

Memory and IO in deep learning

Lecture 12 — CS 577 Deep Learning

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Computer Science
Illinois Institute of Technology

November 6, 2024

Lec 13 is a seminar

Memory and IO in deep learning

So far...

Lecture 12 — CS 577 Deep Learning

- Backprop
- 2D Conv
- lower to Linear Alg
- Parallelize seq model
- RNN → Transformer

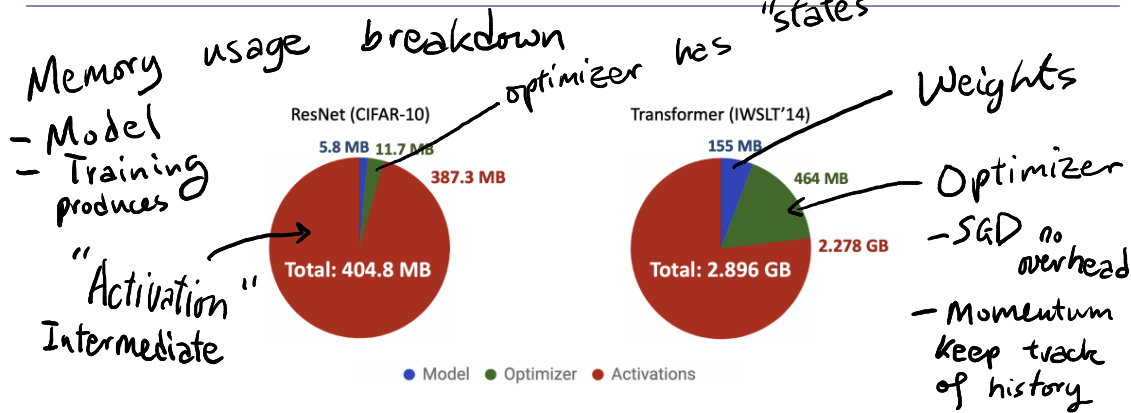
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No discussion of memory so far

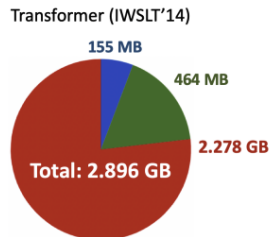
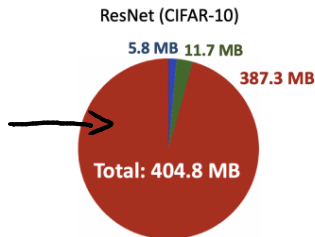
The memory wall



From Sohoni et al. 2019 “Low-memory neural network training: A technical report”

The memory wall

*Biggest
piece of
pie*



● Model ● Optimizer ● Activations

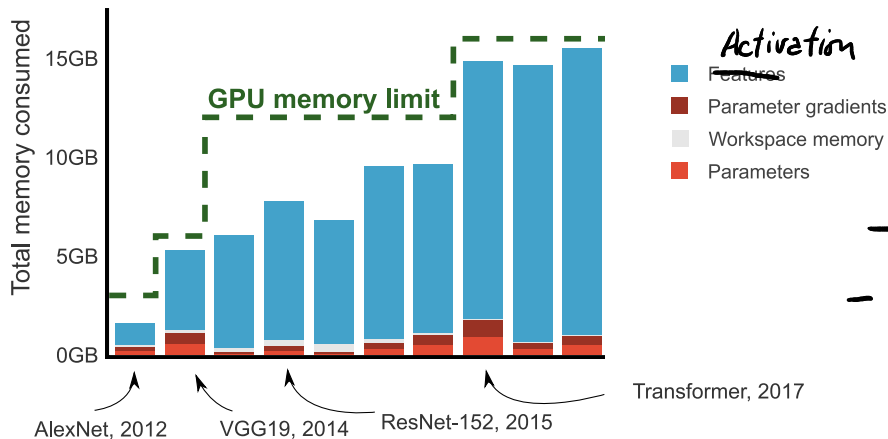
From Sohoni et al. 2019 “Low-memory neural network training: A technical report”

The memory wall

DL practitioners fill up

the
memory
capacity

- Big batch
- Big model

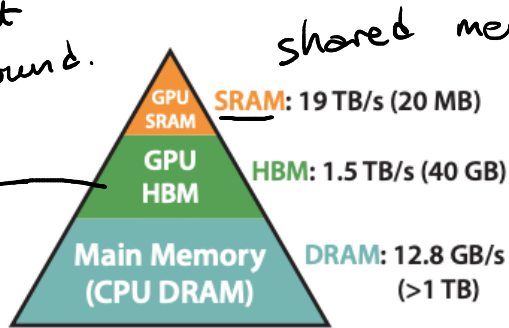


From Jain et al. 2020 “Checkmate: Breaking the memory wall with optimal tensor rematerialization”

Flash attention

IO input-output
moving data around.

"off-chip"
more space
but slow

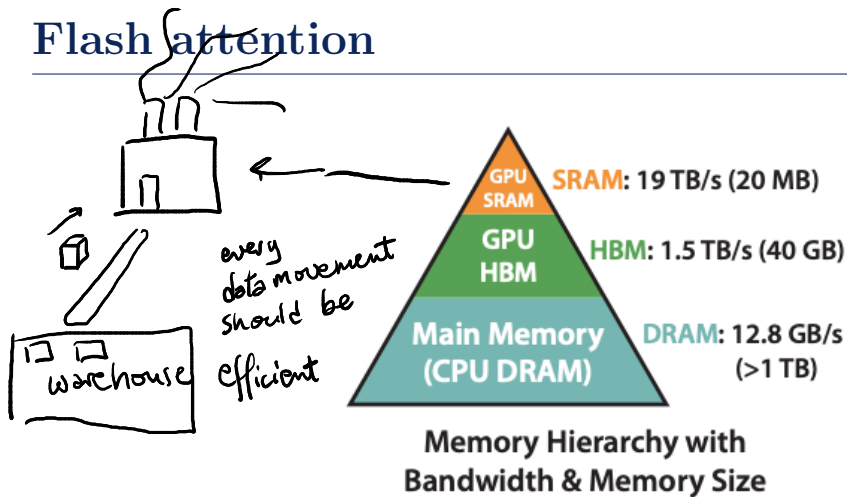


shared memory on
chip
physical
close
to compute

Memory Hierarchy with
Bandwidth & Memory Size

From Dao et al. 2022 "FlashAttention: Fast and memory-efficient exact attention with io-awareness"

Flash Attention



From Dao et al. 2022 "FlashAttention: Fast and memory-efficient exact attention with io-awareness"

Memory and IO

- DL workloads often memory limited
- Moving data (IO) is costly

Roadmap for today

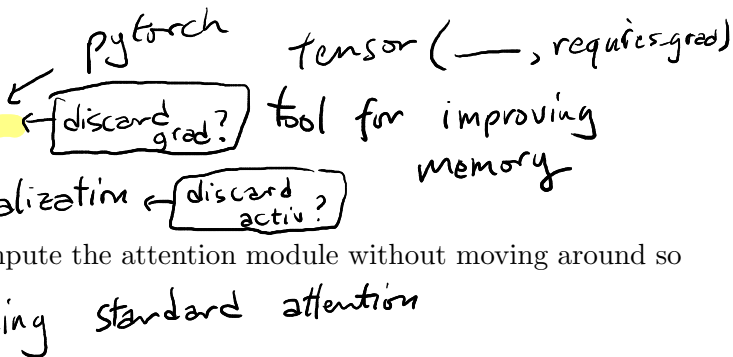
Memory:

- Warm-up: `requires_grad`
- Gradient checkpointing

IO:

- FlashAttention: how to compute the attention module without moving around so much data

Next: `requires_grad`



Size of NumPy array

```
1 import numpy as np
2 import sys
3
4 n = 1000
5 X_np = np.random.randn(n,n)
6 sys.getsizeof(X_np)
7
8 # >>> 8000128      # <- unit in bytes
```

Array in C

```
1 double *X;  
2  
3 X = (double *)malloc(n * n * sizeof(double));
```

```
1 n*n*8
```

```
2  
3 # >>> 8000000
```

$\approx 8 \text{ Mb}$

RAM

8 bytes
in 1 float 64
double

$1000 \times 1000 \times 8$

Size of NumPy array

```
1 import numpy as np
2 import sys
3
4 n = 1000
5 X_np = np.random.randn(n,n)
6 sys.getsizeof(X_np)
7
8 # >>> 8000128      # <--- extra bytes for metadata
9
10
11 n*n*8      # <--- size_of_float64 times num_of_elements_in_X_np
12
13 # >>> 8000000
```

Aside: Size of PyTorch array

```
1 import torch
2
3 n = 1000
4 X_torch = torch.randn(n,n)
5 sys.getsizeof(X_torch.untyped_storage())
6
7 # >>> 4000072
```

reference ↙

```
1 n*n*4      # <--- size_of_float32 times num_of_elements_in_X_torch
2
3 # >>> 4000000
```

bf16 - google brain

- Quantization: save memory by making things less precise

tracemalloc

Allows tracking only memory allocated by numpy

```
1 import tracemalloc
2
3 # [...]
4 print("Simple example")
5
6 start_trace()
7
8 a = 1.0*np.zeros((n,n))    # n = 1000
9
10 print_trace_stats(snapshot_trace())
11 end_trace()
12 # >>> Simple example
13 # >>> memory allocated: 8 MB
```

track memory allocated by a module
numpy

$$\begin{bmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{bmatrix}$$

$$(1000 \times 1000 \times 8)$$



tracemalloc

Allows tracking only memory allocated by numpy

```
1 import tracemalloc
2
3 # [...]
4 print("No discarding")
5 start_trace()
6
7 a = 1.0*np.zeros((n,n))      # n = 1000
8 b = a*a
9 c = np.sum(b,axis=1)
10
11 print_trace_stats(snapshot_trace())
12 end_trace()
13 # >>> No discarding
14 # >>> memory allocated: 16 MB
```

8 MB

8 MB

1000×8

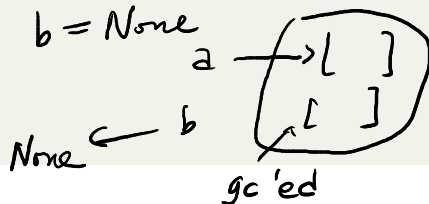
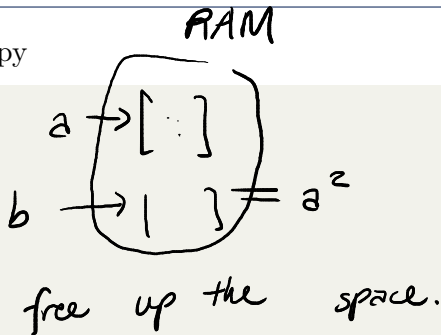
8 kb

16.008

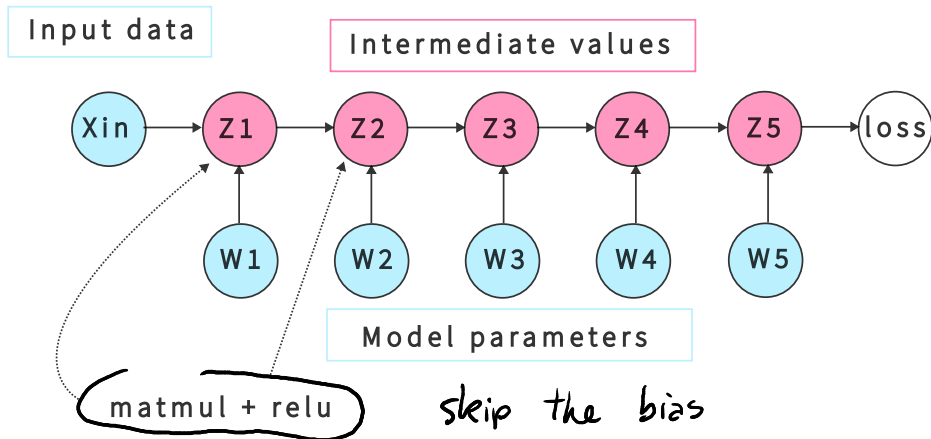
tracemalloc

Allows tracking only memory allocated by numpy

```
1 import tracemalloc
2
3 # [...]
4 print("Discarding")
5 start_trace()
6
7 a = 1.0*np.zeros((n,n))      # n = 1000
8 b = a*a
9 c = np.sum(b,axis=1)
10 b = None
11
12 print_trace_stats(snapshot_trace())
13 end_trace()
14 # >>> With discarding
15 # >>> memory allocated: 8 MB
```

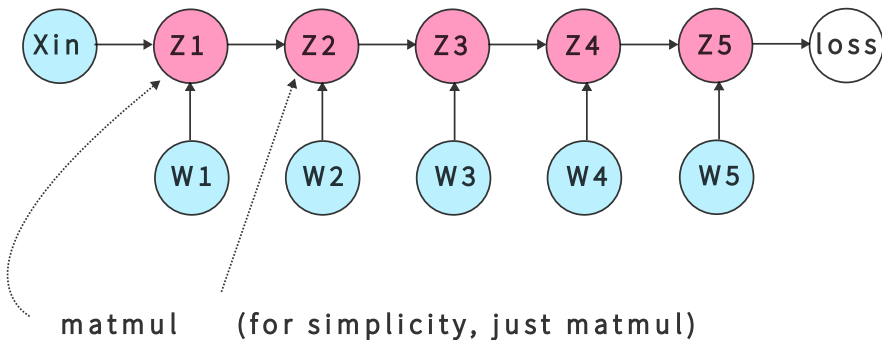


What is needed to calculate the backward?

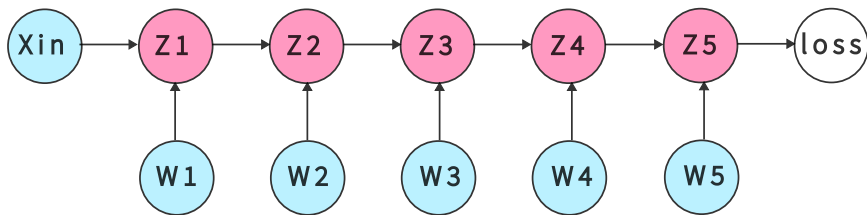


What is needed to calculate the backward?

Not a good model, but simple enough
for memory analysis



What is needed to calculate the backward?

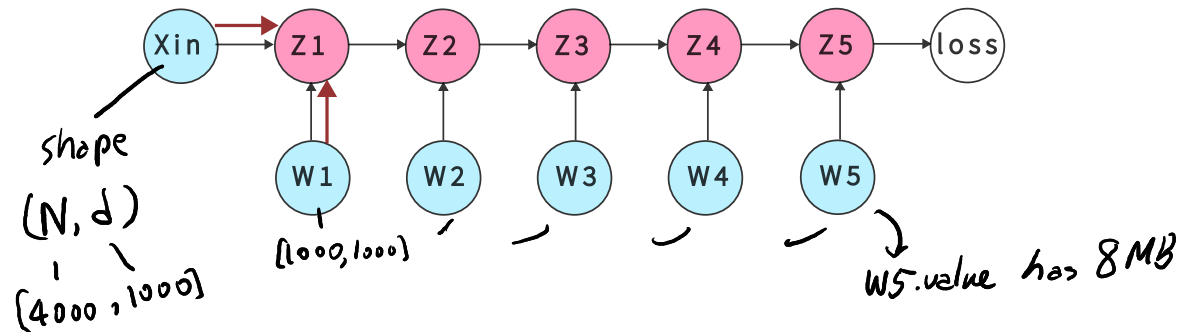


What is needed to calculate the backward?

$$z1.shape = [\underbrace{4000}_{\text{batch-size}}, 1000]$$

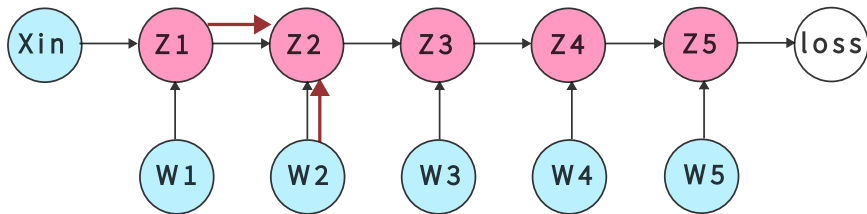
$$Z1 = \text{ag.matmul}(Xin, W1)$$

32 MB



What is needed to calculate the backward?

$$Z2 = \text{ag.matmul}(Z1, W2)$$



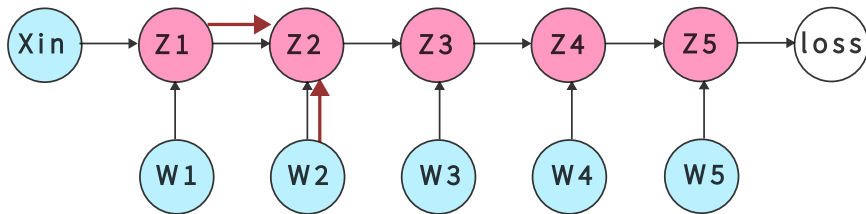
Z2.value — 32 MB
.grad — 32 MB
total 64 MB
per layer

What is needed to calculate the backward?

(Inside constructor for Z2)...

```
self.value = 1.0*value  
self.grad = np.zeros_like(self.value)
```

← *wasted*

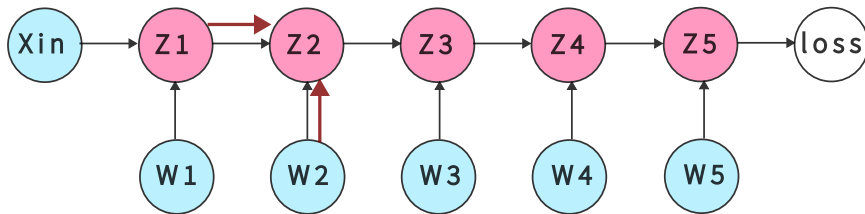


Array sizes!

(Inside constructor for Z2)...

```
self.value = 1.0*value  
self.grad = np.zeros_like(self.value)
```

64 MB



What is needed to calculate the backward?

```
1 def forward(x, weights):  
2     for w in weights:  
3         x = ag.matmul(x, w)  
4     return ag.sum(x)
```


What is needed to calculate the backward?

```
1 def forward_traced(x, weights):
2     start_trace() # tracing
3     mem_usage = [] # tracing
4     for w in weights:
5         x = ag.matmul(x, w)
6         mem_usage.append(snapshot_trace()) # tracing
7     l = ag.sum(x)
8     mem_usage.append(snapshot_trace()) # tracing
9     end_trace() # tracing
10    return l, mem_usage
```

64 MB

128 MB

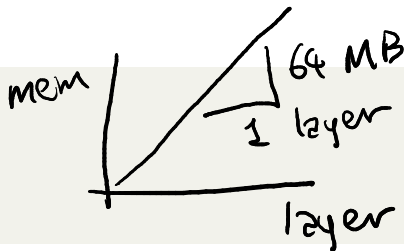
⋮

What is needed to calculate the backward?

```
1 for i, trace_stats in enumerate(mem_usage_forward):  
2     print(f"layer {i}")  
3     print_trace_stats(trace_stats)
```

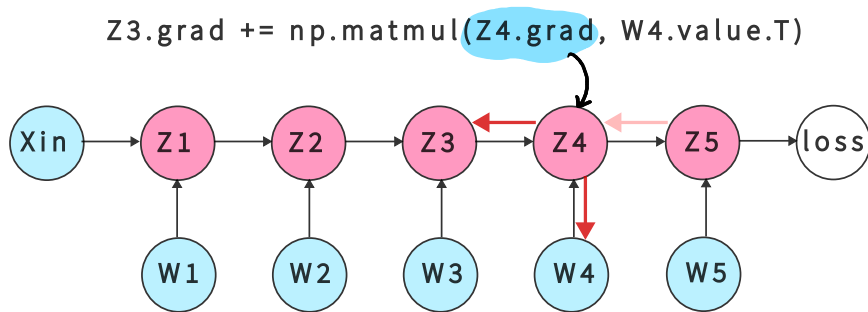
Output:

```
1 layer 0  
2 memory allocated: 64 MB  
3 layer 1  
4 memory allocated: 128 MB  
5 layer 2  
6 memory allocated: 192 MB
```



Observation: double the amount of memory actually needed!

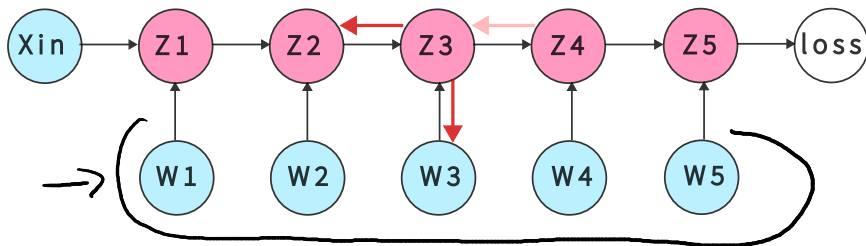
What is needed to calculate the backward?



`W4.grad += np.matmul(Z3.value.T, Z4.grad)`

What is needed to calculate the backward?

```
Z2.grad += np.matmul(Z3.grad, W3.value.T)
```



```
W3.grad += np.matmul(Z2.value.T, Z3.grad)
```

Z4.grad never used again

Backward

```
1     def backward(self):
2         self.grad = np.array(1.0)
3
4         topo_order = self.topological_sort()
5
6         for node in reversed(topo_order):
7             node._backward()
8         return None
```

Backward with tracing

```
1  def backward(self):
2      self.grad = np.array(1.0)
3
4      topo_order = self.topological_sort()
5
6      start_trace() # tracing
7      mem_usage = [] # tracing
8
9      for node in reversed(topo_order):
10         node._backward()
11         mem_usage.append(snapshot_trace()) # tracing
12     end_trace() # tracing
13     return mem_usage
```

Backward with tracing

```
1 for i, trace_stats in enumerate(mem_usage_backward):  
2     print(f"backward step {i}")  
3     print_trace_stats(trace_stats)
```

Output:

```
1 backward step 0  
2 memory allocated: 0 MB  
3 backward step 1  
4 memory allocated: 0 MB  
5 backward step 2  
6 memory allocated: 0 MB
```

*allocated
everything
already*

Observation: After calling backward on a tensor, its grad is no longer needed

Backward with tracing

```
1 for i, trace_stats in enumerate(mem_usage_backward):  
2     print(f"backward step {i}")  
3     print_trace_stats(trace_stats)
```

Output:

```
1 backward step 0  
2 memory allocated: 0 MB  
3 backward step 1  
4 memory allocated: 0 MB  
5 backward step 2  
6 memory allocated: 0 MB
```

Observation: After calling backward on a tensor, its grad is no longer needed

Next: Shift the task of initialize the grad to the backward pass

Keeping track of grad — is it needed?

Constructor

```
1 class Tensor: # Tensor with grads
2     def __init__(self,
3         value,
4         # [...]
5
6         self.value = 1.0*value
7         self.grad = np.zeros_like(self.value) # <---- WASTEFUL!
```

Keeping track of grad — is it needed?

```
1  class Tensor: # Tensor with grads
2      def __init__(self,
3                  value,
4                  requires_grad=False, # <-- Flag for keeping grad
5                  # [...])
6
7      self.value = 1.0*value
8
9      self.grad = None
10     if self.requires_grad:
11         self.grad = np.zeros_like(self.value)
```

Keeping track of grad — is it needed?

```
1  class Tensor: # Tensor with grads
2      def __init__(self,
3                  value,
4                  requires_grad=False, # <-- Flag for keeping grad
5                  # [...])
6
7      self.value = 1.0*value
8
9      self.grad = None
10     if self.requires_grad:
11         self.grad = np.zeros_like(self.value)
12 # [...]
13
14 weights = [ag.Tensor(0.02*np.random.randn(dim_hidden, dim_hidden),
15                  requires_grad = True) for _ in range(num_layers)]
16 #
```

Keeping track of grad — is it needed?

```
1 class Tensor: # Tensor with grads
2     def __init__(self,
3                   value,
4                   requires_grad=False, # <-- Flag for keeping grad
5                   # [...])
6
7         self.value = 1.0*value
8
9         self.grad = None
10        if self.requires_grad:
11            self.grad = np.zeros_like(self.value)
12    # [...]
13
14    for w in weights:
15        x = ag.matmul(x, w)
16        # x.requires_grad == False by default
```

Problem: during backward, we might encounter `None`'s when we should expect `grad`.

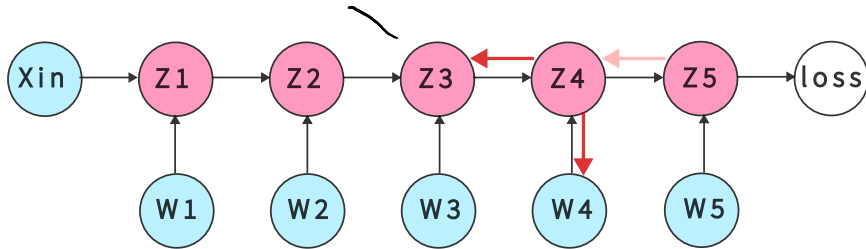
What is needed to calculate the backward?

is None



assume somehow we initialized this

```
Z3.grad += np.matmul(Z4.grad, W4.value.T)
```



```
W4.grad += np.matmul(Z3.value.T, Z4.grad)
```

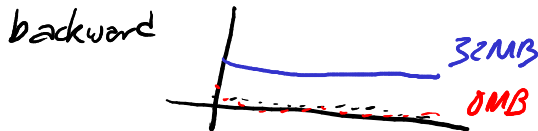
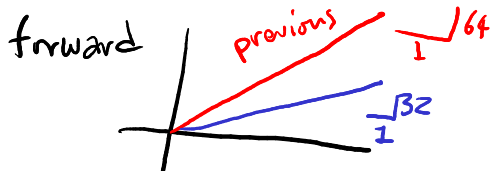
this is fine

Exercise 1: discarding the grad

```
1 # inside ag.__matmul__
2     def _backward():
3         # YOUR CODE HERE FOR initializing the grad
4
5         self.grad += np.matmul(output.grad, other.value.T)
6         other.grad += np.matmul(self.value.T, output.grad)
7
8         # YOUR CODE HERE FOR discarding the grad
9         return None
```

and `def sum(-)'s`
`_backward`

If your answer is correct, then the “sanity checks” should have the expected output.

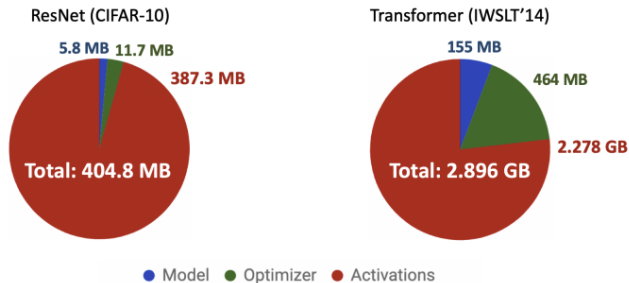


The memory wall

- We've reduced the memory consumption of forward by a factor 2 without incurring much additional backward memory burden.

The memory wall

- We've reduced the memory consumption of forward by a factor 2 without incurring much additional backward memory burden.
- But recall that...



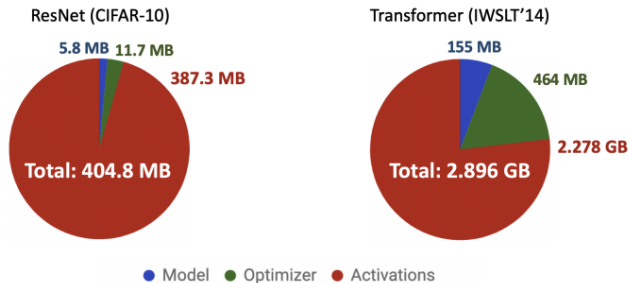
From Sohoni et al. 2019 “Low-memory neural network training: A technical report”

The memory wall

- We've reduced the memory consumption of forward by a factor 2 without incurring much additional backward memory burden.

The memory wall

- We've reduced the memory consumption of forward by a factor 2 without incurring much additional backward memory burden.
- But recall that...



From Sohoni et al. 2019 “Low-memory neural network training: A technical report”

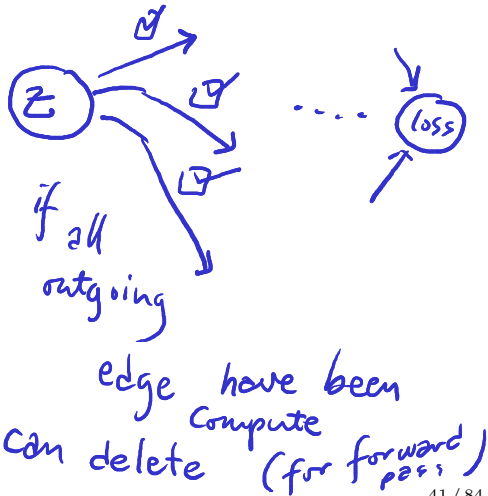
The memory wall

Can we do something about this?

```
1 layer 0
2 memory allocated: 32 MB
3 layer 1
4 memory allocated: 65 MB
5 layer 2
6 memory allocated: 98 MB
7 layer 3
8 memory allocated: 131 MB
9 layer 4
10 memory allocated: 163 MB
11 ...
```

Tensor Rematerialization

- Discard the activations as soon as you can



Tensor Rematerialization

- Discard the activations as soon as you can
- “Beam” them back/recompute them only when you need them



From Berman et al. 1995 “Star Trek: Voyager”

Tensor Rematerialization

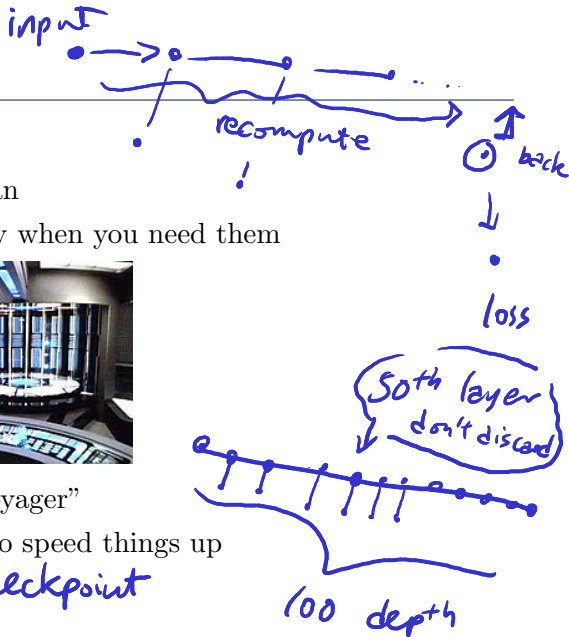
- Discard the activations as soon as you can
- “Beam” them back/recompute them only when you need them



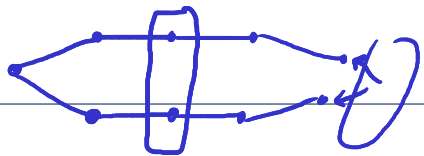
From Berman et al. 1995 “Star Trek: Voyager”

- Save *some* activations as “checkpoints” to speed things up

only recompute from checkpoint



Tensor Rematerialization



Mix
of
Experts

- Discard the activations as soon as you can
- “Beam” them back/recompute them only when you need them

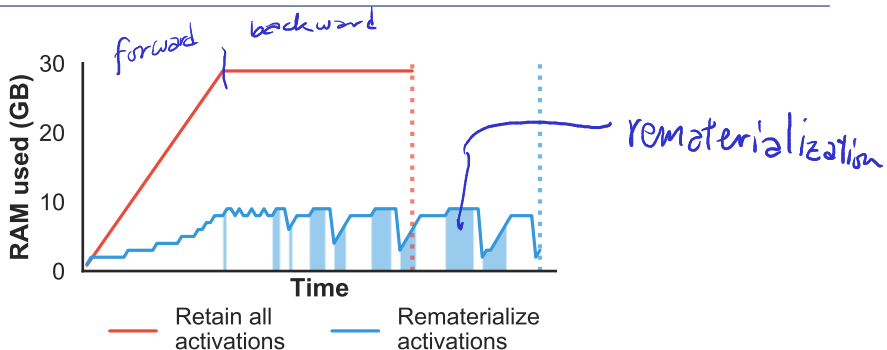


From Berman et al. 1995 “Star Trek: Voyager”

- Save *some* activations as “checkpoints” to speed things up

Tensor Rematerialization

$$h^{(1)} \rightarrow h^{(2)} \rightarrow h^{(3)}$$

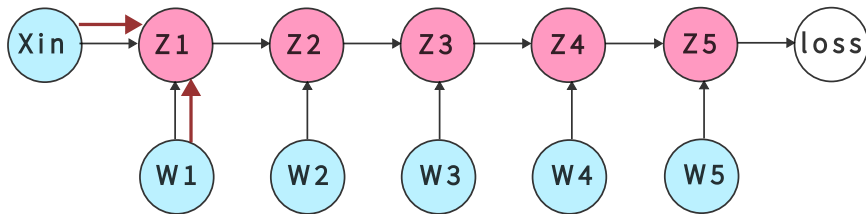


From Jain et al. 2020 “Checkmate: Breaking the memory wall with optimal tensor rematerialization”

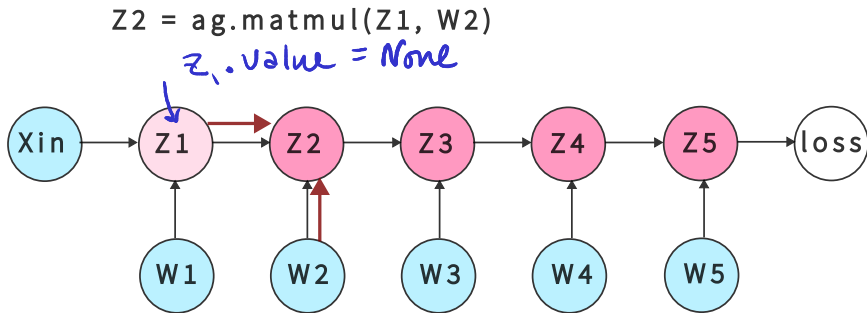
- Also known as gradient checkpoint, activation checkpointing, recomputation...

Rematerialization: forward phase

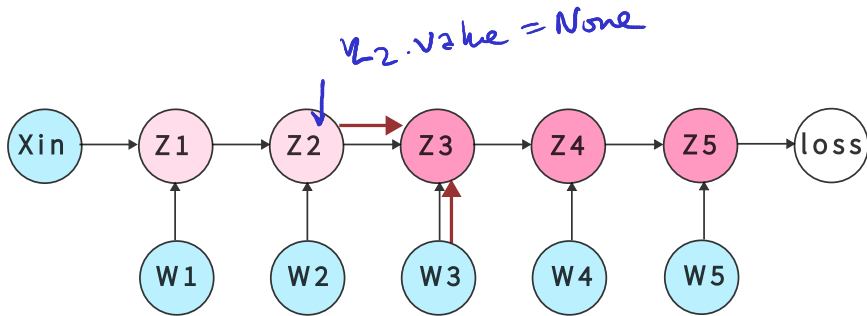
$Z1 = \text{ag.matmul}(X_{in}, W1)$



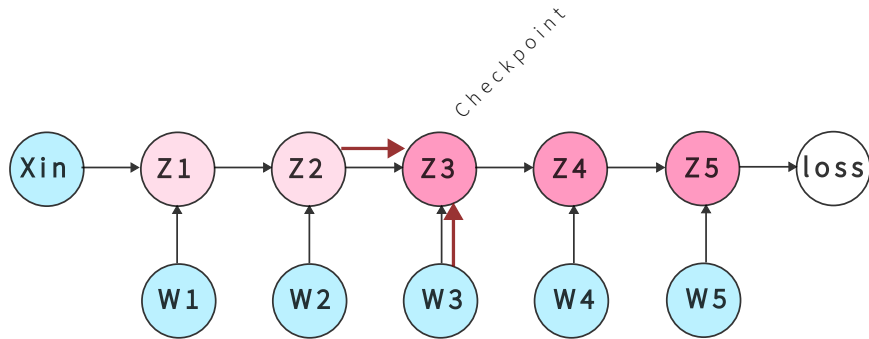
Rematerialization: forward phase



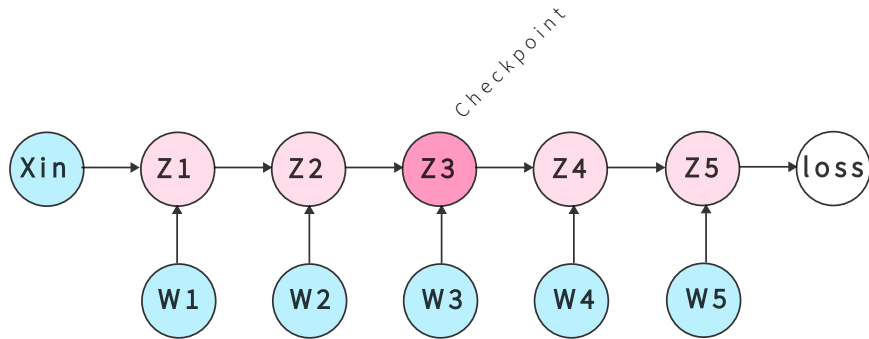
Rematerialization: forward phase



Rematerialization: forward phase

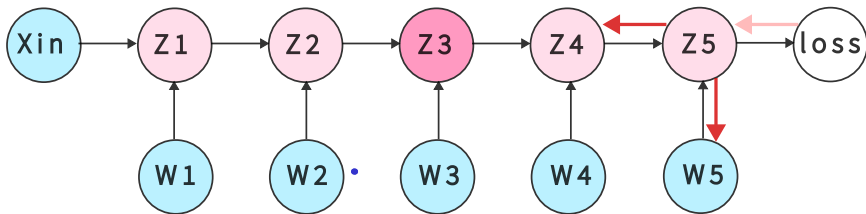


Rematerialization: forward phase



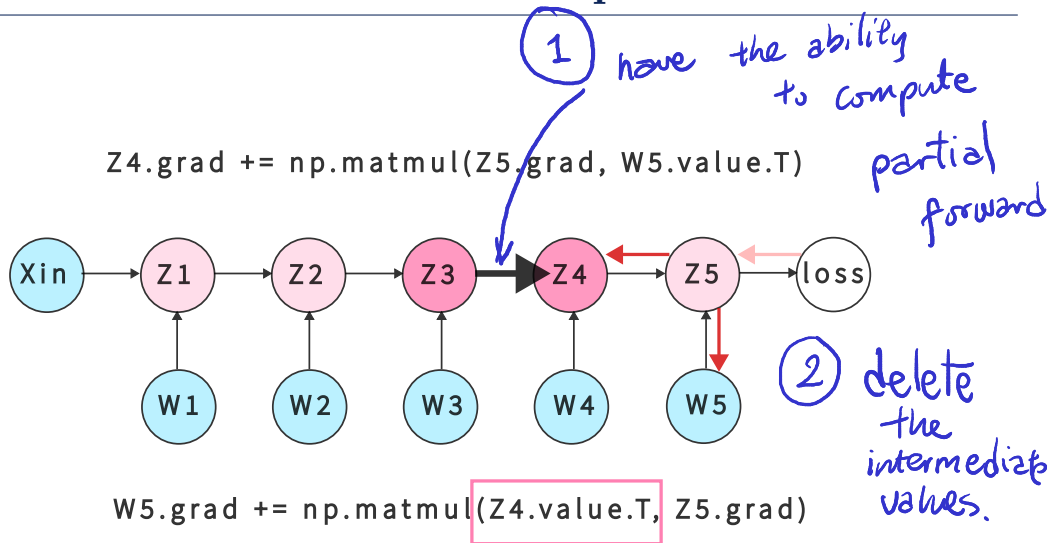
Rematerialization: backward phase

Z4.grad += np.matmul(Z5.grad, W5.value.T)



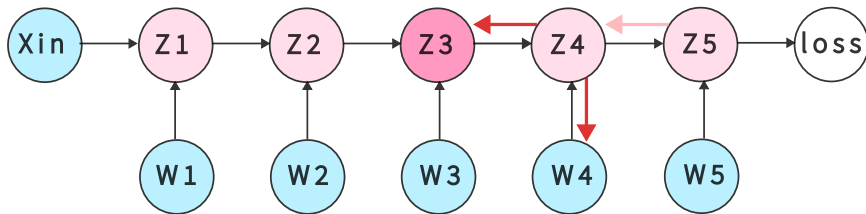
W5.grad += np.matmul(Z4.value.T, Z5.grad)

Rematerialization: backward phase



Rematerialization: backward phase

```
Z3.grad += np.matmul(Z4.grad, W4.value.T)
```



```
W4.grad += np.matmul(Z3.value.T, Z4.grad)
```


Exercise 2: rematerialization

```
1 class Tensor: # Tensor with grads
2     def __init__(self,
3                     value,
4                     requires_grad=False,
5                     rematerializer = None, # None means don't
6     rematerialize, KEEP
7     # [...]
```

partial forward

None
means
checkpoint
this tensor
no discard.

- pass information
to each node
a function to
recompute itself.

Exercise 2: rematerialization

```
1 def forward_traced_with_rematerializer(x, weights):
2     start_trace()
3     mem_usage = [] # tracing
4
5     checkpoints = [5] # these layers are checkpoints
6
7     farthest_checkpoint = 0 # this is the input data
8     x_at_farthest_checkpoint = x
9
10    for i, w in enumerate(weights): # main training loop
11        if i in checkpoints:
12            x = ag.matmul(x, w)
13            farthest_checkpoint = i
14            x_at_farthest_checkpoint = x
15 # [...]
```

Diagram and Annotations:

- A horizontal line with 10 dots represents a sequence of operations. The first dot is labeled x_{in} with a vertical line pointing to it.
- The 6th dot is circled and labeled "checkpoint" with a curved arrow pointing to it.
- Handwritten blue annotations with arrows point to specific lines in the code:
 - "rematerializer = None" points to line 12.
 - "update check" points to line 13.
 - "keep pointer alive" points to line 14.

Exercise 2: rematerialization $ag \leftrightarrow pytorch$

$numpy \leftrightarrow ATEN$

```
1  for i, w in enumerate(weights): # main training loop
2      if i in checkpoints:
3          x = ag.matmul(x, w)
4          farthest_checkpoint = i
5          x_at_farthest_checkpoint = x
6      else:
7          def _rematerializer():
8              xval = x_at_farthest_checkpoint.value
9              for w in weights[farthest_checkpoint:(i+1)]:
10                 xval = np.matmul(xval, w.value)
11             return xval
12         x = ag.matmul(x, w)
13         x.rematerializer = _rematerializer
```

not
checkpoint

do
with
plain

recipe for
reconstructing
x

numpy
to avoid
Autograd

Exercise 2: task 1: rematerialize!

```
1     def backward(self):
2         # [...]
3         for node in reversed(topo_order):
4             # YOUR CODE HERE FOR rematerializing "input.value", if
           ( it is none )
5
6         node._backward()
```

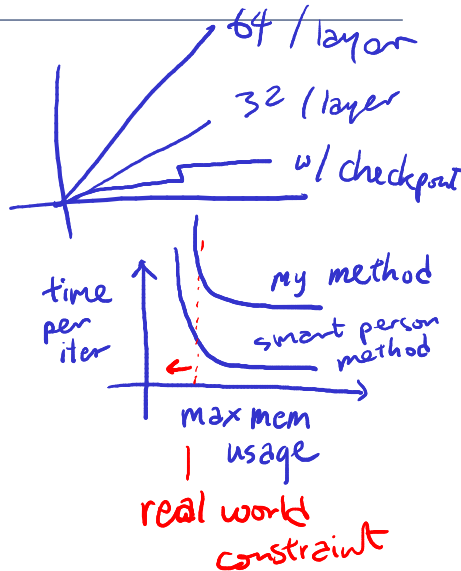
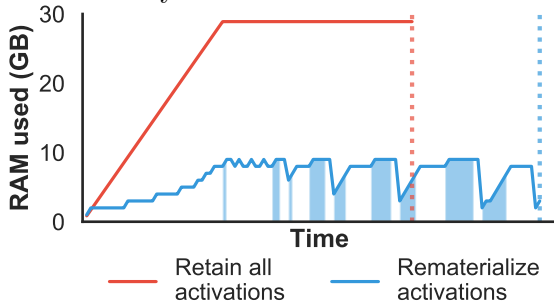
should see inputs whose values
are rematerialization

Exercise 2: task 2: discard!

```
1     def __matmul__(self, other):
2         # [...]
3         def _backward():
4             # [...]
5             self.grad += np.matmul(output.grad, other.value.T)
6             other.grad += np.matmul(self.value.T, output.grad)
7
8             # YOUR CODE HERE FOR discarding activations for "self"
and "other"
9
10            # hint: add a helper function to make it neater
11            # hint: see "discard_value_if_has_rematerializer" below
12            # [lines skipped ...]
13            return None
14
15            output._backward = _backward
16            # YOUR CODE HERE FOR discarding activations for "self" and "
other"
```

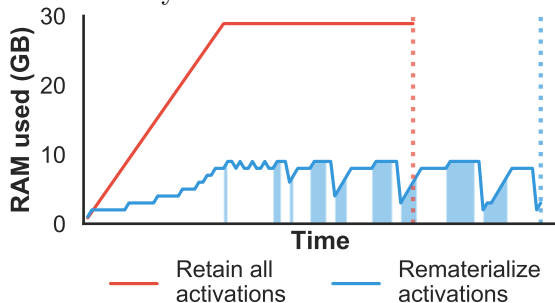
Summary

- Less memory used in the forward



Summary

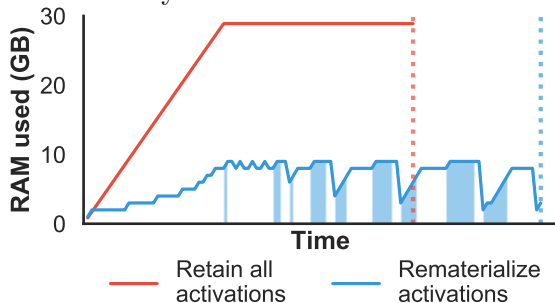
- Less memory used in the forward



- More computation (for rematerialization).
(75 matmuls w/ rematerialization vs. 30 matmuls w/o rematerialization).

Summary

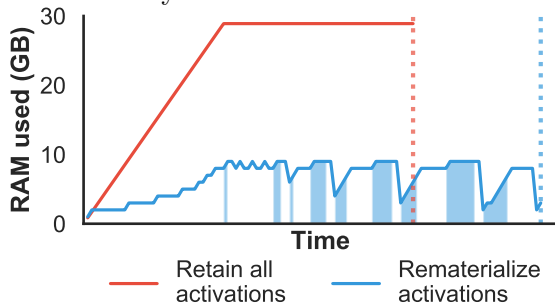
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- **Question:** what about more complicated computational graph?

Summary

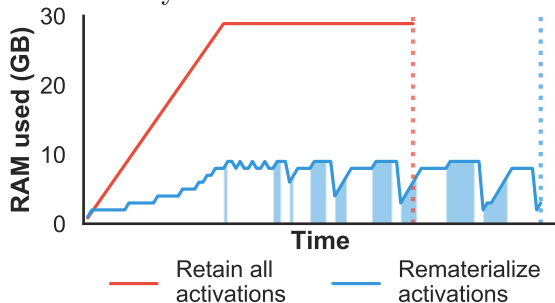
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- **Question:** what about more complicated computational graph?
- **Question:** optimal way of selecting the checkpoints?

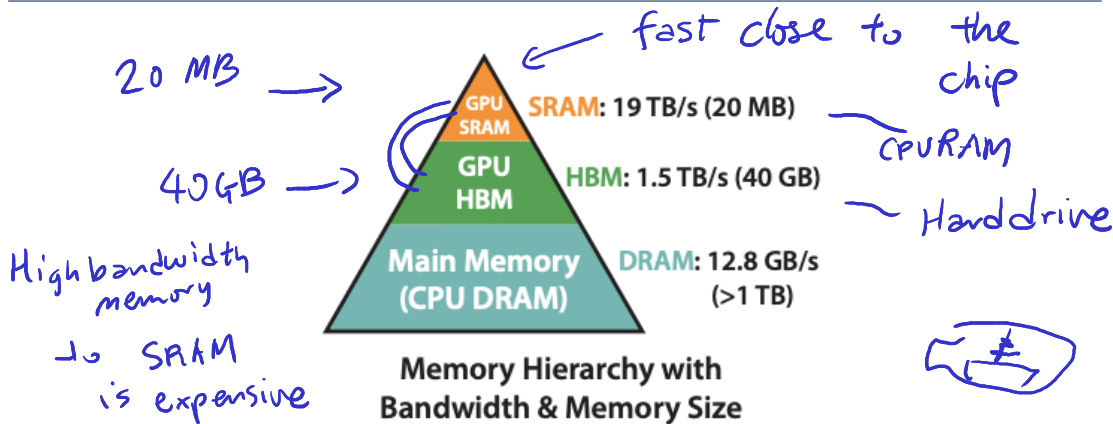
Summary

- Less memory used in the forward



- More computation (for rematerialization).
(75 matmuls w/ rematerialization vs. 30 matmuls w/o rematerialization).
- **Question:** what about more complicated computational graph?
- **Question:** optimal way of selecting the checkpoints?
- **Next:** IO and FlashAttention

Flash attention



From Dao et al. 2022 “FlashAttention: Fast and memory-efficient exact attention with io-awareness”

Self-attention

$$X = \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right] \left\{ \begin{array}{l} C \text{ context} \\ \text{Seq_len} \\ \text{leftmost dimension} \end{array} \right.$$

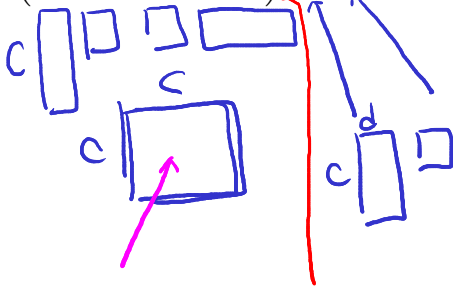
embedding

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax} \left(\mathbf{X} \mathbf{W}^{(Q)} \mathbf{W}^{(K)\top} \mathbf{X}^\top \right) \mathbf{X} \mathbf{W}^{(V)} \in \mathbb{R}^{d \times C}.$$

C = want this to be very large (more tokens)

d = (moderately large) ~ 700



Huge $1,000,000 = C \gg d = 700$

Self-attention

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax} \left(\mathbf{X} \mathbf{W}^{(Q)} \mathbf{W}^{(K)\top} \mathbf{X}^\top \right) \mathbf{X} \mathbf{W}^{(V)} \in \mathbb{R}^{d \times C}.$$

- parameters

$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

Self-attention

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- parameters

$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

- (“ Q , K , V ” stands for “query”, “key”, “value”, respectively)
where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

Self-attention

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax} \left(\mathbf{X} \mathbf{W}^{(Q)} \mathbf{W}^{(K)\top} \mathbf{X}^\top \right) \mathbf{X} \mathbf{W}^{(V)} \in \mathbb{R}^{d \times C}.$$

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$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

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where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

- “seq-2-seq”: maps the sequence \mathbf{X} to another sequence $\text{attention}(\mathbf{X}; \theta)$

$\mathbb{R}^{C \times d}$
 \downarrow
 $\mathbb{R}^{C \times d}$

Self-attention

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax}\left(\underbrace{\mathbf{X}\mathbf{W}^{(Q)}}_{\mathbf{Q}} \underbrace{\mathbf{W}^{(K)\top} \mathbf{X}^\top}_{\mathbf{K}^\top}\right) \underbrace{\mathbf{X}\mathbf{W}^{(V)}}_{\mathbf{V}} \in \mathbb{R}^{d \times C}.$$

- parameters

$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

- (“ Q, K, V ” stands for “query”, “key”, “value”, respectively)
where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

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- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax}\left(\underbrace{\mathbf{Q}\mathbf{K}^\top}_{\mathbf{S}}\right)\mathbf{V} \in \mathbb{R}^{d \times C}.$$

- parameters

$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

- (“ Q , K , V ” stands for “query”, “key”, “value”, respectively)
where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

- “seq-2-seq”: maps the sequence \mathbf{X} to another sequence $\text{attention}(\mathbf{X}; \theta)$

Self-attention

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \underbrace{\text{softmax}\left(\underbrace{\mathbf{Q}\mathbf{K}^\top}_{\mathbf{S}}\right)}_{\mathbf{P}=\text{softmax}(\mathbf{S})} \mathbf{V} \in \mathbb{R}^{d \times C}.$$

- parameters

$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

- (“ Q , K , V ” stands for “query”, “key”, “value”, respectively)
where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

- “seq-2-seq”: maps the sequence \mathbf{X} to another sequence $\text{attention}(\mathbf{X}; \theta)$



row
Stochastic

Self-attention

- Let $\mathbf{X} \in \mathbb{R}^{C \times d}$ (note everything is transposed compared to last time)

$$\text{attention}(\mathbf{X}; \theta) := \text{softmax}(\mathbf{Q}\mathbf{K}^\top) \mathbf{V} \in \mathbb{R}^{d \times C}.$$

- parameters

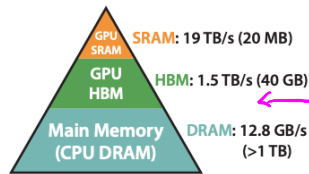
$$\theta^{(\text{att})} = [\mathbf{W}^{(Q)}, \mathbf{W}^{(K)}, \mathbf{W}^{(V)}]$$

- (“ Q , K , V ” stands for “query”, “key”, “value”, respectively)
where

$$\mathbf{W}^{(Q)} \text{ and } \mathbf{W}^{(K)} \text{ and } \mathbf{W}^{(V)} \in \mathbb{R}^{d \times d}.$$

- “seq-2-seq”: maps the sequence \mathbf{X} to another sequence $\text{attention}(\mathbf{X}; \theta)$

Flash attention



Memory Hierarchy with Bandwidth & Memory Size

small enough
loop over block

$P_{i,j}$

$C = 1,000,000$

1: Compute $S = QK^T$

2: $P = \text{softmax}(S)$

3: $O = PV$

Q, K, V

Algorithm 0 Standard Attention Implementation

Require: Matrices $Q, K, V \in \mathbb{R}^{N \times d}$ in HBM.

- 1: Load Q, K by blocks from HBM, compute $S = QK^T$, write S to HBM.
- 2: Read S from HBM, compute $P = \text{softmax}(S)$, write P to HBM.
- 3: Load P and V by blocks from HBM, compute $O = PV$, write O to HBM.
- 4: Return O .

rather move

Cd

Many read & write of C^2 sized matrix

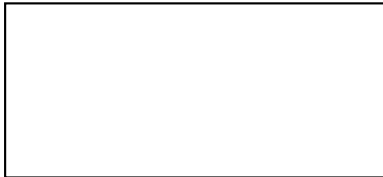
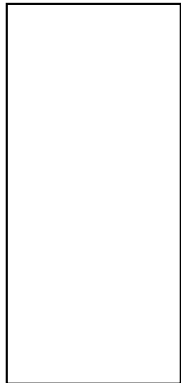
Tiling

$$d \ll C$$

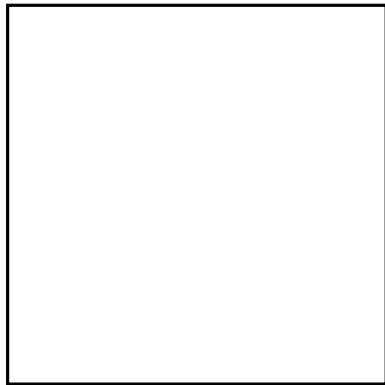
Q \downarrow

K^T

S

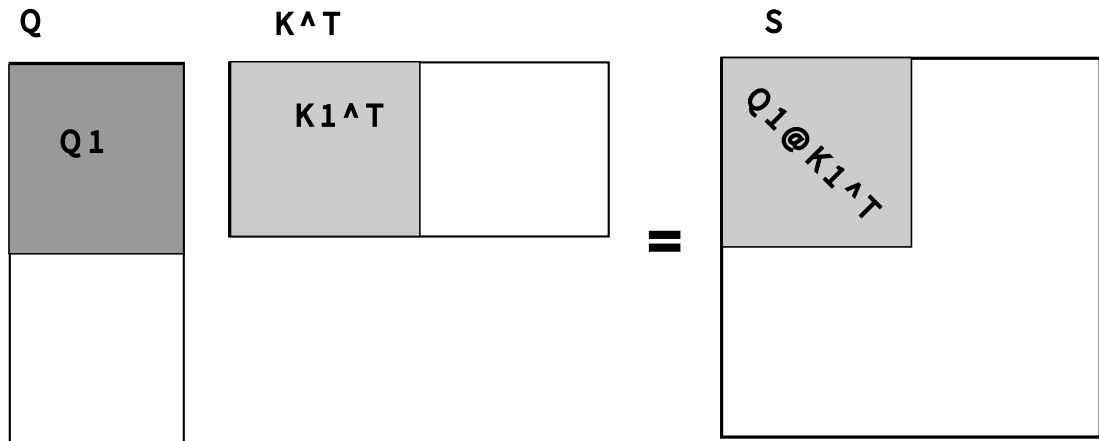


$=$

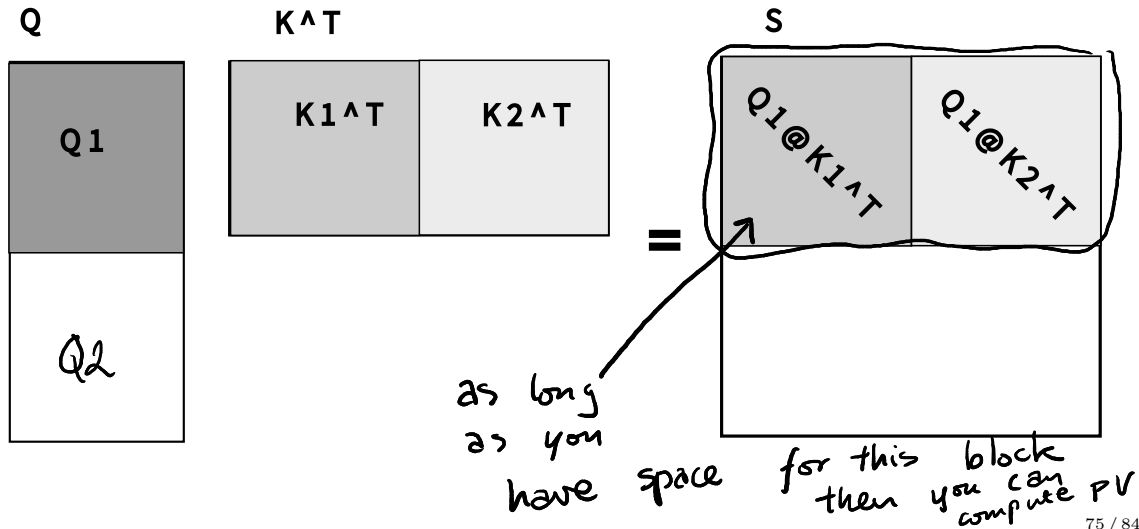


$$Q = X W^{(q)}$$

Tiling



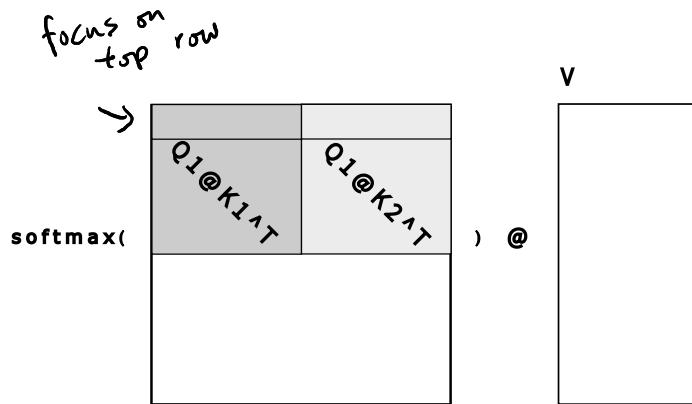
Tiling



Tiling

$$\text{softmax}\left(\begin{array}{c|c} \text{S} & \\ \hline \begin{array}{cc} Q_1 @ K_1^T & Q_1 @ K_2^T \end{array} & \\ \hline \end{array} \right) @ \begin{array}{c} \text{V} \\ \hline \end{array} = 0$$

Tiling



Online softmax

$$\text{softmax} \left(\begin{array}{c} s = \text{first row of } S \\ \boxed{s1} \quad \boxed{s2} \\ \vdots \end{array} \right) @ V$$

Online softmax

```
1 C = 100
2
3 s = np.random.rand(C)      = top row
4
5 I1 = np.arange(0, C//2)
6 I2 = np.arange(C//2, C)
7 s1 = s[I1] ← left
8 s2 = s[I2] ← right
9
10 s = np.hstack([s1,s2]) # make sure we didn't make a silly error
```

Online softmax

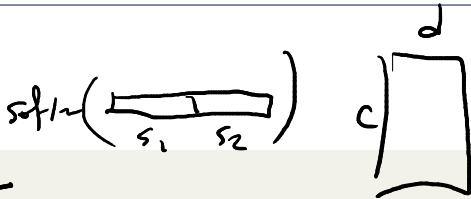
```
1 def softmax(z):  
2     expz = np.exp(z)  
3     normalizer = np.sum(expz)  
4     return expz / normalizer, normalizer
```

$$\sum \exp(s^{(\cdot)})$$

probability vector

normalizer

Online softmax



```
1 d = 3
2 np.random.seed(42)
3 V = np.random.randn(C, d) ←
4
5 p, n = softmax(s)
6 p @ V
7 # >>> array([ 0.13778369, -0.16034761,  0.04310764])
```

Online softmax

$$\boxed{\text{softmax}(s) V} \quad \textcircled{\otimes}$$

What if

```
1 # block 1
2 p1, n1 = softmax(s1)
3 0 = p1 @ V[I1,:]
4
5 # block 2
6 p2, n2 = softmax(s2)
7 0 = None # YOUR CODE HERE
8 0
```

$$\text{softmax}(s_1) @ \boxed{} V[I_1,:] = 0_1$$

$$\text{softmax}(s_2) @ \boxed{} V[I_2,:] = 0_2$$

How can we relate this back?

Online softmax

$$s = \left[\underbrace{s^1 \ s^2}_{s_1}, \underbrace{s^3 \ s^4}_{s_2} \right]$$

softmax

$$\begin{matrix} s_1 \\ \text{"} \\ [s^1 \ s^2] \end{matrix}$$

s_2

```
1 # block 1
2 p1, n1 = softmax(s1)
3 0 = p1 @ V[I1,:]
4
5 # block 2
6 p2, n2 = softmax(s2)
7 0 = None # YOUR CODE HERE
8 0
```

$$\text{softmax}(s_1) = \left(\begin{array}{c} \frac{\exp(s^1)}{\exp(s^1) + \exp(s^2)} \\ \frac{\exp(s^2)}{\exp(s^1) + \exp(s^2)} \end{array} \right)$$

$$\frac{n_1}{n_1 + n_2} = \exp(s^1) + \dots + \exp(s^4)$$

Online softmax

$$\frac{[\exp(s^{(1)}), \exp(s^{(2)})]}{n_1}$$

$$\text{softmax}(s) = \left[\frac{n_1}{(n_1 + n_2)} \text{softmax}(s_1), \right.$$

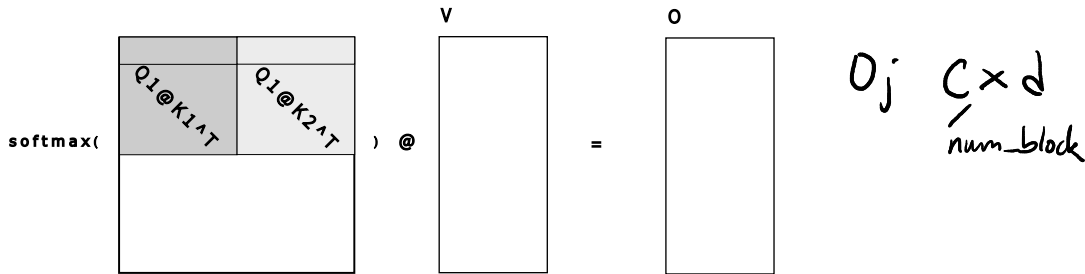
```
1 # block 1
2 p1, n1 = softmax(s1)
3 0 = p1 @ V[I1,:]
4
5 # block 2
6 p2, n2 = softmax(s2)
7 0 = None # YOUR CODE HERE
8 0
```

$$\exp(s^{(1)}) + \dots + \exp(s^{(n)})$$

1-st half

$$\frac{n_2}{n_1 + n_2} \cdot \text{softmax}(s_2) \Big]$$




Summary



- Load Q_i, K_j, V_j one block at a time
- Compute $S_{ij} = Q_i K_j^T$ ($S = QK$ usually)
- Compute $\text{softmax}(S_{ij}) V_j$
- Update O_j using online softmax

small enough you can compute on chip

References I

-  Dao, Tri, Dan Fu, Stefano Ermon, Atri Rudra, and Christopher Ré (2022). “FlashAttention: Fast and memory-efficient exact attention with io-awareness”. In: *Advances in Neural Information Processing Systems* 35, pp. 16344–16359.
-  Jain, Paras, Ajay Jain, Aniruddha Nrusimha, Amir Gholami, Pieter Abbeel, Joseph Gonzalez, Kurt Keutzer, and Ion Stoica (2020). “Checkmate: Breaking the memory wall with optimal tensor rematerialization”. In: *Proceedings of Machine Learning and Systems* 2, pp. 497–511.
-  Sohoni, Nimit S, Christopher R Aberger, Megan Leszczynski, Jian Zhang, and Christopher Ré (2019). “Low-memory neural network training: A technical report”. In: *arXiv preprint arXiv:1904.10631*.