Deep Learning - MAI

Theory - Transformers

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Disclaimer:

Many of the works this lesson is based on have not been thoroughly replicated yet. Conclusions and interpretations may be unreliable.

Context

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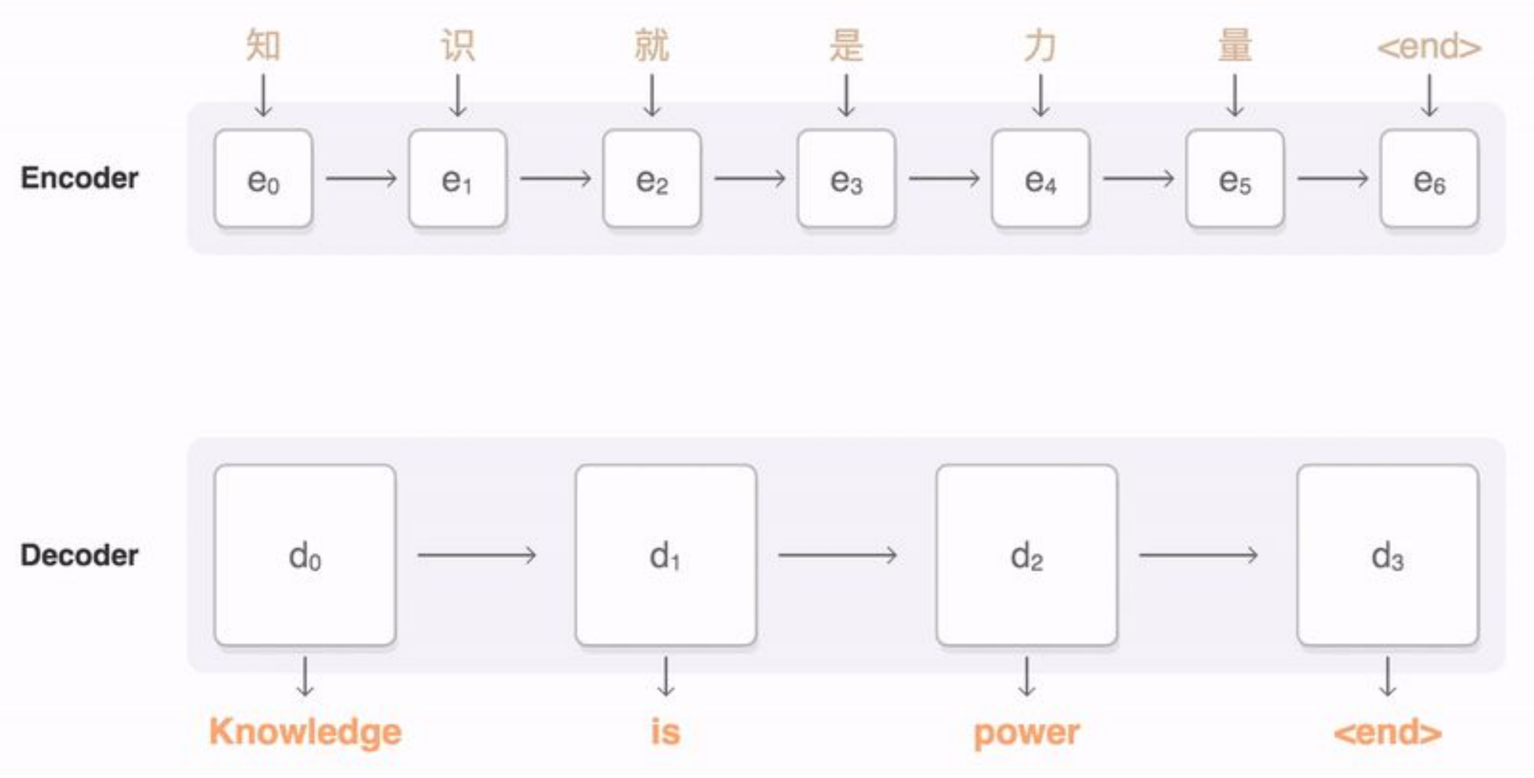
From Encoder-Decoder to Attention

- seq2seq limitations
  - Full sentence into a fixed-sized, unique embedding (bottleneck)
  - Different parts of the decoder focus on different parts of the input

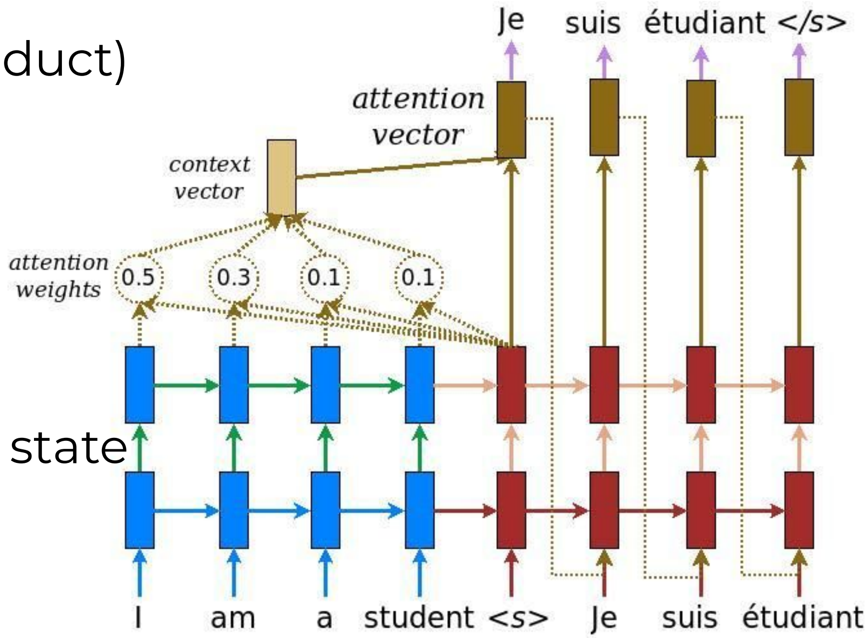
- Solution: Attention
  - Let each decoder step decide which part of the input use

Attention overview



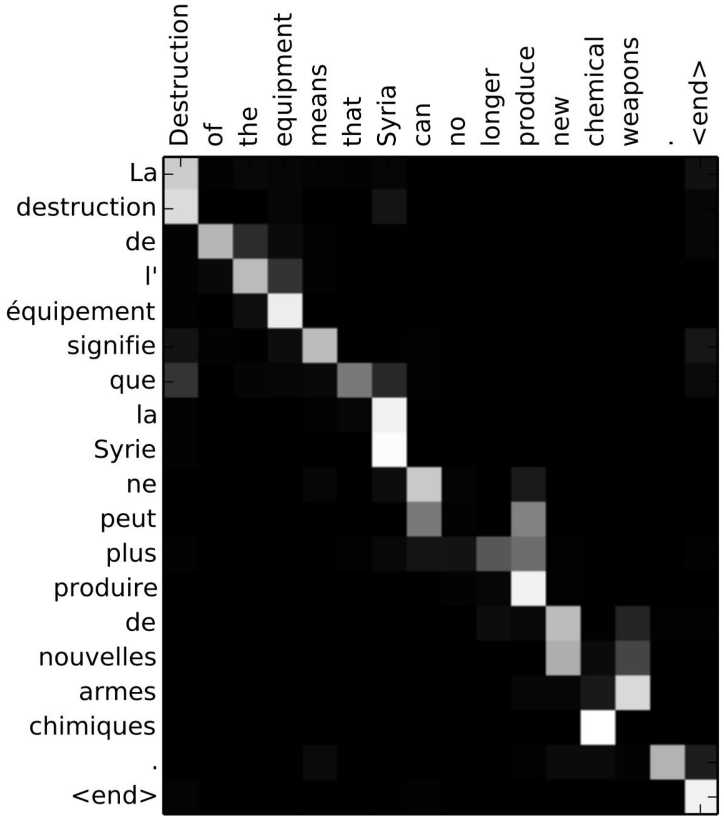
Seq2seq with attention

- Each decoder state
  - Scores prev. hidden states (dot product)
  - Turn into probabilities (softmax)
  - Sum to make the **context vec**.
  - Concatenate with hidden decoder state
  - Output and fed to next step



Why seq2seq with attention

- Enables one different context for each decoding step
  - No fix-sized bottleneck
- Provides shortcuts (better gradient flows)
- More fine-grained -> better interpretability



Attention to Transformers

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The limits of RNNs

- The main challenges of RNNs
  - Distances (long, short or both?)
  - Directionality (data accessibility)
  - Lack of focus specificity (all look the same)
  - Poor parallelization
- How can we solve that?
  - As long as we work with **sequences**, is tough
  - Memory is hard to implement
  - Computational dependencies by sequential design

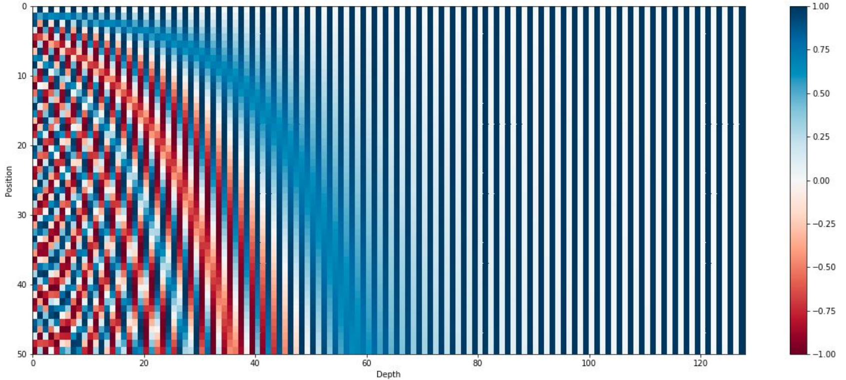
The Attention revolution

- What if we get rid of the sequence? What if attention is enough?
  - No more sequences, no more memory, no more dependencies
  - Meet the Transformers
- Closer to fully connected than RNNs.
- All tokens processed concurrently (instead of recurrently)
  - *Sets* instead of sequences
  - Self-attention for focus

Transformers and ~~Order~~ Position

- We need to keep some notion of position
  - Add order information on the input token embedding
  - Token representation changes with position
- *Positional encoding* through Sinusoidal functions
  - Add the position vector to each embedding
  - Provides consistent distances in the embedding space
    - Regardless of sequence length
    - Bounded range of values
    - Deterministic

50 positions
128 embedding
[-1,1] range



Self-attention

“A mechanism relating different positions of a single sequence in order to compute a representation of the sequence.”

Ashish Vaswani @ Google Brain

Why attention works

- Pseudo-limited connectivity (learnt sparsity, dense computation)
- What should be computed together with input X?
- Learn and use a ‘mask’
  - **Query** for what you want
  - Use **Keys** to match the query
  - Return the **Value** associated
- Let’s do it weightedly, through matrix multiply

Basic attention

- Three weight matrices (**Q**,**K**,**V**) learnt
- Dot product from input embedding of token *X* and **Q**,**K**,**V** matrices
  - **Q**,**K**,**V** vectors for token *X*
- Attention of token *X* on token *Y*:
  - Dot product between **Q** vector of *X* and **K** vector of *Y*
  - Normalize (sqr vec. length + softmax)
  - Multiply prob. by **V** vector of *Y* and sum -> output!

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

Multiple Embedding Spaces

- Multi-headed attention
- Learn different sets of Q,K,V matrices
- Each provides a different view on the data (enforceable on att. weights)
- On output
  - Concat all output embeddings in feature dim.
  - Multiply by another learnt matrix
- Attention heads can be computed in parallel

Computing in Parallel

- Attention relates inputs at arbitrary distance within **constant** num. ops
- ByteNet does so within a **logarithmic** num. ops (dilated convolutions)
- Convs s2s does so within a **linear** num. ops
- Retaining memory is more complicated as this grows

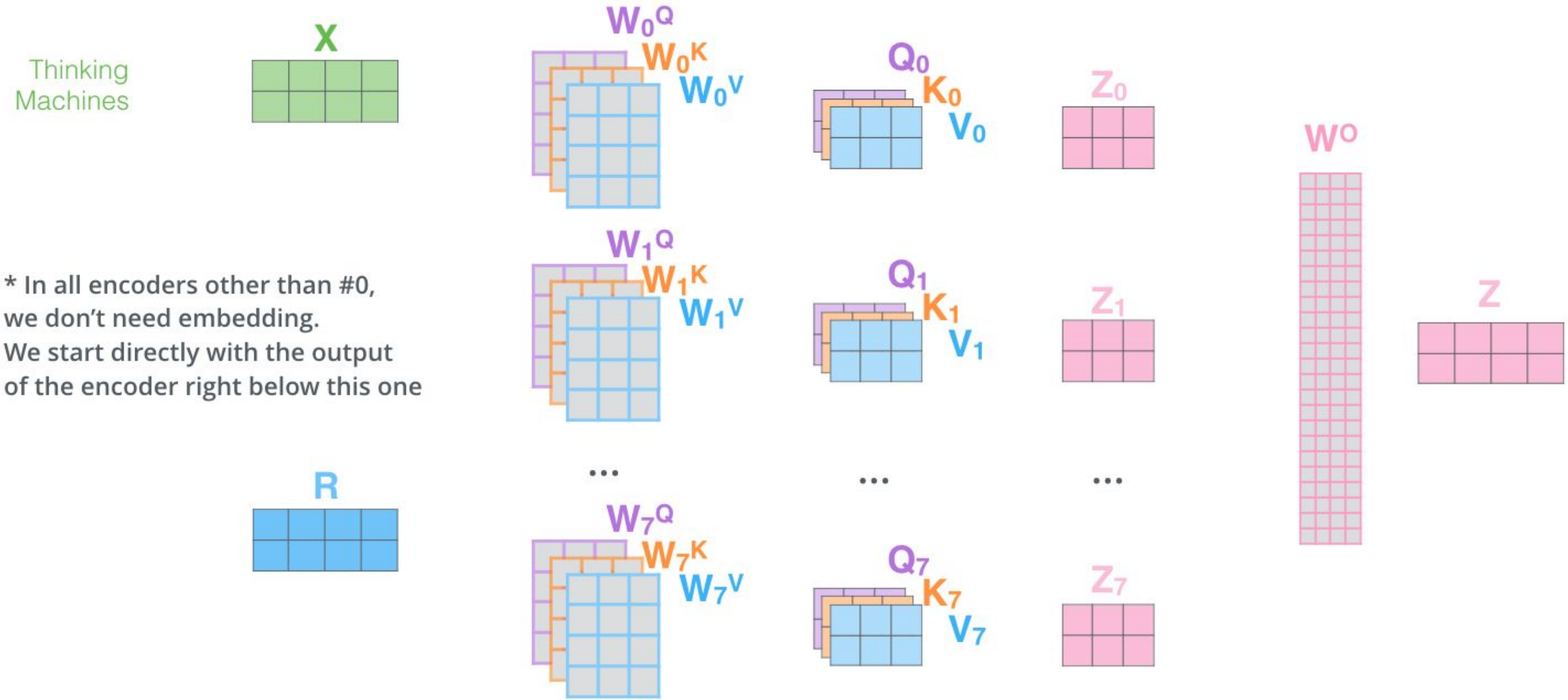
1) This is our input sentence*

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

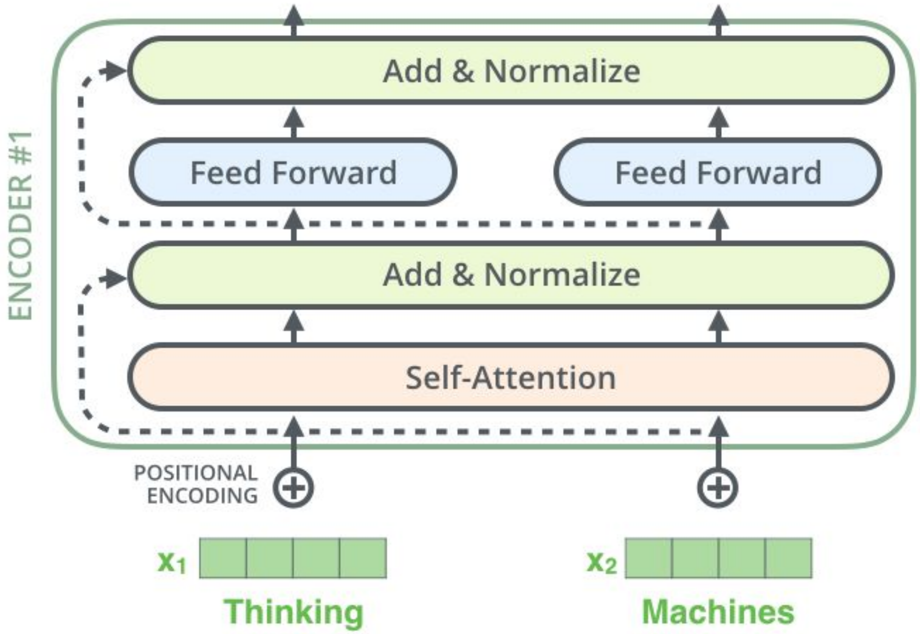
5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer



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

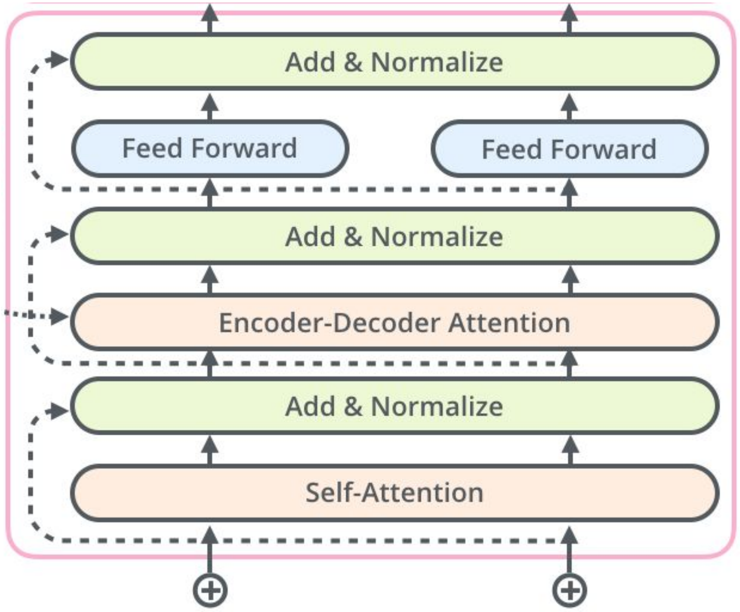
The Encoder block

- Self-Attention + Feed Forward
- Both with
  - Residual connection
  - Layer normalization
- Stack several of these blocks



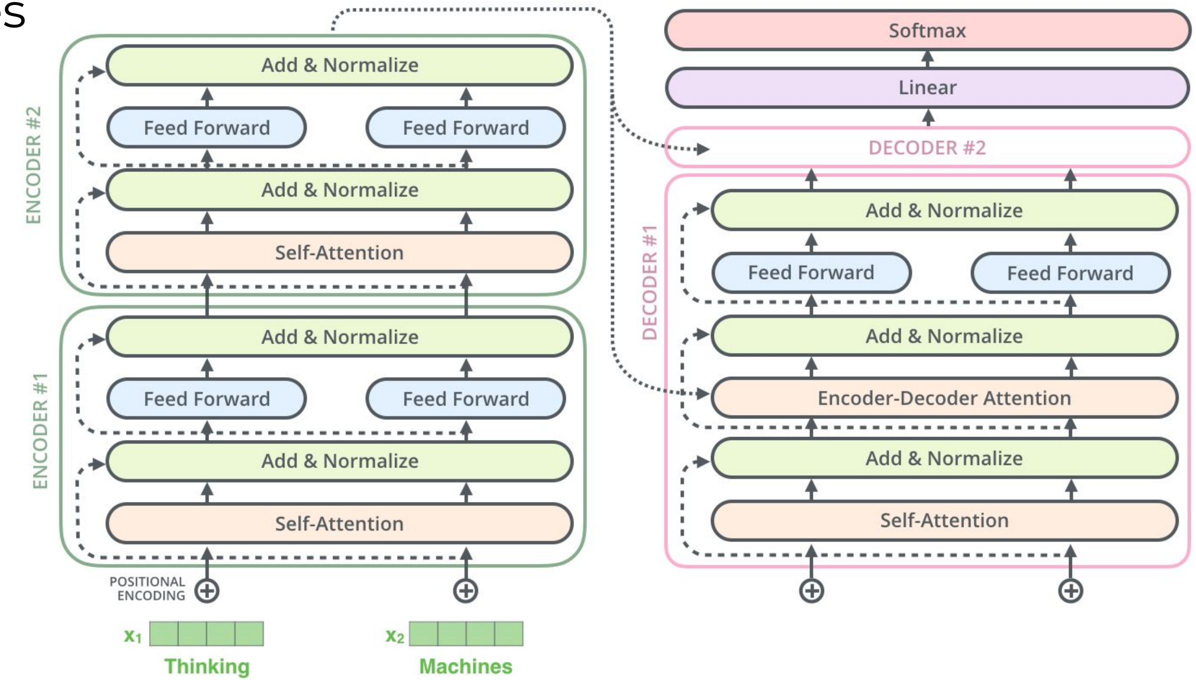
The Decoder block

- Same components as encoder
  - Self-Attention in the past only (mask out previous tokens)
  - Encoder-Decoder attention (**K** & **V** from encoder)
  - Feed Forward, Residual & Norm
- Input: Special token, then previous token (also with pos. encoding)



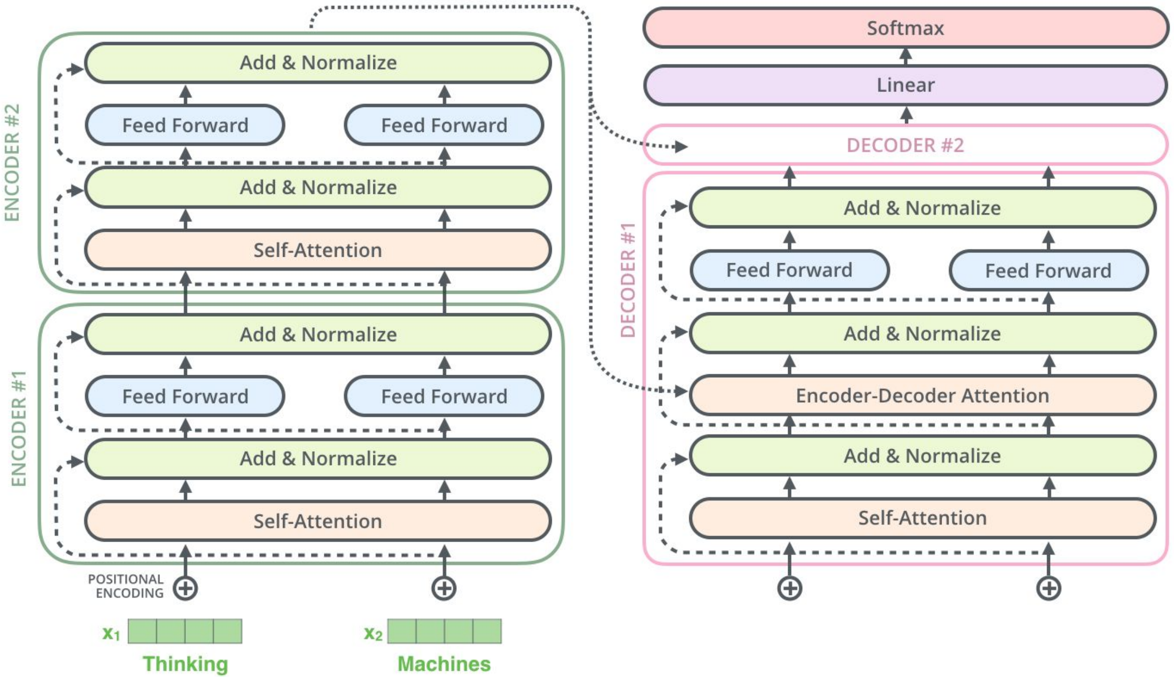
From input to output

- Linear layer for logits (dictionary length!)
- Softmax for probabilities



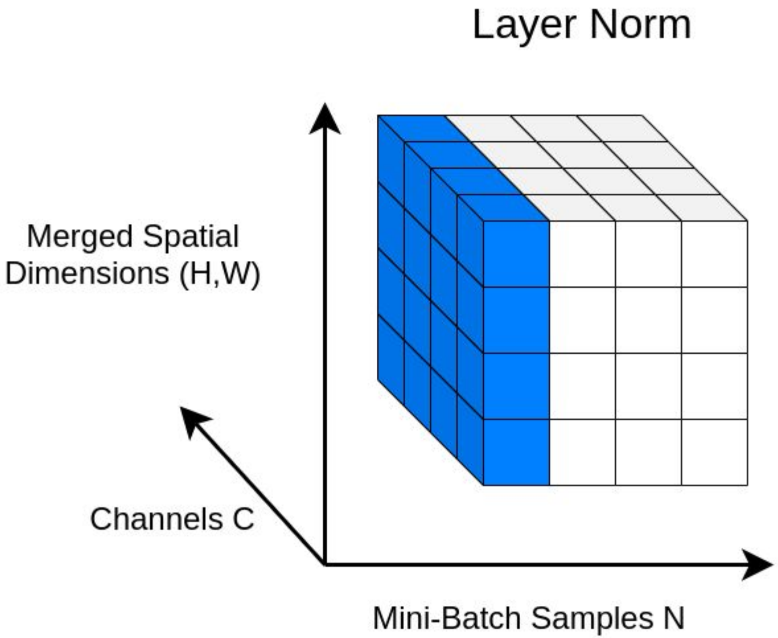
General Transformers

- Without positional encoding, a transformer is a fully connected NN with focus



Layer Normalization

- ❖ Normalize sample-wise
- ❖ Compute mean and std-dev across spatial dimensions (1 for sequences) and channels



Loss & Training

- A transformer outputs a vector of probabilities a number of times (?)
  - Cross entropy loss against golden probabilities*
- Batch training requires padding
- As with RNNs
  - Greedy search (explore one path only)
  - Beam search (explore *n* branches on each step)

Transformer details

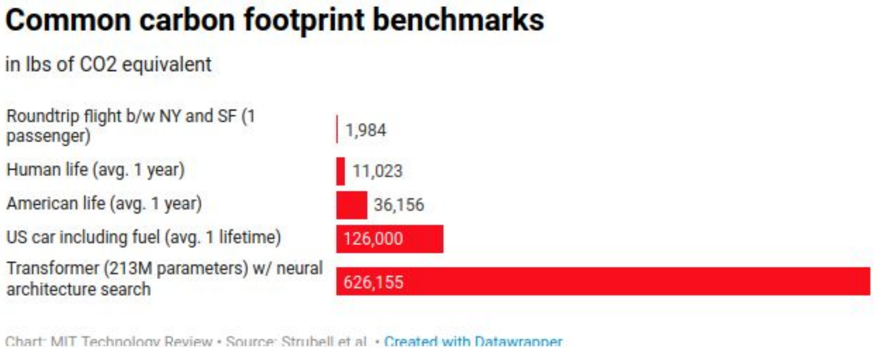
- In the original paper
    - Adam optimizer. Warm-up round and then decay
    - Dropout on residual connections, embeddings sums and pos. enc.
    - Label smoothing

Limitations of Transformers

- Reduced resolution (averaging attention)
  - Multi-head to circumvent
- Sequence length
  - All tokens must be computed concurrently (for context)
- Computational cost / Complexity
  - All relations are learnt (quadratic self-attention complexity). No limited connectivity by design.

A serious issue

- Transformers are efficient, but costly
  - Worthy trade-off?
  - Measuring efficiency
- Interpretability (too many heads)
- Google ethical crisis (Gebru, Bengio, ...)
  - Stochastic parrots
- Interpretability (too many heads) & Bias (too many data)



[63,64,73,74,75]

Fancy Transformers

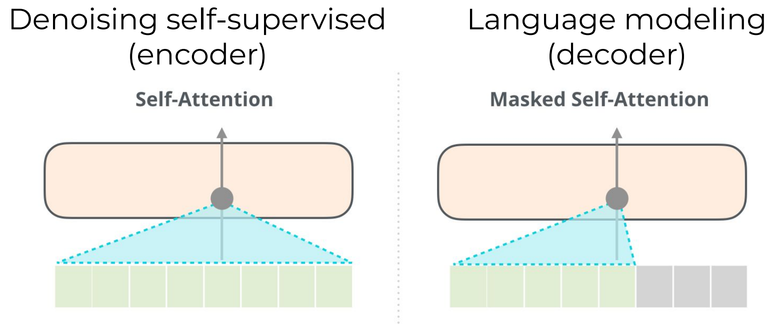
Beyond Encoder-Decoder

- Encoder-Decoder was inherited from RNN times
- Transformers (aka self-attention) is beyond that
- What works:
  - Pre-train heavy (as in Google-level, Millions of $)
  - Fine-tune for everything
- The story goes: GPT - BERT - GPT2 - GPT3 - ....
- Tell me how do you pre-train and...

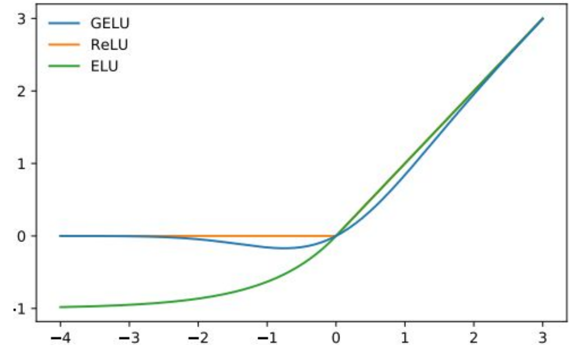
[68,69,76]

The two (main) sides

- Encoder only (BERT)
  - Bidirectional Transformer
  - Gain context (classification↑)
- Decoder only (GPT family)
  - Left to Right Transformer
  - Gain auto-regression (generation↑)



- GELU instead of ReLU
  - Gaussian Error Linear Unit



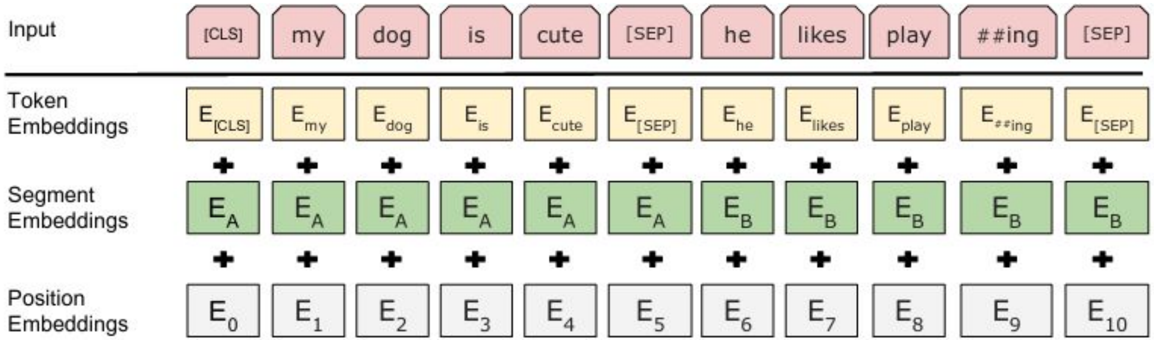
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

HPAI HIGH PERFORMANCE ARTIFICIAL INTELLIGENCE

[68,69,76]

Famous Transformers: BERT

- For text generation: Encoder only
- Special token to separate sentences, and embedded id (+pos. enc.)
- Train two tasks concurrently
  - Masked LM: Mask 15% of tokens, and try to predict them
  - NSP (Sentence prediction): Is the follow up sentence correct?



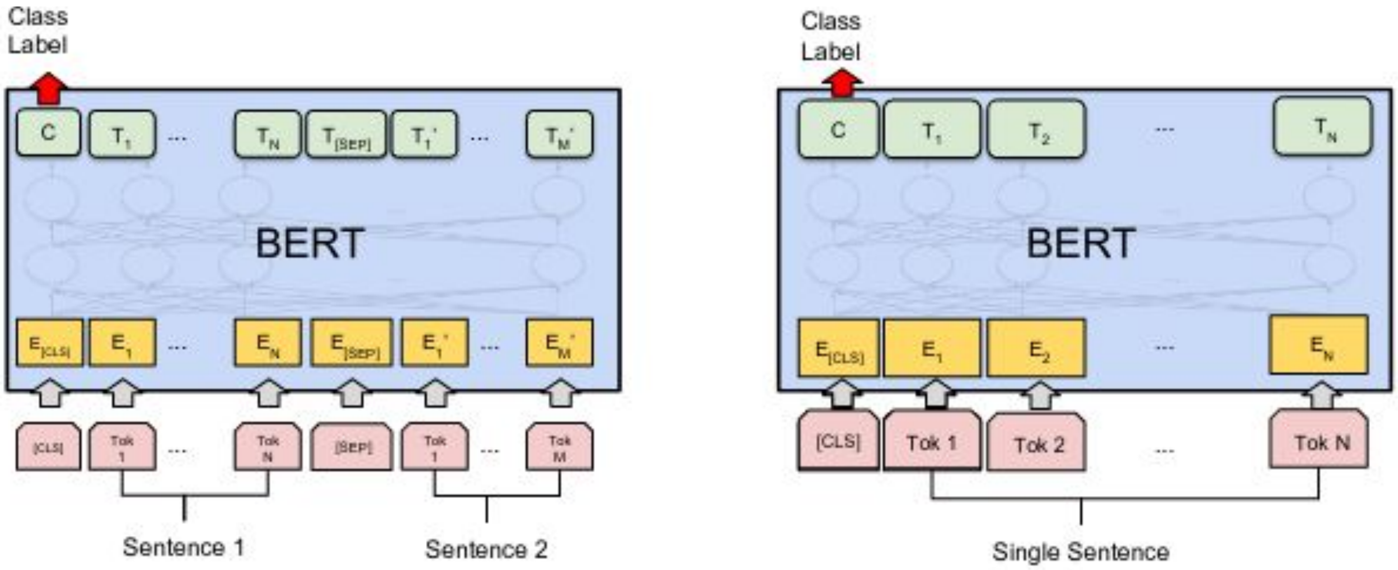
[65,66]

Famous Transformers: BERT

- Pre-train (bulk text) + fine-tuning (paraphrasing, QA, classification, ...)
- BERT-base:
  - 6 blocks, 12 encoder blocks, 110M params (4 TPUs 4 days)
- BERT-large
  - 12 blocks, 16 encoder blocks, 340M params (16 TPUs 4 days)
- Fine-tuning: 1 TPU 1 hour

[65,66]

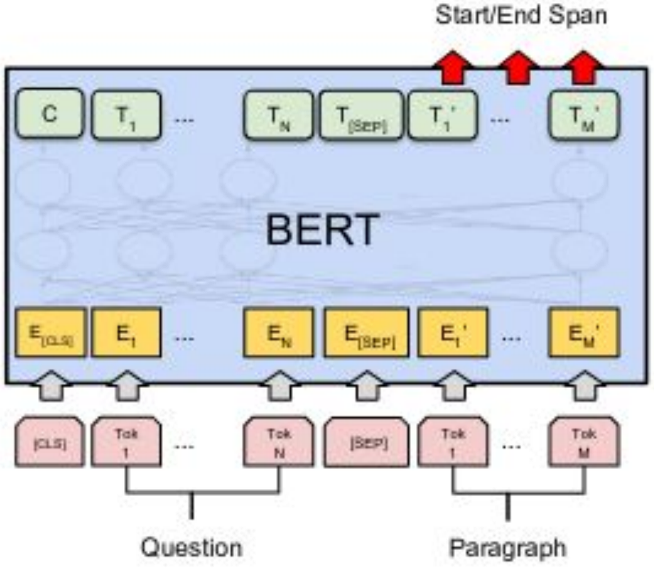
Famous Transformers: BERT



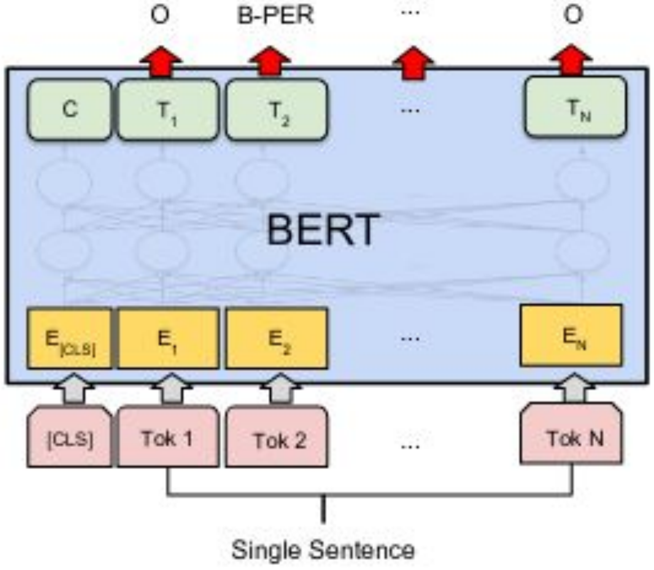
(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG

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

Famous Transformers: BERT



(c) Question Answering Tasks:
SQuAD v1.1



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

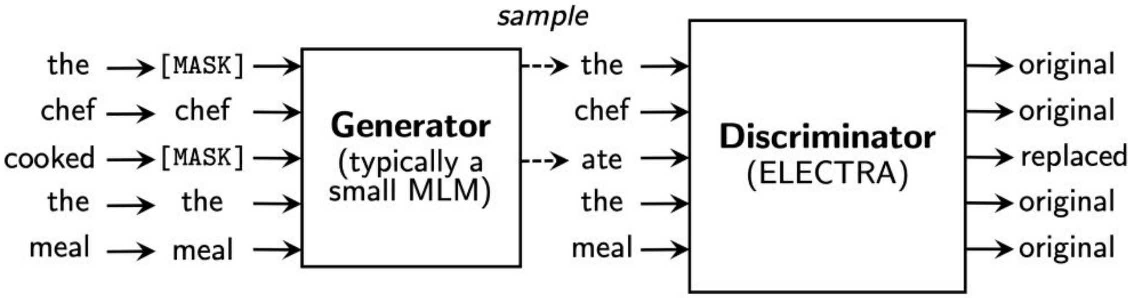
Famous Transformers: GPT

- GPT
  - Pretrain + fine-tune (117 M params)
- GPT2
  - More data, 48 blocks, zero-shot task/transfer (1,500 M params)
  - 1024 tokens
- GPT3 (& DALL-E)
  - More data, 96 blocks, 96 heads, (175 B params)
  - 2048 tokens

[67,78]

Pre-training Transformers like GANs

- Masked Language Model (BERT)
  - Limited token efficiency
  - Differences between train/test
- Electra
  - Generator / Discriminator scheme (keep the later)
  - Validate each token
  - Full token efficiency
  - Faster (12x)



[79,80]

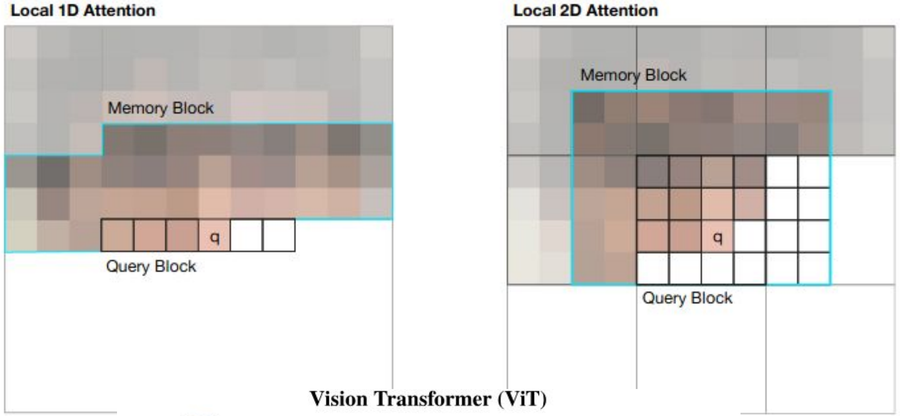
Vision Transformers (ViTs)

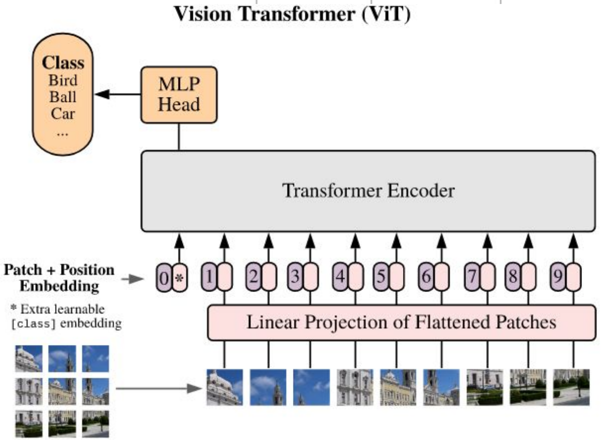
- Lack inductive biases implicit in CNNs
  - Translation invariance (weight sharing)
  - Locality (limited connectivity)
- **These can be learnt from enough data** (14M - 300M samples)
  - Mitigable by knowledge distillation - soft labels - noisy student (?)
- Each pixel attending to each other pixel is unfeasible
  - Several local self-attention mechanisms are being proposed

[70,72]

Vision Transformers (ViTs)

- Doing CNNs with Transformers
  - Self-attention limited spatially
  - Images flattened to 1D
  - Positional encodings
  - Attention bottlenecks
  - Autoencoders





[70,71,77,78]

So what are Transformers?

- Great models for processing data which can be represented as a set of independent numerical features
  - More powerful and smarter version of FFN nets
  - If computation and data availability allows!
- Capable of including location info through Positional Encodings
- Can be good for sequences (the shorter the better). Not for streams, recursion and hierarchies.
- The biggest hammer out there right now

[78,81,82]

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