Deep Learning - MAI

Theory - Transformers

Dario Garcia Gasulla
dario.garcia@bsc.es

Disclaimer:

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

Context

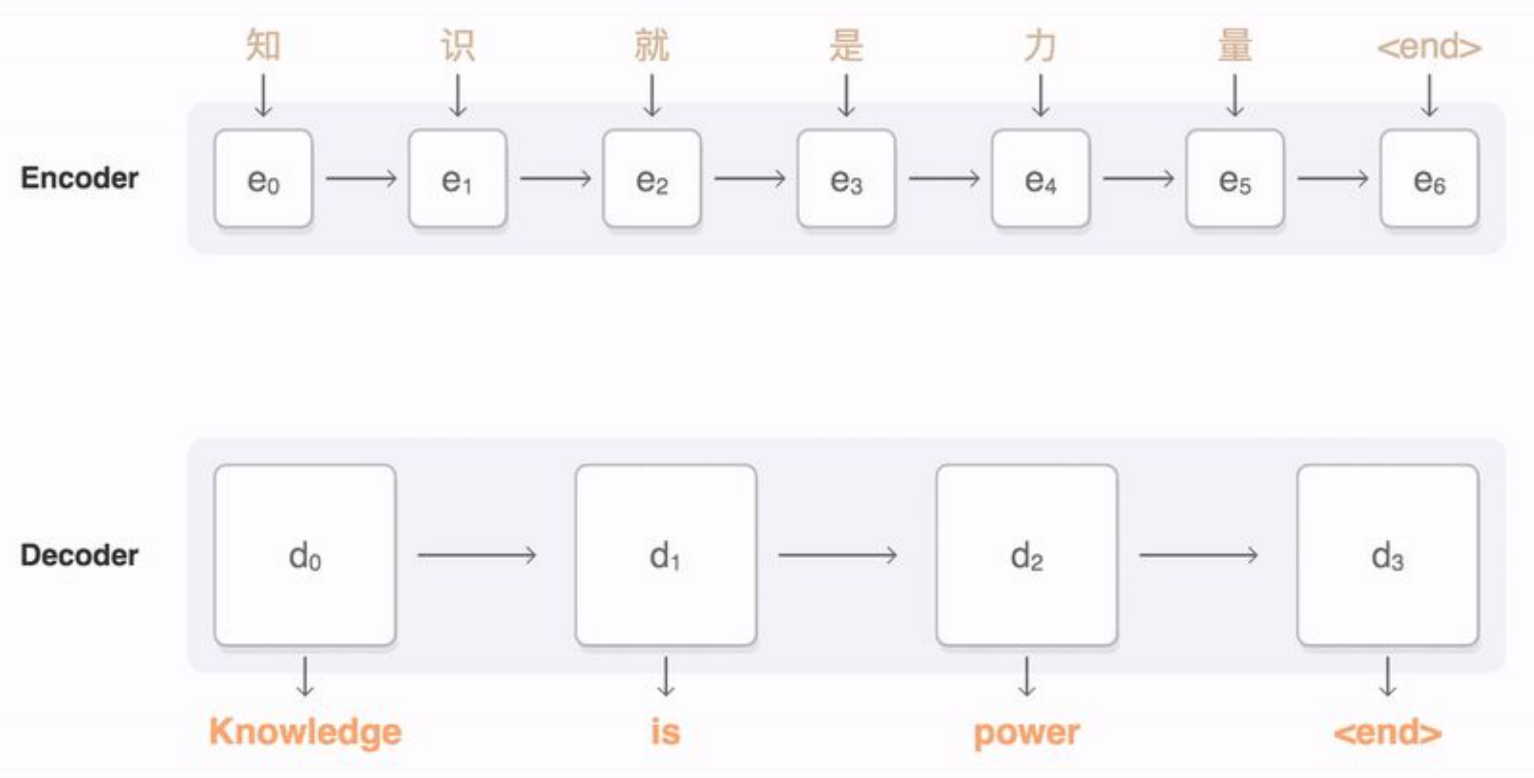
Dario Garcia Gasulla
dario.garcia@bsc.es

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

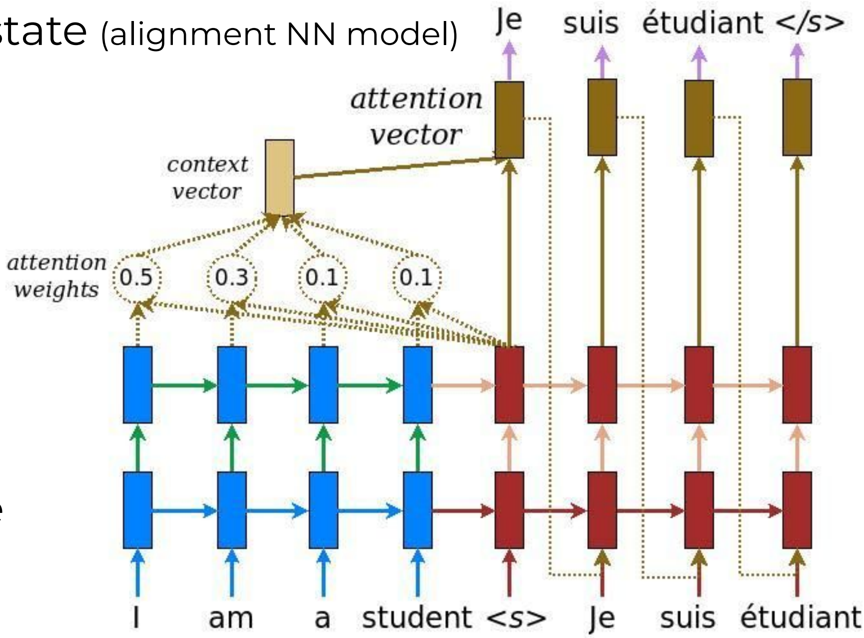
- Solution: Attention
  - Let each decoder step decide which part of the input use

Attention overview



Seq2seq with attention

- Each decoder state
  - Scores enc. hidden states w/ dec. prev. state (alignment NN model)
  - Turn into probabilities (softmax)
  - Dot prod. w/ hidden enc. states
  - Sum to make the fix-len **context vec**
  - Concatenate with hidden decoder state
  - Output and fed to next step



Attention to Transformers

Dario Garcia Gasulla
dario.garcia@bsc.es

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**, hardly
    - Memory is hard to implement
    - Computational dependencies by sequential design

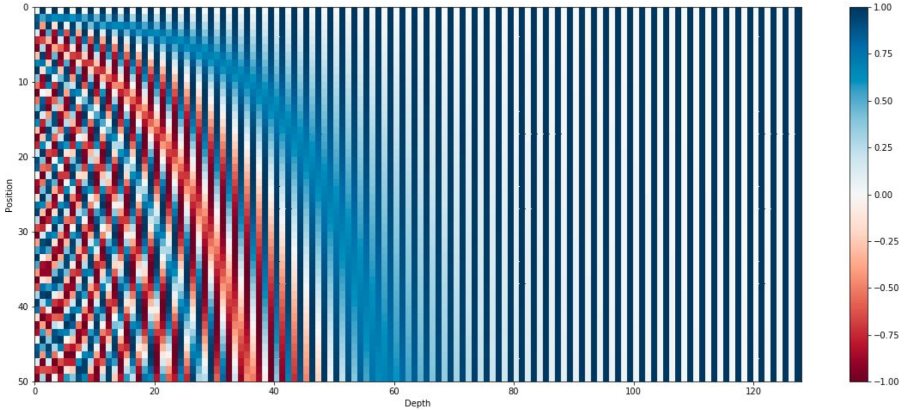
The Attention revolution

- 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)
  - Inputs are *sets* instead of sequences
  - Self-attention for focus

Transformers and ~~Order~~ Position

- Sets? Some notion of position is valuable
  - Add order information on the input token embedding space
  - Token representation changes with position
- *Positional encoding* through Sinusoidal functions
  - Add the position vector to each embedding (residual to keep alive)
    - Saves params
    - Orthogonal wrt embedding?
    - Concentrated in a few positions
  - Provides consistent distances
    - Regardless of sequence length
    - Bounded range of values
    - Deterministic

50 positions
128 embedding
[-1,1] range



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[54,55]

How basic attention works

- We want to process is all, but we cannot. Can we?
  - Pseudo-limited connectivity (learnt sparsity, dense computation)
- Every input token has its own embedding
- All tokens stacked (e.g., word embeddings) are the input
- Length of token is arbitrary (e.g., 512)
- Number of tokens defined by dataset (fixed)

Why attention works

- For all **X** ∈ tokens, for all **Y** ∈ tokens: What is the relevance of **Y** for **X**?
- Learn all combinations, and use a ‘mask’ to select
  - **Query** for what you want to match (current token X)
  - **Keys** to match the query with (other tokens Y)
  - **Value** to be returned (relevance between both)
- Let’s do it weightedly, through matrix multiply
  - No dependencies. Parallelism!

3 not-so-little matrices

- Three weight matrices (**Q**,**K**,**V**) learnt
  - One row per input token
  - Arbitrary length (typically smaller dimensionality than token)
- **Q** & **K** matrices store the sorted & relative importance of pairs of tokens
- **V** matrix stores the information about the token itself
- With **Q** & **K** we get a relevance [0,1], used to weight **V**

Basic attention

- Attention of token *X* on token *Y* (all with all):
  - Dot product between **Q** vector of *X* and **K** vector of *Y*
  - Stabilize gradients (div. square root of vector length)
  - Normalize (apply softmax)

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

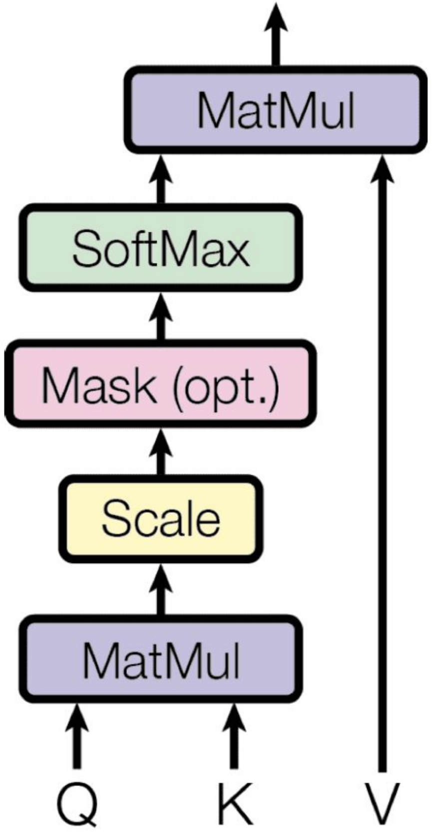
  - Multiply by **V** vector of *Y* (weighting Y by relevance of Y w.r.t X)
  - Sum over all *Y* -> output for *X*
  - In: 1 Token embedding, 1 Q row, K matrix (n T.E.), V matrix (n T.E.) // Out: 1 vector

Multiple Embedding Spaces

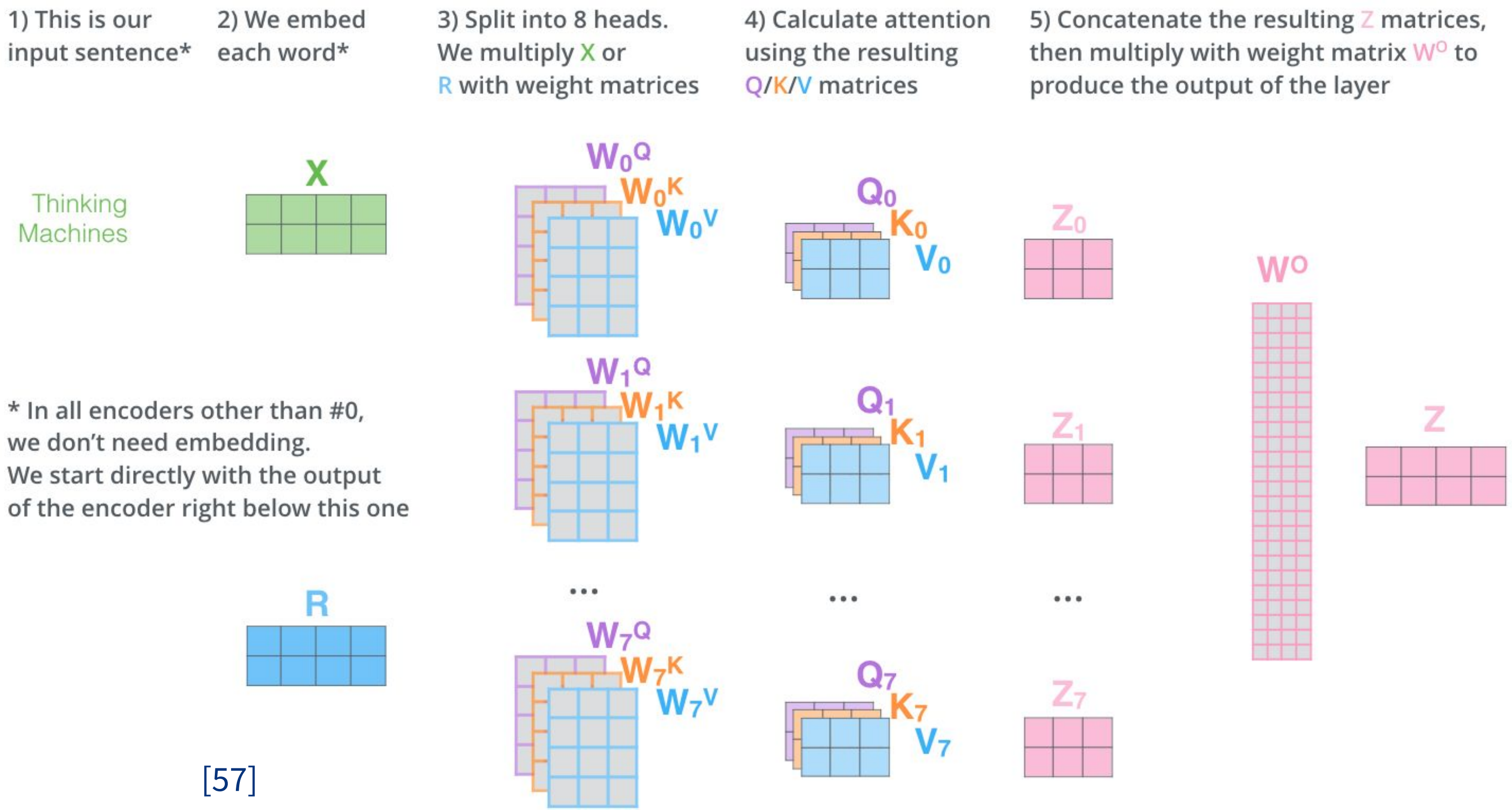
- Multi-headed attention
- Learn different sets of Q,K,V matrices
- Each provides a different view on the data (enforceable on att. weights)
- On output
  - Concat all output embeddings in feature dimension
  - Multiply by another learnt matrix to fit dimensionality
- Attention heads can be computed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

Computing in Parallel

- Attention relates inputs at arbitrary distance within **constant** num. ops
  - Close or far away, it's the same
  - Fully-connected style (all with all)
- 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

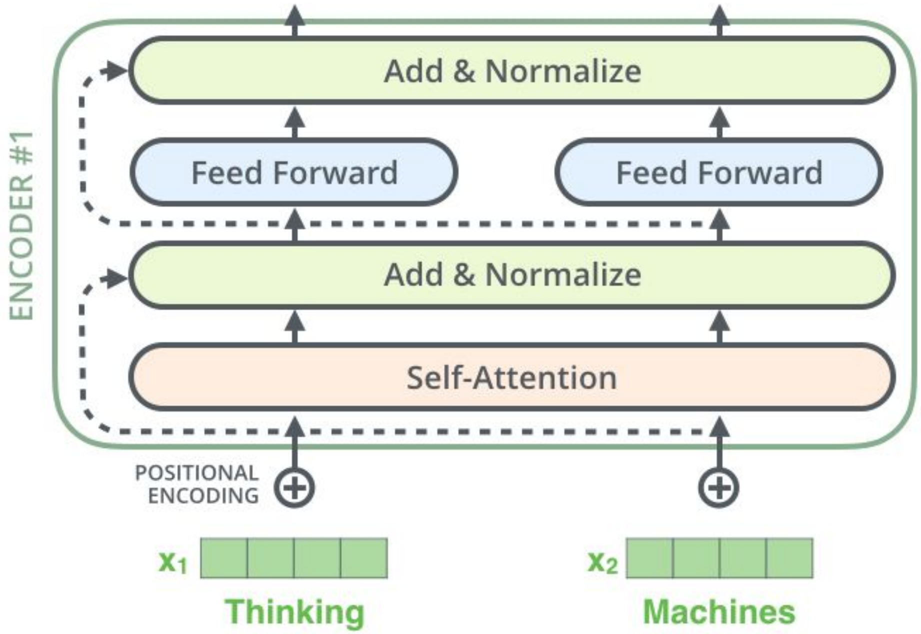


Visual Summary



The Encoder block

- Self-Attention + Feed Forward
  - Each token follows its own path
- Both with
  - Residual connection
    - To self-attend or not
  - Layer normalization
    - Sample-wise layer-wide mean and var.
- Stack several of these blocks

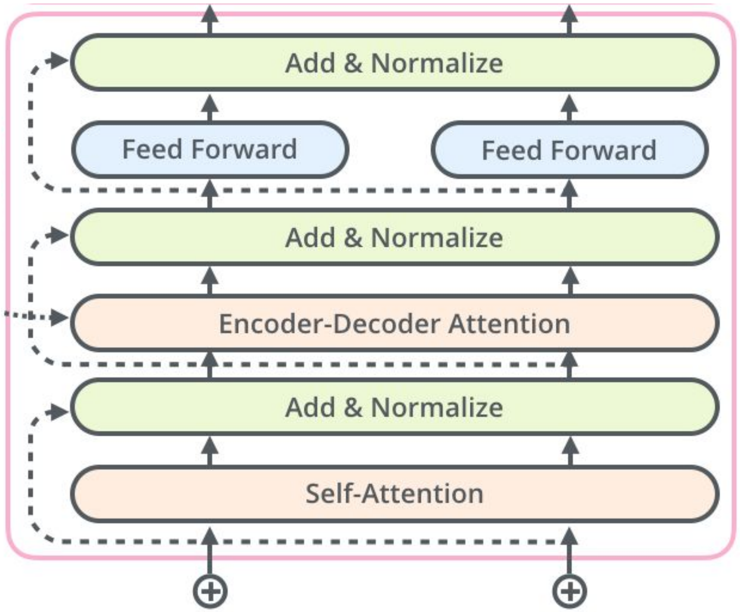


The Decoder block

- Same components as encoder
  - Self-Attention in the past only

    (mask out future tokens, unidirectional)
  - Encoder-Decoder attention

    (**K** & **V** from encoder, **Q** from prev dec.)
  - Feed Forward, Residual & Norm
- Input: Special token, then previous token (also with pos. encoding)

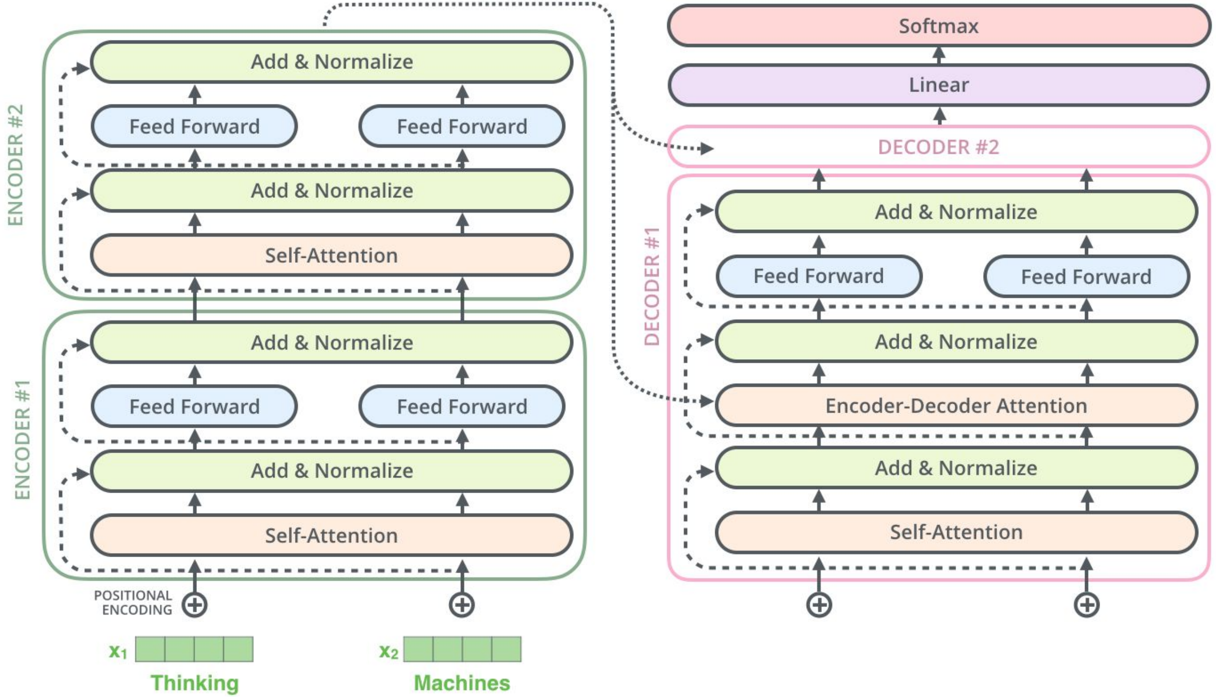


Self-attention: Look at what has been decoded
Encoder-Decoder Attention: Look at the original input

[57,85]

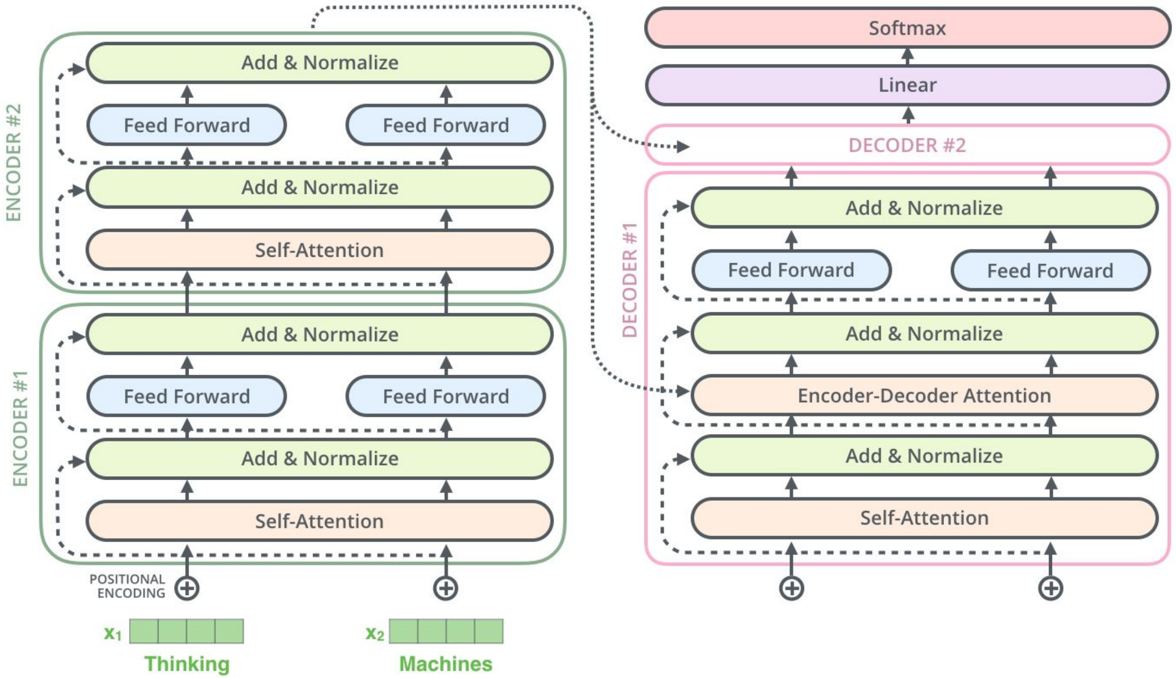
From input to output

- Linear layer
  - Creates logits
  - Dictionary length
- Softmax
  - Probabilities



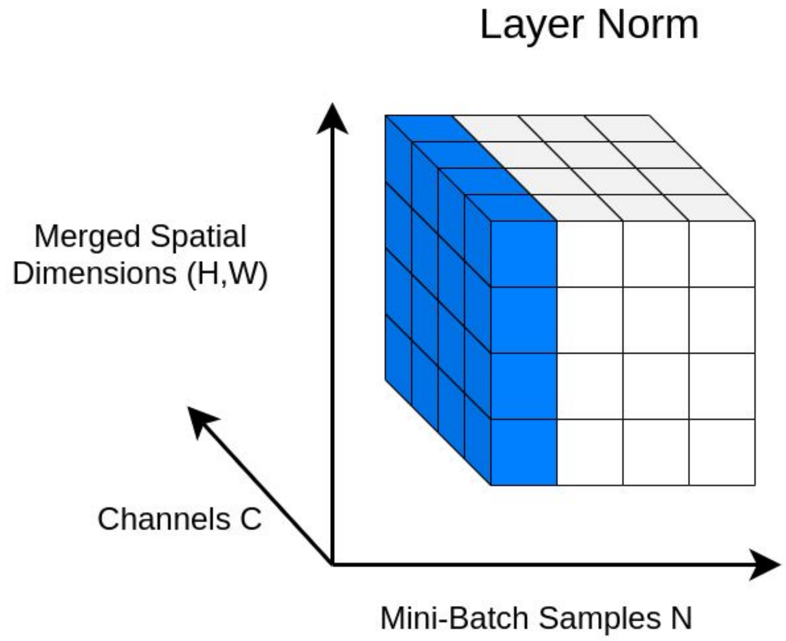
General Transformers

- Without Pos. Enc., and a single attention head, transformer is a fully connected NN, with 3 vectors of weights per input



Layer Normalization

- Normalize sample-wise
  - Batch independent
  - Unique across layer
- Compute mean and std-dev across spatial dimensions (1 for sequences) and channels



[56, 56bis]

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, and due to their masks, decoders use
  - Greedy search (explore one path only)
  - Beam search (explore *n* branches on each step)

Transformer details

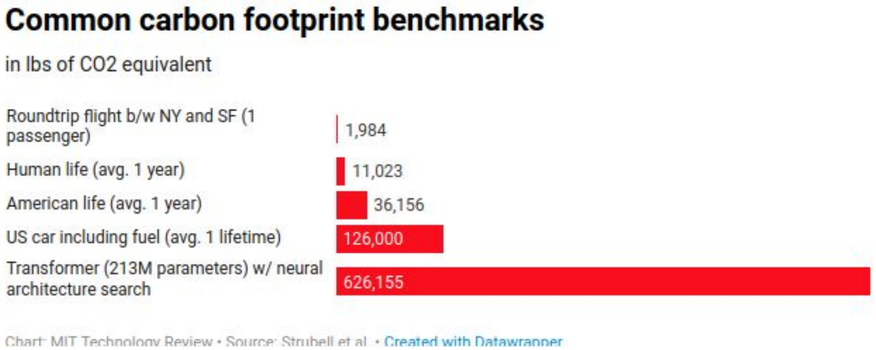
- In the original paper
  - Adam optimizer. Warm-up round and then decay
  - Dropout on residual connections, embeddings sums and pos. enc.
  - Label smoothing (One-hot vector enc + uniform distr. [0,1])

Limitations of Transformers

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

A serious issue

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



On the Dangers of Stochastic Parrots: Can Language Models Be Too Big?

[63,64,73,74,75]

Fancy Transformers

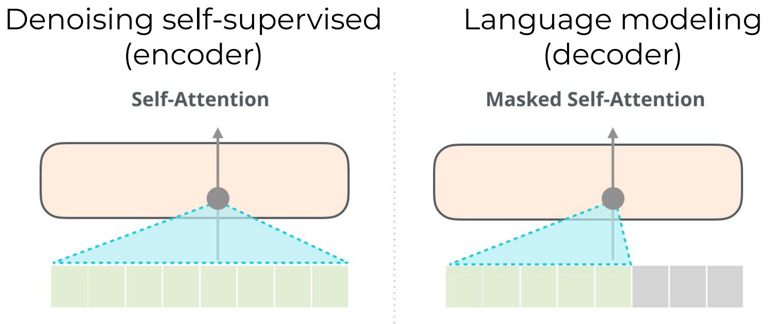
Beyond Encoder-Decoder

- 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...

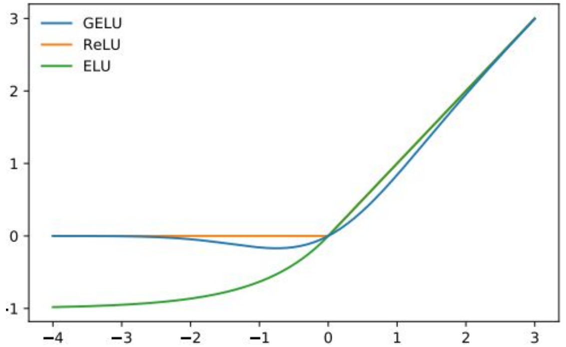
[68,69,76]

The two (main) sides

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



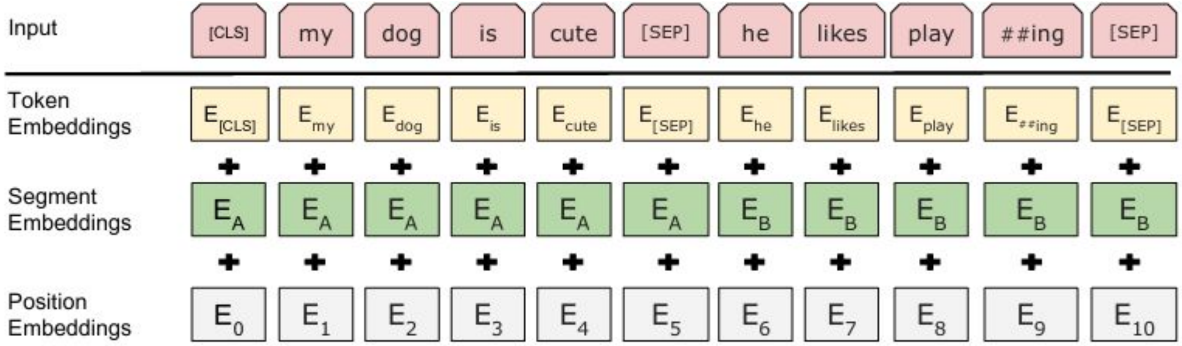
- GELU instead of ReLU
  - Gaussian Error Linear Unit



[68,69,76]

Famous Transformers: BERT

- For text generation: Encoder only
  - Token embedding
  - Special token to separate sentences
  - Sentence embedding
  - Pos. encoding



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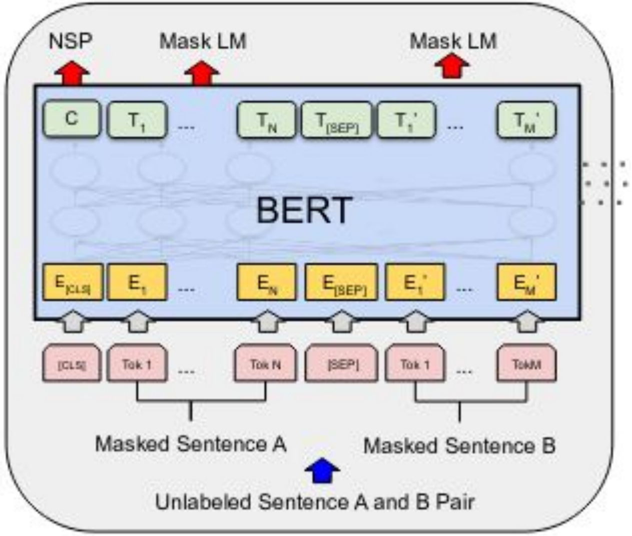
[65,66]

Famous Transformers: BERT

- Train two tasks **concurrently**
  - Masked LM: Mask 15% of tokens, and try to predict them
  - NSP (Sentence prediction): Is the follow up sentence correct?
    - Different relation than LM
  - Corpus: Books and Wikipedia
    - Long sentences and contexts



[65,66]

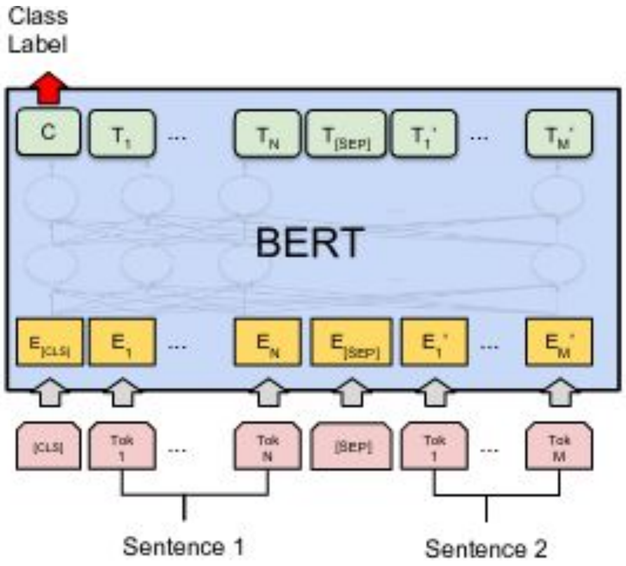
Famous Transformers: BERT

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

[65,66]

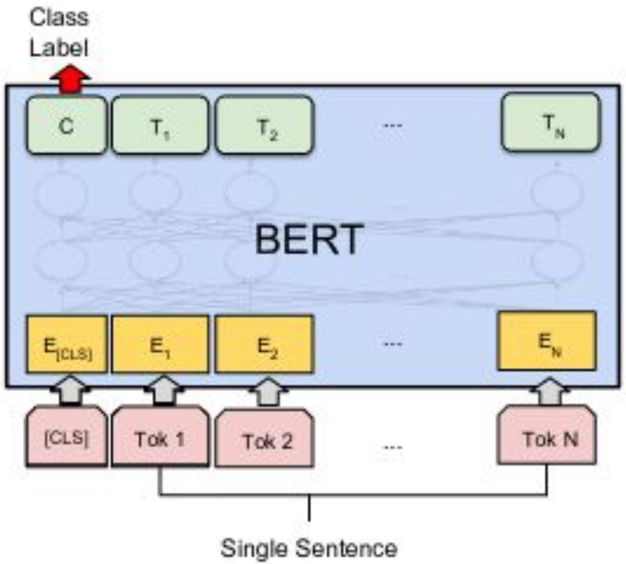
Fine-tuning BERT

- 2 sentence in / 1 class out



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

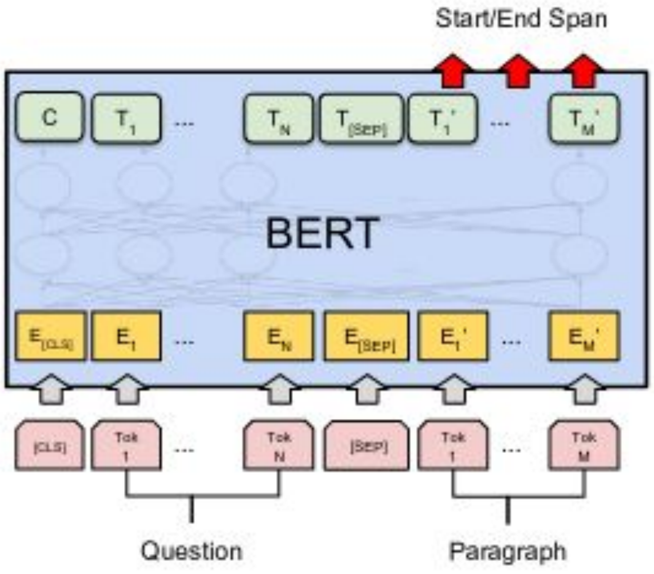
- 1 sentence in / 1 class out



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

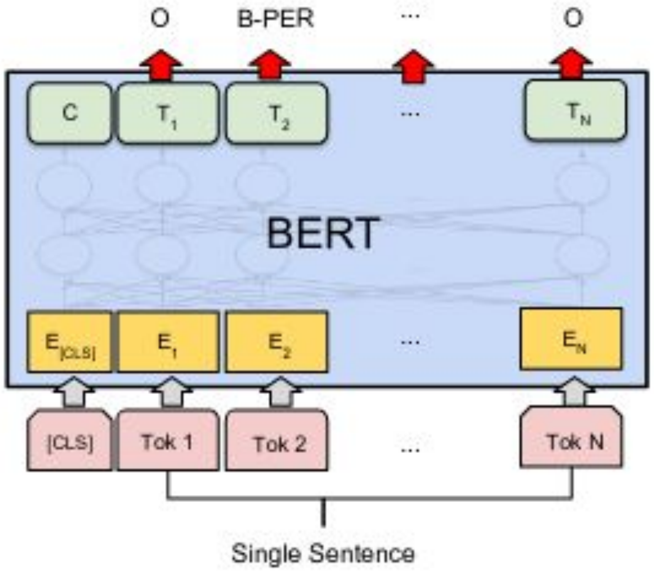
Fine-tuning BERT

- N sentence in / 1 sentence out



(c) Question Answering Tasks:
SQuAD v1.1

- 1 sentence in / 1 sentence out



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

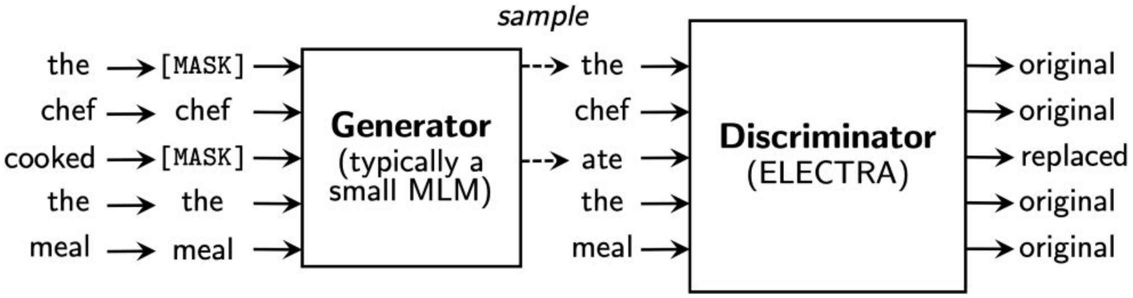
Famous Transformers: GPT

Masked decoder only!

- 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

Pre-training Transformers like GANs

- Masked Language Model (BERT)
  - Limited token efficiency due to Mask (less info per token)
  - Differences between train/test (Mask is gone)
- Electra
  - Generator / Discriminator scheme (keep the later)
  - Validate each token
  - Full token efficiency
  - Faster (12x)



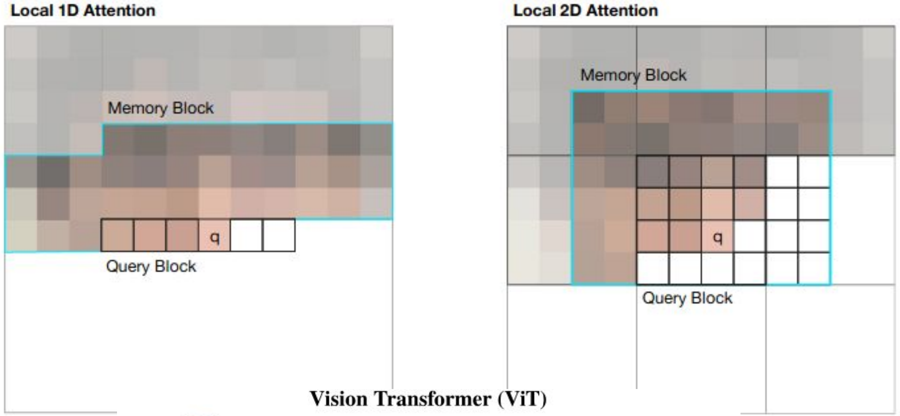
Vision Transformers (ViTs)

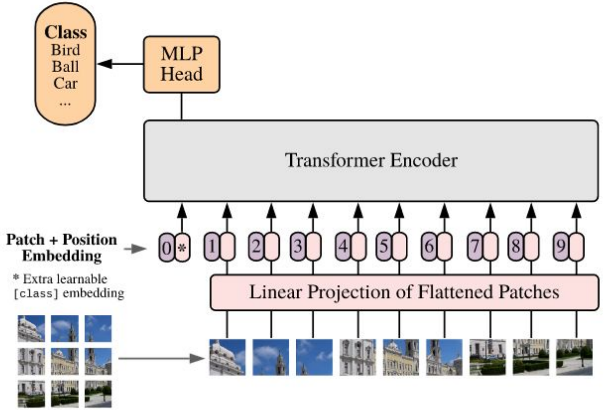
- Lack inductive biases implicit in CNNs
  - Translation invariance (weight sharing)
  - Locality (limited connectivity)
- **These can be learnt from enough data** (14M - 300M samples)
  - Mitigable by knowledge distillation - soft labels - noisy student (?)
- Each pixel attending to each other pixel 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]

References

References

[53] Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. "Attention is all you need." arXiv preprint arXiv:1706.03762 (2017).
[54] https://kazemnejad.com/blog/transformer_architecture_positional_encoding/
[55] https://timodenk.com/blog/linear-relationships-in-the-transformers-positional-encoding/
[56] https://theaisummer.com/transformer/
[56bis] https://arxiv.org/abs/1607.06450
[57] http://jalammar.github.io/illustrated-transformer/
[58] https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/

References

[59] http://nlp.seas.harvard.edu/2018/04/03/attention.html
[60] Kalchbrenner, Nal, Lasse Espeholt, Karen Simonyan, Aaron van den Oord, Alex Graves, and Koray Kavukcuoglu. "Neural machine translation in linear time." arXiv preprint arXiv:1610.10099 (2016).
[61] http://vandergoten.ai/2018-09-18-attention-is-all-you-need/
[62] Dai, Z., Yang, Z., Yang, Y., Carbonell, J., Le, Q. V., & Salakhutdinov, R. (2019). Transformer-xl: Attentive language models beyond a fixed-length context. arXiv preprint arXiv:1901.02860.
[63] Strubell, E., Ganesh, A., & McCallum, A. (2019). Energy and policy considerations for deep learning in NLP. arXiv preprint arXiv:1906.02243.
[64] https://www.technologyreview.com/2019/06/06/239031/training-a-single-ai-model-can-emit-as-much-carbon-as-five-cars-in-their-lifetimes/

References

[65] https://medium.com/@samia.khalid/bert-explained-a-complete-guide-with-theory-and-tutorial-3ac9ebc8fa7c

[66] Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2018). Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805.

[67] https://medium.com/walmartglobaltech/the-journey-of-open-ai-gpt-models-32d95b7b7fb2

[68] https://medium.com/@shoray.goel/gelu-gaussian-error-linear-unit-4ec59fb2e47c

[69] http://jalammar.github.io/illustrated-gpt2/

[70] Dosovitskiy, A., Beyer, L., Kolesnikov, A., Weissenborn, D., Zhai, X., Unterthiner, T., ... & Houlsby, N. (2020). An image is worth 16x16 words: Transformers for image recognition at scale. arXiv preprint arXiv:2010.11929.

References

[71] Parmar, N., Vaswani, A., Uszkoreit, J., Kaiser, L., Shazeer, N., Ku, A., & Tran, D. (2018, July). Image transformer. In International Conference on Machine Learning (pp. 4055-4064). PMLR.
[72] Touvron, H., Cord, M., Douze, M., Massa, F., Sablayrolles, A., & Jégou, H. (2020). Training data-efficient image transformers & distillation through attention. arXiv preprint arXiv:2012.12877.
[73] Bender, E. M., Gebru, T., McMillan-Major, A., & Shmitchell, S. (2021, March). On the Dangers of Stochastic Parrots: Can Language Models Be Too Big?🦜. In Proceedings of the 2021 ACM Conference on Fairness, Accountability, and Transparency (pp. 610-623).
[74] Dong, Y., Cordonnier, J. B., & Loukas, A. (2021). Attention is Not All You Need: Pure Attention Loses Rank Doubly Exponentially with Depth. arXiv preprint arXiv:2103.03404.

References

[75] Peter Henderson, Jieru Hu, Joshua Romoff, Emma Brunskill, Dan Jurafsky, and Joelle Pineau. 2020. Towards the Systematic Reporting of the Energy and Carbon Footprints of Machine Learning. Journal of Machine Learning Research 21, 248(2020), 1–43. http://jmlr.org/papers/v21/20-312.html
[76] https://hannes-stark.com/assets/transformer_survey.pdf
[77] Jaegle, A., Gimeno, F., Brock, A., Zisserman, A., Vinyals, O., & Carreira, J. (2021). Perceiver: General Perception with Iterative Attention. arXiv preprint arXiv:2103.03206.
[78] https://www.youtube.com/watch?v=PtdpWC7Sr98
[79] https://medium.com/dair-ai/bert-is-extremely-inefficient-this-is-how-to-solve-it-688b09350f10
[80] Clark, K., Luong, M. T., Le, Q. V., & Manning, C. D. (2020). Electra: Pre-training text encoders as discriminators rather than generators. arXiv preprint arXiv:2003.10555.

References

[81] Hahn, M. Theoretical limitations of self-attention in neural sequence models.Trans. Assoc.Comput. Linguistics, 8:156–171, 2020.URL https://transacl.org/ojs/index.php/tacl/article/view/1815.
[82] Tran, K. M., Bisazza, A., and Monz, C. The importance of being recurrent for modeling hierarchical structure. In Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing, Brussels, Belgium, October 31 - November 4, 2018, pp. 4731–4736. URL https://www.aclweb.org/anthology/D18-1503/.
[83] https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a
[84] https://machinelearningmastery.com/the-transformer-model/
[85]
https://towardsdatascience.com/transformers-explained-visually-part-3-multi-head-attention-deep-dive-1c1ff1024853

Dario Garcia-Gasulla (BSC)

dario.garcia@bsc.es

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