Advanced stochastic methods. Adaptivity and variance reduction

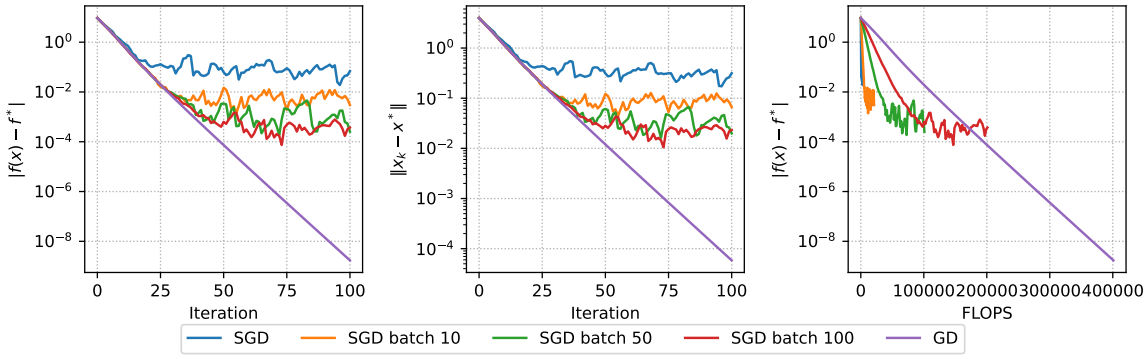
Seminar

Optimization for ML. Faculty of Computer Science. HSE University

Main problem of SGD

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

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:

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

- $\mathbb{E}[Z_\alpha] = \alpha\mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$
- $\mathsf{var}(Z_\alpha) = \alpha^2 \left(\mathsf{var}(X) + \mathsf{var}(Y) - 2\mathsf{cov}(X, Y)\right)$
  - 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 γ.
- Linear convergence rate, simple proof.

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

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

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

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

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

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

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

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.

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: $\frac{L\|x^{(0)}-x^\star\|^2}{2k}$
  - 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 $f(x^{(0)}) - f^\star$ 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.
- 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 $j = 1, \ldots, p$:

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

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

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 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 $j = 1, \ldots, p$:

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

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

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 α:

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

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

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

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

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.