Transformers 1

Ling 282/482: Deep Learning for Computational Linguistics

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Fall 2024

Today's Plan

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

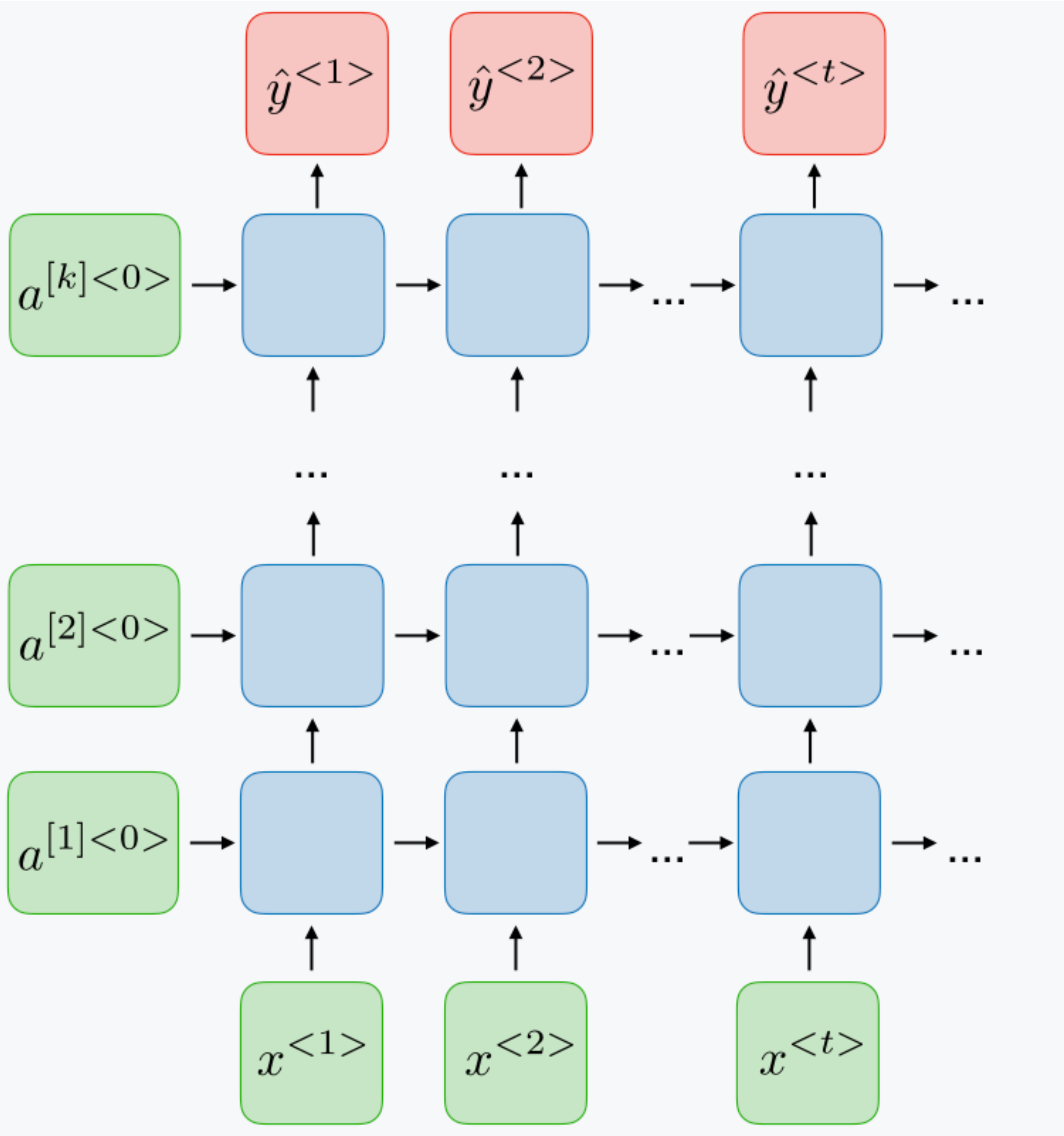
Limitations of Recurrent Models

RNNs Unrolling

- Recall: RNNs are “unrolled” across time, same operation at each step
- This has at least two issues:
  - Creates **long computation chains** 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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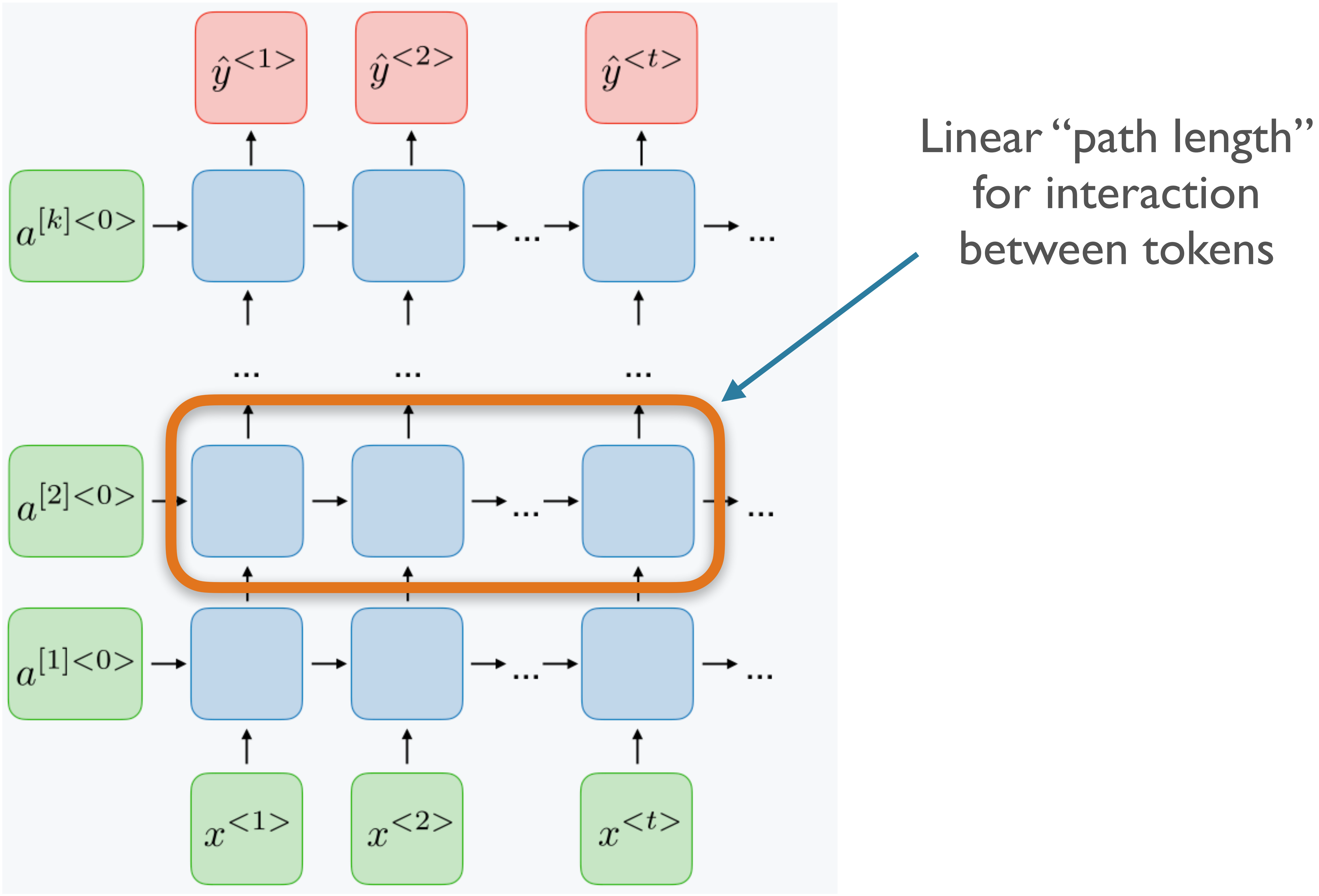

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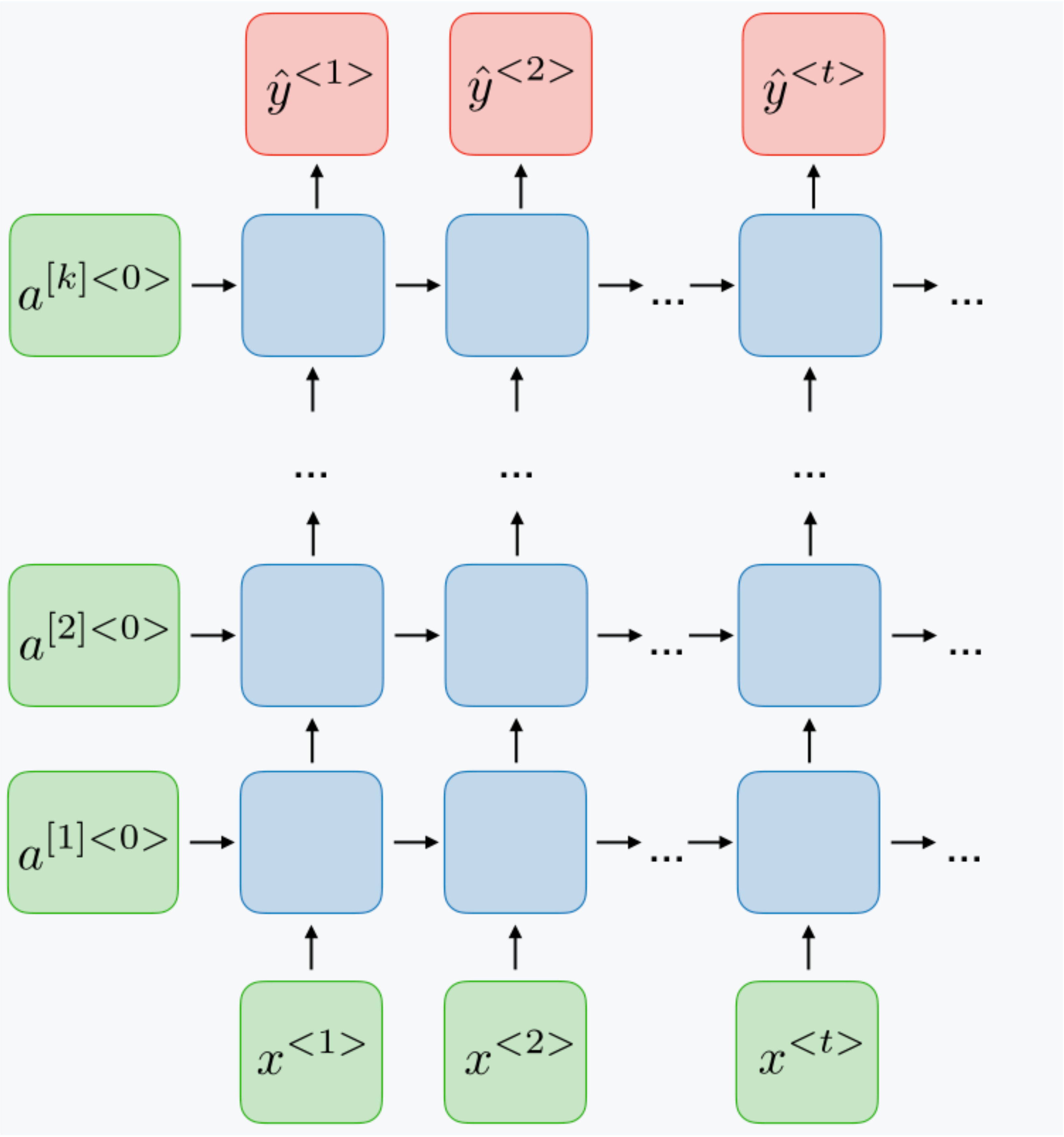
Lack of Parallelizability

- 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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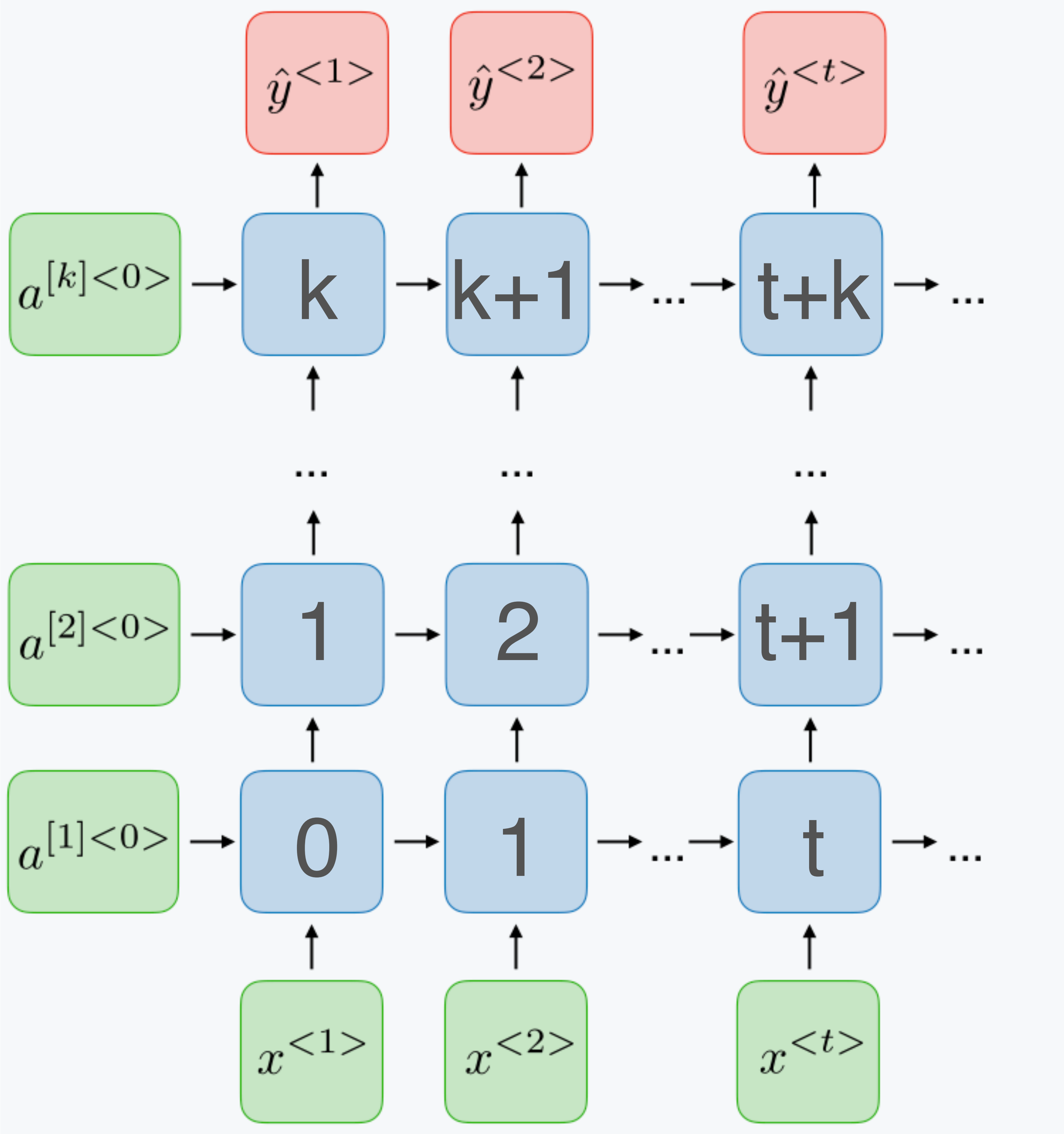

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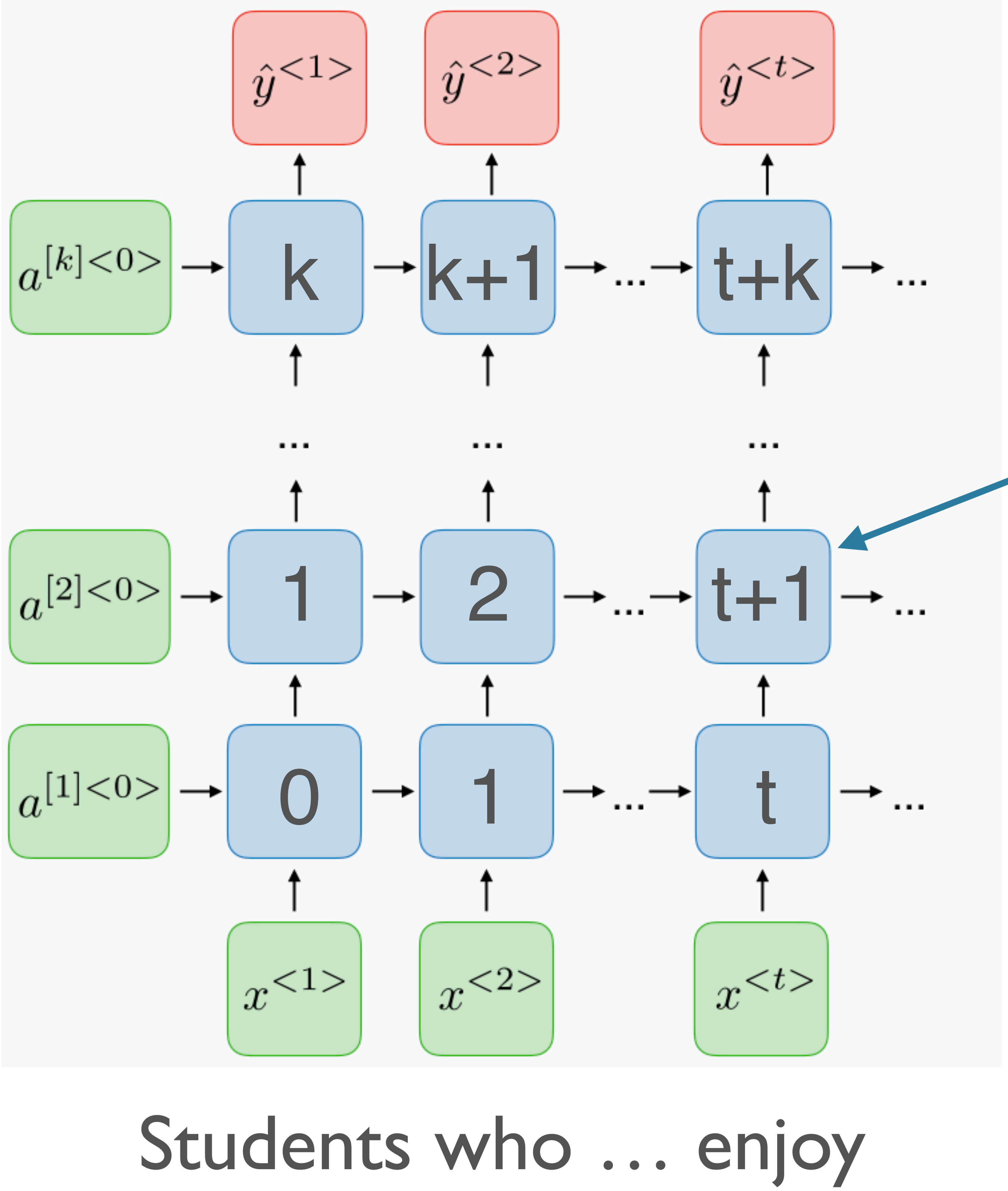

Number of computation steps required: linear in sequence length

Transformer Architecture

Attention Is All You Need

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Paper link

(but see Annotated and Illustrated Transformer)

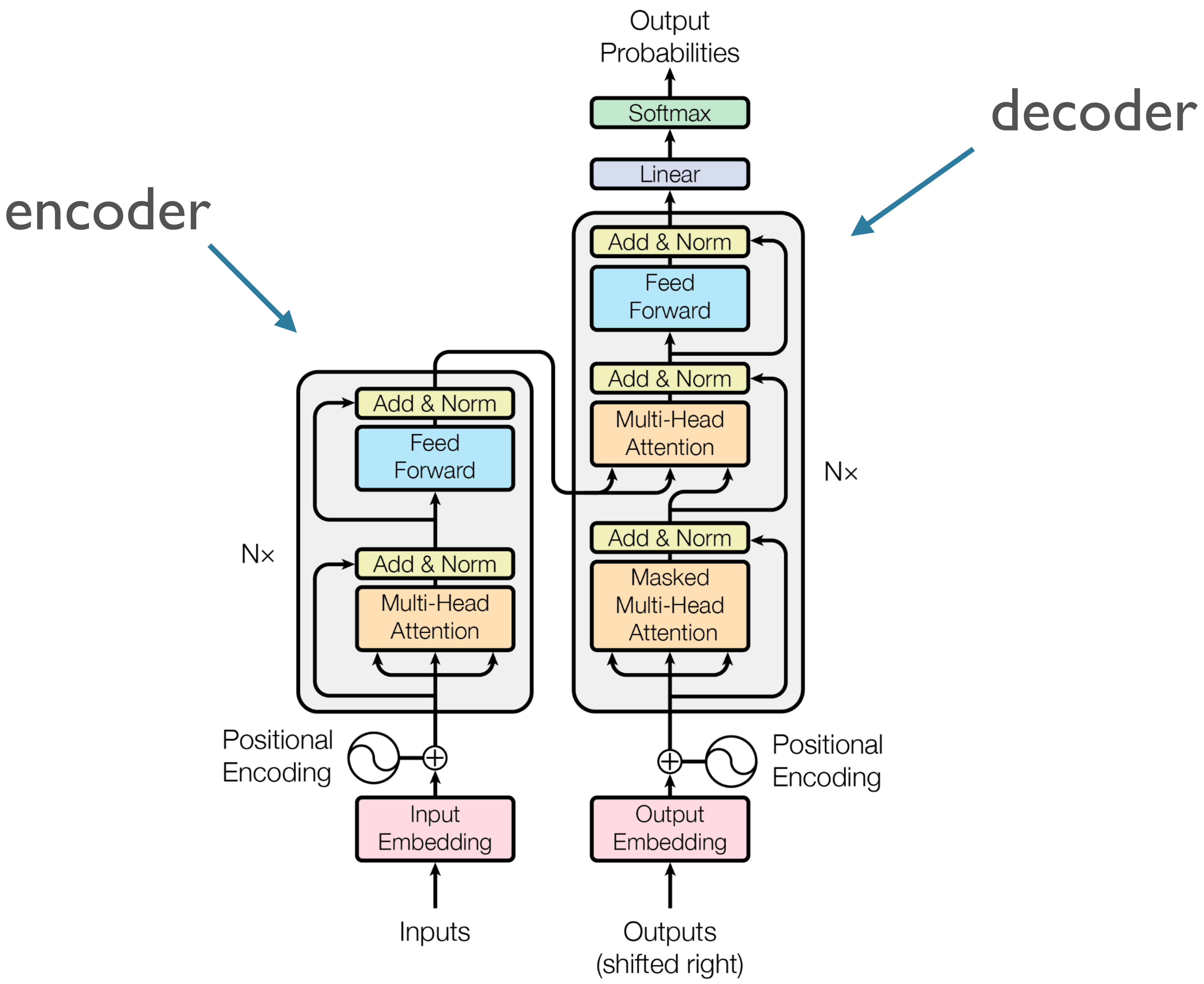
Abstract

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.

Key Idea

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

Full Model


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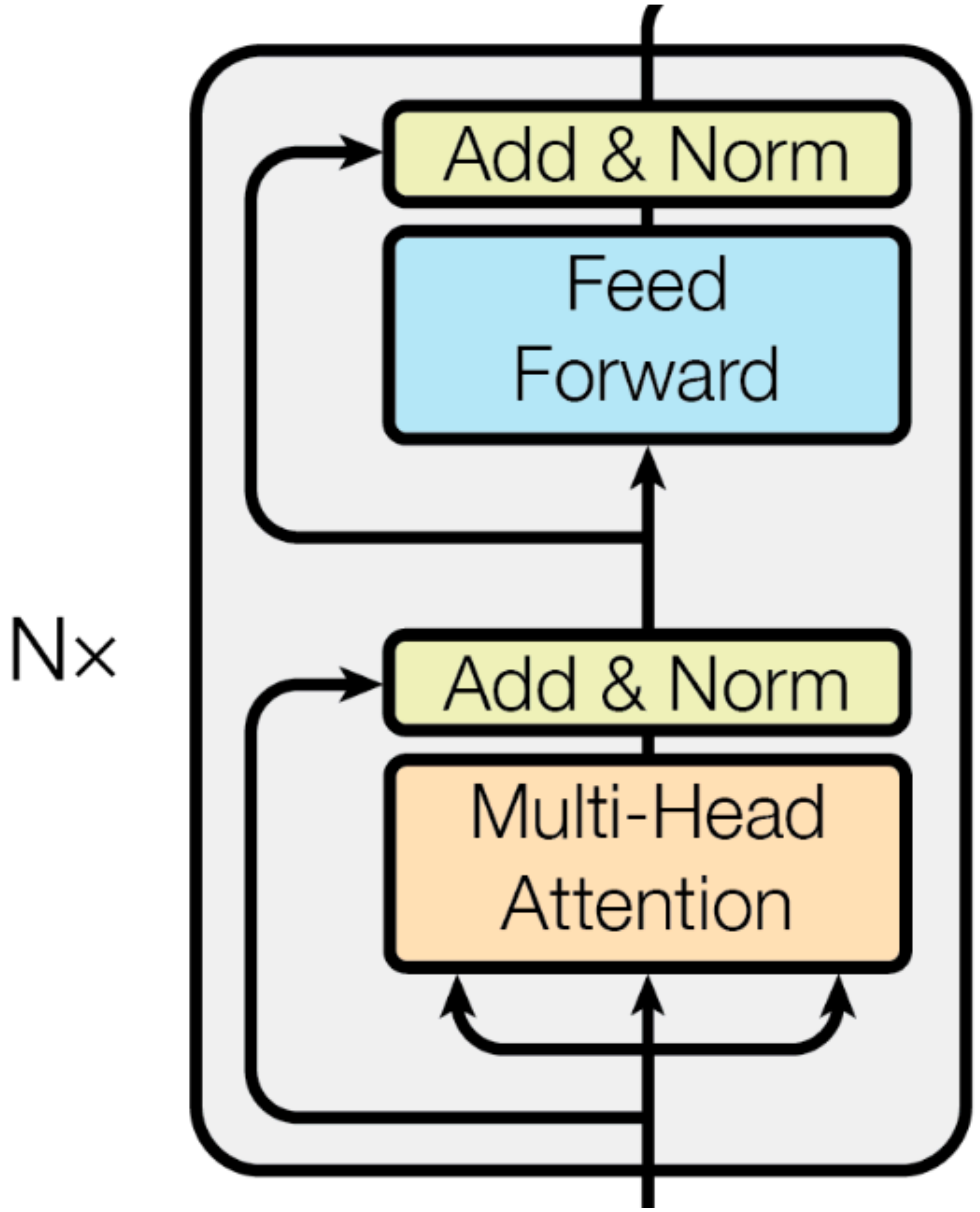
Multi-Head
Attention
N×
Positional
Encoding
Positional
Encoding
Input
Embedding
Output
Embedding
Inputs
Outputs
(shifted right)
encoder
decoder

Transformer Block



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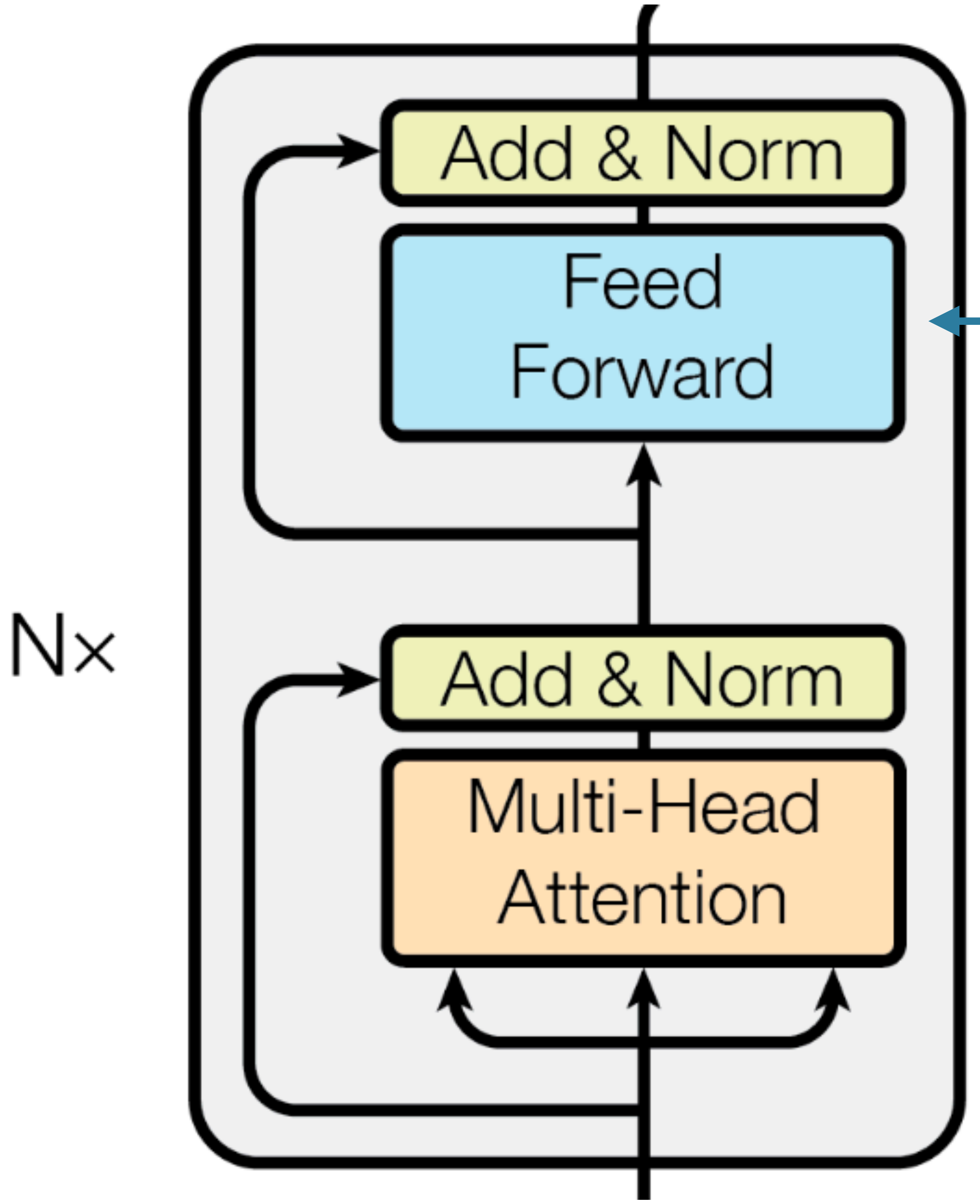

Single layer, applied to each position

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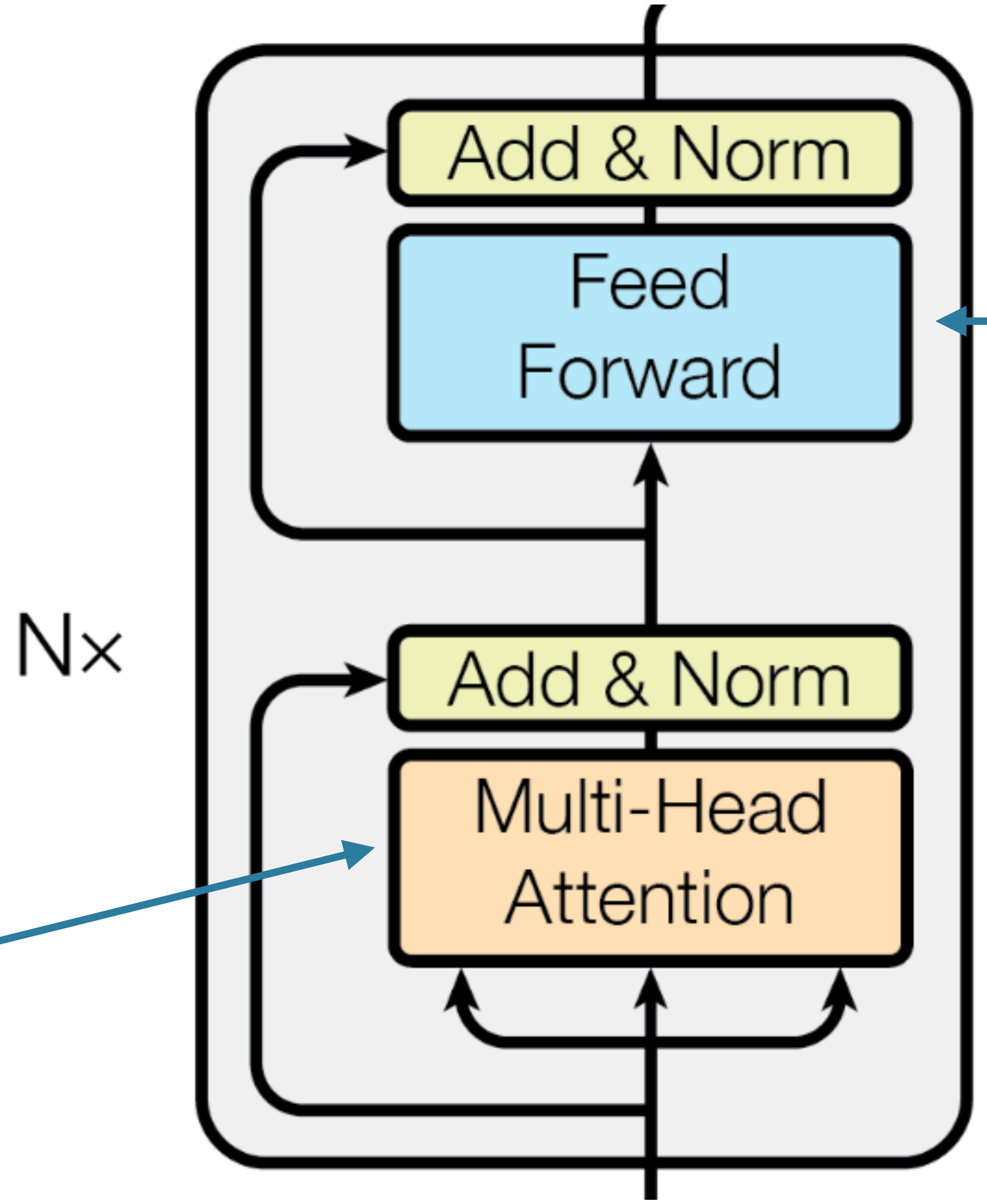

Single layer, applied to each position

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

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$$\alpha_j = q \cdot k_j$$

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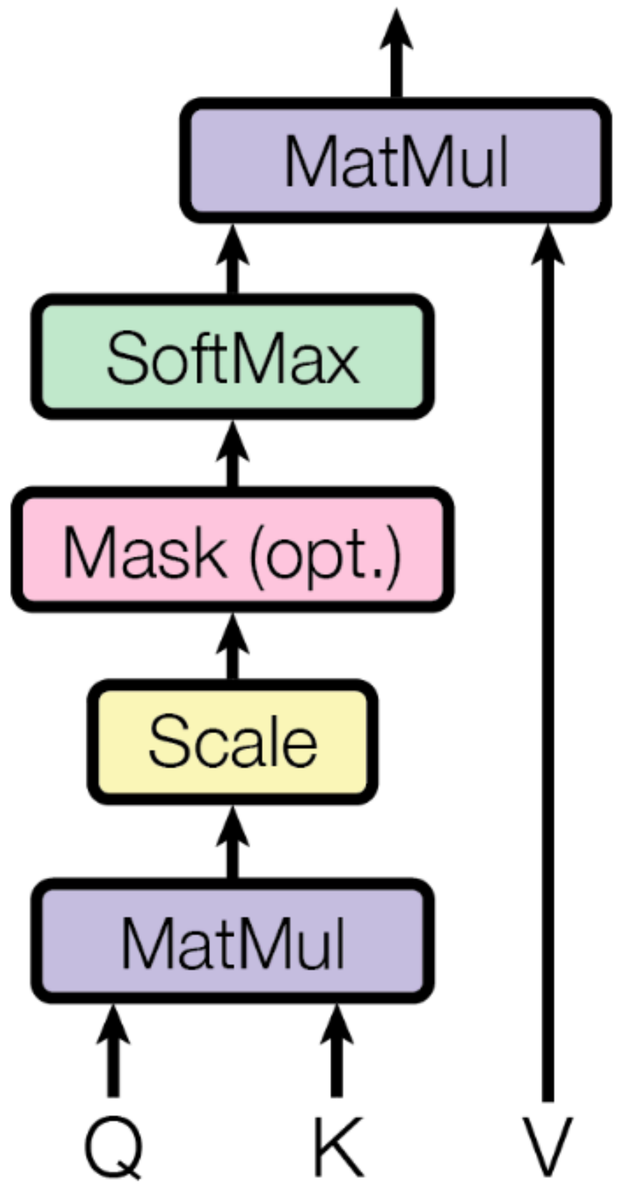

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- **Each vector** at each position **transformed into a query, key, value**
  - Linearly transformed, to be different “views”

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

- 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 (normalization: see paper for motivation)
- **Softmax along *rows***: converts raw scores to **probability distribution**

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Self-Attention: Details

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- 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)
- See here for 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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$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head_1}, \ldots, \mathrm{head_h})W^O$$
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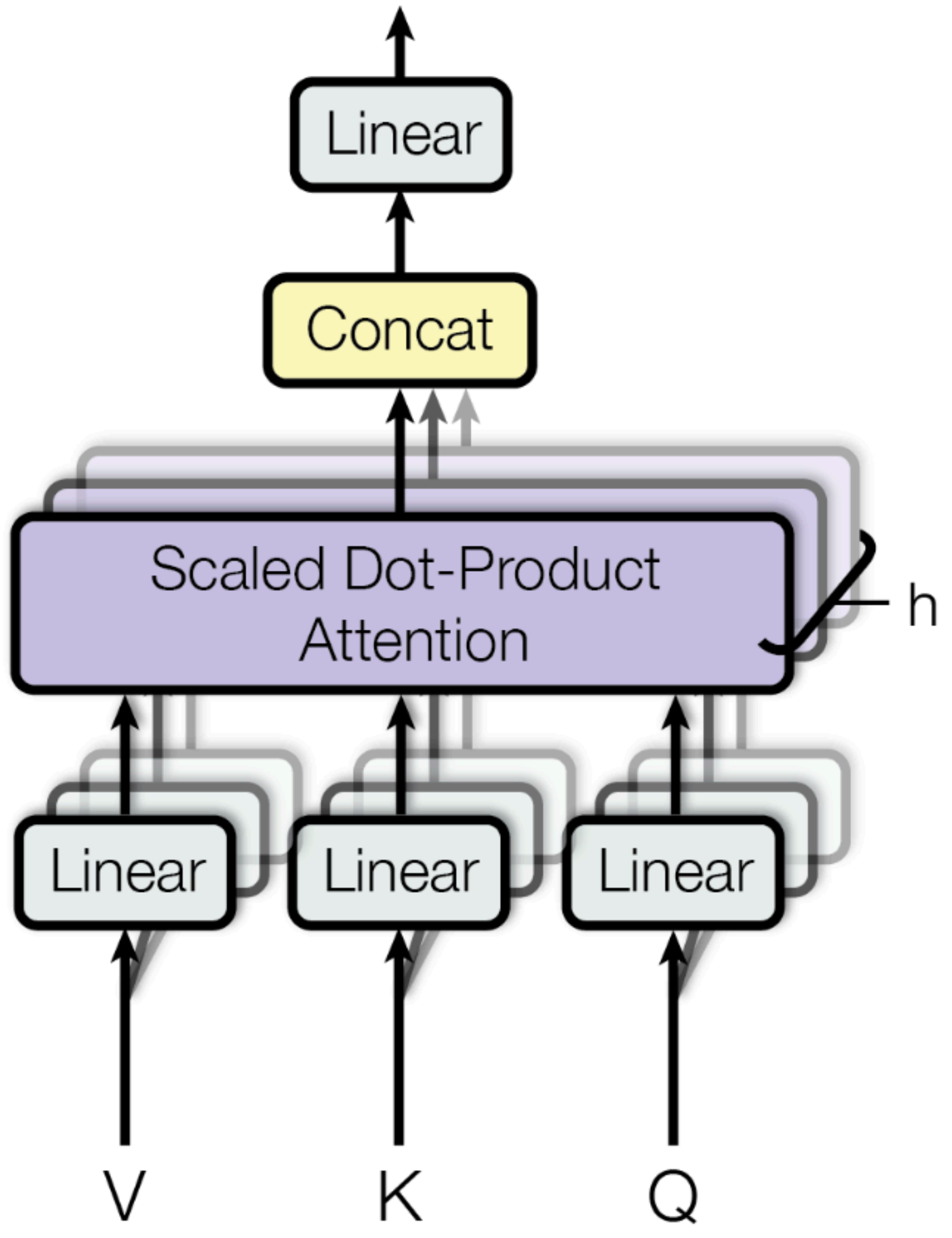

Problem With Self-Attention

- Attention is **order-independent**
  - If we shuffle the sequence we get the **same output!**

Representing Order

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- Represented via **positional encodings**

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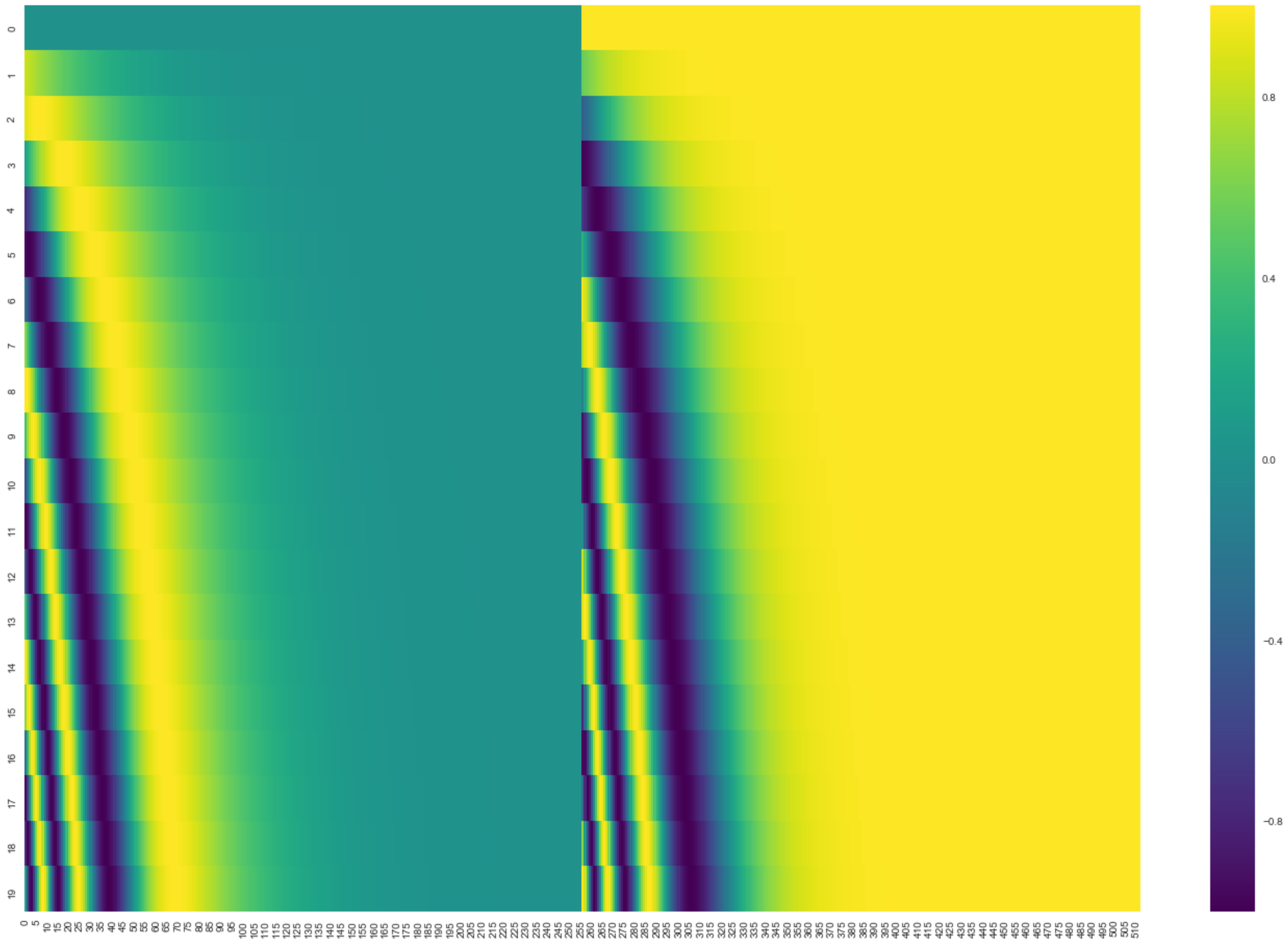

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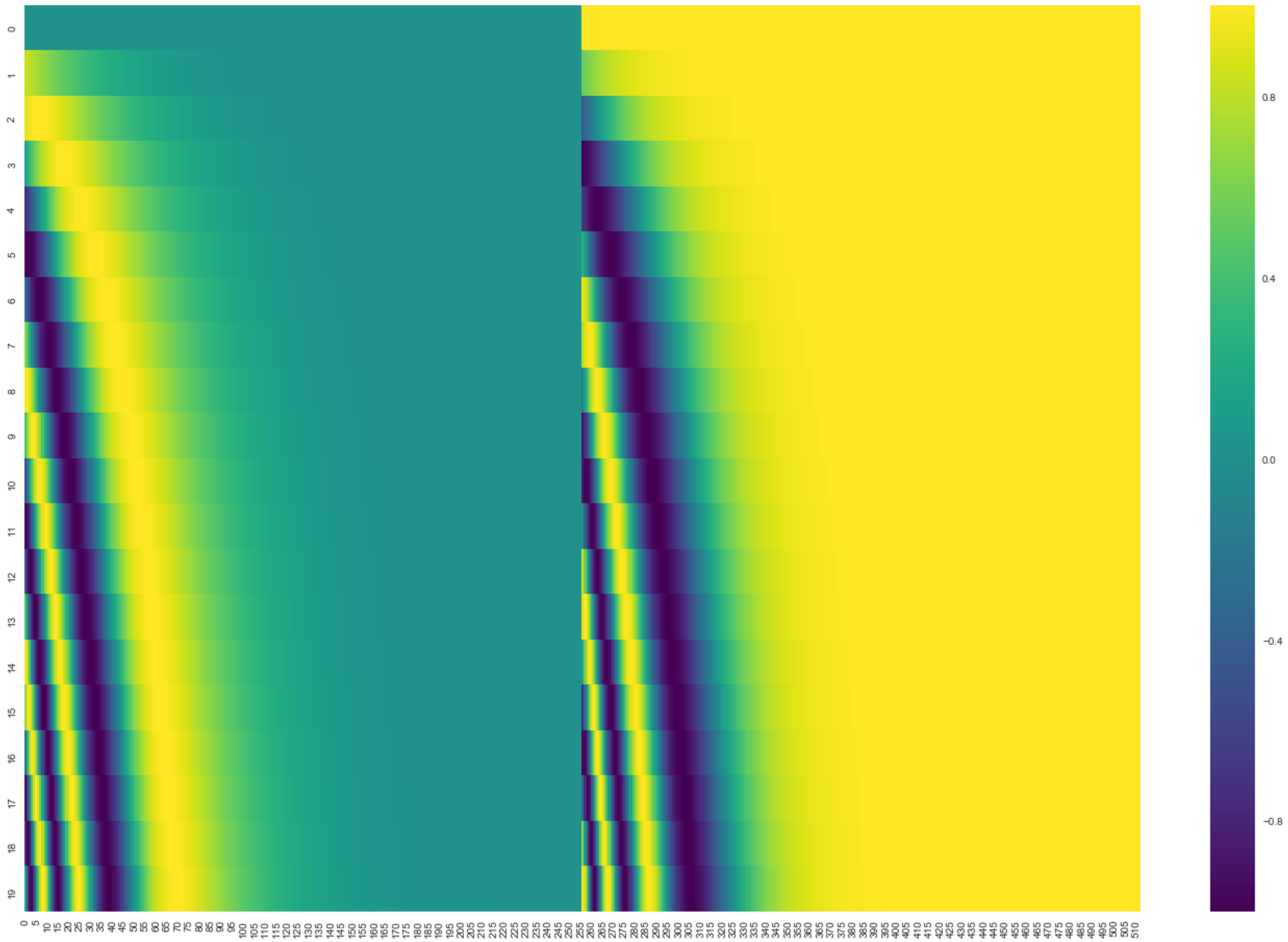

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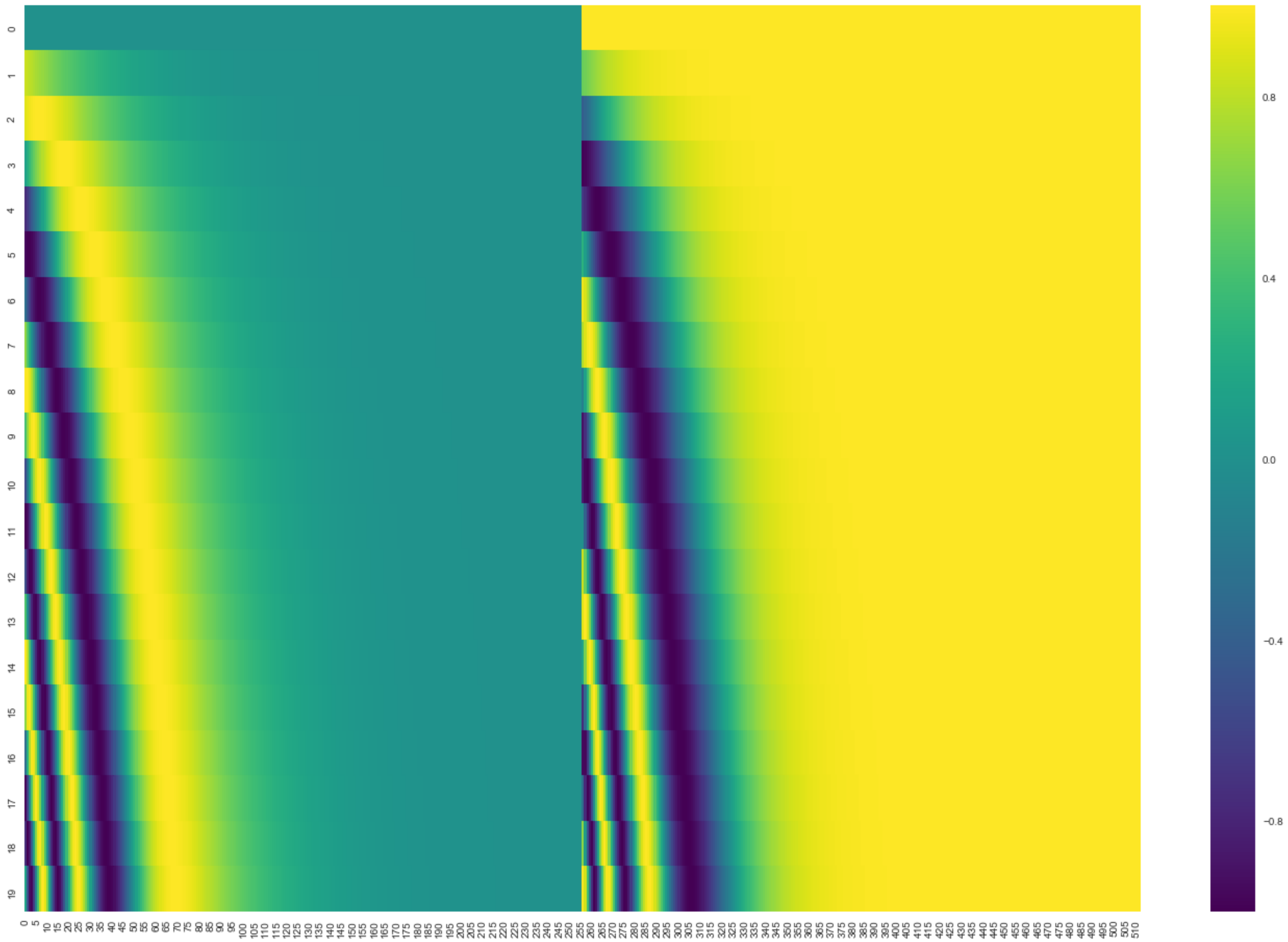

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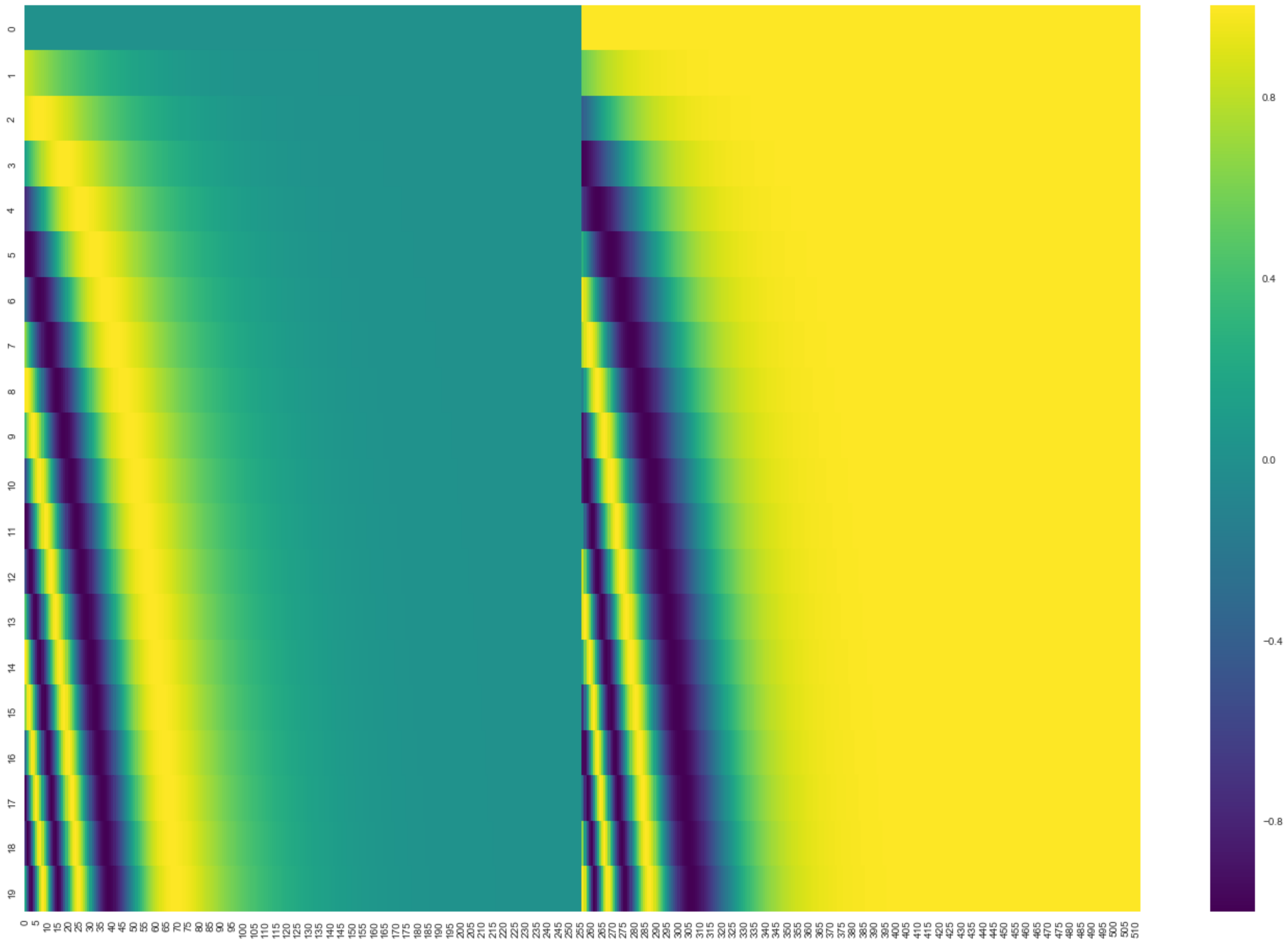

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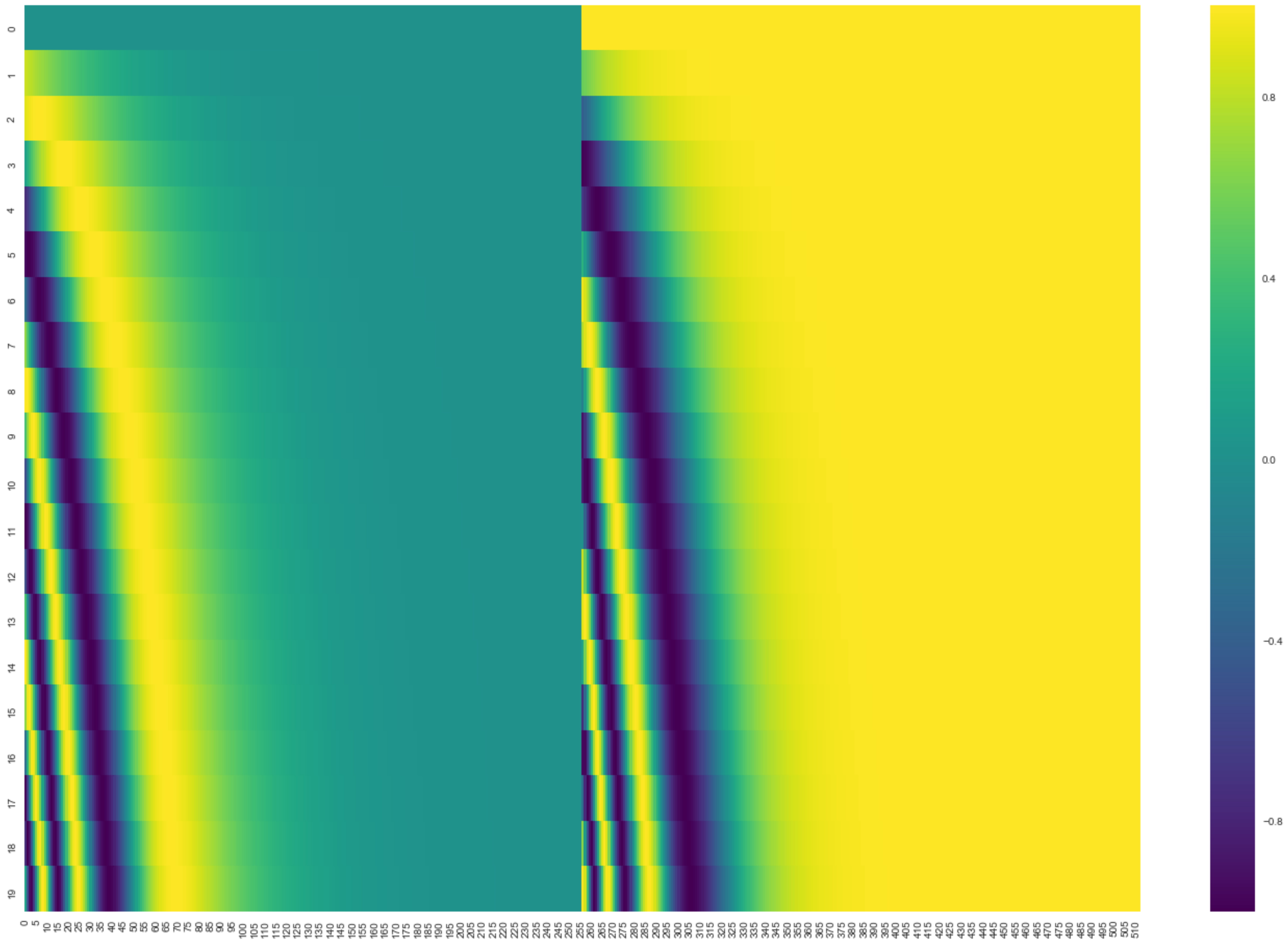

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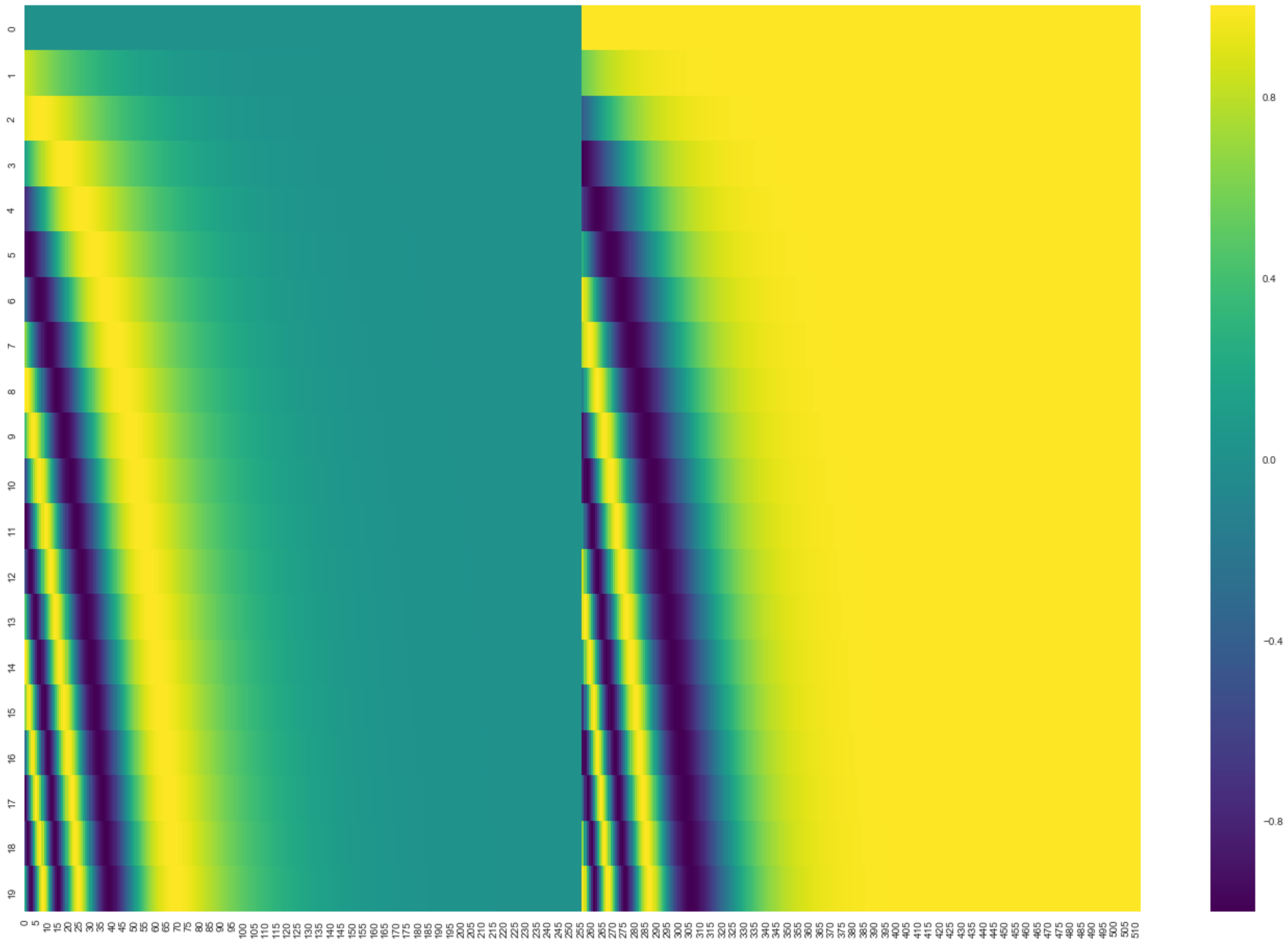
- Can be **fixed/pre-defined** (see right) or **entirely learned**



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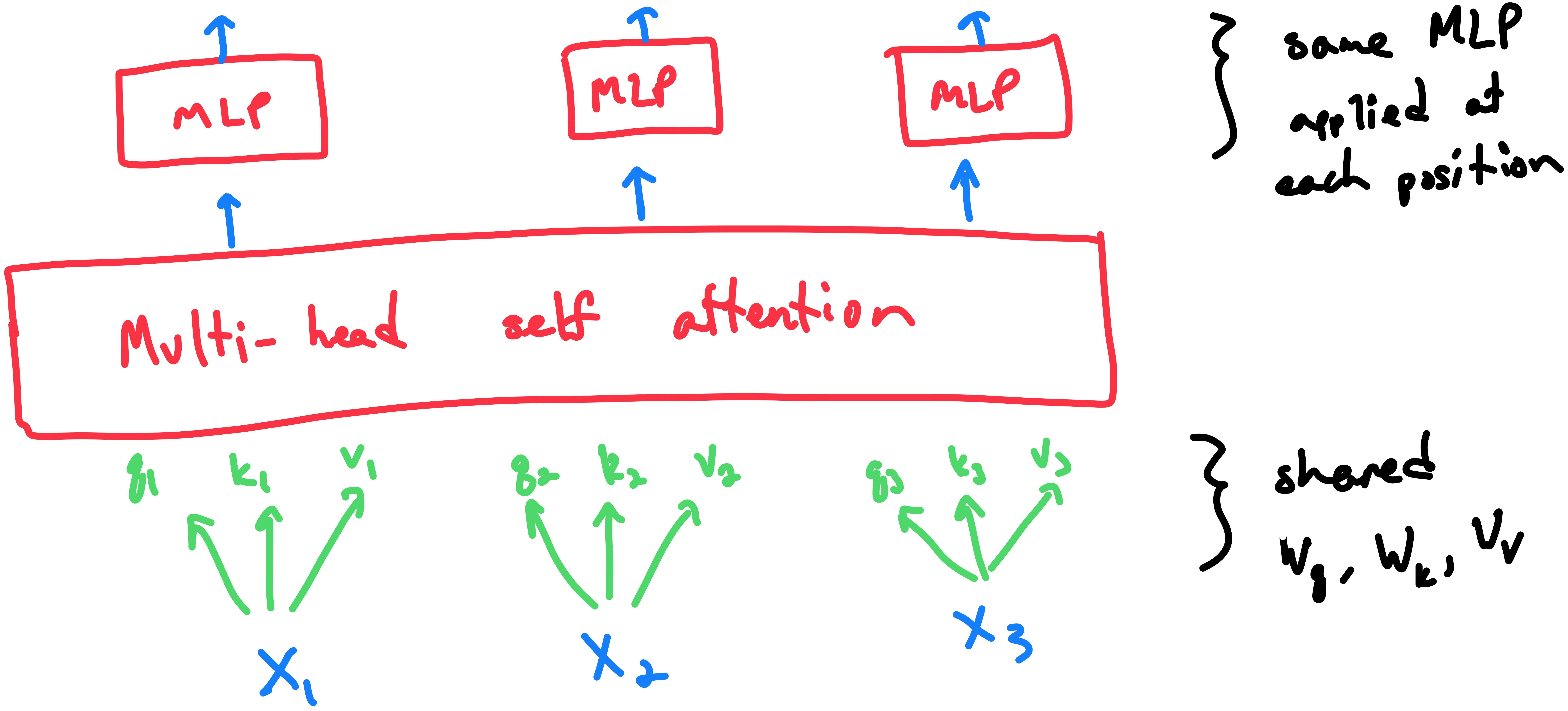
Fixed vs Learned Positional Encoding

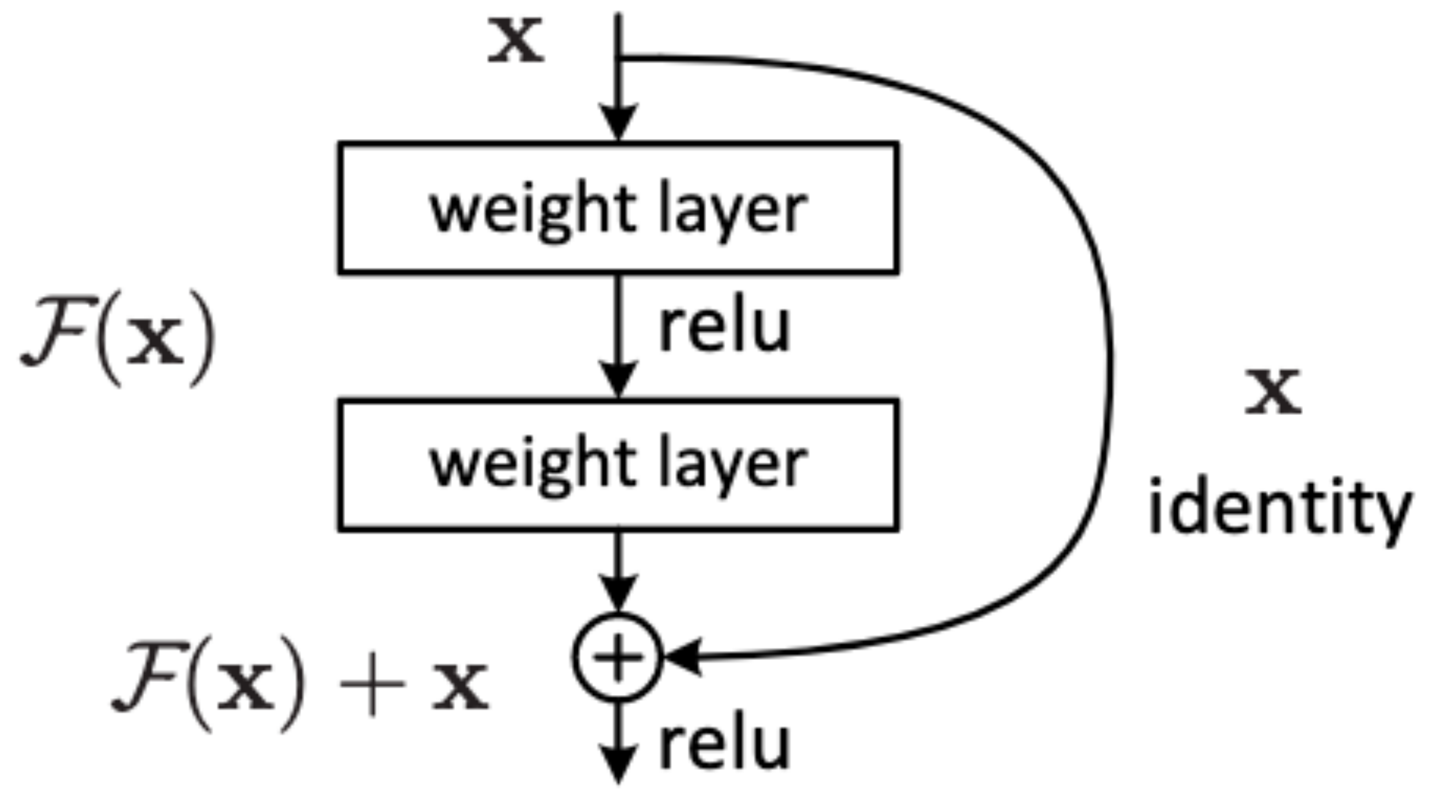
- Fixed:
  - No need to be learned
  - Guaranteed to be **unique to position**
  - Generalizes to **longer sequence lengths** (in theory at least)
- Learned:
  - Might learn **more useful encodings** of position than e.g. sinusoidal
  - **Can't extrapolate** to longer sequence lengths
  - (This has become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

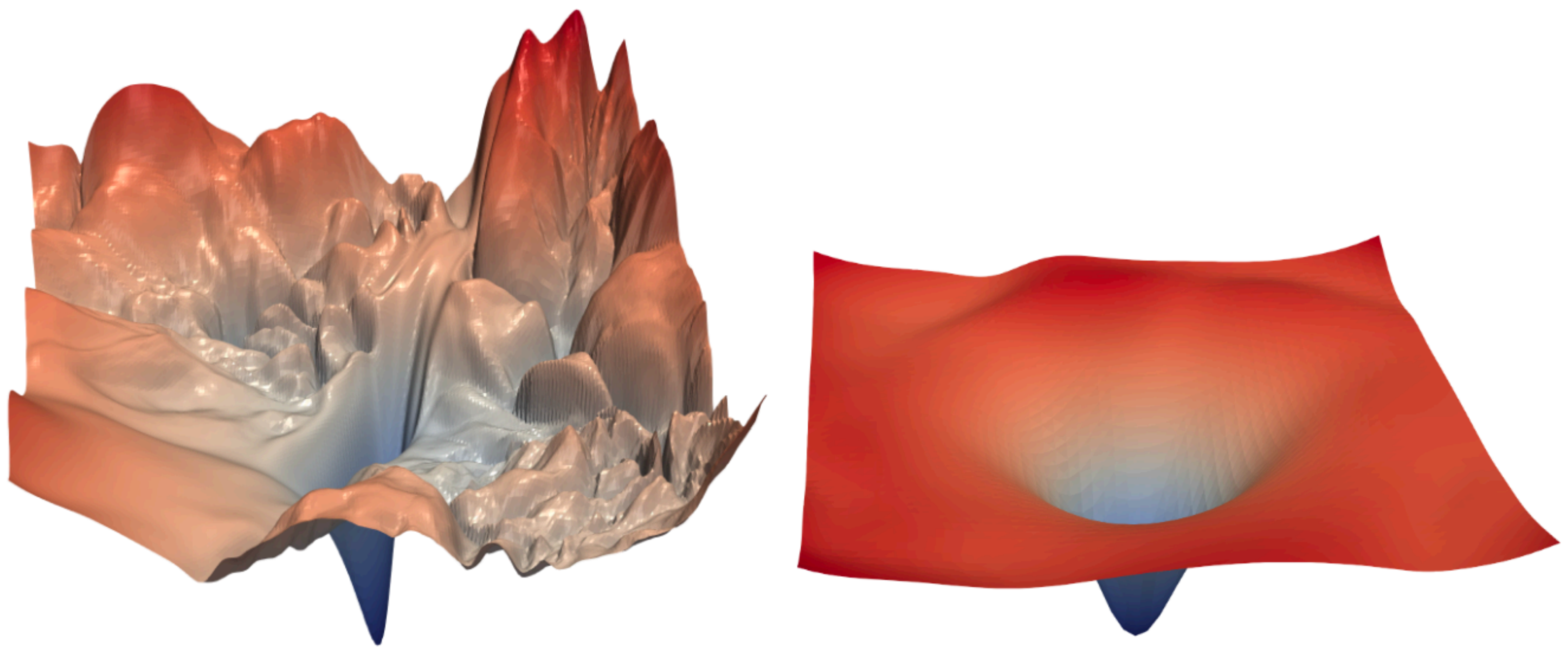
Basic Transformer Encoder Block



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

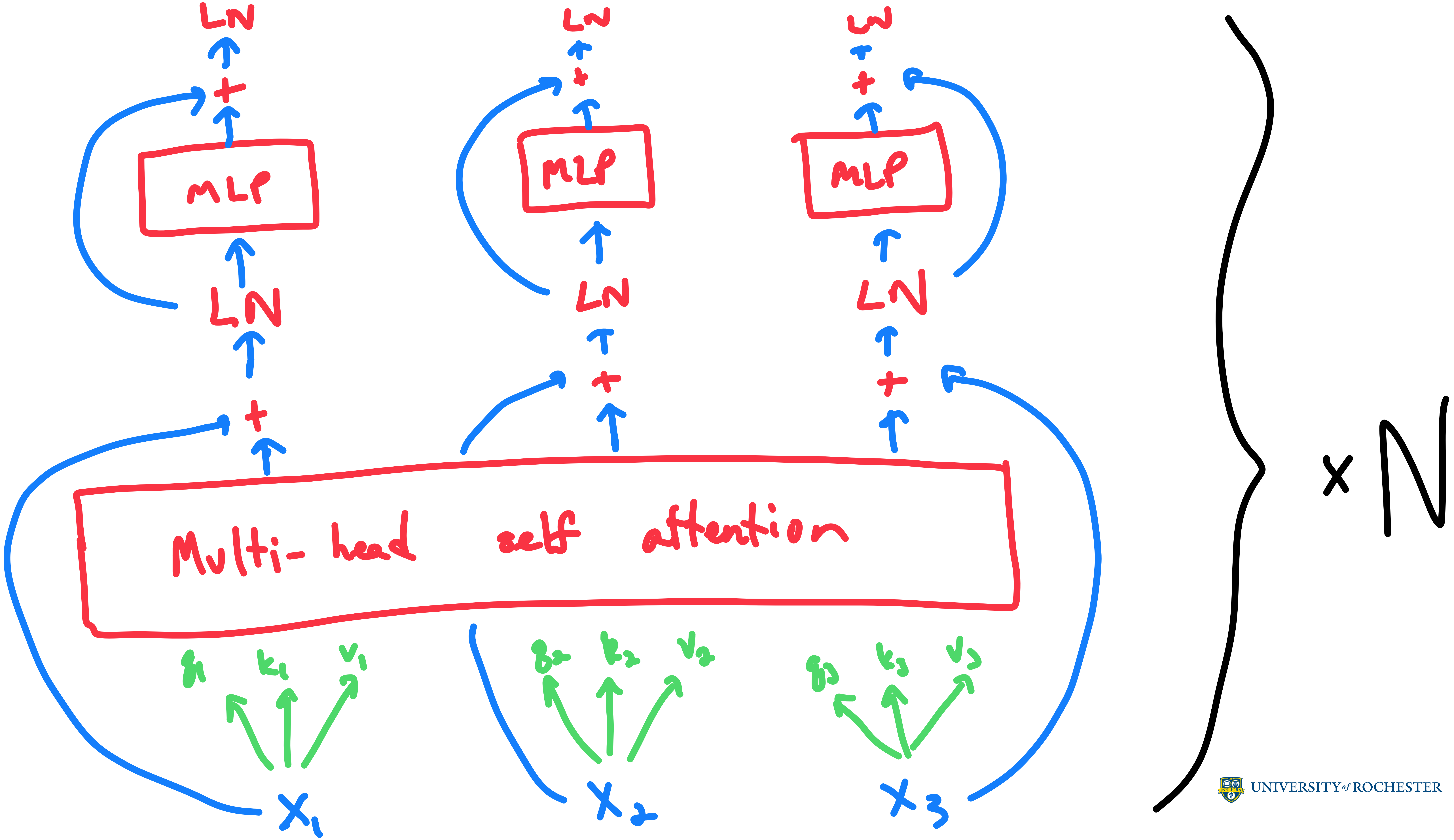
Final Ingredients: Layer Normalization

- 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	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$
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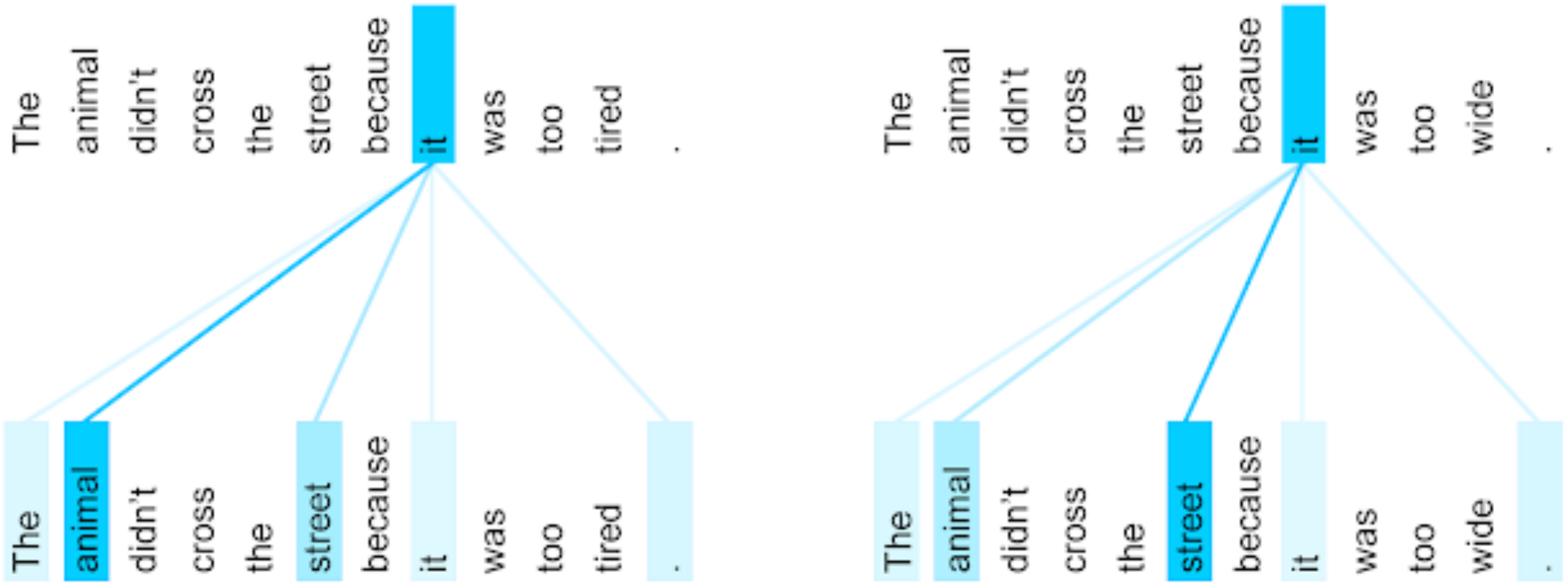
More on why important later

Attention Visualization: Coreference?



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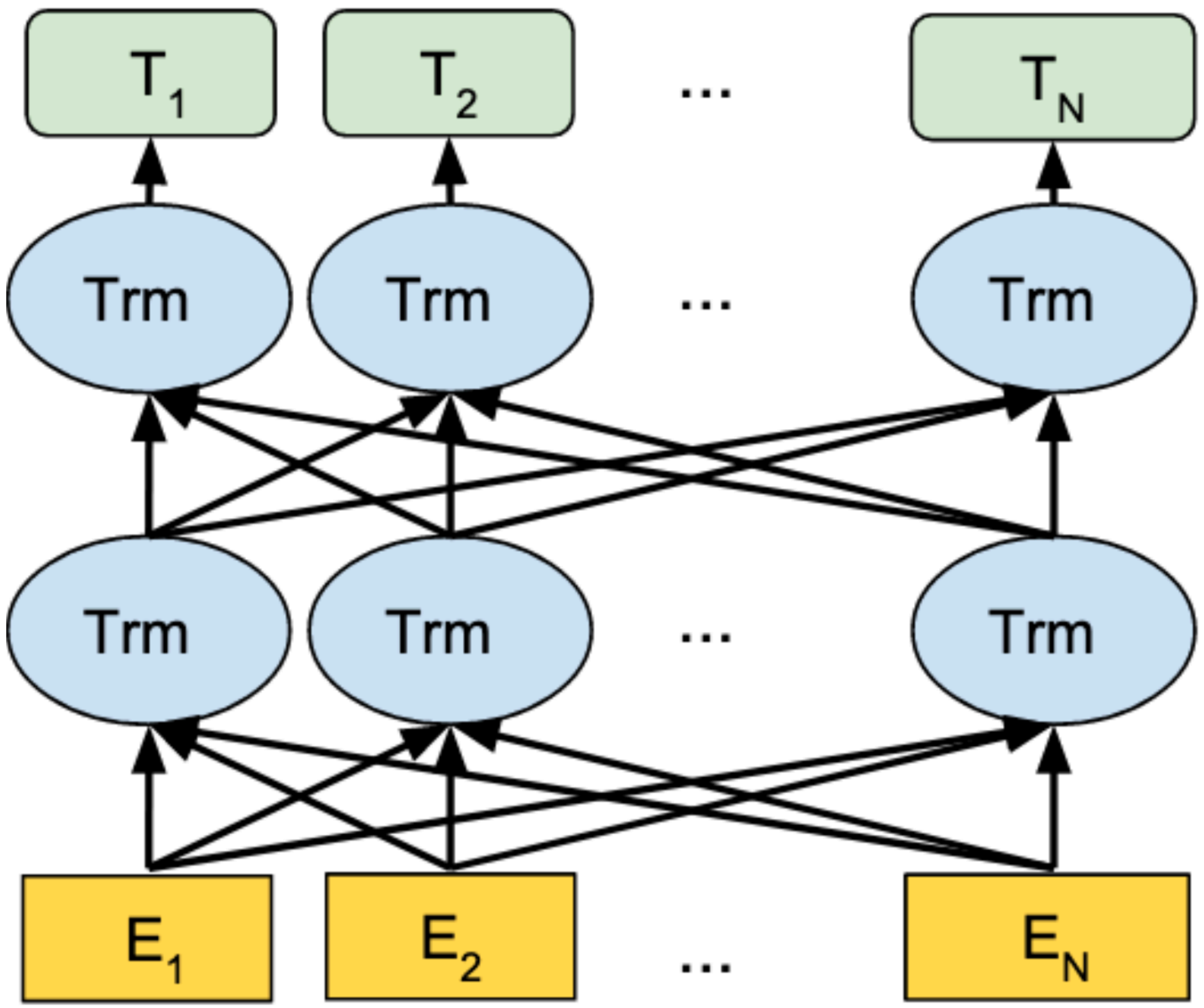
Transformer: Path Lengths + Parallelism



source (BERT paper)

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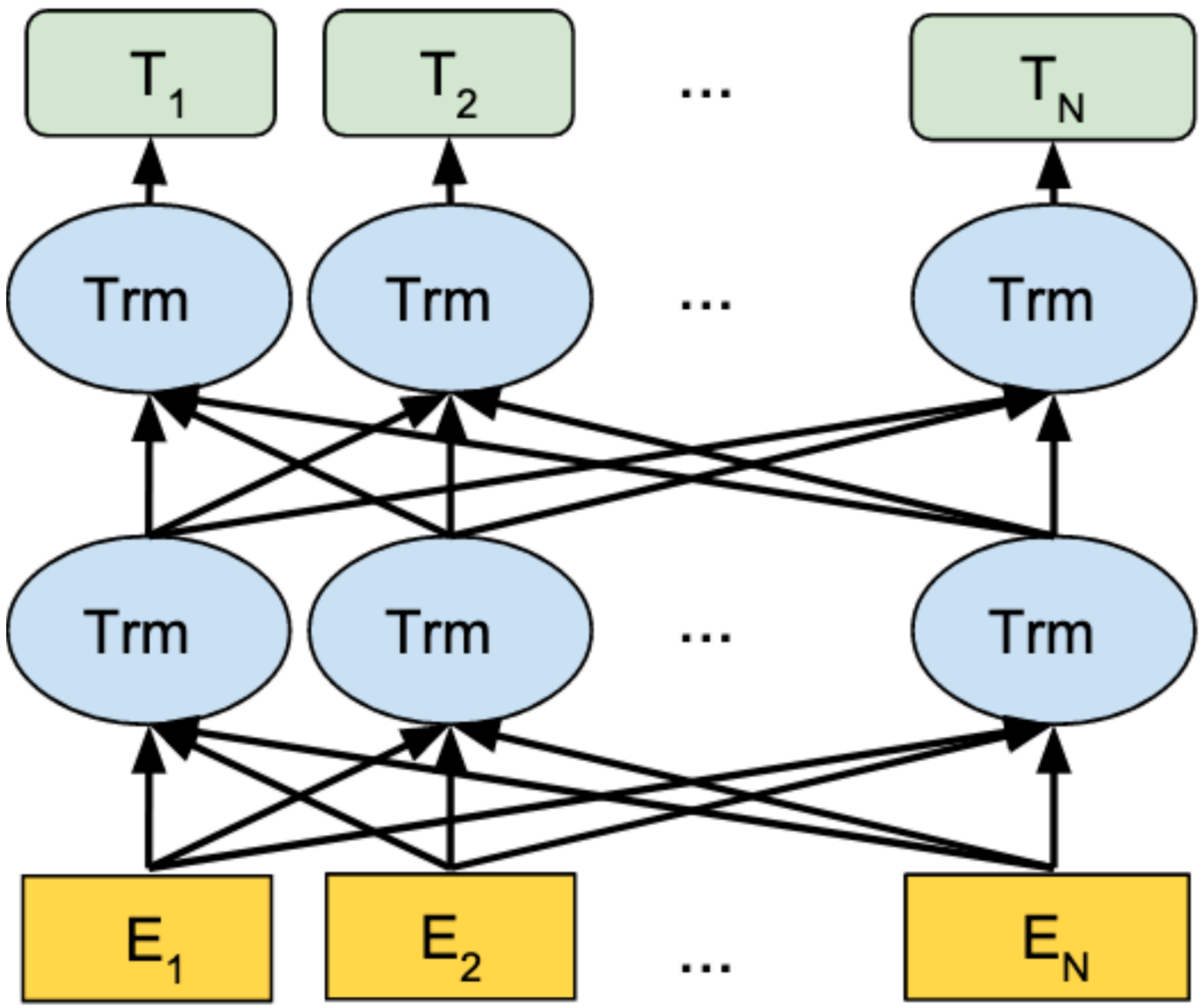


Path lengths between tokens: 1 (constant, not linear)

source (BERT paper)

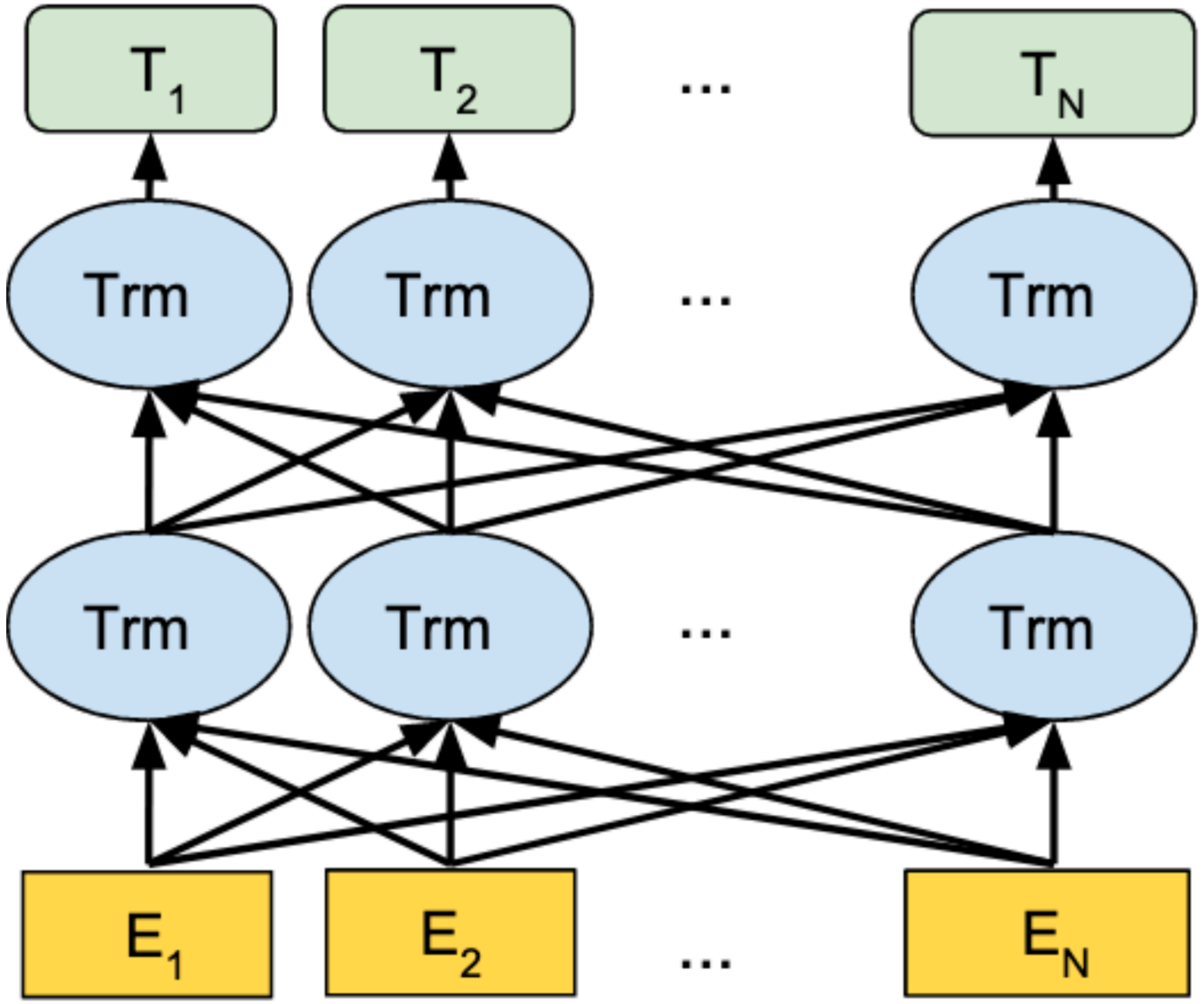
Transformer: Path Lengths + Parallelism

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: **direct connection** to all other tokens

Next Time

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