Variance reduction for stochastic gradient descent

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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 $f(x)$.

Results for Gradient Descent

Stochastic iterations are n times faster, but how many iterations are needed?

If ∇f is Lipschitz continuous then we have:

Assumption	Deterministic Gradient Descent	Stochastic Gradient Descent
PL	$O(\log(1/\varepsilon))$	$O(1/\varepsilon)$
Convex	$O(1/\varepsilon)$	$O(1/\varepsilon^2)$
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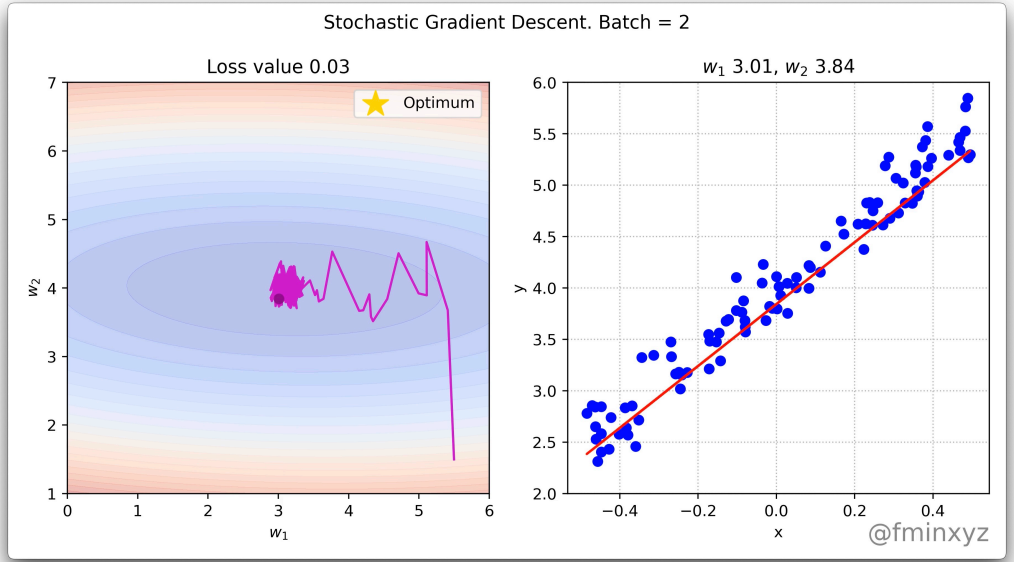
- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

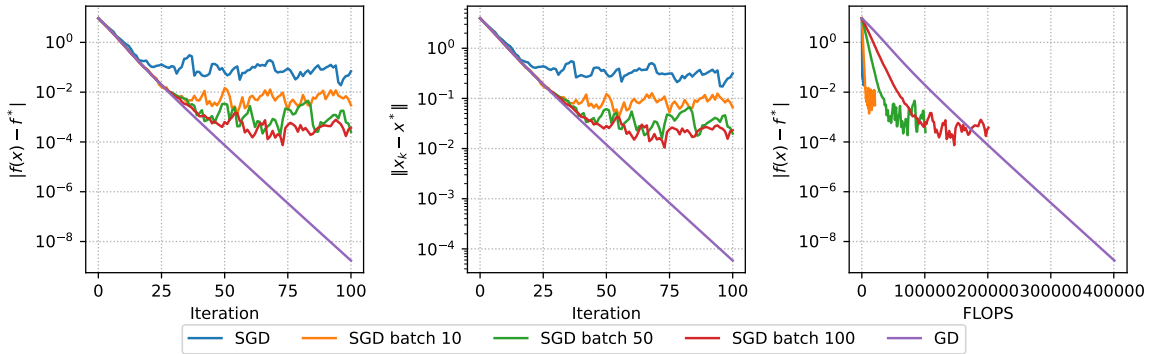
SGD with constant stepsize does not converge



Main problem of SGD

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

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



Variance reduction methods

Key idea of variance reduction

Principle: reducing variance of a sample of X by using a sample from another random variable Y with known expectation:

$$Z_\alpha = \alpha(X - Y) + \mathbb{E}[Y]$$

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$

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Application to gradient estimation ?

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- $X - Y = \nabla f_{i_k}(x^{(k-1)}) - \nabla f_{i_k}(\tilde{x})$

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$$g_{i_k}^{(k)} = \nabla f_{i_k}(x^{(k-1)}) \quad \text{(most recent gradient of } f_{i_k}\text{)}$$

Set all other $g_i^{(k)} = g_i^{(k-1)}$, $i \neq i_k$, i.e., these stay the same

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- Isn't it expensive to average all these gradients? Basically just as efficient as SGD, as long we're clever:

$$x^{(k)} = x^{(k-1)} - \alpha_k \underbrace{\left(\frac{1}{n} g_i^{(k)} - \frac{1}{n} g_i^{(k-1)} + \underbrace{\frac{1}{n} \sum_{i=1}^{n} g_i^{(k-1)}}_{\text{old table average}} \right)}_{\text{new table average}}$$

SAG convergence

Assume that $f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$, where each f_i is differentiable, and ∇f_i is Lipschitz with constant L.

Denote $\bar{x}^{(k)} = \frac{1}{k}\sum_{l=0}^{k-1} x^{(l)}$, the average iterate after $k-1$ steps.

Theorem

SAG, with a fixed step size $\alpha = \frac{1}{16L}$, and the initialization

$$g_i^{(0)} = \nabla f_i(x^{(0)}) - \nabla f(x^{(0)}), \quad i = 1, \dots, n$$

satisfies

$$\mathbb{E}[f(\bar{x}^{(k)})] - f^\star \leq \frac{48n}{k}[f(x^{(0)}) - f^\star] + \frac{128L}{k}\|x^{(0)} - x^\star\|^2$$

where the expectation is taken over random choices of indices.

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  - SAG: $\frac{48n[f(x^{(0)})-f^\star]+128L\|x^{(0)}-x^\star\|^2}{k}$
- So the first term in SAG bound suffers from a factor of n; authors suggest smarter initialization to make $f(x^{(0)}) - f^\star$ small (e.g., they suggest using the result of n SGD steps).

SAG convergence

Assume further that each f_i is strongly convex with parameter μ.

Theorem

SAG, with a step size $\alpha = \frac{1}{16L}$ and the same initialization as before, satisfies

$$\mathbb{E}[f(x^{(k)})] - f^\star \leq \left(1 - \min\left(\frac{\mu}{16L}, \frac{1}{8n}\right)\right)^k \left(\frac{3}{2}\left(f(x^{(0)}) - f^\star\right) + \frac{4L}{n}\|x^{(0)} - x^\star\|^2\right)$$

Notes:

- This is linear convergence rate $\mathcal{O}(\gamma^k)$ for SAG. Compare this to $\mathcal{O}(\gamma^k)$ for GD, and only $\mathcal{O}\left(\frac{1}{k}\right)$ for SGD.

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- Like GD, we say SAG is adaptive to strong convexity.
- Proofs of these results not easy: 15 pages, computed-aided!

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$$f_{i_k}(x^{k+1}) \leq f_{i_k}(x^k) + \nabla f_{i_k}(x^k)(x^{k+1} - x^k) + \frac{L}{2}\|x^{k+1} - x^k\|_2^2$$

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- For the generalized linear models (this includes LogReg, LLS) you need to store much less memory $\mathcal{O}(n)$ instead of $\mathcal{O}(pn)$.

$$f_i(w) = \varphi(w^T x_i) \leftrightarrow \nabla f_i(w) = \varphi'(w^T x_i) x_i$$

SAG non-uniform sampling

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- When selecting components with a probability proportional to L_i, the constant L can be reduced from $\max_i L_i$ to $\bar{L} = \sum_i L_i / N$:

$$
\begin{aligned}
g(x) &= \frac{1}{n} \sum_{i=1}^{n} f_i(x) \\
&= \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \frac{f_i(x)}{L_i} \\
&= \frac{1}{\sum_k L_k} \sum_{i=1}^{n} \sum_{j=1}^{L_i} \left(\sum_k \frac{L_k}{n} \frac{f_i(x)}{L_i} \right)
\end{aligned}
$$

With this approach, the component with a larger value of L_i is selected more often.

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- The step size α_k and the convergence rate of the method are determined by the constant L for $f(x)$, where $L = \max_{1 \le i \le n} L_i$, L_i is the Lipschitz constant for the function f_i
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- Two parameters: length of epochs + step-size α.
- Linear convergence rate, simple proof.

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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- 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 $j = 1, \ldots, p$:

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- 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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- 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:

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

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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.

AdamW decouples weight decay from the gradient adaptation step.

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

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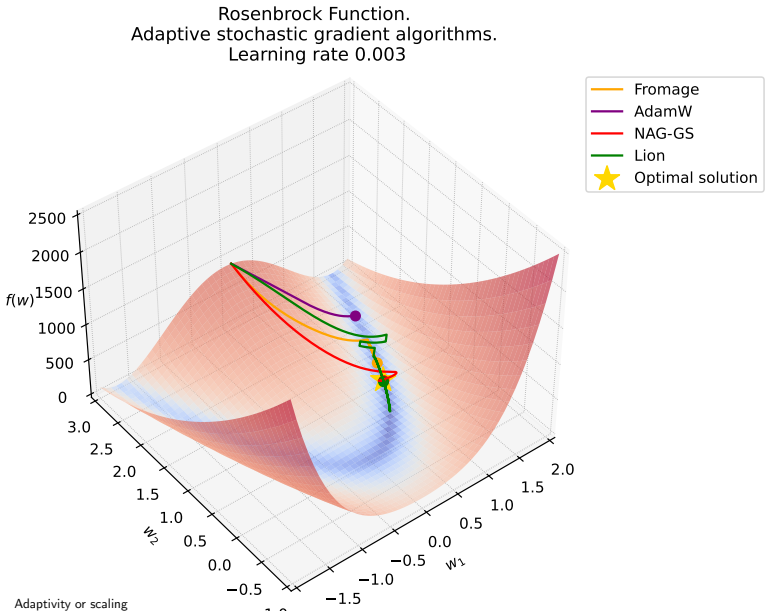
$$x_j^{(k)} = x_j^{(k-1)} - \alpha \left(\frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon} + \lambda x_j^{(k-1)} \right)$$

Notes:

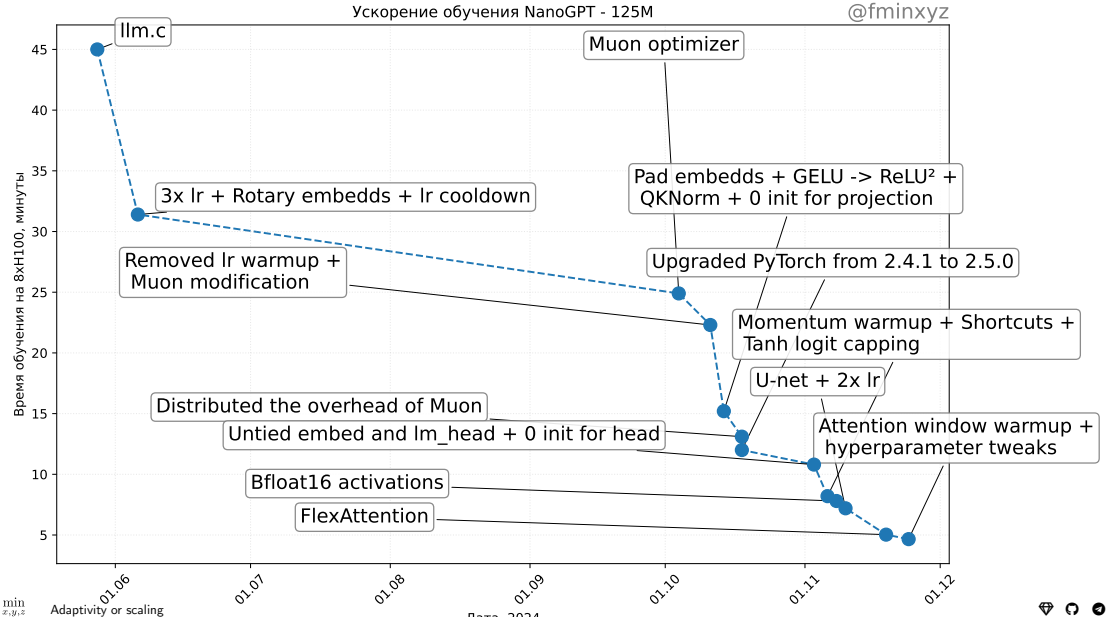
- The weight decay term $\lambda x_j^{(k-1)}$ is added *after* the adaptive gradient step.
- Widely adopted in training transformers and other large models. Default choice for huggingface trainer.

A lot of them


Rosenbrock Function.
Adaptive stochastic gradient algorithms.
Learning rate 0.003
Fromage
AdamW
NAG-GS
Lion
Optimal solution
f(w)
2500
2000
1500
1000
500
0
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
w2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
w1

How to compare them? 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.

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:

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Simplified concept:

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2. Update statistics $L_k = \beta L_{k-1} + (1-\beta) G_k G_k^T$ and $R_k = \beta R_{k-1} + (1-\beta) G_k^T G_k$.

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

Muon [3]

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

[3] Deriving Muon