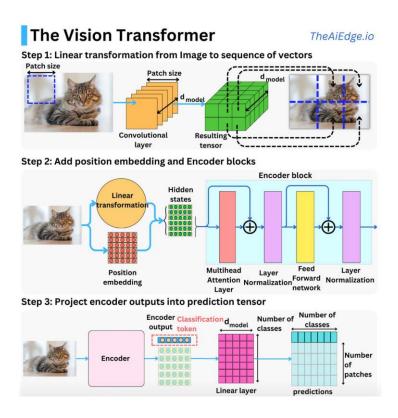
prompt: externally given initial sequence for running start and context on which to build rest of sequence (prompt engineering)



Output Probabilities

# Image Classification with Vision Transformer

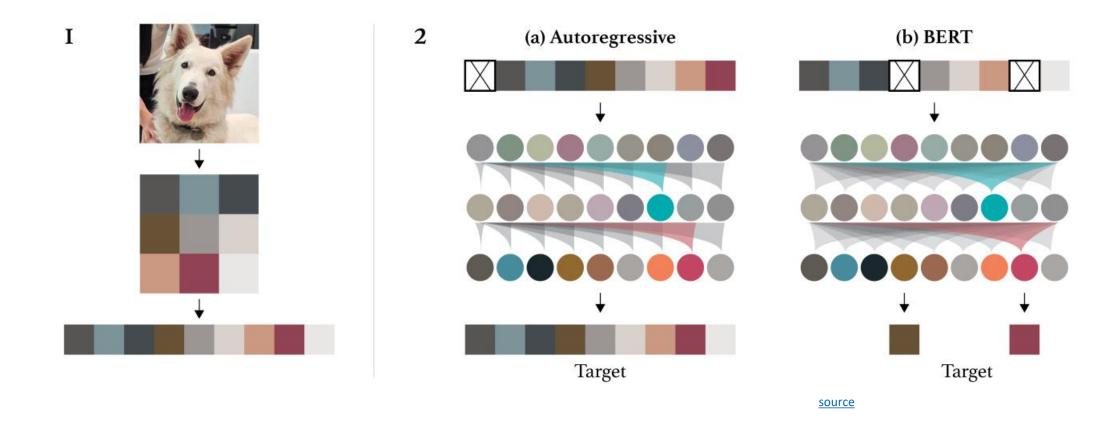




formulation as sequential problem: split image into patches (tokens) and flatten, add positional embeddings

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

# Pixel Generation (iGPT)



# Open-Source Implementations

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

more powerful:

nanoGPT, LitGPT