

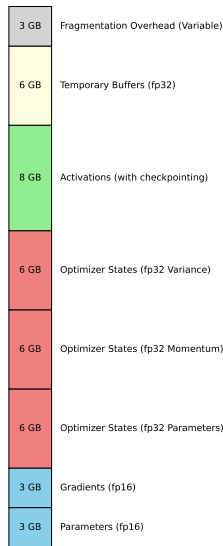
Large models training

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University



GPT-2 training Memory footprint



Example: 1.5B parameter GPT-2 model needs 3GB for weights in 16-bit precision but can't be trained on a 32GB GPU using Tensorflow or PyTorch. Major memory usage during training includes optimizer states, gradients, parameters, activations, temporary buffers, and fragmented memory.

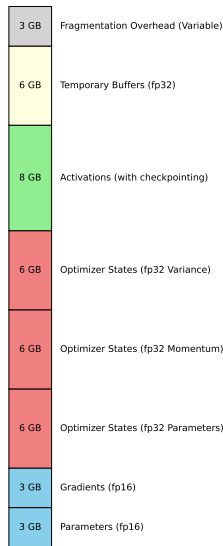
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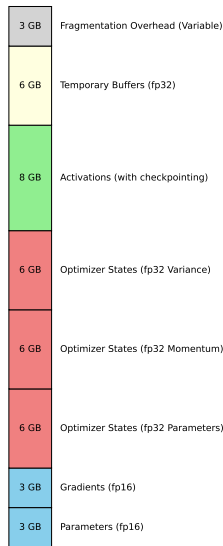
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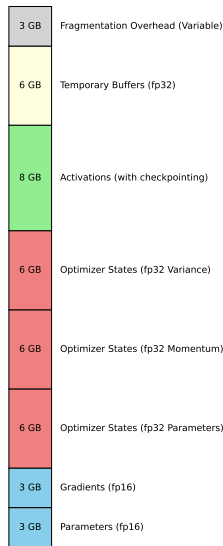
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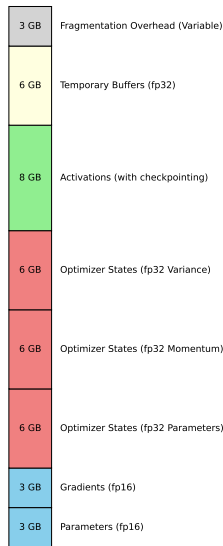
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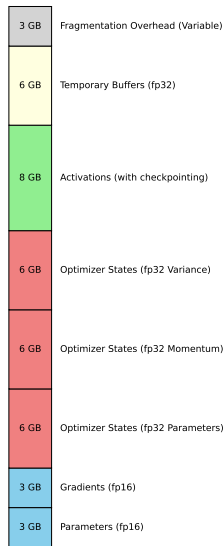
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- Activation checkpointing can reduce activation memory by about 50%, with a 33% recomputation overhead.

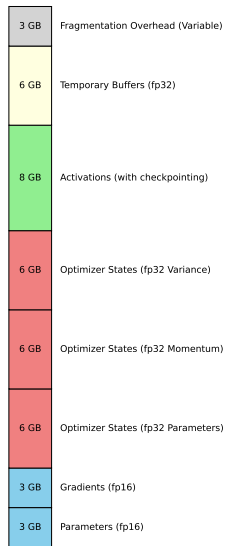
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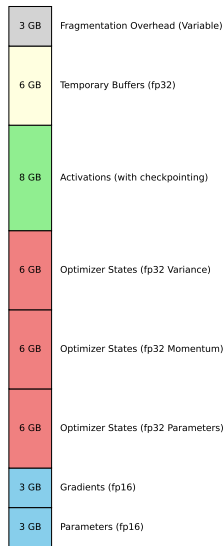
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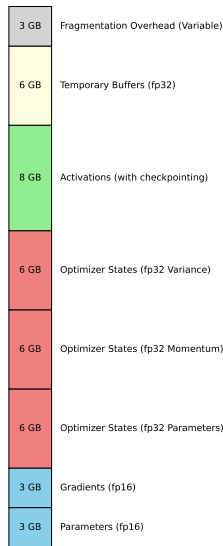
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- Store intermediate results; e.g., gradient all-reduce operations fuse gradients into a single buffer.
- For large models, temporary buffers can consume substantial memory (e.g., 6GB for 1.5B parameter model with fp32 buffer).

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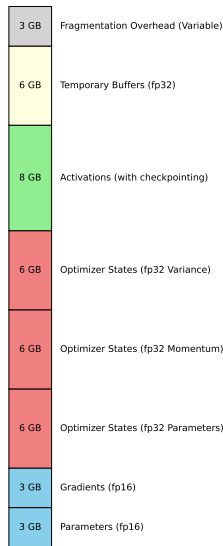
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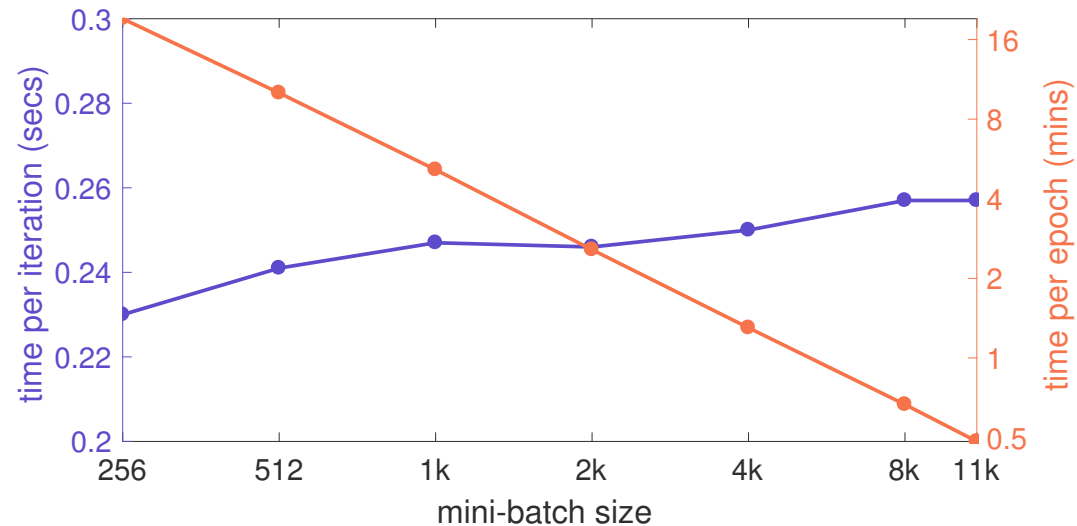
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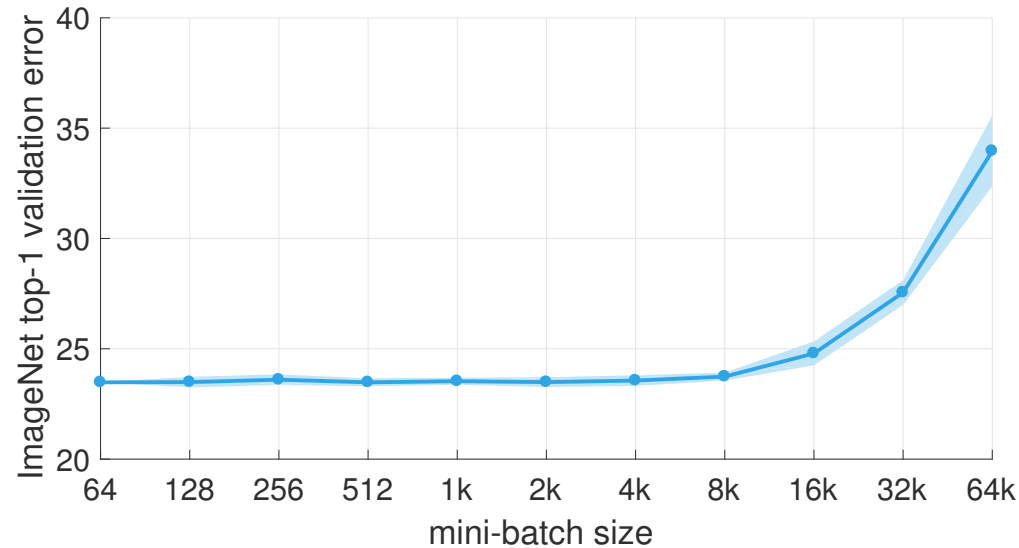
- Memory fragmentation can cause out-of-memory issues despite available memory, as contiguous blocks are required.
- In some cases, over 30% of memory remains unusable due to fragmentation.

Large batch training ¹



¹Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Large batch training ²



²Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Large batch training ³

Effective batch size (kn)	α	top-1 error (%)
256	0.05	23.92 ± 0.10
256	0.10	23.60 ± 0.12
256	0.20	23.68 ± 0.09
8k	$0.05 \cdot 32$	24.27 ± 0.08
8k	$0.10 \cdot 32$	23.74 ± 0.09
8k	$0.20 \cdot 32$	24.05 ± 0.18
8k	0.10	41.67 ± 0.10
8k	$0.10 \cdot \sqrt{32}$	26.22 ± 0.03

Comparison of learning rate scaling rules. ResNet-50 trained on ImageNet. A reference learning rate of $\alpha = 0.1$ works best for $kn = 256$ (23.68% error). The linear scaling rule suggests $\alpha = 0.1 \cdot 32$ when $kn = 8k$, which again gives best performance (23.74% error). Other ways of scaling α give worse results.

³Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Linear and square root scaling rules

When training with large batches, the learning rate must be adjusted to maintain convergence speed and stability. The **linear scaling rule**⁴ suggests multiplying the learning rate by the same factor as the increase in batch size:

$$\alpha_{\text{new}} = \alpha_{\text{base}} \cdot \frac{\text{Batch Size}_{\text{new}}}{\text{Batch Size}_{\text{base}}}$$

The **square root scaling rule**⁵ proposes scaling the learning rate with the square root of the batch size increase:

$$\alpha_{\text{new}} = \alpha_{\text{base}} \cdot \sqrt{\frac{\text{Batch Size}_{\text{new}}}{\text{Batch Size}_{\text{base}}}}$$

Authors claimed, that it suits for adaptive optimizers like Adam, RMSProp and etc. while linear scaling rule serves well for SGD.

⁴Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

⁵Learning Rates as a Function of Batch Size: A Random Matrix Theory Approach to Neural Network Training

Gradual warmup⁶

Gradual warmup helps to avoid instability when starting with large learning rates by slowly increasing the learning rate from a small value to the target value over a few epochs. This is defined as:

$$\alpha_t = \alpha_{\max} \cdot \frac{t}{T_w}$$

where t is the current iteration and T_w is the warmup duration in iterations. In the original paper, authors used first 5 epochs for gradual warmup.

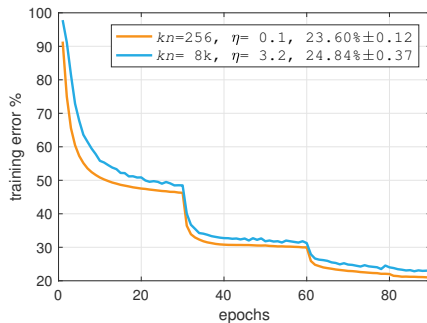


Figure 1: no warmup

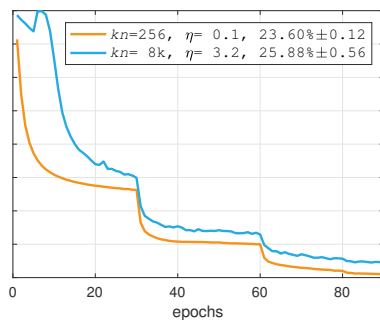


Figure 2: constant warmup

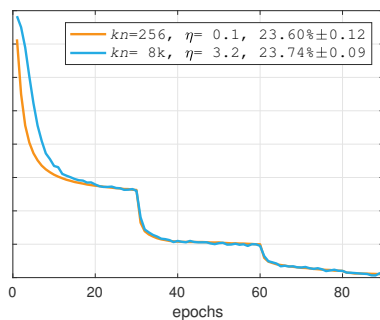


Figure 3: gradual warmup

⁶Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Gradient accumulation

Gradient accumulation allows the effective batch size to be increased without requiring larger memory by accumulating gradients over several mini-batches:

Without gradient accumulation

```
for i, (inputs, targets) in enumerate(data):
    outputs = model(inputs)
    loss = criterion(outputs, targets)
    loss.backward()

    optimizer.step()
    optimizer.zero_grad()
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    optimizer.step()  
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```

With gradient accumulation

```
for i, (inputs, targets) in enumerate(data):  
    outputs = model(inputs)  
    loss = criterion(outputs, targets)  
    loss.backward()  
    if (i+1) % accumulation_steps == 0:  
        optimizer.step()  
        optimizer.zero_grad()
```

Data Parallel training

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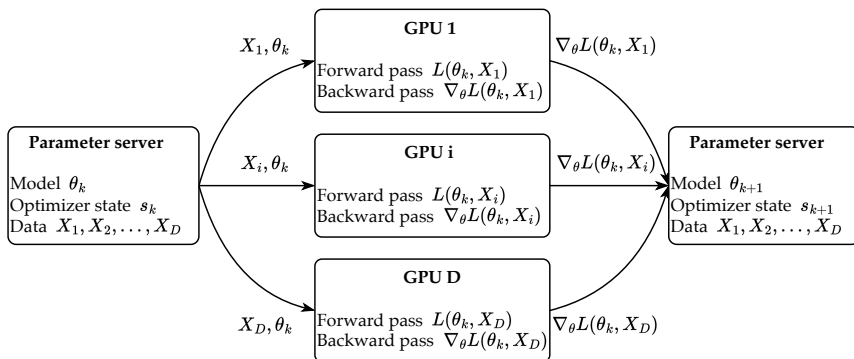
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Per device batch size: b . Overall batchsize: Db . Data parallelism involves splitting the data across multiple GPUs, each with a copy of the model. Gradients are averaged and weights updated synchronously:



Distributed Data Parallel training

Distributed Data Parallel (DDP) ⁷ extends data parallelism across multiple nodes. Each node computes gradients locally, then synchronizes with others. Below one can find differences from the PyTorch site. This is used by default in 🐍Accelerate library.

DataParallel	DistributedDataParallel
More overhead; model is replicated and destroyed at each forward pass	Model is replicated only once
Only supports single-node parallelism	Supports scaling to multiple machines
Slower; uses multithreading on a single process and runs into Global Interpreter Lock (GIL) contention	Faster (no GIL contention) because it uses multiprocessing

⁷Getting Started with Distributed Data Parallel

Naive model parallelism

Model parallelism divides the model across multiple GPUs. Each GPU handles a subset of the model layers, reducing memory load per GPU. Allows to work with the models, that won't fit in the single GPU. Poor resource utilization.

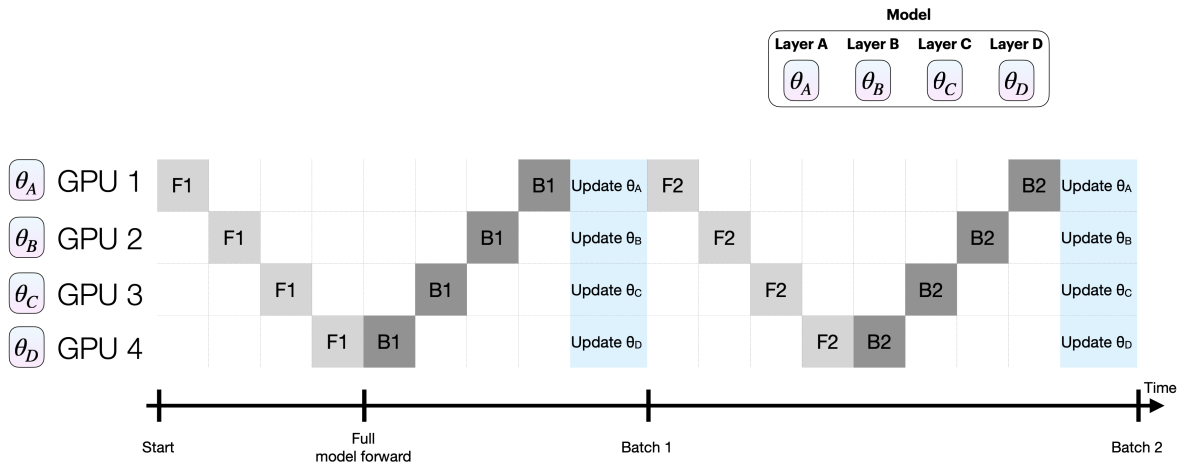
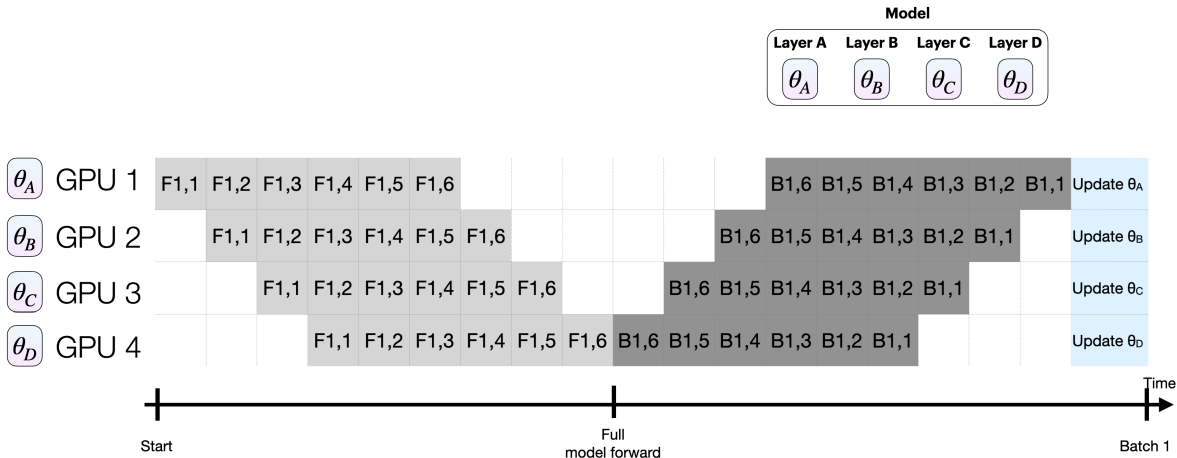


Figure 5: Model parallelism

Pipeline model parallelism (GPipe) ⁸

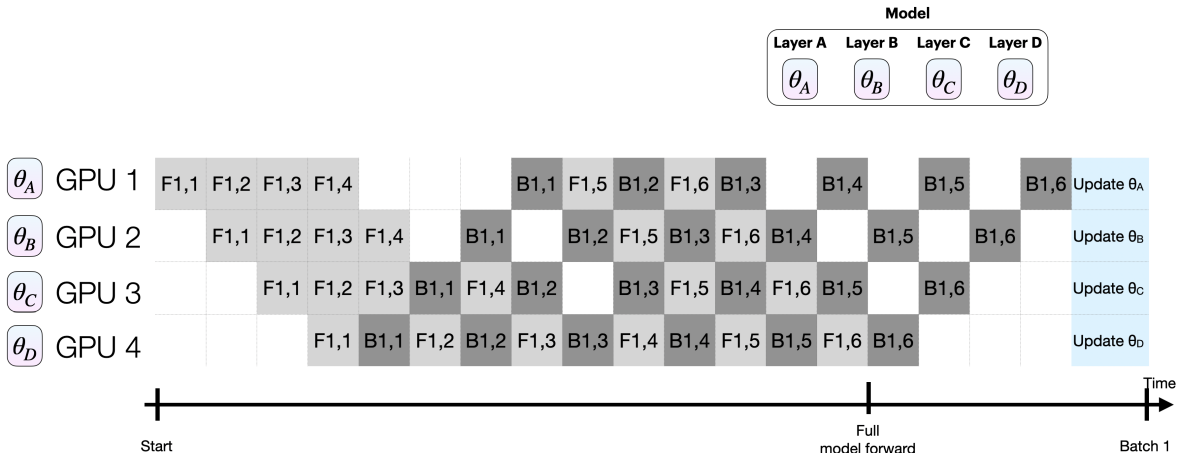
GPipe splits the model into stages, each processed sequentially. Micro-batches are passed through the pipeline, allowing for overlapping computation and communication:



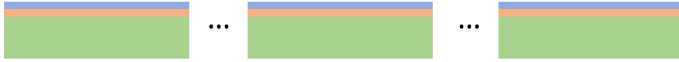



⁸GPipe: Efficient Training of Giant Neural Networks using Pipeline Parallelism

Pipeline model parallelism (PipeDream) ⁹

PipeDream uses asynchronous pipeline parallelism, balancing forward and backward passes across the pipeline stages to maximize utilization and reduce idle time:

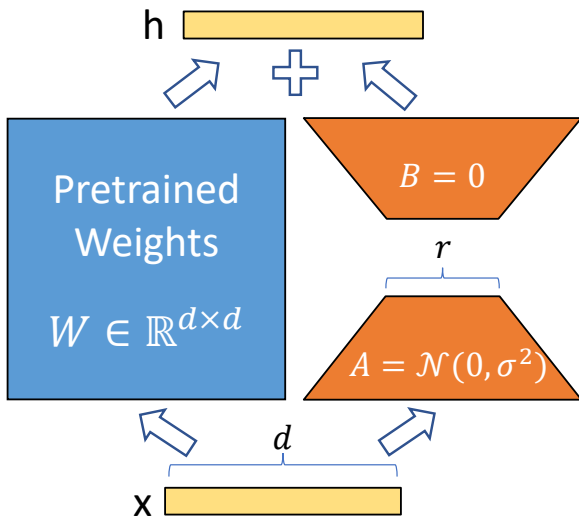


⁹PipeDream: Generalized Pipeline Parallelism for DNN Training

	gpu ₀ ... gpu _i ... gpu _{N-1}	Memory Consumed	K=12 $\Psi=7.5\text{B}$ $N_d=64$
Baseline		$(2 + 2 + K) * \Psi$	120GB
P _{os}		$2\Psi + 2\Psi + \frac{K * \Psi}{N_d}$	31.4GB
P _{os+g}		$2\Psi + \frac{(2+K)*\Psi}{N_d}$	16.6GB
P _{os+g+p}		$\frac{(2+2+K)*\Psi}{N_d}$	1.9GB

■ Parameters
 ■ Gradients
 ■ Optimizer States

¹⁰ZeRO: Memory Optimizations Toward Training Trillion Parameter Models

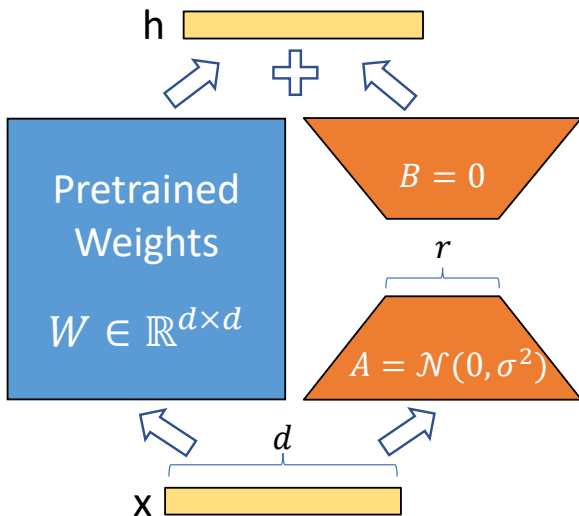


LoRA reduces the number of parameters by approximating weight matrices with low-rank factorization:

$$W_{\text{new}} = W + \Delta W$$

where $\Delta W = AB^T$, with A and B being low-rank matrices. This reduces computational and memory overhead while maintaining model performance.

- A is initialized as usual, while B is initialized with zeroes in order to start from identity mapping

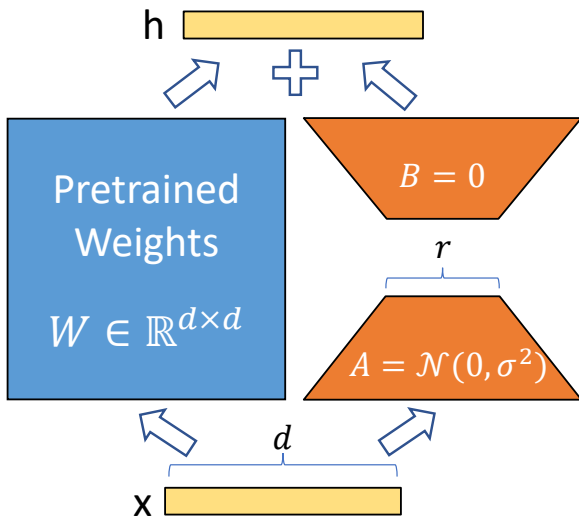


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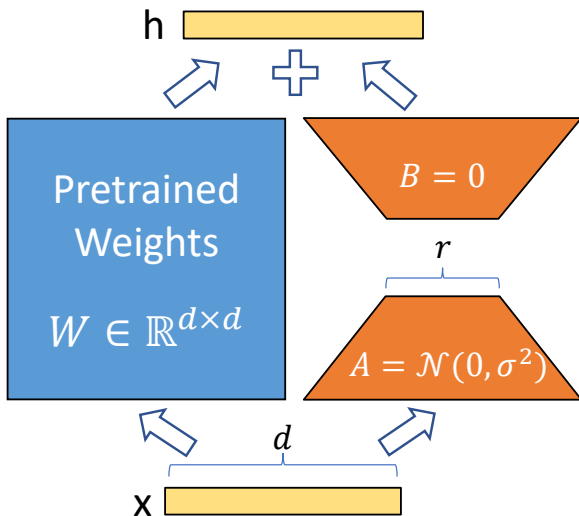


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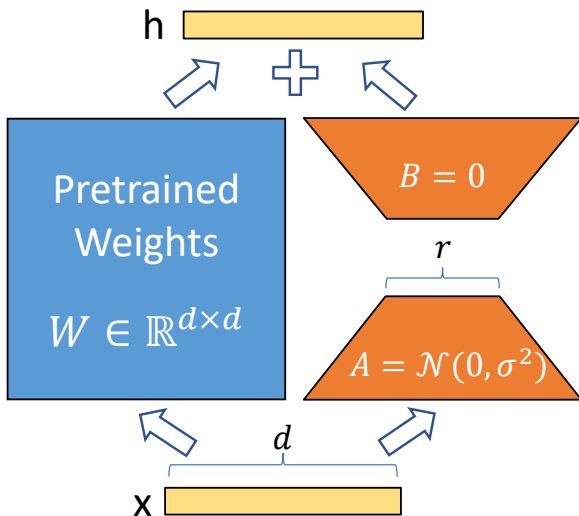
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¹¹LoRA: Low-Rank Adaptation of Large Language Models



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Feedforward Architecture

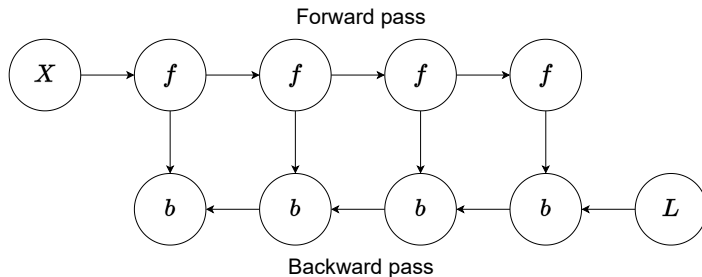


Figure 6: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an f . The gradient of the loss with respect to the activations and parameters marked with b .

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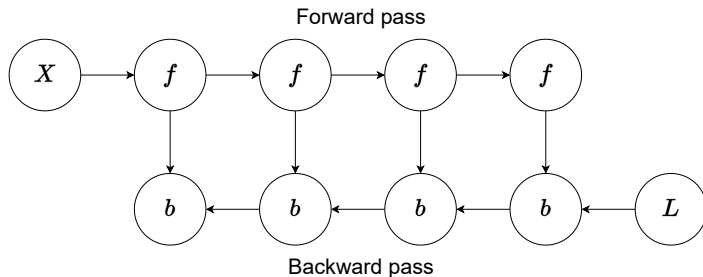


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! Important

The results obtained for the f nodes are needed to compute the b nodes.

Vanilla backpropagation

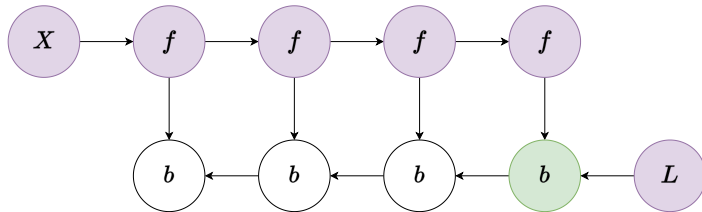


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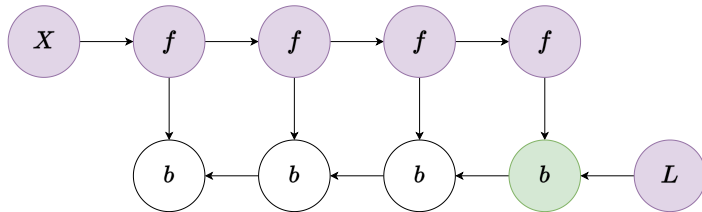


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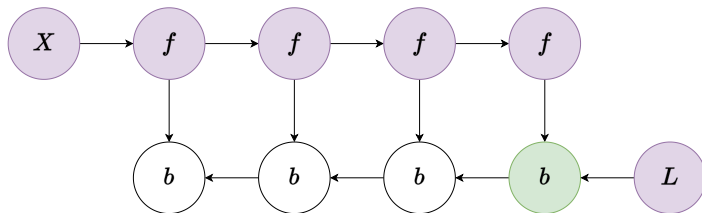


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- Optimal in terms of computation: it only computes each node once.
- High memory usage. The memory usage grows linearly with the number of layers in the neural network.

Memory poor backpropagation

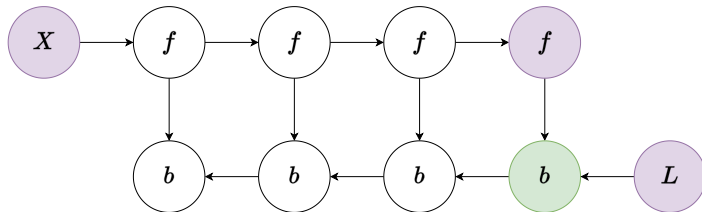


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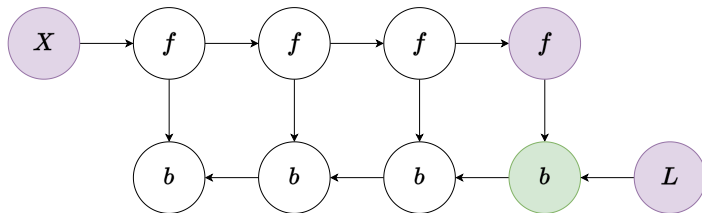


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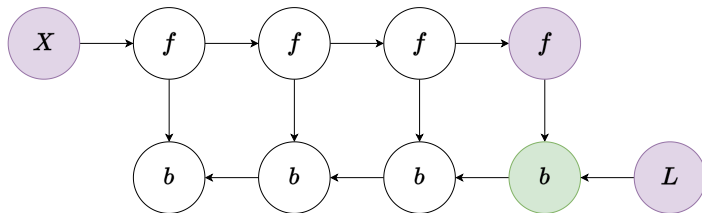


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- Optimal in terms of memory: there is no need to store all activations in memory.
- Computationally inefficient. The number of node evaluations scales with n^2 , whereas it vanilla backprop scaled as n : each of the n nodes is recomputed on the order of n times.

Checkpointed backpropagation

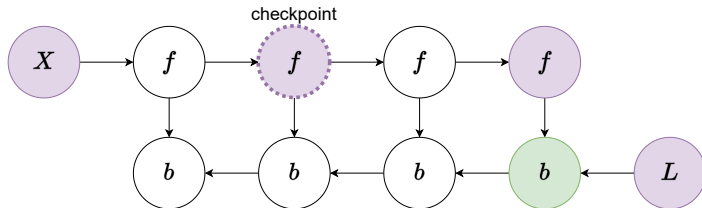


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Checkpointed backpropagation

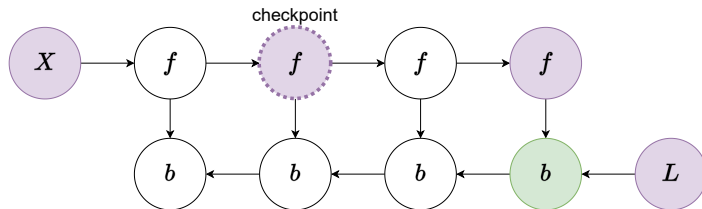


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- Trade-off between the **vanilla** and **memory poor** approaches. The strategy is to mark a subset of the neural net activations as checkpoint nodes, that will be stored in memory.

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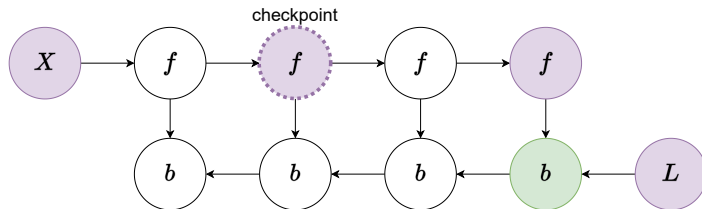


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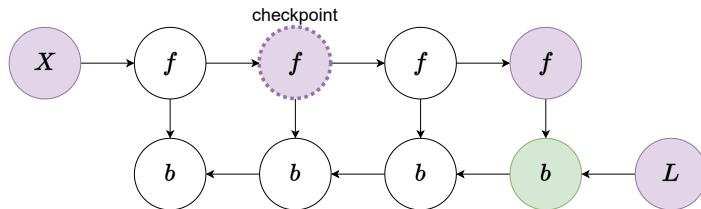


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- Faster recalculation of activations f . We only need to recompute the nodes between a b node and the last checkpoint preceding it when computing that b node during backprop.

Checkpointed backpropagation

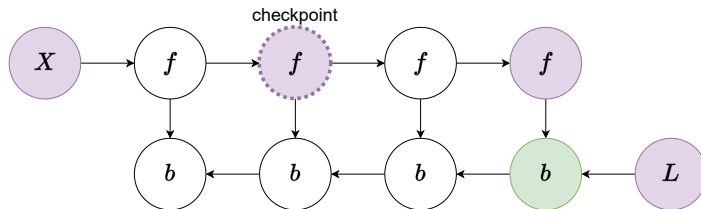


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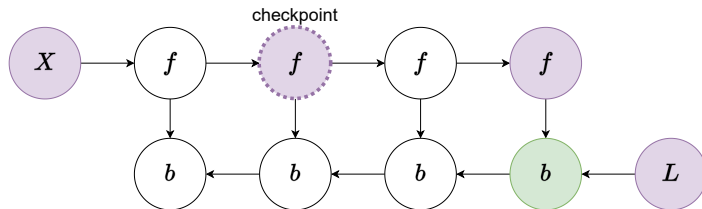




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- Memory consumption depends on the number of checkpoints. More effective than **vanilla** approach.

Gradient checkpointing visualization

The animated visualization of the above approaches 

An example of using a gradient checkpointing 

Split the weight matrix into 2 well clustered factors ¹²

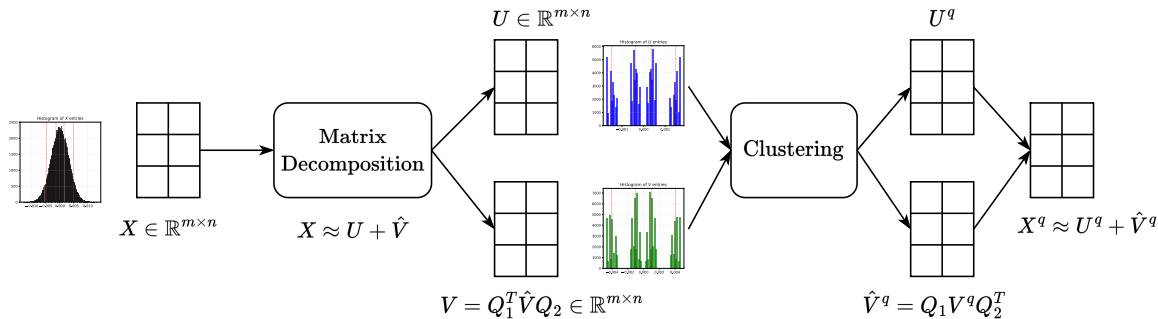


Figure 10: Scheme of post-training quantization approach.

¹²Quantization of Large Language Models with an Overdetermined Basis