

# Advanced stochastic methods. Adaptivity and variance reduction

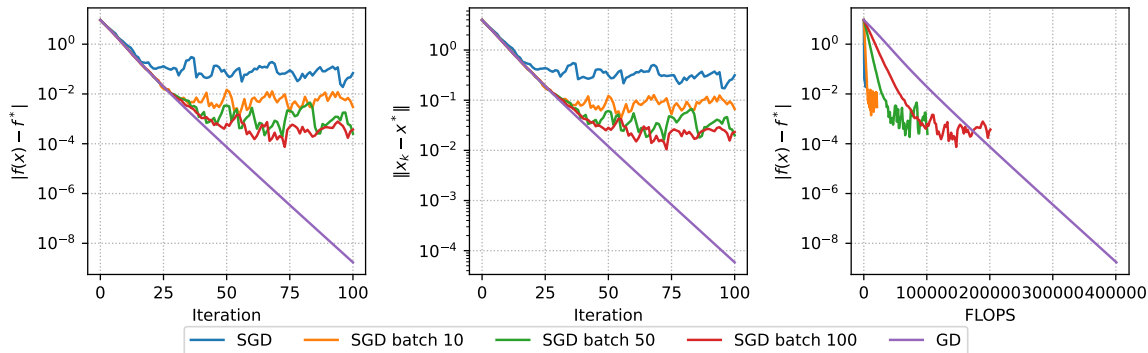
## Seminar

Optimization for ML. Faculty of Computer Science. HSE University

# Main problem of SGD

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

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



# 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:

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

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$
- $\text{var}(Z_\alpha) = \alpha^2 (\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y))$ 
  - If  $\alpha = 1$ : no bias
  - If  $\alpha < 1$ : potential bias (but reduced variance).
- Useful if  $Y$  is positively correlated with  $X$ .

## Application to gradient estimation ?

- SVRG: Let  $X = \nabla f_{i_k}(x^{(k-1)})$  and  $Y = \nabla f_{i_k}(\tilde{x})$ , with  $\alpha = 1$  and  $\tilde{x}$  stored.
- $\mathbb{E}[Y] = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\tilde{x})$  full gradient at  $\tilde{x}$ ;
- $X - Y = \nabla f_{i_k}(x^{(k-1)}) - \nabla f_{i_k}(\tilde{x})$

# SVRG (Stochastic Variance Reduced Gradient; Johnson, and Zhang, 2013)

- **Initialize:**  $\tilde{x} \in \mathbb{R}^d$
- **For**  $i_{epoch} = 1$  **to** # of epochs
  - Compute all gradients  $\nabla f_i(\tilde{x})$ ; store  $\nabla f(\tilde{x}) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\tilde{x})$
  - Initialize  $x_0 = \tilde{x}$
  - **For**  $t = 1$  **to** length of epochs ( $m$ )
    - $x_t = x_{t-1} - \alpha \left[ \nabla f(\tilde{x}) + \left( \nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(\tilde{x}) \right) \right]$
    - Update  $\tilde{x} = x_t$

## Notes:

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

## SAG (Stochastic average gradient, Schmidt, Le Roux, and Bach 2013)

- Maintain table, containing gradient  $g_i$  of  $f_i$ ,  $i = 1, \dots, n$
- Initialize  $x^{(0)}$ , and  $g_i^{(0)} = \nabla f_i(x^{(0)})$ ,  $i = 1, \dots, n$
- At steps  $k = 1, 2, 3, \dots$ , pick random  $i_k \in \{1, \dots, n\}$ , then let

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

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

- Update

$$x^{(k)} = x^{(k-1)} - \alpha_k \frac{1}{n} \sum_{i=1}^n g_i^{(k)}$$

- 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:

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

# SAG convergence

Assume that  $f(x) = \frac{1}{n} \sum_{i=1}^n f_i(x)$ , where each  $f_i$  is differentiable, and  $\nabla f_i$  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

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

where the expectation is taken over random choices of indices.

# SAG convergence

- Result stated in terms of the average iterate  $\bar{x}^{(k)}$ , but also can be shown to hold for the best iterate  $x_{best}^{(k)}$  seen so far.
- This is  $\mathcal{O}\left(\frac{1}{k}\right)$  convergence rate for SAG. Compare to  $\mathcal{O}\left(\frac{1}{k}\right)$  rate for GD, and  $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$  rate for SGD.
- But, the constants are different! Bounds after  $k$  steps:
  - GD:  $\frac{L\|x^{(0)} - x^*\|^2}{2k}$
  - SAG:  $\frac{48n[f(x^{(0)}) - f^*] + 128L\|x^{(0)} - x^*\|^2}{k}$
- 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).

# SAG convergence

Assume further that each  $f_i$  is strongly convex with parameter  $\mu$ .

## Theorem

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

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

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



## 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.
- The learning rate of rare informative features diminishes slowly.
- 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  $j = 1, \dots, p$ :

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

$$x_j^{(k)} = x_j^{(k-1)} - \alpha \frac{g_j^{(k)}}{\sqrt{v_j^{(k)} + \epsilon}}$$

### Notes:

- 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  $\alpha$ :

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

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

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

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

### Notes:

- Adadelta adapts learning rates based on a moving window of gradient updates, rather than accumulating all past gradients. This way, learning rates adjusted are more robust to changes in model's dynamics.
- 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)

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

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

$$v_j^{(k)} = \beta_2 v_j^{(k-1)} + (1 - \beta_2) (g_j^{(k)})^2$$

$$\hat{m}_j = \frac{m_j^{(k)}}{1 - \beta_1^k}, \quad \hat{v}_j = \frac{v_j^{(k)}}{1 - \beta_2^k}$$



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

### Notes:

- Adam is suitable for large datasets and high-dimensional optimization problems.
- It corrects the bias towards zero in the initial moments seen in other methods like RMSProp, making the estimates more accurate.
- Highly popular in training deep learning models, owing to its efficiency and straightforward implementation.
- However, the proposed algorithm in initial version does not converge even in convex setting (later fixes

# Computational experiments

Let's look at computational experiments for

- SGD, SAG and SVRG in JAX .
- SVRG in JAX for VAE .