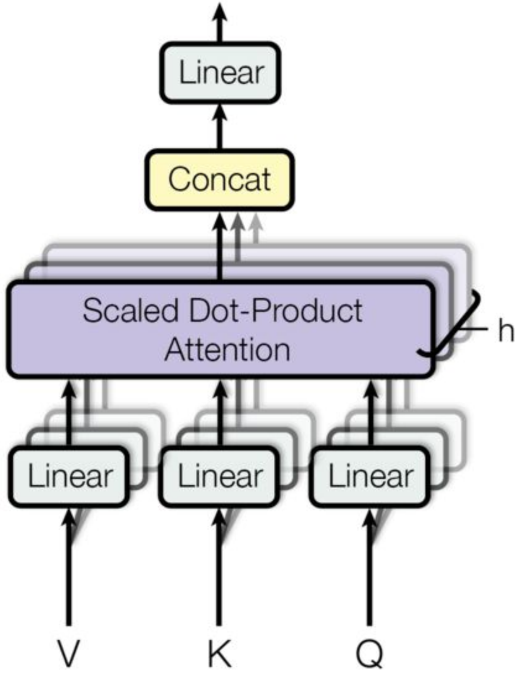
(Better) understanding the scaled dot-product multi-headed self-attention

Understanding multi-headed self-attention

- Might seem intimidating, but the individual parts are rather simple
  - The easiest way to understand **multi-headed** self-attention is to understand a *single-headed* one



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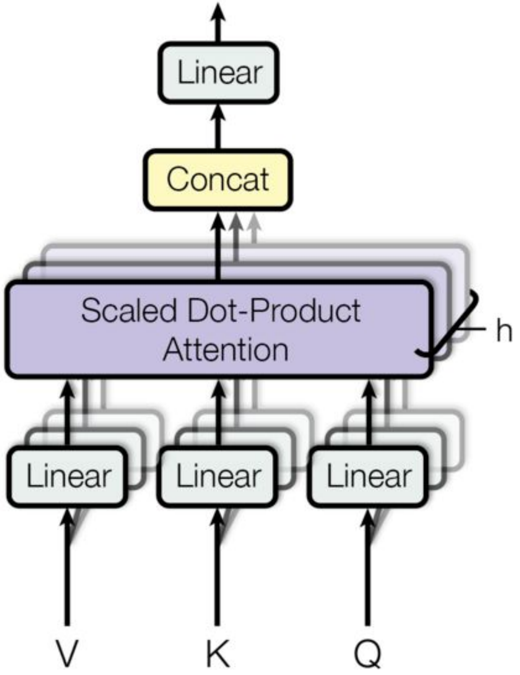

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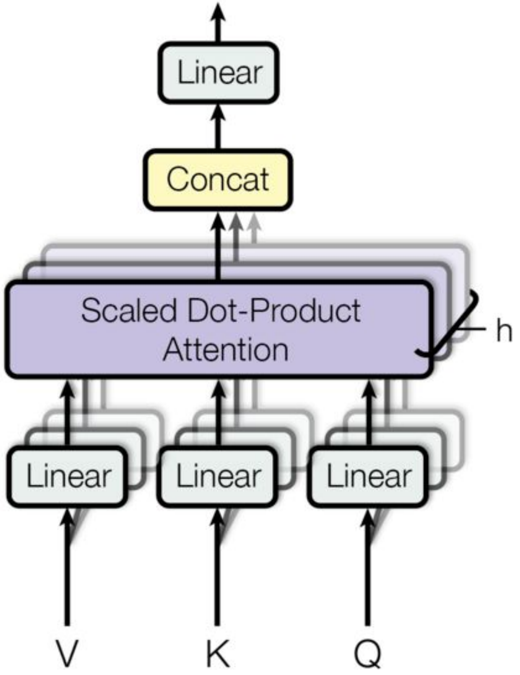


For a single pair of token positions

$$a_{ij} = \mathrm{softmax}(\frac{\mathbf{q}_i \mathbf{k}_j^\top}{\sqrt{d_k}}) = \frac{\exp(\mathbf{q}_i \mathbf{k}_j^\top)}{\sqrt{d_k} \sum_{r \in S_i} \exp(\mathbf{q}_i \mathbf{k}_r^\top)}$$

A *personal* view on Self-Attention (SA)

A powerful blending machine on steroids

A *personal* view on Self-Attention (SA)

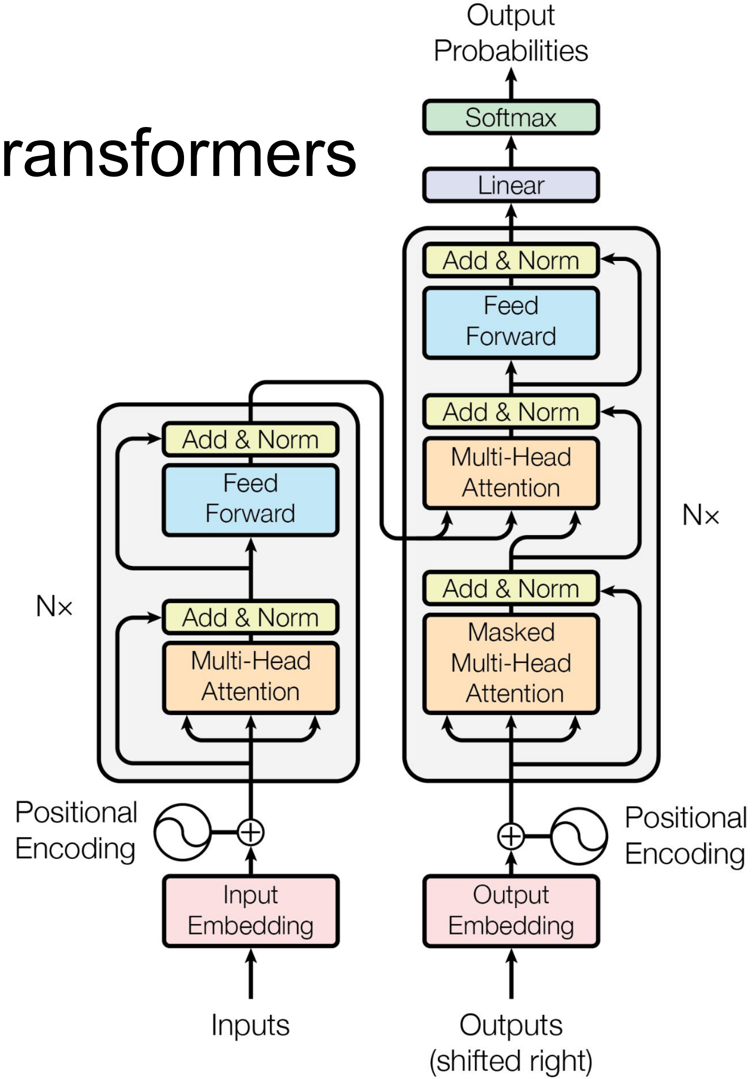
A powerful blending machine on steroids (gradients)

What are all the query / key / value abstractions, and why are they needed?

Why is multi-headed attention needed?

(Are they needed eventually?)

Tips for easier understanding SA in transformers



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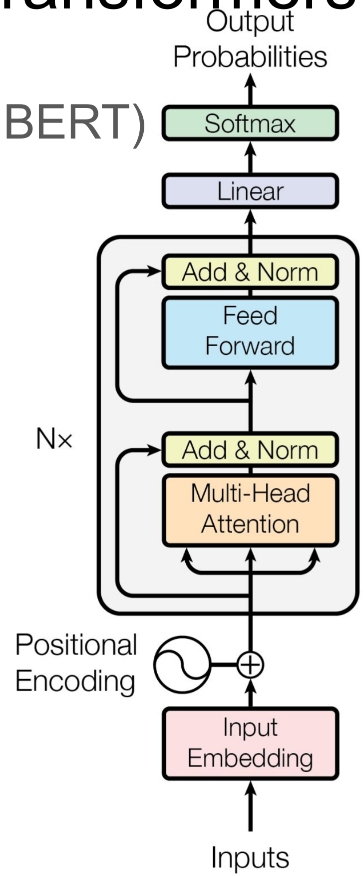

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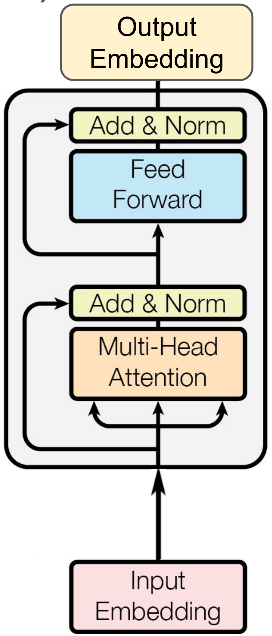

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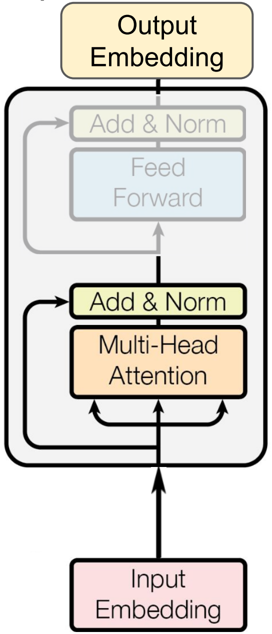

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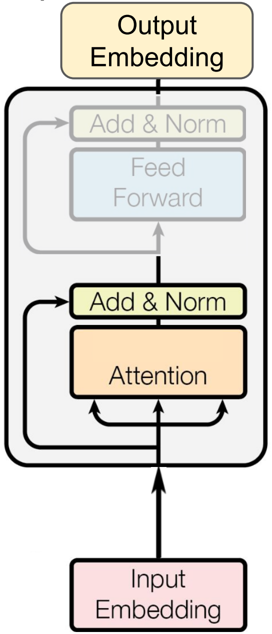

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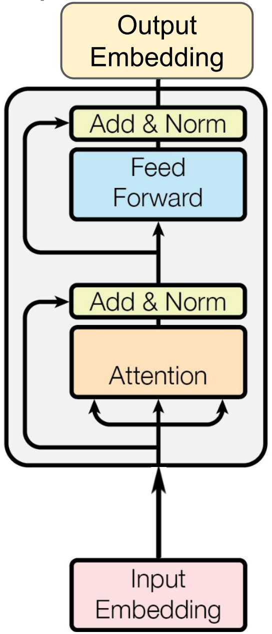

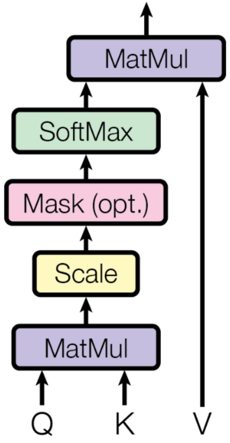

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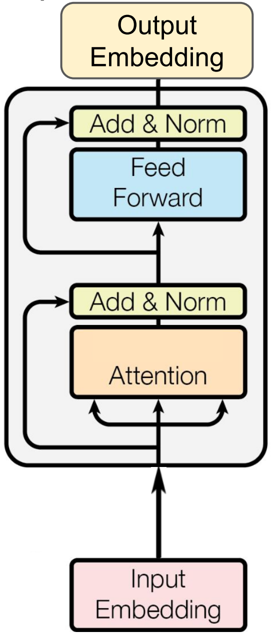

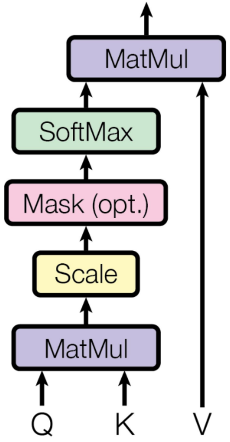

- If X contains the input embeddings then we have:
  - $Q = X W_Q$
  - $K = X W_K$
  - $V = X W_V$

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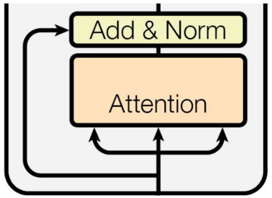
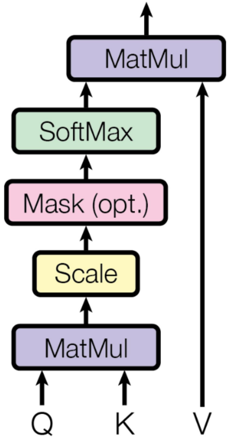
What is the role of the value transformation?

- At each layer, it allows for new semantic aspects to enter the representations
  - It adds on top of the already calculated one via the residual connection





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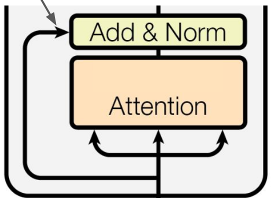

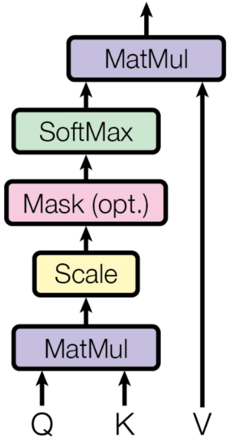

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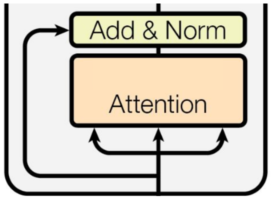

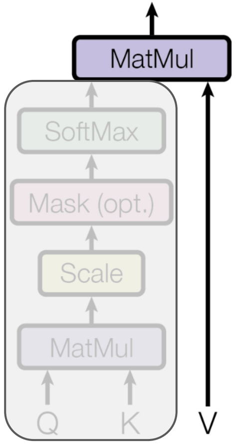

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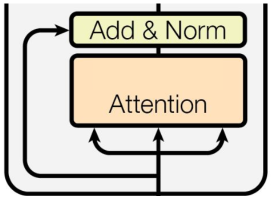

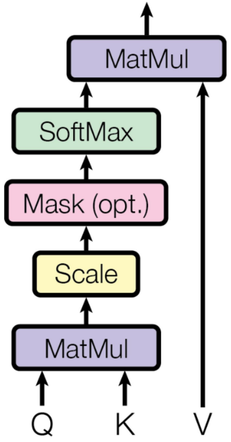

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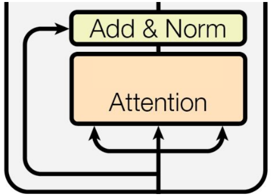

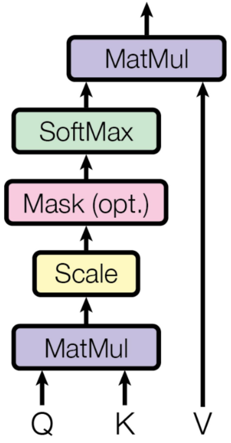

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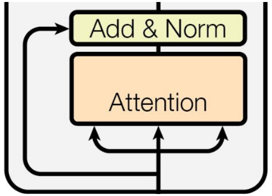

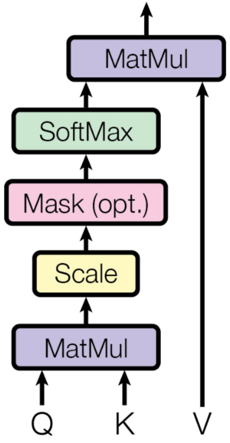

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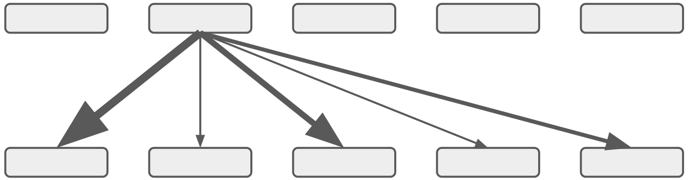

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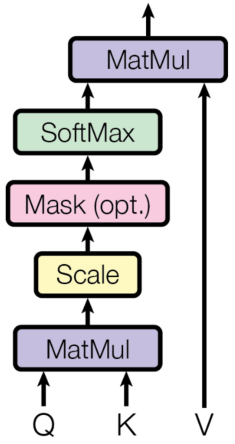

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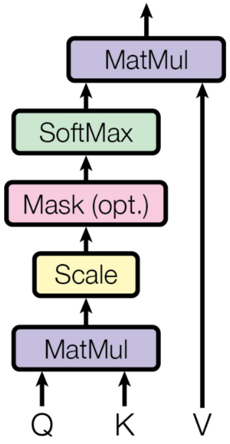

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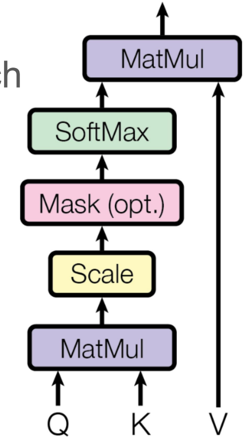

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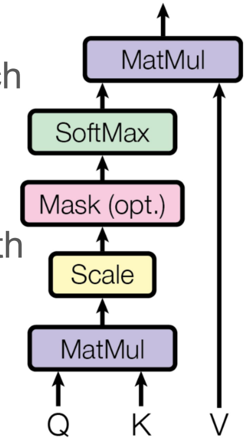

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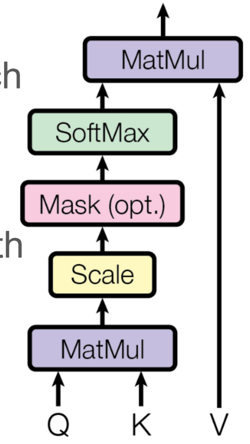
  - A single transformation ($W_{QK} \approx W_Q W_K$) could do the job as well as $(XW_Q)(W_K X^T) = X(W_Q W_K)X^T$
    - Disentangling is, however more effective when W_* has more rows than columns



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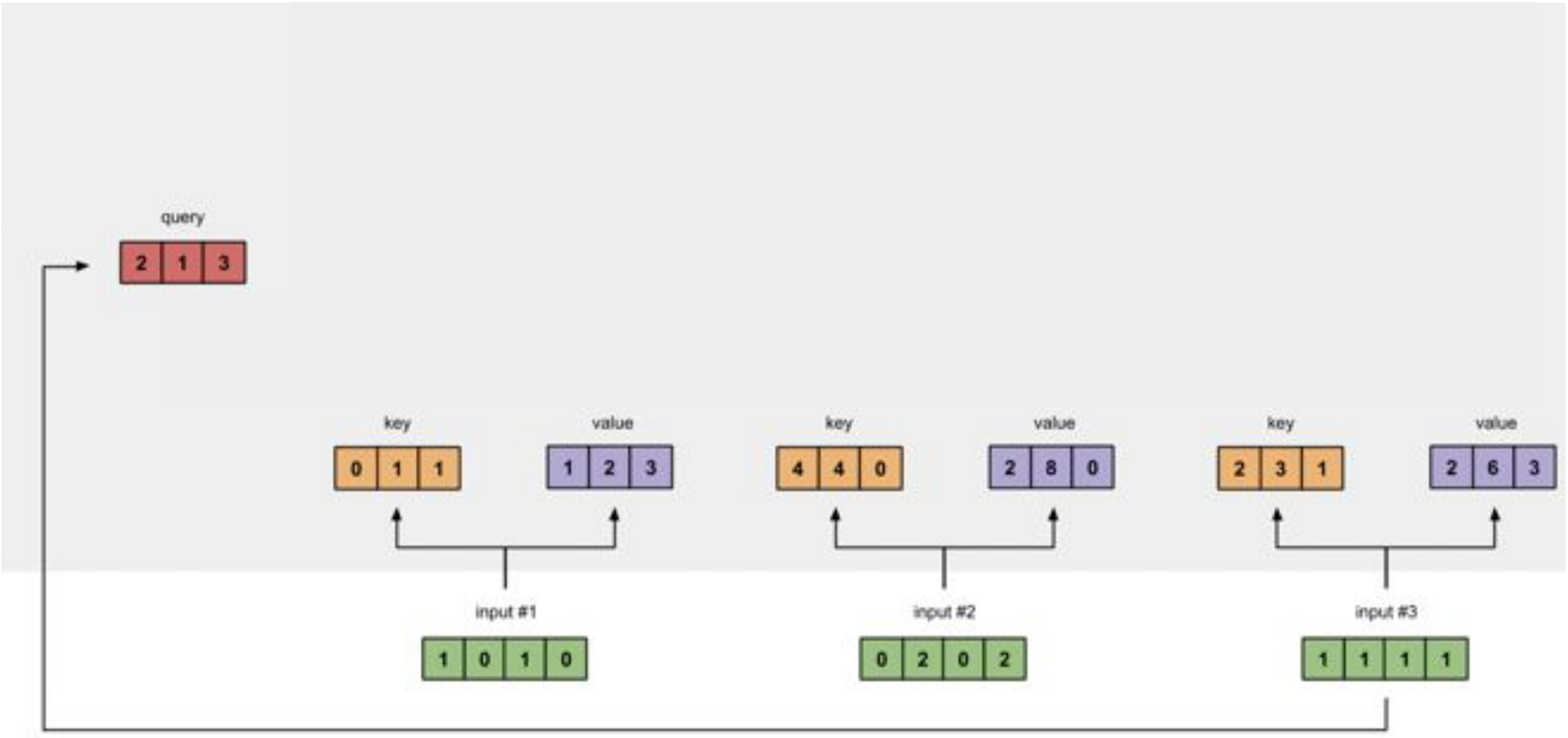

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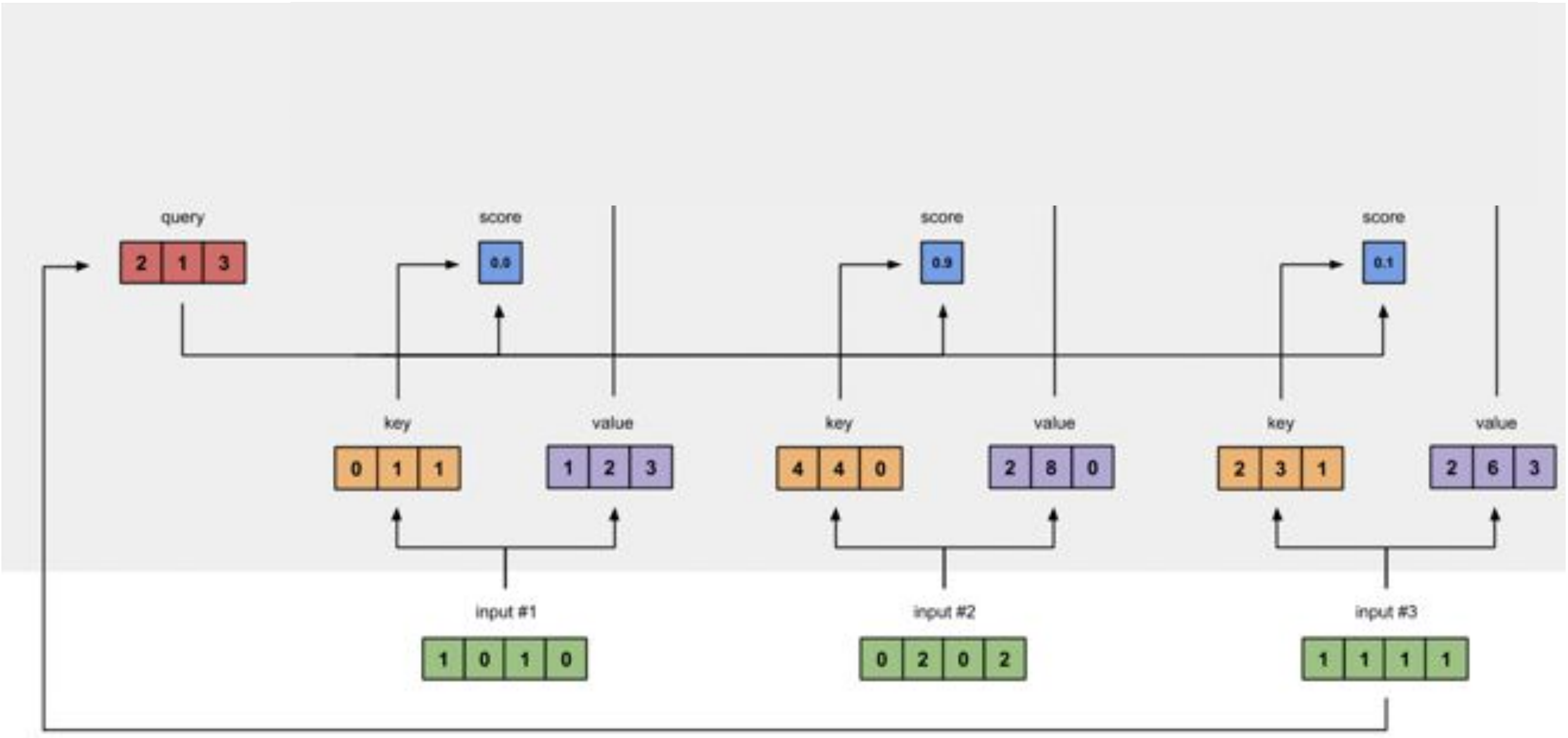

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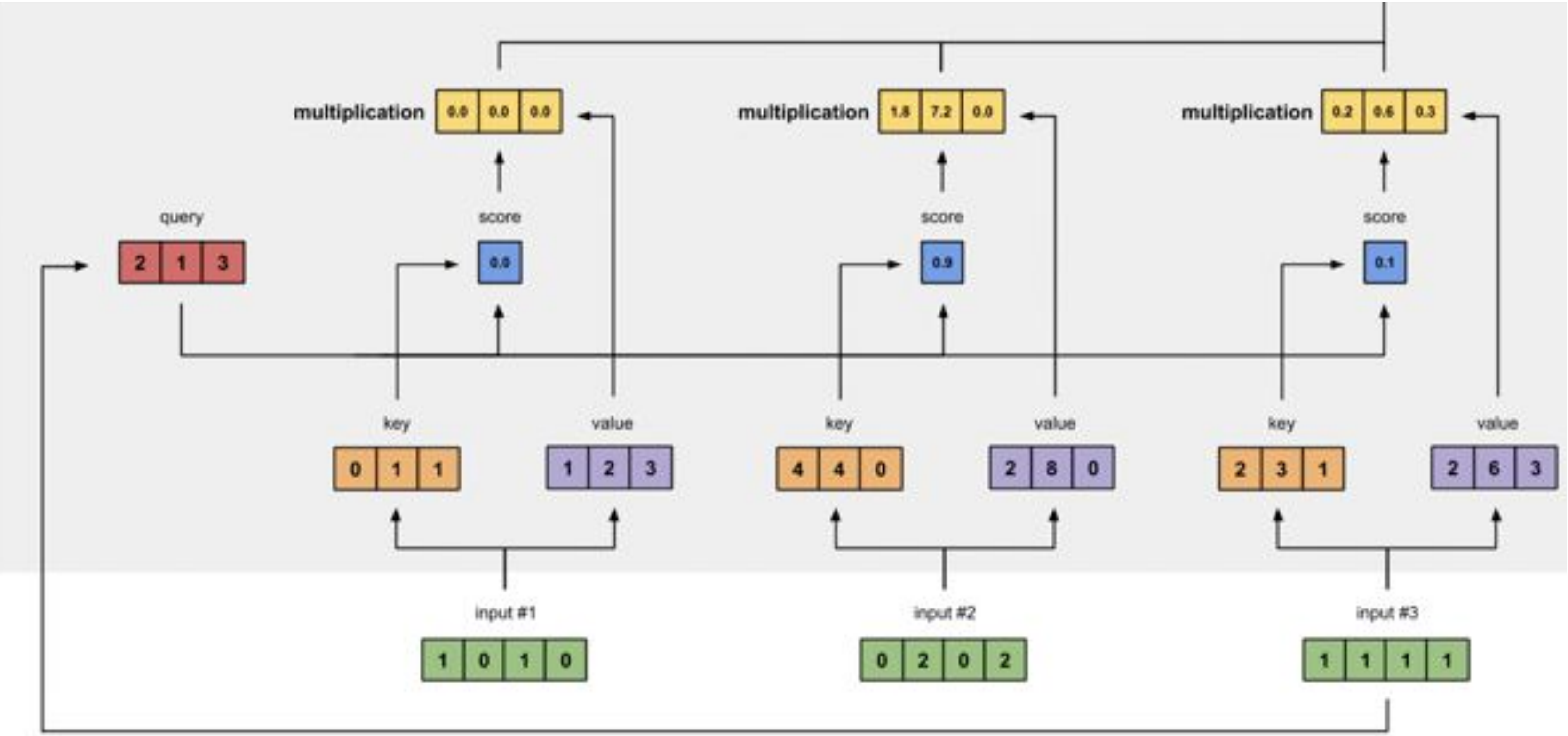

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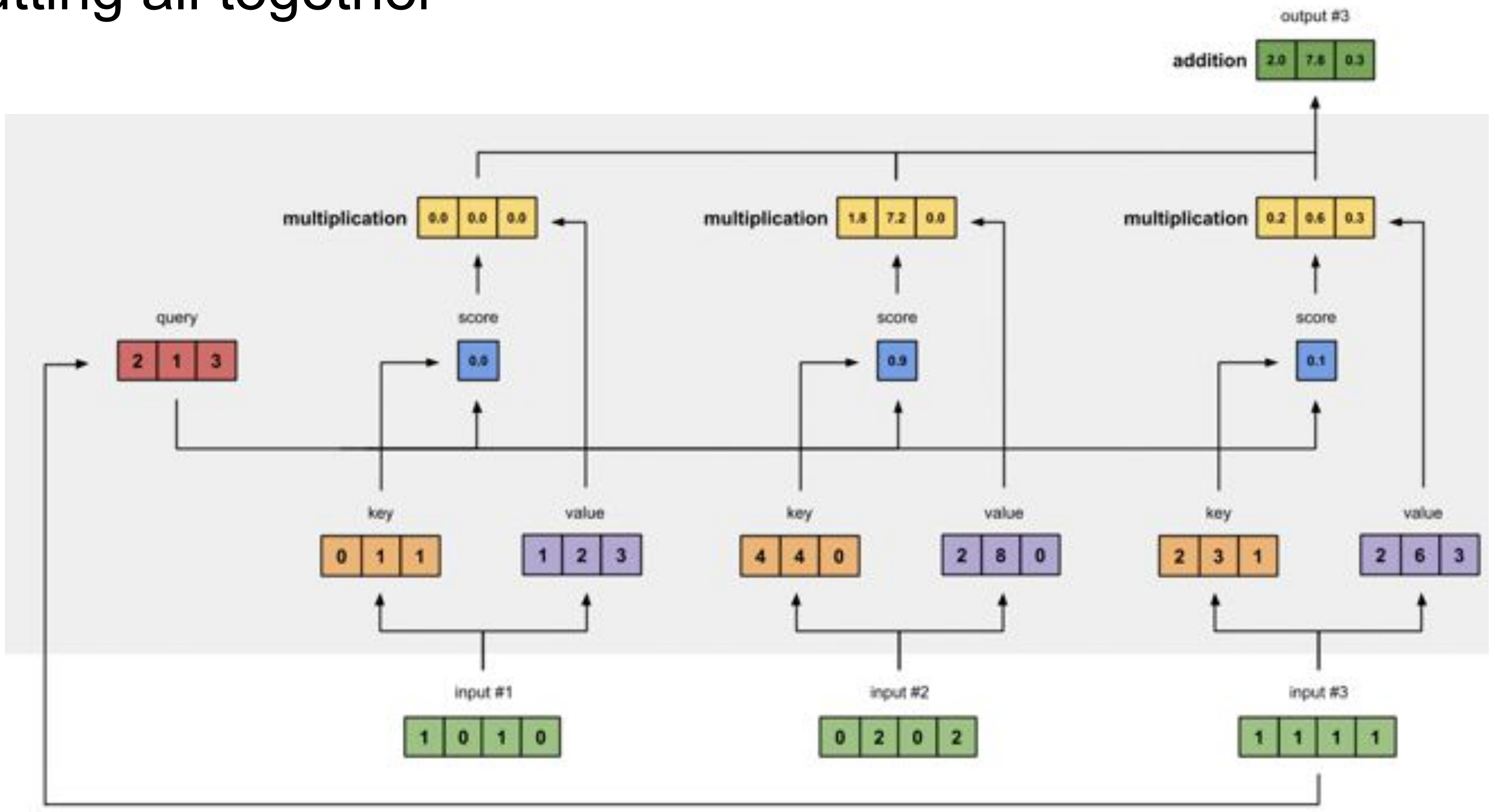
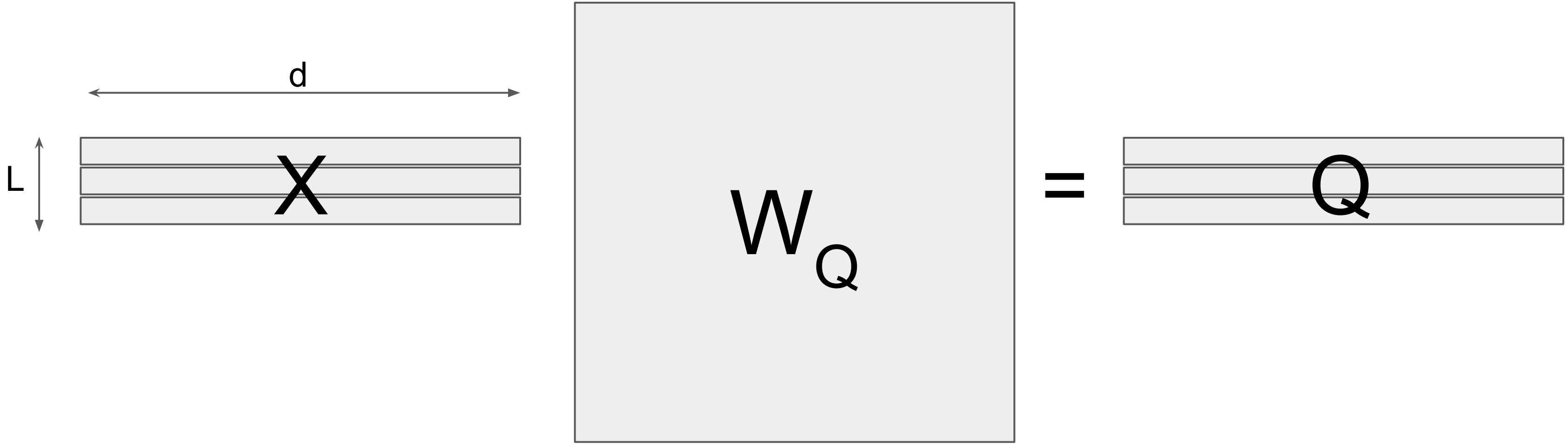


The multi-headed SA

- Hidden dimension *d* is treated as a composition of *h*x*(d/h)* subrepresentations
  - E.g. the 768 dimensional vectors of BERT-base can be viewed as a concatenation of 12 independent 64 dimensional representations
  - With slicing all the attention heads are calculated simultaneously



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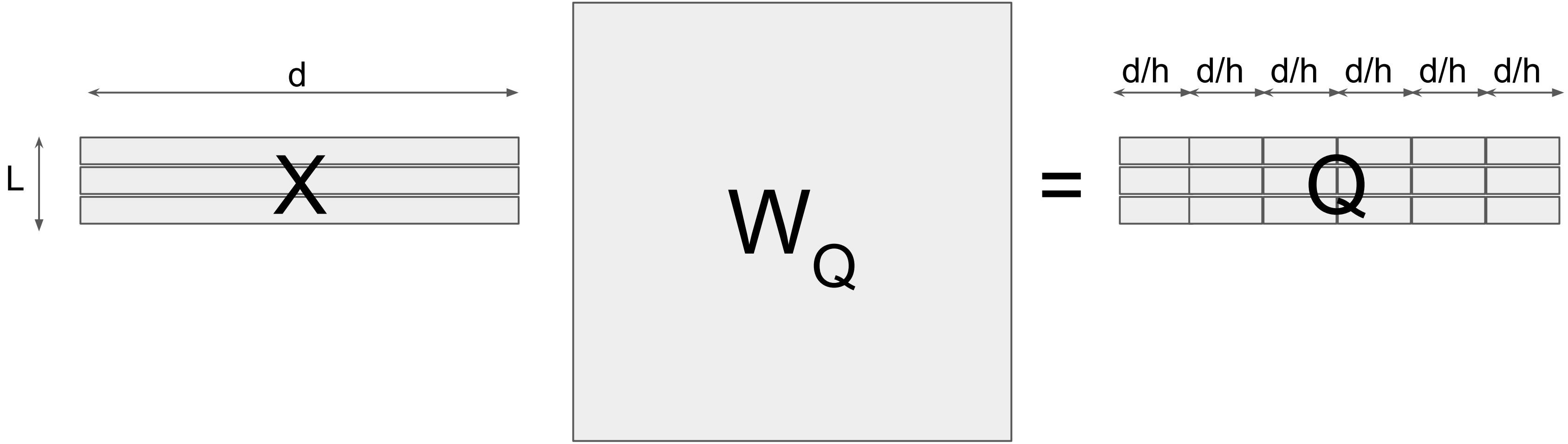

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  - Question: Could another attention module maybe decide how to mix the individual SA heads?

The case of MHSA

- Actually, most of the SAs can be omitted, only a few does the ‘heavy lifting’
  - “*pruning 38 out of 48 encoder heads results in a [marginal] drop*” (Voita et al., 2019)
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Parameters (in Millions)	**Depth**	**Multi-head Attention**	**Fake-English**	**Russian**	**Δ**
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- OTOH, “reducing the amount of heads also decreases finetuning performance” (Geiping & Goldstein, 2022)

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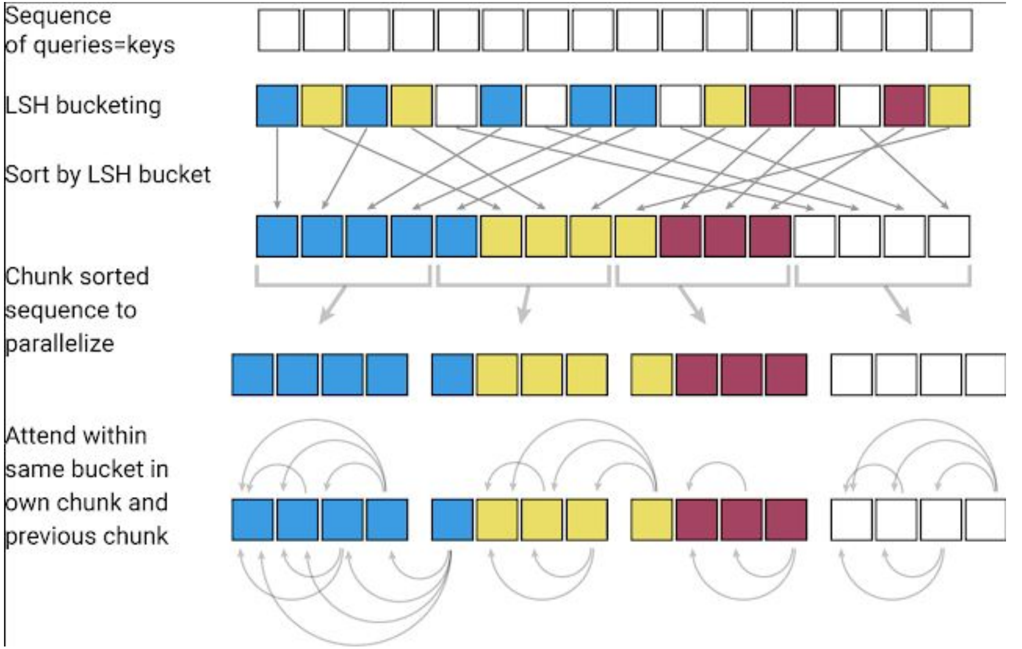
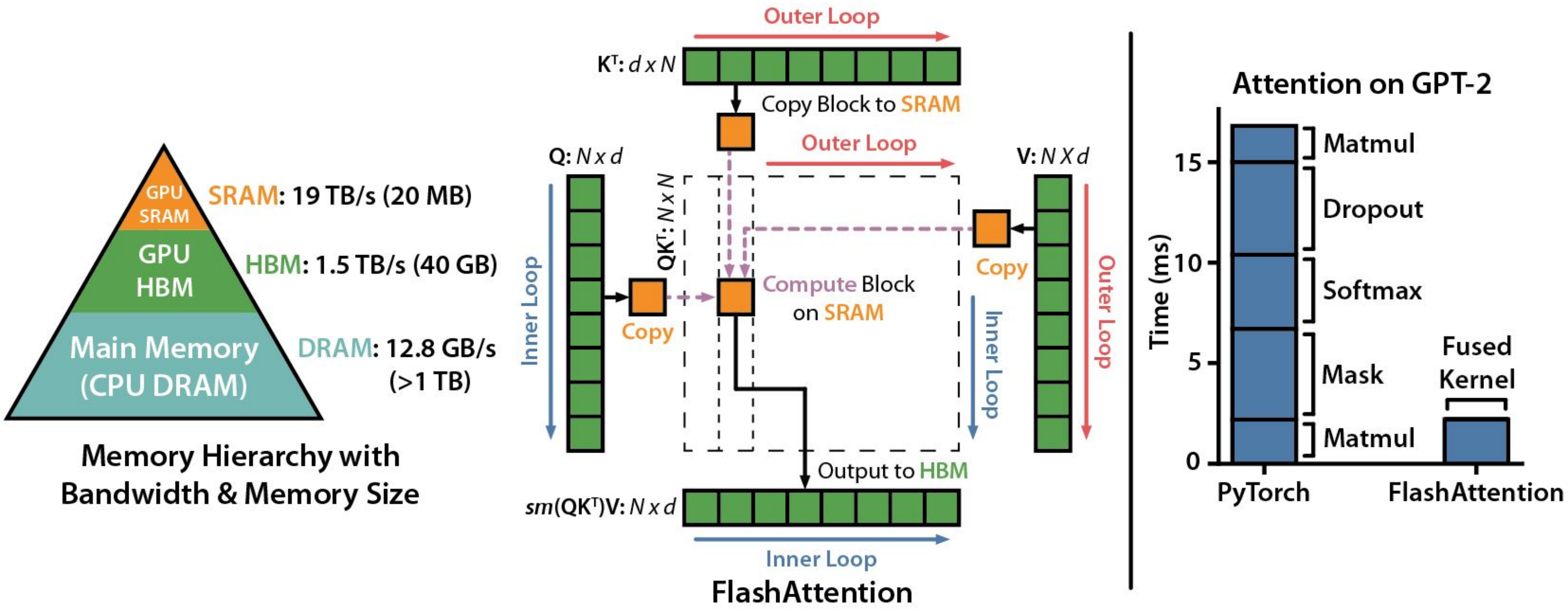
132.78	12	12	79.0	65.7	13.3

Extensions to SA – Reformer

- For an input of length L, there are L^2 a_{ij} scores to compute :(
- Reformer: LSH to the rescue

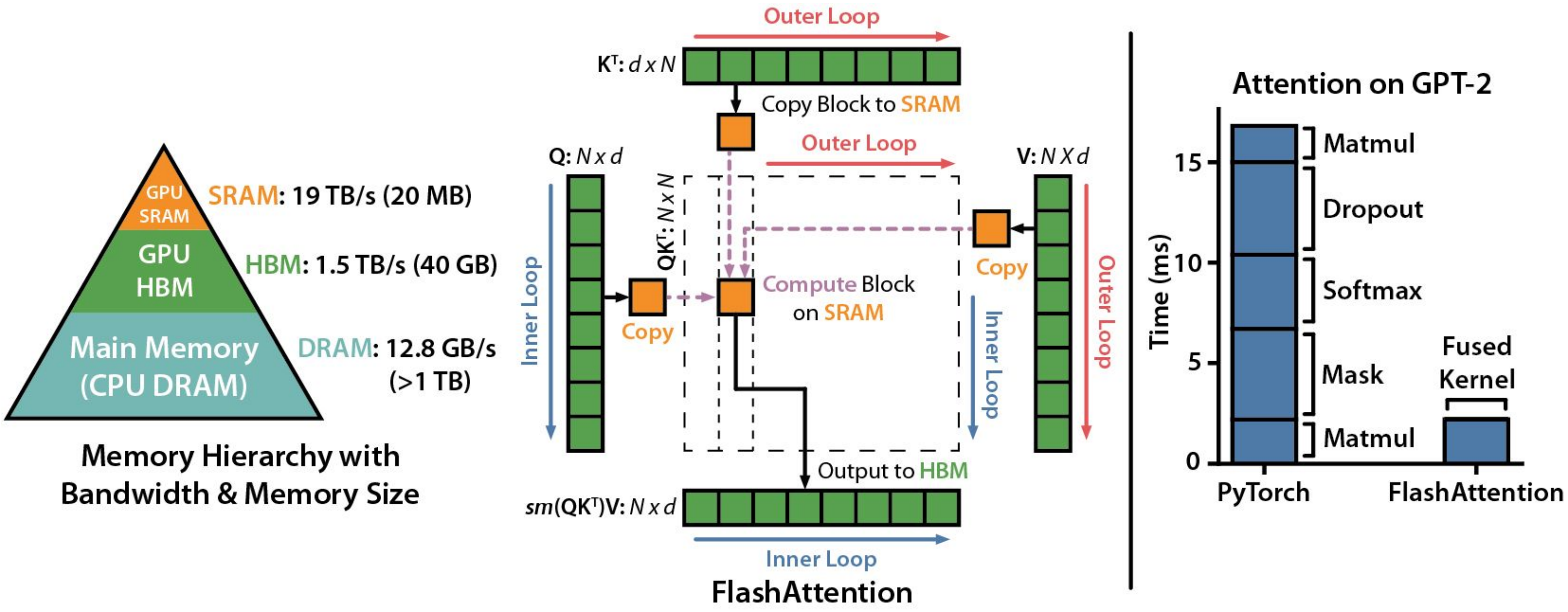


Extensions to SA – FlashAttention (Hua et al., 2022)



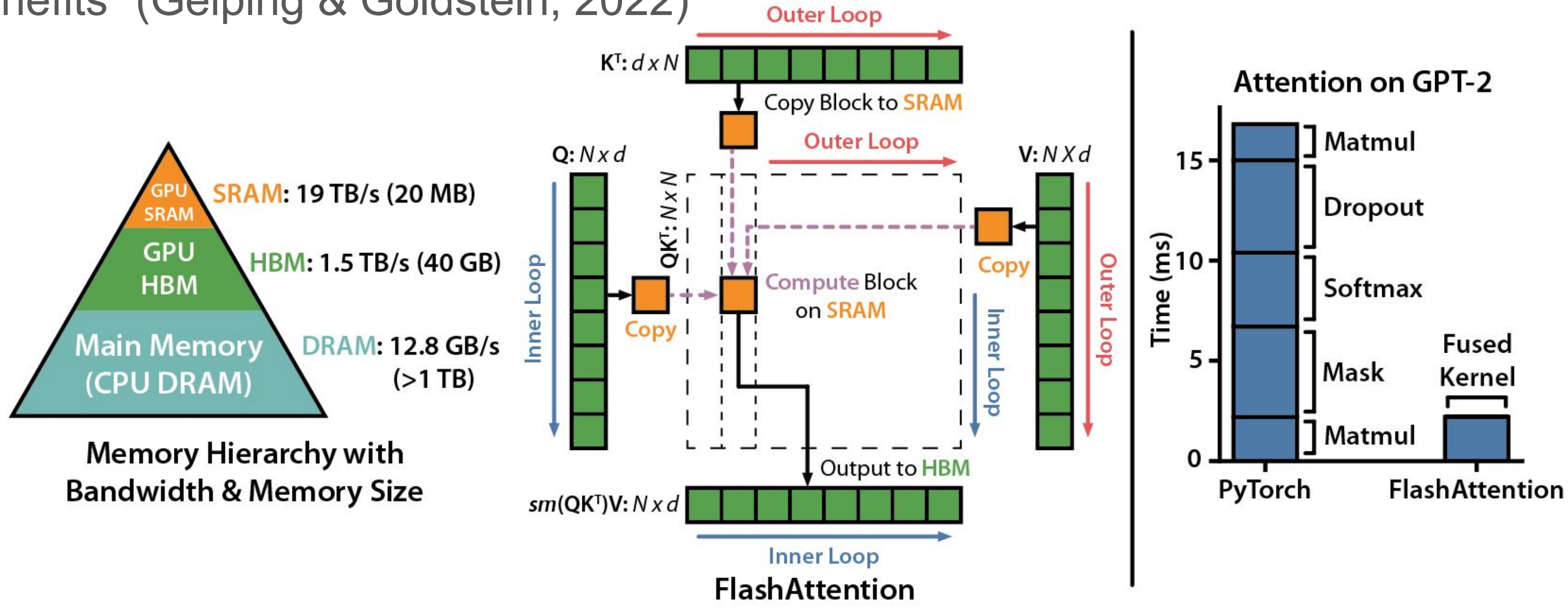
Extensions to SA – FlashAttention (Hua et al., 2022)

- Performs more FLOPs actually, but faster I/O, causing a speedup near up to 10x



Extensions to SA – FlashAttention (Hua et al., 2022)

- Performs more FLOPs actually, but faster I/O, causing a speedup near up to 10x
- OTOH, "we implement the recently proposed FLASH mechanism, but find no benefits" (Geiping & Goldstein, 2022)

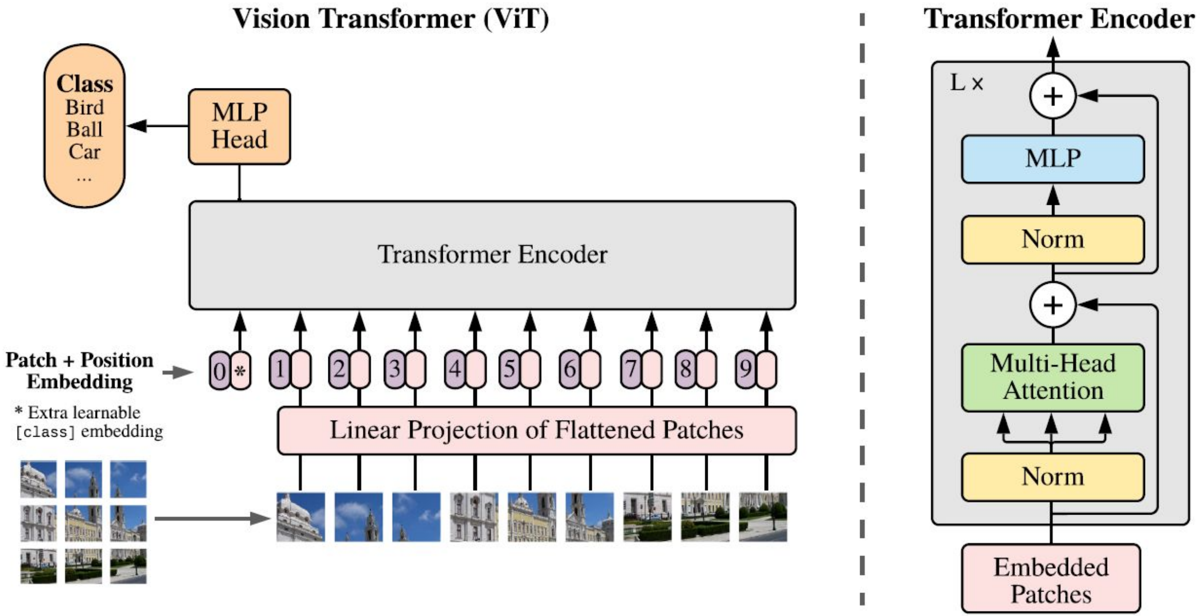


Further extensions

- DeBERTa: Relies on a disentangled attention mechanism
- RWKV: a combination of RNNs and transformers (with linear attention)
- Linformer
- Nystromformer
- Longformer
- Performer
- *former
- …

Attention in ViT

- Transformers (w/o positional embeddings) are meant for sets not sequences
    - There is (certain) evidence that the matter of the order words does not much



Further useful readings

- https://nlp.seas.harvard.edu/2018/04/03/attention.html
- https://lilianweng.github.io/posts/2023-01-27-the-transformer-family-v2
- https://jalammar.github.io/illustrated-transformer/
- https://stats.stackexchange.com/questions/421935/what-exactly-are-keys-queries-and-values-in-attention-mechanisms
- **Cross-Lingual Ability of Multilingual BERT: An Empirical Study**
- **Analyzing Multi-Head Self-Attention: Specialized Heads Do the Heavy Lifting, the Rest Can Be Pruned**