An Introduction to FlashAttention

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Outline

Outline

Attention and Its Bottleneck I

- The Transformer architecture proposed by Vaswani et al.2017) has become dominant in modern deep learning.
- However, scaling Transformers to long contexts remains challenging due to their attention operations, which have high computation and memory complexity in sequence length (discussed later in this presentation).
- Many prior works have attempted to address this challenge, among which **FlashAttention** (Dao et al.2022) is one of the most well-known.

Attention and Its Bottleneck II

- In these slides, we introduce FlashAttention and its subsequent variants.
- To better understand this challenge, we first analyze the standard forward and backward calculations of the attention operation.
- We then identify the key bottleneck in attention.
- Finally, we derive the FlashAttention algorithm and show how it resolves this bottleneck.

Outline

Attention Operations I

- 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.

Attention Operations II

- In (1), the SoftMax function is applied on each row z of an input matrix in the following way,

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

Attention Operations III

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

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

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

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

Attention Operations IV

- 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,

$$\text{MultiHead}(Q = \tilde{Z}, K = \tilde{Z}, V = \tilde{Z}).$$

Attention Operations V

- 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

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

Attention Operations VI

- Because the multi-head situation is similar to the single case, for our discussion we assume $h = 1$ (i.e., one head). Under this assumption, d/h reduces to d, so we use d to denote the per-head dimension in this document.
- 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

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

Attention Operations VII

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

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

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

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

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

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

Attention Operations VIII

where $\tilde{Z}, \tilde{Z}^{\text{out}} \in \mathbf{R}^{T \times d}$ 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.

Attention Operations IX

- The following graph shows the connection between variables:

Attention Operations X

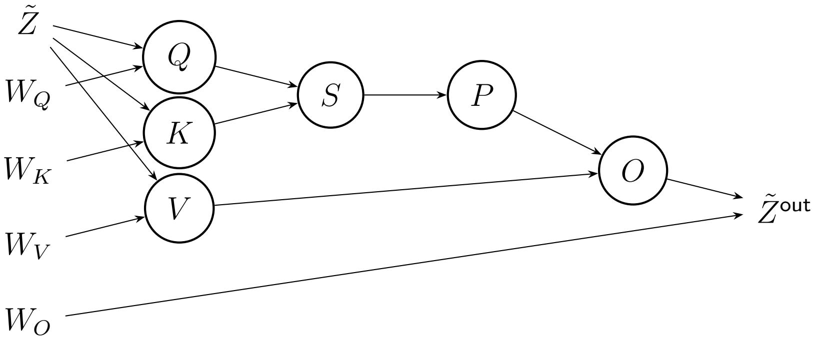


Figure 1: The computation graph of attention.

Attention Operations XI

- From the graph, we can clearly see that

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

  is a sub-graph.
- We can treat (11) as a general component for the use in (5) and other places.

Attention Operations XII

- Therefore, in this document, we focus on the efficient forward and backward computation of

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

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

Outline

The Need to Derive Backward Calculation I

- 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.

The Need to Derive Backward Calculation II

- 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.

The Need to Derive Backward Calculation III

- Subsequently, we derive the backward calculation of attention.

Backward Pass: Problem Setup I

- 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

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

Backward Pass: Problem Setup II

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

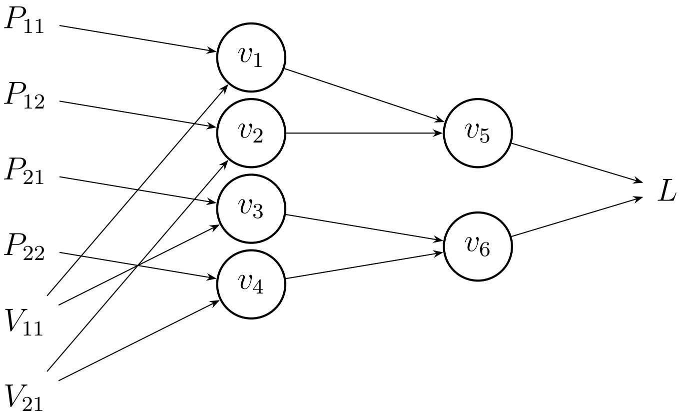
$$\frac{\partial L}{\partial Q}, \quad \frac{\partial L}{\partial K}, \quad \text{and} \quad \frac{\partial L}{\partial V}.$$

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

Gradient with Respect to V I

- We begin by deriving the gradient with respect to the value matrix $V \in \mathbf{R}^{T \times d}$.
- From (9),
$$O_{ik} = \sum_{j=1}^{T} P_{ij} V_{jk}, \tag{13}$$
for $i = 1, \ldots, T$ and $k = 1, \ldots, d$.
- 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.

Gradient with Respect to V II



Gradient with Respect to V III

- 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

Gradient with Respect to V IV

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

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

Gradient with Respect to V V

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

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

- We can represent (15) in the following matrix form

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

Gradient with Respect to V VI

because of

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

Gradient with Respect to P I

- 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

$$O_{ik} = \sum_{j'=1}^{T} P_{ij'} V_{j'k},$$

for $i = 1, \ldots, T$ and $k = 1, \ldots, d$.

Gradient with Respect to P II

- 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

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

Gradient with Respect to P III

because of

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

Gradient with Respect to S I

- 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.

Gradient with Respect to S II

- The following computational graph gives an illustration of $T = 2$.

$$
\begin{tikzcd}
S_{11} \arrow[rr] \arrow[rrd] & & P_{11} \\
S_{12} \arrow[rr] \arrow[rru] & & P_{12} \\
S_{21} \arrow[rr] \arrow[rrd] & & P_{21} \\
S_{22} \arrow[rr] \arrow[rru] & & P_{22}
\end{tikzcd}
$$

Gradient with Respect to S III

- 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

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

Gradient with Respect to S IV

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

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

Gradient with Respect to S V

- 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

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

Gradient with Respect to S VI

- 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,

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

Gradient with Respect to S VII

- Substituting (20) into (19) gives

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

Gradient with Respect to S VIII

- 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

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

Gradient with Respect to S IX

where $\mathbf{1} \in \mathbf{R}^T$ 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

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

Gradient with Respect to S X

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

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

Gradient with Respect to S XI

- Thus, we can rewrite (23) as

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

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

Gradient with Respect to Q and K I

- 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

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

Gradient with Respect to Q and K II

- The results derived earlier for

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

directly lead us to have

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

Summary of Backward Calculation I

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

$$
\begin{aligned}
\frac{\partial L}{\partial V} &= P^\top \frac{\partial L}{\partial O} \in \mathbf{R}^{T\times d} \\
\frac{\partial L}{\partial P} &= \frac{\partial L}{\partial O} V^\top \in \mathbf{R}^{T\times T}
\end{aligned}
$$

Summary of Backward Calculation II

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

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

$$\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S} K \in \mathbf{R}^{T \times d}$$

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

Outline

Memory Accesses in Attention I

- 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.

Memory Accesses in Attention II

- We need

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

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

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

- As in general

$$T \gg d^1,$$

even though the output

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

Memory Accesses in Attention III

is smaller, storing $T \times T$ intermediate matrices is the main difficulty.

[1] d is the per-head dimension.

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

- 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:

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

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

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

- load the matrix in (29) for calculating

$$\text{SoftMax}(QK^\top)V \in \mathbf{R}^{T\times d}.$$

- 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.

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

- 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.

Memory Versus Computation I

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

$$
\begin{aligned}
QK^\top &: 2T^2d, \\
\text{SoftMax}(QK^\top) &: 3T^2, \\
\text{SoftMax}(QK^\top)V &: 2T^2d.
\end{aligned}
$$

Memory Versus Computation II

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

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

  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.

Memory Versus Computation III

- This GPU sustains up to 312 tera floating point operations per second (TFLOPS) for half-precision floating-point format (FP16) operations[2].
- 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).

Memory Versus Computation IV

- 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).

Memory Versus Computation V

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

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

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

- 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):

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

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

- 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.

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

- 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,

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

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

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

and write the result to secondary memory, and

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

- load (32) from secondary memory twice to compute

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

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

- 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.

Backward Pass: Computational Complexity I

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

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

Backward Pass: Computational Complexity II

$$\gamma = \text{rowsum}\left(\frac{\partial L}{\partial O} \odot O\right) : 2Td,$$

$$\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S} K : 2T^2 d,$$

$$\frac{\partial L}{\partial K} = \left(\frac{\partial L}{\partial S}\right)^\top Q : 2T^2 d.$$

- The total computational cost for the backward pass is

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

Outline

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

- Now we assume that the main memory is sufficient to store

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

- 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.

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

- 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:
  - Load $Q, K,$ and V to main memory.

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

- For $i = 1, \ldots, T$, calculate

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

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

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

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

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

- By this way, the number of memory accesses is reduced to

$$O(Td).$$

because we never load/store any $T \times T$ matrices.

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

- Unfortunately, our assumption that $T \times d$ matrices can be stored in main memory is often untrue.
- We discuss the situation of

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

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.

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

- A possible strategy is to calculate $|I|$ rows together:

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

  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).

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

- We also need to store the intermediate blocks of

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

or

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

which requires

$$|I| \times T$$

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

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

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

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

- 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).

FlashAttention I

- 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

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

FlashAttention II

- 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.

FlashAttention III

- 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

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

FlashAttention IV

- We have

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

- If we sequentially generate each term, there is no need to store the intermediate sub-matrix in (37).

FlashAttention V

- In this situation, the algorithm can be as follows.
- For $i = 1, \ldots, T_r$
  - For $j = 1, \ldots, T_c$

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

  - 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. $O_{I,:} \in \mathbf{R}^{|I| \times d}$

FlashAttention VI

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

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

FlashAttention VII

- We also need that

$$|I| \text{ as large as possible,}$$

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.

FlashAttention VIII

- 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

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

- This value is smaller than the one we had earlier in (39).

FlashAttention IX

- 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

FlashAttention X

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

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

FlashAttention XI

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 $\forall t \in J_1 \cup \cdots \cup J_{j-1}$,

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

FlashAttention XII

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

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

FlashAttention XIII

- When handling j, we get

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

so we can update (47) by

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

FlashAttention XIV

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

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

FlashAttention XV

- Then (46) becomes,

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

FlashAttention XVI

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.
- For $i = 1, \ldots, T_r$
  - Load $Q_{I_i,:}$
  - For $j = 1, \ldots, T_c$

    Set

$$\Delta_{I_i}^{\text{old}} = \begin{cases} \Delta_{I_i} & \text{if } j > 1 \\ \mathbf{0} & \text{otherwise} \end{cases}$$

FlashAttention XVII

Load $K_{J_j,:}$ and calculate

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

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

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

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

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

FlashAttention XVIII

- 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.

FlashAttention XIX

- By our trick in (46), the number of memory accesses is the same as the algorithm analyzed in (42) and (45),

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

FlashAttention and FlashAttention-2 I

- FlashAttention was first introduced in Dao et al.2022).
- Later Dao2024) proposed an improved version FlashAttention-2.
- Interestingly, what we described earlier is FlashAttention-2.

FlashAttention and FlashAttention-2 II

- In the original FlashAttention, the algorithm is as follows.
- For $j = 1, \ldots, T_c$
  - Load $V_{J_j,:}$ and $K_{J_j,:}$
  - For $i = 1, \ldots, T_r$

    Load Δ_{I_i} and $Q_{I_i,:}$, and calculate

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

$$\Delta_{I_i}^{\text{old}} = \begin{cases} \Delta_{I_i} & \text{if } j > 1 \\ \mathbf{0} & \text{otherwise} \end{cases}$$

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

FlashAttention and FlashAttention-2 III

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

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

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

FlashAttention and FlashAttention-2 IV

- 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

FlashAttention and FlashAttention-2 V

- 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.

FlashAttention and FlashAttention-2 VI

- 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.

Outline

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

- 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.

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

- We can now conduct the following procedure:
  - Load

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

  - For $i = 1, \ldots, T$ calculate:

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

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

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

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

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

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

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

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

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

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

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

- The total memory access cost is

  $$O(Td),$$

  since we never load/store any $T \times T$ matrices.

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

- 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.

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

- 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.

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

- The calculation for $|I|$ rows is as follows:

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

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

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

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

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

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

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

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

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

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

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

and

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

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

- 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

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

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

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.

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

- Thus, the largest possible $|I|$ is

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

and the total number of memory accesses is

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

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

FlashAttention Backward Pass I

- 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.

FlashAttention Backward Pass II

- 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

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

FlashAttention Backward Pass III

- 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

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

FlashAttention Backward Pass IV

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

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

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

$$P_{I,:} = \text{Diag}(\Delta_I)^{-1} \exp\left(Q_{I,:}\left[K^\top_{J_1,:} \quad \cdots \quad K^\top_{J_{T_c},:}\right]\right), \tag{71}$$

where $\text{Diag}(\Delta_I)$ denotes the diagonal matrix with the elements of Δ_I on its diagonal.

FlashAttention Backward Pass V

- 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

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

- 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).

FlashAttention Backward Pass VI

- 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

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

FlashAttention Backward Pass VII

- 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

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

FlashAttention Backward Pass VIII

- 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 $\partial L / \partial S_{I,:}$.

FlashAttention Backward Pass IX

- 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.

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

FlashAttention Backward Pass X

- 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 $\partial L / \partial K_{J,:}$.

FlashAttention Backward Pass XI

- From (63), using (75) and $K_{J_j,:}$, we have

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

FlashAttention Backward Pass XII

- 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).

FlashAttention Backward Pass XIII

- 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 γ_I. Because γ_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 $Q_{I,:}$.

FlashAttention Backward Pass XIV

- Finally, we have the following algorithm.
- 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 $j = 1, \ldots, T_c$

FlashAttention Backward Pass XV

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

$$
\begin{aligned}
P_{I_i,J_j} &= \text{Diag}(\Delta_{I_i})^{-1} \exp(Q_{I_i,:}K_{J_j,:}^\top) \\
\frac{\partial L}{\partial V_{J_j,:}} &\leftarrow \frac{\partial L}{\partial V_{J_j,:}} + P_{I_i,J_j}^\top \frac{\partial L}{\partial O_{I_i,:}} \\
\frac{\partial L}{\partial S_{I_i,J_j}} &= P_{I_i,J_j} \odot \left(\frac{\partial L}{\partial O_{I_i,:}} V_{J_j,:}^\top - \boldsymbol{\gamma}_{I_i} \mathbf{1}^\top \right) \\
\frac{\partial L}{\partial K_{J_j,:}} &\leftarrow \frac{\partial L}{\partial K_{J_j,:}} + \frac{\partial L}{\partial S_{I_i,J_j}}^\top Q_{I_i,:} \\
\frac{\partial L}{\partial Q_{I_i,:}} &\leftarrow \frac{\partial L}{\partial Q_{I_i,:}} + \frac{\partial L}{\partial S_{I_i,J_j}} K_{J_j,:}
\end{aligned}
$$

FlashAttention Backward Pass XVI

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

FlashAttention Backward Pass XVII

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.

FlashAttention Backward Pass XVIII

- 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.

FlashAttention Backward Pass XIX

- 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).

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

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

- For $j = 1, \ldots, T_c$
  - Load $K_{J_j,:}$ and $V_{J_j,:}$
  - For $i = 1, \ldots, T_r$

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

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

. . . (rest omitted for now)

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

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

- In (80), the same γ_{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.

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

- 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 $i = 1, \ldots, T_r$

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

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

$$
\begin{aligned}
P_{I_i,J_j} &= \mathrm{Diag}(\Delta_{I_i})^{-1} \exp(Q_{I_i,:} K_{J_j,:}^\top) \\
\frac{\partial L}{\partial V_{J_j,:}} &\leftarrow \frac{\partial L}{\partial V_{J_j,:}} + P_{I_i,J_j}^\top \frac{\partial L}{\partial O_{I_i,:}} \\
\frac{\partial L}{\partial S_{I_i,J_j}} &= P_{I_i,J_j} \odot \left(\frac{\partial L}{\partial O_{I_i,:}} V_{J_j,:}^\top - \boldsymbol{\gamma}_{I_i} \mathbf{1}^\top \right) \\
\frac{\partial L}{\partial K_{J_j,:}} &\leftarrow \frac{\partial L}{\partial K_{J_j,:}} + \frac{\partial L}{\partial S_{I_i,J_j}}^\top Q_{I_i,:}
\end{aligned}
$$

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

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

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.

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

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

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

- 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

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

- 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

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

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

- 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.

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

- 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.

Outline

Gradient with Respect to W_O and O I

- 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

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

Gradient with Respect to W_O and O II

- 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

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

Gradient with Respect to W_O and O III

- The results derived earlier for

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

directly lead us to have

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

Gradients with Respect to W_Q, W_K, and W_V I

- 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).

Gradients with Respect to W_Q, W_K, and W_V II

- Thus we directly have

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

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

- From (6),

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

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

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

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

- 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.

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

- Thus, applying the chain rule gives

$$\frac{\partial L}{\partial \tilde{Z}_{i\ell}} = \sum_{k=1}^{d} \frac{\partial L}{\partial Q_{ik}} \frac{\partial Q_{ik}}{\partial \tilde{Z}_{i\ell}} + \sum_{k=1}^{d} \frac{\partial L}{\partial K_{ik}} \frac{\partial K_{ik}}{\partial \tilde{Z}_{i\ell}} + \sum_{k=1}^{d} \frac{\partial L}{\partial V_{ik}} \frac{\partial V_{ik}}{\partial \tilde{Z}_{i\ell}}$$

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

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

- 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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