# Self-attention Does Not Need $O(n^2)$ Memory

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#### ABSTRACT

We present a very simple algorithm for attention that requires O(1) memory with respect to sequence length and an extension to self-attention that requires  $O(\log n)$  memory. This is in contrast with the frequently stated belief that self-attention requires  $O(n^2)$  memory. While the time complexity is still  $O(n^2)$ , device memory rather than compute capability is often the limiting factor on modern accelerators. Thus, reducing the memory requirements of attention allows processing of longer sequences than might otherwise be feasible. We provide a practical implementation for accelerators that requires  $O(\sqrt{n})$  memory, is numerically stable, and is within a few percent of the runtime of the standard implementation of attention. We also demonstrate how to differentiate the function while remaining memory-efficient. For sequence length 16384, the memory overhead of self-attention is reduced by 59X for inference and by 32X for differentiation.

# 1 Introduction

Attention (Bahdanau et al., 2015) is widely used in modern neural architectures. In particular, it is the heart of the Transformer architecture (Vaswani et al., 2017), which has revolutionized Natural Language Processing (Devlin et al., 2019), and found wide-spread adoption across several research areas since then.

Given a query  $q \in \mathbb{R}^d$  and lists of keys and values  $k_1, \dots, k_n$  and  $v_1, \dots, v_n \in \mathbb{R}^d$  of length n, attention is defined as follows:

$$s_i = \operatorname{dot}(q, k_i), \qquad s_i' = \frac{e^{s_i}}{\sum_j e^{s_j}}, \qquad \operatorname{attention}(q, k, v) = \sum_i v_i s_i'.$$

The result of the attention operation for a single query, is hence a weighted sum of the value vectors, where the weights are the softmax of the dot products of the query and the keys.

The straight-forward implementation of the attention operation above requires us to first compute and remember  $s_i$  for all i, leading to a O(n) time and memory complexity for each query. Transformers use *self-attention*, which issues a separate query for each position in the sequence, so the overall time and space complexity is  $O(n^2)$ .

In many works the quadratic time and space complexity of self-attention has been used as the motivation for the investigation of variants of the original attention mechanism and architectures with more favorable complexity classes (Kitaev et al., 2020; Roy et al., 2021; Zaheer et al., 2020; Choromanski et al., 2020; Wang et al., 2020; Ren et al., 2021; Child et al., 2019; Tay et al., 2021; Wang et al., 2020; Ma et al., 2021; Shen et al., 2021). Modern accelerator hardware, such as GPUs and TPUs, are often memory constrained for applications in deep learning, while compute is relatively cheap. So the space complexity of transformers is a particular concern, c.f. Kitaev et al. (2020); Roy et al. (2021); Zaheer et al. (2020).

In this work, we present new algorithms for attention and self-attention that require only constant memory and logarithmic memory, respectively. The basic algorithm is very simple; but it requires a trick to make it numerically feasible (see Section 3). We also present an implementation in JAX (Bradbury et al., 2018), which runs efficiently on TPUs, and requires  $O(\sqrt{n})$  memory for self-attention (see Section 4).

Our algorithm still requires  $O(n^2)$  time complexity for self-attention and O(n) time complexity for single-query attention, and the various efficient, long-context attention mechanisms introduced recently remain an interesting al-

ternative to (dense) attention. However, the memory-efficient algorithm for attention may allow us to reconsider architecture choices, or scale to new datasets that require longer, dense attention. For example, the Perceiver architecture (Jaegle et al., 2021) does not use self-attention, but only attends once over the input with a fixed number of queries - and the authors still report scalability limits due to the memory demand of attention. Using memory-efficient attention over the input would address this limitation.

# 2 Algorithm

First, we present the algorithm for the attention operation with a single query and extend the algorithm to self-attention at the end of this Section. We observe that the division by  $\sum_j e^{s_j}$  can be moved to the very end of the attention operation using the distributive law:

$$s_i = \text{dot}(q, k_i), \qquad s_i' = e^{s_i}, \qquad \text{attention}(q, k, v) = \frac{\sum_i v_i s_i'}{\sum_j s_j'}.$$

This can be computed with constant memory: The memory overhead of this algorithm consists of a vector  $v^* \in \mathbb{R}^d$  and a scalar  $s^* \in \mathbb{R}$ , both initialized with 0. Given the query q, keys  $k_1, \ldots, k_n$  and values  $v_1, \ldots, v_n$ , we process the keys and values in sequence. Given a key value pair  $k_i$ ,  $v_i$ , we compute  $s_i = \text{dot}(q, k_i)$  and update  $v^* \leftarrow v^* + v_i e^{s_i}$  and  $s^* \leftarrow s^* + e^{s_i}$ . After processing all keys and values, we divide  $\frac{v^*}{s^*}$  to get the final result.

The analysis of space complexity assumes that inputs are given in a particular order: we first read the query, and then a list of *pairs* of keys and values. If the inputs are provided in a different order, we have to additionally store an index into the sequence, requiring  $O(\log n)$  memory instead.

To extend this algorithm to *self*-attention, we compute the results to all queries sequentially. This requires just one additional index into the list of queries, giving rise to the  $O(\log n)$  memory complexity. Note that the operation produces outputs that are linear in the size of the number of queries, i.e., O(n), which is not counted towards the space complexity.

# 3 Numerical Stability

The formulation of standard attention that we presented in the Introduction, as well as our memory-efficient algorithm, are not numerically stable when using floating point arithmetic, because the softmax exponentiates the scores. For  $scores \ge 89$  the exponentiation results in inf (for bfloat16 and float32), which will be carried through to the final result of the attention operation. In practice, the softmax is implemented by subtracting the maximum score from all scores. This does not change the result of the softmax, but avoids this numerical problem.

Our incremental computation of the sum of exponentiated scores (and the values times the scores) does not immediately allow for the same trick, as the maximum may depend on the last score in the sequence. But the subtraction cannot be delayed either, since the scores must be exponentiated before they can be added to the cumulative sum.

To resolve this problem, we introduce an additional scalar, which keeps track of the maximum score that the incremental algorithm has seen so far, and we renormalize the sums of exponentiated values as needed: We initialize the vector  $v^* \in \mathbb{R}^d$  and scalar  $s^* \in \mathbb{R}$  with 0, and  $m^*$  with  $-\inf$ . As before, given a key value pair  $k_i$ ,  $v_i$ , we compute  $s_i = \det(q, k_i)$ , but then the algorithm differs slightly from Section 2. We first compute  $m_i = \max(m^*, s_i)$  and update  $v^* \leftarrow v^* e^{m^* - m_i} + v_i e^{s_i - m_i}$  and  $s^* \leftarrow s^* e^{m^* - m_i} + e^{s_i - m_i}$  and  $m^* \leftarrow m_i$ . After processing all keys and queries, we divide  $\frac{v^*}{s^*}$  to get the final result.

## 4 An Implementation For GPUs/TPUs

In this section, we provide a version of the algorithm above that exploits the massive parallelism of modern hardware, such as GPUs or TPUs. The naive algorithm above is is not trivial to parallelize for a compiler, as the incremental sum introduces a dependency across all keys and values.

We present the entire implementation, including the support for multiple attention heads and memory-efficient differentiation in Figure 1. The implementation does not optimize strictly for memory efficiency, but instead aims to strike a balance between simplicity, computational efficiency, and memory requirements.

To exploit the parallelism available in modern hardware, we split the computation into chunks at the cost of some additional memory. In the out loop (line 56f), we split the queries in to chunks of constant size, resulting in a linear

```
import functools, jax, math
  from jax import numpy as jnp
   def _query_chunk_attention(query, key, value, precision, key_chunk_size=4096):
     """Multi-head dot product attention with a limited number of queries."""
     num_kv, num_heads, k_features = key.shape
     v_features = value.shape[-1]
8
     key_chunk_size = min(key_chunk_size, num_kv)
     query = query / jnp.sqrt(k_features)
9
10
     @functools.partial(jax.checkpoint, prevent_cse=False)
11
     def summarize_chunk(query, key, value):
12
       attn_weights = jnp.einsum('qhd,khd->qhk', query, key, precision=precision)
13
       max_score = jnp.max(attn_weights, axis=-1, keepdims=True)
14
       max_score = jax.lax.stop_gradient(max_score)
15
       exp_weights = jnp.exp(attn_weights - max_score)
16
       exp_values = jnp.einsum('vhf,qhv->qhf', value, exp_weights, precision=precision)
17
       return (exp_values, exp_weights.sum(axis=-1),
18
               max_score.reshape((query.shape[0], num_heads)))
19
20
21
     def chunk_scanner(chunk_idx):
       key_chunk = jax.lax.dynamic_slice(
22
           key, (chunk_idx, 0, 0),
23
            slice_sizes=(key_chunk_size, num_heads, k_features))
24
       value_chunk = jax.lax.dynamic_slice(
25
           value, (chunk_idx, 0, 0),
26
            slice_sizes=(key_chunk_size, num_heads, v_features))
27
       return summarize_chunk(query, key_chunk, value_chunk)
28
29
     chunk_values, chunk_weights, chunk_max = jax.lax.map(
30
31
         chunk_scanner, xs=jnp.arange(0, num_kv, key_chunk_size))
32
     global_max = jnp.max(chunk_max, axis=0, keepdims=True)
33
     max_diffs = jnp.exp(chunk_max - global_max)
34
     chunk_values *= jnp.expand_dims(max_diffs, axis=-1)
35
     chunk_weights *= max_diffs
36
37
     all_values = chunk_values.sum(axis=0)
38
     all_weights = jnp.expand_dims(chunk_weights, -1).sum(axis=0)
39
     return all_values / all_weights
40
41
   def attention(query, key, value, precision=jax.lax.Precision.HIGHEST,
42
                  query_chunk_size=1024):
43
      """Memory-efficient multi-head dot product attention."""
44
     num_q, num_heads, q_features = query.shape
45
46
     def chunk_scanner(chunk_idx, _):
47
       query_chunk = lax.dynamic_slice(
48
           query, (chunk_idx, 0, 0),
49
           slice_sizes=(min(query_chunk_size, num_q), num_heads, q_features))
50
       return (chunk_idx + query_chunk_size,
51
                _query_chunk_attention(query_chunk, key, value, precision=precision))
52
53
54
     _, res = jax.lax.scan(
         chunk_scanner, init=0, xs=None, length=math.ceil(num_q / query_chunk_size))
55
     return res.reshape(num_q, num_heads, value.shape[-1])
56
```

Figure 1: Implementation of memory-efficient attention suited for TPUs.

Sequence length	$n = 2^{8}$	$2^{10}$	$2^{12}$	$2^{14}$	$2^{16}$	$2^{18}$	$2^{20}$
Size of inputs and outputs	160KB	640KB	2.5MB	10MB	40MB	160MB	640MB
Memory overhead of standard attention	270KB	4.0MB	64MB	1GB	OOM	OOM	OOM
Memory overhead of memory-efficient att.	270KB	4.0MB	16MB	17MB	21MB	64MB	256MB
Compute time on TPUv2	0.15ms	0.24ms	1.8ms	24ms	381ms	5.96s	95.2s
Approximate relative compute speed	+2%	-1%	-5%	-8%	-	-	-

Table 2: Memory and time requirements of self-attention during **inference**.

number of iterations. In each iteration of the outer loop, we call \_query\_chunk\_attention, which itself processes the keys and values in chunks (lines 23 to 33). The chunks are processed sequentially and each chunk is summarized independently (lines 14 to 21). Assuming a chunk size of  $\sqrt{n}$  for the keys and values, we hence obtain  $\sqrt{n}$  summaries, giving rise to the  $O(\sqrt{n})$  memory complexity.

After the summaries are computed, they need to be rescaled (lines 35 to 38) along the lines of Section 3, before we return the values divided by the weights (line 42). The result of each iteration of the outer loop is directly written to the output tensor res (line 56), so that no additional memory is consumed across iterations. (A multi-stage summarization approach could achieve  $O(\log n)$  but would complicate the implementation.)

While a constant chunk size for the queries and a chunk size of  $\sqrt{n}$  for the keys and values is optimal for memory consumption, the runtime is also affected by the choice of chunk size in practice, which is heavily affected by the choice of hardware. Ultimately, we have to leave this trade-off to the programmer, and expose the chunk sizes as arguments query\_chunk\_size and key\_chunk\_size. In Figure 1 we provide default values for the chunk sizes that lead to minimal runtime impact (on TPUv2), while still providing significant memory savings.

# 5 Empirical Analysis

#### 5.1 Inference

In Table 2 we compare the memory requirements and the compute time of the memory-efficient attention implementation and the Flax implementation of attention (Heek et al. (2020), see flax/linen/attention.py). The size of inputs and outputs includes the query, key, and value tensors of dtype bfloat16, and the output tensor of dtype float32. We measure the memory overhead as the TPUs peak memory in excess of the input and output tensors. All computations were done on a single TPUv2 chip with 8GB memory. For this experiment, we only use one attention head.

Our memory-efficient implementation of attention removes the memory bottleneck of self-attention, scaling at least to a sequence length of 1M. At this length the algorithm is multiplying over 1T combinations of queries and keys. The time complexity is still quadratic.

The "approximate relative compute speed" of the implementations was averaged over 100 runs (10k runs for  $n=2^8$ ) for both implementations—but the numbers still fluctuated across multiple runs of the evaluation and we only provide them to demonstrate that the runtime performance is roughly similar. Please note that this experiment analyzes the attention operation in isolation; the measured relative performance is not necessarily the same when the operations are embedded in larger architectures. In fact, we observed a slight increase in steps/sec of about 4% when training a small Transformer.

For all cases where the standard attention would not OOM (i.e. require > 8GB device memory), we checked that the results of the two implementations are within  $1.5 \times 10^{-7}$  for vectors drawn from a normal distribution with standard deviation 1 and within  $6.5 \times 10^{-7}$  when the vectors drawn from a uniform distribution (measured as the maximal absolute difference of any dimension in a self-attention over sequence length  $2^{14}$ ).

### 5.2 Differentiation

During the forward pass our algorithm saves memory by summarizing parts of the attention matrix sequentially, allowing it to forget the parts of the attention matrix it has summarized already. A naive application of differentiation would have to store all those intermediate results and our algorithm would loose its memory advantage entirely. So we apply checkpointing (Chen et al., 2016) in line 13 to the function that summarizes the individual chunks. The intermediate results can thus be forgotten during the forward pass and recomputed during backpropagation.

Sequence length	$n = 2^{8}$	$2^{10}$	$2^{12}$	$2^{14}$	$2^{16}$	$2^{18}$	$2^{20}$
Size of inputs and outputs	192KB	768KB	2.9MB	12MB	47MB	188MB	750MB
Memory overhead of standard attention	532KB	8.0MB	128MB	2.0GB	OOM	OOM	OOM
Memory overhead of memory-eff. att.	532KB	8.0MB	41MB	64MB	257MB	1.0GB	4.0GB
Compute time on TPUv2	0.18ms	0.61ms	8.2ms	122ms	1.9s	30.9s	493s
Approximate relative compute speed	-7%	-29%	-44%	-44%	-	-	-

Table 3: Memory and time requirements of self-attention during **differentiation**. Note that the slowdown in compute speed is expected due to checkpointing.

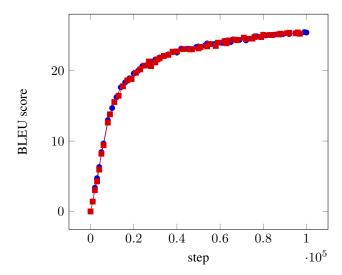


Figure 4: BLEU scores of a two Transformer models trained with standard attention (red rectangles) and memory-efficient attention (blue circles).

In Table 3 we compare runtime and peak memory during differentiation of our implementation to standard attention. We used the same setting as for the forward pass, but applied jax.grad to an arbitrarily chosen loss function (the sum of the results). The relative compute speed was reduced by almost 2X compared to standard attention. This is expected when using checkpointing since some values must be recomputed during backpropagation.

Note that applying checkpointing to the standard attention algorithm would not achieve these results. The standard algorithm with checkpointing would forget the attention matrix after it is formed; our algorithm never forms the attention matrix at all.

# 5.3 Training

We integrated our memory-efficient implementation into a simple Transformer architecture provided in the Flax library, and ran the WMT en-de translation experiment with the standard attention module and with the memory-efficient attention module. Throughout the training, the two implementations behaved almost identically. After 100K training steps, the evaluation accuracy reached 62.69 for the memory-efficient implementation and 62.59 for the standard implementation. This demonstrates that our memory-efficient implementation of self-attention can be used to replace existing implementations. Figure 4 illustrates that both models resulted in very similar BLEU scores. We used the default settings for the WMT en-de experiment as given in the Flax implementation, except that we had to deactivate example packing to simplify the masking code. This also required us to lower the learning rate to 0.005.

#### 6 Conclusion

This paper presents a simple trick to reduce the memory requirement of (self-)attention dramatically, which appears to have been simply overlooked by the community. We hope that this short paper raises awareness of the fact that attention is not intrinsically memory-hungry, which may allow us to revisit some of the design choices in popular neural architectures.

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