

A whimsical illustration featuring a white Corgi dog and a yellow rubber duck. They are standing on a surface that resembles a 3D wireframe plot of a function, with peaks and valleys colored in a rainbow gradient from blue to red. The background is a soft, hazy sky. A semi-transparent white box contains the title and author information.

# 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:

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

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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:

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

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  $f(x)$ .

## 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  $\epsilon$  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  $j = 1, \dots, p$ :

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

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- RMSProp divides the learning rate for a weight by a running average of the magnitudes of recent gradients for that weight.
- 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  $\alpha$ :

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

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

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

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

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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) <sup>1</sup> <sup>2</sup>

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

EMA: 
$$m_j^{(k)} = \beta_1 m_j^{(k-1)} + (1 - \beta_1) g_j^{(k)}$$
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Bias correction: 
$$\hat{m}_j = \frac{m_j^{(k)}}{1 - \beta_1^k}$$
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- Гораздо лучше работает для языковых моделей, чем для задач компьютерного зрения - почему?

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<sup>1</sup>Adam: A Method for Stochastic Optimization

<sup>2</sup>On the Convergence of Adam and Beyond



## AdamW (Loshchilov & Hutter, 2017)

Addresses a common issue with  $\ell_2$  regularization in adaptive optimizers like Adam. Standard  $\ell_2$  regularization adds  $\lambda\|x\|^2$  to the loss, resulting in a gradient term  $\lambda x$ . In Adam, this term gets scaled by the adaptive learning rate  $(\sqrt{\hat{v}_j} + \epsilon)$ , coupling the weight decay to the gradient magnitudes.

AdamW decouples weight decay from the gradient adaptation step.

Update rule:

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### Notes:

- The weight decay term  $\lambda x_j^{(k-1)}$  is added *after* the adaptive gradient step.
- 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



## How to compare them? AlgoPerf benchmark <sup>3 4</sup>

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

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<sup>3</sup>Benchmarking Neural Network Training Algorithms

<sup>4</sup>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

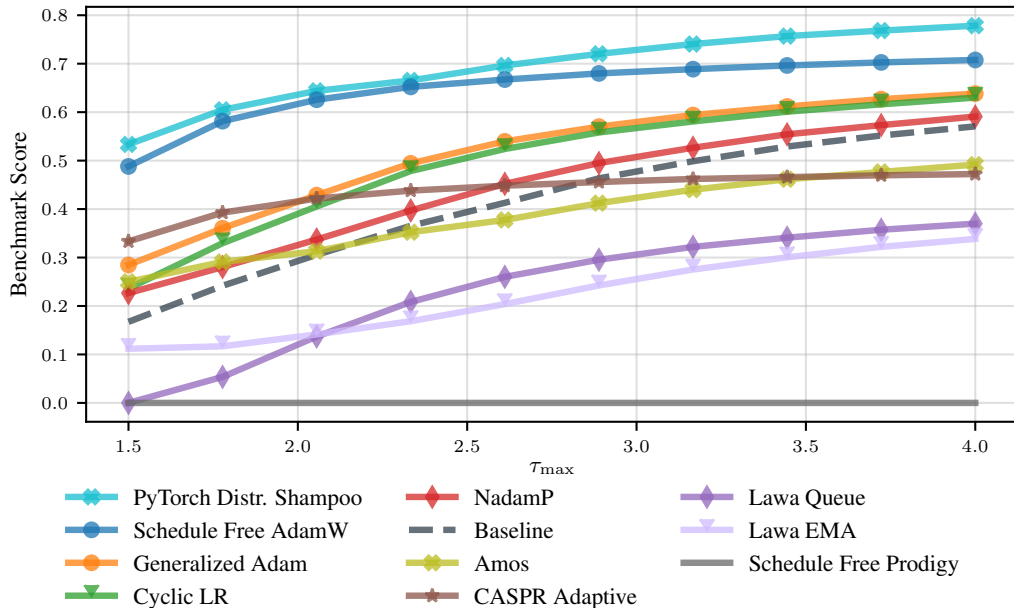
Submission	Line	Score
PYTORCH DISTRIBUTED SHAMPOO		0.7784
SCHEDULE FREE ADAMW		0.7077
GENERALIZED ADAM		0.6383
CYCLIC LR		0.6301
NADAMP		0.5909
BASELINE		0.5707
AMOS		0.4918
CASPR ADAPTIVE		0.4722
LAWA QUEUE		0.3699
LAWA EMA		0.3384
SCHEDULE FREE PRODIGY		0

(a) External tuning leaderboard



(b) External tuning performance profiles

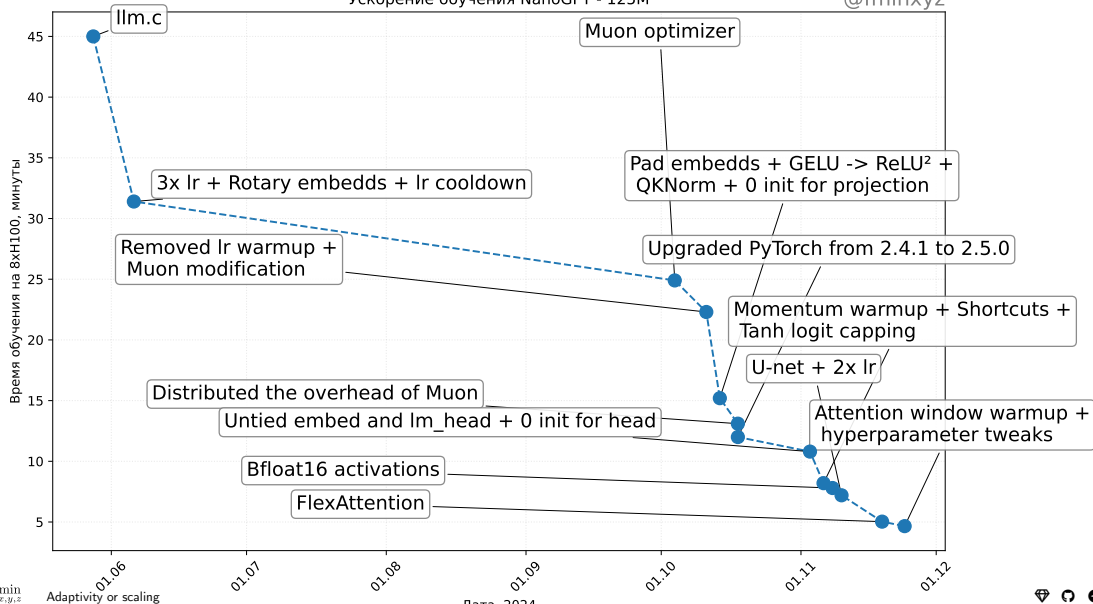
# AlgoPerf benchmark



# NanoGPT speedrun

Ускорение обучения NanoGPT - 125M

@fminxyz



## 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.

**Core Idea:** Approximates the full-matrix AdaGrad pre conditioner using efficient matrix structures, specifically Kronecker products.

For a weight matrix  $W \in \mathbb{R}^{m \times n}$ , the update involves preconditioning using approximations of the statistics matrices  $L \approx \sum_k G_k G_k^T$  and  $R \approx \sum_k G_k^T G_k$ , where  $G_k$  are the gradients.

Simplified concept:

1. Compute gradient  $G_k$ .

**Notes:**

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

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- Requires careful implementation for efficiency (e.g., efficient computation of inverse matrix roots, handling large matrices).
- Variants exist for different tensor shapes (e.g., convolutional layers).

$$\begin{aligned}W_{t+1} &= W_t - \eta(G_t G_t^\top)^{-1/4} G_t (G_t^\top G_t)^{-1/4} \\&= W_t - \eta(US^2U^\top)^{-1/4} (USV^\top)(VS^2V^\top)^{-1/4} \\&= W_t - \eta(US^{-1/2}U^\top)(USV^\top)(VS^{-1/2}V^\top) \\&= W_t - \eta US^{-1/2}SS^{-1/2}V^\top \\&= W_t - \eta UV^\top\end{aligned}$$

## Neural network training

# Optimization for Neural Network training

Neural network is a function, that takes an input  $x$  and current set of weights (parameters)  $w$  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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$$\mathcal{NN}(\mathbf{w}, x) = \sigma_L \circ w_L \circ \dots \circ \sigma_1 \circ w_1 \circ x \quad \mathbf{w} = (W_1, b_1, \dots W_L, b_L),$$



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

## 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



Training a Neural Network on Fashion MNIST.  
79510 trainable parameters.



## 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:

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