



Some notes about scalable algorithms

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Introduction to Data Science. Skoltech

Stochastic Gradient Descent

Example: multidimensional scaling problem

Suppose, we have a pairwise distance matrix for N d -dimensional objects $D \in \mathbb{R}^{N \times N}$. Given this matrix, our goal is to recover the initial coordinates $W_i \in \mathbb{R}^d$, $i = 1, \dots, N$.

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Link to a nice visualization ♣, where one can see, that gradient-free methods handle this problem much slower, especially in higher dimensions.

Question

Is it somehow connected with PCA?

Example: multidimensional scaling problem



Figure 1: Link to the animation

Finite-sum problem

We consider classic finite-sample average minimization:

$$\min_{x \in \mathbb{R}^p} f(x) = \min_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n f_i(x)$$

The gradient descent acts like follows:

$$x_{k+1} = x_k - \frac{\alpha_k}{n} \sum_{i=1}^n \nabla f_i(x) \quad (\text{GD})$$

- Convergence with constant α or line search.

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Let's/ switch from the full gradient calculation to its unbiased estimator, when we randomly choose i_k index of point at each iteration uniformly:

$$x_{k+1} = x_k - \alpha_k \nabla f_{i_k}(x_k) \quad (\text{SGD})$$

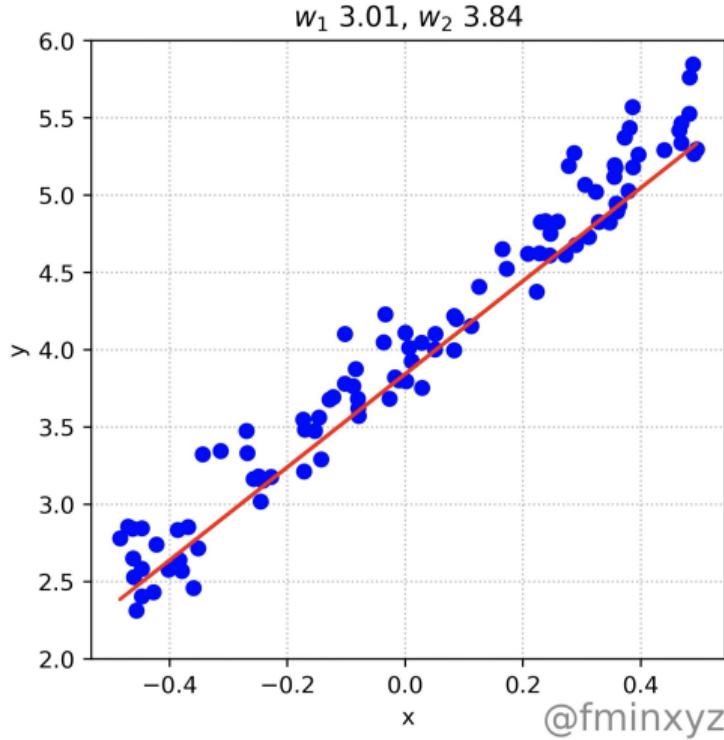
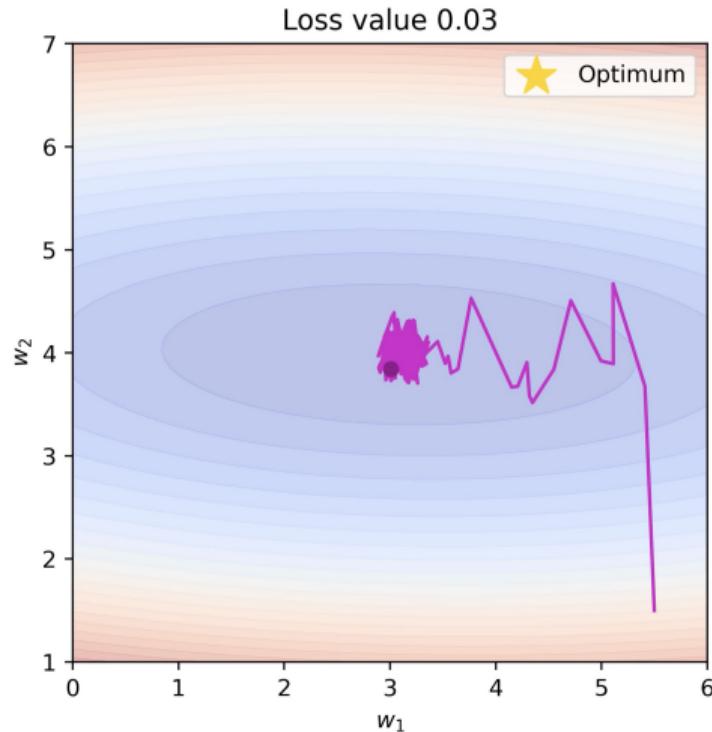
With $p(i_k = i) = \frac{1}{n}$, the stochastic gradient is an unbiased estimate of the gradient, given by:

$$\mathbb{E}[\nabla f_{i_k}(x)] = \sum_{i=1}^n p(i_k = i) \nabla f_i(x) = \sum_{i=1}^n \frac{1}{n} \nabla f_i(x) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(x) = \nabla f(x)$$

This indicates that the expected value of the stochastic gradient is equal to the actual gradient of $f(x)$.

Typical behaviour

Stochastic Gradient Descent. Batch = 2



@fminxyz

Main problem of SGD

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Strongly convex binary logistic regression. m=200, n=10, mu=1.



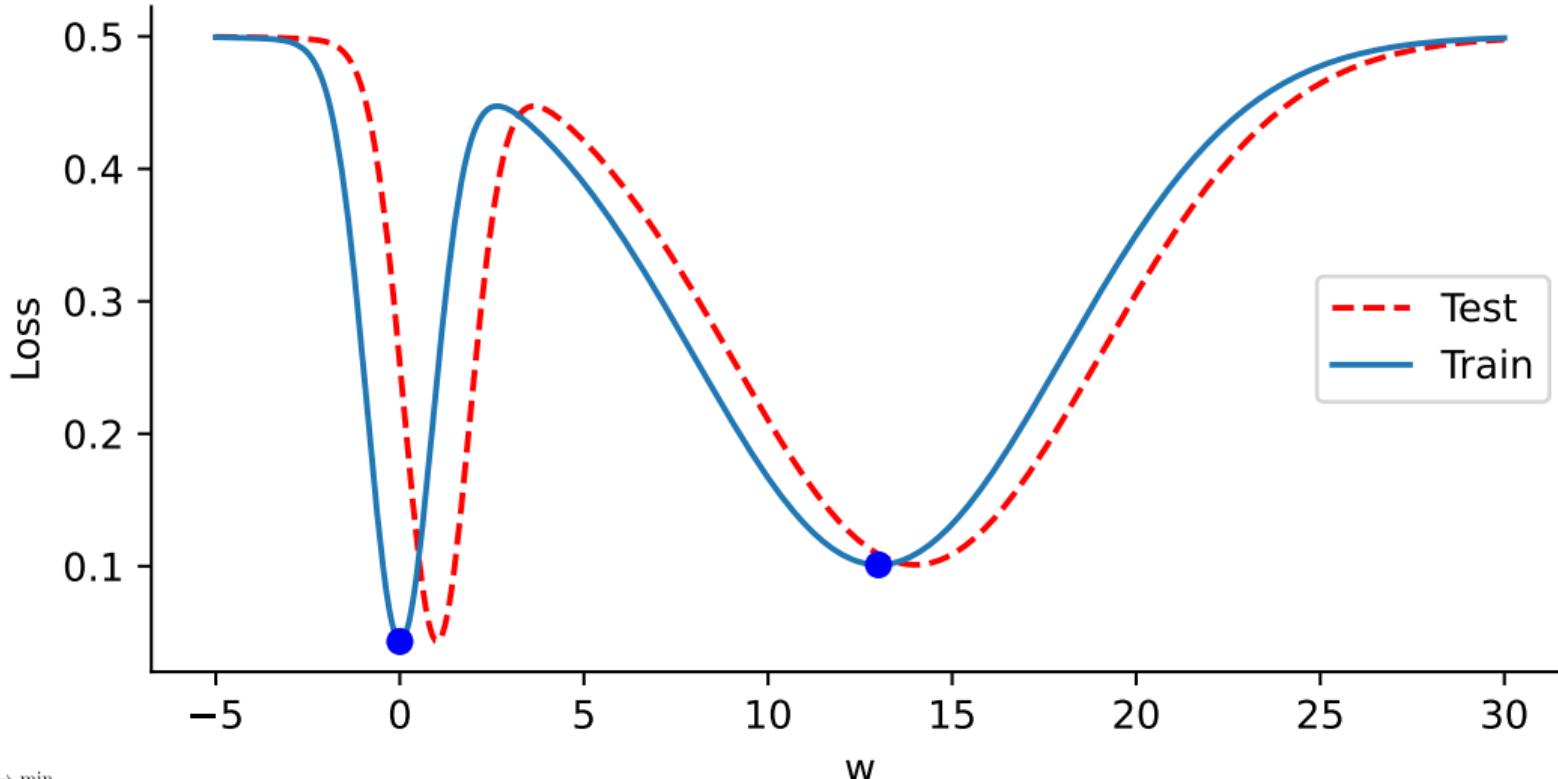
Wide vs narrow local minima

Узкие и широкие локальные минимумы



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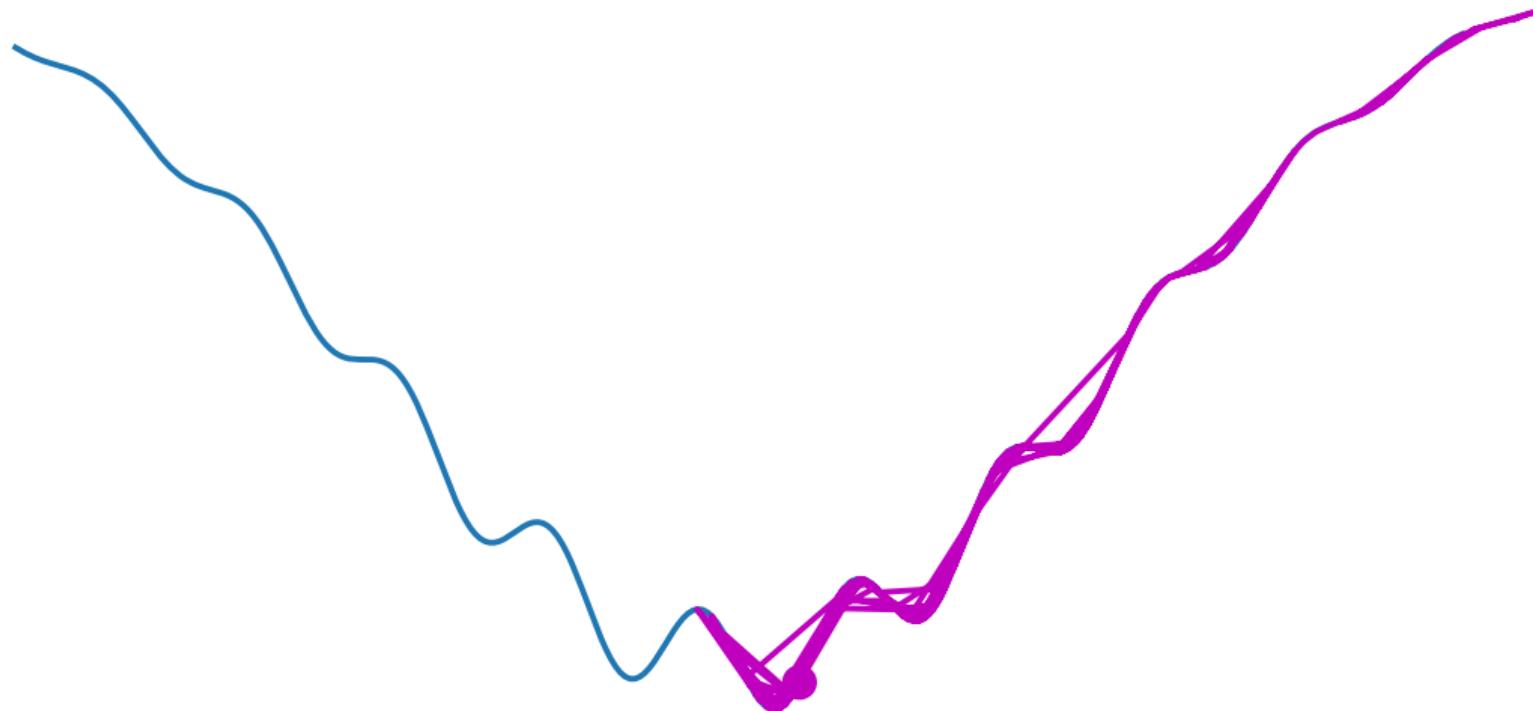
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Узкие и широкие локальные минимумы



Stochasticity allows to escape local minima

Стохастический градиентный спуск
выпрыгивает из локальных минимумов



Local divergence can also be beneficial

Градиентный спуск с большим шагом
избегает узкого локального минимума



Adaptivity or scaling

Adagrad (Duchi, Hazan, and Singer 2010)

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \dots, p$:

$$v_j^{(k)} = v_j^{k-1} + (g_j^{(k)})^2$$
$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

Notes:

- AdaGrad does not require tuning the learning rate: $\alpha > 0$ is a fixed constant, and the learning rate decreases naturally over iterations.

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- Can drastically improve over SGD in sparse problems.
- Main weakness is the monotonic accumulation of gradients in the denominator. AdaDelta, Adam, AMSGrad, etc. improve on this, popular in training deep neural networks.
- The constant ϵ is typically set to 10^{-6} to ensure that we do not suffer from division by zero or overly large step sizes.

RMSProp (Tieleman and Hinton, 2012)

An enhancement of AdaGrad that addresses its aggressive, monotonically decreasing learning rate. Uses a moving average of squared gradients to adjust the learning rate for each weight. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$ and update rule for $j = 1, \dots, p$:

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1 - \gamma)(g_j^{(k)})^2$$

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

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- Allows for a more nuanced adjustment of learning rates than AdaGrad, making it suitable for non-stationary problems.
- Commonly used in training neural networks, particularly in recurrent neural networks.

Adadelta (Zeiler, 2012)

An extension of RMSProp that seeks to reduce its dependence on a manually set global learning rate. Instead of accumulating all past squared gradients, Adadelta limits the window of accumulated past gradients to some fixed size w . Update mechanism does not require learning rate α :

$$v_j^{(k)} = \gamma v_j^{(k-1)} + (1 - \gamma)(g_j^{(k)})^2$$

$$\tilde{g}_j^{(k)} = \frac{\sqrt{\Delta x_j^{(k-1)} + \epsilon}}{\sqrt{v_j^{(k)} + \epsilon}} g_j^{(k)}$$

$$x_j^{(k)} = x_j^{(k-1)} - \tilde{g}_j^{(k)}$$

$$\Delta x_j^{(k)} = \rho \Delta x_j^{(k-1)} + (1 - \rho)(\tilde{g}_j^{(k)})^2$$

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- The method does not require an initial learning rate setting, making it easier to configure.
- Often used in deep learning where parameter scales differ significantly across layers.

Adam (Kingma and Ba, 2014)

Combines elements from both AdaGrad and RMSProp. It considers an exponentially decaying average of past gradients and squared gradients. Update rule:

$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1 - \beta_1) g_j^{(k)}$$

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1 - \beta_2) (g_j^{(k)})^2$$

$$\hat{m}_j = \frac{m_j^{(k)}}{1 - \beta_1^k}, \quad \hat{v}_j = \frac{v_j^{(k)}}{1 - \beta_2^k}$$

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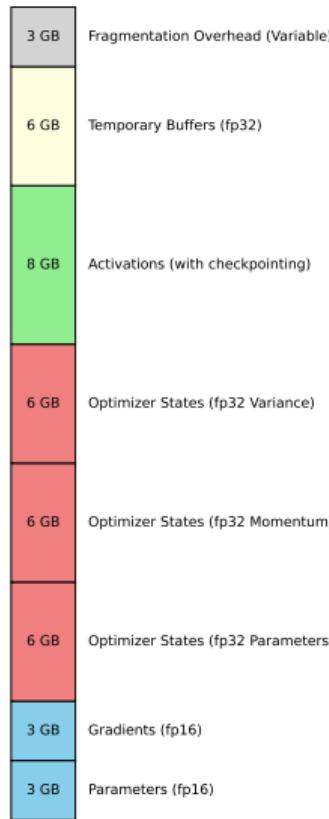
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- Highly popular in training deep learning models, owing to its efficiency and straightforward implementation.
- However, the proposed algorithm in initial version does not converge even in convex setting (later fixes)

GPT-2 training Memory footprint

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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.

Model States:

- Optimizer states (e.g., Adam) require memory for time-averaged momentum and gradient variance.

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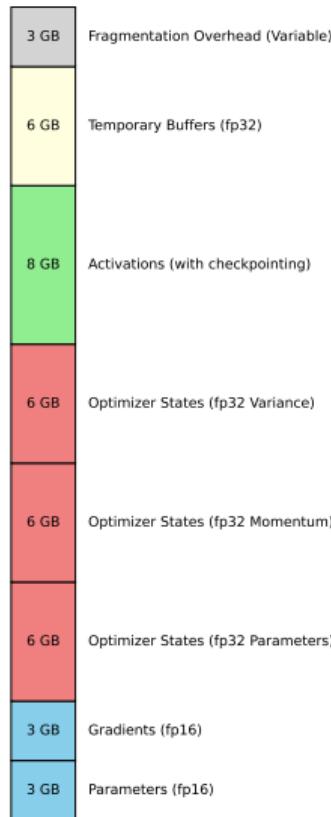
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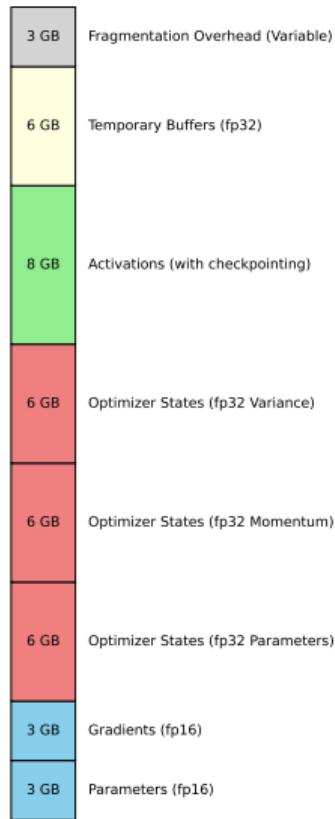
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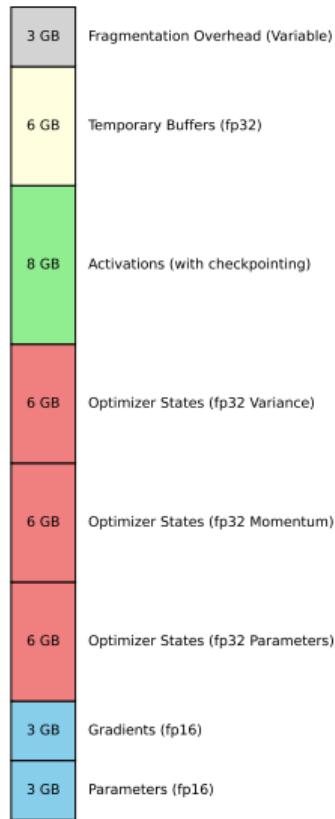
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- Activation checkpointing can reduce activation memory by about 50%, with a 33% recomputation overhead.

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Memory Fragmentation:

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- In some cases, over 30% of memory remains unusable due to fragmentation.

 Simple annotated MNIST exercise

 A quick introduction to Optuna

MultiGPU training

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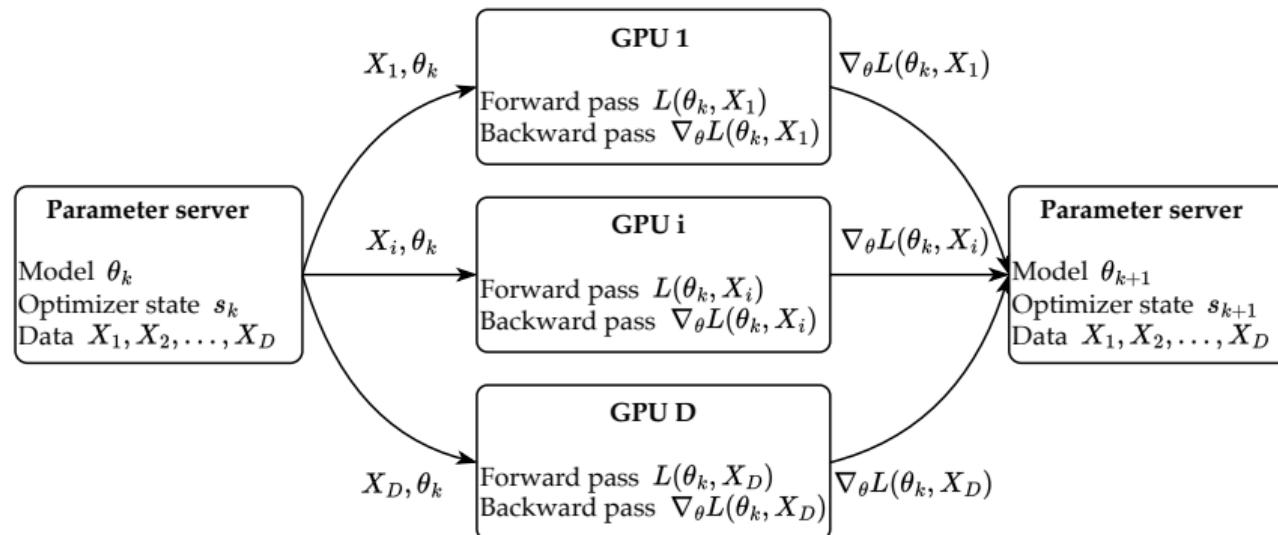
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Per device batch size: b . Overall batchsize: D_b . Data parallelism involves splitting the data across multiple GPUs, each with a copy of the model. Gradients are averaged and weights updated synchronously:



Distributed Data Parallel training

Distributed Data Parallel (DDP)¹ 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

¹Getting Started with Distributed Data Parallel

Naive model parallelism

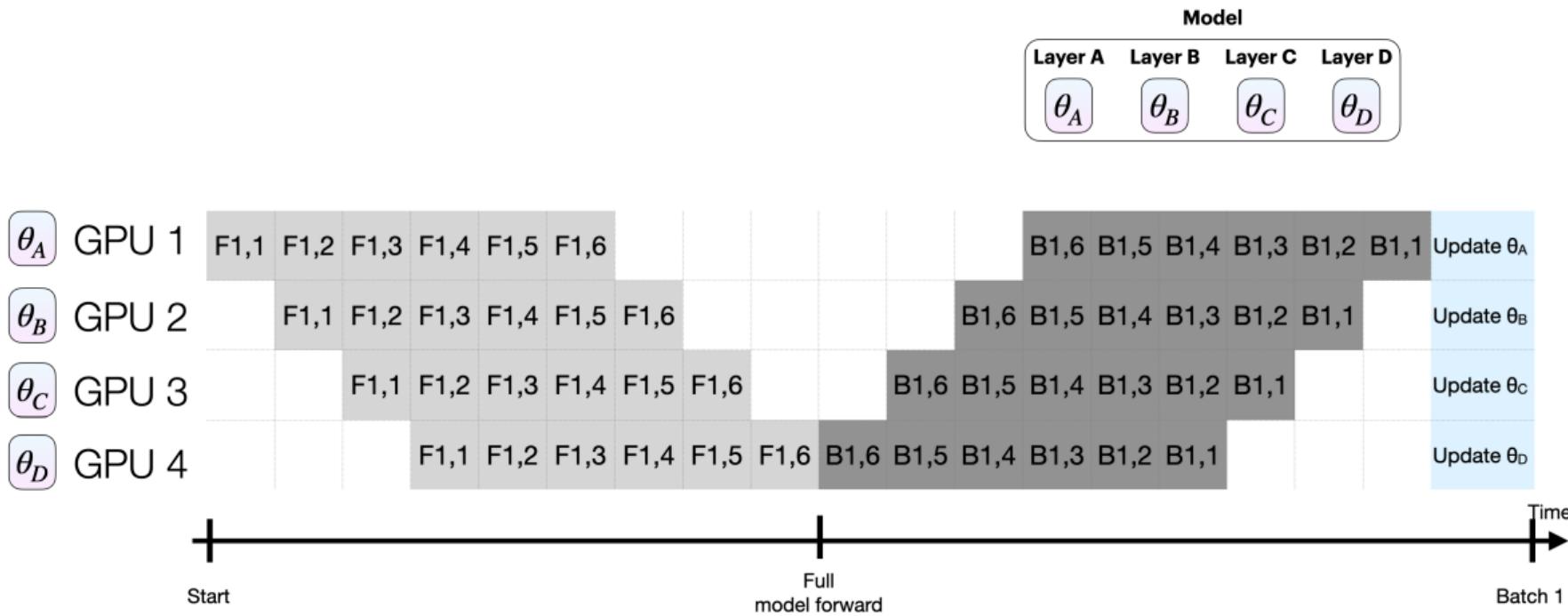
Model parallelism divides the model across multiple GPUs. Each GPU handles a subset of the model layers, reducing memory load per GPU. Allows to work with the models, that won't fit in the single GPU Poor resource utilization.



Figure 4: Model parallelism

Pipeline model parallelism (GPipe)²

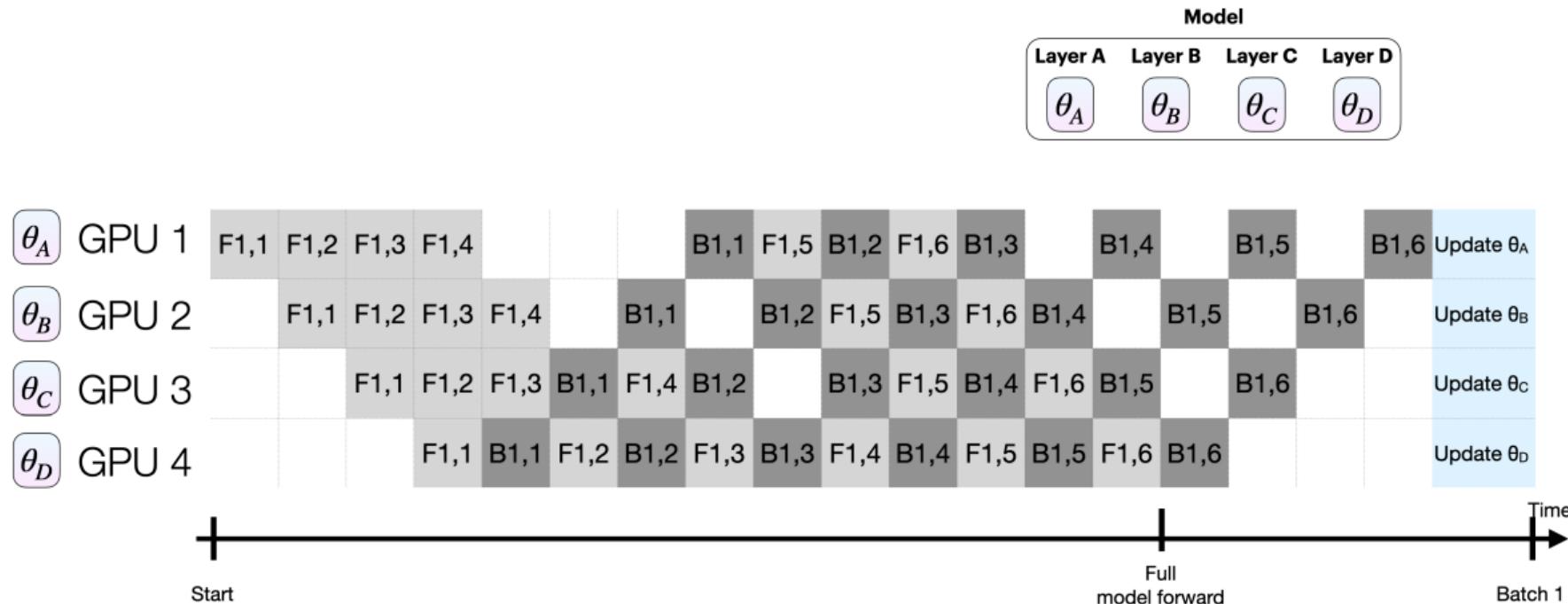
GPipe splits the model into stages, each processed sequentially. Micro-batches are passed through the pipeline, allowing for overlapping computation and communication:



²GPipe: Efficient Training of Giant Neural Networks using Pipeline Parallelism

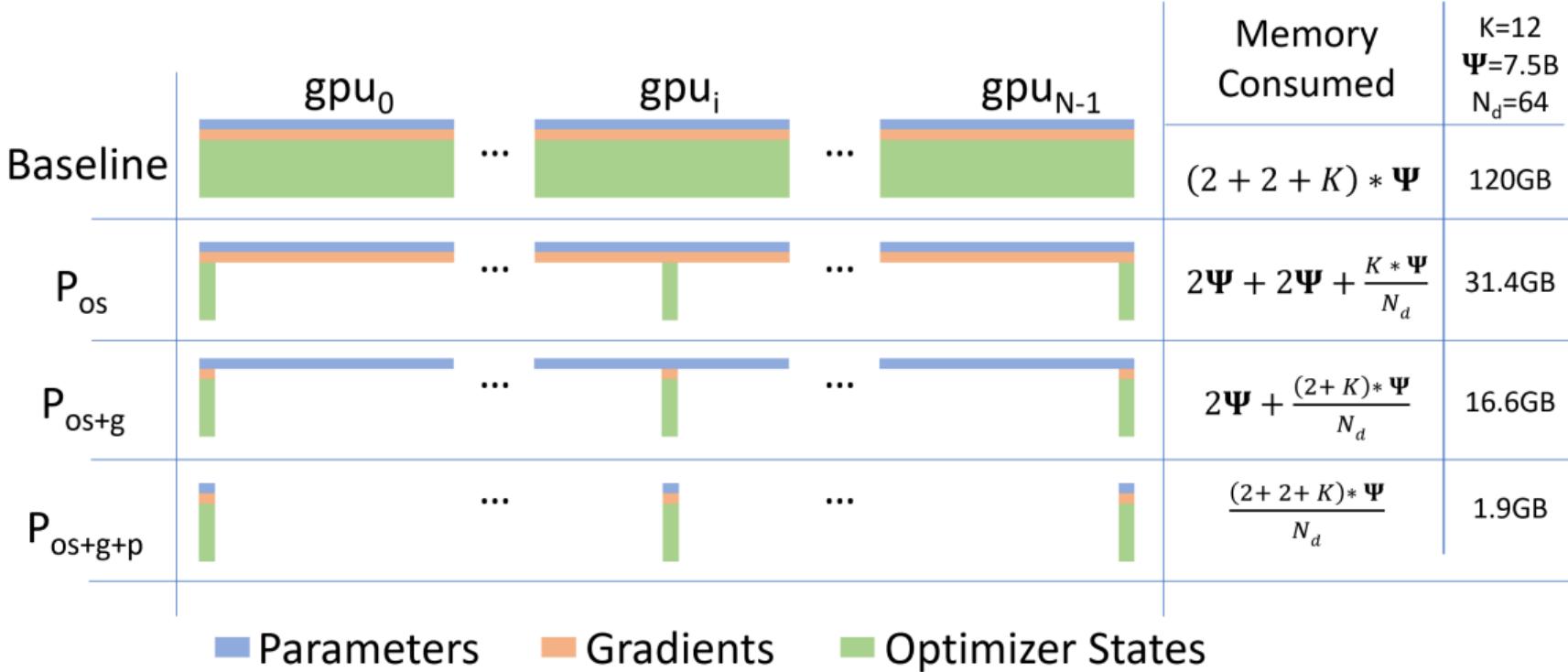
Pipeline model parallelism (PipeDream)³

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



³PipeDream: Generalized Pipeline Parallelism for DNN Training

ZeRO⁴



⁴ZeRO: Memory Optimizations Toward Training Trillion Parameter Models

LoRA⁵



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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$$h = W_{\text{new}}x = Wx + \Delta Wx = Wx + AB^Tx$$

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Feedforward Architecture



Figure 5: 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 .

Feedforward Architecture



Figure 5: 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 .

! Important

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

Vanilla backpropagation

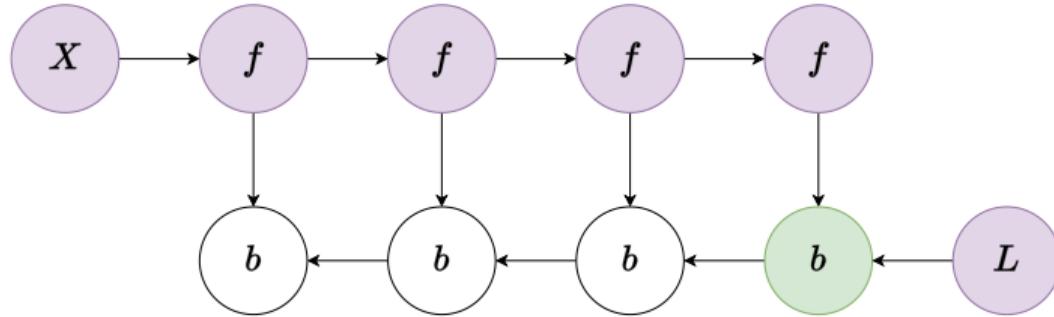


Figure 6: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Vanilla backpropagation



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- All activations f are kept in memory after the forward pass.

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 - Optimal in terms of computation: it only computes each node once.

Vanilla backpropagation

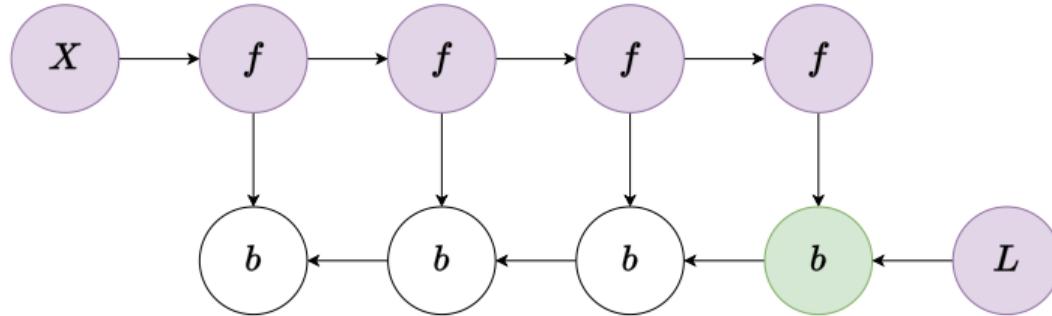


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- All activations f are kept in memory after the forward pass.
 - Optimal in terms of computation: it only computes each node once.
 - High memory usage. The memory usage grows linearly with the number of layers in the neural network.

Memory poor backpropagation



Figure 7: 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.

Memory poor backpropagation

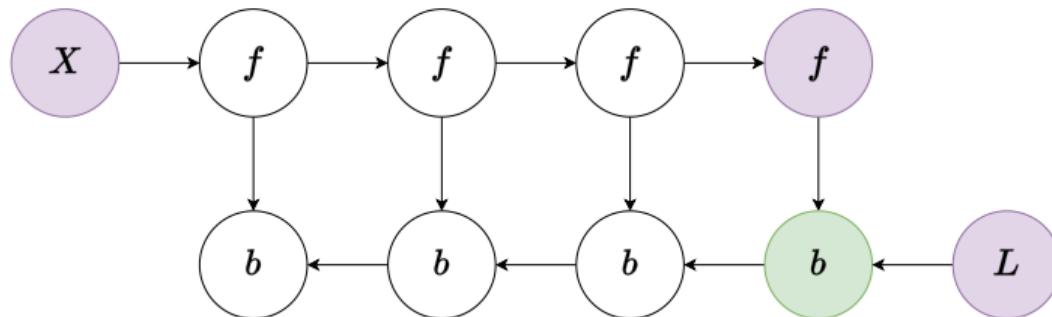


Figure 7: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

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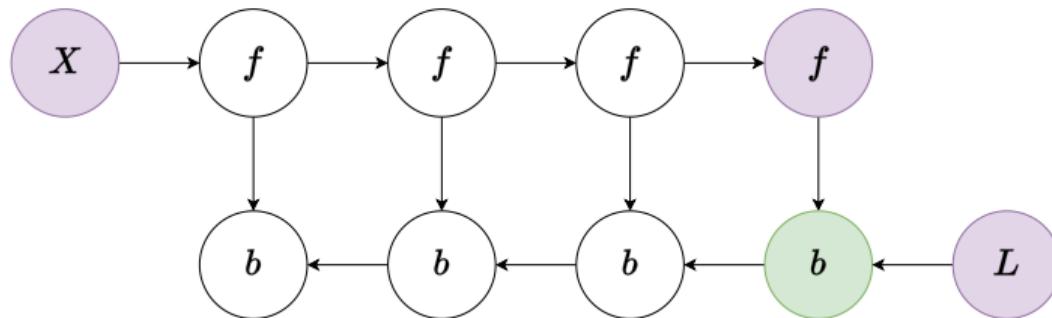


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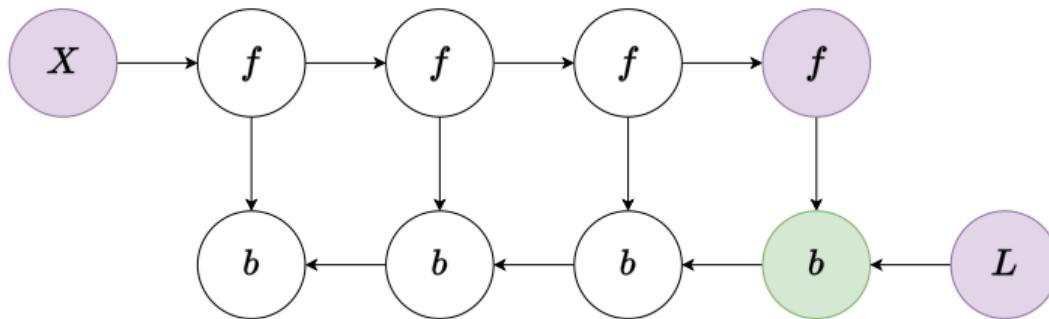


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- Each activation f is recalculated as needed.
 - Optimal in terms of memory: there is no need to store all activations in memory.
- Computationally inefficient. The number of node evaluations scales with n^2 , whereas vanilla backprop scaled as n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

Checkpointed backpropagation



Figure 8: 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.

Checkpointed backpropagation



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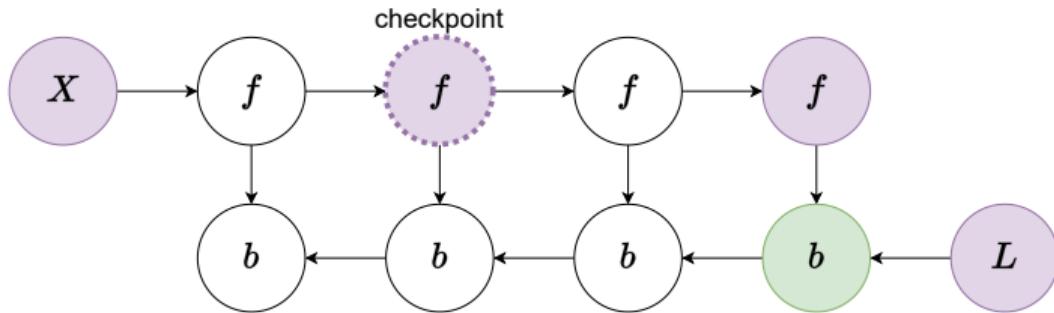


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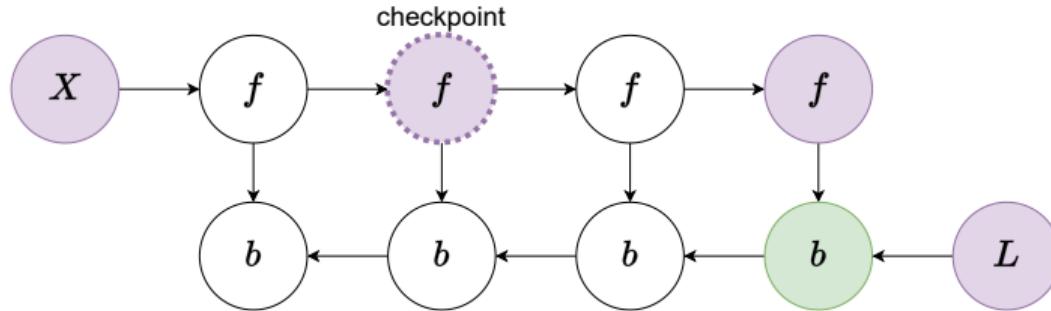


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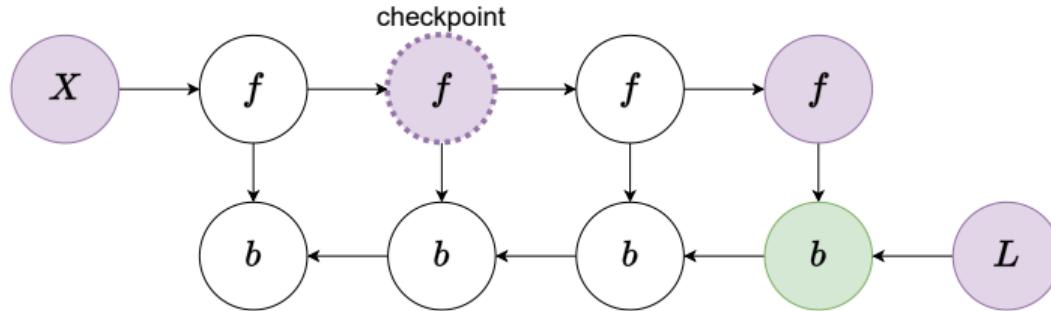


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 - Faster recalculation of activations f . We only need to recompute the nodes between a b node and the last checkpoint preceding it when computing that b node during backprop.
 - Memory consumption depends on the number of checkpoints. More effective than **vanilla** approach.

Gradient checkpointing visualization

The animated visualization of the above approaches 

An example of using a gradient checkpointing 

Quantization

Split the weight matrix into 2 well clustered factors⁶



Figure 9: Scheme of post-training quantization approach.

⁶Quantization of Large Language Models with an Overdetermined Basis