Transformers, I

LING 574 Deep Learning for NLP

Shane Steinert-Threlkeld

Announcements

- Shapes, shapes, shapes:
  - In your code, annotate the shape that each Tensor should have (see e.g. `forward` in hw3/ref/word2vec.py)
  - If you get a shape error, print out the shape of each Tensor (via .value and .grad)
  - These are the most common issues and biggest pain point in ML land
- HW4: use floating-point numbers for bag-of-words counts, e.g.
  - NOT [1, 0, 0, 3], but [1.0, 0.0, 0.0, 3.0]
- Cross entropy loss: $$\frac{1}{\text{batch-size}} \sum_{\text{row}_i} \text{c-ent}(\text{labels}[\text{row}_i], \text{probabilities}[\text{row}_i])$$

Today's Plan

- Attention
- Limitations of Recurrent Models
- Transformers: building blocks
  - Self-attention
  - Encoder architecture

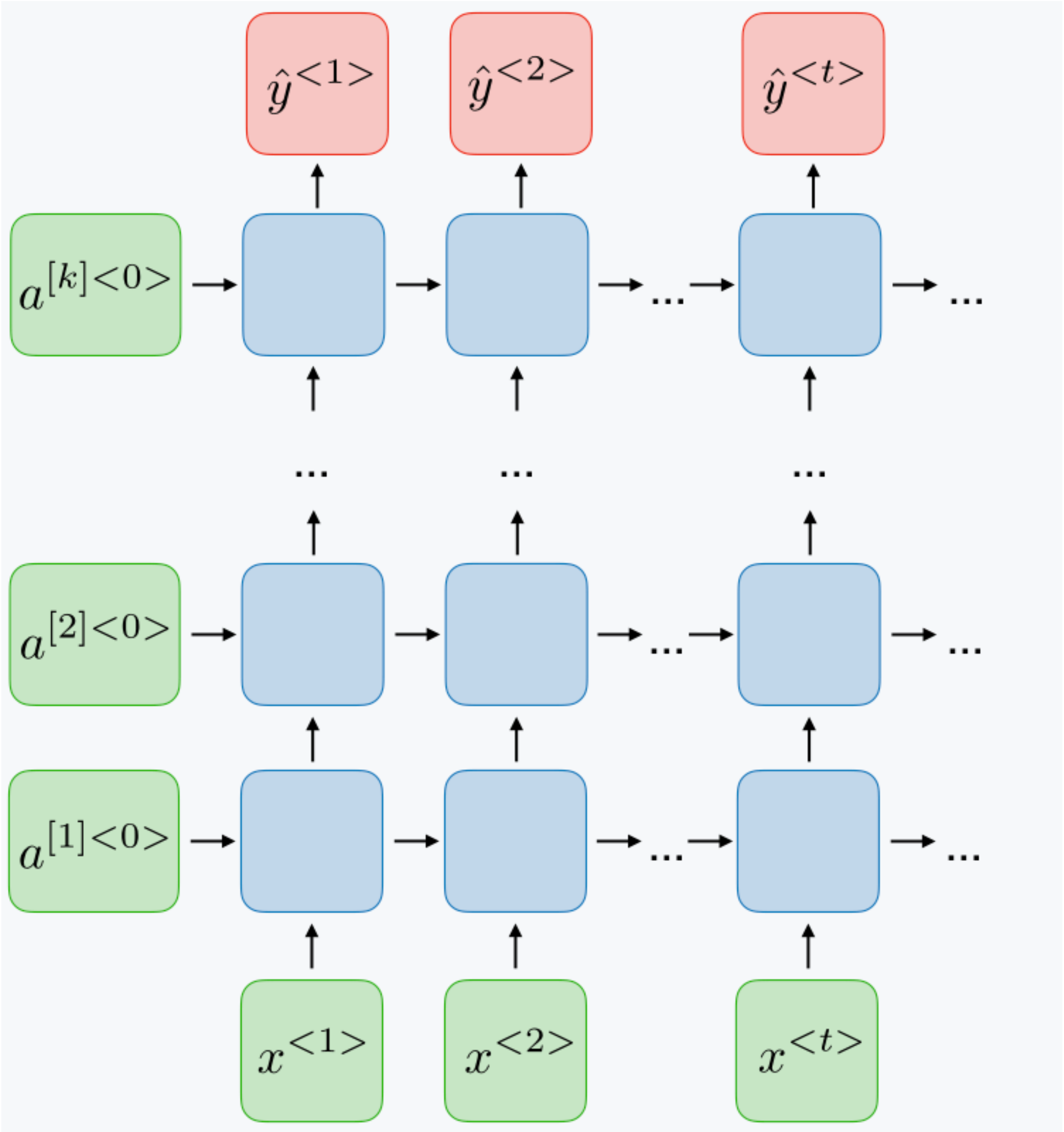
Limitations of Recurrent Models

RNNs Unrolling

- Recall: RNNs are “unrolled” across time, same operation at each step
- This has at least two issues:
  - Creates “long path lengths” between sequence positions
  - Not parallelizable

Long Path Lengths

- Gating mechanisms help RNNs learn long distance dependencies, by alleviating the vanishing gradient problem
- But: still takes a linear number of computations for one token to influence another
  - Long-distance dependencies are still hard!



Students who … enjoy

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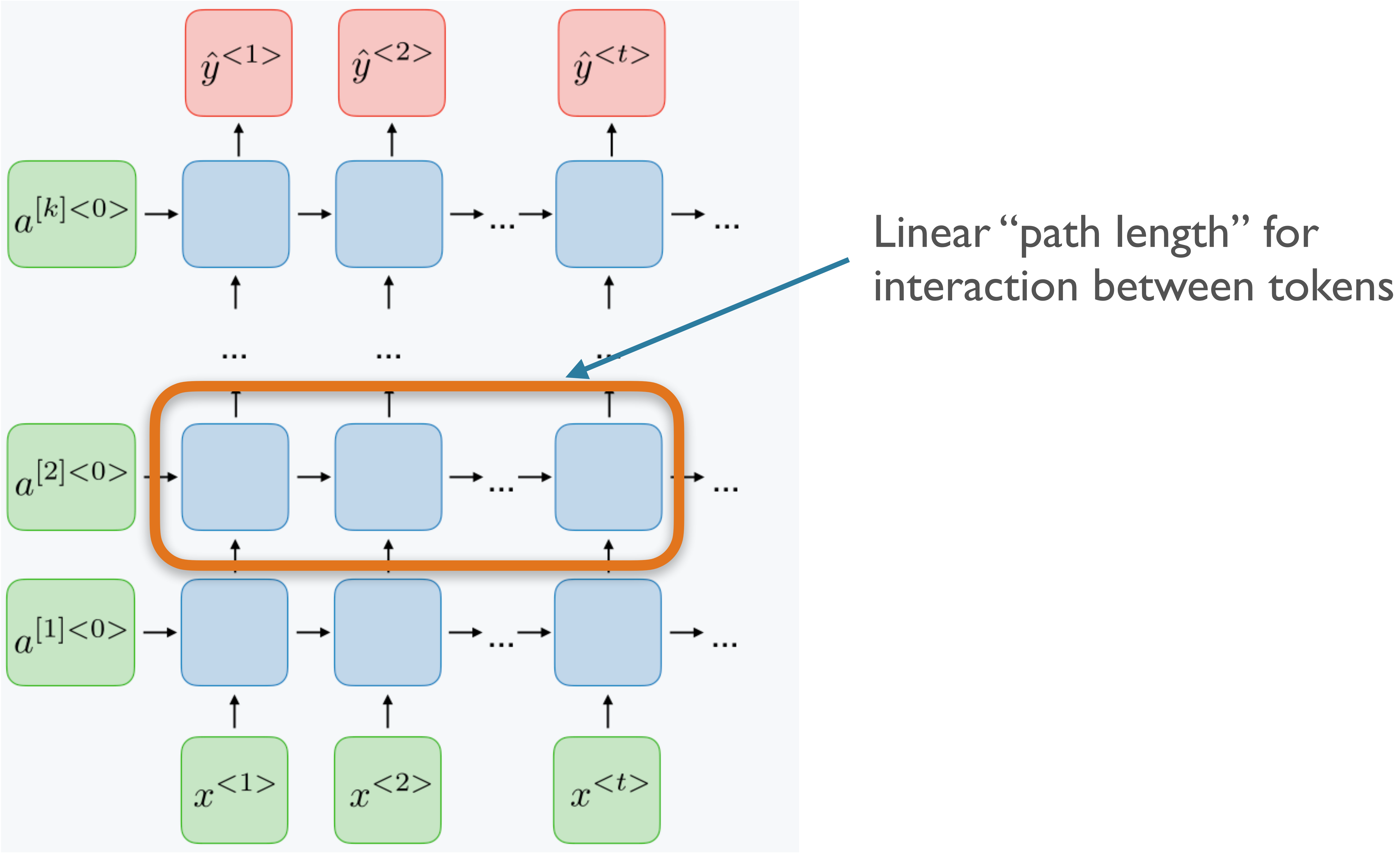

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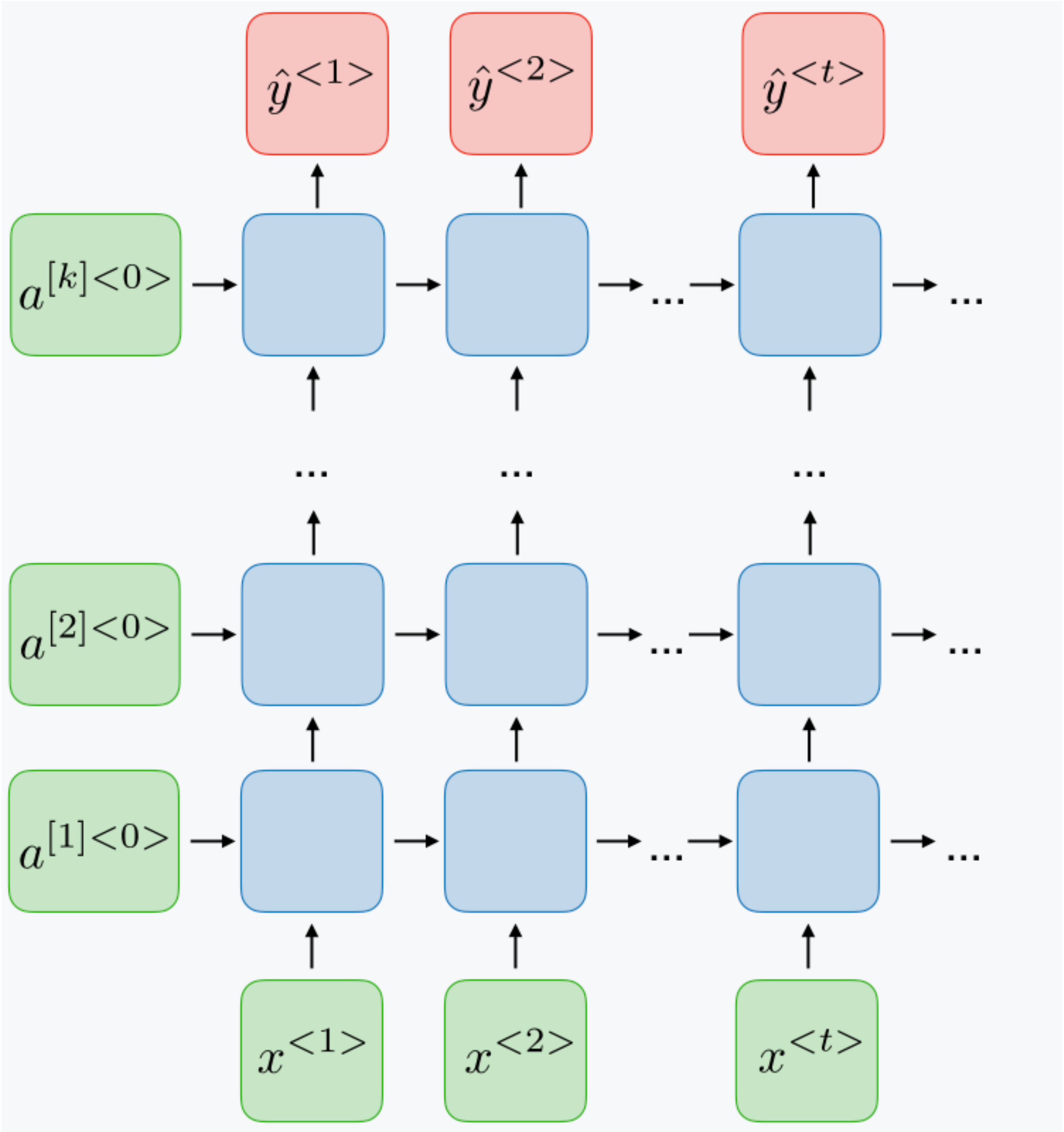
Lack of Parallelizability

- Modern hardware (e.g. GPUs) are very good at doing *independent* computations in parallel
- RNNs are inherently serial:
  - Cannot compute future time steps without the past
- Bottleneck that makes scaling up difficult



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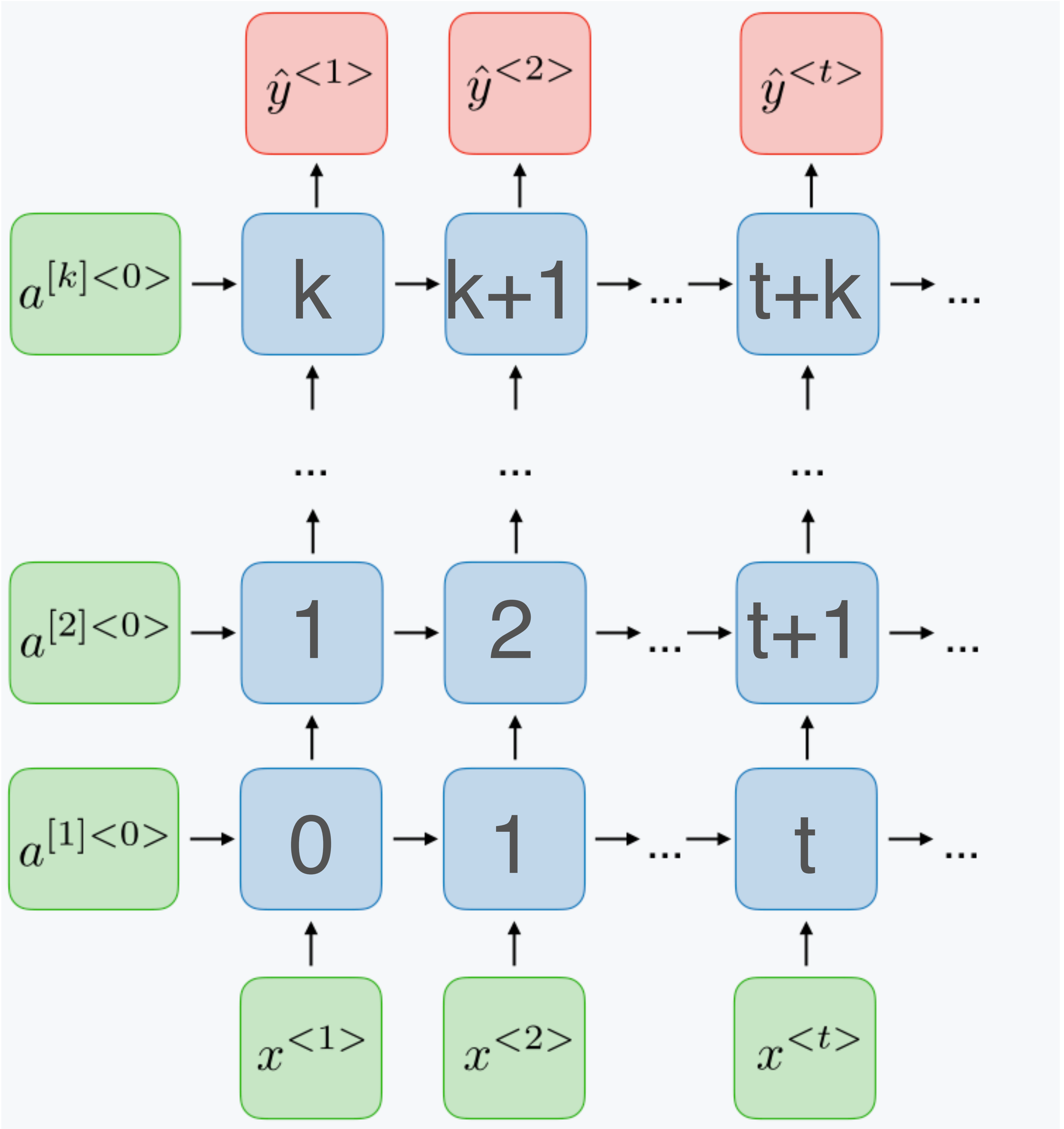

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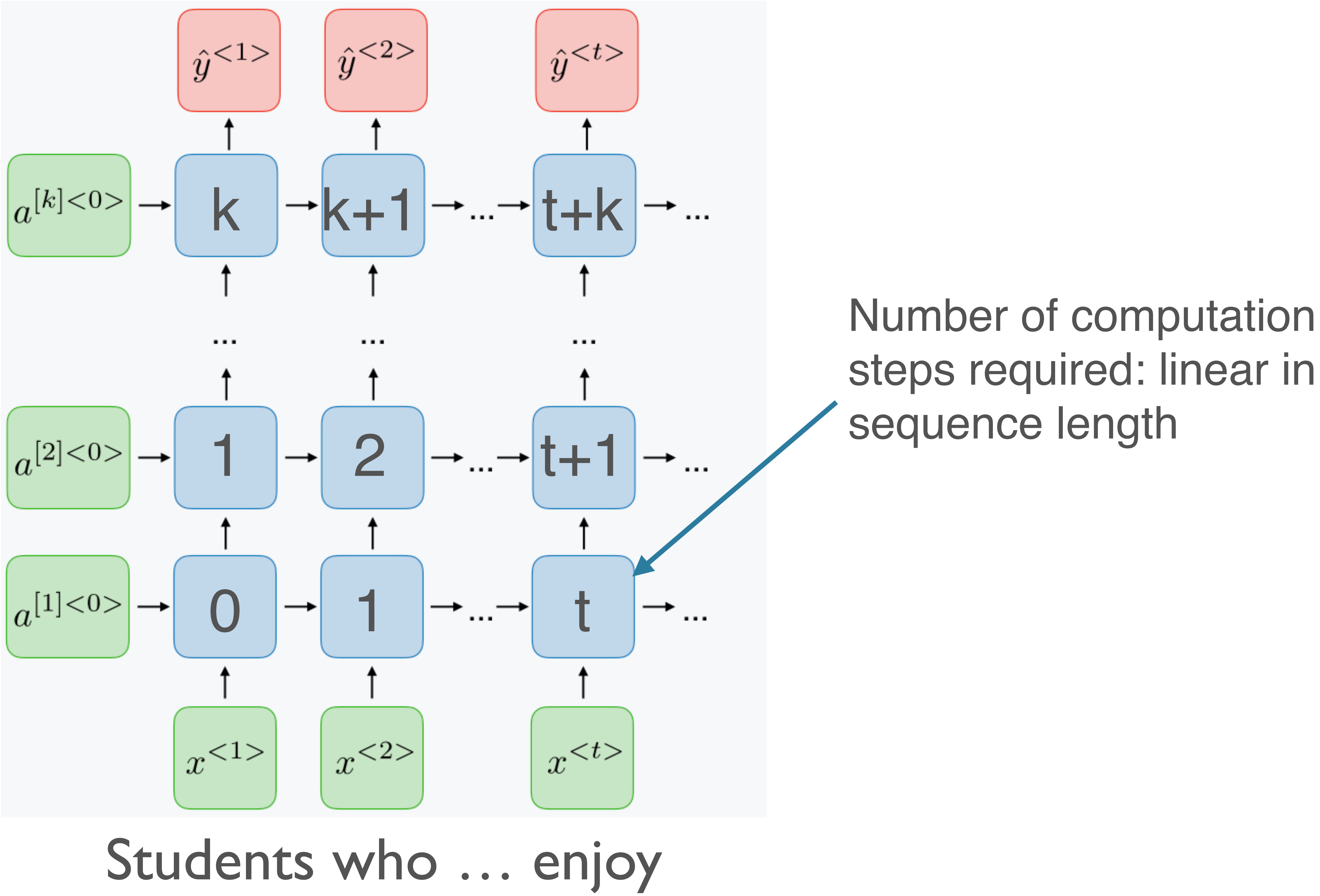

Transformer Architecture

Attention Is All You Need

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Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.0 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature.

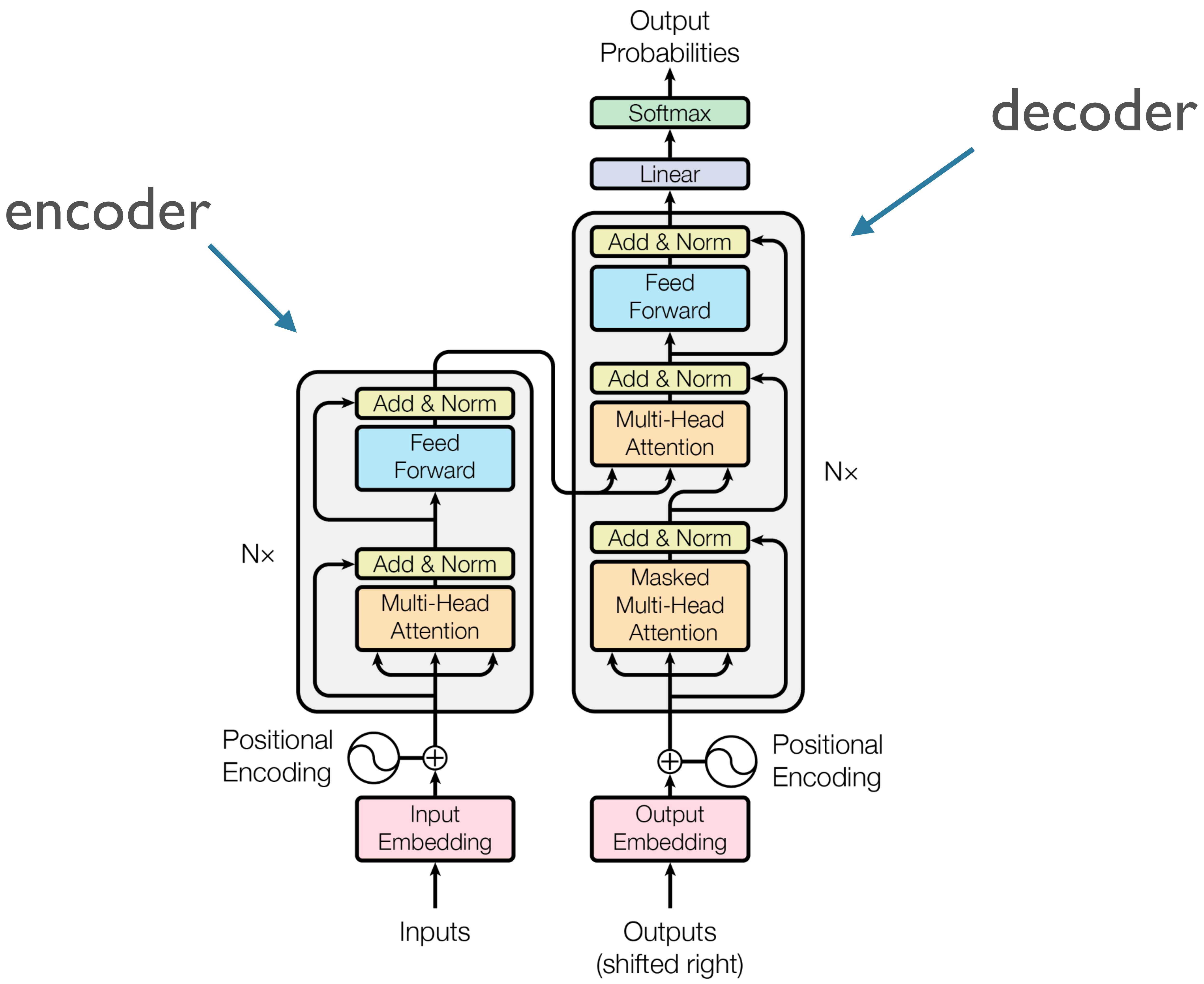
Paper link

(but see Annotated and Illustrated Transformer)

Key Idea

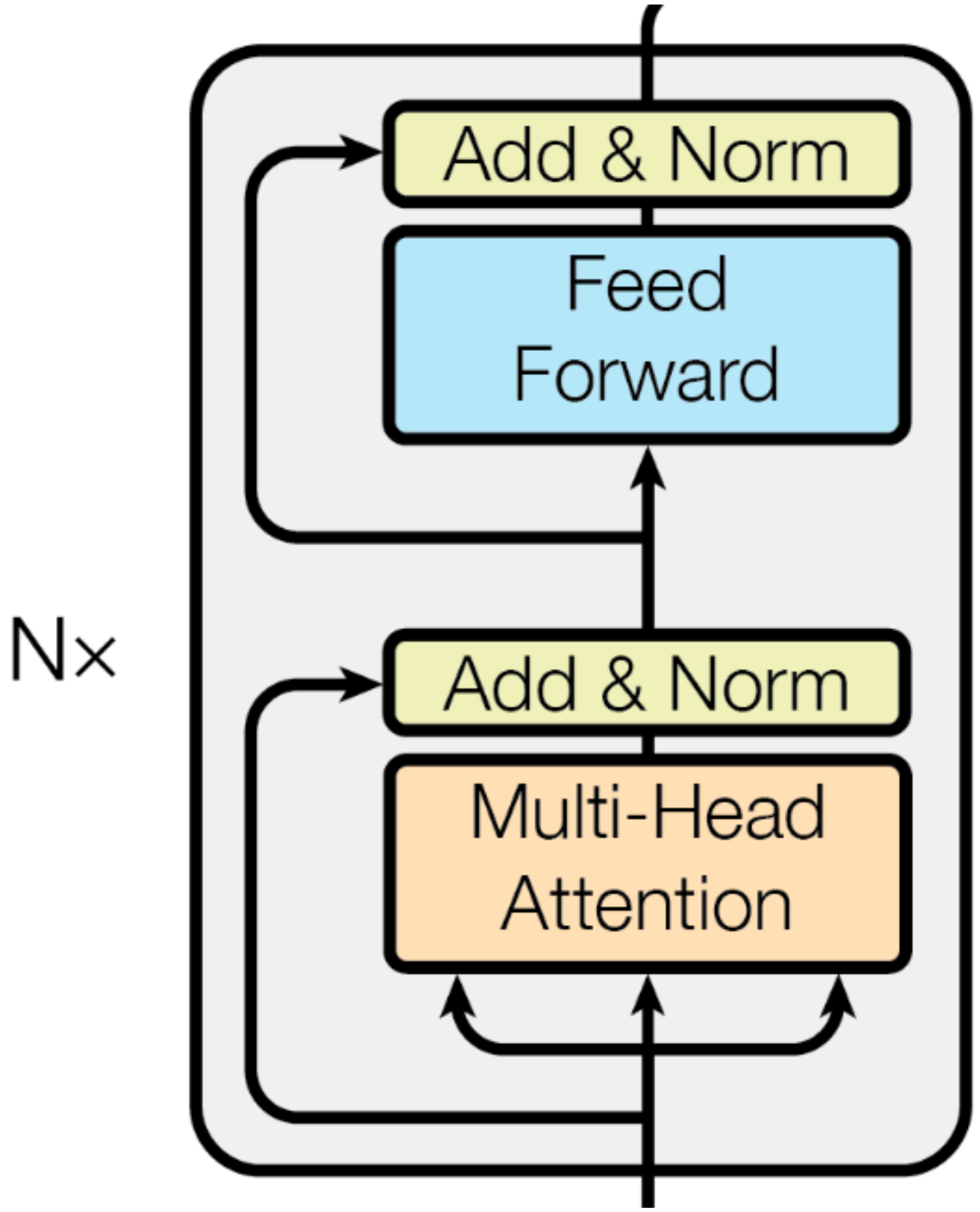
- Recurrence: not parallelizable, long “path lengths”
- *Attention*:
  - Parallelizable, short path lengths
- Transformer: “replace” recurrence with attention mechanism
  - Subtle issues in making this work, which we we will see

Full Model



encoder
decoder
Output
Probabilities
Softmax
Linear
Add & Norm
Feed
Forward
Add & Norm
Multi-Head
Attention
Add & Norm
Masked
Multi-Head
Attention
Nx
Add & Norm
Feed
Forward
Add & Norm
Multi-Head
Attention
Nx
Positional
Encoding
Positional
Encoding
Input
Embedding
Output
Embedding
Inputs
Outputs
(shifted right)

Transformer Block



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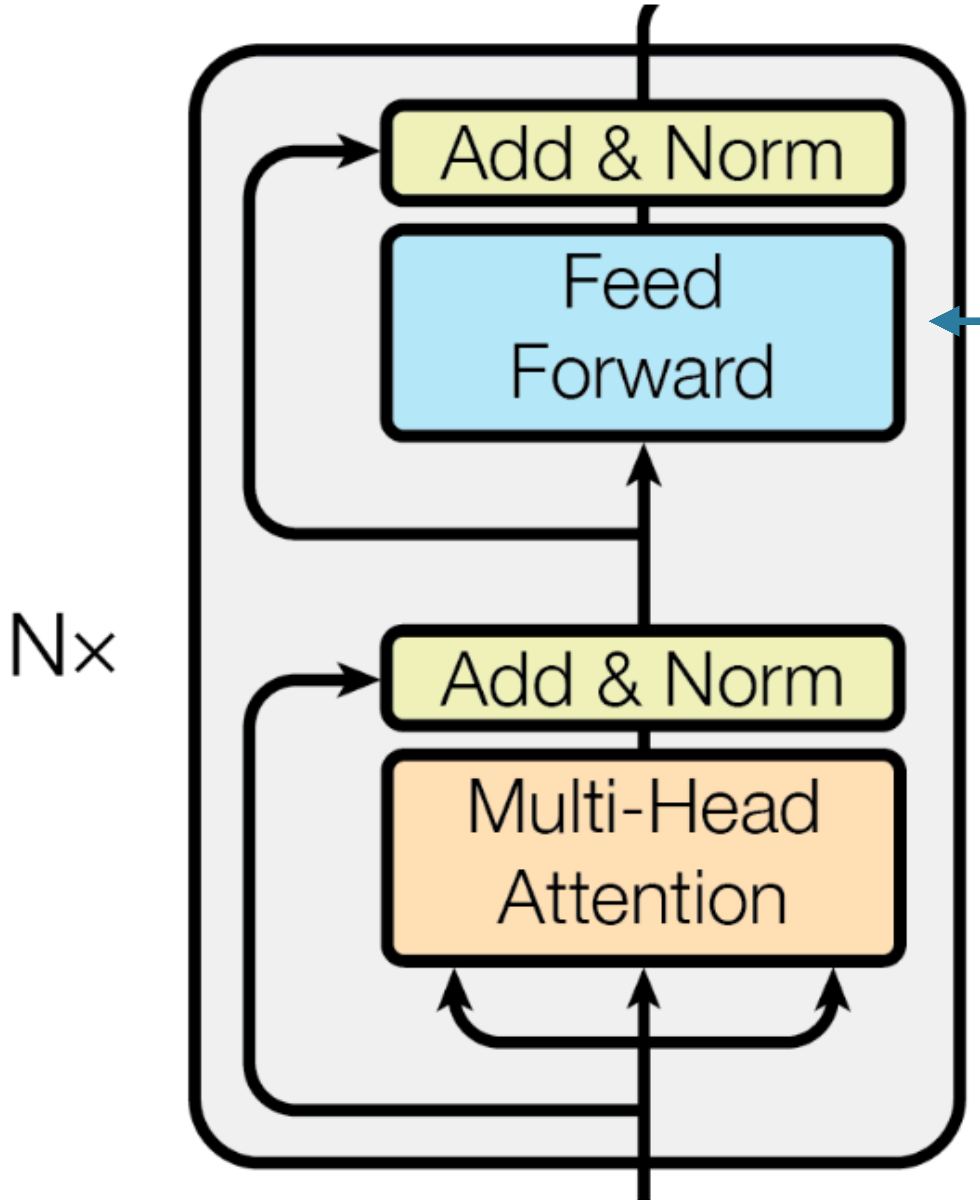

Single layer, applied to each position

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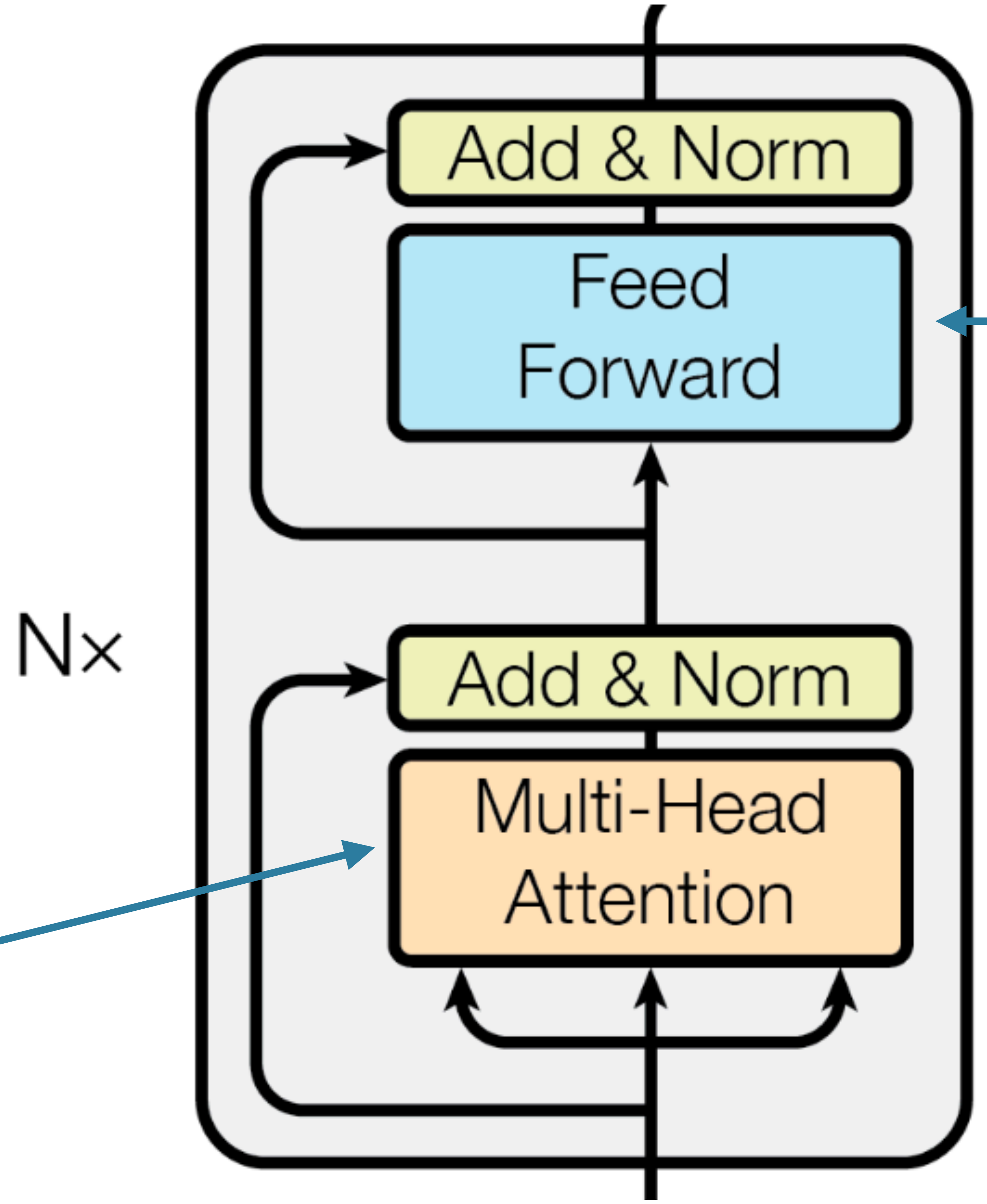

Single layer, applied to each position

What's this?

Scaled Dot-Product Attention

- Recall:

- Putting it together: (keys/values in matrices) $$\text{Attention}(q, K, V) = \sum_j \frac{e^{q \cdot k_j}}{\sum_i e^{q \cdot k_i}} v_j$$

- Stacking *multiple* queries: (and scaling) $$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

Scaled Dot-Product Attention

- Recall:

$$\alpha_j = q \cdot k_j$$

$$e_j = e^{\alpha_j} / \Sigma_j e^{\alpha_j}$$

$$c = \Sigma_j e_j v_j$$

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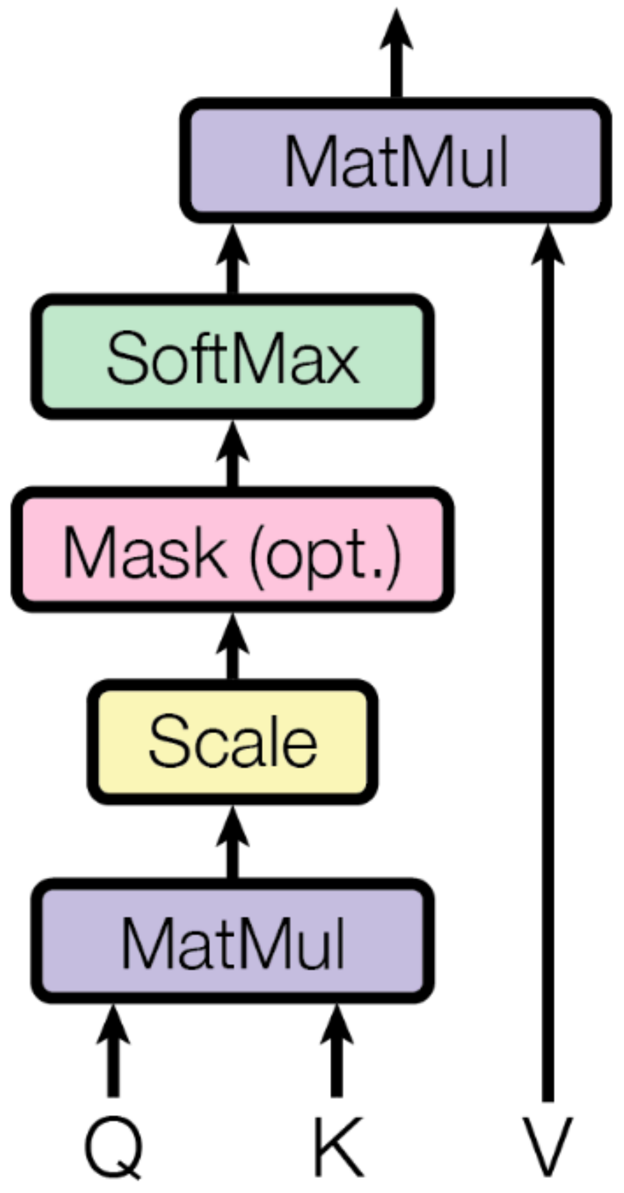

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- Transformer: *self*-attention
  - Every (token) position attends to every other position [including self!]
  - Caveat: in the encoder, and only by default
    - Mask in decoder to attend only to previous positions [next time]
      - Used for generation [NMT, LM, etc]

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- So vector at each position is a query
  - And a key, and a value
  - Linearly transformed, to be different "views"

Self-Attention, Details

- Every token attends to every other token
- X: [seq_len, embedding_dim]
  - XW_q: queries
  - XW_k: keys
  - XW_v: values
  - Each W is [embedding_dim, embedding_dim] learned matrix

Self-Attention: Details

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

- Q = XW_q, K = XW_k, V = XW_v
  - K^T: [embedding_dim, seq_len]
  - QK^T: [seq_len, seq_len]
    - Dot-product of rows of Q with columns of K
    - $(QK^T)_{ij} = q_i \cdot k_j$
- Scaled by sq-rt of hidden dimension [see paper for motivation]
- Softmax: along *rows*, gets the weights

Self-Attention: Details

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

- Softmax output: each row has weights
  - How much q_i should pay attention to each v_j
- Matrix multiplication with V: output is [seq_len, embedding_dim]
  - Each row: weighted average of the v_j (rows of V)
  - Each row: the weight sum attention value for each query (each input token)
- [NB: a more explicit notation, if you like: https://namedtensor.github.io/]

Multi-headed Attention

- So far: a *single* attention mechanism.
- Could be a bottleneck: need to pay attention to different vectors *for different reasons*
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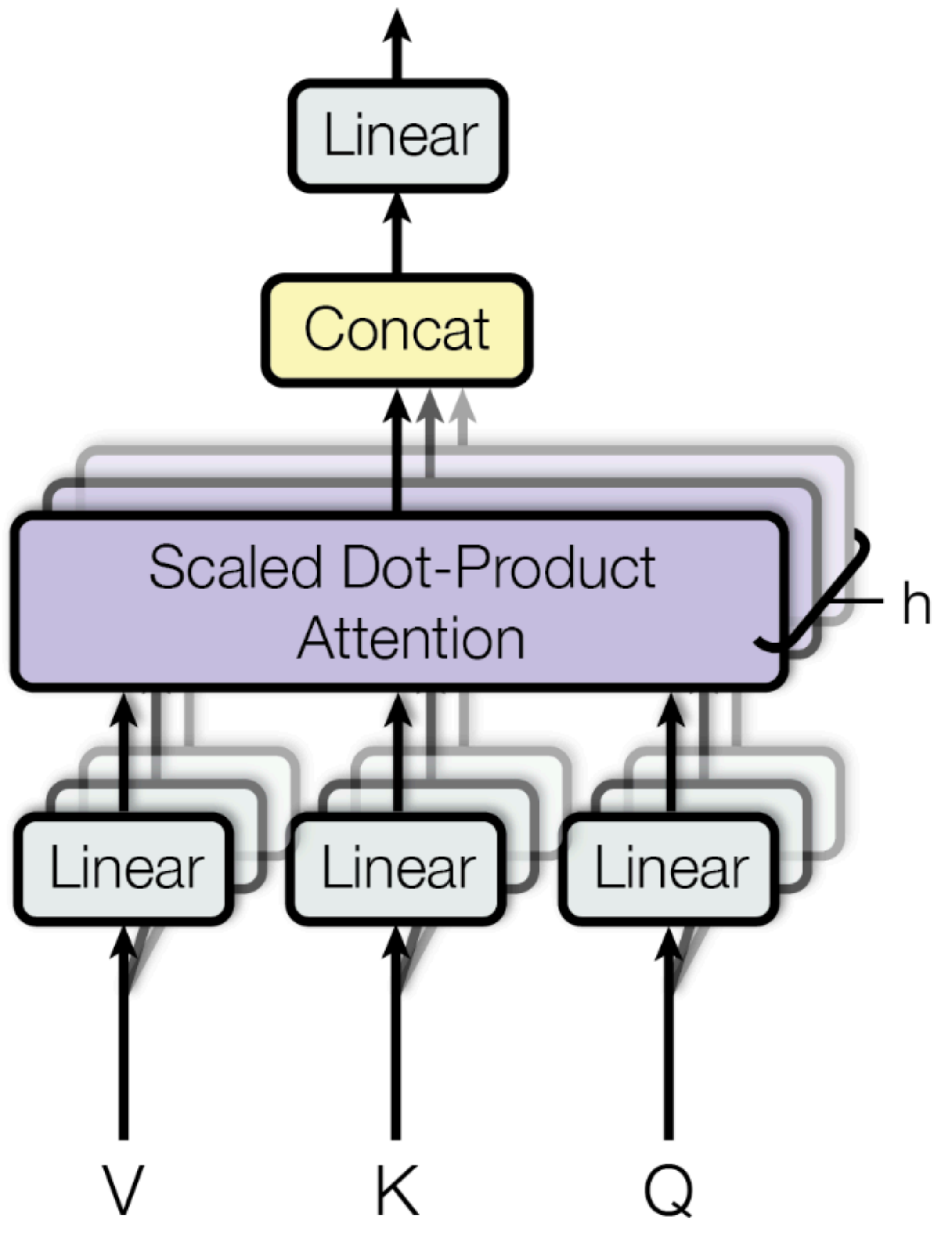

Problem With Self-Attention

- Attention is order-independent
  - If we shuffle Q, K, V, we get the same output!

Representing Order

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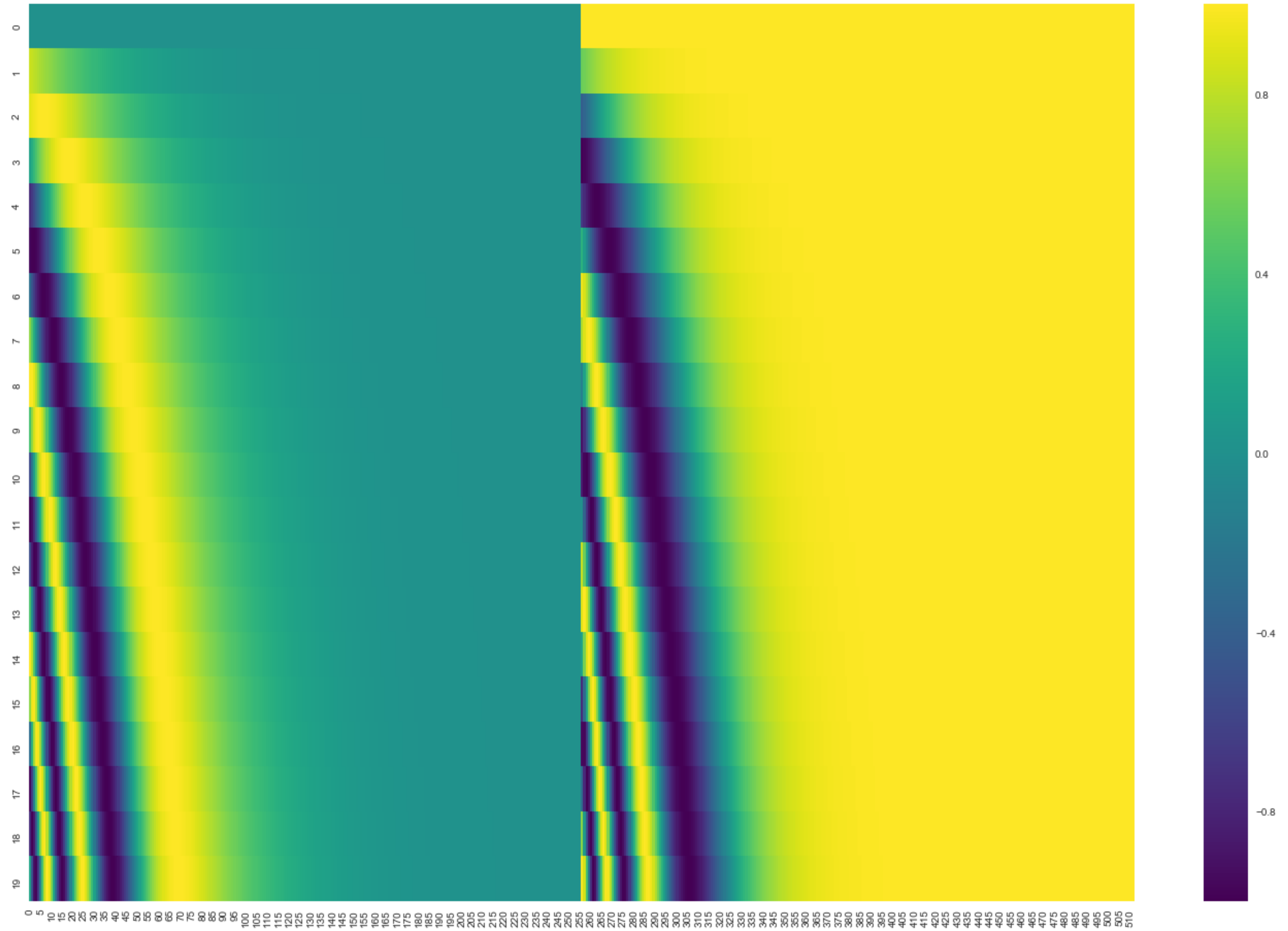

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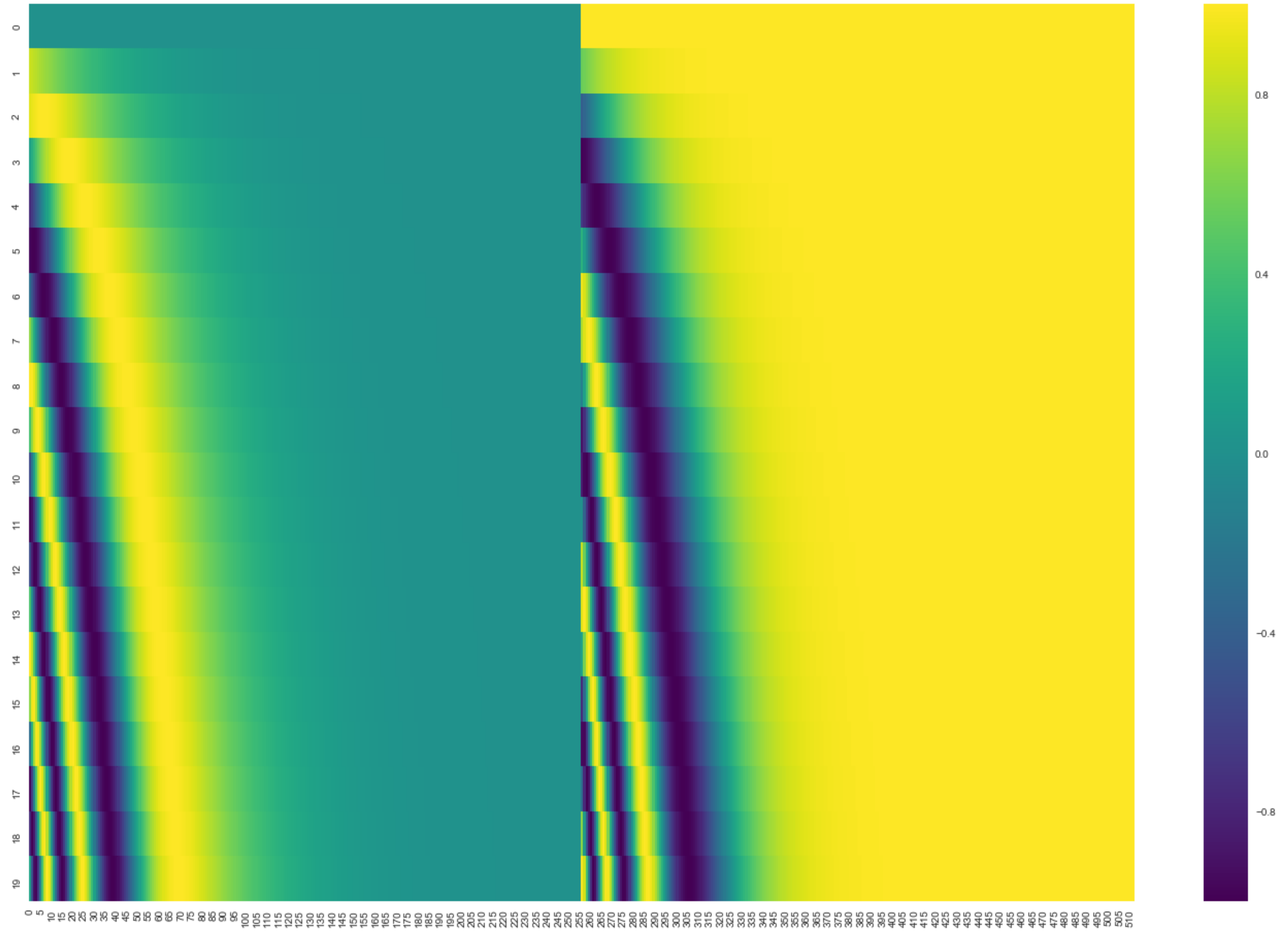

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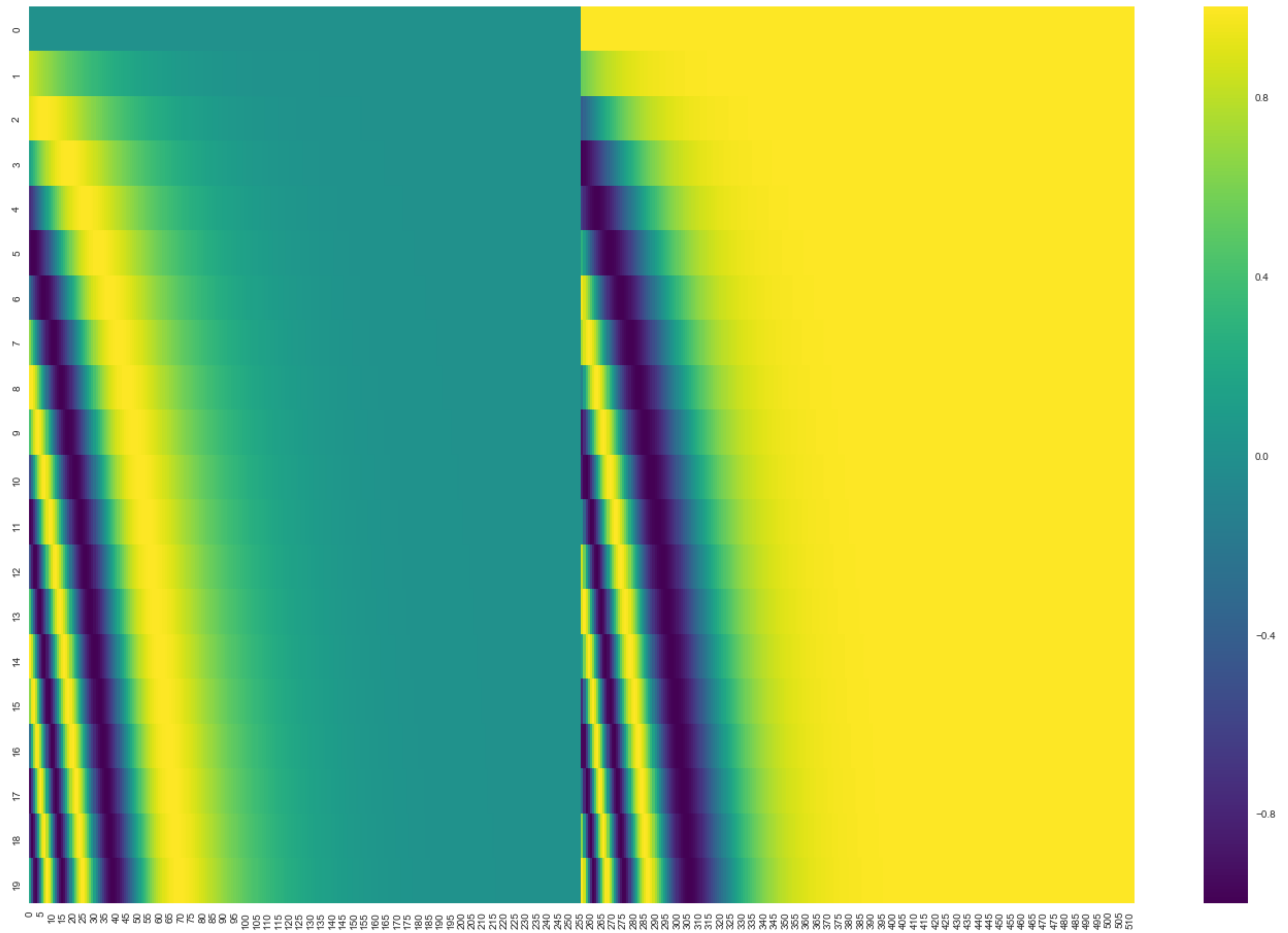

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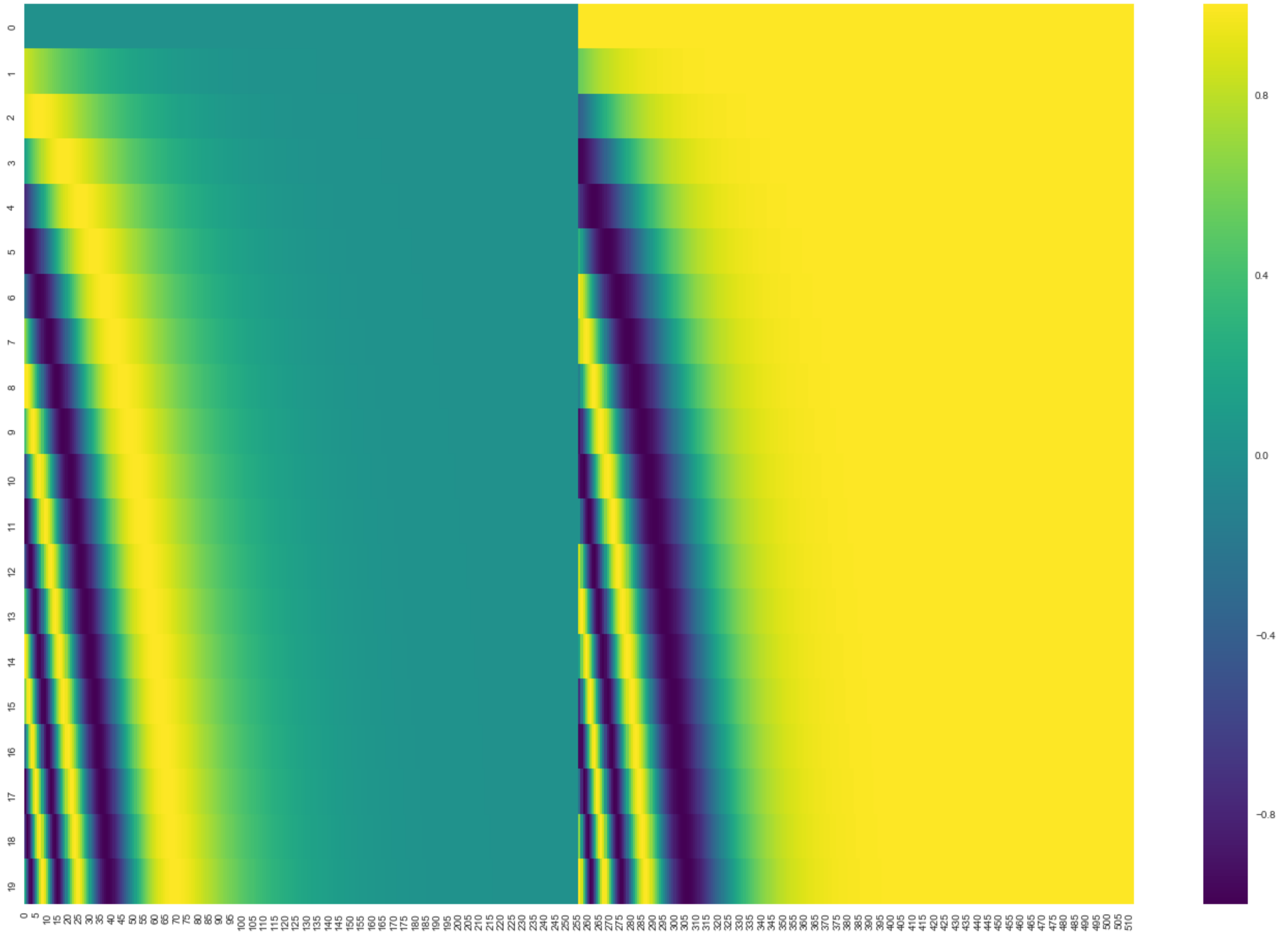

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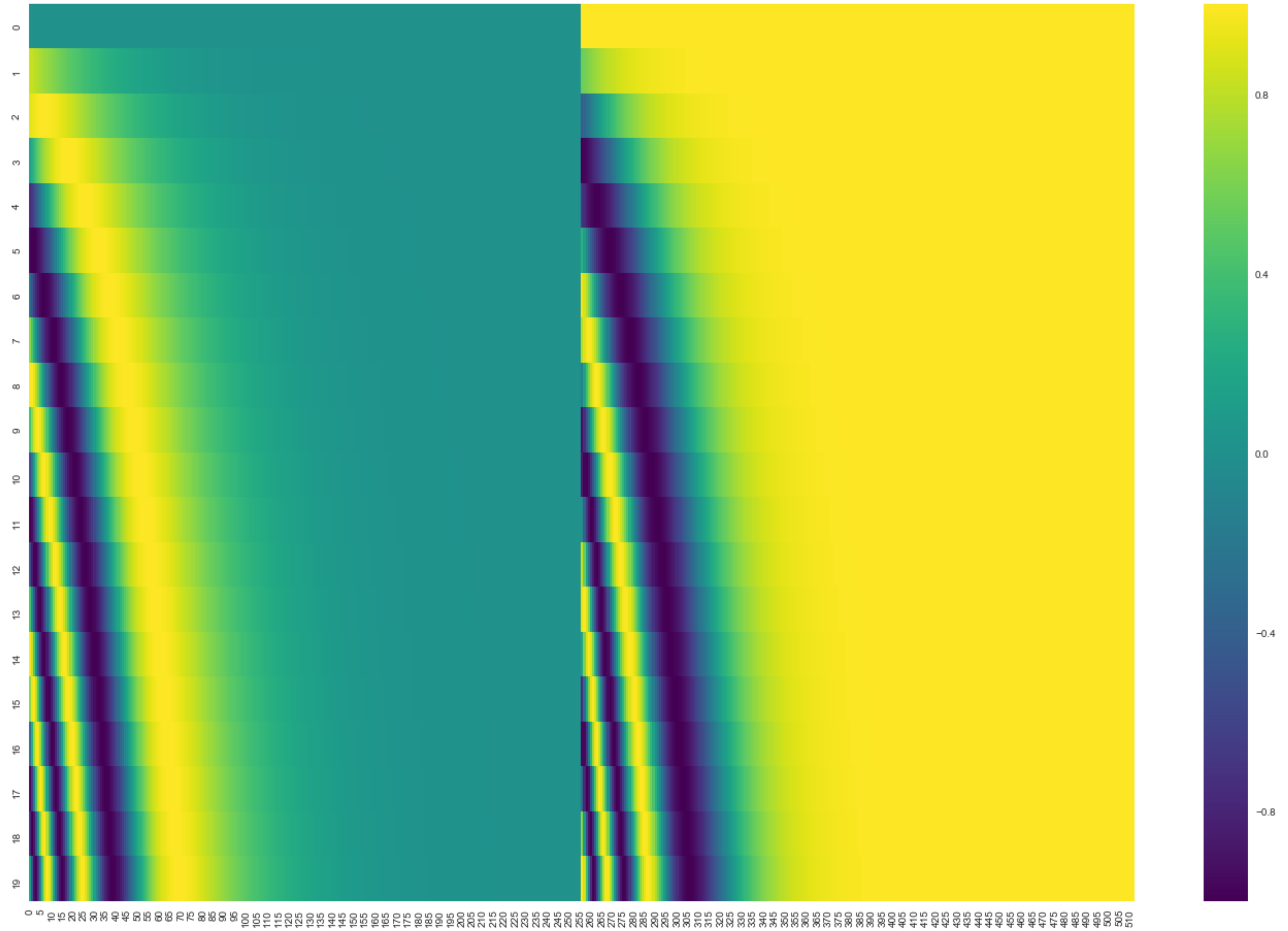

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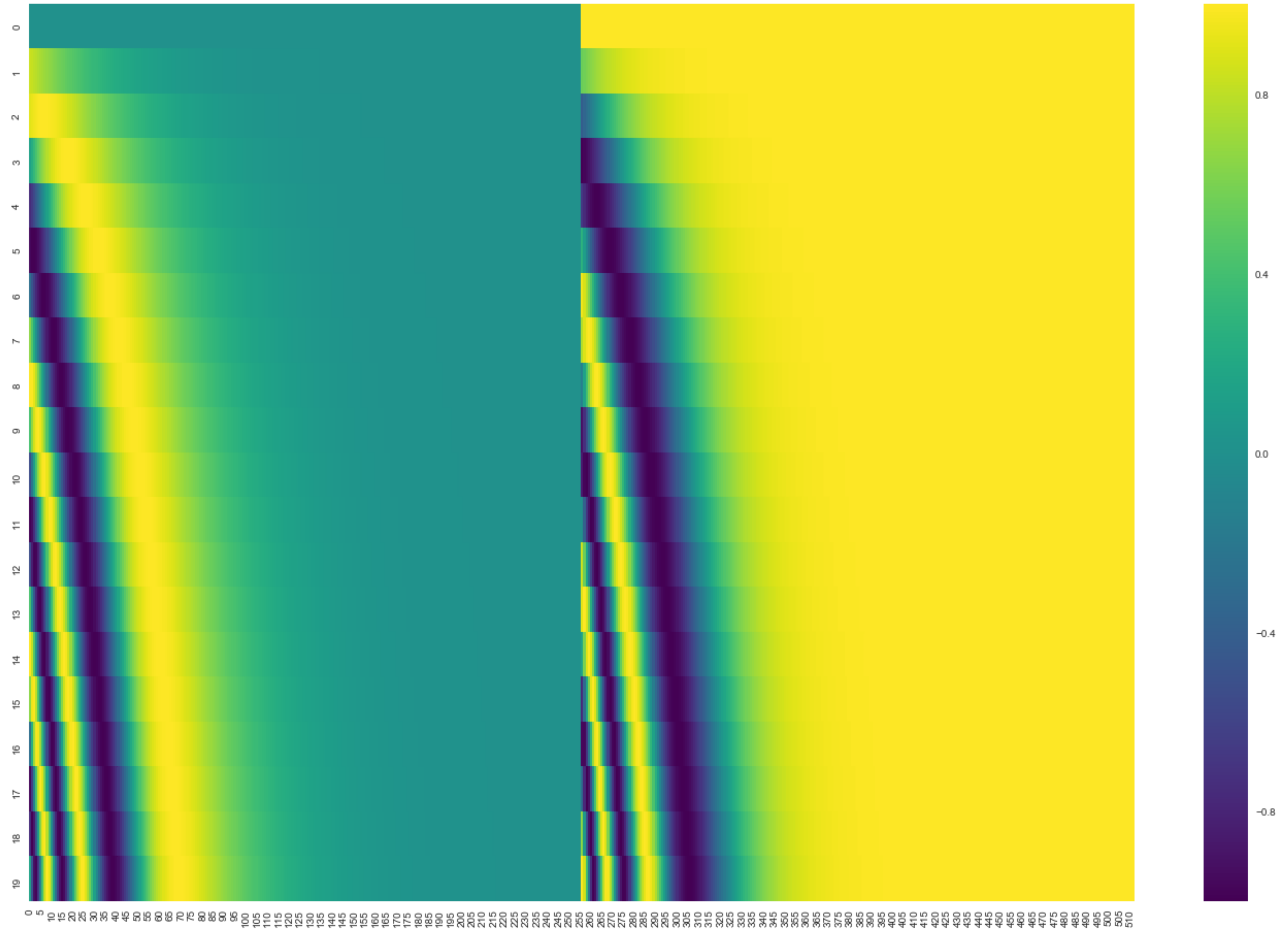
- Can be fixed/pre-defined [see right] or entirely learned



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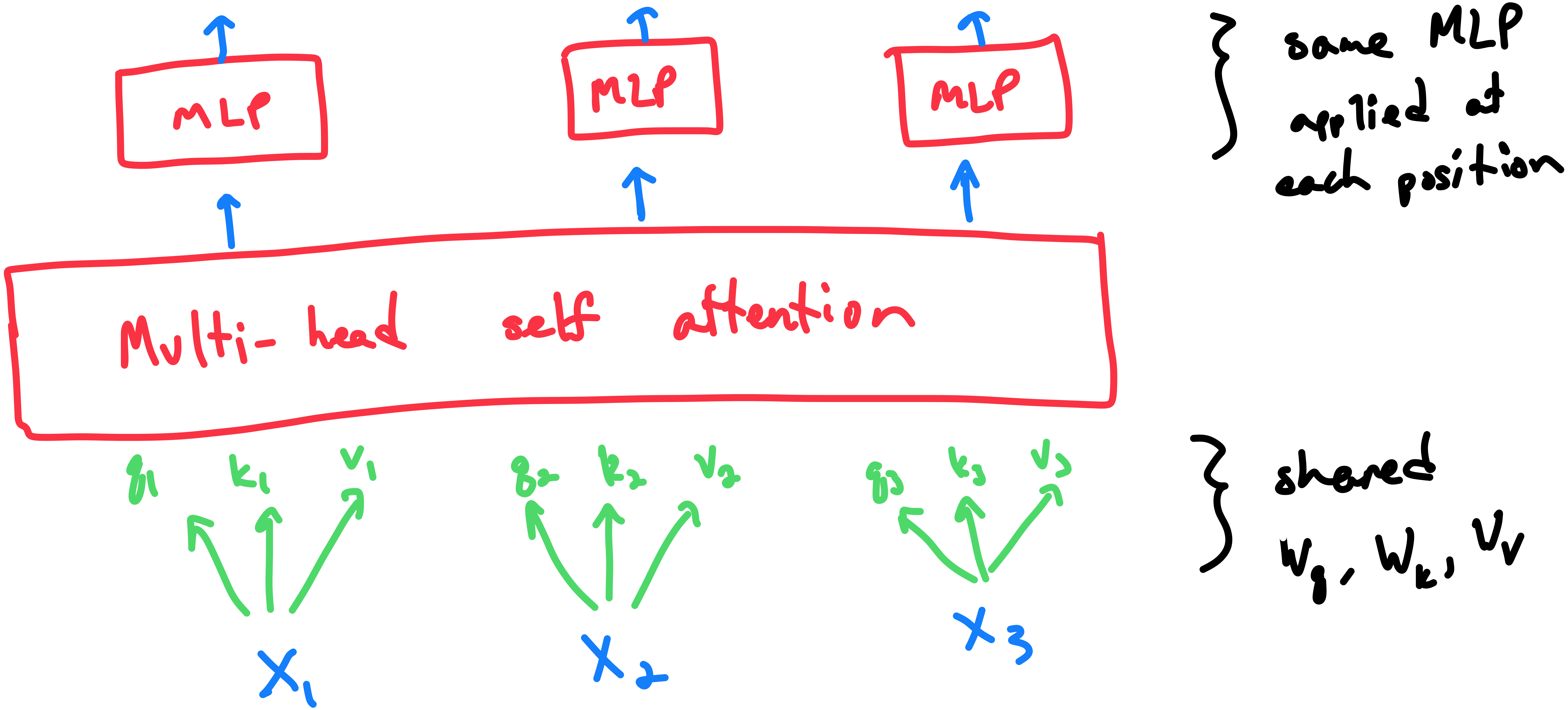
Fixed vs Learned Positional Encoding

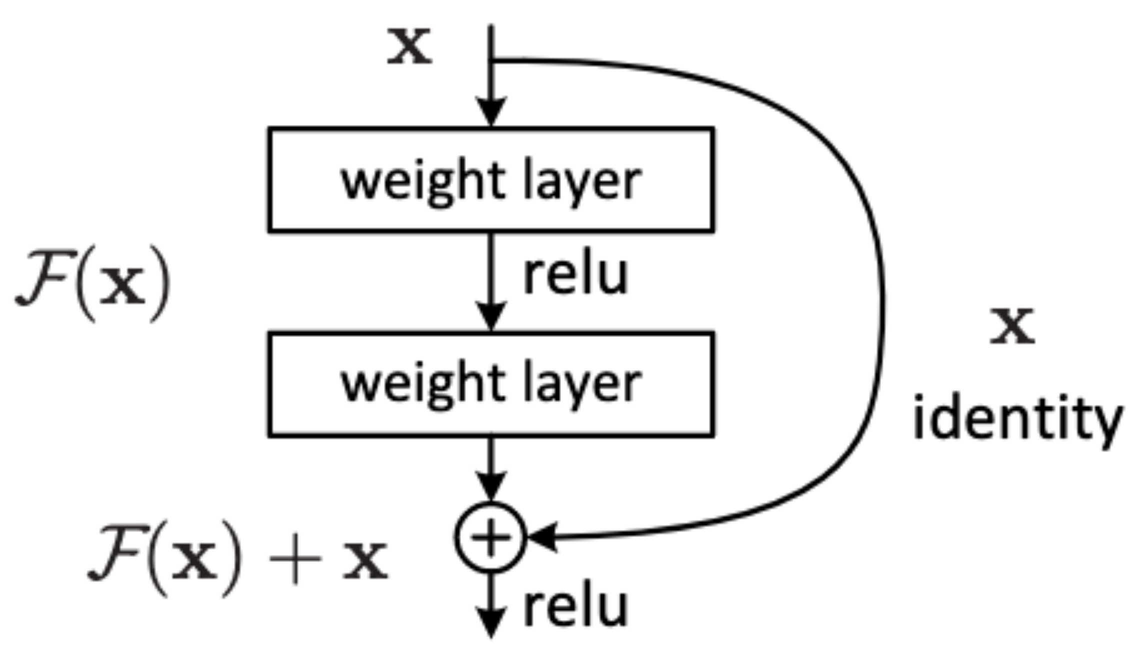
- Fixed:
  - No need to be learned
  - Guaranteed to be unique to position
  - Generalizes to longer sequence lengths (in theory at least)
- Learned:
  - Might learn more useful encodings of position than e.g. sinusoidal
  - Can't extrapolate to longer sequence lengths
  - [This has become the default/norm]
- Fancier ways of representing positional info: rotary embeddings, learned bias of distance, fixed bias of distance (ALiBi)

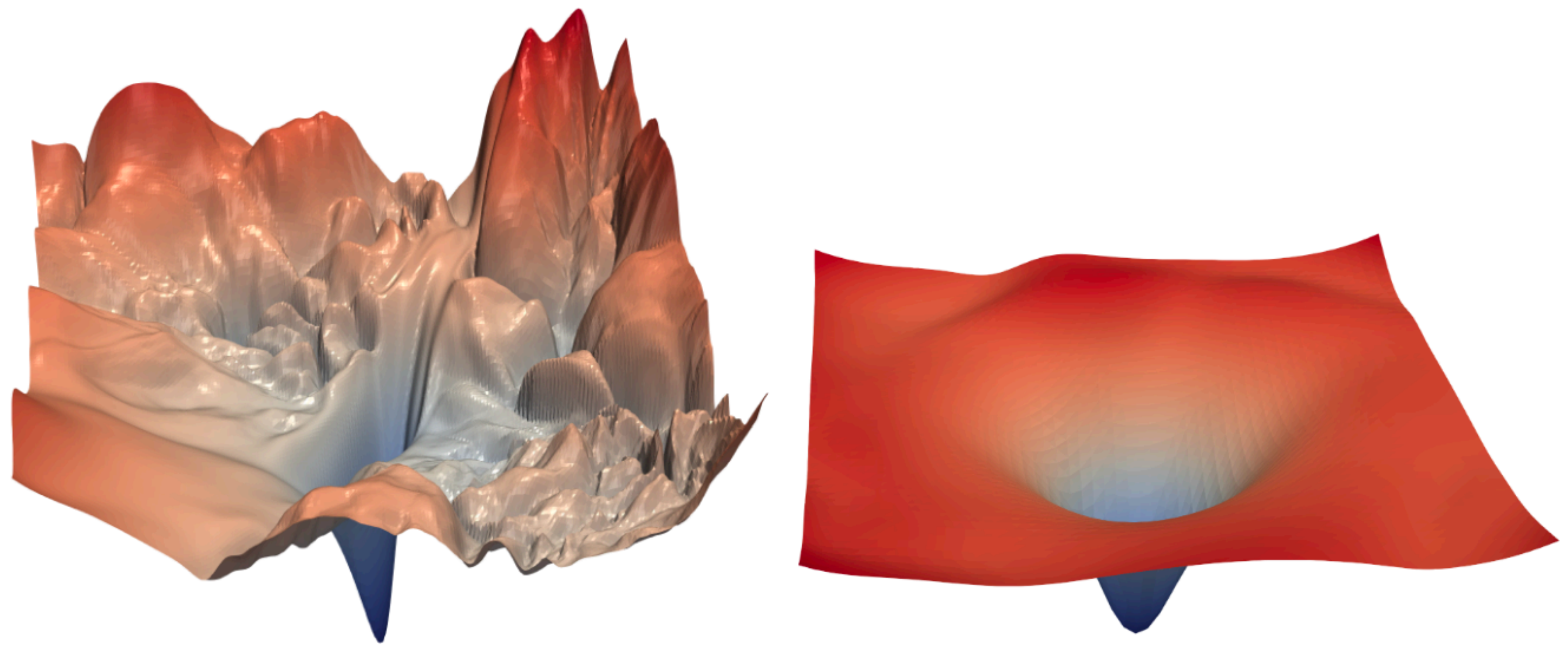
Basic Transformer Encoder Block



Final Ingredients: Residual Connections

- Core idea: add a "skip" connection around neural building blocks
- Replace $f(x)$ with $x + f(x)$
- Makes training work much better, by smoothing out loss surface
- In Transformer: residual connection around both self-attention and feed-forward blocks
- Used widely now: FFNNs, CNNs, RNNs, Transformers, …





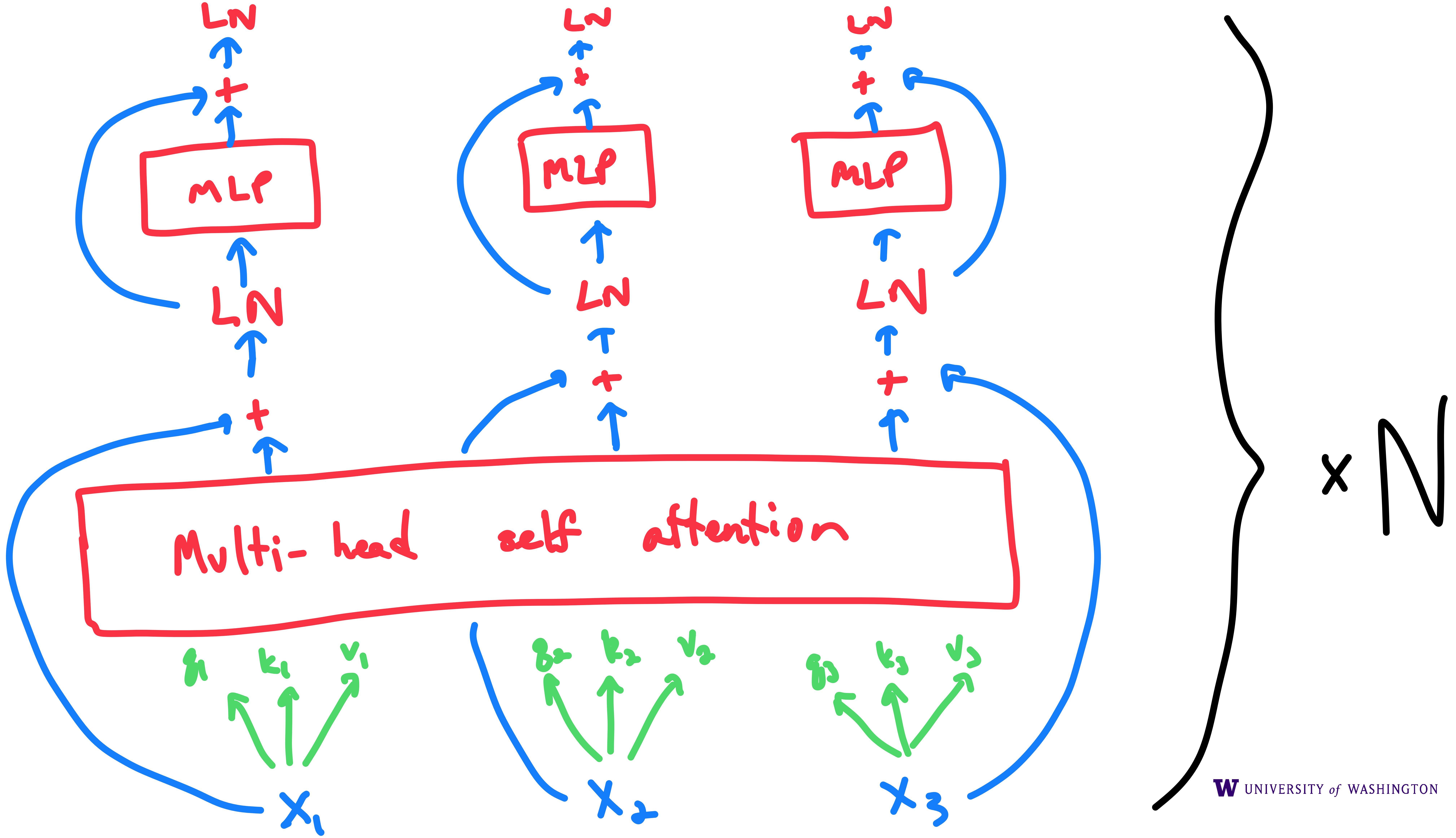
(a) without skip connections (b) with skip connections

source

Final Ingredients: Layer Normalization

- Normalizing inputs: subtract mean, divide by standard deviation
  - Makes new mean 0, new standard deviation 1
  - Widely used in many kinds of statistical modeling [e.g. predictors in linear regression], including in NNs
- Layer norm: to each row x of a matrix [a batch]: $$LN(x) = \frac{x - \mu}{\sigma + \epsilon}\gamma + \beta$$
  - Where μ is mean, σ is std dev
  - γ, β are learned scaling parameters [but often omitted entirely]

Full Transformer Encoder Block



Initial WMT Results

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
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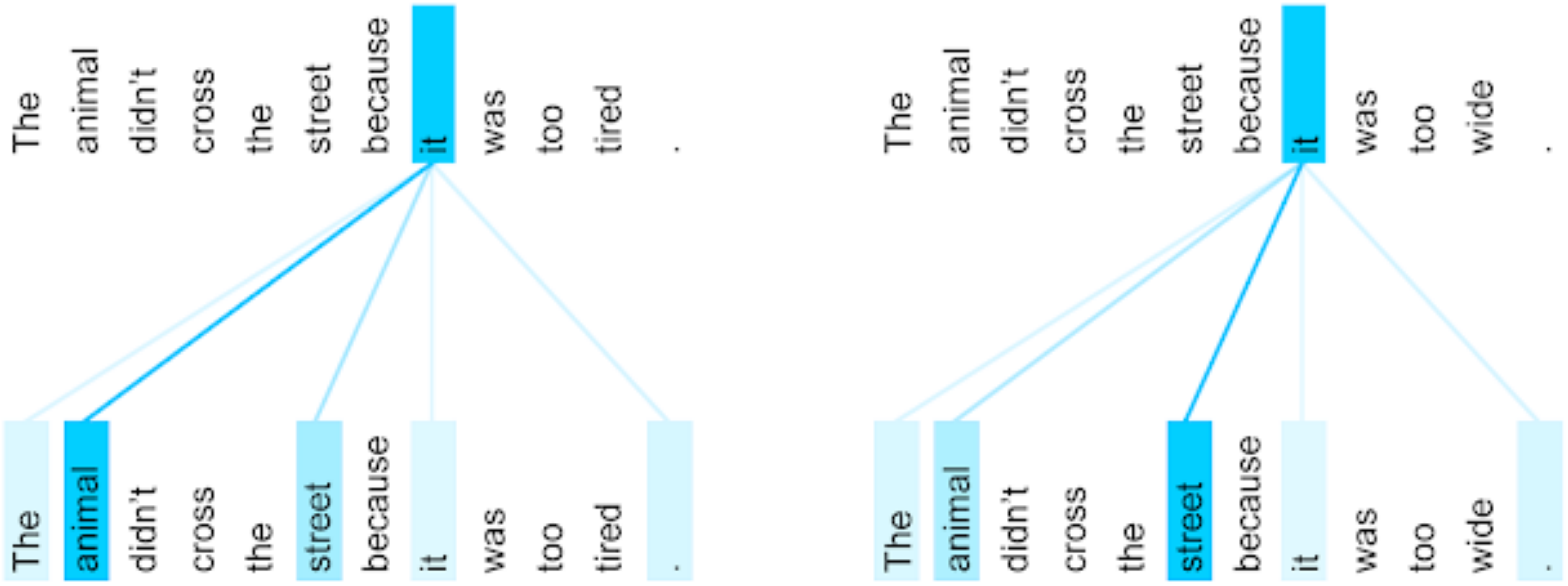
More on why important later

Attention Visualization: Coreference?



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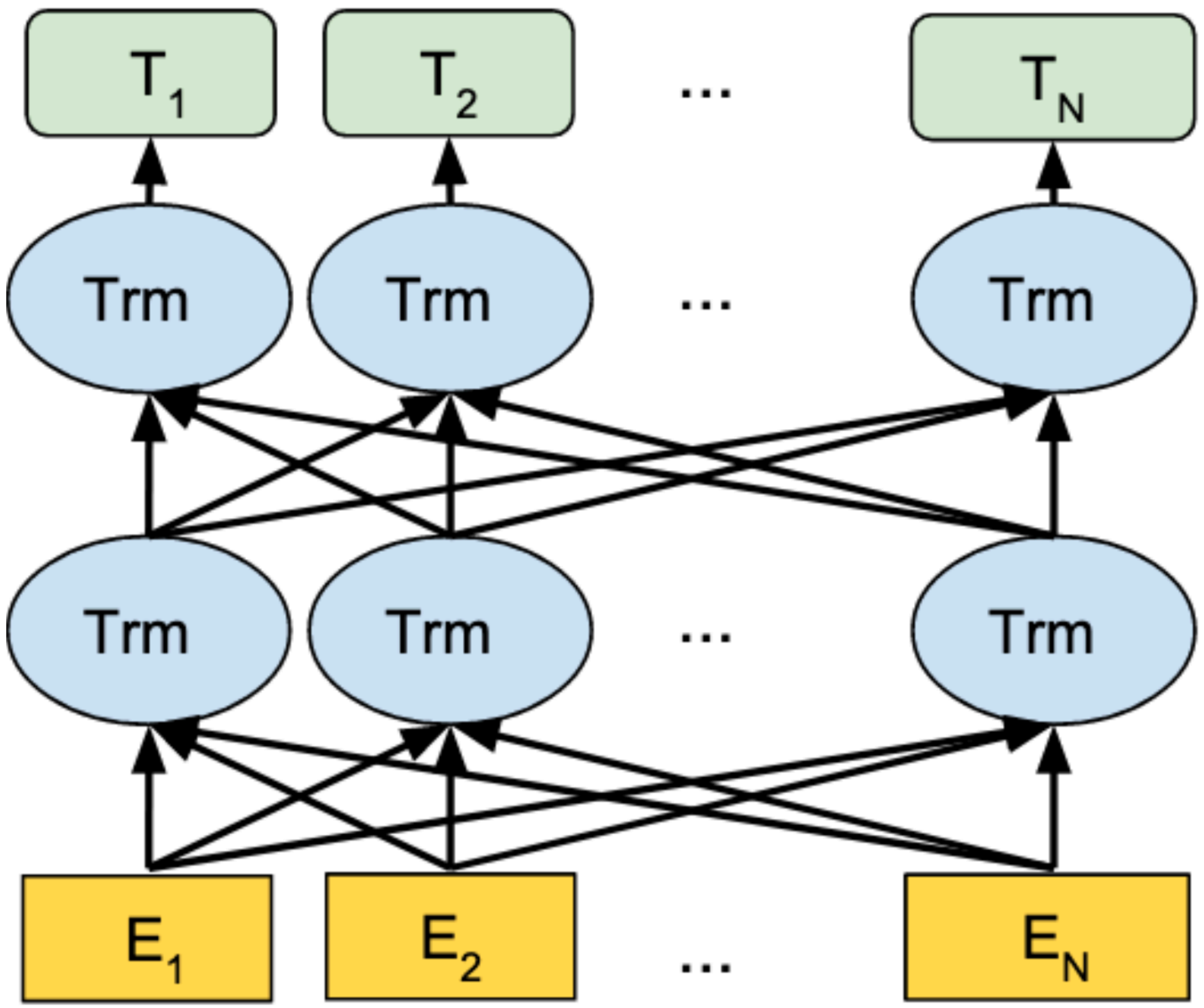
Transformer: Path Lengths + Parallelism



source (BERT paper)

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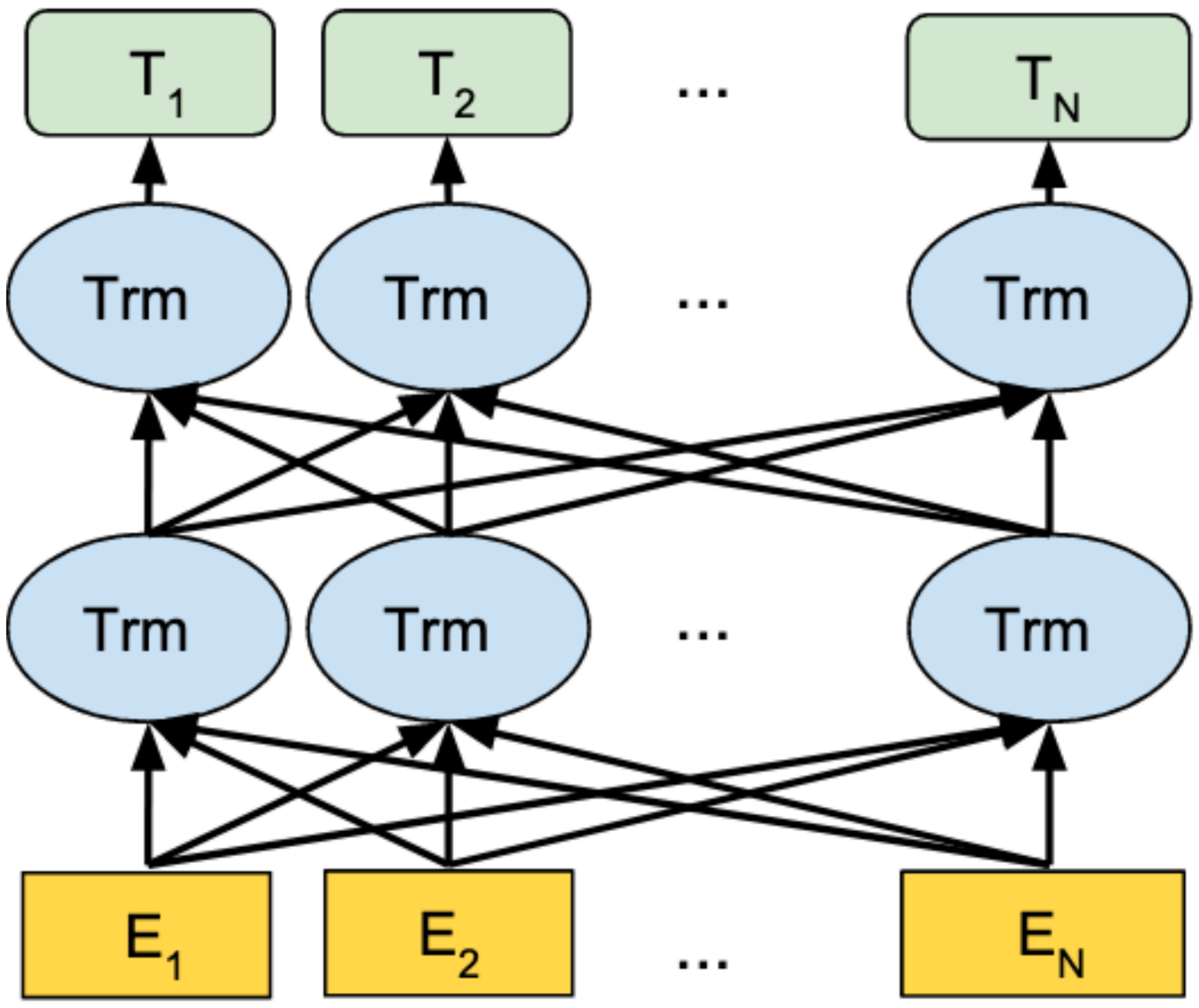


Path lengths between tokens: 1
[constant, not linear]

source (BERT paper)

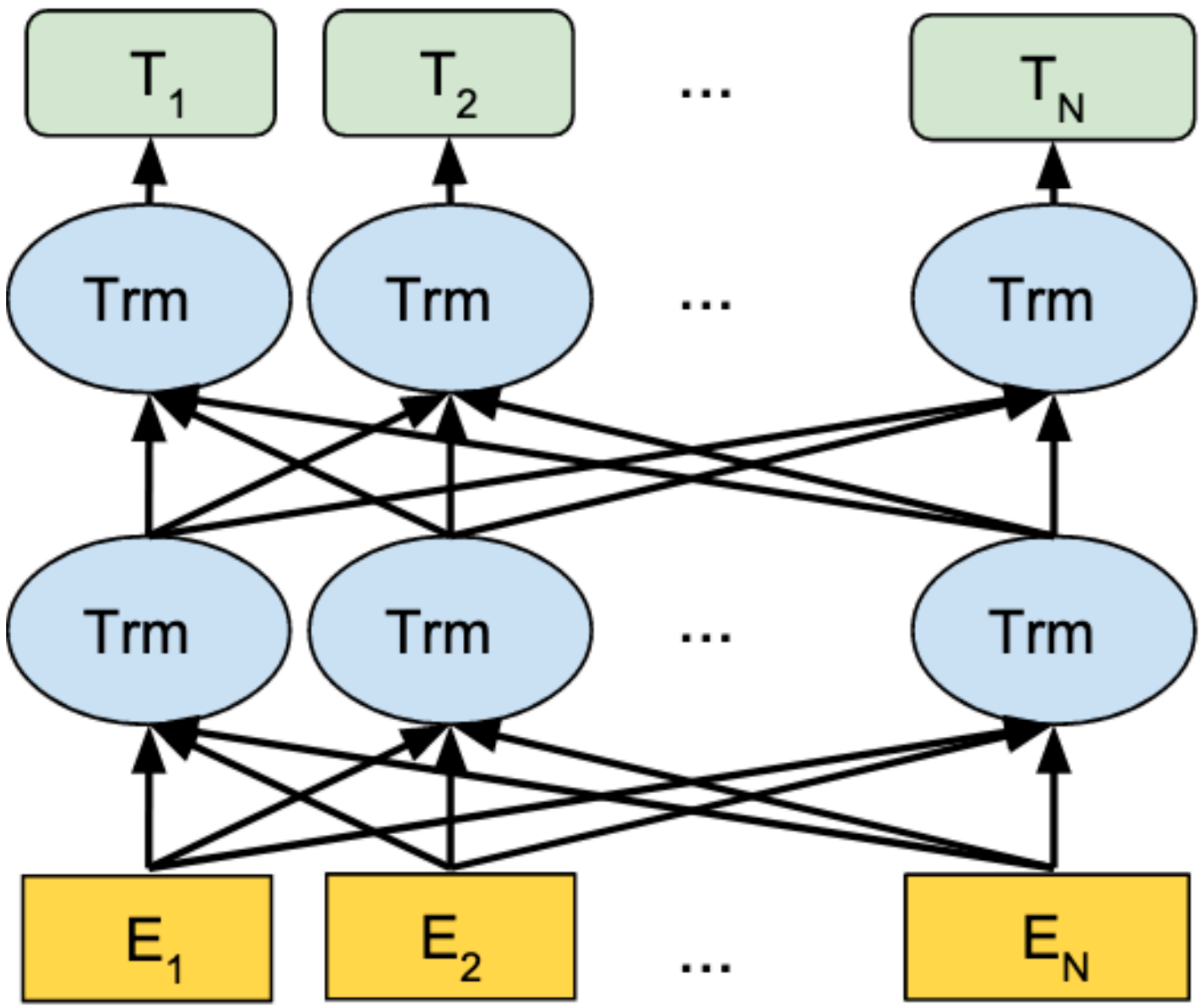
Transformer: Path Lengths + Parallelism

Computation order:

Entire second layer: 1

Entire first layer: 0

Also not linear in sequence length! Can be parallelized.



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Transformer: Summary

- *Entirely* feed-forward
  - Therefore massively parallelizable
  - RNNs are inherently sequential, a parallelization bottleneck
- (Self-)attention everywhere
- Long-term dependencies:
  - LSTM: has to maintain representation of early item
  - Transformer: very short “path-lengths”

Next Time

- A deeper look at the *decoder* block of a Transformer
  - Attention masks
- Subword tokenization