Distributed Optimization for Machine Learning

Lecture 20 - Memory footprint of GPT and mixed precision training

ECE 5290/7290 & ORIE 5290

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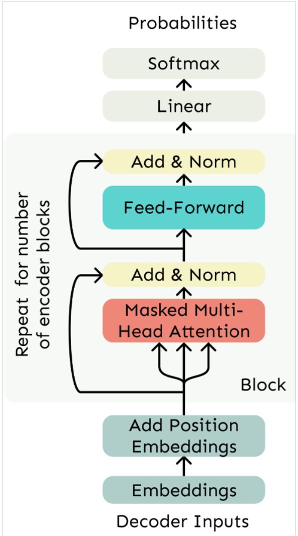
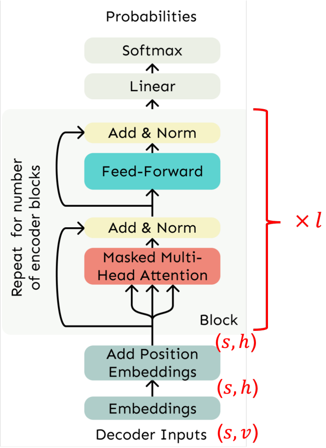
GPT: Generative pre-trained transformer

- A generative pre-trained transformer (GPT) is a type of LLMs.
- GPT is based on the decoder-only transformer.
- Each block consists of:
  - Self-attention
  - Add & Norm
  - Feed-forward
  - Add & Norm
- We will analyze the parameters, memories, and computation costs for decoder-only transformer.



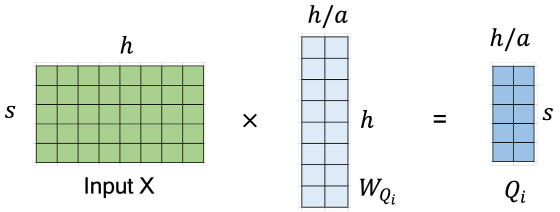
Notations for GPT

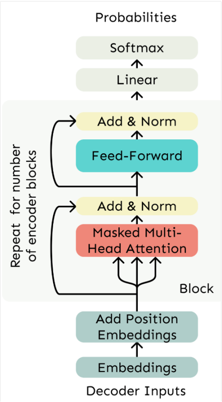
- Number of the transformer layers: ℓ
- Sequence length: s
- Vocabulary size: v
- Embedding representation dims: h



Multi-head self-attention computations

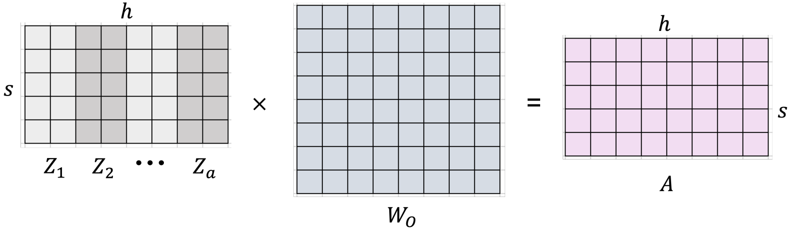
- Number of heads: a
- Dims of each W_{Q_i}, W_{K_i} and W_{V_i}: $h \times \frac{h}{a}$





Multi-head self-attention memory

- Number of heads: a
- Dims of each W_O: $h \times h$
- Dims of each W_{Q_i}, W_{K_i} and W_{V_i}: $h \times \frac{h}{a}$



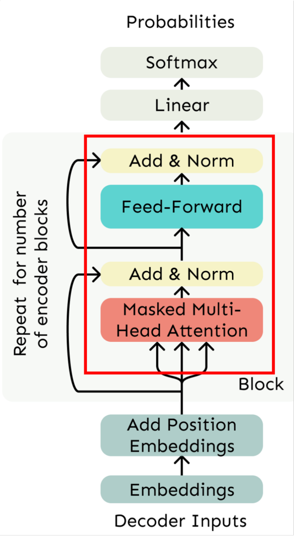
We need to store $\mathbf{W}_Q, \mathbf{W}_K, \mathbf{W}_V$ and $\mathbf{W}_O$, which is in total $4h^2$

$$3 \times \frac{h^2}{\alpha} \times \alpha = 3h^2 \quad \text{and} \quad h^2$$

Feed-forward layer memory

$$X' = \mathrm{ReLU}(A \cdot W_1 + b_1) \cdot W_2 + b_2$$

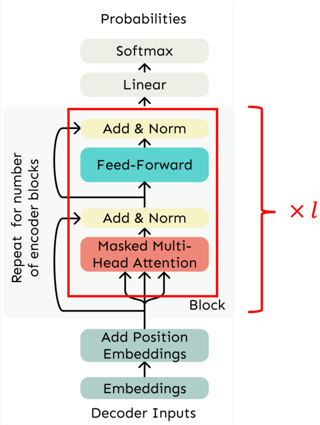
- Dims of W_1: $h \times 4h$
- Dims of each W_2: $4h \times h$
- We need to store W_1 and W_2 : $8h^2$
- The storage of b_1 and b_2 can be ignored



Transformer block memory

- Multi-head attentions: $4h^2$
- Feed-forward layers: $8h^2$
- ℓ layers of attentions:

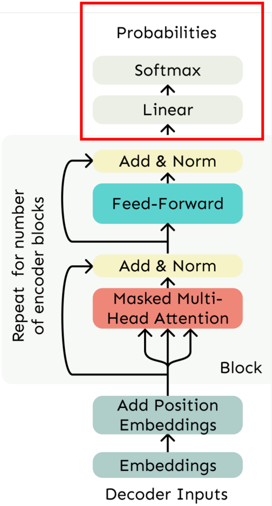
$$(4h^2 + 8h^2) \times \ell = 12\ell h^2$$



Probability predictions memory

$$p = \mathrm{Softmax}(X \cdot \mathbf{W}_V + b_v)$$

- Dimension of $\mathbf{W}_V$: $h \times v$
- We need to store $\mathbf{W}_V$: hv parameters
- b_V can be ignored

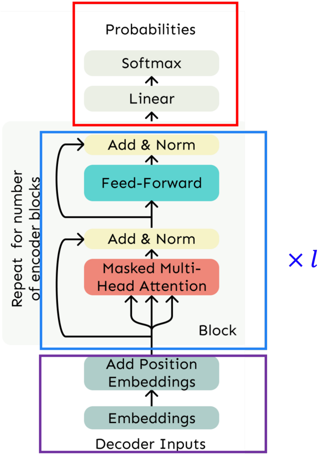


Total number of parameters in GPT

- Embeddings: vh
- Attention blocks: $12\ell h^2$
- Probability predictions: vh

Total parameters:

$$12\ell h^2 + 2vh$$



Example: LLaMA parameters

- Now we compare our theoretical evaluations with the LLaMA model.
- $12\ell h^2 + 2vh$ is a very accurate estimation.

Actual params	**Embedding h**	**Attention layers ℓ**	**Vocab size v**	**Estimated params**
6.7B	4096	32	32000	6,704,594,944
13.0B	5120	40	32000	12,910,592,000
32.5B	6656	60	32000	32,323,665,920
65.2B	8192	80	32000	64,948,797,440

Table: Comparison of actual and estimated parameters for LLaMA models

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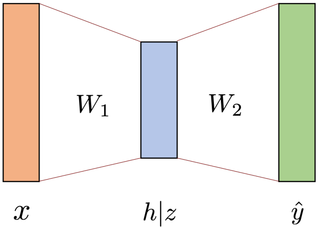
From parameters to memory usage

- We now know how to compute the **total number of parameters**:

$$N_{\text{params}} = 12\ell h^2 + 2vh$$

- But model **size alone doesn't tell the full story.**
- During training or inference, we must also consider:
  - Parameter storage (weights)
  - Optimizer states and gradients
  - Intermediate activation functions
  - KV cache for attention
- These determine the **true memory footprint** of a model.

Warmup: Linear neural network with batch gradient



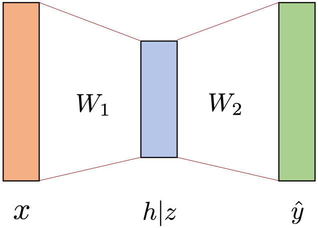
dims:	d	input dimension
	(p, d)	W_1
	p	hidden dimension
	(q, p)	W_2
	q	output dimension

Forward:

$$
\begin{aligned}
h_b &= W_1 x_b, \\
z_b &= \sigma(h_b), \\
y_b &= W_2 z_b, \\
f &= \frac{1}{B} \sum_{b=1}^{B} \mathcal{L}(y_b)
\end{aligned}
$$

Store $\{h_b, z_b, y_b\}_{b=1}^{B}$ during forward pass

Warmup: Linear neural network with batch gradient



dims:		
	d	input dimension
	(p, d)	W_1
	p	hidden dimension
	(q, p)	W_2
	q	output dimension

Backward:

$$\frac{\partial f}{\partial W_2} = \frac{1}{B}\sum_{b=1}^{B} \frac{\partial \mathcal{L}}{\partial y_b} z_b^\top,$$

$$\frac{\partial f}{\partial z_b} = W_2^\top \frac{\partial \mathcal{L}}{\partial y_b},$$

$$\frac{\partial f}{\partial h_b} = \frac{\partial f}{\partial z_b} \odot \sigma'(h_b),$$

$$\frac{\partial f}{\partial W_1} = \frac{1}{B}\sum_{b=1}^{B} \frac{\partial f}{\partial h_b} x_b^\top$$

Store $\nabla_{W_1} f(W_1)$ and $\nabla_{W_2} f(W_2)$ during backward pass

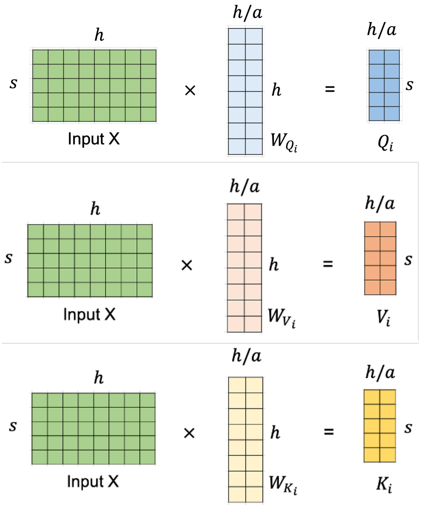
Memory decomposition of training LLMs

$$\textbf{Memory} = \underbrace{\text{Model}}_{\text{weights}} + \underbrace{\text{Gradients}}_{\text{backprop}} + \underbrace{\text{Optimizer States}}_{\text{e.g., Adam m,v}} + \underbrace{\text{Activations}}_{\text{forward/backward pass}}$$

Model Parameters P	Gradients P	Optimizer States $2P$	Activations (?)

Typical memory usage breakdown in training large models.

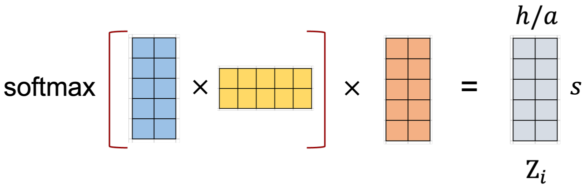
Activations in multi-head self-attention



Store α copies of $\mathbf{Q}_i$, $\mathbf{K}_i$, and $\mathbf{V}_i$

$$3 \times \frac{sh}{\alpha} \times \alpha = 3sh$$

Activations in multi-head self-attention



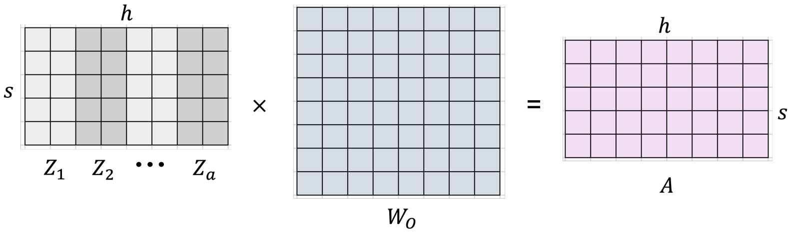
- Given $\mathbf{Q}_i$, $\mathbf{K}_i$, and $\mathbf{V}_i \in \mathbb{R}^{s \times h/\alpha}$, one head self-attention is

$$\mathrm{Attn}(\mathbf{Q}_i, \mathbf{K}_i, \mathbf{V}_i) \;=\; \mathrm{softmax}\left(\frac{\mathbf{Q}_i \mathbf{K}_i^\top}{\sqrt{h/a}}\right) \mathbf{V}_i$$

- Store $\mathbf{Q}_i \mathbf{K}_i^\top$ with s^2 parameters;
- Store $\mathrm{softmax}(\mathbf{Q}_i \mathbf{K}_i^\top)$ with s^2 parameters;
- Store $\mathrm{softmax}\left(\frac{\mathbf{Q}_i \mathbf{K}_i^\top}{\sqrt{h/a}}\right) \mathbf{V}_i$ with sh/a parameters;

Activations in multi-head self-attention

- Number of heads: a
- Dims of each W_O: $h \times h$
- Dims of each W_{Q_i}, W_{K_i} and W_{V_i}: $h \times \frac{h}{a}$

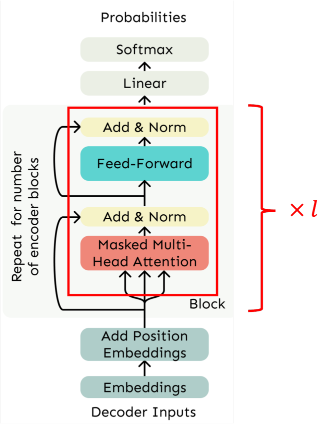


We need to store **A**, which is in total *sh*

Activations in Transformer block

- Multi-head attentions: $5sh + 2s^2a$
- Feed-forward layers: $9sh$
- ℓ layers of attentions:

$$(2s^2a + 14sh) \times \ell$$

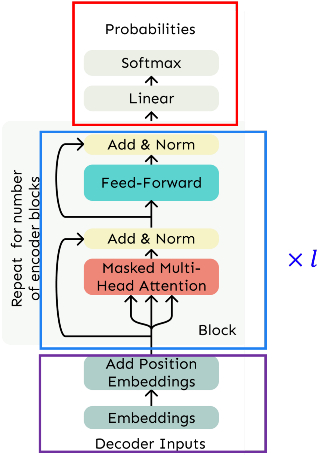


Total number of activations in GPT

- Number of the transformer layers: ℓ
- Sequence length: s
- Embedding representation dims: h
- Embedding activations: sh
- Self-attention activations: $(2s^2\alpha + 14sh) \times \ell$
- Probability activations: $2sv$

Total parameters with batch size b:

$$(2s^2a + 14sh) \times \ell \times b$$



Total memory of training LLMs

$$\textbf{Memory} = \underbrace{\text{Model}}_{\text{weights}} + \underbrace{\text{Gradients}}_{\text{backprop}} + \underbrace{\text{Optimizer States}}_{\text{e.g., Adam m,v}} + \underbrace{\text{Activations}}_{\text{forward/backward pass}}$$

Model Parameters P	Gradients P	Optimizer States $2P$	Activations (?)

$$\left(48\ell h^2 \quad + \quad b\ell(2s^2a + 14sh)\right) \quad \times \quad 4 \text{ Bytes (32 bits)}$$

- When hidden state h is large, the model dominates the memory
- If batch-size b or sequence length s is large, the activation dominates
- The activation-incurred memory cannot be ignored

Memory estimation for GPT-3

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

- GPT-3 has 175B parameters; its model consumes

$$4 \times 175 \times 10^9 \text{ Bytes} = 700\,\text{GB}$$

- Its gradients take 700 GB; optimizer states take 1.4 TB.
- GPT has sequence length $s = 2048$. When $b = 1$, its activation takes 444 GB (63% of the model).
- When $b = 128$, its activation is 81 times the model size.

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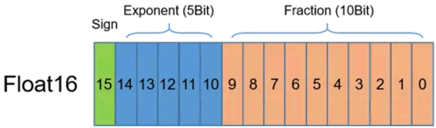
Memory analysis of GPT

Mixed precision training

Full precision training and low precision training

- Full precision training (e.g., FP32)
  - each parameter takes 4 Bytes
  - used in training most DNNs; very precise
  - takes a lot of computations and memories
- Low precision training (e.g., FP16)
  - each parameter takes 2 Bytes
  - train larger models due to computational and memory efficiency
  - not precise enough; overflow and underflow occur occasionally

Float 16 (FP16) precision



- **Sign**: 1 bit; 0 for positive and 1 for negative
- **Exponent**: 5 bits; range: 00001(1)-11110(30); value: $2^{-14} \sim 2^{15}$

$$\text{Example:} \quad 00111(7) \quad \longrightarrow \quad 2^{7-15} = 2^{-8}$$

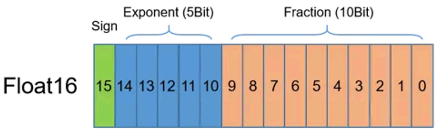
where -15 is the offset

- **Fraction**: 10 bits;

$$\begin{aligned} \text{Example:} \quad 1001000000 \quad &\longrightarrow \quad 1.1001000000 \\ &\longrightarrow \quad 1 + 576/1024 = 1.5625 \end{aligned}$$

where binary 1001000000 translates into decimal 576

Float 16 (FP16) precision



- **Translation law**

$$(-1)^{\text{sign}} \times 2^{\text{exponent}-15} \times (1 + \frac{\text{fraction}}{1024})$$

- **Largest positive number**:

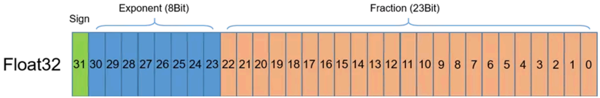
$$(-1)^0 \times 2^{15} \times (1 + \frac{1023}{1024}) = 65504$$

The range of FP16 is $[-65504, +65504]$.

- **Smallest positive number**:

$$(-1)^0 \times 2^{-14} \times (0 + \frac{1}{1024}) \approx 2^{-24}$$

Float 32 (FP32) precision



- **Sign**: 1 bit; 0 for positive and 1 for negative
- **Exponent**: 8 bits; range: 00000001(1) - 11111110(254);
  Bias: 127, hence the exponent value is $2^{-126} \sim 2^{127}$.

$$\text{Example:} \quad 01111111(127) \quad \longrightarrow \quad 2^{127-127} = 2^0 = 1$$

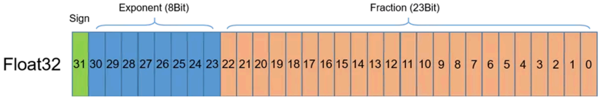
- **Fraction**: 23 bits;

$$\text{Example:} \quad 10010000000000000000000 \quad \rightarrow \quad 1.10010000000000000000000$$

$$\rightarrow \quad 1 + \frac{10010000000000000000000}{2^{23}} = 1 + \frac{4718592}{8388608} = 1.5625$$

where binary 10010000000000000000000 translates into 4718592.

Float 32 (FP32) precision



- **Translation law**

$$(-1)^{\text{sign}} \times 2^{\text{exponent}-127} \times (1 + \frac{\text{fraction}}{2^{23}})$$

- **Range**: $[-3.40282 \times 10^{38}, +3.40282 \times 10^{38}]$

- **Smallest positive number**: 1.17549×10^{-38}

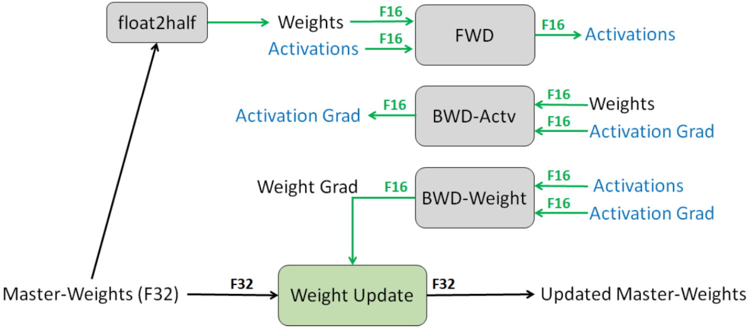
- FP 32 is much more powerful than FP 16; but takes more memory

Mixed precision training

- When both FP32 and FP16 are used in training, we get **Mixed precision training**; see (`micikevicius2017mixed`)
- Save memory and computations without hurting performance
- Three key techniques:
  - FP32 weight copies
  - Loss scaling
  - Arithmetic precision

Technique I - FP32 weight copies

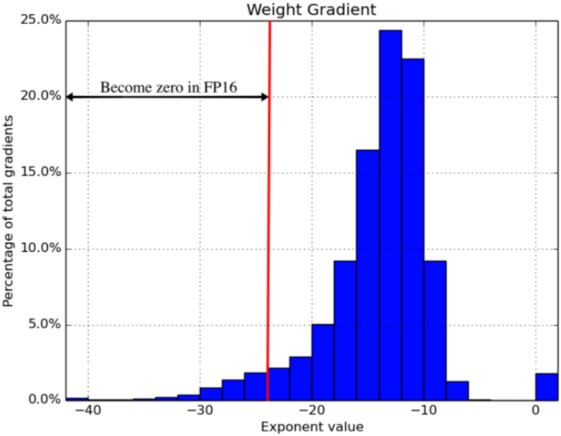
- An FP32 weight copy is maintained and updated with gradient



Technique I - FP32 weight copies

- Reason I: **maintain small values in the weight update**
- Weight update = learning rate $\times$ gradient; typically very small in late phase
- Values less than $2^{-24} \approx 5.96 \times 10^{-8}$ become 0 when using FP16
- About 5% values are less than 2^{-24}

FP32 weight copies



Technique I - FP32 weight copies

- Reason II: **big value-to-update ratio**
- The resolution in each period is shown as follows[1]

Min	Max	interval
0	2^{-13}	2^{-24}
2^{-13}	2^{-12}	2^{-23}
2^{-12}	2^{-11}	2^{-22}
2^{-11}	2^{-10}	2^{-21}
2^{-10}	2^{-9}	2^{-20}
2^{-9}	2^{-8}	2^{-19}
2^{-8}	2^{-7}	2^{-18}
2^{-7}	2^{-6}	2^{-17}
2^{-6}	2^{-5}	2^{-16}
2^{-5}	2^{-4}	2^{-15}
2^{-4}	$\frac{1}{8}$	2^{-14}
$\frac{1}{8}$	$\frac{1}{4}$	2^{-13}
$\frac{1}{4}$	$\frac{1}{2}$	2^{-12}
$\frac{1}{2}$	1	2^{-11}
1	2	2^{-10}
2	4	2^{-9}
4	8	2^{-8}
8	16	2^{-7}
16	32	2^{-6}
32	64	2^{-5}
64	128	2^{-4}
128	256	$\frac{1}{8}$
256	512	$\frac{1}{4}$
512	1024	$\frac{1}{2}$
1024	2048	1
2048	4096	2
4096	8192	4
8192	16384	8
16384	32768	16
32768	65519	32
65519	∞	∞

[1]This figure is from wikipedia

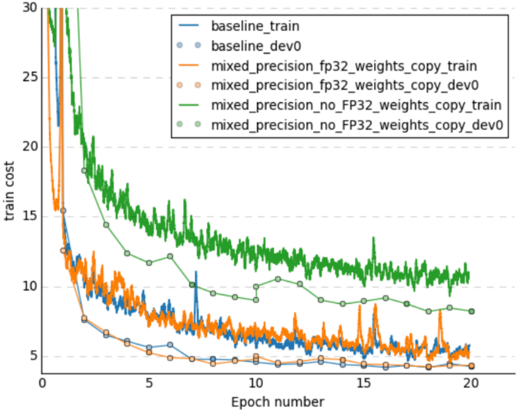
Technique I - FP32 weight copies

- If the value-to-update ratio is bigger than $2^{11} = 2048$, it holds that

$$\text{value} + \text{update} = \text{value}$$

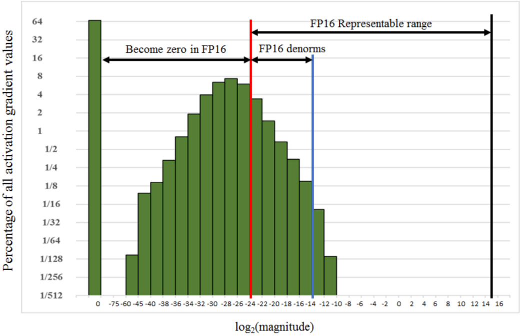
- The update has no influence on the value
- For reasons I and II, we maintain FP32 copies for both the weight and weight decay

Technique I - FP32 weight copies



Technique II - Loss scaling

- FP16 representation range $[2^{-24}, 2^{15}]$
- The activation gradient is typically very small; most values are smaller than 2^{-24}



Technique II - Loss scaling

- Scale-up the loss value before the back-propagation
- Unscale the gradient after back-propagation but before the update

$$g(x) = \frac{\partial L}{\partial x} = \frac{1}{c}\frac{\partial (c \cdot L)}{\partial x}$$

- Effectively shift the gradient value to the FP representation range
- Tricky to choose the scale-up coefficient
- $c = 8$ typically works

Technique II - Loss scaling

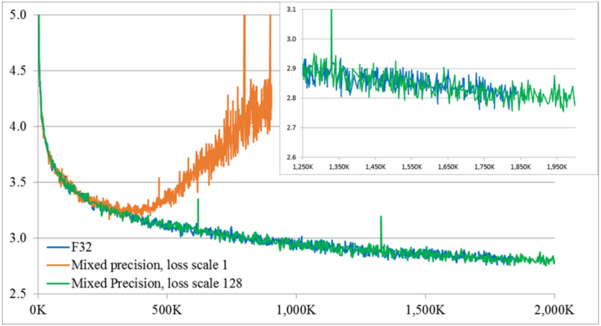


Figure: bigLSTM training perplexity.

- Mixed-precision training with loss scale 128 (green) closely matches full-precision (F32, blue) performance.
- Without appropriate loss scaling (loss scale 1, orange), training diverges due to numerical underflow in gradients.

Technique III - Arithmetic precision

- Not as important as the above two techniques
- Three key computation steps: vector dot-products; reductions; point-wise operations
- It is suggested in (`micikevicius2017mixed`) that vector dot-products and reductions are read and written in FP16 but carried out in FP32
- Point-wise operations can be carried in FP16

Numerical studies

Table 1: ILSVRC12 classification top-1 accuracy.

Model	Baseline	Mixed Precision	Reference
AlexNet	56.77%	56.93%	(Krizhevsky et al., 2012)
VGG-D	65.40%	65.43%	(Simonyan and Zisserman, 2014)
GoogLeNet (Inception v1)	68.33%	68.43%	(Szegedy et al., 2015)
Inception v2	70.03%	70.02%	(Ioffe and Szegedy, 2015)
Inception v3	73.85%	74.13%	(Szegedy et al., 2016)
Resnet50	75.92%	76.04%	(He et al., 2016b)

Table 2: Detection network average mean precision.

Model	Baseline	MP without loss-scale	MP with loss-scale
Faster R-CNN	69.1%	68.6%	69.7%
Multibox SSD	76.9%	diverges	77.1%

- Across various architectures, **mixed precision training** achieves accuracy comparable to or slightly higher than full precision.
- For detection networks, **loss scaling is essential** — without it, training may diverge (e.g., Multibox SSD).

Nvidia AMP[2]

AMP FOR PYTORCH

As simple as two lines of code

Wrap the model and optimizer

```
model, optimizer = amp.initialize(model, optimizer)
```

Apply automatic loss scaling and backpropagate with scaled loss

```
with amp.scaled_loss(loss, optimizer) as scaled_loss:
    scaled_loss.backward()
```

[2] https://nvlabs.github.io/iccv2019-mixed-precision-tutorial/

Nvidia AMP[3]: An example

```
import torch
import amp
model = ...
optimizer = ...
model, optimizer = amp.initialize(model, optimizer, opt_level="O1")
for data, label in data_iter:
    out = model(data)
    loss = criterion(out, label)
    optimizer.zero_grad()
    with amp.scaled_loss(loss, optimizer) as scaled_loss:
        scaled_loss.backward()
optimizer.step()
```

allows AMP to perform automatic casting

replaces `loss.backward()`

[3] https://nvlabs.github.io/iccv2019-mixed-precision-tutorial/

Case study: Mixed-precision Adam

- Adam is an optimization method widely-used in training LLMs
- Adam states use $33\% \sim 75\%$ memories
- For example, Adam states use 11GB for GPT2 and 41GB for T5
- It is urgent to reduce the memory footprint caused by Adam states

Case study: 8-bit Adam optimizer

- Recall the Adam optimizer

$$
\begin{aligned}
g_k &= \nabla F(x_k; \xi_k) \\
m_k &= \beta_1 m_{k-1} + (1-\beta_1) g_k \\
s_k &= \beta_2 s_{k-1} + (1-\beta_2) g_k \odot g_k \\
x_{k+1} &= x_k - \frac{\gamma}{\sqrt{s_k} + \epsilon} \odot m_k
\end{aligned}
$$

- 8-bit only supports $2^8 = 256$ values; much less than FP16 and FP32

- (`dettmers2021`) develops 8-bit Adam optimizer with block-wise quantization and dynamic quantization

8-bit optimizer procedure

- Quantize and store Adam states with 8 bit
- When updating and using state, dequantize it to FP32, update the weight, and quantize back to 8 bit
- 8-bit to 32-bit conversion element-by-element in registers; no additional temporary memory

Performance for common benchmarks

Optimizer	Task	Data	Model	Metric†	Time	Mem saved
32-bit AdamW	GLUE	Multiple	RoBERTa-Large	88.9	–	Reference
32-bit AdamW	GLUE	Multiple	RoBERTa-Large	88.6	17h	0.0 GB
32-bit Adafactor	GLUE	Multiple	RoBERTa-Large	**88.7**	24h	1.3 GB
8-bit AdamW	GLUE	Multiple	RoBERTa-Large	**88.7**	**15h**	**2.0 GB**
32-bit Momentum	CLS	ImageNet-1k	ResNet-50	77.1	–	Reference
32-bit Momentum	CLS	ImageNet-1k	ResNet-50	77.1	118h	0.0 GB
8-bit Momentum	CLS	ImageNet-1k	ResNet-50	**77.2**	**116 h**	**0.1 GB**
32-bit Adam	MT	WMT'14+16	Transformer	29.3	–	Reference
32-bit Adam	MT	WMT'14+16	Transformer	29.0	126h	0.0 GB
32-bit Adafactor	MT	WMT'14+16	Transformer	29.0	127h	0.3 GB
8-bit Adam	MT	WMT'14+16	Transformer	**29.1**	**115h**	**1.1 GB**
32-bit Momentum	MoCo v2	ImageNet-1k	ResNet-50	67.5	–	Reference
32-bit Momentum	MoCo v2	ImageNet-1k	ResNet-50	67.3	30 days	0.0 GB
8-bit Momentum	MoCo v2	ImageNet-1k	ResNet-50	**67.4**	**28 days**	**0.1 GB**
32-bit Adam	LM	Multiple	Transformer-1.5B	9.0	308 days	0.0 GB
32-bit Adafactor	LM	Multiple	Transformer-1.5B	**8.9**	316 days	5.6 GB
8-bit Adam	LM	Multiple	Transformer-1.5B	9.0	**297 days**	**8.5 GB**
32-bit Adam	LM	Multiple	GPT3-Medium	10.62	795 days	0.0 GB
32-bit Adafactor	LM	Multiple	GPT3-Medium	10.68	816 days	1.5 GB
8-bit Adam	LM	Multiple	GPT3-Medium	**10.62**	**761 days**	**1.7 GB**
32-bit Adam	Masked-LM	Multiple	RoBERTa-Base	3.49	101 days	0.0 GB
32-bit Adafactor	Masked-LM	Multiple	RoBERTa-Base	3.59	112 days	0.7 GB
8-bit Adam	Masked-LM	Multiple	RoBERTa-Base	**3.48**	**94 days**	**1.1 GB**

†**Metric**: GLUE=Mean Accuracy/Correlation. CLS/MoCo = Accuracy. MT=BLEU. LM=Perplexity.

Enable training larger models

	Largest finetunable Model (parameters)	
GPU size in GB	32-bit Adam	8-bit Adam
6	RoBERTa-base (110M)	RoBERTa-large (355M)
11	MT5-small (300M)	MT5-base (580M)
24	MT5-base (580M)	MT5-large (1.2B)
24	GPT-2-medium (762M)	GPT-2-large (1.5B)

- **Observation:** Using 8-bit Adam enables fine-tuning of models up to **three times larger** on the same GPU memory.
- This highlights the **scalability benefits of memory-efficient optimizers**, allowing larger models to be trained on same hardware.

Recap and fine-tuning

- What we have talked about today?
  - ⇒ What is the number of parameters in GPTs?
  - ⇒ What is the memory complexity in GPTs
  - ⇒ How to perform memory-efficient training of GPTs?

Welcome anonymous survey!