



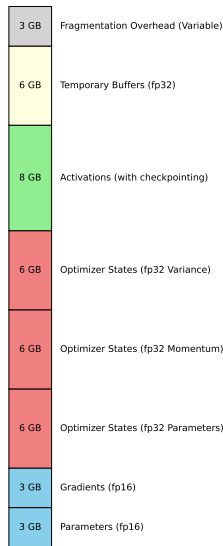
Large models training. Bonus: newton and quasinewton methods

Daniil Merkulov

Applied Math for Data Science. Sberuniversity.

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.

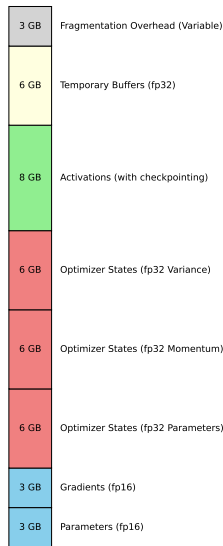
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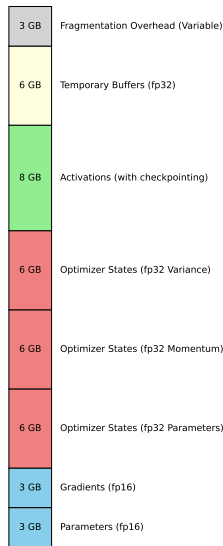
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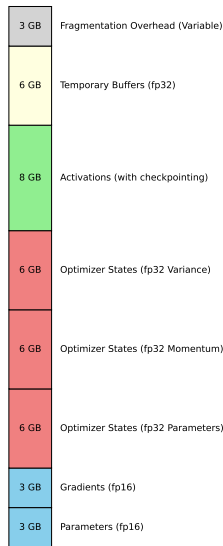
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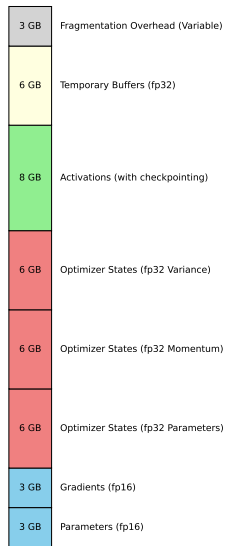
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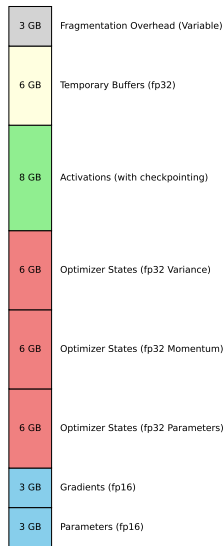
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Residual Memory Consumption:

- Activations: Significant memory usage, e.g., 1.5B parameter GPT-2 model with sequence length 1K and batch size 32 requires ~60GB.
- Activation checkpointing can reduce activation memory by about 50%, with a 33% recomputation overhead.

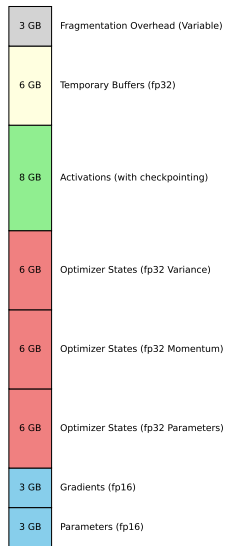
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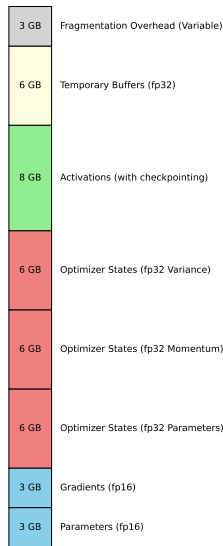
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- Store intermediate results; e.g., gradient all-reduce operations fuse gradients into a single buffer.

Memory Fragmentation:



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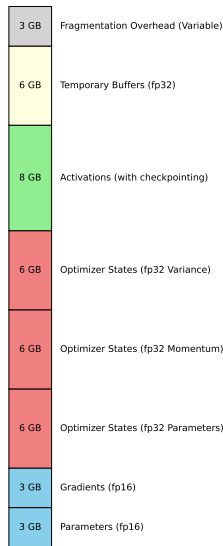
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- Store intermediate results; e.g., gradient all-reduce operations fuse gradients into a single buffer.
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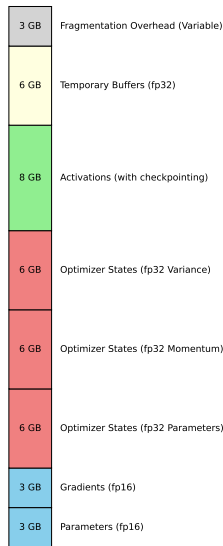
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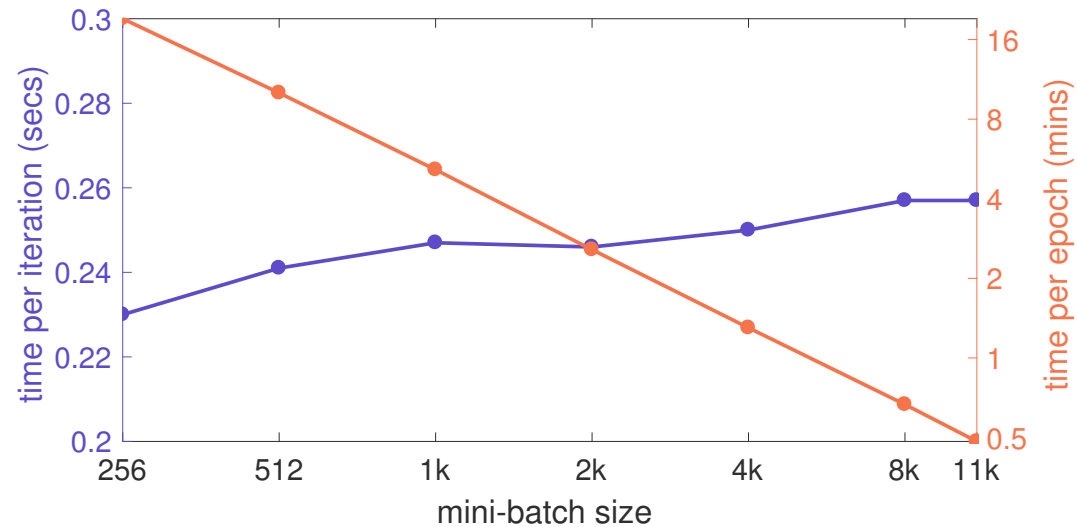
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Memory Fragmentation:

- 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.

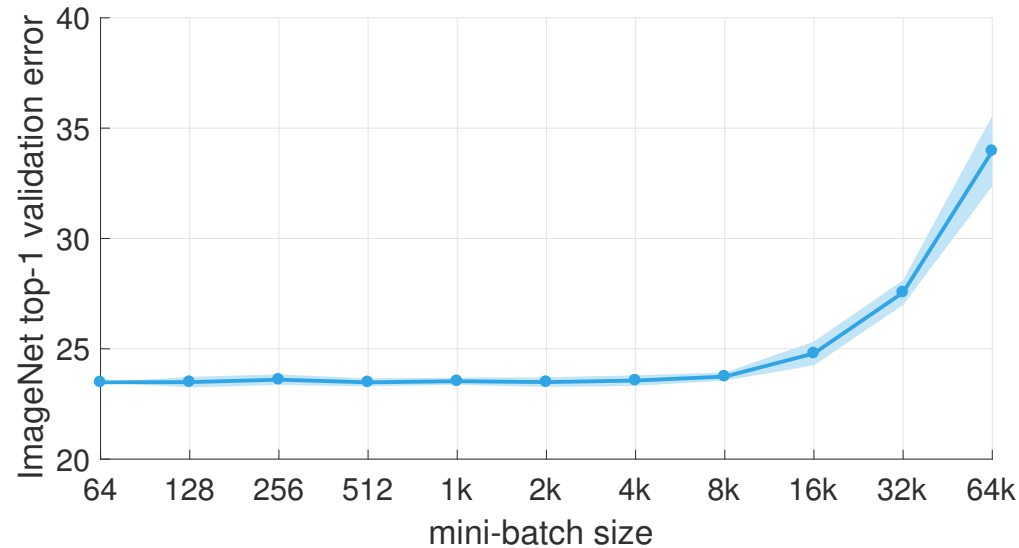
Large batch training

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.

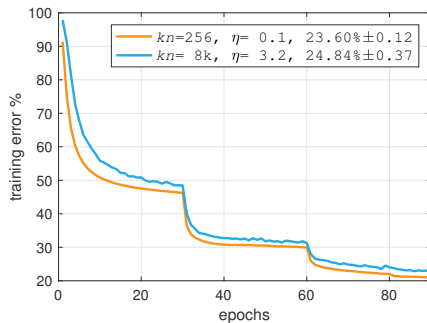


Figure 1: no warmup

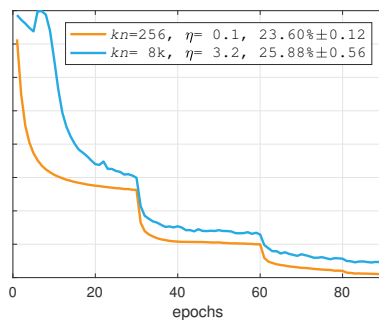


Figure 2: constant warmup

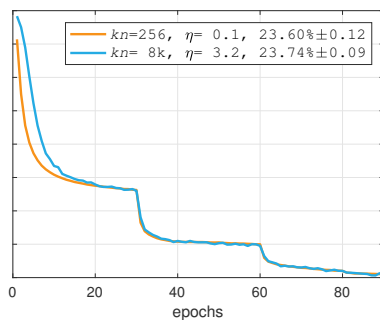


Figure 3: gradual warmup

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()  
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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()
```

MultiGPU training

Data Parallel training

1. Parameter server sends the full copy of the model to each device

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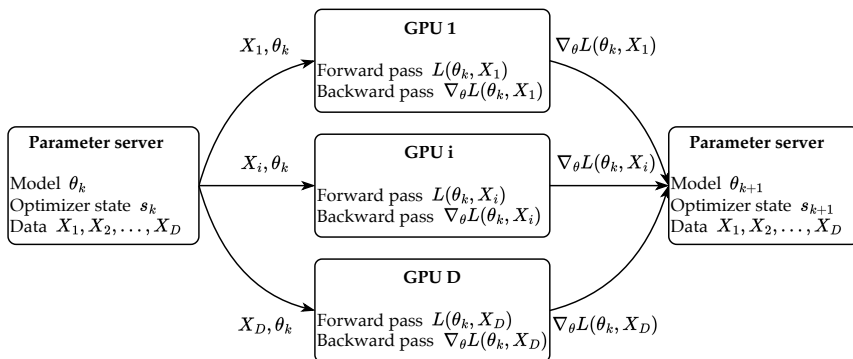
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Per device batch size: b . Overall batchsize: Db . Data parallelism involves splitting the data across multiple GPUs, each with a copy of the model. Gradients are averaged and weights updated synchronously:



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.

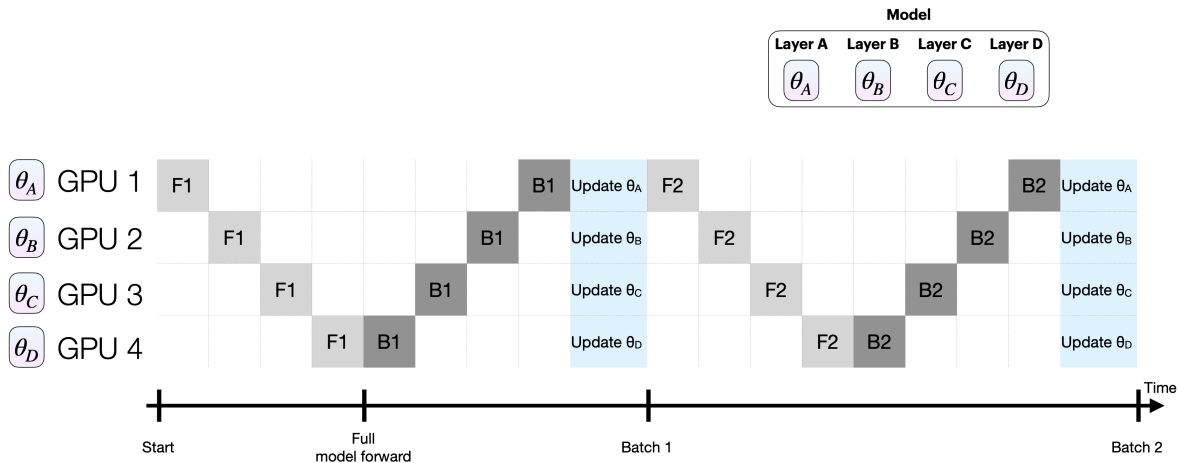


Figure 5: Model parallelism

	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

Automatic Mixed Precision training

Two copies of the models needed to be stored - fp32 and fp16 (fp8). Rewrite the computational graph with respect to the following idea:

Numerically-Safe plus
Performance Critical
(always in fp16/fp8)

Convolution & Matmul

In accelerate:

Numerically-Neutral
(Context-Dependent)

Max, min

Numerically-Safe
(Conditional,
Context-Dependent)

Activations

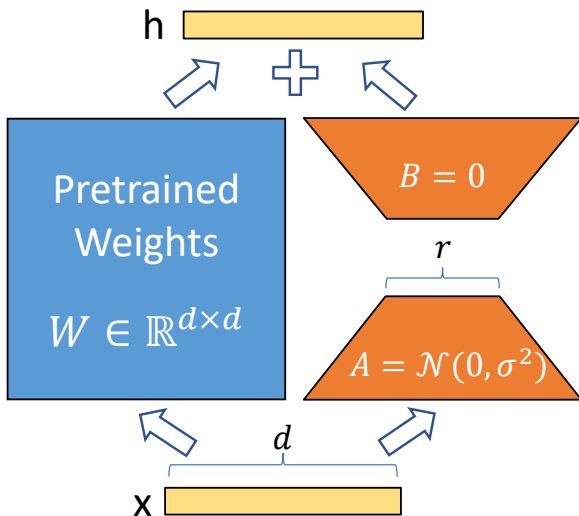
Numerically-Dangerous
(Always in fp32)

Exp, Log, Pow, Softmax,
Reduction Sum, Mean

```
torch.cuda.amp.autocast(dtype=torch.float16)(model_forward_func)
```

or

```
torch.autocast(device_type=self.device.type, dtype=torch.bfloat16)(model_forward_func)
```

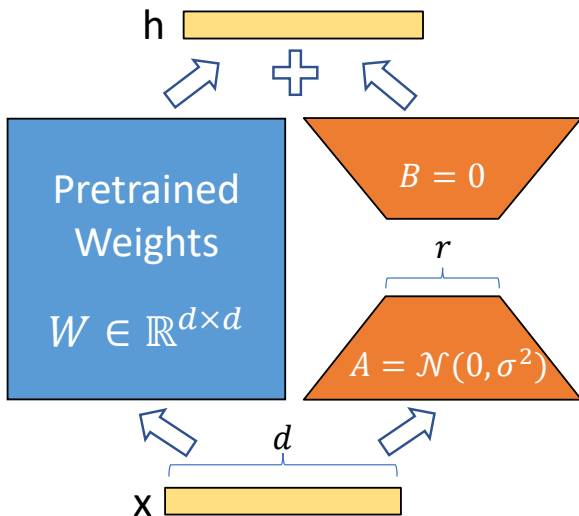


LoRA reduces the number of parameters by approximating weight matrices with low-rank factorization:

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

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

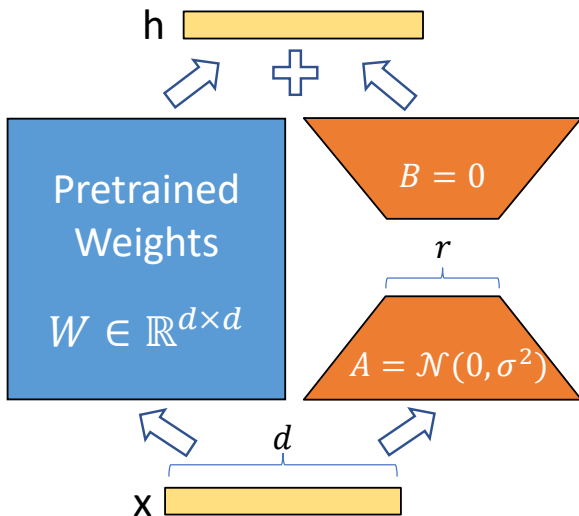


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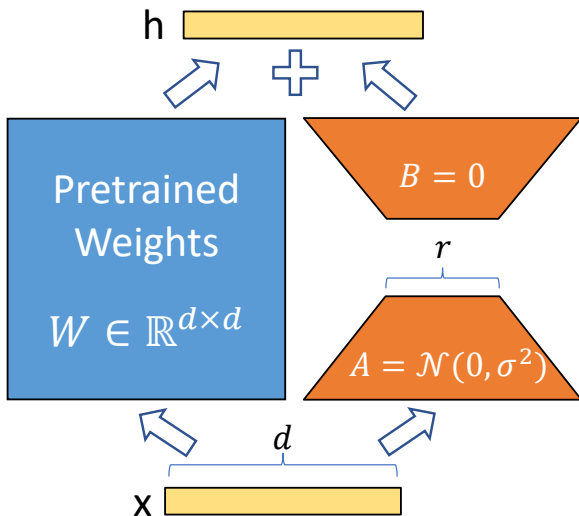


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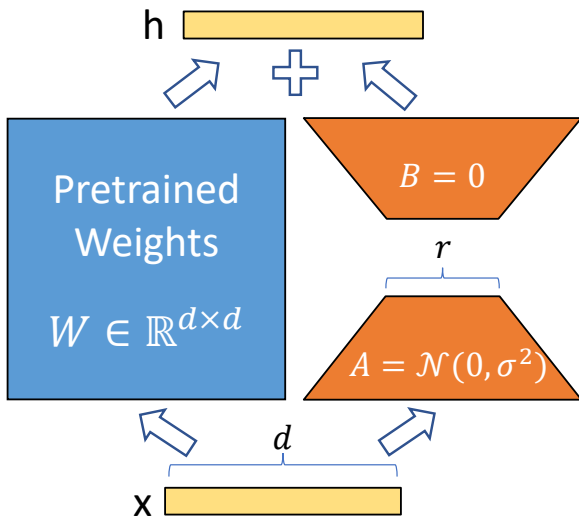
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$$h = W_{\text{new}}x = Wx + \Delta Wx = Wx + AB^Tx$$

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Feedforward Architecture

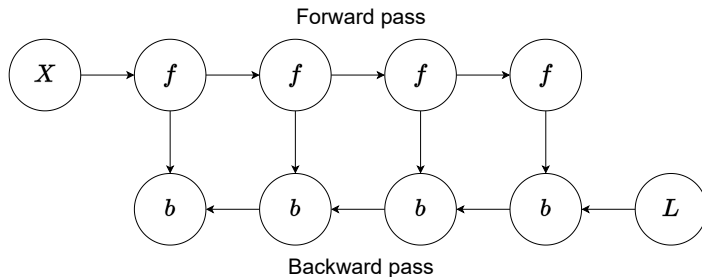


Figure 6: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The activations marked with an f . The gradient of the loss with respect to the activations and parameters marked with b .

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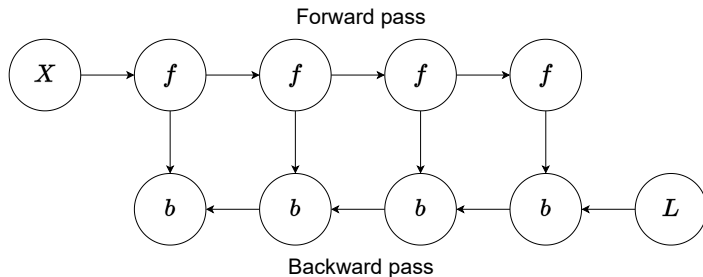


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! Important

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

Vanilla backpropagation



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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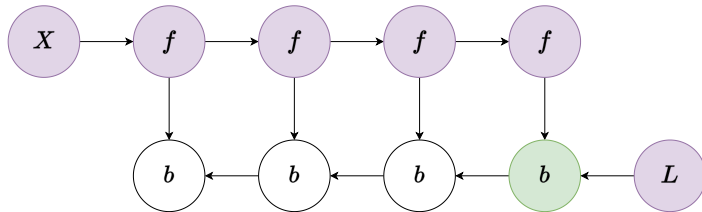


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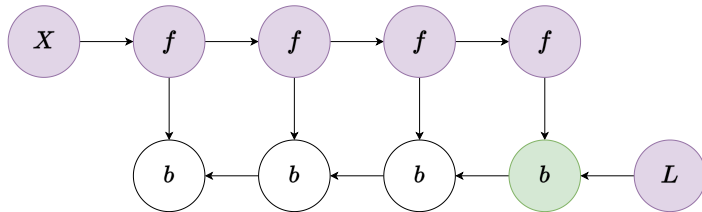


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- Optimal in terms of computation: it only computes each node once.
- High memory usage. The memory usage grows linearly with the number of layers in the neural network.

Memory poor backpropagation

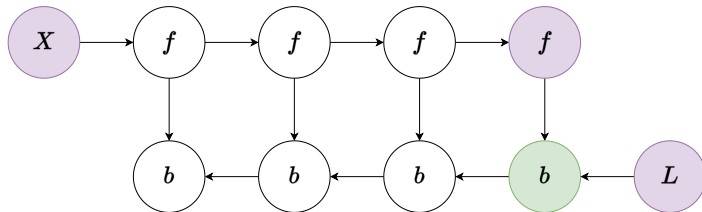


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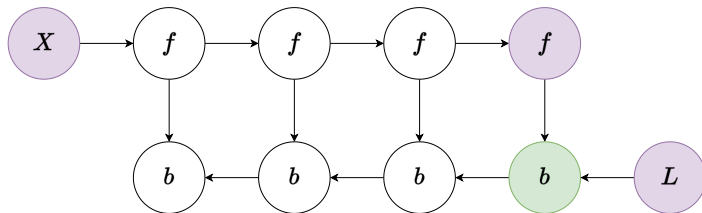


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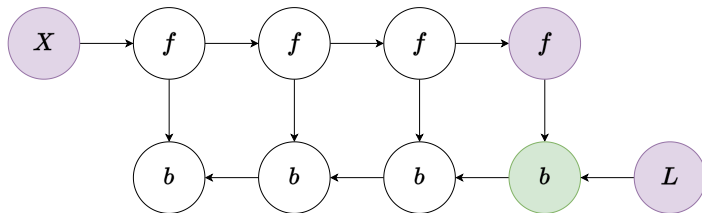


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- Each activation f is recalculated as needed.
- Optimal in terms of memory: there is no need to store all activations in memory.
- Computationally inefficient. The number of node evaluations scales with n^2 , whereas it vanilla backprop scaled as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

Checkpointed backpropagation



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Checkpointed backpropagation

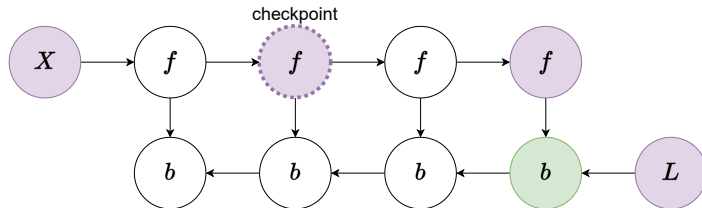


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- Trade-off between the **vanilla** and **memory poor** approaches. The strategy is to mark a subset of the neural net activations as checkpoint nodes, that will be stored in memory.

Checkpointed backpropagation

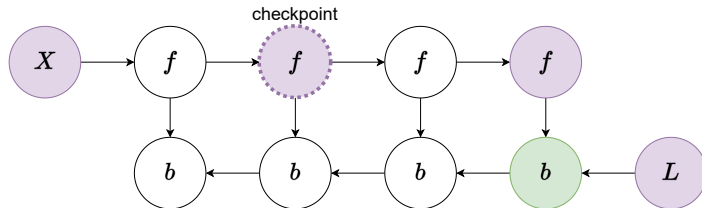


Figure 9: Computation graph for obtaining gradients for a simple feed-forward neural network with n layers. The purple color indicates nodes that are stored in memory.

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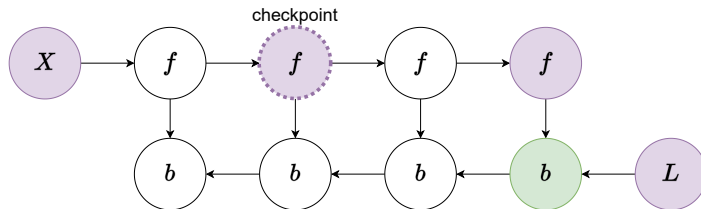


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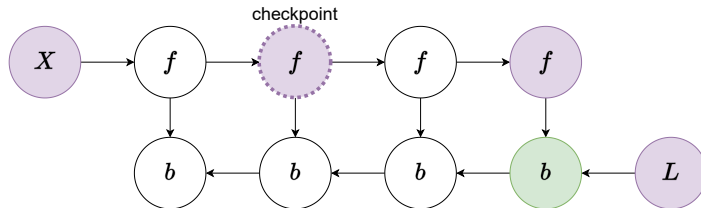


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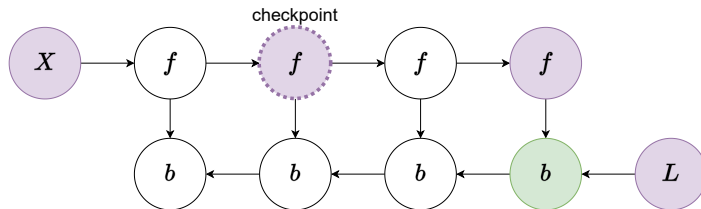


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- Memory consumption depends on the number of checkpoints. More effective than **vanilla** approach.

Gradient checkpointing visualization

The animated visualization of the above approaches 

An example of using a gradient checkpointing 

Quantization

Split the weight matrix into 2 well clustered factors ¹²

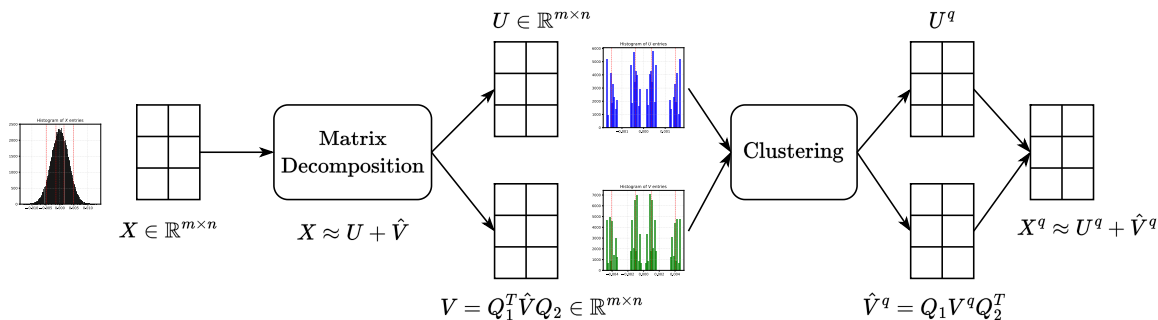


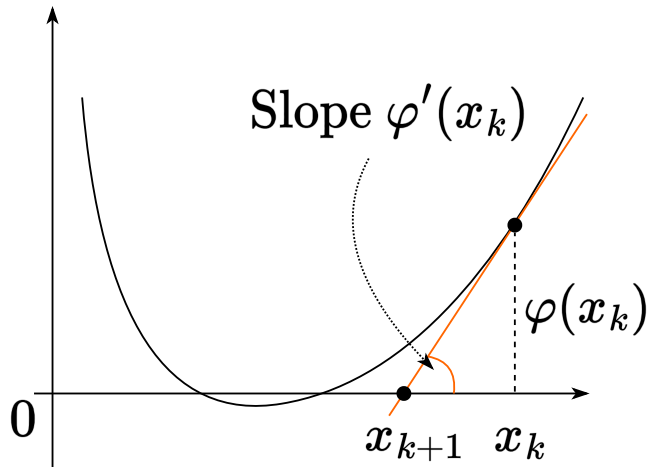
Figure 10: Scheme of post-training quantization approach.

¹²Quantization of Large Language Models with an Overdetermined Basis

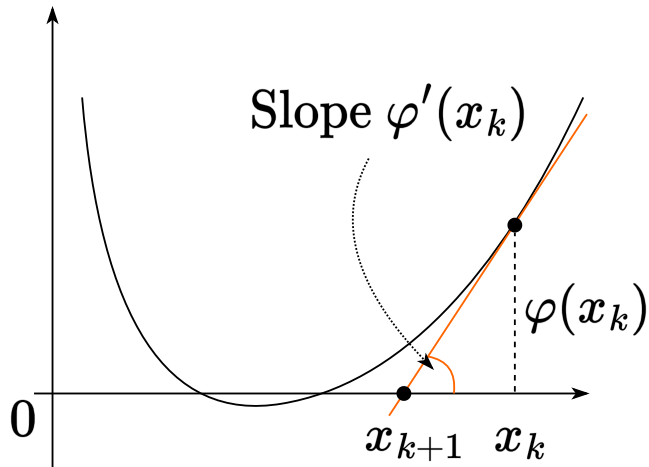
Newton method

Idea of Newton method of root finding

Consider the function $\varphi(x) : \mathbb{R} \rightarrow \mathbb{R}$.



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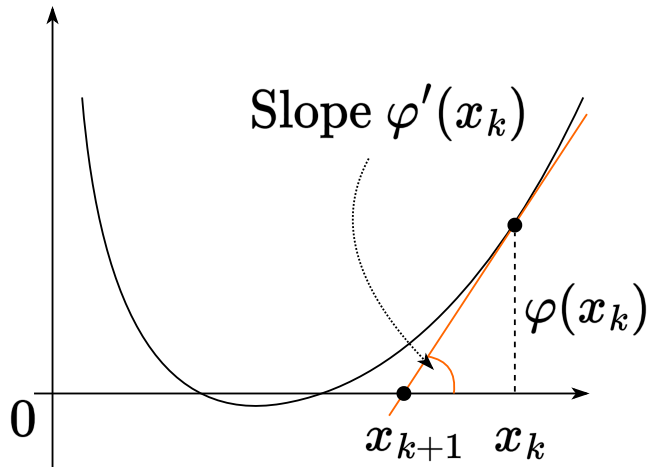
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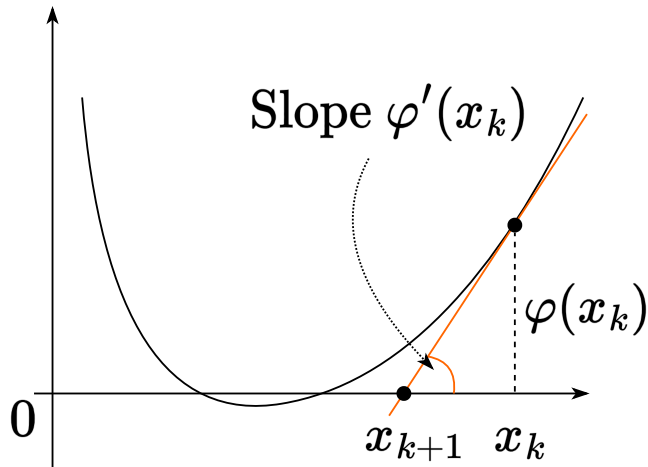
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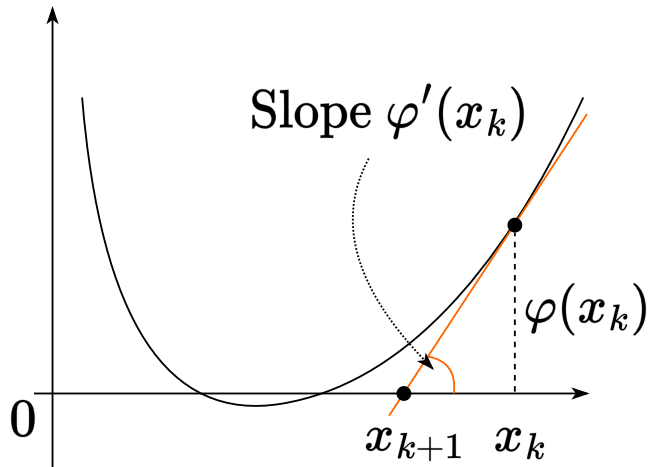
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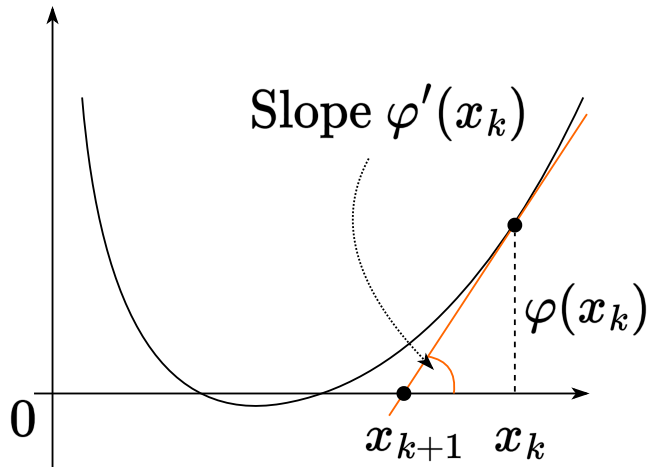
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$$x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

^aLiterally we aim to solve the problem of finding stationary points $\nabla f(x) = 0$

Newton method as a local quadratic Taylor approximation minimizer

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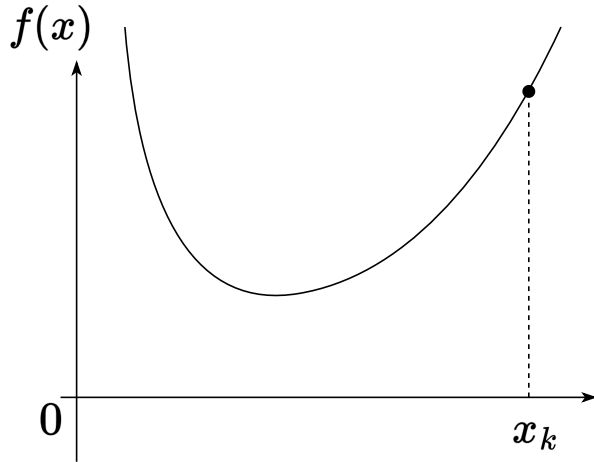
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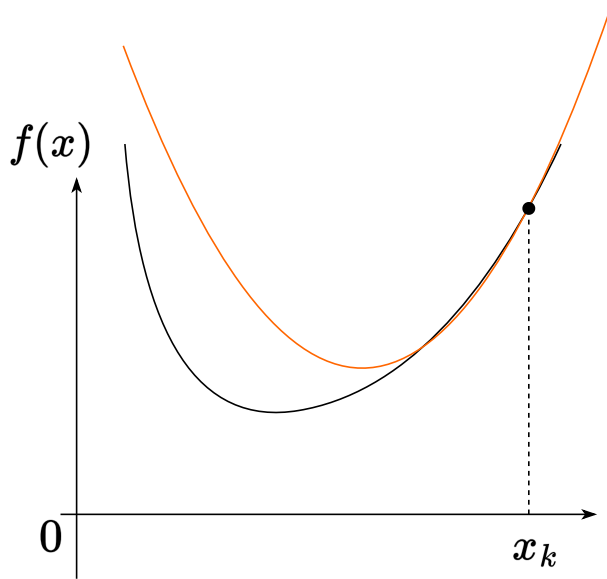
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Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

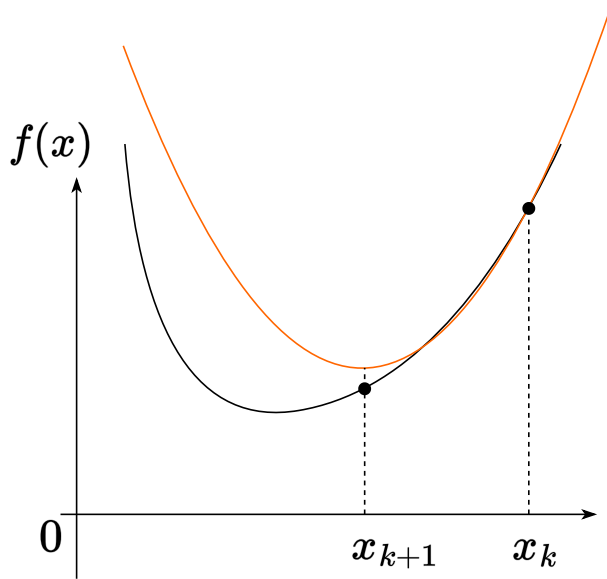
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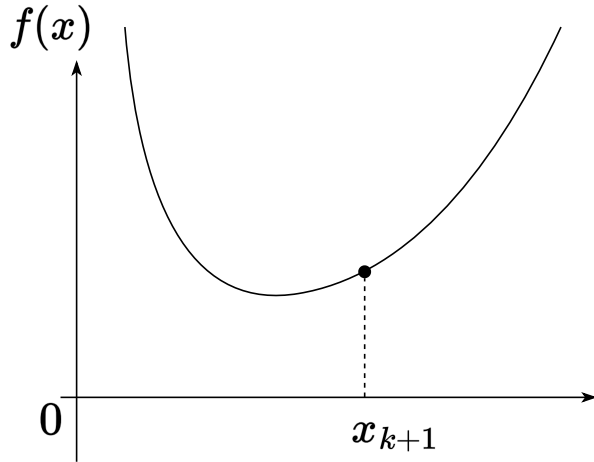
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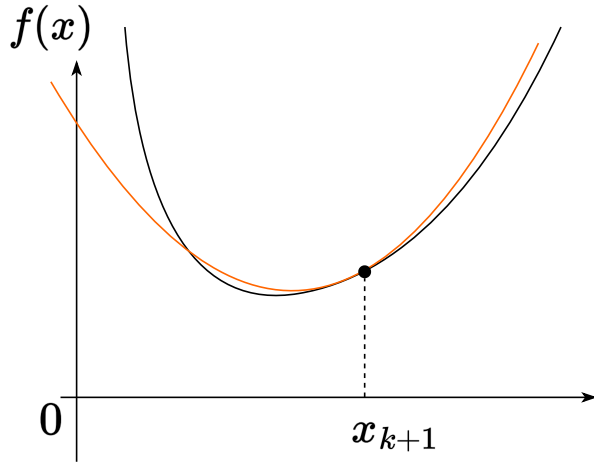
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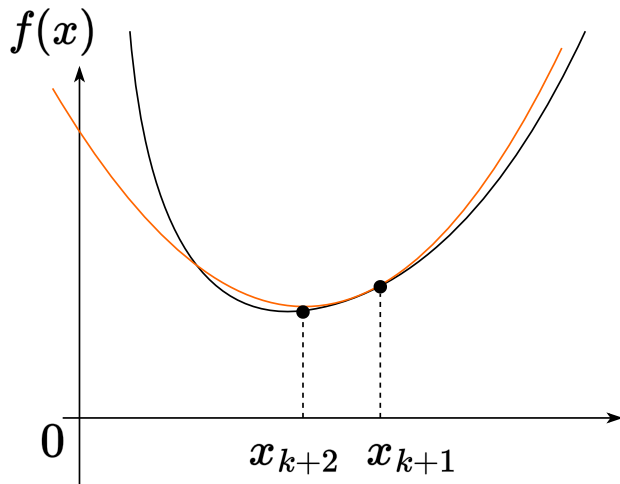
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Newton method as a local quadratic Taylor approximation minimizer



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Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at \mathbb{R}^n , for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M -Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Thus, we have an important result: Newton's method for the function with Lipschitz positive-definite Hessian converges **quadratically** near ($\|x_0 - x^*\| < \frac{2\mu}{3M}$) to the solution.

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

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This shows that the progress made by Newton's method is independent of problem scaling. This property is not shared by the gradient descent method!

Summary

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- it is necessary to solve linear systems: $\mathcal{O}(n^3)$ operations
- the Hessian can be degenerate at x^*
- the hessian may not be positively determined \rightarrow direction $-(f''(x))^{-1}f'(x)$ may not be a descending direction

Newton

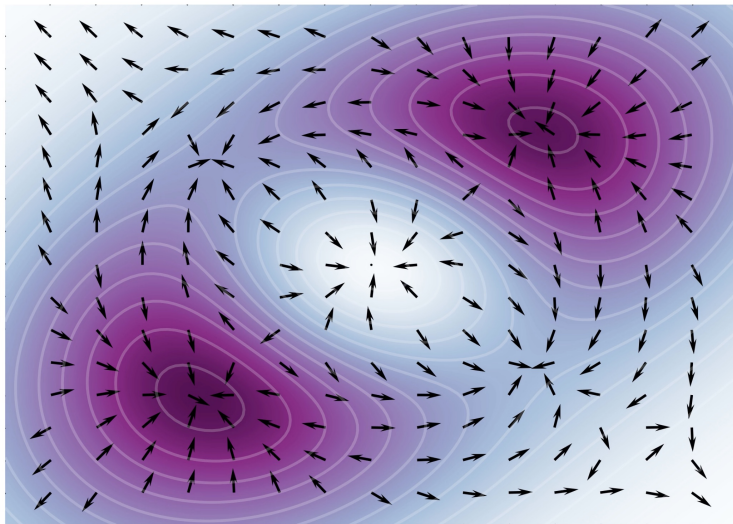



Figure 17: Animation 

Newton method problems

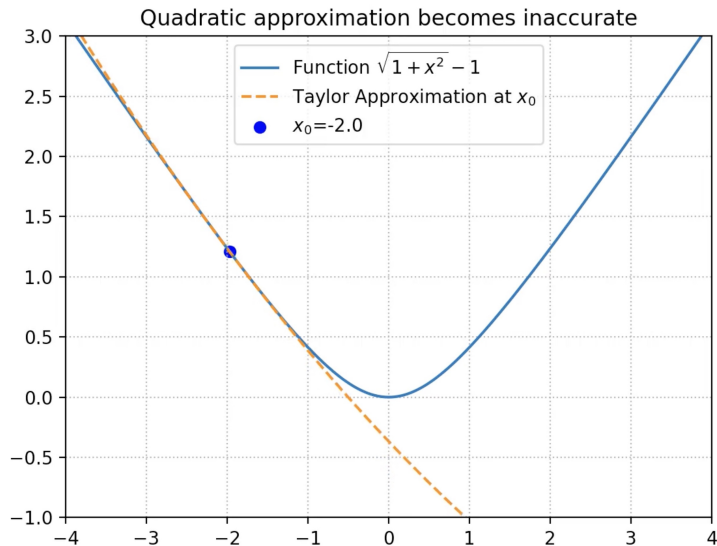


Figure 18: Animation

The idea of adaptive metrics

Given $f(x)$ and a point x_0 . Define

$B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0 . Here we presume the existence of a distance function $d(x, x_0)$.

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Let us assume that the distance is defined locally by some metric A :

$$d(x, x_0) = (x - x_0)^\top A(x - x_0)$$

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$B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0 . Here we presume the existence of a distance function $d(x, x_0)$.

$$x^* = \arg \min_{x \in B_\varepsilon(x_0)} f(x)$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$s = \lim_{\varepsilon \rightarrow 0} \frac{x^* - x_0}{\varepsilon}$$

Let us assume that the distance is defined locally by some metric A :

$$d(x, x_0) = (x - x_0)^\top A (x - x_0)$$

Let us also consider first order Taylor approximation of a function $f(x)$ near the point x_0 :

$$f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \quad (1)$$

Now we can explicitly pose a problem of finding s , as it was stated above.

$$\begin{aligned} \min_{\delta x \in \mathbb{R}^n} & f(x_0 + \delta x) \\ \text{s.t. } & \delta x^\top A \delta x = \varepsilon^2 \end{aligned}$$

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Which means, that new direction of steepest descent is nothing else, but $A^{-1} \nabla f(x_0)$.

(1) . . . Indeed, if the space is isotropic and $A = I$, we immediately have gradient descent formula, while Newton method uses local Hessian as a metric matrix.    36

Quasi-Newton methods

Quasi-Newton methods intuition

For the classic task of unconditional optimization $f(x) \rightarrow \min_{x \in \mathbb{R}^n}$ the general scheme of iteration method is written as:

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Note here that if we take a single matrix of $B_k = I_n$ as B_k at each step, we will exactly get the gradient descent method.

The general scheme of quasi-Newton methods is based on the selection of the B_k matrix so that it tends in some sense at $k \rightarrow \infty$ to the truth value of the Hessian $\nabla^2 f(x_k)$.

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \dots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$

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- $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$

Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + \alpha uu^T$$

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Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + a u u^T$$

The secant equation $B_{k+1} d_k = \Delta y_k$ yields:

$$(a u^T d_k) u = \Delta y_k - B_k d_k$$

This only holds if u is a multiple of $\Delta y_k - B_k d_k$. Putting $u = \Delta y_k - B_k d_k$, we solve the above,

$$a = \frac{1}{(\Delta y_k - B_k d_k)^T d_k},$$

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which leads to

$$B_{k+1} = B_k + \frac{(\Delta y_k - B_k d_k)(\Delta y_k - B_k d_k)^T}{(\Delta y_k - B_k d_k)^T d_k}$$

called the symmetric rank-one (SR1) update or Broyden method.

Symmetric Rank-One Update with inverse

How can we solve

$$B_{k+1}d_{k+1} = -\nabla f(x_{k+1}),$$

in order to take the next step? In addition to propagating B_k to B_{k+1} , let's propagate inverses, i.e., $C_k = B_k^{-1}$ to $C_{k+1} = (B_{k+1})^{-1}$.

Sherman-Morrison Formula:

The Sherman-Morrison formula states:

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1}u}$$

Thus, for the SR1 update, the inverse is also easily updated:

$$C_{k+1} = C_k + \frac{(d_k - C_k \Delta y_k)(d_k - C_k \Delta y_k)^T}{(d_k - C_k \Delta y_k)^T \Delta y_k}$$

In general, SR1 is simple and cheap, but it has a key shortcoming: it does not preserve positive definiteness.

Davidon-Fletcher-Powell Update

We could have pursued the same idea to update the inverse C :

$$C_{k+1} = C_k + auu^T + bv v^T.$$

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$$C_{k+1} = C_k + a u u^T + b v v^T.$$

Multiplying by Δy_k , using the secant equation $d_k = C_k \Delta y_k$, and solving for a , b , yields:

$$C_{k+1} = C_k - \frac{C_k \Delta y_k \Delta y_k^T C_k}{\Delta y_k^T C_k \Delta y_k} + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

Woodbury Formula Application

Woodbury then shows:

$$B_{k+1} = \left(I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k} \right) B_k \left(I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k} \right) + \frac{\Delta y_k \Delta y_k^T}{\Delta y_k^T d_k}$$

This is the Davidon-Fletcher-Powell (DFP) update. Also cheap: $O(n^2)$, preserves positive definiteness. Not as popular as BFGS.

Broyden-Fletcher-Goldfarb-Shanno update

Let's now try a rank-two update:

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Putting $u = \Delta y_k$, $v = B_k d_k$, and solving for a, b we get:

$$B_{k+1} = B_k - \frac{B_k d_k d_k^T B_k}{d_k^T B_k d_k} + \frac{\Delta y_k \Delta y_k^T}{d_k^T \Delta y_k}$$

called the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update.

Broyden-Fletcher-Goldfarb-Shanno update with inverse

Woodbury Formula

The Woodbury formula, a generalization of the Sherman-Morrison formula, is given by:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

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Applied to our case, we get a rank-two update on the inverse C :

$$C_{k+1} = C_k + \frac{(d_k - C_k \Delta y_k) d_k^T}{\Delta y_k^T d_k} + \frac{d_k (d_k - C_k \Delta y_k)^T}{\Delta y_k^T d_k} - \frac{(d_k - C_k \Delta y_k)^T \Delta y_k}{(\Delta y_k^T d_k)^2} d_k d_k^T$$

$$C_{k+1} = \left(I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k} \right) C_k \left(I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k} \right) + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

This formulation ensures that the BFGS update, while comprehensive, remains computationally efficient, requiring $O(n^2)$ operations. Importantly, BFGS update preserves positive definiteness. Recall this means $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$. Equivalently, $C_k \succ 0 \Rightarrow C_{k+1} \succ 0$

Code

- Open In Colab

Code

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