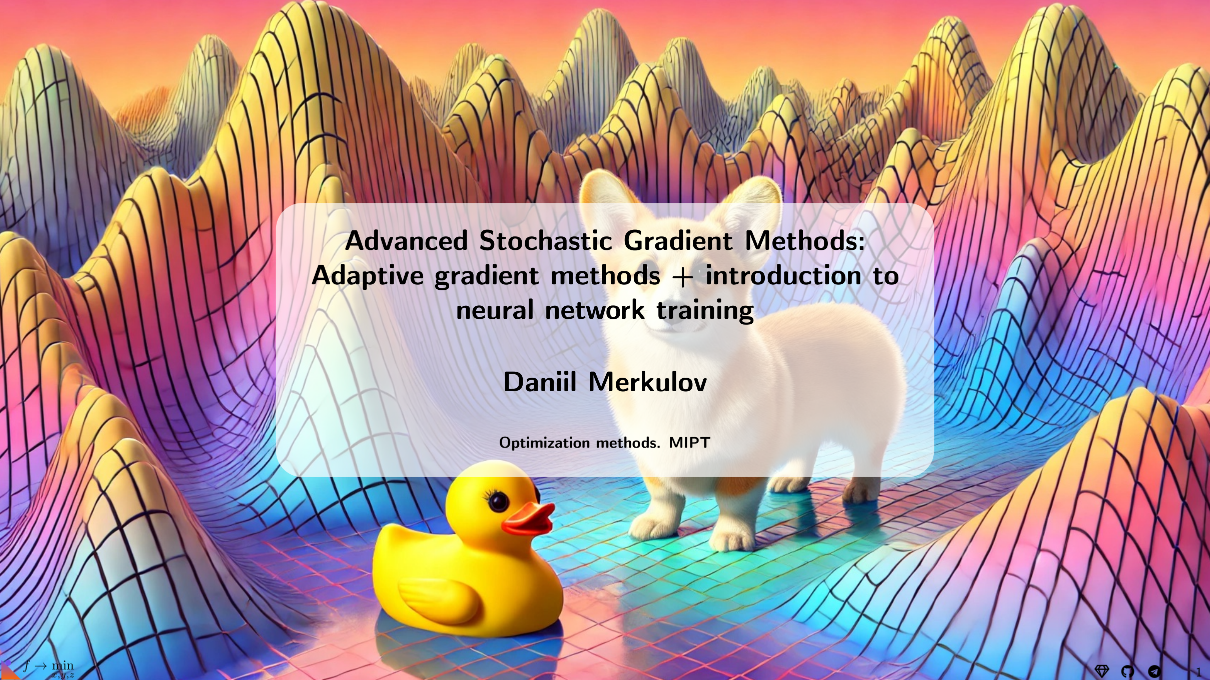

Advanced Stochastic Gradient Methods: Adaptive gradient methods + introduction to neural network training

Daniil Merkulov

Optimization methods. MIPT

Finite-sum problem

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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:

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

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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:

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

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 $f(x)$.

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
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x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}
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- 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 $j = 1, \dots, p$:

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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:

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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) [1] [2]

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

EMA:

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- Гораздо лучше работает для языковых моделей, чем для задач компьютерного зрения - почему?

[1] Adam: A Method for Stochastic Optimization

[2] On the Convergence of Adam and Beyond

AdamW (Loshchilov & Hutter, 2017)

Addresses a common issue with ℓ_2 regularization in adaptive optimizers like Adam. Standard ℓ_2 regularization adds $\lambda\|x\|^2$ to the loss, resulting in a gradient term λx. In Adam, this term gets scaled by the adaptive learning rate $\left(\sqrt{\hat{v}_j} + \epsilon\right)$, coupling the weight decay to the gradient magnitudes.

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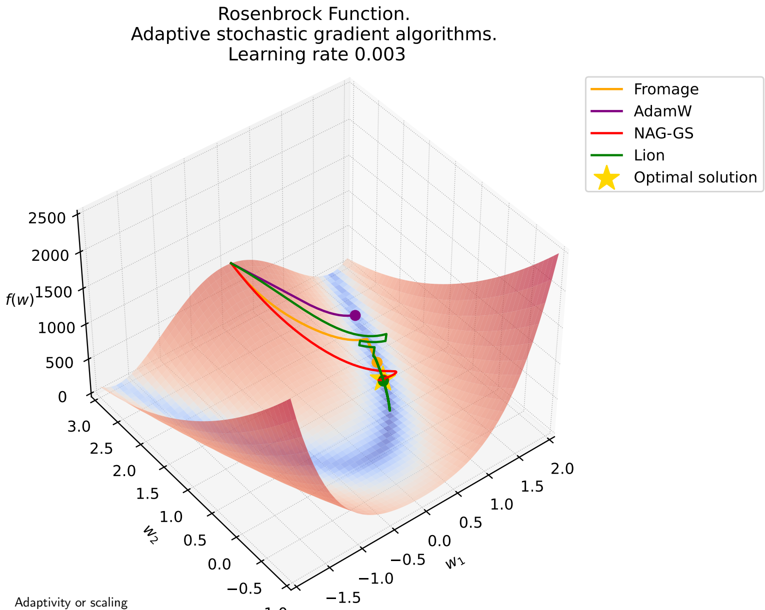
- Widely adopted in training transformers and other large models. Default choice for huggingface trainer.

A lot of them



Rosenbrock Function.
Adaptive stochastic gradient algorithms.
Learning rate 0.003
Fromage
AdamW
NAG-GS
Lion
Optimal solution
2500
2000
$f(w)$1500
1000
500
0
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
w_2
2.0
1.5
1.0
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w_1

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- **Computational Cost:** Scoring required $\sim 49,240$ total hours on 8x NVIDIA V100 GPUs (avg. ~ 3469h/external, ~ 1847h/self-tuning submission).

[3] Benchmarking Neural Network Training Algorithms

[4] Accelerating neural network training: An analysis of the AlgoPerf competition

AlgoPerf benchmark

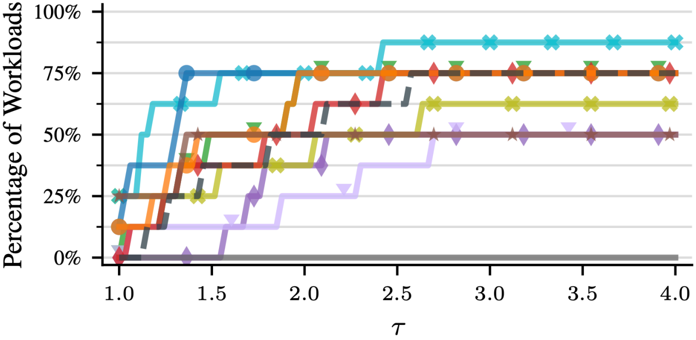
Summary of *fixed* base workloads in the AlgoPerf benchmark. Losses include cross-entropy (CE), mean absolute error (L1), and Connectionist Temporal Classification loss (CTC). Additional evaluation metrics are structural similarity index measure (SSIM), (word) error rate (ER & WER), mean average precision (mAP), and bilingual evaluation understudy score (BLEU). The \runtime budget is that of the external tuning ruleset, the self-tuning ruleset allows $3\times$ longer training.

Task	Dataset	Model	Loss	Metric	Validation Target	Runtime Budget
Clickthrough rate prediction	CRITEO 1TB	DLRMSMALL	CE	CE	0.123735	7703
MRI reconstruction	FASTMRI	U-NET	L1	SSIM	0.7344	8859
Image classification	IMAGENET	ResNet-50	CE	ER	0.22569	63,008
		ViT	CE	ER	0.22691	77,520
Speech recognition	LIBRISPEECH	Conformer	CTC	WER	0.085884	61,068
		DeepSpeech	CTC	WER	0.119936	55,506
Molecular property prediction	OGBG	GNN	CE	mAP	0.28098	18,477
Translation	WMT	Transformer	CE	BLEU	30.8491	48,151

AlgoPerf benchmark

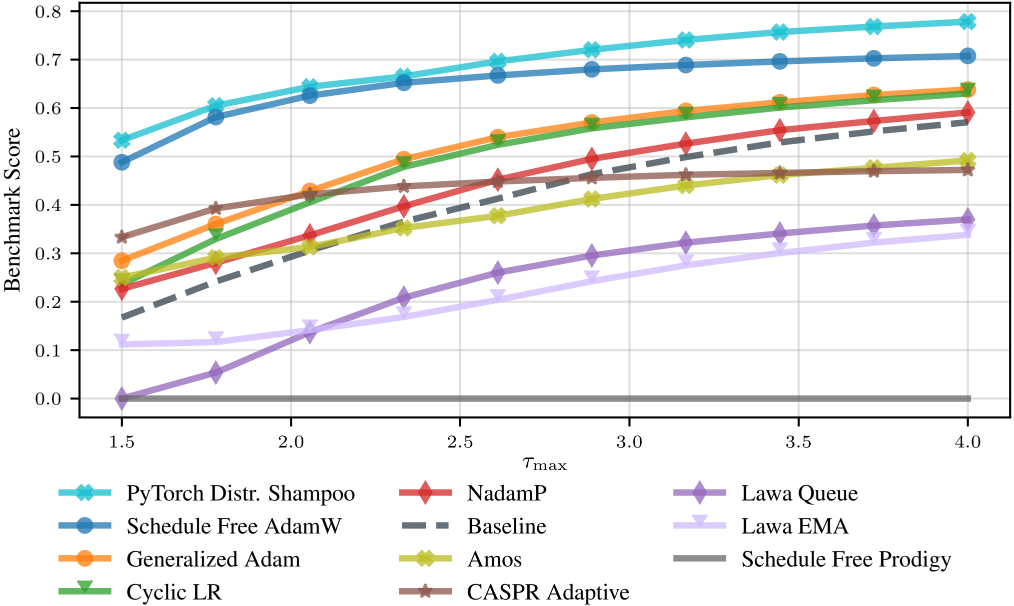
Submission	Line	Score
PyTorch Distributed Shampoo		0.7784
Schedule Free AdamW		0.7077
Generalized Adam		0.6383
Cyclic LR		0.6301
NadamP		0.5909
Baseline		0.5707
Amos		0.4918
CASPR Adaptive		0.4722
LAWA Queue		0.3699
LAWA EMA		0.3384
Schedule Free Prodigy		0

(a) External tuning leaderboard

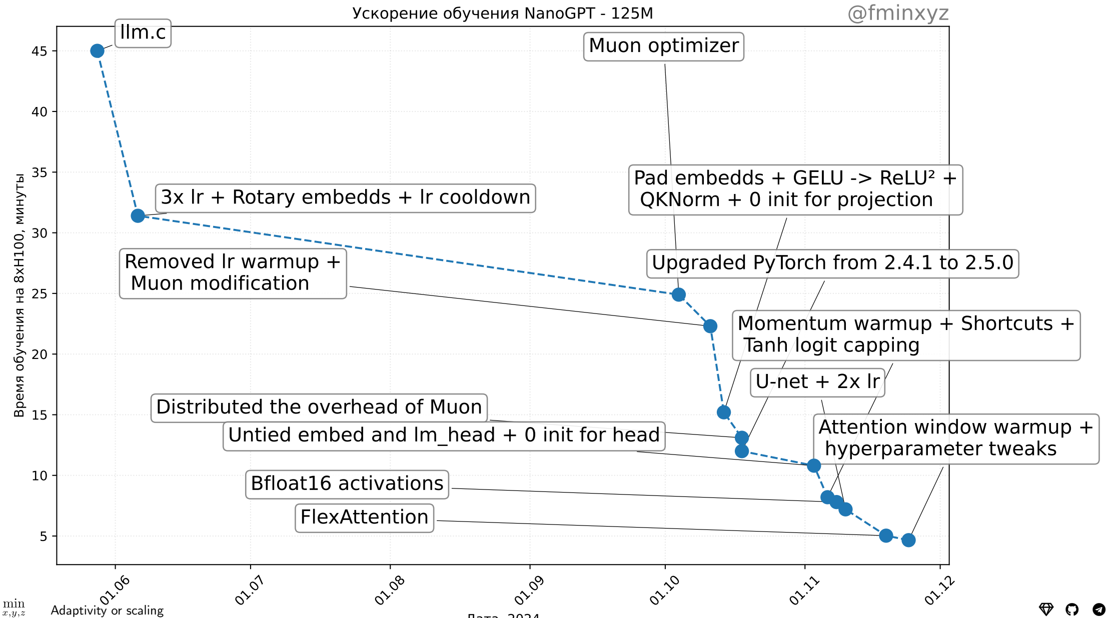


(b) External tuning performance profiles

AlgoPerf benchmark



NanoGPT speedrun



Shampoo (Gupta, Anil, et al., 2018; Anil et al., 2020)

Stands for **S**tochastic **H**essian-**A**pproximation **M**atrix **P**reconditioning for **O**ptimization **O**f deep networks. It's a method inspired by second-order optimization designed for large-scale deep learning.

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- Variants exist for different tensor shapes (e.g., convolutional layers).

Muon [5]

$$
\begin{aligned}
W_{t+1} &= W_t - \eta (G_t G_t^\top)^{-1/4} G_t (G_t^\top G_t)^{-1/4} \\
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[5] Deriving Muon

Neural network training

Optimization for Neural Network training

Neural network is a function, that takes an input x and current set of weights (parameters) $\mathbf{w}$ and predicts some vector as an output. Note, that a variety of feed-forward neural networks could be represented as a series of linear transformations, followed by some nonlinear function (say, ReLU (x) or sigmoid):

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$$\mathcal{N}\mathcal{N}(\mathbf{w}, x) = \sigma_L \circ w_L \circ \dots \circ \sigma_1 \circ w_1 \circ x \qquad \mathbf{w} = \left(W_1, b_1, \dots W_L, b_L\right),$$

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$$L(\mathbf{w}, X, y) \to \min_{\mathbf{w}} \qquad \frac{1}{N} \sum_{i=1}^{N} l(\mathbf{w}, x_i, y_i) \to \min_{\mathbf{w}}$$

Loss functions

In the context of training neural networks, the loss function, denoted by $l(\mathbf{w}, x_i, y_i)$, measures the discrepancy between the predicted output $\mathcal{NN}(\mathbf{w}, x_i)$ and the true output y_i. The choice of the loss function can significantly influence the training process. Common loss functions include:

Mean Squared Error (MSE)

Used primarily for regression tasks. It computes the square of the difference between predicted and true values, averaged over all samples.

$$\text{MSE}(\mathbf{w}, X, y) = \frac{1}{N}\sum_{i=1}^{N}(\mathcal{NN}(\mathbf{w}, x_i) - y_i)^2$$

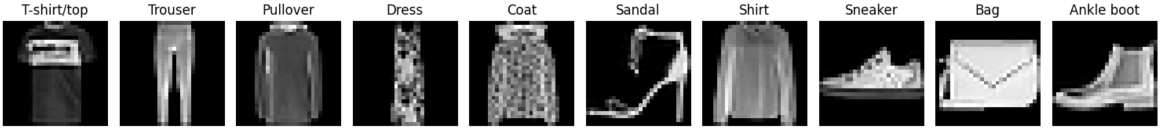
Cross-Entropy Loss

Typically used for classification tasks. It measures the dissimilarity between the true label distribution and the predictions, providing a probabilistic interpretation of classification.

$$\text{Cross-Entropy}(\mathbf{w}, X, y) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{C} y_{i,c}\log(\mathcal{NN}(\mathbf{w}, x_i)_c)$$

where $y_{i,c}$ is a binary indicator (0 or 1) if class label c is the correct classification for observation i, and C is the number of classes.

Simple example: Fashion MNIST classification problem



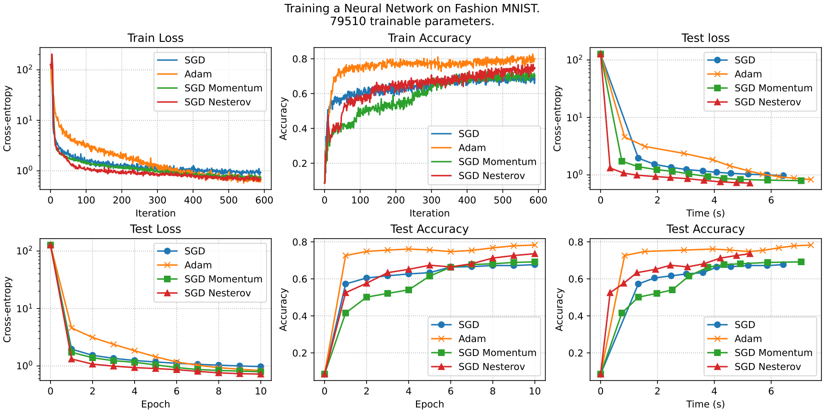


Рис. 2: Open in colab

GPT-2 training Memory footprint

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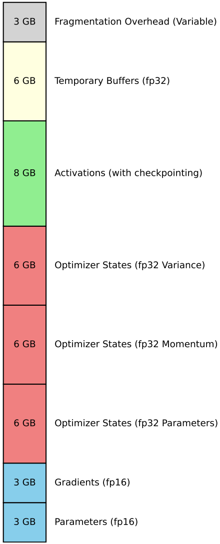

Example: 1.5B parameter GPT-2 model needs 3GB for weights in 16-bit precision but can't be trained on a 32GB GPU using Tensorflow or PyTorch. Major memory usage during training includes optimizer states, gradients, parameters, activations, temporary buffers, and fragmented memory.

Model States:

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

Memory Requirements Example:

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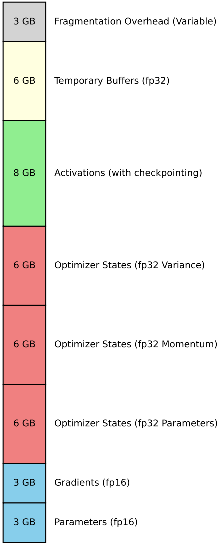

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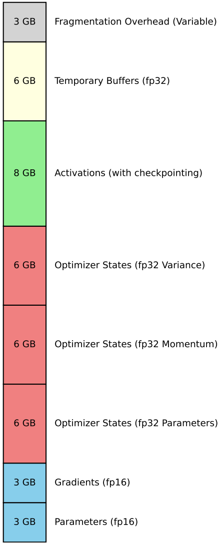

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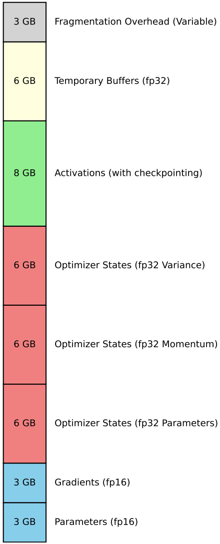

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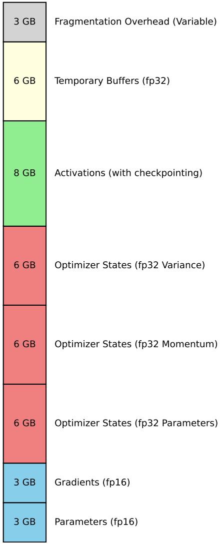

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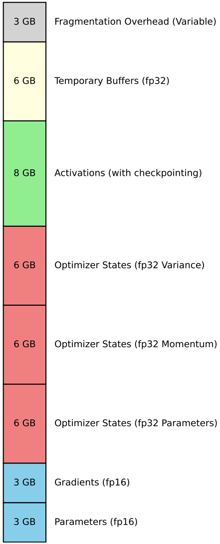

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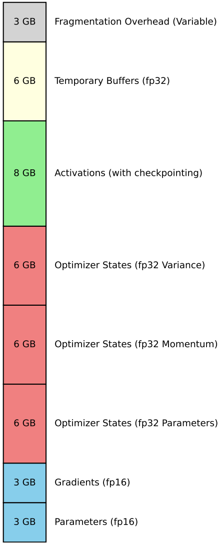

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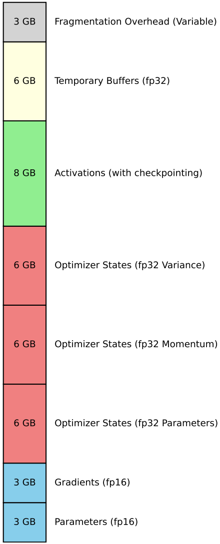

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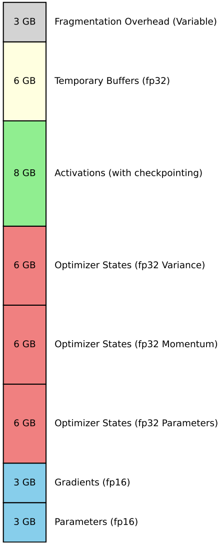

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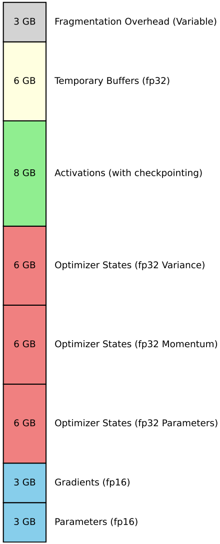

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- In some cases, over 30% of memory remains unusable due to fragmentation.