

CME 307 / MS&E 311 / OIT 676: Optimization

Acceleration, Stochastic Gradient Descent, and Variance Reduction

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Convergence of gradient descent

unconstrained minimization: find $x \in \mathbf{R}^n$ to solve

$$\text{minimize } f(x) \quad (1)$$

where $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is convex and differentiable

we analyzed gradient descent (GD) on this problem:

- ▶ a point x is ϵ -suboptimal if $f(x) - f^* \leq \epsilon$
- ▶ when f is L -smooth and μ -PL (or μ -strongly convex), we showed GD converges to sub-optimality ϵ in at most

$$T = \mathcal{O} \left(\kappa \log \left(\frac{1}{\epsilon} \right) \right) \text{ iterations,}$$

where $\kappa := \frac{L}{\mu}$ is the condition number

Acceleration: motivation

Definition

a *first-order method* uses only a first-order oracle for $f : \mathbf{R}^n \rightarrow \mathbf{R}$ (i.e., gradient and function evaluation) to minimize $f(x)$

GD $x \leftarrow x - \alpha \nabla f(x)$ is a first-order method

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Q: is GD the best first-order method for L -smooth, μ -strongly convex functions?

A: no! Nemirovski and Yudin showed a *lower-bound* of

$$T_{\text{opt}} = \Omega \left(\sqrt{\kappa} \log \left(\frac{1}{\epsilon} \right) \right) \text{ iterations}$$

to find an ϵ -suboptimal point of *any* L -smooth, μ -strongly convex function

notice: same rate as CG if f is quadratic

A worst-case quadratic function

the lower bound can be obtained by constructing a particularly hard problem instance using quadratic functions

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- ▶ easier to work in the infinite dimensional-space $\ell^2(\mathbf{R})$, which consists of vectors x of infinite length, satisfying

$$\|x\|^2 = \sum_{j=1}^{\infty} x_j^2 < \infty$$

A worst-case quadratic function

the lower bound can be obtained by constructing a particularly hard problem instance using quadratic functions

- ▶ easier to work in the infinite dimensional-space $\ell^2(\mathbf{R})$, which consists of vectors x of infinite length, satisfying

$$\|x\|^2 = \sum_{j=1}^{\infty} x_j^2 < \infty$$

- ▶ the (family of) evil quadratic functions (parametrized by $\mu > 0$ and $\kappa_f > 1$) is

$$f(x) = \frac{\mu(\kappa_f - 1)}{8} \left((x_1 - 1)^2 + \sum_{j=1}^{\infty} (x_j - x_{j+1})^2 \right) + \frac{\mu}{2} \|x\|^2,$$

source: Section 2.1, Nesterov, 2018

The lower bound

Using the family of quadratics on the preceding slide, the following theorem may be shown

Theorem (Nesterov Theorem 2.1.13)

Let $\mu > 0$, $\kappa_f > 1$. Suppose \mathcal{M} is a first-order method such that for any input function f , \mathcal{M} generates a sequence satisfying

$$x_k \in x_0 + \text{span}\{\nabla f(x_0), \dots, \nabla f(x_k)\}, \quad \forall k$$

Then there exists a L -smooth, μ -strongly convex function with $L/\mu = \kappa_f$ such that the sequence output by \mathcal{M} applied to f satisfies

$$\|x_k - x_\star\|^2 \geq \left(\frac{\sqrt{\kappa_f} - 1}{\sqrt{\kappa_f} + 1} \right)^{2k} \|x_0 - x_\star\|^2,$$

$$f(x_k) - f(x_\star) \geq \frac{\mu}{2} \left(\frac{\sqrt{\kappa_f} - 1}{\sqrt{\kappa_f} + 1} \right)^{2k} \|x_0 - x_\star\|^2$$

Accelerated Gradient Descent

Nesterov's accelerated gradient method (AGD)

- ▶ a first-order method
- ▶ that matches the lower bound

so, converges faster than GD (esp. on ill-conditioned functions)

(one variant of) Nesterov's AGD:

1. Choose $x_0, y_0 \in \mathbf{R}^n$
2. for $k = 0, 1, \dots, T$,

$$\begin{aligned}x_{k+1} &= y_k - \alpha \nabla f(y_k) \\ y_{k+1} &= x_{k+1} + \beta (x_{k+1} - x_k)\end{aligned}$$

3. Return x_{k+1}

achieves lower bound when $\alpha = \frac{1}{L}$, $\beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$

source: Section 2.2, Nesterov, 2018

GD vs. AGD: numerical example

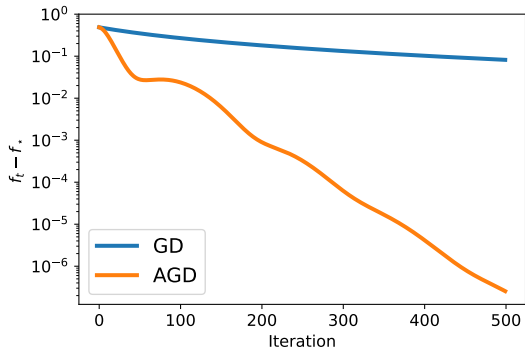
goal is to solve the logistic regression problem

$$\text{minimize} \quad \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-b_i a_i^T x)) + \frac{1}{m} \|x\|^2$$

with variable x on rcv1 dataset, with data matrix $A \in \mathbf{R}^{20,242 \times 47,236}$ and labels $b \in \mathbf{R}^{20,242}$

- ▶ GD and AGD both use theoretically-chosen stepsizes:
 - ▶ GD is run with stepsize $\frac{1}{L}$, which for this example equals 4
 - ▶ AGD is run with $\alpha = \frac{1}{L}$ and $\beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$
- ▶ here strong convexity $\mu = \frac{1}{m}$ from the regularizer

GD vs. AGD results



AGD summary and closing remarks

- ▶ AGD is theoretically optimal among first-order methods for L -smooth and μ -strongly convex functions
- ▶ converges to ϵ -suboptimality in at most

$$\mathcal{O} \left(\sqrt{\kappa} \log \left(\frac{1}{\epsilon} \right) \right) \text{ iterations}$$

- ▶ despite its elegance, AGD is rarely used in practice (quasi-Newton methods work better and are more stable)
- ▶ conceptual foundation for useful accelerated gradient methods like FISTA and Katyusha

Outline

Stochastic optimization

Finite sum minimization

Minimizing a sum

finite sum minimization: solve

$$\text{minimize } \frac{1}{m} \sum_{i=1}^m f_i(x)$$

examples:

- ▶ least squares: $f_i(x) = (a_i^T x - b_i)^2$
- ▶ logistic regression: $f_i(x) = \log(1 + \exp(-b_i a_i^T x))$
- ▶ maximum likelihood estimation: $f_i(x)$ is -loglik of observation i given parameter x
- ▶ machine learning: f_i is misfit of model x on example i

Minimizing a sum

finite sum minimization: solve

$$\text{minimize } \frac{1}{m} \sum_{i=1}^m f_i(x)$$

with variable $x \in \mathbf{R}^n$

quandary:

- ▶ solving a problem with *more data* should be *easier*
- ▶ but complexity of algorithms increases with m !

goal: find algorithms that work *better* given *more data*
(or at least, not worse)

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idea: throw away data! (cleverly)

Minimizing an expectation

Stochastic optimization: solve

$$\text{minimize } \mathbb{E}f(x) = \mathbb{E}_{\omega}f(x; \omega)$$

with variable $x \in \mathbf{R}^n$

- ▶ random loss function f
- ▶ or equivalently, function $f(\cdot; \omega)$ of random variable ω

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examples: *data* $\omega = (a, b)$ is random

- ▶ least squares: $f(x; \omega) = (a^T x - b)^2$
- ▶ logistic regression: $f(x; \omega) = \log(1 + \exp(-ba^T x))$
- ▶ maximum likelihood estimation: $f(x; \omega)$ is -loglik of observation ω given parameter x
- ▶ machine learning: $f(x; \omega)$ is misfit of model x on example ω

minimize test loss, not just training loss

Stochastic optimization: applications

- ▶ machine learning
 - ▶ stochastic objective represents test error rather than (finite sum) training set error
 - ▶ e.g., in physics-informed neural networks (PINNs), objective is integral over domain
- ▶ stochastic control
 - ▶ flying an airplane: ω represents wind and other weather conditions
 - ▶ trading a large portfolio slowly to reduce market impact: ω represents exogenous moves of asset prices

Stochastic optimization: what distribution?

stochastic optimization problem

$$\begin{array}{ll} \text{minimize} & \mathbb{E}_{\omega \sim \mu_{\Omega}} [f(\omega, x)] \\ \text{variable} & x \in \mathbf{R}^n \end{array} \quad (2)$$

with $f(\omega, x) : \Omega \times \mathbf{R}^n$ convex, $\Omega \subseteq \mathbf{R}^n$, ω a random variable distributed according to probability measure μ_{Ω}

objective is expected cost under the randomness due to ω :

$$\mathbb{E}_{\omega \sim \mu_{\Omega}} [f(\omega, x)] = \int_{\Omega} f(\omega; x) d\mu_{\Omega}(\omega)$$

Stochastic optimization: examples

1. $n = 1, \Omega = \mathbf{R}$, and $f(\omega, x) = (x - \omega)^2$.

$$\text{minimize } \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}} [(x - \omega)^2]$$

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then x_{\star} = the median of $\mu_{\mathbf{R}}$

3. $\Omega = \mathbf{R}^n$, $\mu_{\mathbf{R}^n} = \frac{1}{m} \sum_{i=1}^m \delta_{\omega_i}$ (discrete distribution with positive measure only on $\omega_1, \dots, \omega_m$) results in the finite sum minimization problem

$$\text{minimize } \frac{1}{m} \sum_{i=1}^m f(\omega_i, x).$$

Stochastic gradient oracle

Definition

a *stochastic gradient oracle* \mathcal{G} , when queried at $x \in \mathbf{R}^n$, produces $g(\omega; x) \in \mathbf{R}^n$ satisfying

$$\mathbb{E}_{\omega \sim \mu_{\Omega}} [g(\omega; x)] = \nabla F(x)$$

i.e., \mathcal{G} produces an unbiased estimate of the true gradient $\nabla F(x)$

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Q: examples of stochastic gradient oracle?

A: minibatch gradient

$$\frac{1}{|S|} \sum_{\omega \in S} \nabla f_i(\omega, x)$$

notation: use $\hat{\nabla} f(x)$ to denote stochastic gradient at x

Stochastic gradient descent (SGD)

SGD:

1. Choose $x_0 \in \mathbf{R}^n$
2. for $k = 0, 1, \dots$
 - i. query \mathcal{G} at x_k to obtain $g(\omega_k, x_k)$
 - ii. compute update:

$$x_{k+1} = x_k - \eta_k g(\omega_k, x_k)$$

- ▶ SGD is not a descent method!
- ▶ SGD exactly the same as GD, except that it uses a stochastic gradient $g(\omega_k, x_k)$ rather than the true gradient
- ▶ selection of stepsize η_k is challenging!

A typical convergence result

Theorem (General SGD convergence)

Consider (2) with smooth and strongly convex f and stochastic gradient oracle satisfying

$$\mathbb{E}_{\omega} \|g(\omega, x)\|^2 \leq M_1 + M_2 \|\nabla F(\omega, x)\|^2.$$

1. for an appropriate fixed stepsize $\eta_k = O(1)$,

$$\lim_{k \rightarrow \infty} \mathbb{E}[f(\omega_k, x_k)] - f_{\star} = O(1)$$

2. for decreasing stepsizes $\eta_k = O(1/k)$,

$$\mathbb{E}[f(\omega_k, x_k)] - f_{\star} = O(1/k)$$

SGD convergence: discussion

- ▶ with fixed stepsize, the algorithm converges to ϵ -sublevel set
- ▶ convergence of SGD requires a decreasing stepsize \implies slow!

contrast to GD, which converges to the exact optimum even with fixed stepsize

analysis is tight: there is a matching lower bound.

Agarwal et al., 2012 shows that for strongly convex problems, any algorithm using a stochastic gradient oracle must make at least $\Omega(1/\epsilon)$ queries to obtain an ϵ -suboptimal point

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don't despair: add more assumptions!

Outline

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Finite sum minimization

Finite-sum minimization

return to finite sum problem:

$$\text{minimize} \quad \frac{1}{m} \sum_{i=1}^m f_i(x), \quad (3)$$

where each f_i is L_i -smooth and convex

why use SGD for finite sum minimization?

- ▶ evaluating minibatch gradient is cheaper per iteration
- ▶ converges faster than GD since each iteration is faster

Convergence of SGD

prove SGD minimizes finite sum (3):

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$$\begin{aligned}\|x_{k+1} - x_\star\|^2 &= \|x_k - x_\star - \eta \widehat{\nabla} f(x_k)\|^2 \\ &= \|x_k - x_\star\|^2 - 2\eta \langle x_k - x_\star, \widehat{\nabla} f(x_k) \rangle + \eta^2 \|\widehat{\nabla} f(x_k)\|^2.\end{aligned}$$

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take expectation wrt $\widehat{\nabla} f(x_k)$:

$$\begin{aligned}\mathbb{E}_k \|x_{k+1} - x_\star\|^2 &= \|x_k - x_\star\|^2 - 2\eta \langle x_k - x_\star, \nabla f(x_k) \rangle + \eta^2 \mathbb{E}_k \|\widehat{\nabla} f(x_k)\|^2 \\ &\leq (1 - \eta\mu) \|x_k - x_\star\|^2 - 2\eta (f(x_k) - f(x_\star)) \\ &\quad + \eta^2 \mathbb{E}_k \|\widehat{\nabla} f(x_k)\|^2\end{aligned}$$

using strong convexity:

$$f(x_\star) \geq f(x_k) + \nabla f(x_k)^T (x_\star - x_k) + \frac{\mu}{2} \|x_\star - x_k\|^2.$$

One-step lemma

we have shown the following progress bound for one step of SGD

Lemma

at iteration k of SGD,

$$\begin{aligned}\mathbb{E}_k \|x_{k+1} - x_\star\|^2 &\leq (1 - \eta\mu) \|x_k - x_\star\|^2 \\ &\quad - 2\eta (f(x_k) - f(x_\star)) + \eta^2 \mathbb{E}_k \|\hat{\nabla} f(x_k)\|^2\end{aligned}$$

how to show convergence? ideas:

- ▶ small/decreasing stepsize η
e.g., Statistical Adaptive Stochastic Gradient Methods
- ▶ bound variance $\mathbb{E}_k \|\hat{\nabla} f(x_k)\|^2$, eg Gower et al., 2019

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let's bound the variance!

Expected smoothness

Definition (Expected smoothness)

f satisfies L -expected smoothness (L -ES) if $\exists L > 0$ such that

$$\mathbb{E} \|\hat{\nabla} f(x) - \hat{\nabla} f(x_*)\|^2 \leq 2L(f(x) - f(x_*))$$

reduces to L -smoothness if we replace $\hat{\nabla}$ by ∇ :

$$f(x) - f(x_*) \geq \frac{1}{2L} \|\nabla f(x) - \nabla f(x_*)\|^2$$

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Corollary

define $\sigma^2 := \mathbb{E} \|\hat{\nabla} f(x_*)\|^2$. then

$$\mathbb{E} \|\hat{\nabla} f(x)\|^2 \leq 4L(f(x) - f(x_*)) + 2\sigma^2, \quad \forall x$$

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under ES, gradient variance is controlled by suboptimality and variance of the gradient at the optimum

L -ES condition for smooth convex functions

Theorem (special case of Gower et al., 2019)

Suppose each f_i is L_i -smooth and convex. Consider mini-batch stochastic gradients $\widehat{\nabla}f = \frac{1}{|S|} \sum_{i \in S} \nabla f_i(x)$ with batch-size $b_g = |S|$. Then

$$\mathbb{E} \|\widehat{\nabla}f(x)\|^2 \leq 4L(f(x) - f(x_*)) + 2\sigma^2,$$

with

$$L = \frac{m(b_g - 1)}{b_g(m - 1)} \frac{1}{m} \sum_{i=1}^m L_i + \frac{m - b_g}{b_g(m - 1)} \max_{1 \leq i \leq m} L_i$$

and

$$\sigma^2 = \frac{m - b_g}{b_g(m - 1)} \frac{1}{m} \sum_{i=1}^m \|\nabla f_i(x_*)\|^2$$

sanity check: $\sigma^2 \rightarrow 0$ as $b_g \rightarrow n$

Back to SGD convergence

using the one-step lemma with μ -strong convexity and L -ES, we find

$$\begin{aligned}\mathbb{E}_k \|x_{k+1} - x_\star\|^2 &\leq (1 - \eta\mu) \|x_k - x_\star\|^2 \\ &\quad + 2\eta(2\eta L - 1)(f(x_k) - f(x_\star)) + \eta^2 2\sigma^2\end{aligned}$$

so, choosing stepsize $\eta \leq \frac{1}{2L}$,

$$\mathbb{E}_k \|x_{k+1} - x_\star\|^2 \leq (1 - \eta\mu) \|x_k - x_\star\|^2 + \eta^2 2\sigma^2$$

SGD convergence contd

apply induction + take total expectation to get

$$\begin{aligned}\mathbb{E}\|x_{k+1} - x_\star\|^2 &\leq (1 - \eta\mu)^{k+1}\|x_0 - x_\star\|^2 + \left(\sum_{j=0}^k (1 - \eta\mu)^j\right) \eta^2 2\sigma^2 \\ &\leq (1 - \eta\mu)^{k+1}\|x_0 - x_\star\|^2 + \frac{\eta 2\sigma^2}{\mu}\end{aligned}$$

by summing the geometric series. choose $\eta \leq \frac{\mu\epsilon}{4\sigma^2}$, so

$$\mathbb{E}\|x_{k+1} - x_\star\|^2 \leq (1 - \eta\mu)^{k+1}\|x_0 - x_\star\|^2 + \frac{\epsilon}{2}$$

we can solve for k to find how many iterations are needed to reach error $\frac{\epsilon}{2}$:

$$k \geq (\eta\mu)^{-1} \log \left(\frac{2(f(x_0) - f(x_\star))}{\epsilon} \right)$$

SGD convergence with fixed stepsize

we have shown

Theorem

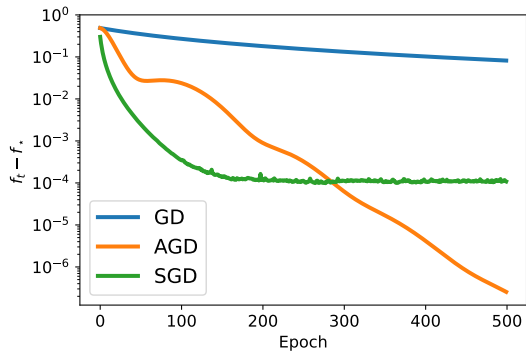
Suppose $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is μ -strongly convex, with an L -ES stochastic gradient oracle. Run SGD with batchsize b_g and fixed stepsize $\eta = \min \left\{ \frac{1}{2L}, \frac{\epsilon\mu}{4\sigma^2} \right\}$. Then for

$k \geq (\eta\mu)^{-1} \log \left(\frac{2(f(x_0) - f(x_*))}{\epsilon} \right)$ iterations,

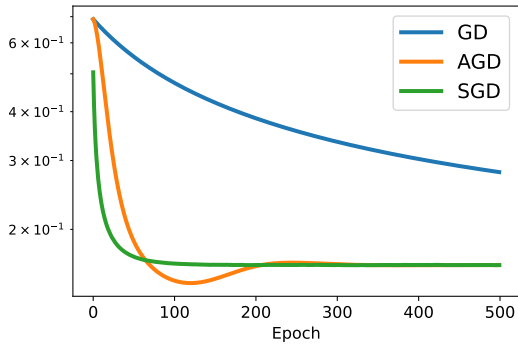
$$\mathbb{E} \|x_k - x_*\|^2 \leq \epsilon$$

- ▶ same convergence rate as we'd get with decreasing stepsize sequence $\eta = \mathcal{O}(1/k)$
- ▶ but motivates variance reduction, which will give linear convergence!

Results: Optimization error



Results: Test error



train faster, generalize better

The gradient is too noisy!

the expected smoothness condition shows the gradient is noisy,

$$\mathbb{E}\|\hat{\nabla}f(x)\|^2 \leq 4L(f(x) - f(x_\star)) + 2\sigma^2,$$

even at x_\star

- ▶ good news: $f(x) - f^\star \rightarrow 0$ as $x \rightarrow x_\star$
- ▶ bad news: $\sigma^2 > 0$ even near x_\star

can we design an algorithm that eliminates this noise as $x \rightarrow x_\star$?

Stochastic Variance Reduced Gradient

Stochastic Variance Reduced Gradient (SVRG) uses a different stochastic gradient

$$g(x) = \hat{\nabla} f(x) - \hat{\nabla} f(x_s) + \nabla f(x_s)$$

where

- ▶ $\hat{\nabla}$ still denotes the minibatch gradient
- ▶ $x_s \in \mathbf{R}^n$ is a reference point
- ▶ $\nabla f(x_s) - \hat{\nabla} f(x_s)$ is a control variate introduced to reduce variance

$g(x) \in \mathbf{R}^n$ is a stochastic gradient at $x \in \mathbf{R}^n$:

$$\mathbb{E}[g(x)] = \nabla f(x) - \nabla f(x_s) + \nabla f(x_s) = \nabla f(x),$$

SVRG algorithm

1. initialize at x_0 and set $x_s = x_0$
2. for $s = 0, \dots, S$
 - 2.1 compute and store $\nabla f(x_s)$
 - 2.2 for $k = 0, \dots, m - 1$

$$x_{k+1}^{(s)} = x_k^{(s)} - \eta \left(\widehat{\nabla} f(x_k^{(s)}) - \widehat{\nabla} f(x_s) + \nabla f(x_s) \right)$$

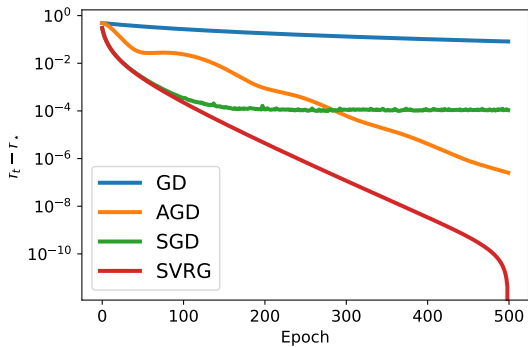
- 2.3 select x_{s+1} by uniformly sampling at random from $\{x_0^{(s)}, \dots, x_{m-1}^{(s)}\}$
 - 2.4 set $x_0^{(s+1)} = x_{s+1}$
3. return x_S

- notice that $\mathbb{E}f_{s+1} = \frac{1}{m} \sum_{i=1}^m f(x_i^{(s)})$ (needed for proof)
- in practice, fine to set $f_{s+1} = f(x_m^{(s)})$ (last iterate)

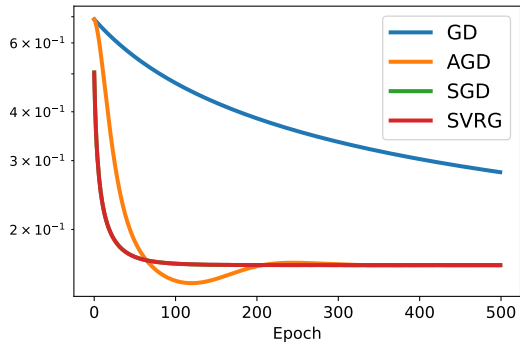
SVRG numerical performance

- ▶ revisit the same logistic regression example
- ▶ run SVRG with step-size $\eta = 4$
- ▶ update snapshot every epoch

Results: Optimization error



Results: Test loss



Using SVRG in practice

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Q: how to choose step-size η ?

A: monitor convergence. theoretical step-size often too small

Q: does SVRG work for non-convex problems like deep learning?

A: alas, no: variance reduction may worsen performance for nonconvex problems!

Some useful identities

recall the following two identities for random variables X, Y :

1. $\mathbb{E}\|X + Y\|^2 \leq 2\mathbb{E}\|X\|^2 + 2\mathbb{E}\|Y\|^2$
2. $\mathbb{E}\|X - \mathbb{E}[X]\|^2 \leq \mathbb{E}\|X\|^2$

Some useful identities

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1. $\mathbb{E}\|X + Y\|^2 \leq 2\mathbb{E}\|X\|^2 + 2\mathbb{E}\|Y\|^2$

2. $\mathbb{E}\|X - \mathbb{E}[X]\|^2 \leq \mathbb{E}\|X\|^2$

(exercise: prove these!)

SVRG reduces variance

variance of $g(x)$ depends on suboptimality of x and x_s

$$\begin{aligned}\mathbb{E}\|g(x)\|^2 &= \mathbb{E}\|g(x) - \widehat{\nabla}f(x_*) + \widehat{\nabla}f(x_*)\|^2 \\&= \mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_*) + \widehat{\nabla}f(x_*) - \widehat{\nabla}f(x_s) + \nabla f(x_s)\|^2 \\&\leq 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_*)\|^2 \\&\quad + 2\mathbb{E}\|\widehat{\nabla}f(x_s) - \widehat{\nabla}f(x_*) - \nabla f(x_s)\|^2 \\&= 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_*)\|^2 \\&\quad + 2\mathbb{E}\|\widehat{\nabla}f(x_s) - \widehat{\nabla}f(x_*) - \mathbb{E}[\widehat{\nabla}f(x_s) - \widehat{\nabla}f(x_*)]\|^2 \\&= 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_*)\|^2 + 2\mathbb{E}\|\widehat{\nabla}f(x_s) - \widehat{\nabla}f(x_*)\|^2 \\&= 4L[f(x) - f(x_*) + f(x_s) - f(x_*)]\end{aligned}$$

hence $\text{Var}(g(x)) \rightarrow 0$ as $f(x) \rightarrow f_*$, $f(x_s) \rightarrow f_*$

How to select x_s ?

to ensure $x, x_s \rightarrow x_*$ (and so $\text{Var}(g(x)) \rightarrow 0$)

- ▶ update x_s as we make progress (so $f(x_s) \rightarrow f(x_*)$)
- ▶ don't update too often, as computing $\nabla f(x_s)$ is expensive

SVRG convergence

Theorem

Run SVRG with $S = \mathcal{O}\left(\log\left(\frac{1}{\epsilon}\right)\right)$ outer iterations, $m = \mathcal{O}(\kappa)$ inner iterations, and fixed stepsize $\eta = \mathcal{O}(1/L)$. Then

$$\mathbb{E}[f(x_S)] - f(x_*) \leq \epsilon.$$

The number of gradient oracle calls is bounded by

$$\mathcal{O}\left((n + \kappa b_g) \log\left(\frac{1}{\epsilon}\right)\right).$$

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- ▶ unlike SGD, SVRG converges linearly to the optimum
- ▶ when $\kappa = \mathcal{O}(n)$, SVRG makes only $\tilde{\mathcal{O}}(nb_g)$ oracle calls, while GD makes $\tilde{\mathcal{O}}(n^2)$ calls. so SVRG reduces the number of calls by n/b_g !

Proof of SVRG convergence

the argument may be broken down into two lemmas. We begin with the following one-step progress bound for outer-iteration s

Lemma (One-step lemma)

Suppose we are at iteration k of outer-iteration s . Then

$$\begin{aligned}\mathbb{E}_k \|x_{k+1}^{(s)} - x_\star\|^2 &\leq \|x_k^{(s)} - x_\star\|^2 + 2\eta(2\eta L - 1)[f(x_k^{(s)}) - f(x_\star)] \\ &\quad + 4\eta^2 L[f(x_s) - f(x_\star)]\end{aligned}$$

Proof of One-step lemma

$$\begin{aligned}\mathbb{E}_k \|x_{k+1}^{(s)} - x_\star\|^2 &= \\ &\|x_k^{(s)} - x_\star\|^2 - 2\eta \langle \nabla f(x_k), x_k - x_\star \rangle + \eta^2 \mathbb{E}_k \|g(x_k)\|^2 \\ &\leq \|x_k^{(s)} - x_\star\|^2 - 2\eta (f(x_k) - f(x_\star)) + \eta^2 \mathbb{E}_k \|g(x_k)\|^2 \\ &\leq \|x_k^{(s)} - x_\star\|^2 - 2\eta (f(x_k) - f(x_\star)) + \\ &\quad 4\eta^2 L[f(x) - f(x_\star) + f(x_s) - f(x_\star)],\end{aligned}$$

where the first inequality uses convexity

$$f(x_k) - f(x_\star) \leq \langle \nabla f(x_k), x_k - x_\star \rangle$$

so, after rearranging

$$\begin{aligned}\mathbb{E}_k \|x_{k+1}^{(s)} - x_\star\|^2 &\leq \|x_k^{(s)} - x_\star\|^2 + 2\eta (2\eta L - 1) [f(x_k^{(s)}) - f(x_\star)] \\ &\quad + 4\eta^2 L[f(x_s) - f(x_\star)]\end{aligned}$$

Outer iteration contraction

the next step is show to the follow contraction result for the outer-iterations.

Lemma (Outer iteration contraction)

Suppose we are in outer iteration s . Then

$$\mathbb{E}_{0:s-1}[f(x_s)] - f(x_*) \leq \left[\frac{1}{\eta\mu(1-2\eta L)m} + \frac{2}{1-2\eta L} \right] (f(x_{s-1}) - f(x_*)),$$

where $\mathbb{E}_{0:s-1}$ denotes the expectation conditioned on outer-iterations 0 through $s-1$.

Proof of outer iteration contraction

summing the inequality in the one-step lemma from $k = 0, \dots, m - 1$,

$$\sum_{k=1}^m \mathbb{E}_k \|x_{k+1}^{(s)} - x_\star\|^2 \leq \sum_{k=0}^{m-1} \|x_k^{(s)} - x_\star\|^2 +$$
$$2\eta m (2\eta L - 1) \frac{1}{m} \sum_{k=0}^{m-1} [f(x_k^{(s)}) - f(x_\star)] + 4m\eta^2 [f(x_{s-1}) - f(x_\star)].$$

Proof of outer iteration contraction

summing the inequality in the one-step lemma from $k = 0, \dots, m - 1$,

$$\begin{aligned} \sum_{k=1}^m \mathbb{E}_k \|x_{k+1}^{(s)} - x_\star\|^2 &\leq \sum_{k=0}^{m-1} \|x_k^{(s)} - x_\star\|^2 + \\ &2\eta m (2\eta L - 1) \frac{1}{m} \sum_{k=0}^{m-1} [f(x_k^{(s)}) - f(x_\star)] + 4m\eta^2 [f(x_{s-1}) - f(x_\star)]. \end{aligned}$$

taking the expectation over all inner-iterations conditioned on outer-iterations 0 through $s - 1$ + cancellation, yields

$$\begin{aligned} \mathbb{E}_{0:s-1} \|x_m^{(s)} - x_\star\|^2 &\leq \|x_{s-1} - x_\star\|^2 + \\ &+ 2\eta m (2\eta L - 1) (\mathbb{E}_{0:s-1} [f(x_s)] - f(x_\star)) + 4m\eta^2 L [f(x_{s-1}) - f(x_\star)]. \end{aligned}$$

Proof contd.

rearranging gives

$$\begin{aligned} & \mathbb{E}_{0:s-1} \|x_s - x_\star\|^2 + 2\eta m (1 - 2\eta L) (\mathbb{E}_{0:s-1} [f(x_s)] - f(x_\star)) \\ & \leq 2 \left(\frac{1}{\mu} + 2m\eta^2 L \right) [f(x_{s-1}) - f(x_\star)], \end{aligned}$$

where we used strong convexity of f

$$\|x_{s-1} - x_\star\|^2 \leq \frac{2}{\mu} (f(x_{s-1}) - f(x_\star))$$

hence (dropping $\mathbb{E}_{0:s-1} \|x_s - x_\star\|^2 \geq 0$)

$$\begin{aligned} & 2\eta m (1 - 2\eta L) (\mathbb{E}_{0:s-1} [f(x_s)] - f(x_\star)) \\ & \leq 2 \left(\frac{1}{\mu} + 2m\eta^2 L \right) [f(x_{s-1}) - f(x_\star)], \end{aligned}$$

and so the claim follows by rearrangement

Finishing the proof

$$\mathbb{E}_{0:s-1}[f(x_{s+1})] - f(x_*) \leq \left[\frac{1}{\eta\mu(1-2\eta L)m} + \frac{2}{1-2\eta L} \right] (f(x_s) - f(x_*))$$

setting $\eta = \frac{1}{10L}$ and $m = 20\frac{\mathcal{L}}{\mu}$, we find

$$\mathbb{E}_{0:s-1}[f(x_s)] - f(x_*) \leq \frac{1}{2} (f(x_{s-1}) - f(x_*))$$

now taking expectations over all outer iterations and recursing,

$$\mathbb{E}[f(x_s)] - f(x_*) \leq \left(\frac{1}{2}\right)^s (f(x_0) - f(x_*)),$$

which gives the theorem after setting $s = O(\log(1/\epsilon))$

SVRG: Final comments

- ▶ variance reduction is a powerful tool for convex finite-sum optimization, as it delivers linear convergence
- ▶ SVRG has motivated the development of better (usually) variance reduced algorithms such as SAGA and Katyusha
- ▶ outside of finite-sum convex optimization, variance reduction hasn't proven to be terribly useful