Advanced stochastic methods. Adaptivity and variance reduction

Daniil Merkulov

Optimization methods. MIPT



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:

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

 $f \rightarrow \min_{x,y,z}$ Finite-sum problem

♥ O Ø 2

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

If ∇f is Lipschitz continuous then we have:

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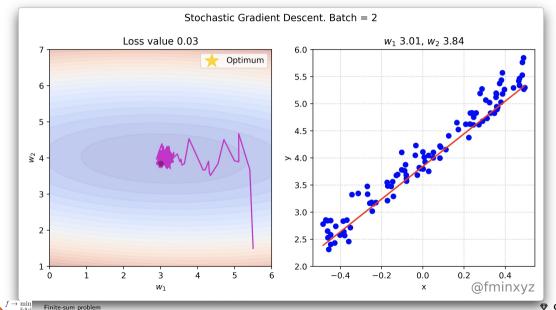
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- Momentum and Quasi-Newton-like methods do not improve rates in stochastic case. Can only improve constant factors (bottleneck is variance, not condition number).

SGD with constant stepsize does not converge

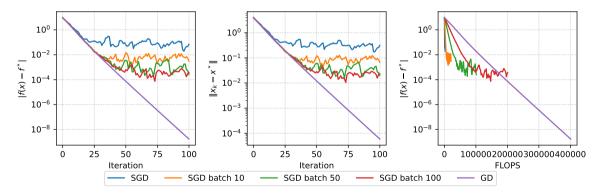


Finite-sum problem

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.



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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- At steps k = 1, 2, 3, ..., pick random $i_k \in \{1, ..., n\}$, then let

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



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• Update

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- SAG gradient estimates are no longer unbiased, but they have greatly reduced variance
- Isn't it expensive to average all these gradients? Basically just as efficient as SGD, as long we're clever:

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





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

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

where the expectation is taken over random choices of indices.



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- But, the constants are different! Bounds after k steps:

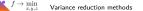


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$$\frac{L \|x^{(0)} - x^{\star}\|^2}{2k}$$



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 - GD: $\frac{L \|x^{(0)} x^{\star}\|^2}{2k}$ • SAG: $\frac{48n[f(x^{(0)}) - f^{\star}] + 128L \|x^{(0)} - x^{\star}\|^2}{k}$



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 - GD: $\frac{L \|x^{(0)} x^{\star}\|^2}{2k}$
 - 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 $f(x^{(0)}) f^*$ small (e.g., they suggest using the result of n SGD steps).

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

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

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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SAG convergence

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- Proofs of these results not easy: 15 pages, computed-aided!



SAGA for quadratics



SAG for binary logistic regression



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- Two gradient evaluations per inner step.
- Two parameters: length of epochs + step-size γ .
- Linear convergence rate, simple proof.

Very popular adaptive method. Let $g^{(k)} = \nabla f_{i_k}(x^{(k-1)})$, and update for $j = 1, \ldots, p$:

$$\begin{aligned} v_j^{(k)} &= v_j^{k-1} + (g_j^{(k)})^2 \\ x_j^{(k)} &= x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}} \end{aligned}$$

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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 $j = 1, \ldots, p$:

$$\begin{aligned} v_j^{(k)} &= \gamma v_j^{(k-1)} + (1-\gamma) (g_j^{(k)})^2 \\ x_j^{(k)} &= x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}} \end{aligned}$$

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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 :

$$\begin{split} v_j^{(k)} &= \gamma v_j^{(k-1)} + (1-\gamma) (g_j^{(k)})^2 \\ \tilde{g}_j^{(k)} &= \frac{\sqrt{\Delta x_j^{(k-1)} + \epsilon}}{\sqrt{v_j^{(k)} + \epsilon}} g_j^{(k)} \\ x_j^{(k)} &= x_j^{(k-1)} - \tilde{g}_j^{(k)} \\ \Delta x_j^{(k)} &= \rho \Delta x_j^{(k-1)} + (1-\rho) (\tilde{g}_j^{(k)})^2 \end{split}$$

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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.

1

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$$\begin{split} m_j^{(k)} &= \beta_1 m_j^{(k-1)} + (1 - \beta_1) g_j^{(k)} \\ v_j^{(k)} &= \beta_2 v_j^{(k-1)} + (1 - \beta_2) (g_j^{(k)})^2 \\ \hat{m}_j &= \frac{m_j^{(k)}}{1 - \beta_1^k}, \quad \hat{v}_j = \frac{v_j^{(k)}}{1 - \beta_2^k} \\ x_j^{(k)} &= x_j^{(k-1)} - \alpha \frac{\hat{m}_j}{\sqrt{\hat{v}_j} + \epsilon} \end{split}$$

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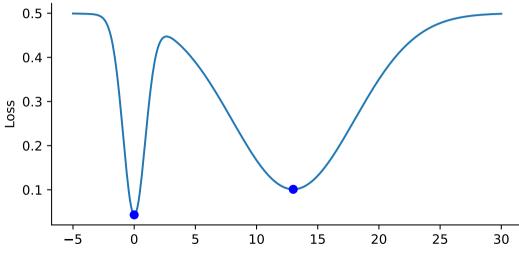
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r - ฐ However, the proposed algorithm in initial version does not converge even in convex setting (later fixes, 👩

Wide vs narrow local minima

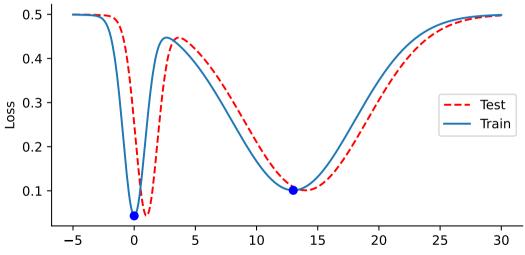
Узкие и широкие локальные минимумы



 $\rightarrow \min_{x,y,z}$ Modern problems

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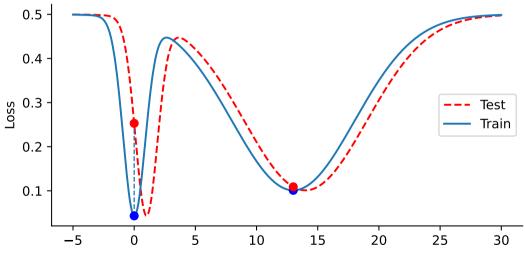
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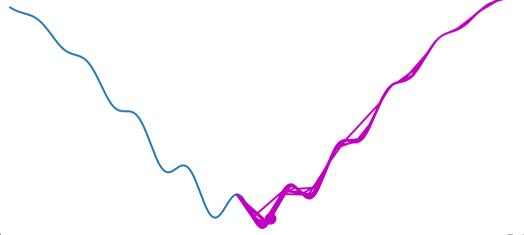
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Stochasticity allows to escape local minima

Стохастический градиентный спуск выпрыгивает из локальных минимумов



Local divergence can also be benefitial

Градиентный спуск с большим шагом избегает узкого локального минимума

