Variance reduction for stochastic gradient methods

Axel Böhm

December 3, 2021

1. Introduction
2. SAG
3. SAGA
4. SVRG

The finite sum probem

A common Task in (supervised) machine learning:

$$\min_{x\in\mathbb{R}^d} f(x) := \frac{1}{n}\sum_{i=1}^{n} \underbrace{f_i(x)}_{\text{loss for } i\text{-th sample}} + \underbrace{\psi(x)}_{\text{regularizer}}$$

where the i-th sample is (a_i, y_i).

Examples:

- linear regression: $f_i(x) = (a_i^T x - y_i)^2$, and $\psi = 0$
- logistic regression: $f_i(x) = \log(1 + e^{-y_i a_i^T x})$, and $\psi = 0$ "sigmoid function" and logistic loss.
- Lasso: f_i as for linear regression but $\psi(x) = \|x\|_1$
- SVM: $f_i(x) = \max\{0, 1 - y_i a_i^T x\}$ and $\psi(x) = \|x\|^2$

Gradient descent

Algorithm (batch) GD

1: **for** $k = 1, 2, \ldots$ **do**
2: $\quad x_{k+1} = x_k - \alpha_k \nabla f(x_k)$

- gradient can be computed via

$$\nabla f(x) = \nabla \left(\sum_{i=1}^{n} f_i(x) \right) = \sum_{i=1}^{n} \nabla f_i(x_k)$$

- good convergence properties
- can be **expensive** if n is large!

Stochastic gradient descent

Algorithm SGD

1: **for** $k = 1, 2, \ldots$ **do**
2: pick i_k uniform at random in $[n]$
3: $x_{k+1} = x_k - \alpha_k \nabla f_{i_k}(x_k)$

We already noticed that:

- unbiased: $\mathbb{E}[\nabla f_{i_k}(x)] = \sum_{i=1}^{n} \mathbb{P}[i = i_k] \nabla f_i(x) = \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(x)$
- large stepsizes fail to suppress variability in the stoch. gradients $\rightarrow$ leads to oscillations
- decreasing stepsizes mitigate this problem but **slows down** convergence (too *conservative*)

Recall SGD (template)

$$x_{k+1} = x_k - \alpha_k g_k$$

- g_k is an unbiased estimator of the true gradient $\nabla F(x_k)$
- convergence depends on **variance** $\mathbb{E}[\|g_k - \nabla F(x_k)\|] \le \sigma_g$ (not strictly necessary)
- vanilla SGD uses $g_k = \nabla f_{i_k}(x_k)$
  issue: σ_g is non-negligible even close to the solution
- **Q:** can we choose g_k in a different way to reduce variability?

Minibatching

Algorithm minibatch SGD

1: **for** $k = 1, 2, \ldots$ **do**
2: pick I_k random subset of $[n]$ with $|I_k| = b$
3: $x_{k+1} = x_k - \alpha_k \sum_{i \in I_k} \nabla f_i(x_k)$

- typically we make a (uniform) *random* choice $i_k \in [n] = \{1, \ldots, n\}$ (or random reshuffling)
- by increasing the size to a **random subset** $I_k \subset [n]$ of size $b \ll n$ we can
  - decrease variance
  - increase cost only moderately,
  - no improvement in the rate

A simple idea

Consider

- estimator X for parameter μ ($\mathbb{E}[X] = \mu$ and $\mathbb{V}[X] = \sigma^2$)
- want to keep unbiased but reduce variance
- find Y such that $\mathbb{E}[Y] = 0$ but $\mathrm{Cov}(X, Y)$ is large and $\tilde{X} = X - Y$
- remains unbiased

$$\mathbb{V}[\tilde{X}] = \mathbb{V}[X] + \mathbb{V}[Y] - 2\,\mathrm{Cov}[X, Y]$$

- can be much smaller than $\mathbb{V}[X]$ if X, Y are highly correlated

Stochastic average gradient (SAG), 2013

- maintain table containing gradients g_i of f_i
- at step $k = 1, 2, \dots$ pick random $i_k \in [n]$ and

$$g_i^k := \nabla f_{i_k}(x^k)$$

  set $g_i^k = g_i^{k-1}$ for all $i \neq i_k$ (remain the same)
- Update

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

- assuming gradients do not change too much along trajectory
- gradient estimator no longer unbiased
- Isn't it expensive to average these gradients?

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

SAG variance reduction

Gradient estimator in SAG:

$$x^{k+1} = x^k - \alpha_k \frac{1}{n}\Big(\underbrace{g_{i_k}^k}_{X} - \underbrace{g_{i_k}^{k-1} - \sum_{i=1}^{n} g_i^k}_{Y}\Big)$$

- While $\mathbb{E}[X] = \nabla f(x^k)$, but $\mathbb{E}[Y] \neq 0 \to$ biased estimator
- X and Y are correlated as $X - Y \to 0$ as
- x^k and x_{k-1} both converge to x^* and
- the last term converges to $\nabla f(x^*) = 0$

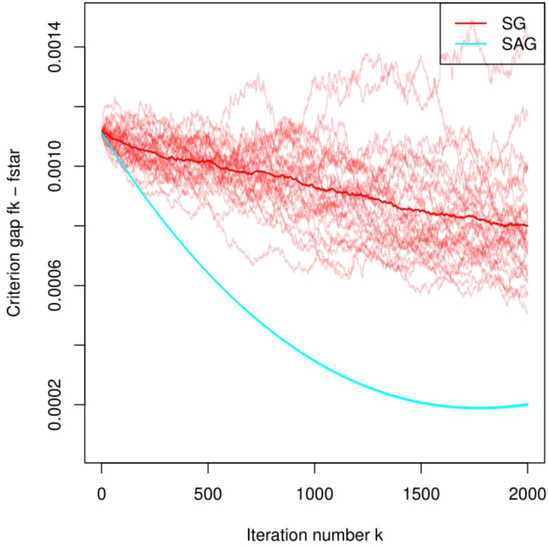
Convergence

As always, initialization plays a role: $D^2 := \|x^0 - x^*\|^2$.

$$\begin{aligned} \text{SAG:} &\quad \frac{n}{k}(f(x^0) - f^*) + \frac{L}{k}D^2 \\ \text{GD:} &\quad \frac{L}{k}D^2 \\ \text{SGD:} &\quad \frac{L}{\sqrt{k}}D^2 \end{aligned}$$

- Achieves linear convergence in the *strongly* convex setting.
- proofs are difficult (and computer-aided)

Same gradient oracle cost as SGD, but same converge rate as GD.



SG
SAG
Criterion gap fk – fstar
0.0002
0.0006
0.0010
0.0014
0
500
1000
1500
2000
Iteration number k

SAGA, 2014

Very similar:

- maintain table containing gradients g_i of f_i
- at step $k = 1, 2, \ldots$ pick random $i_k \in [n]$ and

$$g_i^k := \nabla f_{i_k}(x^k)$$

  set $g_i^k = g_i^{k-1}$ for all $i \neq i_k$ (remain the same)
- Update

$$x^{k+1} = x^k - u\alpha_k \left(g_{i_k}^k - g_{i_k}^{k-1} + \frac{1}{n} \sum_{i=1}^{n} g_i^k \right)$$

- estimator now **unbiased**!

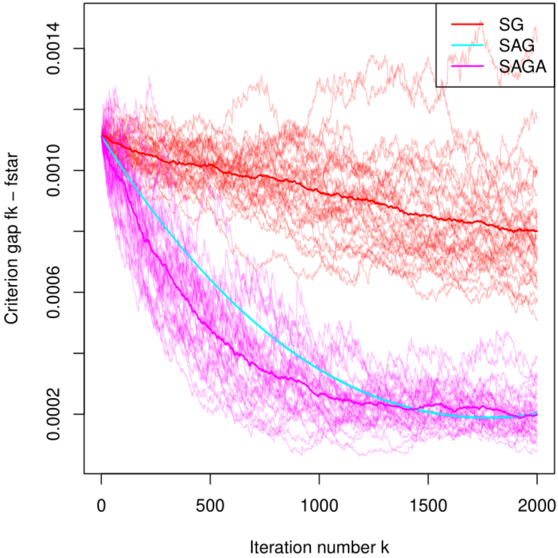
For Comparison

SAGA gradient estimate:

$$g_{i_k}^k - g_{i_k}^{k-1} + \frac{1}{n}\sum_{i=1}^{n} g_i^k$$

SAGA gradient estimate:

$$\frac{1}{n} g_{i_k}^k - \frac{1}{n} g_{i_k}^{k-1} + \frac{1}{n}\sum_{i=1}^{n} g_i^k$$


SG
SAG
SAGA
Criterion gap fk – fstar
0.0002
0.0006
0.0010
0.0014
0
500
1000
1500
2000
Iteration number k

Stochastic Variance Reduced Gradient (SVRG), 2013

Algorithm SVRG

for $k = 1, 2, \ldots$ **do**
  Set $x^1 = \tilde{x} = \tilde{x}^k$
  Compute $\tilde{\mu} := \nabla f(\tilde{x})$ //update snapshot
  for $l = 1, 2, \ldots, m$ **do** //m iterations per epoch
    pick i_l uniform at random in $[n]$
    Set $x^{l+1} = x^l - \alpha(\nabla f_{i_l}(x^l) - \nabla f_{i_l}(\tilde{x}) + \tilde{\mu})$
  $\tilde{x}^{k+1} = x^{m+1}$

- Does **not** need to **store** full table of gradients.
- requires *batch* gradient computation every *epoch*
- per iteration cost is comparable to that of SGD if $m \geq n$
- convergence rates similar to SAGA, but simpler analysis.

SVRG

key idea: by storing old point we can

$$\underbrace{\nabla f_{i_k}(x^k) - \nabla f_{i_k}(x^{\text{old}})}_{\to 0 \text{ if } x \approx x^{\text{old}}} + \underbrace{\nabla f(x^{\text{old}})}_{\to 0 \text{ if } x^{\text{old}}}$$

- is an unbiased estimate of $\nabla f(x^k)$
- converges to 0 (meaning reduced variability) if $x^k \approx x^{\text{old}} \approx x^*$

SVRG: Theorem

Theorem

Assume each f_i is convex and L-smooth, and F is μ-strongly convex. Choose m large enough s.t. $\rho = \frac{1}{\mu\alpha(1-2L\alpha)m} + \frac{2L\alpha}{1-2L\alpha} < 1$, then

$$\mathbb{E}[F(x_s^{old}) - F(x^*)] \leq \rho^s [F(x_0^{old}) - F(x^*)]$$

Computational cost:

- per epoch: $(m + n)$
- complexity: $(n + \kappa)\log(1/\epsilon)$

SVRG: Convergence Proof

Denote $g_s^k = \nabla f_{i_l}(x_s^k) - \nabla f_{i_l}(x_s^{old}) + \nabla F(x_s^{old})$. Conditioning on everythong prior to x_s^{k+1} we get

$$\begin{aligned}\mathbb{E}[\|x_s^{k+1} - x^*\|^2] &= \mathbb{E}[\|x_s^k - \alpha g_s^k - x^*\|^2] \\ &= \|x_s^k - x^*\|^2 - 2\alpha(x_s^k - x^*)^T\mathbb{E}[g_s^t] + \alpha^2\mathbb{E}[\|g_s^k\|^2] \\ &= \|x_s^k - x^*\|^2 - 2\alpha(x_s^k - x^*)^T\nabla F(x_s^t) + \alpha^2\mathbb{E}[\|g_s^k\|^2] \\ &\leq \|x_s^k - x^*\|^2 - 2\alpha(F(x_s^k) - F(x^*)) + \alpha^2\mathbb{E}[\|g_s^k\|^2]\end{aligned}$$

- **key step:** control $\mathbb{E}[\|g_s^k\|^2]$

Comparison

SVRG	GD	SGD
$(n+\kappa)\log(1/\epsilon)$	$n\kappa\log(1/\epsilon)$	κ^2/ϵ