An Introduction to FlashAttention

Chin-Hui Chu*[1], Ya-Xu Liu*[1,2], and Chih-Jen Lin[1,2]

[1]National Taiwan University
{r12944041, d08944012}@ntu.edu.tw
cjlin@cise.ntu.edu.tw

[2]Mohamed bin Zayed University of Artificial Intelligence
{yaxu.liu, chihjen.lin}@mbzuai.ac.ae

1 Introduction

The Transformer architecture proposed by Vaswani et al. [2017] has become dominant in modern deep learning. However, scaling to long contexts remains challenging because attention operations in the transformer have high computation and memory complexity in sequence length. Among many approaches addressing this challenge, FlashAttention [Dao et al., 2022] is highly effective by reducing the number of memory accesses.

While the original FlashAttention paper and some existing materials[1,2,3,4] provide basic concepts, they either lack certain details or are not self-contained. This document offers a comprehensive and self-contained introduction of FlashAttention suitable for the teaching purpose.

Main components of this document are as follows.

- We provide complete mathematical derivations for both forward and backward passes of the attention operation.
- We analyze the memory access patterns in standard attention and identify that some intermediate matrices create a memory bottleneck.
- We derive the FlashAttention algorithm step by step, showing how block-wise computation and efficient softmax calculation address the identified bottleneck.

This document as well as the same contents in a slide form are available at https://www.csie.ntu.edu.tw/~cjlin/papers/flashattention.

*These authors contributed equally to this work

[1]https://gordicaleksa.medium.com/eli5-flash-attention-5c44017022ad

[2]https://courses.cs.washington.edu/courses/cse599m/23sp/notes/flashattn.pdf

[3]https://damek.github.io/random/basic-idea-behind-flash-attention/

[4]https://dev.to/lewis_won/flashattention-by-hand-34im

2 Standard Attention: Forward Calculation

2.1 Attention Operations

We first recall the forward calculation of the attention defined in Vaswani et al. [2017],

$$\text{Attention}(Q, K, V) := \text{SoftMax}(\frac{QK^\top}{\sqrt{d}})V, \tag{1}$$

where $Q, K, V \in \mathbf{R}^{T\times d}$ are the input matrices, T is the sequence length, and d is the embedding dimension. In (1), the SoftMax function is applied on each row $\boldsymbol{z}$ of an input matrix in the following way,

$$\text{SoftMax}(\mathbf{z}) = \begin{bmatrix} \frac{\exp(z_1)}{\sum_j \exp(z_j)} \\ \vdots \\ \frac{\exp(z_T)}{\sum_j \exp(z_j)} \end{bmatrix}. \tag{2}$$

However, instead of performing (1), Vaswani et al. [2017] found it more beneficial to perform multi-head attention,

$$\text{MultiHead}(Q, K, V) := \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W_O, \tag{3}$$

where h, a divisor of d, is the number of heads, and

$$\begin{aligned} \text{head}_i &= \text{Attention}(QW_Q^i, KW_K^i, VW_V^i) \\ &= \text{SoftMax}(\frac{QW_Q^i(KW_K^i)^\top}{\sqrt{d}})VW_V^i \in \mathbf{R}^{T\times d/h}. \end{aligned}$$

Here $\forall i, W_Q^i, W_K^i, W_V^i \in \mathbf{R}^{d\times d/h}$ and $W_O \in \mathbf{R}^{d\times d}$ are trainable weight matrices. Moreover, attention is most commonly used in the self-attention setting, where Q, K, V come from the same input matrix $\tilde{Z} \in \mathbf{R}^{T\times d}$, that is, $\text{MultiHead}(Q = \tilde{Z}, K = \tilde{Z}, V = \tilde{Z})$. Then, we have the multi-head self-attention,

$$\begin{aligned} &\text{MultiHeadSelfAttention}(\tilde{Z}) \\ &:= \text{MultiHead}(Q = \tilde{Z}, K = \tilde{Z}, V = \tilde{Z}) \\ &= \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W_O, \end{aligned} \tag{4}$$

where

$$\begin{aligned} \text{head}_i &= \text{Attention}(\tilde{Z}W_Q^i, \tilde{Z}W_K^i, \tilde{Z}W_V^i) \\ &= \text{SoftMax}(\frac{\tilde{Z}W_Q^i(\tilde{Z}W_K^i)^\top}{\sqrt{d}})\tilde{Z}W_V^i \in \mathbf{R}^{T\times d/h}. \end{aligned}$$

Because the multi-head situation is similar to the single case, for our discussion we assume $h = 1$ (i.e., one head). If we follow Dao et al. [2022] to abuse the notation by redefining Q, K, V as $Q := \tilde{Z}W_Q, K := \tilde{Z}W_K, V := \tilde{Z}W_V$, then what we calculate is

$$\text{Attention}(Q, K, V)W_O. \tag{5}$$

For later discussion, we further decompose the computation in (5) into the following steps:

$$Q = \tilde{Z}W_Q, K = \tilde{Z}W_K, V = \tilde{Z}W_V, \tag{6}$$

$$S = QK^\top, \tag{7}$$

$$P = \mathrm{SoftMax}(S), \tag{8}$$

$$O = PV, \tag{9}$$

$$\tilde{Z}^{\mathrm{out}} = OW_O, \tag{10}$$

where $\tilde{Z}, \tilde{Z}^{\mathrm{out}} \in \mathbf{R}^{T\times d}$ are the input and output matrices, while $Q, K, V, O \in \mathbf{R}^{T\times d}$ and $S, P \in \mathbf{R}^{T\times T}$ denote the intermediate results. The following graph shows the connection between variables:

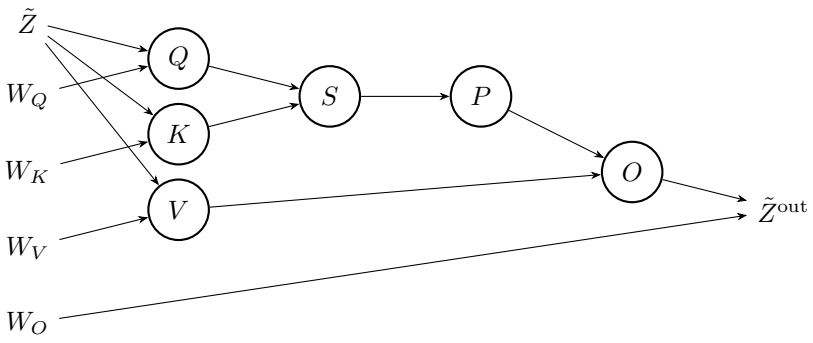


Figure 1: The computation graph of attention.

From the graph, we can clearly see that

$$O = \mathrm{Attention}(Q, K, V) \tag{11}$$

is a sub-graph. We can treat (11) as a general component for the use in (5) and other places. Therefore, in this document, we focus on the efficient forward and backward computation of

$$\begin{aligned}&\text{input: } Q, K, V,\\ &\text{output: } O = \mathrm{Attention}(Q, K, V),\end{aligned}$$

which includes (7)-(9). In the Appendix, we extend the derivation to cover (10) and (6).

3 Standard Attention: Backward Calculation

3.1 The Need to Derive Backward Calculation

Modern machine learning tools apply automatic differentiation to compute gradients through backpropagation. Thus, for any given network architecture, we generally do not need to derive explicit backward operations. However, as attention is often the bottleneck in the entire computation, explicitly implementing the backward operation improves the efficiency. In addition, memory-efficient attention algorithms such as FlashAttention typically have a low-level implementation invoked by higher-level frameworks such as PyTorch or TensorFlow. The automatic differentiation functionality of general-purpose deep learning frameworks may not be able to access low-level implementations, so cannot automatically generate the necessary gradient operations. Subsequently, we derive the backward calculation of attention.

3.2 Backward Pass: Problem Setup

We assume that, in the forward calculation, the output matrix O from (11) is passed to subsequent operations, and a scalar-valued loss L is computed at the end. During backward propagation, the attention operation receives from its subsequent operations the gradient

$$\frac{\partial L}{\partial O} \in \mathbf{R}^{T\times d}. \tag{12}$$

With (12), our objective is to compute the gradients with respect to the input matrices Q, K, and V,

$$\frac{\partial L}{\partial Q}, \quad \frac{\partial L}{\partial K}, \quad \text{and} \quad \frac{\partial L}{\partial V}.$$

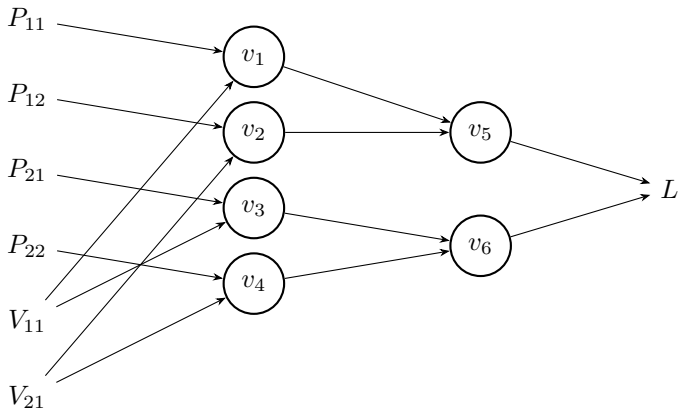
We derive the gradients by applying the chain rule backward through (9), (8), and (7).

3.3 Gradient with Respect to V

We begin by deriving the gradient with respect to the value matrix $V \in \mathbf{R}^{T\times d}$. From (9),

$$O_{ik} = \sum_{j=1}^{T} P_{ij}V_{jk}, \quad \text{for } i = 1,\dots,T \text{ and } k = 1,\dots,d. \tag{13}$$

We observe that each element V_{jk} influences all output elements O_{ik} in the k-th column of O. The following computational graph illustrates this relationship for a simplified $T = 2, d = 1$ case.



The intermediate nodes in the graph represent the following computations:

$$\begin{aligned} v_1 &= P_{11}V_{11}, & v_2 &= P_{12}V_{21}, \\ v_3 &= P_{21}V_{11}, & v_4 &= P_{22}V_{21}, \\ v_5 &= v_1 + v_2 = O_{11}, & v_6 &= v_3 + v_4 = O_{21}. \end{aligned}$$

To find the gradient of the loss L with respect to an element, such as V_{11}, we apply the chain rule

and sum the contributions from all paths through which V_{11} affects L.

$$\begin{aligned}\frac{\partial L}{\partial V_{11}} &= \frac{\partial L}{\partial v_5}\frac{\partial v_5}{\partial v_1}\frac{\partial v_1}{\partial V_{11}} + \frac{\partial L}{\partial v_6}\frac{\partial v_6}{\partial v_3}\frac{\partial v_3}{\partial V_{11}} \\ &= \frac{\partial L}{\partial O_{11}} \cdot 1 \cdot P_{11} + \frac{\partial L}{\partial O_{21}} \cdot 1 \cdot P_{21} \\ &= \sum_{i=1}^{T} \frac{\partial L}{\partial O_{i1}} P_{i1}. \end{aligned} \tag{14}$$

For an arbitrary element V_{jk}, we can generalize (14) to

$$\frac{\partial L}{\partial V_{jk}} = \sum_{i=1}^{T} \frac{\partial L}{\partial O_{ik}}\frac{\partial O_{ik}}{\partial V_{jk}} = \sum_{i=1}^{T} \frac{\partial L}{\partial O_{ik}} P_{ij}. \tag{15}$$

We can represent (15) in the following matrix form

$$\frac{\partial L}{\partial V} = P^\top \frac{\partial L}{\partial O} \in \mathbf{R}^{T \times d},$$

because of

$$\left(P^\top \frac{\partial L}{\partial O}\right)_{jk} = \sum_{i=1}^{T} (P^\top)_{ji} \left(\frac{\partial L}{\partial O}\right)_{ik} = \sum_{i=1}^{T} \frac{\partial L}{\partial O_{ik}} P_{ij}.$$

3.4 Gradient with Respect to P

The derivation for $\partial L/\partial P$ is similar to $\partial L/\partial V$, since both appear in the matrix multiplication $O = PV$. An element P_{ij} influences outputs through

$$O_{ik} = \sum_{j'=1}^{T} P_{ij'} V_{j'k}, \quad \text{for } i = 1, \ldots, T \text{ and } k = 1, \ldots, d.$$

Applying the chain rule gives

$$\frac{\partial L}{\partial P_{ij}} = \sum_{k=1}^{d} \frac{\partial L}{\partial O_{ik}}\frac{\partial O_{ik}}{\partial P_{ij}} = \sum_{k=1}^{d} \frac{\partial L}{\partial O_{ik}} V_{jk}. \tag{16}$$

We can represent (16) in the following matrix form

$$\frac{\partial L}{\partial P} = \frac{\partial L}{\partial O} V^\top \in \mathbf{R}^{T \times T}, \tag{17}$$

because of

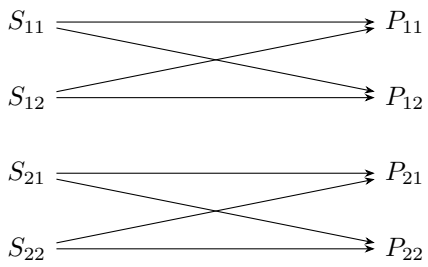
$$\left(\frac{\partial L}{\partial O} V^\top\right)_{ij} = \sum_{k=1}^{d} \left(\frac{\partial L}{\partial O}\right)_{ik} (V^\top)_{kj} = \sum_{k=1}^{d} \frac{\partial L}{\partial O_{ik}} V_{jk}. \tag{18}$$

3.5 Gradient with Respect to S

From (8), next we should derive the gradient with respect to the matrix $S \in \mathbf{R}^{T\times T}$. Given

$$\frac{\partial L}{\partial P} \in \mathbf{R}^{T\times T},$$

we propagate this gradient through the softmax operation defined in (8). We note that softmax operation independently normalizes each row of S to form the corresponding row of P. The following computational graph gives an illustration of $T = 2$.



In the graph, S_{11} affects the loss L through both P_{11} and P_{12}, so the chain rule yields

$$\frac{\partial L}{\partial S_{11}} = \frac{\partial L}{\partial P_{11}}\frac{\partial P_{11}}{\partial S_{11}} + \frac{\partial L}{\partial P_{12}}\frac{\partial P_{12}}{\partial S_{11}}.$$

Since $\partial L/\partial P$ is known from (17), it remains to compute

$$\frac{\partial P_{1k}}{\partial S_{11}}, \text{ for } k = 1, 2.$$

We defer the derivation and instead check the general form of

$$\frac{\partial L}{\partial S_{ij}} \quad \forall i, j = 1, \ldots, T.$$

Because S_{ij} affects the loss L through all elements in row i of P, the chain rule yields

$$\frac{\partial L}{\partial S_{ij}} = \sum_{k=1}^{T} \frac{\partial L}{\partial P_{ik}}\frac{\partial P_{ik}}{\partial S_{ij}}. \tag{19}$$

To compute the partial derivatives $\partial P_{ik}/\partial S_{ij}$, we take the logarithm of both sides of the softmax expression

$$P_{ik} = \frac{e^{S_{ik}}}{\sum_{\ell=1}^{T} e^{S_{i\ell}}}$$

to obtain

$$\ln P_{ik} = S_{ik} - \ln \sum_{\ell=1}^{T} e^{S_{i\ell}}.$$

Then,

$$\frac{1}{P_{ik}}\frac{\partial P_{ik}}{\partial S_{ij}} = \delta_{kj} - \frac{e^{S_{ij}}}{\sum_{\ell=1}^{T} e^{S_{i\ell}}} = \delta_{kj} - P_{ij},$$

where

$$\delta_{kj} = \begin{cases} 1 & \text{if } k = j, \\ 0 & \text{otherwise.} \end{cases}$$

Therefore,

$$\frac{\partial P_{ik}}{\partial S_{ij}} = \begin{cases} P_{ik}(1 - P_{ik}) & \text{if } k = j, \\ -P_{ik}P_{ij} & \text{if } k \neq j. \end{cases} \tag{20}$$

Substituting (20) into (19) gives

$$\begin{aligned} \frac{\partial L}{\partial S_{ij}} &= \frac{\partial L}{\partial P_{ij}} P_{ij}(1 - P_{ij}) + \sum_{k:k\neq j} \frac{\partial L}{\partial P_{ik}}(-P_{ik}P_{ij}) \\ &= P_{ij}\left(\frac{\partial L}{\partial P_{ij}} - \sum_{k=1}^{T} P_{ik}\frac{\partial L}{\partial P_{ik}}\right). \end{aligned} \tag{21}$$

By defining

$$\gamma_i = \sum_{k=1}^{T} P_{ik}\frac{\partial L}{\partial P_{ik}}, \tag{22}$$

$$\boldsymbol{\gamma} = \text{rowsum}\left(\frac{\partial L}{\partial P} \odot P\right) \in \mathbf{R}^T, \tag{23}$$

we can further write (21) in a matrix form

$$\frac{\partial L}{\partial S} = P \odot \left(\frac{\partial L}{\partial P} - \boldsymbol{\gamma}\mathbf{1}^\top\right) \in \mathbf{R}^{T\times T}, \quad \text{where } \mathbf{1} \in \mathbf{R}^T \text{ is the vector of all ones.}$$

We note that (23) requires $O(T^2)$ operations. To reduce the number of operations, we rewrite (23) to use

$$O \in \mathbf{R}^{T\times d} \quad \text{and} \quad \frac{\partial L}{\partial O} \in \mathbf{R}^{T\times d}.$$

Substituting (17) into (22) and applying (13), we have

$$\begin{aligned} \sum_{k=1}^{T} P_{ik}\frac{\partial L}{\partial P_{ik}} &= \sum_{k=1}^{T} P_{ik}\sum_{l=1}^{d}\frac{\partial L}{\partial O_{il}}V_{kl} \\ &= \sum_{l=1}^{d}\frac{\partial L}{\partial O_{il}}\sum_{k=1}^{T} P_{ik}V_{kl} \\ &= \sum_{l=1}^{d}\frac{\partial L}{\partial O_{il}}O_{il}. \end{aligned}$$

Thus, we can rewrite (23) as

$$\boldsymbol{\gamma} = \text{rowsum}\left(\frac{\partial L}{\partial O} \odot O\right) \in \mathbf{R}^T. \tag{24}$$

The number of operations is reduced to $O(Td)$.

3.6 Gradient with Respect to Q and K

From (7), next we derive

$$\frac{\partial L}{\partial Q} \in \mathbf{R}^{T\times d} \quad \text{and} \quad \frac{\partial L}{\partial K} \in \mathbf{R}^{T\times d}.$$

We note that (7) is in a similar form to (9), where they are respectively

$$S = QK^\top \quad \text{and} \quad O = PV.$$

The results derived earlier for

$$\frac{\partial L}{\partial V} \quad \text{and} \quad \frac{\partial L}{\partial P}$$

directly lead us to have

$$\begin{aligned}
\frac{\partial L}{\partial Q} &= \frac{\partial L}{\partial S}(K^T)^T = \frac{\partial L}{\partial S}K, \\
\frac{\partial L}{\partial K} &= \left(\frac{\partial L}{\partial (K^T)}\right)^T = \left(Q^T\frac{\partial L}{\partial S}\right)^T = \left(\frac{\partial L}{\partial S}\right)^T Q.
\end{aligned}$$

3.7 Summary of Backward Calculation

From the given $\partial L/\partial O \in \mathbf{R}^{T\times d}$, a summary of operations is as follows:

$$\begin{aligned}
&\frac{\partial L}{\partial V} = P^\top \frac{\partial L}{\partial O} \in \mathbf{R}^{T\times d} \\
&\frac{\partial L}{\partial P} = \frac{\partial L}{\partial O}V^\top \in \mathbf{R}^{T\times T} \\
&\frac{\partial L}{\partial S} = P \odot \left(\frac{\partial L}{\partial P} - \boldsymbol{\gamma}\mathbf{1}^\top\right) \in \mathbf{R}^{T\times T}, \\
&\text{where} \quad \boldsymbol{\gamma} = \text{rowsum}\left(\frac{\partial L}{\partial O} \odot O\right) \in \mathbf{R}^T \\
&\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S}K \in \mathbf{R}^{T\times d} \\
&\frac{\partial L}{\partial K} = \left(\frac{\partial L}{\partial S}\right)^\top Q \in \mathbf{R}^{T\times d}
\end{aligned}$$

4 The Bottleneck on Memory Usage and Access

4.1 Memory Accesses in Attention

We assume that our machine has only two layers of memory:

- main memory, and
- secondary memory.

If an operand is not available in main memory, we must transport it from secondary memory. Now consider (11) and check intermediate values during computation. We need

$$QK^\top \in \mathbf{R}^{T\times T} \tag{25}$$

$$\mathrm{SoftMax}(QK^\top) \in \mathbf{R}^{T\times T} \tag{26}$$

$$\mathrm{SoftMax}(QK^\top)V \in \mathbf{R}^{T\times d} \tag{27}$$

As in general $T \gg d$, even though the output $\mathrm{SoftMax}(QK^\top)V \in \mathbf{R}^{T\times d}$ is smaller, storing $T \times T$ intermediate matrices is the main difficulty.

4.2 Insufficient Memory to Store $T \times T$ Intermediate Matrices

Our first analysis is to assume that $T \times T$ matrices cannot be stored in the main memory, and check the need to move these matrices. If we consider (25)-(27) as independent operations, immediately we see the following major memory accesses:

- write
$$QK^\top \in \mathbf{R}^{T\times T} \tag{28}$$
to secondary memory,
- load the matrix (28) from secondary memory to calculate
$$\mathrm{SoftMax}(QK^\top) \tag{29}$$
and write results back to secondary memory, and
- load the matrix in (29) for calculating
$$\mathrm{SoftMax}(QK^\top)V \in \mathbf{R}^{T\times d}.$$

We assume that even though storing a $T \times T$ matrix in main memory is not possible, the computer has a way to sequentially work on part of the input data in main memory and gradually generate/save part of the whole output to secondary memory. It is just like that we do matrix-matrix products all the time, but never worry that our highest-level memory (i.e., registers) is insufficient to store operands. Now we conclude that a naive implementation of attention leads to

$$4 \times T^2 \tag{30}$$

accesses between main and secondary memory.

4.3 Memory Versus Computation

We see attention involves the following operations and list their respective cost.

$$QK^\top : 2T^2d,$$
$$\mathrm{SoftMax}(QK^\top) : 3T^2,$$
$$\mathrm{SoftMax}(QK^\top)V : 2T^2d.$$

Thus, the total computational cost is around $4T^2d$. With (30), we see that if

$$4T^2d \times \text{ cost per operation} < 4T^2 \times \text{ cost per memory access},$$

then attention is memory bounded. We give the following example.

- Consider $T = 1,024$ and $d = 64$, and assume that we run on an A100 80GB SXM GPU.
- This GPU sustains up to 312 tera floating point operations per second (TFLOPS) for half-precision floating-point format (FP16) operations.[5]
- The GPU is equipped with 80 GB of high-bandwidth memory (HBM), corresponding to the secondary memory in our setting and offering a memory bandwidth of 2.04 tera bytes per second (TB/s).
- Then, the total computational cost is

$$\frac{4 \times 1024^2 \times 64 \text{ FLOPs}}{312 \text{ TFLOPS}} \approx 0.86 \ \mu\text{s}.$$

- The total memory-access cost is

$$\frac{4 \times 1024^2 \times 2 \text{ bytes}}{2.04 \text{ TB/s}} \approx 3.74 \ \mu\text{s}.$$

  Note that we assume each value is stored in FP16 (two bytes).

Based on the above discussion, we should reduce memory accesses in order to accelerate the attention operation.

4.4 Backward Pass: Insufficient Memory to Store $T \times T$ Intermediate Matrices

The backward pass also requires computing and storing $T \times T$ intermediate matrices as in the forward pass. Specifically, we derived the following $T \times T$ intermediate gradients in (16) and (21):

$$\frac{\partial L}{\partial P} \quad \text{and} \quad \frac{\partial L}{\partial S} \in \mathbf{R}^{T \times T}.$$

As in the forward pass, our first analysis assumes that $T \times T$ matrices cannot be stored in main memory. Under this assumption, the major memory accesses are as follows.

- load $P \in \mathbf{R}^{T \times T}$ from secondary memory (stored during forward pass) to compute

$$\frac{\partial L}{\partial V} = P^\top \frac{\partial L}{\partial O} \in \mathbf{R}^{T \times d},$$

- compute and write

$$\frac{\partial L}{\partial P} = \frac{\partial L}{\partial O} V^\top \in \mathbf{R}^{T \times T} \tag{31}$$

  to secondary memory,

[5] https://www.nvidia.com/content/dam/en-zz/Solutions/Data-Center/a100/pdf/nvidia-a100-datasheet-nvidia-us-2188504-web.pdf

- load P and (31) from secondary memory to compute

$$\frac{\partial L}{\partial S} = P \odot \left(\frac{\partial L}{\partial P} - \boldsymbol{\gamma} \mathbf{1}^\top \right) \in \mathbf{R}^{T \times T}, \tag{32}$$

  and write the result to secondary memory, and

- load (32) from secondary memory twice to compute

$$\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S} K \in \mathbf{R}^{T \times d},$$
$$\frac{\partial L}{\partial K} = \left(\frac{\partial L}{\partial S} \right)^\top Q \in \mathbf{R}^{T \times d}.$$

We assume that although storing a complete $T \times T$ matrix in main memory is not possible, the computer can sequentially process parts of the input data to gradually generate the output. A simple count of load and write operations in the above procedure indicates approximately $7 \times T^2$ accesses between main and secondary memory for the $T \times T$ intermediate matrices.

4.5 Backward Pass: Computational Complexity

The computational cost of operations involved in the backward pass is as follows.

$$\frac{\partial L}{\partial V} = P^\top \frac{\partial L}{\partial O} : 2T^2 d,$$
$$\frac{\partial L}{\partial P} = \frac{\partial L}{\partial O} V^\top : 2T^2 d,$$
$$\frac{\partial L}{\partial S} = P \odot \left(\frac{\partial L}{\partial P} - \boldsymbol{\gamma} \mathbf{1}^\top \right) : 2T^2,$$

$$\boldsymbol{\gamma} = \mathrm{rowsum}\left(\frac{\partial L}{\partial O} \odot O \right) : 2Td,$$
$$\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S} K : 2T^2 d,$$
$$\frac{\partial L}{\partial K} = \left(\frac{\partial L}{\partial S} \right)^\top Q : 2T^2 d.$$

The total computational cost for the backward pass is

$$8T^2 d + 2T^2 + 2Td.$$

5 Flash Attention: Forward Calculation

5.1 Situation When Storing $T \times d$ Matrices Is Possible

Now we assume that the main memory is sufficient to store $T \times d$ matrices such as $Q, K,$ and V. Let us develop strategies to reduce the number of memory accesses in (30). In particular, we would like to avoid loading and storing intermediate results. That is, we should generate the attention results "part by part." All we need is to sequentially store the finished part back to the secondary memory. We can conduct the following procedure:

Algorithm 1 Row-wise forward pass

Load $Q, K,$ and V to main memory.
For $i = 1, \ldots, T$, calculate

$$Q_{i,:}K^\top \in \mathbf{R}^{1\times T} \tag{33}$$

$$\mathrm{SoftMax}(Q_{i,:}K^\top) \in \mathbf{R}^{1\times T} \tag{34}$$

$$\mathrm{SoftMax}(Q_{i,:}K^\top)V \in \mathbf{R}^{1\times d} \tag{35}$$

and store the ith row of the output matrix to the secondary memory.

By this way, the number of memory accesses is reduced to $O(Td)$. because we never load/store any $T \times T$ matrices.

5.2 Situation When Storing $T \times d$ Matrices Is Not Possible

Unfortunately, our assumption that $T \times d$ matrices can be stored in main memory is often untrue. We discuss the situation of $d \le M \le Td$, where M is the size of the main memory. Then in (33)-(35), we must load the whole K and V once even for calculating just one output row. A possible strategy is to calculate $|I|$ rows together:

$$\mathrm{SoftMax}(Q_{I,:}K^\top)V, \tag{36}$$

where I is the block of rows that we intend to calculate. In calculating (36), we must access $|I|$ rows of Q, and the whole K and V (by row blocks). We also need to store the intermediate blocks of

$$Q_{I,:}K^\top, \tag{37}$$

or

$$\mathrm{SoftMax}\left(Q_{I,:}K^\top\right), \tag{38}$$

which requires $|I| \times T$ space. If we assume (38) overwrites the space of (37), then the largest possible $|I|$ is

$$\frac{M}{T},$$

where M is the size of the main memory. Thus the total number of memory accesses is

$$O(\frac{T}{M/T}) \times O(Td) = O(\frac{T^3 d}{M}). \tag{39}$$

In the above discussion, we see that the main bottleneck is to store the intermediate matrix in (37). Because the number of rows in (37) is a large number T, $|I|$ must be small. Thus we get a large first term in (39).

5.3 FlashAttention

To reduce the number of memory accesses, let us see if we may avoid storing the intermediate matrix in (37). Assume that we split Q to the following row-block form:

$$\begin{bmatrix} Q_{I_1,:} \\ \vdots \\ Q_{I_{T_r},:} \end{bmatrix} \tag{40}$$

with

$$|I_1| = \cdots = |I_{T_r}|.$$

For K, V, we respectively split them to

$$\begin{bmatrix} K_{J_1,:} \\ \vdots \\ K_{J_{T_c},:} \end{bmatrix}, \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{T_c},:} \end{bmatrix}. \tag{41}$$

Similarly, we assume that $|J_1| = \cdots = |J_{T_c}|$. We explain later why the split of Q should be different from that of K, V, even though they have the same size. In our discussion, we let I, J be any one of $|I_1|, \ldots, |I_{T_r}|$ and $|J_1|, \ldots, |J_{T_c}|$, respectively. We have

$$\begin{aligned} &\text{SoftMax}(Q_{I,:} \begin{bmatrix} K_{J_1,:}^\top & \cdots & K_{J_{T_c},:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{T_c},:} \end{bmatrix} \\ =&\text{SoftMax}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_{T_c},:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{T_c},:} \end{bmatrix} \end{aligned}$$

If there is no SoftMax, we can see the result is

$$(Q_{I,:}K_{J_1,:}^\top)V_{J_1,:} + \cdots + (Q_{I,:}K_{J_{T_c},:}^\top)V_{J_{T_c},:}.$$

We have

$$\begin{gathered} (Q_{I,:}K_{J_1,:}^\top)V_{J_1,:} \in \mathbf{R}^{|I| \times d}, \\ \vdots \\ (Q_{I,:}K_{J_{T_c},:}^\top)V_{J_{T_c},:} \in \mathbf{R}^{|I| \times d}. \end{gathered}$$

If we sequentially generate each term, there is no need to store the intermediate sub-matrix in (37). In this situation, the algorithm can be as follows.

Algorithm 2 Block-wise forward pass (without SoftMax)

For $i = 1, \ldots, T_r$

For $j = 1, \ldots, T_c$

$$O_{I_i,:} = O_{I_i,:} + (Q_{I_i,:}K_{J_j,:}^\top)V_{J_j,:}. \tag{42}$$

Save $O_{I_i,:}$ to secondary memory.

At any time point we must store the following **four** blocks in main memory

1. $Q_{I,:} \in \mathbf{R}^{|I| \times d}$
2. $O_{I,:} \in \mathbf{R}^{|I| \times d}$
3. $K_{J,:} \in \mathbf{R}^{|J| \times d}$ **or** $V_{J,:} \in \mathbf{R}^{|J| \times d}$

Note that we only need space for storing one of them. It can be overwritten once used.

4. $Q_{I,:}K_{J,:}^\top \in \mathbf{R}^{|I|\times|J|}$

We assume that (42) does not require extra space to store the intermediate result $(Q_{I_i,:}K_{J_j,:}^\top)V_{J_j,:}$. This is possible as any resulting element or sub-matrix can be immediately used to update O. Therefore, we select $|I|$ and $|J|$ to satisfy

$$|I|d < \frac{M}{4}, \quad |J|d < \frac{M}{4}, \quad |I||J| < \frac{M}{4}. \tag{43}$$

We also need that $|I|$ as large as possible, so K, V are less frequently loaded. The reason is that for any I, we must access the whole K, V. If we choose

$$|I| = \left\lfloor \frac{M}{4d} \right\rfloor \text{ and } |J| = \min(\left\lfloor \frac{M}{4d} \right\rfloor, d) \tag{44}$$

then (43) holds. The condition (44) indicates that we choose $|I|$ and $|J|$ differently. We consider the largest possible $|I|$ while having $|J|$ to satisfy (43). This situation explains why in (40) and (41), Q is split differently from K and V. In the end, the number of memory accesses is

$$\frac{T}{|I|} \times O(Td) = O(\frac{T}{M/d}) \times O(Td) = O(\frac{T^2d^2}{M}). \tag{45}$$

This value is smaller than the one we had earlier in (39). Unfortunately, we need the whole intermediate matrix in (37) because the SoftMax function involves all elements in each row. A crucial observation is that we hope to have

$$\begin{aligned}
&\text{SoftMax}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_j,:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_j,:} \end{bmatrix} = \\
&\boldsymbol{v} \odot (\text{SoftMax}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_{j-1},:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{j-1},:} \end{bmatrix}) \\
&+ \boldsymbol{w} \odot \left(\text{SoftMax}(Q_{I,:}K_{J_j,:}^\top)V_{J_j,:}\right),
\end{aligned} \tag{46}$$

where $\odot$ is the component-wise product and $\boldsymbol{v}, \boldsymbol{w} \in \mathbf{R}^{|I|}$ are two vectors. If $\boldsymbol{v}, \boldsymbol{w}$ are easily available, then we can do an operation similar to (42). We discuss why $\boldsymbol{w}$ can be easily calculated. While $\boldsymbol{w}$ is a vector, we give an illustration to get one of its components. We have $\forall t \in J_1 \cup \cdots \cup J_{j-1}$,

$$\frac{\exp(z_t)}{\sum_{s\in J_1\cup\cdots\cup J_j}\exp(z_s)} = \underbrace{\left(\frac{\sum_{s\in J_1\cup\cdots\cup J_{j-1}}\exp(z_s)}{\sum_{s\in J_1\cup\cdots\cup J_j}\exp(z_s)}\right)}_{\boldsymbol{v}} \frac{\exp(z_t)}{\sum_{s\in J_1\cup\cdots\cup J_{j-1}}\exp(z_s)},$$

and $\forall t \in J_j$,

$$\frac{\exp(z_t)}{\sum_{s\in J_1\cup\cdots\cup J_j}\exp(z_s)} = \underbrace{\left(\frac{\sum_{s\in J_j}\exp(z_s)}{\sum_{s\in J_1\cup\cdots\cup J_j}\exp(z_s)}\right)}_{\boldsymbol{w}} \frac{\exp(z_t)}{\sum_{s\in J_j}\exp(z_s)}.$$

Clearly, all we need is to maintain

$$\sum_{s\in J_1\cup\cdots\cup J_j} \exp(z_s). \tag{47}$$

When handling j, we get

$$\sum_{s\in J_j} \exp(z_s),$$

so we can update (47) by

$$\sum_{s\in J_1\cup\cdots\cup J_j} \exp(z_s) = \sum_{s\in J_1\cup\cdots\cup J_{j-1}} \exp(z_s) + \sum_{s\in J_j} \exp(z_s).$$

This $O(|I|)$ cost for storing (47) in main memory is affordable. To have an algorithm, let's define

$$\begin{aligned}
&\Delta_I^{\text{old}} = \exp(\text{'s row sum}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_{j-1},:}^\top \end{bmatrix})\\
&\Delta_I = \exp(\text{'s row sum}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_j,:}^\top \end{bmatrix})\\
&\hat{\Delta}_I = \exp(Q_{I,:}K_{J_j,:}^\top)\text{'s row sum}
\end{aligned}$$

Then (46) becomes,

$$\begin{aligned}
&\frac{\Delta_I^{\text{old}}}{\Delta_I} \odot (\text{SoftMax}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_{j-1},:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{j-1},:} \end{bmatrix})\\
&+ \frac{\hat{\Delta}_I}{\Delta_I} \odot \left(\text{SoftMax}(Q_{I,:}K_{J_j,:}^\top)V_{J_j,:}\right)\\
=&\frac{\Delta_I^{\text{old}}}{\Delta_I} \odot (\text{SoftMax}(\begin{bmatrix} Q_{I,:}K_{J_1,:}^\top & \cdots & Q_{I,:}K_{J_{j-1},:}^\top \end{bmatrix}) \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{j-1},:} \end{bmatrix})\\
&+ \frac{\mathbf{1}}{\Delta_I} \odot \left(\exp(Q_{I,:}K_{J_j,:}^\top)V_{J_j,:}\right),
\end{aligned}$$

where the fraction denotes element-wise division and $\mathbf{1} \in \mathbf{R}^{|I|}$ is the all-ones vector. Finally, we have the following algorithm.

Algorithm 3 A flash attention implementation (FlashAttention-2 in Dao, 2024)

For $i = 1, \ldots, T_r$

Load $Q_{I_i,:}$

For $j = 1, \ldots, T_c$

if $j > 1$

$\Delta_{I_i}^{\text{old}} = \Delta_{I_i}$

else

$\Delta_{I_i}^{\text{old}} = \mathbf{0}$

Load $K_{J_j,:}$

$$P_{I_i,J_j} = \exp(Q_{I_i,:} K_{J_j,:}^\top) \tag{48}$$

$$\Delta_{I_i} = \Delta_{I_i}^{\text{old}} + \text{rowsum}(P_{I_i,J_j}) \tag{49}$$

Load $V_{J_j,:}$ to overwrite $K_{J_j,:}$

$$O_{I_i,:} \leftarrow \frac{\Delta_{I_i}^{\text{old}}}{\Delta_{I_i}} \odot O_{I_i,:} + \frac{\mathbf{1}}{\Delta_{I_i}} \odot (P_{I_i,J_j} V_{J_j,:})$$

Save $O_{I_i,:}$ and Δ_{I_i} to secondary memory.

At first glance, Δ_I is a working array, so we do not need to keep it. However, we show later that the backward calculation also needs Δ. Thus we must save it to the secondary memory. For (48), we can calculate $Q_{I_i,:} K_{J_j,:}^\top$ first and calculate the exp value of each component. Thus, we only need space for one matrix. By our trick in (46), the number of memory accesses is the same as the algorithm analyzed in (42) and (45),

$$O(\frac{T^2 d^2}{M}). \tag{50}$$

5.4 FlashAttention and FlashAttention-2

FlashAttention was first introduced in Dao et al. [2022]. Later Dao [2024] proposed an improved version FlashAttention-2. Interestingly, what we described earlier is FlashAttention-2. In the original FlashAttention, the algorithm is as follows.

Algorithm 4 A flash attention implementation (FlashAttention in Dao et al., 2022)

For $j = 1, \ldots, T_c$

Load $V_{J_j,:}$ and $K_{J_j,:}$

For $i = 1, \ldots, T_r$

Load $\Delta_{I_i}, Q_{I_i,:}$

$P_{I_i,J_j} = \exp(Q_{I_i,:} K_{J_j,:}^\top)$

if $j > 1$

$\Delta_{I_i}^{\text{old}} = \Delta_{I_i}$

else

$\Delta_{I_i}^{\text{old}} = \mathbf{0}$

$\Delta_{I_i} = \Delta_{I_i}^{\text{old}} + \text{rowsum}(P_{I_i,J_j})$

Load $O_{I_i,:}$ to overwrite $Q_{I_i,:}$

$$O_{I_i,:} \leftarrow \frac{\Delta_{I_i}^{\text{old}}}{\Delta_{I_i}} \odot O_{I_i,:} + \frac{\mathbf{1}}{\Delta_{I_i}} \odot (P_{I_i,J_j} V_{J_j,:})$$

Save $O_{I_i,:}, \Delta_{I_i}$ to secondary memory

A comparison with FlashAttention-2 shows that here i and j are swapped. Like FlashAttention-2, FlashAttention also maintains four matrices in the main memory

1. $K_{J,:} \in \mathbf{R}^{|J| \times d}$
2. $V_{J,:} \in \mathbf{R}^{|J| \times d}$
3. $Q_{I,:} \in \mathbf{R}^{|I| \times d}$ or $O_{I,:} \in \mathbf{R}^{|I| \times d}$

   Note that we only need space for storing one of them. It can be overwritten once used.
4. $Q_{I,:} K_{J,:}^\top \in \mathbf{R}^{|I| \times |J|}$

In the inner loop, we now need to load two matrices, and save one matrix and one vector, from/to secondary memory, respectively. However, the earlier version (i.e., FlashAttention-2) needs to load only two matrices. The main issue is that FlashAttention sequentially uses

$$O_{I_i,:}, \forall i$$

in the inner loop, but we cannot afford to store them. Thus, we must save $O_{I_i,:}$ back to secondary memory. Another issue is that we must ensure that the save operation of $O_{I_i,:}$ is finished before the load operation in iteration $i+1$. The reason is to free space for loading $Q_{I_{i+1},:}$ or P. The above discussion explains why FlashAttention-2 is more memory efficient than FlashAttention.

6 Flash Attention: Backward Calculation

6.1 Backward Pass: Situation When Storing $T \times d$ Matrices Is Possible

Now we assume that the main memory is sufficient to store

$$T \times d \text{ matrices such as } Q, K, V, \text{ and } \frac{\partial L}{\partial O}.$$

To avoid loading and storing $T \times T$ matrices, as in the forward pass, we devise a strategy to generate results in a row-wise setting. We can now conduct the following procedure:

Algorithm 5 Row-wise backward pass

Load

$$Q, K, V, O, \frac{\partial L}{\partial O} \in \mathbf{R}^{T \times d}$$

For $i = 1, \ldots, T$

$$P_{i,:} = \mathrm{SoftMax}(Q_{i,:} K^\top) \in \mathbf{R}^{1 \times T} \tag{51}$$

$$\frac{\partial L}{\partial V} \leftarrow \frac{\partial L}{\partial V} + P_{i,:}^\top \frac{\partial L}{\partial O_{i,:}} \in \mathbf{R}^{T \times d} \tag{52}$$

$$\frac{\partial L}{\partial P_{i,:}} = \frac{\partial L}{\partial O_{i,:}} V^\top \in \mathbf{R}^{1 \times T} \tag{53}$$

$$\gamma_i = \mathrm{rowsum}\left(\frac{\partial L}{\partial O_{i,:}} \odot O_{i,:} \right) \in \mathbf{R} \tag{54}$$

$$\frac{\partial L}{\partial S_{i,:}} = P_{i,:} \odot \left(\frac{\partial L}{\partial P_{i,:}} - \gamma_i \mathbf{1}^\top \right) \in \mathbf{R}^{1 \times T} \tag{55}$$

$$\frac{\partial L}{\partial Q_{i,:}} = \frac{\partial L}{\partial S_{i,:}} K \in \mathbf{R}^{1 \times d} \tag{56}$$

$$\frac{\partial L}{\partial K} \leftarrow \frac{\partial L}{\partial K} + \frac{\partial L}{\partial S_{i,:}}^\top Q_{i,:} \in \mathbf{R}^{T \times d} \tag{57}$$

Store the resulting gradient $\partial L / \partial Q, \partial L / \partial K$ and $\partial L / \partial V$ to the secondary memory.

The total memory access cost is $O(Td)$, since we never load/store any $T \times T$ matrices.

6.2 Backward Pass: Situation When Storing $T \times d$ Matrices Is Not Possible

We discuss the implementation of the backward pass under the situation of

$$d \leq M \leq Td,$$

where M is the size of the main memory. Similar to the forward calculation, we can no longer store $T \times d$ matrices such as K. Therefore in (51)–(56), for every row we must expensively load the whole K, V, $\partial L / \partial V$, and $\partial L / \partial K$. A possible strategy to reduce the memory access is to calculate $|I|$ rows together. The calculation for $|I|$ rows is as follows:

$$P_{I,:} = \mathrm{SoftMax}(Q_{I,:} K^\top) \in \mathbf{R}^{|I| \times T}, \tag{58}$$

$$\frac{\partial L}{\partial V} \leftarrow \frac{\partial L}{\partial V} + P_{I,:}^\top \frac{\partial L}{\partial O_{I,:}} \in \mathbf{R}^{T \times d}, \tag{59}$$

$$\frac{\partial L}{\partial P_{I,:}} = \frac{\partial L}{\partial O_{I,:}} V^\top \in \mathbf{R}^{|I| \times T}, \tag{60}$$

$$\boldsymbol{\gamma}_I = \mathrm{rowsum}\left(\frac{\partial L}{\partial O_{I,:}} \odot O_{I,:} \right) \in \mathbf{R}^{|I|}, \tag{61}$$

$$\frac{\partial L}{\partial S_{I,:}} = P_{I,:} \odot \left(\frac{\partial L}{\partial P_{I,:}} - \boldsymbol{\gamma}_I \mathbf{1}^\top \right) \in \mathbf{R}^{|I| \times T}, \tag{62}$$

$$\frac{\partial L}{\partial Q_{I,:}} = \frac{\partial L}{\partial S_{I,:}} K \in \mathbf{R}^{|I| \times d}, \tag{63}$$

$$\frac{\partial L}{\partial K} \leftarrow \frac{\partial L}{\partial K} + \frac{\partial L}{\partial S_{I,:}}^\top Q_{I,:} \in \mathbf{R}^{T \times d}. \tag{64}$$

In calculating (58)–(64), we must access

$$|I| \text{ rows of } Q, \frac{\partial L}{\partial O}, \text{ and } O, \tag{65}$$

and

$$\text{the whole } K, V, \frac{\partial L}{\partial V}, \text{ and } \frac{\partial L}{\partial K} \text{ (by row blocks)}. \tag{66}$$

We also need to store the intermediate blocks of

$$P_{I,:} = \text{SoftMax}(Q_{I,:} K^\top) \in \mathbf{R}^{|I| \times T}, \tag{67}$$

$$\frac{\partial L}{\partial P_{I,:}} = \frac{\partial L}{\partial O_{I,:}} V^\top \in \mathbf{R}^{|I| \times T}, \tag{68}$$

and

$$\frac{\partial L}{\partial S_{I,:}} = P_{I,:} \odot \left(\frac{\partial L}{\partial P_{I,:}} - \boldsymbol{\gamma}_I \mathbf{1}^\top \right) \in \mathbf{R}^{|I| \times T}, \tag{69}$$

which requires $2 \times |I| \times T$ space because (69) can overwrite either (67) or (68). As the memory access in (65) cost $O(|I|d)$ and we can control the block size in (66), the $2 \times |I| \times T$ for (67)–(68) is the bottleneck. Thus, the largest possible $|I|$ is

$$\frac{M}{2T},$$

and the total number of memory accesses is

$$O\left(\frac{T}{M/(2T)} \right) \times O(Td) = O\left(\frac{T^3 d}{M} \right), \tag{70}$$

which is the same as (39) for the forward pass.

6.3 FlashAttention Backward Pass

To reduce the number of memory accesses in (70), we identify that the bottleneck is the storage of the intermediate matrices in (67) and (68). This bottleneck is similar to what we encountered in the forward pass, where we addressed it by splitting the $|I| \times T$ matrices into smaller sub-matrices and sequentially using them. We adopt the same strategy in the backward pass, and examine whether the calculations from (58) to (64) can be performed under this strategy. For Q, O and $\partial L / \partial O$, we respectively split them into

$$\begin{bmatrix} Q_{I_1,:} \\ \vdots \\ Q_{I_{T_r},:} \end{bmatrix}, \begin{bmatrix} O_{I_1,:} \\ \vdots \\ O_{I_{T_r},:} \end{bmatrix}, \begin{bmatrix} \frac{\partial L}{\partial O_{I_1,:}} \\ \vdots \\ \frac{\partial L}{\partial O_{I_{T_r},:}} \end{bmatrix},$$

with

$$|I_1| = \cdots = |I_{T_r}|.$$

For $K, V, \partial L/\partial K$ and $\partial L/\partial V$, we respectively split them into

$$\begin{bmatrix} K_{J_1,:} \\ \vdots \\ K_{J_{T_c},:} \end{bmatrix}, \begin{bmatrix} V_{J_1,:} \\ \vdots \\ V_{J_{T_c},:} \end{bmatrix}, \begin{bmatrix} \frac{\partial L}{\partial K_{J_1,:}} \\ \vdots \\ \frac{\partial L}{\partial K_{J_{T_c},:}} \end{bmatrix}, \begin{bmatrix} \frac{\partial L}{\partial V_{J_1,:}} \\ \vdots \\ \frac{\partial L}{\partial V_{J_{T_c},:}} \end{bmatrix},$$

with

$$|J_1| = \cdots = |J_{T_c}|.$$

For $P_{I,:}$ in (58), since we already calculated and stored

$$\Delta = \mathrm{rowsum}\left(\exp\left(QK^\top\right)\right)$$

in (49), from (67) we can express $P_{I,:}$ as follows:

$$P_{I,:} = \mathrm{Diag}(\Delta_I)^{-1} \exp\left(Q_{I,:}\begin{bmatrix} K_{J_1,:}^\top & \cdots & K_{J_{T_c},:}^\top \end{bmatrix}\right), \tag{71}$$

where $\mathrm{Diag}(\Delta_I)$ denotes the diagonal matrix with the elements of Δ_I on its diagonal. Thus, while $P_{I,:} \in \mathbf{R}^{|I| \times T}$ is too large to be stored, we can calculate each block $P_{I,J}$ sequentially

$$P_{I,J} = \mathrm{Diag}(\Delta_I)^{-1} \exp(Q_{I,:}K_{J,:}^\top) \in \mathbf{R}^{|I| \times |J|}. \tag{72}$$

Although this strategy works for (58), we must check that $P_{I,J_1}, \ldots, P_{I,J_{T_c}}$ blocks can be sequentially used in the remaining calculation (59)–(64). For $\partial L/\partial V$, from (59) and (71), we have

$$P_{I,:}^\top \frac{\partial L}{\partial O_{I,:}} = \begin{bmatrix} P_{I,J_1}^\top \\ \vdots \\ P_{I,J_{T_c}}^\top \end{bmatrix} \frac{\partial L}{\partial O_{I,:}} = \begin{bmatrix} P_{I,J_1}^\top \frac{\partial L}{\partial O_{I,:}} \\ \vdots \\ P_{I,J_{T_c}}^\top \frac{\partial L}{\partial O_{I,:}} \end{bmatrix}.$$

If we split $\partial L/\partial V$ to row blocks corresponding to $J_1, \ldots, J_{T_c}$, then (59) becomes to sequentially calculate

$$\left(\frac{\partial L}{\partial V}\right)_{J,:} \leftarrow \left(\frac{\partial L}{\partial V}\right)_{J,:} + P_{I,J}^\top \frac{\partial L}{\partial O_{I,:}}. \tag{73}$$

By this way, we need only $P_{I,J}$ each time instead of the whole $P_{I,:}$. Next, for $\partial L/\partial P_{I,:}$ in (60), we have

$$\begin{aligned} \frac{\partial L}{\partial P_{I,:}} &= \frac{\partial L}{\partial O_{I,:}} V^\top \\ &= \frac{\partial L}{\partial O_{I,:}} \begin{bmatrix} V_{J_1,:}^\top & \cdots & V_{J_{T_c},:}^\top \end{bmatrix} \in \mathbf{R}^{|I| \times T}. \end{aligned}$$

We cannot store an $|I| \times T$ matrix, but instead we calculate one block at a time:

$$\frac{\partial L}{\partial P_{I,J}} = \frac{\partial L}{\partial O_{I,:}} V_{J,:}^\top \in \mathbf{R}^{|I| \times |J|}. \tag{74}$$

We then see where $\partial L/\partial P_{I,:}$ is used. It is in (62) for calculating $\partial L/\partial S_{I,:}$. Recall that $\partial L/\partial S_{I,:} \in \mathbf{R}^{|I|\times T}$ is too large to be stored. From (72) and (74), each time we calculate one block as follows.

$$\begin{aligned}\frac{\partial L}{\partial S_{I,J}} &= P_{I,J} \odot \left(\frac{\partial L}{\partial P_{I,J}} - \boldsymbol{\gamma}_I \mathbf{1}^\top\right) \\ &= P_{I,J} \odot \left(\frac{\partial L}{\partial O_{I,:}} V_{J,:}^\top - \boldsymbol{\gamma}_I \mathbf{1}^\top\right) \in \mathbf{R}^{|I|\times|J|}.\end{aligned} \tag{75}$$

From (75), there is no need to store $\partial L/\partial P_{I,J}$ as we can directly apply $\partial L/\partial O_{I,:}$ and $V_{J,:}^\top$ for the calculation. We also need to check how to compute $\boldsymbol{\gamma}_I$. From (24), we know that $\boldsymbol{\gamma}_I$ can be computed with

$$\boldsymbol{\gamma}_I = \text{rowsum}\left(\frac{\partial L}{\partial O_{I,:}} \odot O_{I,:}\right) \in \mathbf{R}^{|I|},$$

which can be calculated before we go through all $\partial L/\partial S_{I,J}$ blocks. Next, we check how to calculate $\partial L/\partial Q_{I,:}$ and $\partial L/\partial K_{J,:}$. From (63), using (75) and $K_{J_j,:}$, we have

$$\begin{aligned}\frac{\partial L}{\partial Q_{I,:}} &= \frac{\partial L}{\partial S_{I,:}} K \\ &= \begin{bmatrix}\frac{\partial L}{\partial S_{I,J_1}} & \cdots & \frac{\partial L}{\partial S_{I,J_{T_c}}}\end{bmatrix} \begin{bmatrix} K_{J_1,:} \\ \vdots \\ K_{J_{T_c},:}\end{bmatrix} \\ &= \sum_{j=1}^{T_c} \frac{\partial L}{\partial S_{I,J_j}} K_{J_j,:}.\end{aligned} \tag{76}$$

By this setting, we no longer need the whole $\partial L/\partial S_{I,:}$. Instead, we sequentially calculate $\partial L/\partial S_{I,J_j}$ via (75) and add

$$\frac{\partial L}{\partial S_{I,J_j}} K_{J_j,:} \quad \text{to} \quad \frac{\partial L}{\partial Q_{I,:}}.$$

For $\partial L/\partial K$, the situation is the same as that for $\partial L/\partial V$ due to the similar form of (59) and (64). Thus, what we do is an update like (73):

$$\frac{\partial L}{\partial K_{J,:}} \leftarrow \frac{\partial L}{\partial K_{J,:}} + \frac{\partial L}{\partial S_{I,J}}^\top Q_{I,:}. \tag{77}$$

In (72)–(77), $O_{I,:}$ is only required for calculating $\boldsymbol{\gamma}_I$. Because $\boldsymbol{\gamma}_I$ is independent of operations on blocks $J_1, \ldots, J_{T_c}$, and can be pre-computed, once we have used $O_{I,:}$, the same space can be available for $Q_{I,:}$. Finally, we have the following algorithm.

Algorithm 6 A flash attention implementation for the backward pass (i, j version)

For $i = 1, \ldots, T_r$

Load $O_{I_i,:}, \partial L/\partial O_{I_i,:},$ and Δ_{I_i}

Compute

$$\boldsymbol{\gamma_{I_i}} = \text{rowsum}\left(\frac{\partial L}{\partial O_{I_i,:}} \odot O_{I_i,:}\right)$$

Load $Q_{I_i,:}$ to overwrite $O_{I_i,:}$

For $j = 1, \ldots, T_c$

Load $K_{J_j,:}$ and $V_{J_j,:}$

$$P_{I_i,J_j} = \text{Diag}(\Delta_{I_i})^{-1} \exp(Q_{I_i,:} K_{J_j,:}^\top)$$

$$\frac{\partial L}{\partial V_{J_j,:}} \leftarrow \frac{\partial L}{\partial V_{J_j,:}} + P_{I_i,J_j}^\top \frac{\partial L}{\partial O_{I_i,:}}$$

$$\frac{\partial L}{\partial S_{I_i,J_j}} = P_{I_i,J_j} \odot \left(\frac{\partial L}{\partial O_{I_i,:}} V_{J_j,:}^\top - \boldsymbol{\gamma}_{I_i} \mathbf{1}^\top\right)$$

$$\frac{\partial L}{\partial K_{J_j,:}} \leftarrow \frac{\partial L}{\partial K_{J_j,:}} + \frac{\partial L}{\partial S_{I_i,J_j}}^\top Q_{I_i,:}$$

$$\frac{\partial L}{\partial Q_{I_i,:}} \leftarrow \frac{\partial L}{\partial Q_{I_i,:}} + \frac{\partial L}{\partial S_{I_i,J_j}} K_{J_j,:}$$

Save $\partial L/\partial V_{J_j,:}$ and $\partial L/\partial K_{J_j,:}$ to secondary memory.

Save $\partial L/\partial Q_{I_i,:}$ to secondary memory.

At any time point of the inner loop, we must store the following blocks in main memory:

1. $Q_{I,:} \in \mathbf{R}^{|I| \times d}$
2. $K_{J,:} \in \mathbf{R}^{|J| \times d}$
3. $V_{J,:} \in \mathbf{R}^{|J| \times d}$
4. $P_{I,J} \in \mathbf{R}^{|I| \times |J|}$ **or** $\partial L/\partial S_{I,J} \in \mathbf{R}^{|I| \times |J|}$
5. $\partial L/\partial O_{I,:} \in \mathbf{R}^{|I| \times d}$
6. $\partial L/\partial Q_{I,:} \in \mathbf{R}^{|I| \times d}$
7. $\partial L/\partial K_{J,:} \in \mathbf{R}^{|J| \times d}$
8. $\partial L/\partial V_{J,:} \in \mathbf{R}^{|J| \times d}$

Similar to the forward pass, we assume that operations in (72)–(77) do not require extra space to store intermediate results, such as

$$P_{I,J} \frac{\partial L}{\partial O_{I,:}}, \frac{\partial L}{\partial O_{I,:}} V_J \text{ and } \left(\frac{\partial L}{\partial S_{I,J}}\right)^\top Q_{I,:},$$

as any results can be immediately used to update the matrix on the left-hand side. Therefore, we select $|I|$ and $|J|$ to satisfy

$$|I|d < \frac{M}{8}, \quad |J|d < \frac{M}{8}, \quad |I||J| < \frac{M}{8}. \tag{78}$$

If we choose

$$|I| = \left\lfloor \frac{M}{8d} \right\rfloor \text{ and } |J| = \min\left(\left\lfloor \frac{M}{8d} \right\rfloor, d \right), \tag{79}$$

then (78) holds. Similar to the forward calculation, under each block I, we must access several $T \times d$ matrices. Thus the number of memory accesses is still

$$\frac{T}{|I|} \times O(Td) = O\left(\frac{T^2 d^2}{M} \right)$$

as in (50).

6.4 FlashAttention Backward Pass: (i, j) Versus (j, i)

What we have derived so far is not yet the FlashAttention backward pass. Recall that in forward FlashAttention, we have a different version by swapping the loop order of i and j. We referred to the i, j version as FlashAttention-2, while the j, i version is referred to as FlashAttention. We showed that the i, j version is slightly more memory efficient. Thus, we would like to check the j, i version of the backward implementation. The procedure is as follows.

Algorithm 7 A draft of flash attention backward pass

For $j = 1, \ldots, T_c$
  Load $K_{J_j,:}$ and $V_{J_j,:}$
  For $i = 1, \ldots, T_r$
    Load $O_{I_i,:}$, $\dfrac{\partial L}{\partial O_{I_i,:}}$, and Δ_{I_i}

$$\boldsymbol{\gamma}_{I_i} = \text{rowsum}\left(\frac{\partial L}{\partial O_{I_i,:}} \odot O_{I_i,:} \right) \tag{80}$$

    ... (rest omitted for now)

In (80), the same $\boldsymbol{\gamma}_{I_i}$ is computed T_c times. As it is independent of J blocks, we can pre-compute it before the main loop. By this way, we can also prevent the frequent loading of O_{I_i}. The new procedure is as follows.

Algorithm 8 A flash attention implementation for the backward pass (j, i version)

For $i = 1, \ldots, T_r$

Load $\partial L/\partial O_{I_i,:}, O_{I_i,:}$

Calculate and save

$$\boldsymbol{\gamma}_{I_i} = \text{rowsum}\left(\frac{\partial L}{\partial O_{I_i,:}} \odot O_{I_i,:}\right)$$

For $j = 1, \ldots, T_c$

Load $K_{J_j,:}$ and $V_{J_j,:}$

For $i = 1, \ldots, T_r$

Load $Q_{I_i,:}, \dfrac{\partial L}{\partial O_{I_i,:}}, \Delta_{I_i}$ and $\boldsymbol{\gamma}_{I_i}$

$$P_{I_i,J_j} = \text{Diag}(\Delta_{I_i})^{-1} \exp(Q_{I_i,:} K_{J_j,:}^\top)$$

$$\frac{\partial L}{\partial V_{J_j,:}} \leftarrow \frac{\partial L}{\partial V_{J_j,:}} + P_{I_i,J_j}^\top \frac{\partial L}{\partial O_{I_i,:}}$$

$$\frac{\partial L}{\partial S_{I_i,J_j}} = P_{I_i,J_j} \odot \left(\frac{\partial L}{\partial O_{I_i,:}} V_{J_j,:}^\top - \boldsymbol{\gamma}_{I_i} \mathbf{1}^\top\right)$$

$$\frac{\partial L}{\partial K_{J_j,:}} \leftarrow \frac{\partial L}{\partial K_{J_j,:}} + \frac{\partial L}{\partial S_{I_i,J_j}}^\top Q_{I_i,:}$$

$$\frac{\partial L}{\partial Q_{I_i,:}} \leftarrow \frac{\partial L}{\partial Q_{I_i,:}} + \frac{\partial L}{\partial S_{I_i,J_j}} K_{J_j,:}$$

Save $\partial L/\partial Q_{I_i,:}$ to secondary memory

Save $\partial L/\partial V_{J_j,:}$ and $\partial L/\partial K_{J_j,:}$ to secondary memory.

The above procedure maintains the following eight blocks in main memory:

1. $Q_{I,:} \in \mathbf{R}^{|I| \times d}$
2. $K_{J,:} \in \mathbf{R}^{|J| \times d}$
3. $V_{J,:} \in \mathbf{R}^{|J| \times d}$
4. $P_{I,J} \in \mathbf{R}^{|I| \times |J|}$ or $\partial L/\partial S_{I,J} \in \mathbf{R}^{|I| \times |J|}$
5. $\partial L/\partial O_{I,:} \in \mathbf{R}^{|I| \times d}$
6. $\partial L/\partial Q_{I,:} \in \mathbf{R}^{|I| \times d}$
7. $\partial L/\partial K_{J,:} \in \mathbf{R}^{|J| \times d}$
8. $\partial L/\partial V_{J,:} \in \mathbf{R}^{|J| \times d}$

The number of blocks is the same as that of the i, j version discussed earlier. Thus they have the same memory consumption. However, the two versions differ in the number of memory accesses. Let us check their respective inner loops. The i, j version requires to

- load $K_{J_j,:} \in \mathbf{R}^{|J| \times d}$, $V_{J_j,:} \in \mathbf{R}^{|J| \times d}$ and
- save $\partial L / \partial K_{J_j,:} \in \mathbf{R}^{|J| \times d}$ and $\partial L / \partial V_{J_j,:} \in \mathbf{R}^{|J| \times d}$.

The j, i version requires to

- load $Q_{I_i,:} \in \mathbf{R}^{|I| \times d}$, $\partial L / \partial O_{I_i,:} \in \mathbf{R}^{|I| \times d}$ and
- save $\partial L / \partial Q_{I_i,:} \in \mathbf{R}^{|I| \times d}$.

Thus, their number of memory accesses is

$$4 \times T_r \times |J| \times d$$

and

$$3 \times T_c \times |I| \times d.$$

If we consider

$$T_r \approx T_c \quad \text{and} \quad |I| \approx |J|,$$

then the j, i version is more memory efficient. Therefore, it is interesting that for the forward calculation, the i, j version is better but the opposite may occur for the backward calculation. Another thing worth noticing is that since the j, i version of backward implementation also maintains eight blocks, the block sizes $|I|$ and $|J|$ should also satisfy (79). However, the setting in Dao et al. [2022] is

$$|I| = \left\lfloor \frac{M}{4d} \right\rfloor \text{ and } |J| = \min\left(\left\lfloor \frac{M}{4d} \right\rfloor, d \right),$$

which we think is incorrect.

7 Appendix

7.1 Gradient with Respect to W_O and O

In (6)–(10), we gave details of multi-head attention, in which

$$\text{input: } Q, K, V \rightarrow \text{output: } O$$

is a sub-process. Here we give full details of gradient calculation by considering

$$\text{input: } \tilde{Z} \rightarrow \text{output: } \tilde{Z}^{\text{out}}.$$

From (10), we derive

$$\frac{\partial L}{\partial W_O} \in \mathbf{R}^{d \times d} \quad \text{and} \quad \frac{\partial L}{\partial O} \in \mathbf{R}^{T \times d}.$$

We note that (10) is in a similar form to (9), where they are respectively

$$\tilde{Z}^{\text{out}} = O W_O \quad \text{and} \quad O = PV.$$

The results derived earlier for

$$\frac{\partial L}{\partial V} \quad \text{and} \quad \frac{\partial L}{\partial P}$$

directly lead us to have

$$\frac{\partial L}{\partial W_O} = O^\top \frac{\partial L}{\partial \tilde{Z}^{\text{out}}} \in \mathbf{R}^{d \times d},$$
$$\frac{\partial L}{\partial O} = \frac{\partial L}{\partial \tilde{Z}^{\text{out}}} W_O^\top \in \mathbf{R}^{T \times d}.$$

7.2 Gradients with Respect to W_Q, W_K, and W_V

From (6), next we derive

$$\frac{\partial L}{\partial W_Q}, \frac{\partial L}{\partial W_K}, \frac{\partial L}{\partial W_V} \in \mathbf{R}^{d\times d}.$$

We note that $Q = \tilde{Z}W_Q$, $K = \tilde{Z}W_K$, and $V = \tilde{Z}W_V$ are all in a similar form to (9). Thus we directly have

$$\begin{aligned}
\frac{\partial L}{\partial W_Q} &= \tilde{Z}^\top \frac{\partial L}{\partial Q} \in \mathbf{R}^{d\times d},\\
\frac{\partial L}{\partial W_K} &= \tilde{Z}^\top \frac{\partial L}{\partial K} \in \mathbf{R}^{d\times d},\\
\frac{\partial L}{\partial W_V} &= \tilde{Z}^\top \frac{\partial L}{\partial V} \in \mathbf{R}^{d\times d}.
\end{aligned}$$

7.3 Gradient with Respect to $\tilde{Z}$

From (6),

$$Q_{ik} = \sum_{\ell=1}^{d} \tilde{Z}_{i\ell}(W_Q)_{\ell k}, \tag{81}$$

$$K_{ik} = \sum_{\ell=1}^{d} \tilde{Z}_{i\ell}(W_K)_{\ell k}, \tag{82}$$

$$V_{ik} = \sum_{\ell=1}^{d} \tilde{Z}_{i\ell}(W_V)_{\ell k}. \tag{83}$$

From Figure 1, $\tilde{Z}$ affects the loss L through elements in Q, K, and V. More specifically, from (81)–(83) and the similar form of (13) in calculating $\partial L/\partial P$, we see $\tilde{Z}_{i\ell}$ affects L through the ith row of Q, K, and V. Thus, applying the chain rule gives

$$\begin{aligned}
\frac{\partial L}{\partial \tilde{Z}_{i\ell}} &= \sum_{k=1}^{d} \frac{\partial L}{\partial Q_{ik}}\frac{\partial Q_{ik}}{\partial \tilde{Z}_{i\ell}} + \sum_{k=1}^{d} \frac{\partial L}{\partial K_{ik}}\frac{\partial K_{ik}}{\partial \tilde{Z}_{i\ell}} + \sum_{k=1}^{d} \frac{\partial L}{\partial V_{ik}}\frac{\partial V_{ik}}{\partial \tilde{Z}_{i\ell}}\\
&= \sum_{k=1}^{d} \frac{\partial L}{\partial Q_{ik}}(W_Q)_{\ell k} + \sum_{k=1}^{d} \frac{\partial L}{\partial K_{ik}}(W_K)_{\ell k} + \sum_{k=1}^{d} \frac{\partial L}{\partial V_{ik}}(W_V)_{\ell k}.
\end{aligned} \tag{84}$$

We can represent (84) in the following matrix form

$$\frac{\partial L}{\partial \tilde{Z}} = \frac{\partial L}{\partial Q}W_Q^\top + \frac{\partial L}{\partial K}W_K^\top + \frac{\partial L}{\partial V}W_V^\top \in \mathbf{R}^{T\times d}.$$

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