



Big Models

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Методы Оптимизации в Машинном Обучении. ФКН ВШЭ

Тренды

Training compute (FLOP)

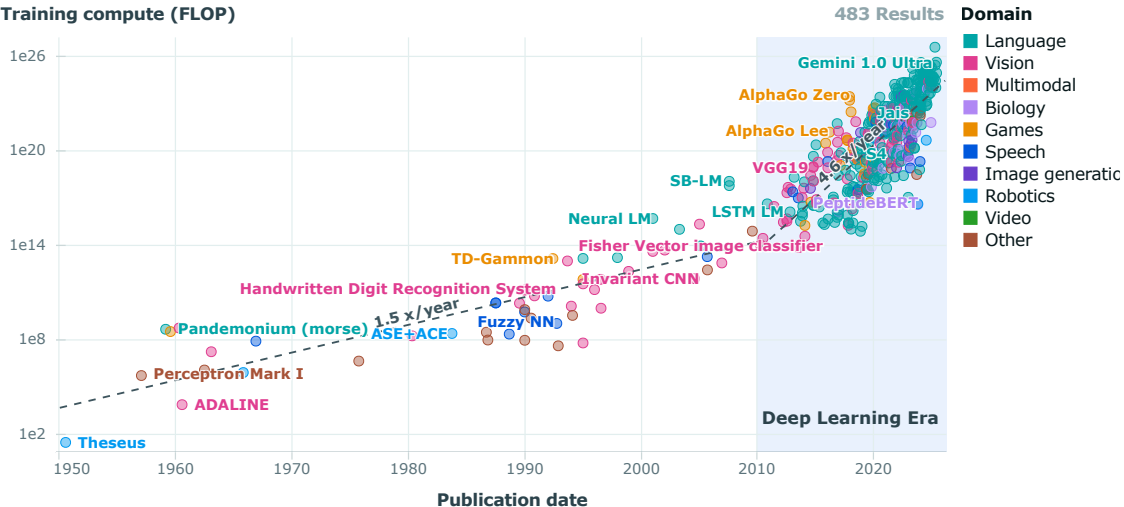


Рисунок 1: Динамика вычислений, необходимых для обучения моделей. Источник

Notable AI Models

Training compute (FLOP)

483 Results

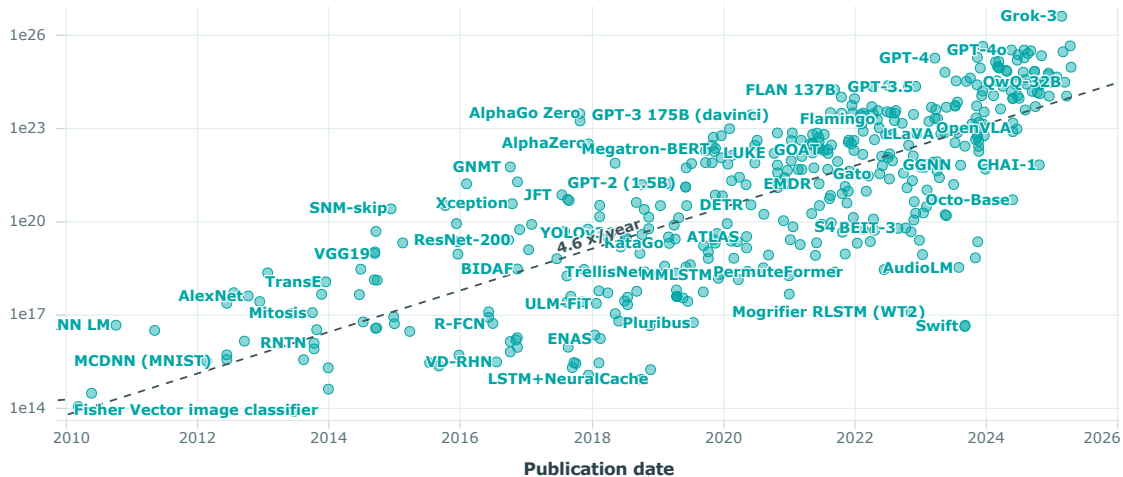


Рисунок 2: Динамика вычислений, необходимых для обучения нейросетевых моделей. Источник

Number of trainable parameters

636 Results

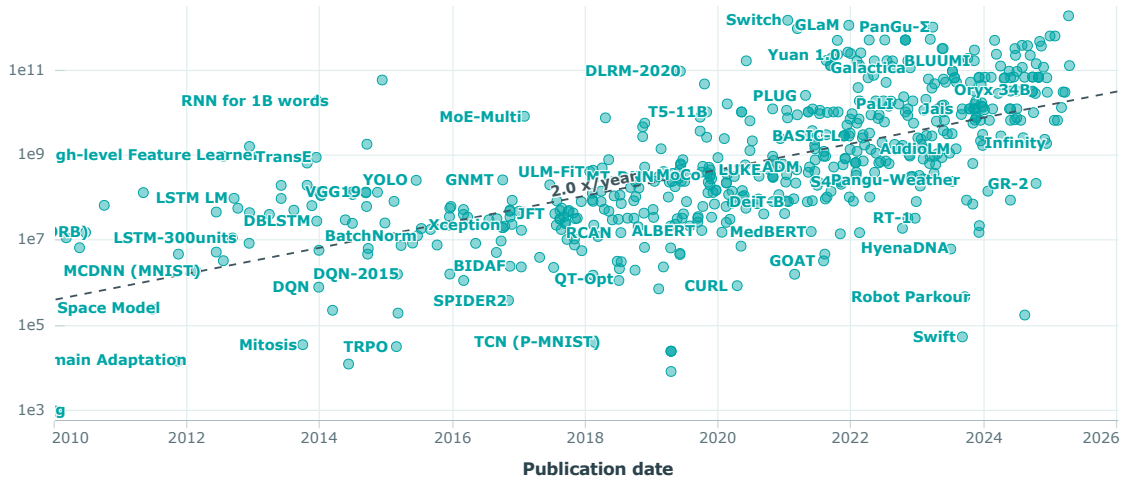


Рисунок 3: Динамика количества обучаемых параметров нейросетевых моделей. Источник

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.

Memory Requirements Example:

Residual Memory Consumption:

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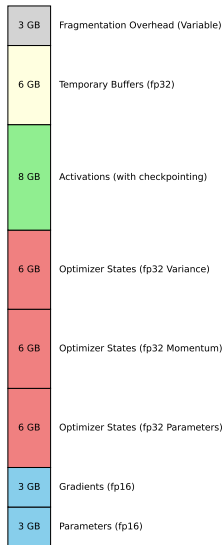
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- Activation checkpointing can reduce activation memory by about 50%, with a 33% recomputation overhead.

GPT-2 training Memory footprint

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Temporary Buffers:

- Store intermediate results; e.g., gradient all-reduce operations fuse gradients into a single buffer.

Memory Fragmentation:



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

Scaling Laws

Scaling Laws ¹

- **Эмпирическое правило:** кросс-энтропия уменьшается по степенному закону

$$L(N, D, C) \propto N^{-\alpha} D^{-\beta} C^{-\gamma}$$

где N — параметры, D — токены, C — FLOPs.

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- Практически scaling-законы помогают подбирать размеры корпуса и останавливать обучение до переобучения.

¹Kaplan et al., 2020

Chinchilla²

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- Вывод: лучше «дольше учить меньшую модель», чем «коротко учить огромную».

²Hoffmann et al., 2022

Chinchilla scaling laws

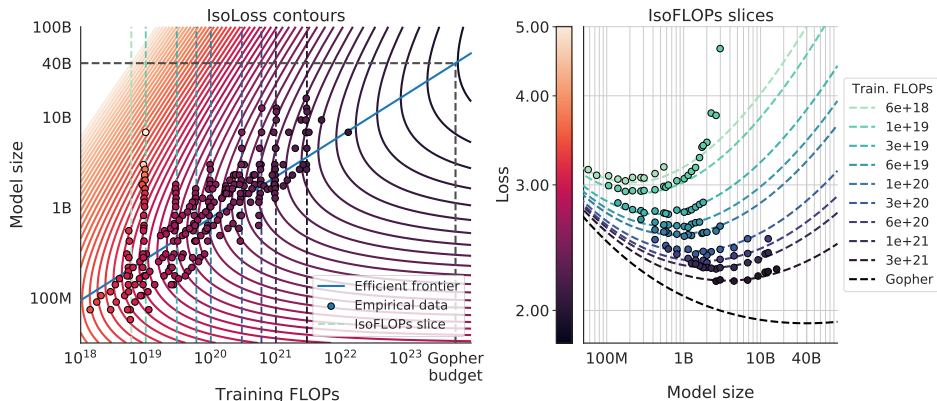


Рисунок 4: Parametric modeling of the loss $L(N, D)$ with contour plot (left) and isoFLOP slices (right). Each isoFLOP slice corresponds to a dashed line in the left plot. The efficient frontier is shown in blue, forming a line in log-log space. The curve intersects each iso-loss contour at the point of minimum FLOPs. The optimal model size for the Gopher FLOP budget is projected to be 40B parameters.

Automatic Mixed Precision (AMP)

Activations³

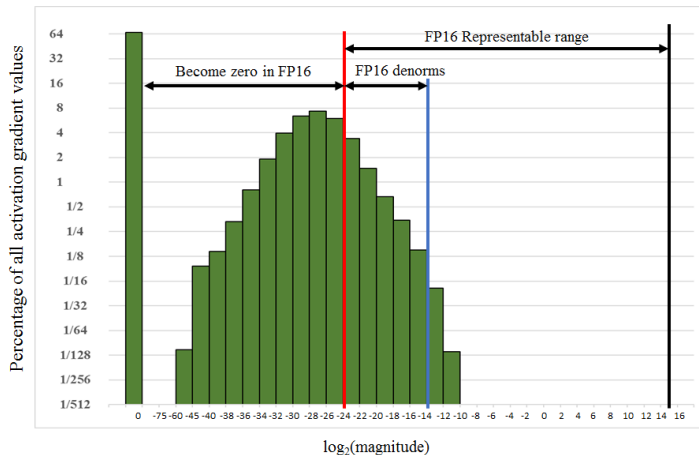


Рисунок 5: Histogram of activation gradient values during the training of Multibox SSD network. Note that the bins on the x-axis cover varying ranges and there's a separate bin for zeros. For example, 2% of the values are in the $[2^{-34}, 2^{-32})$ range, 2% of values are in the $[2^{-24}, 2^{-23})$ range, and 67% of values are zero.

³Mixed Precision Training

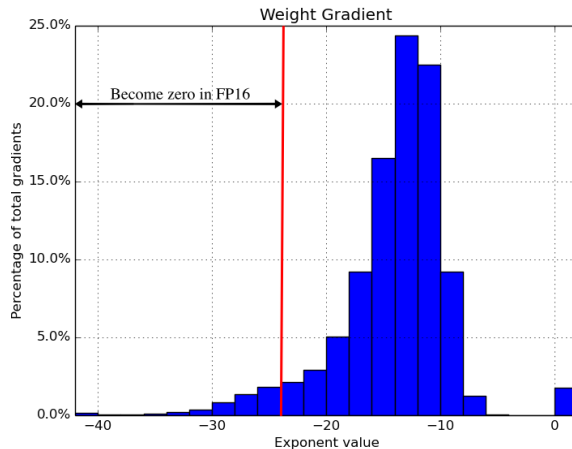
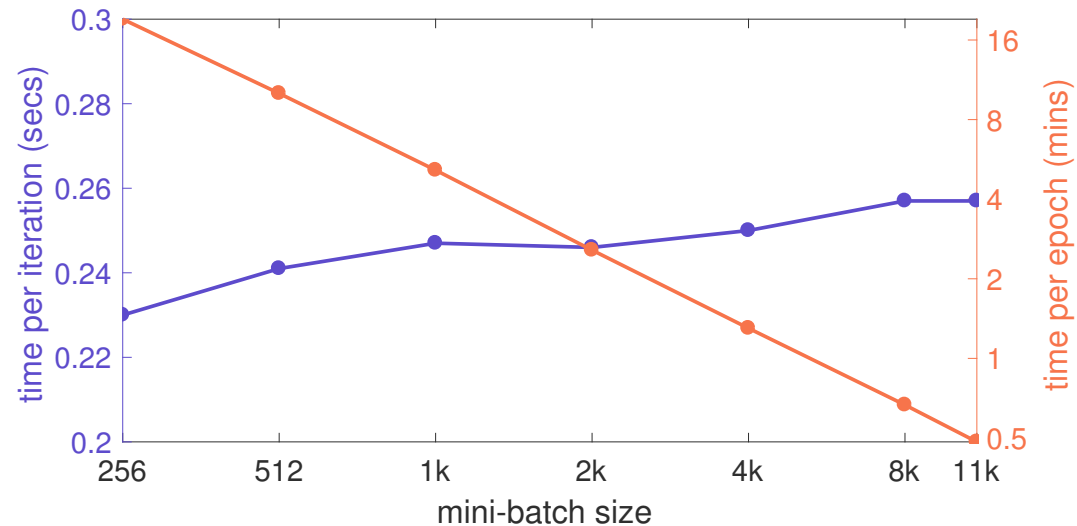


Рисунок 6: Histogram for the exponents of weight gradients for DeepSpeech 2 model (215 M parameters) training on Mandarin speech recognition. The gradients are sampled every 4,000 iterations during training for all the layers in the model.

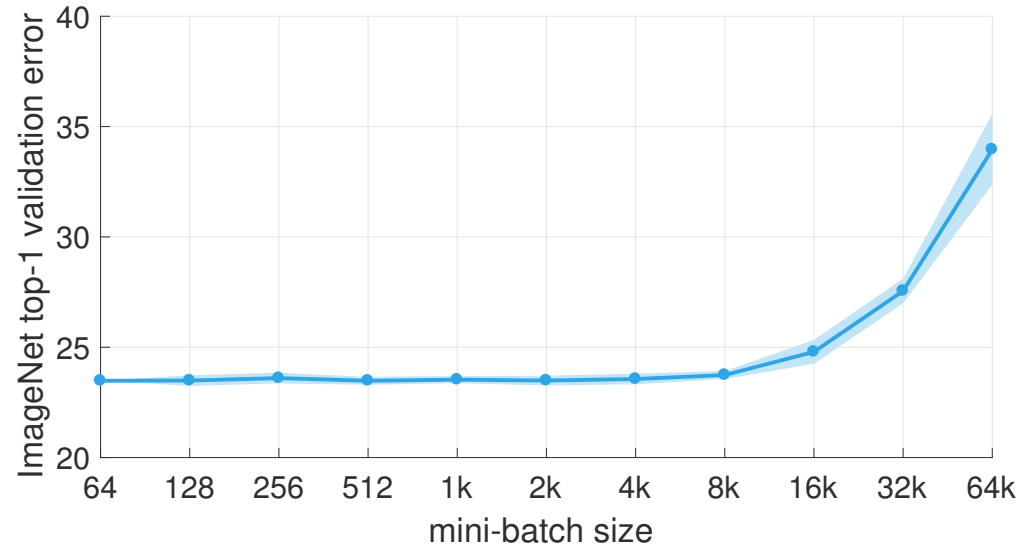
Large batch training

Large batch training⁵



⁵Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Large batch training⁶



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

Large batch training ⁷

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.

⁷Accurate, 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**⁸ 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**⁹ proposes scaling the learning rate with the square root of the batch size increase:

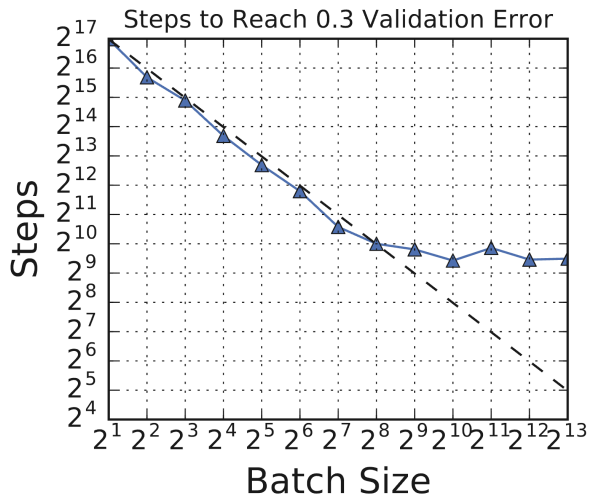
$$\alpha_{\text{new}} = \alpha_{\text{base}} \cdot \sqrt{\frac{\text{Batch Size}_{\text{new}}}{\text{Batch Size}_{\text{base}}}}$$

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

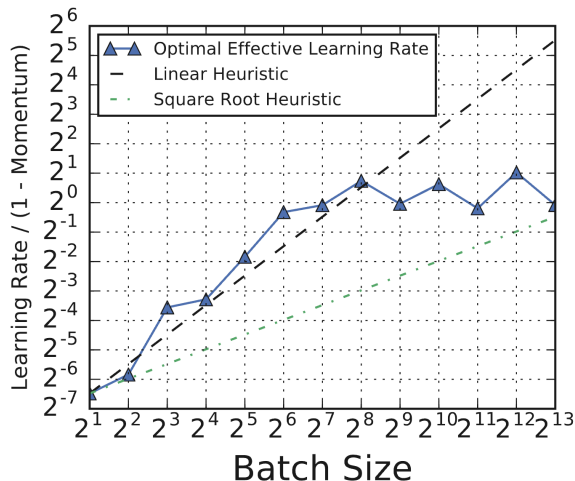
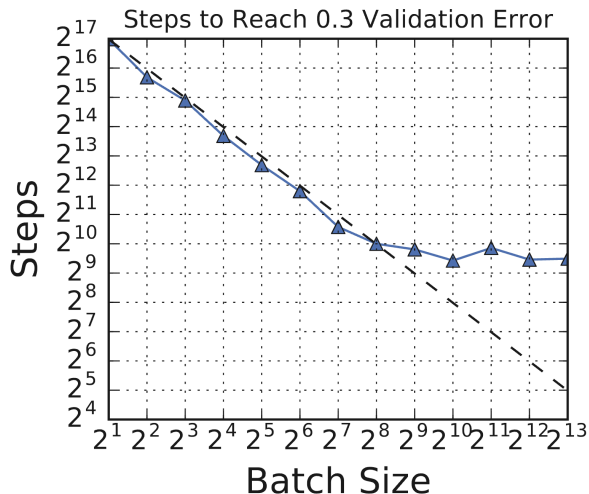
⁸Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

⁹Learning Rates as a Function of Batch Size: A Random Matrix Theory Approach to Neural Network Training

Batch size scaling



Batch size scaling



Gradual warmup¹⁰

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.

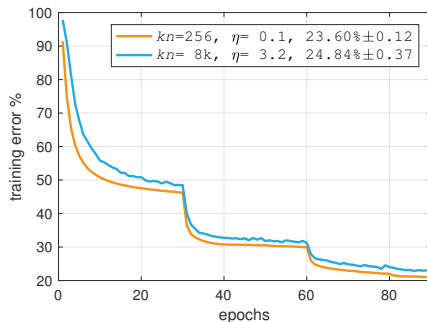


Рисунок 7: no warmup

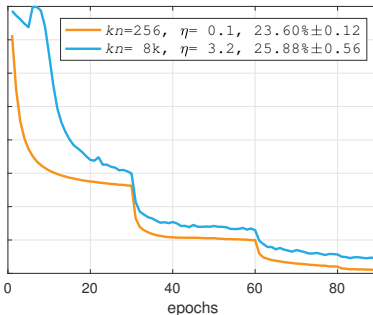


Рисунок 8: constant warmup

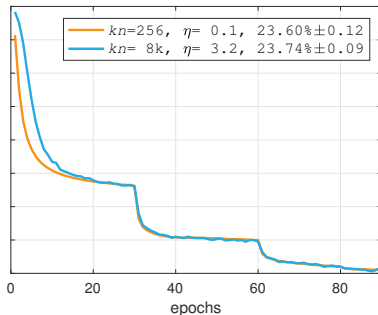
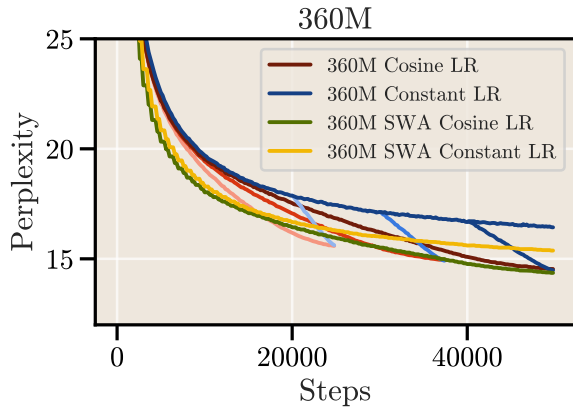
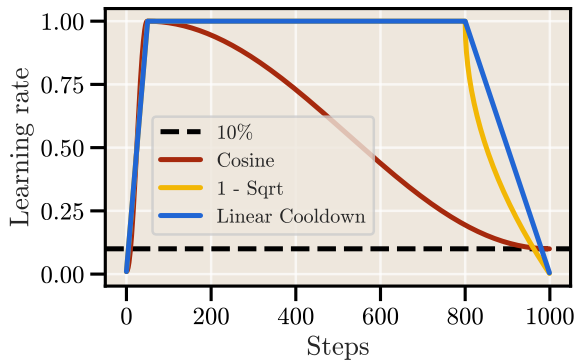


Рисунок 9: gradual warmup

¹⁰ Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour

Cooldown^{11 12}



¹¹Scaling Laws and Compute-Optimal Training Beyond Fixed Training Durations

¹²Scaling Vision Transformers

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()  
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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()
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MultiGPU training

Data Parallel training

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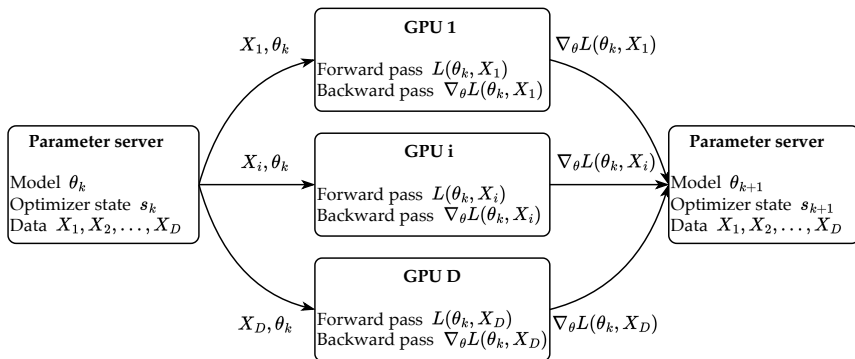
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Per device batch size: b . Overall batchsize: Db . Data parallelism involves splitting the data across multiple GPUs, each with a copy of the model. Gradients are averaged and weights updated synchronously:



Distributed Data Parallel training

Distributed Data Parallel (DDP) ¹³ 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

¹³Getting 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.

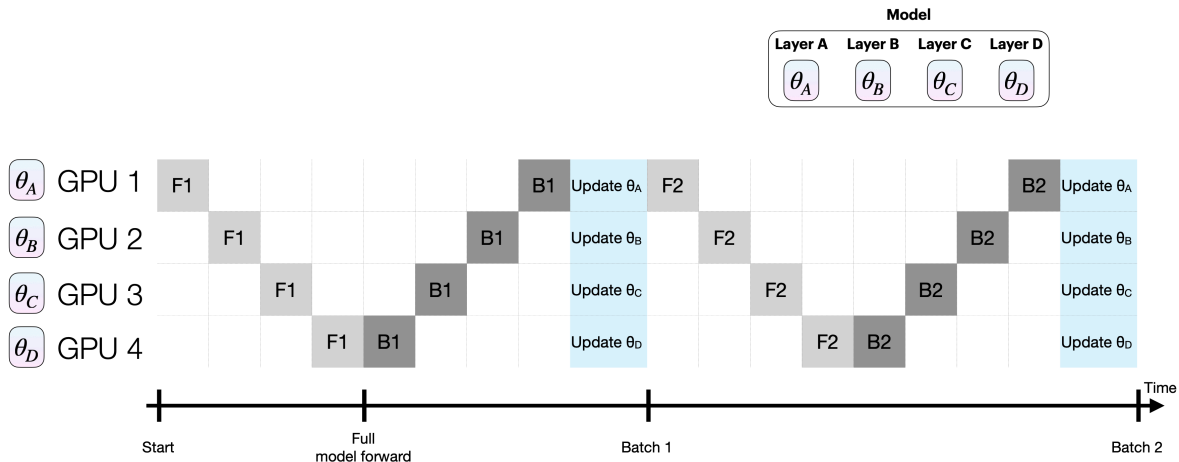
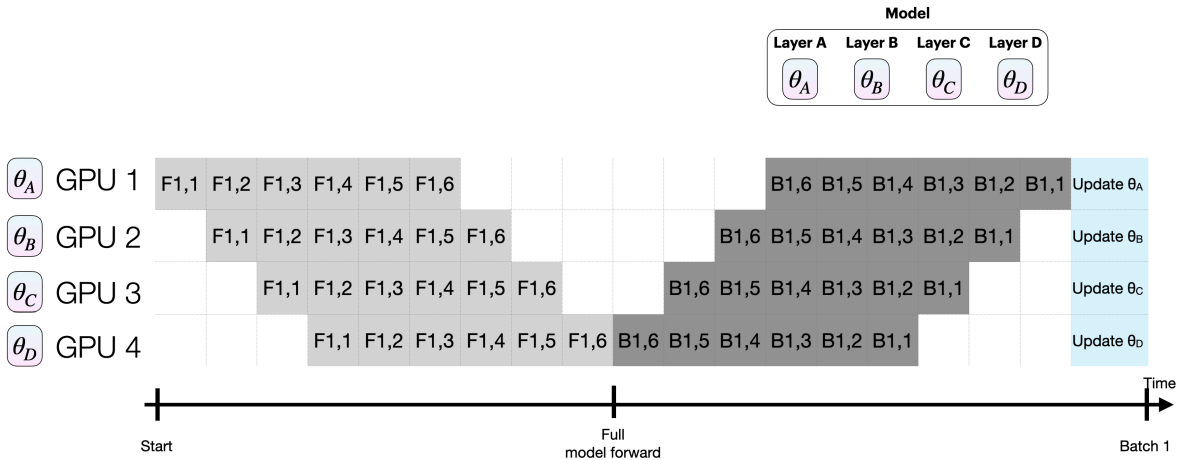


Рисунок 11: Model parallelism

Pipeline model parallelism (GPipe)¹⁴

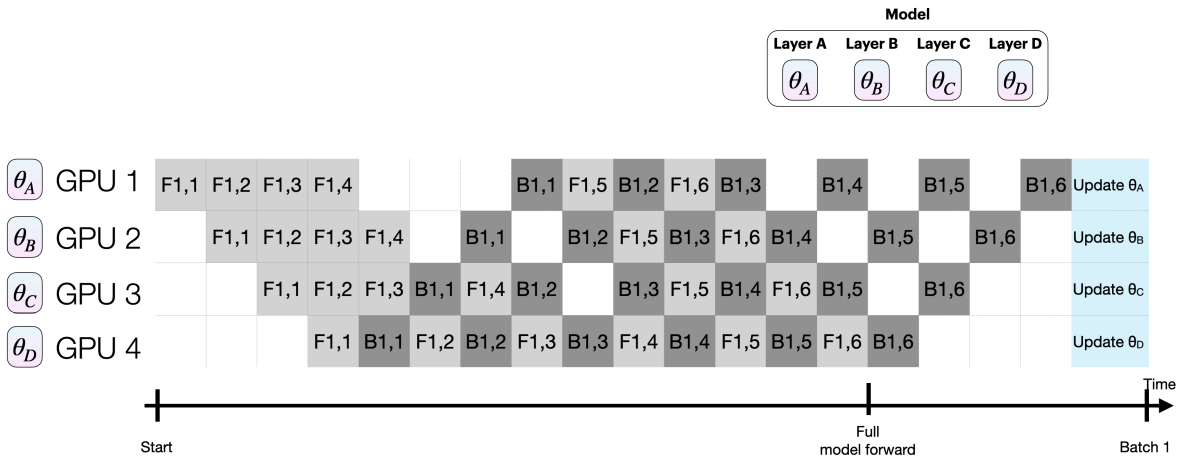
GPipe splits the model into stages, each processed sequentially. Micro-batches are passed through the pipeline, allowing for overlapping computation and communication:



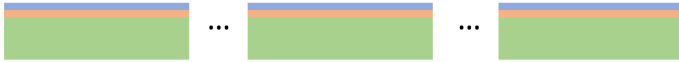



¹⁴GPipe: Efficient Training of Giant Neural Networks using Pipeline Parallelism

Pipeline model parallelism (PipeDream) ¹⁵

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



¹⁵PipeDream: 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

FSDP (Fully Sharded Data Parallel) ¹⁷

- Шардинг параметров, градиентов и состояний оптимизатора по процессам → экономия **7x памяти** относительно DDP.

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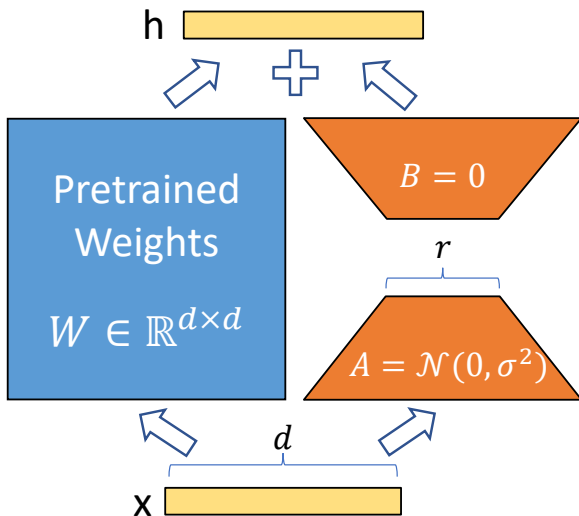
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- Поддержка CPU-offload, mixed-precision, активационного checkpointinga.
- Минимальный пример:

```
import torch
from torch.distributed.fsdp import FullyShardedDataParallel as FSDP
torch.cuda.set_device(device_id)
sharded_module = FSDP(my_module)
optim = torch.optim.SGD(sharded_module.parameters(), lr=0.0001)
x = sharded_module(x, y=3, z=torch.Tensor([1]))
loss = x.sum()
loss.backward()
optim.step()
```

¹⁷PyTorch docs

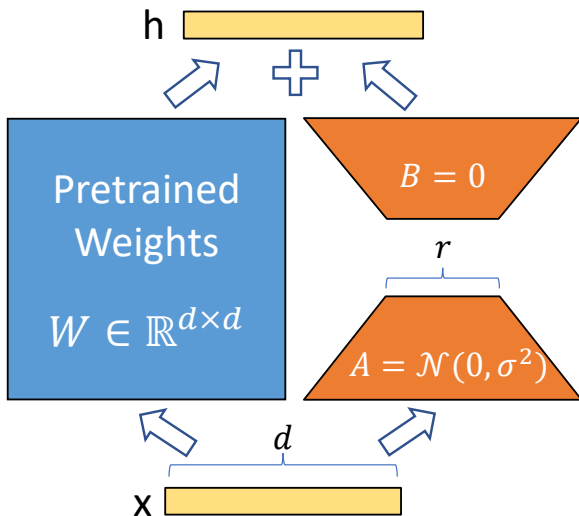


LoRA reduces the number of parameters by approximating weight matrices with low-rank factorization:

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

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

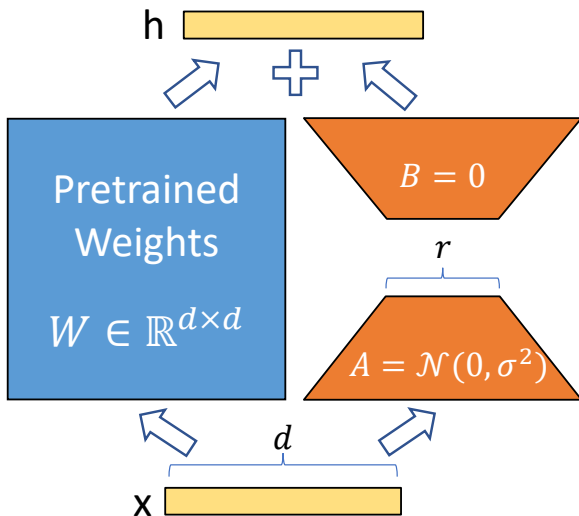


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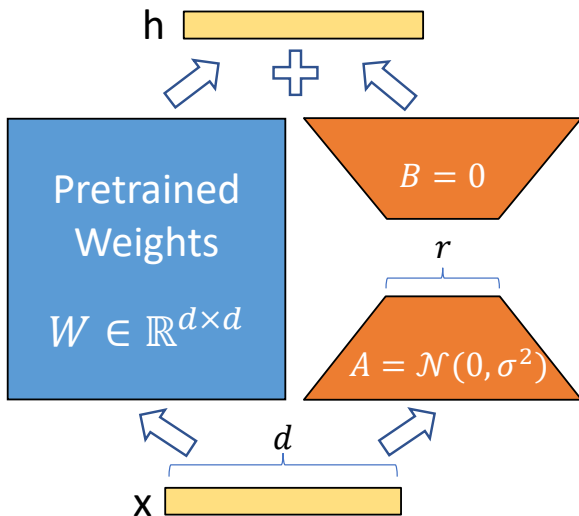


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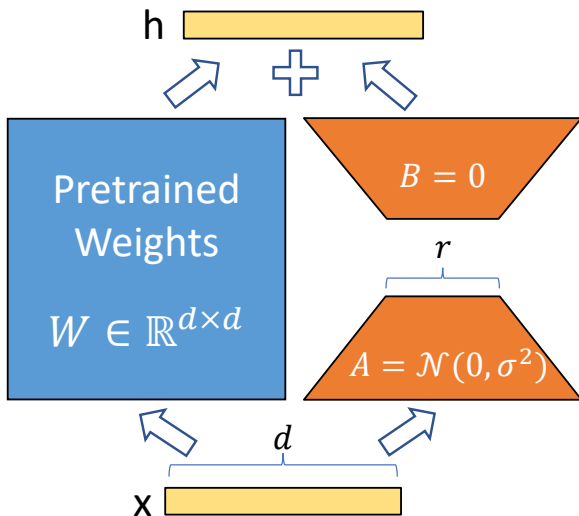


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$$h = W_{\text{new}}x = Wx + \Delta Wx = Wx + AB^Tx$$

Feedforward Architecture

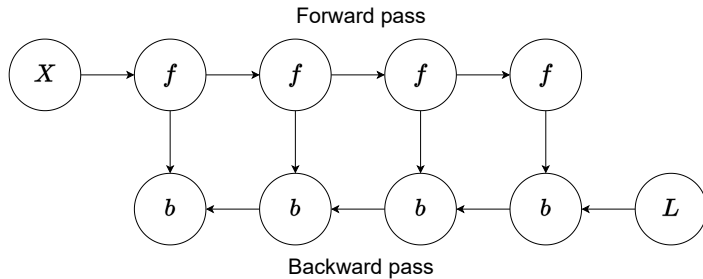


Рисунок 12: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an f . The gradient of the loss with respect to the activations and parameters marked with b .

Feedforward Architecture

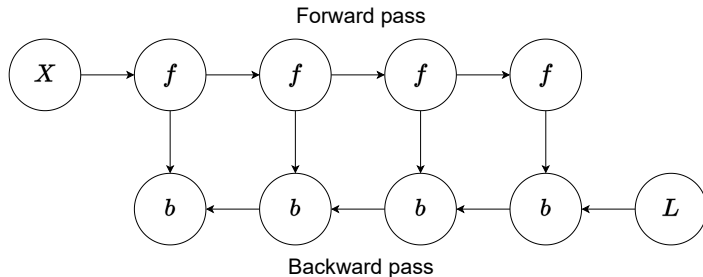


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! Важное уведомление

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

Vanilla backpropagation

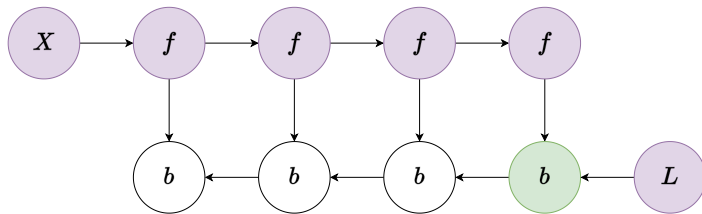


Рисунок 13: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Vanilla backpropagation

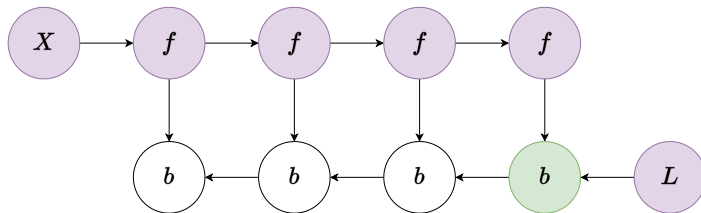


Рисунок 13: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

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

Vanilla backpropagation

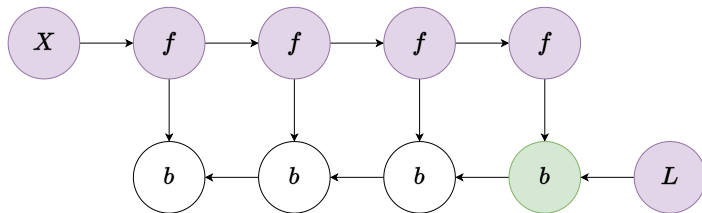


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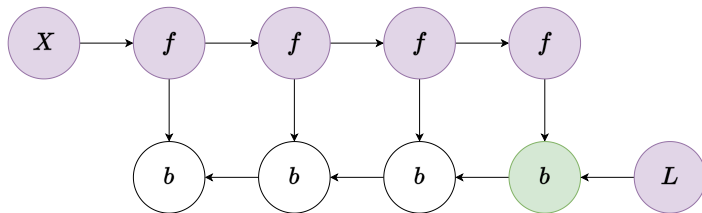


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- Optimal in terms of computation: it only computes each node once.

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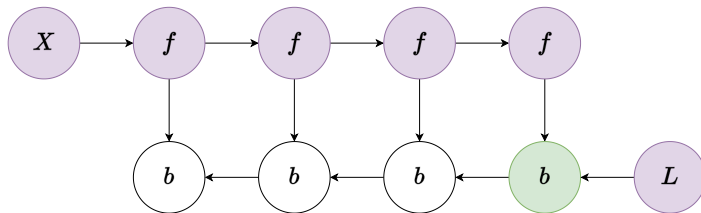


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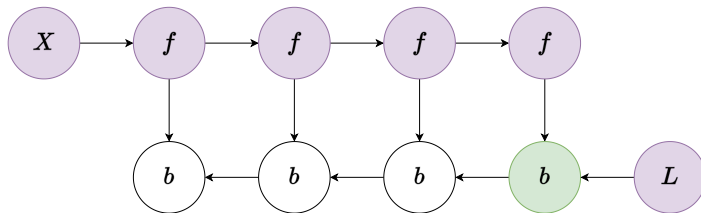


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- All activations f are kept in memory after the forward pass.
- Optimal in terms of computation: it only computes each node once.
- High memory usage. The memory usage grows linearly with the number of layers in the neural network.

Memory poor backpropagation

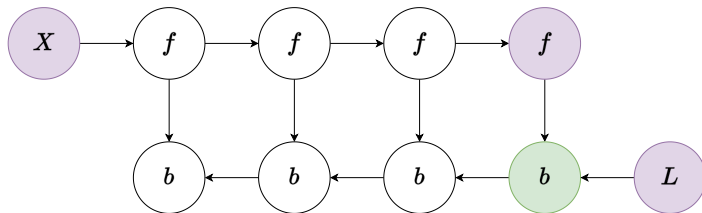


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Memory poor backpropagation

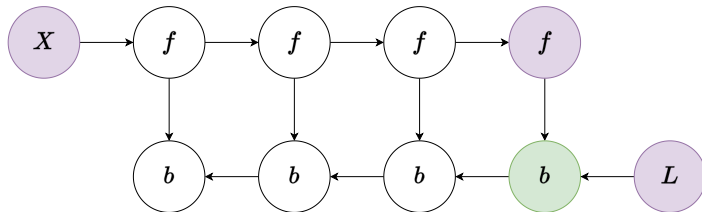


Рисунок 14: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- Each activation f is recalculated as needed.

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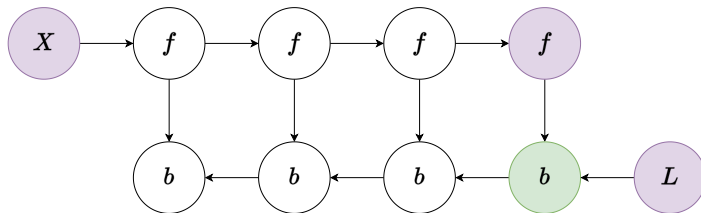


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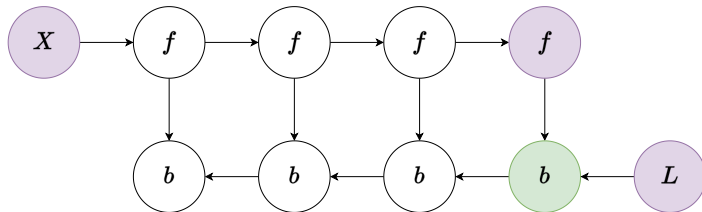


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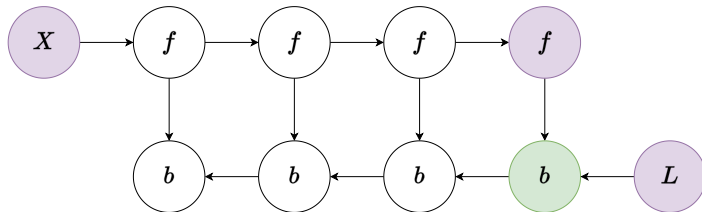


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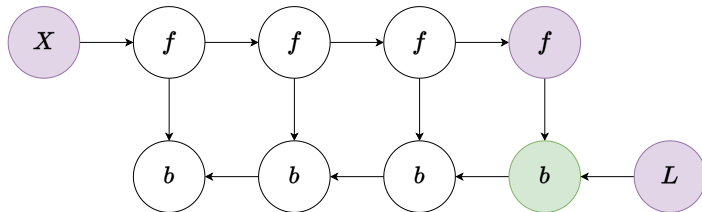


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- Each activation f is recalculated as needed.
- Optimal in terms of memory: there is no need to store all activations in memory.
- Computationally inefficient. The number of node evaluations scales with n^2 , whereas it vanilla backprop scaled as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

Checkpointed backpropagation

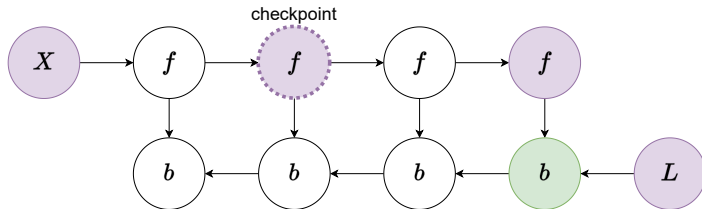


Рисунок 15: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

Checkpointed backpropagation

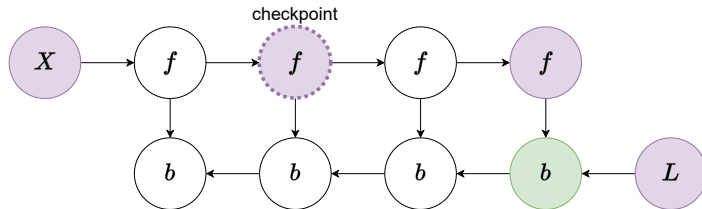


Рисунок 15: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

- 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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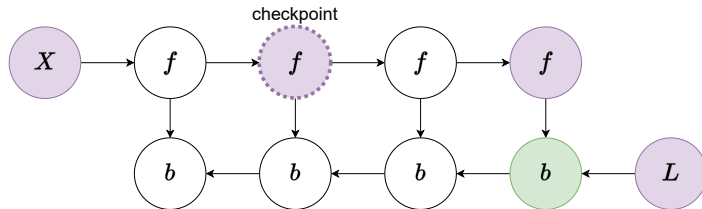


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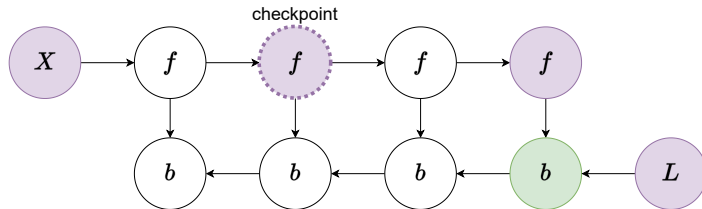


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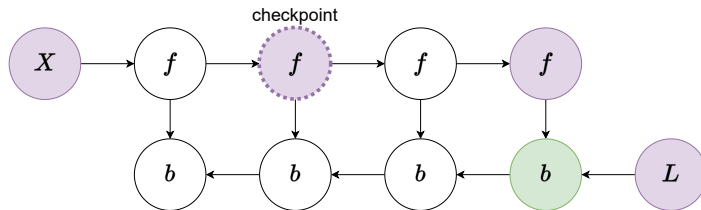


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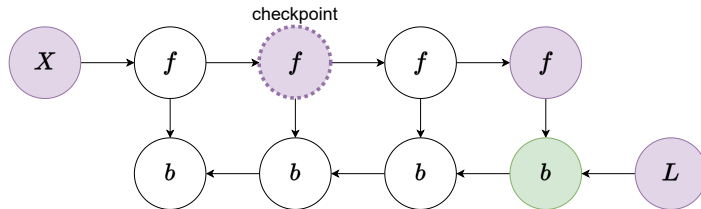




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- Faster recalculation of activations f . We only need to recompute the nodes between a b node and the last checkpoint preceding it when computing that b node during backprop.
- Memory consumption depends on the number of checkpoints. More effective 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 factors ¹⁹

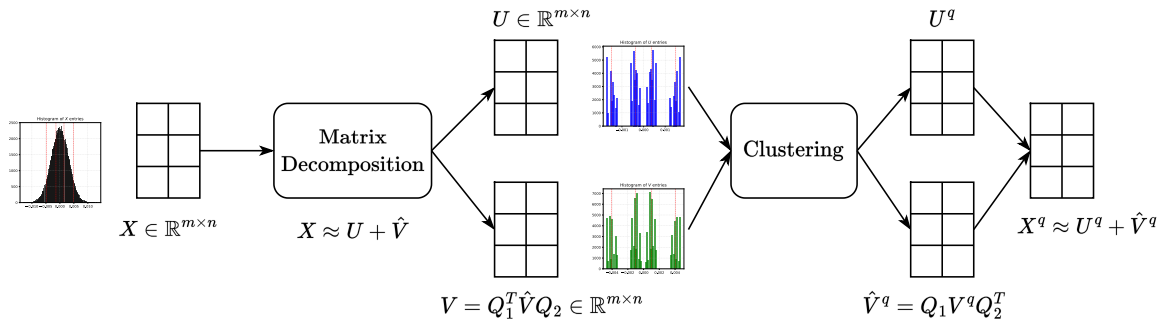


Рисунок 16: Scheme of post-training quantization approach.

¹⁹Quantization of Large Language Models with an Overdetermined Basis