

# CME 307/MSE 311: Optimization

## Acceleration, Stochastic Gradient Descent, and Variance Reduction

Professor Udell

Management Science and Engineering  
Stanford

February 14, 2024

## Convergence of gradient descent

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

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

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

we analyzed gradient descent (GD) on this problem:

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

## 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

**Q:** is GD the best first-order method for  $L$ -smooth,  $\mu$ -strongly convex functions?

## 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

**Q:** is GD the best first-order method for  $L$ -smooth,  $\mu$ -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  $\epsilon$ -suboptimal point of *any*  $L$ -smooth,  $\mu$ -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

## 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

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

## 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,  $\mu$ -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

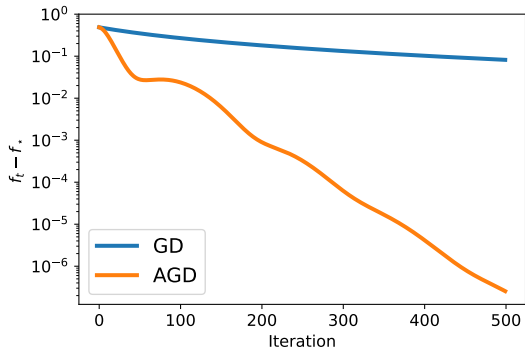
goal is to solve the logistic regression problem

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

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  $\mu$ -strongly convex functions
- ▶ converges to  $\epsilon$ -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)



## 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)

idea:

## 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)

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  $\omega$

## 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  $\omega$

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  $\omega$  given parameter  $x$
- ▶ machine learning:  $f(x; \omega)$  is misfit of model  $x$  on example  $\omega$

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:  $\omega$  represents wind and other weather conditions
  - ▶ trading a large portfolio slowly to reduce market impact:  $\omega$  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,  $\Omega \subseteq \mathbf{R}^n$ ,  $\omega$  a random variable distributed according to probability measure  $\mu_{\Omega}$

objective is expected cost under the randomness due to  $\omega$ :

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

## Stochastic optimization: examples

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

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

## Stochastic optimization: examples

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

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

then  $x_{\star} =$



## Stochastic optimization: examples

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

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

then  $x_{\star} = \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$  and  $f_{\star} = \text{Var}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$ .

## Stochastic optimization: examples

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

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

then  $x_{\star} = \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$  and  $f_{\star} = \text{Var}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$ .

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

$$\text{minimize } \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}} [|x - \omega|]$$

## Stochastic optimization: examples

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

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

then  $x_{\star} = \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$  and  $f_{\star} = \text{Var}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$ .

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

$$\text{minimize } \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}} [|x - \omega|]$$

then  $x_{\star} =$

## Stochastic optimization: examples

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

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

then  $x_{\star} = \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$  and  $f_{\star} = \text{Var}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$ .

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

$$\text{minimize } \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}} [|x - \omega|]$$

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

## Stochastic optimization: examples

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

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

then  $x_{\star} = \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$  and  $f_{\star} = \text{Var}_{\omega \sim \mu_{\mathbf{R}}}[\omega]$ .

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

$$\text{minimize } \mathbb{E}_{\omega \sim \mu_{\mathbf{R}}} [|x - \omega|]$$

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  $\nabla F(x)$

## 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  $\nabla F(x)$

## 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  $\nabla F(x)$

**Q:** examples of stochastic gradient oracle?



## 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  $\nabla F(x)$

**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  $\eta_k$  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  $\epsilon$ -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  $\epsilon$ -suboptimal point

## SGD convergence: discussion

- ▶ with fixed stepsize, the algorithm converges to  $\epsilon$ -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  $\epsilon$ -suboptimal point

**don't despair:** add more assumptions!

# Outline

Stochastic optimization

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):



## Convergence of SGD

prove SGD minimizes finite sum (3):

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

## Convergence of SGD

prove SGD minimizes finite sum (3):

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

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

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

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  $\nabla$ :

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

## 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  $\nabla$ :

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

### Corollary

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

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

## 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  $\nabla$ :

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

### Corollary

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

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

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  $\mu$ -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

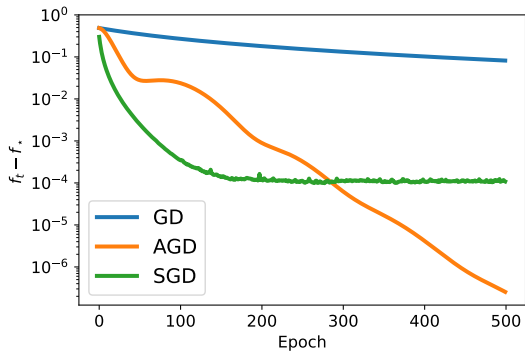
Suppose  $f : \mathbf{R}^n \rightarrow \mathbf{R}$  is  $\mu$ -strongly convex, with an  $L$ -ES stochastic gradient oracle. Run SGD with batchsize  $b_g$  and fixed stepsize  $\eta = \min \left\{ \frac{1}{2L}, \frac{\epsilon\mu}{4\sigma^2} \right\}$ . Then for

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

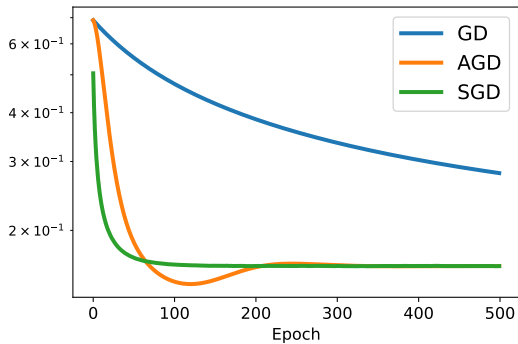
$$\mathbb{E} \|x_k - x_*\|^2 \leq \epsilon$$

- ▶ 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  $x_S$

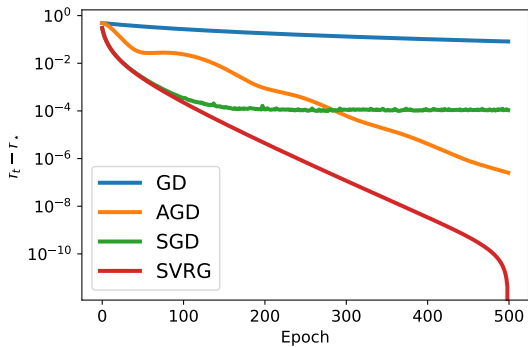
- notice that  $\mathbb{E}f_{s+1} = \frac{1}{m} \sum_{i=1}^m f(x_i^{(s)})$  (needed for proof)
- in practice, fine to set  $f_{s+1} = f(x_m^{(s)})$  (last iterate)



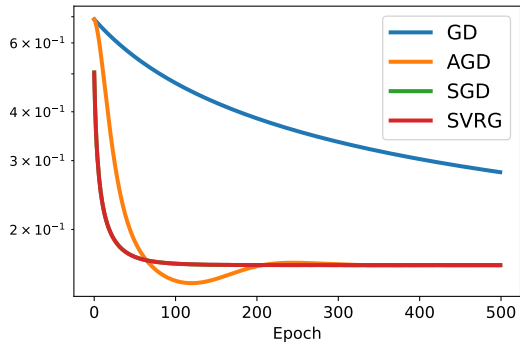
## SVRG numerical performance

- ▶ 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

## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

**A:** not obvious even from theory (below). often use  $m \approx n/b_g$  where  $b_g$  is batchsize used to compute stochastic gradient update every 1–2 epochs

## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

**A:** not obvious even from theory (below). often use  $m \approx n/b_g$  where  $b_g$  is batchsize used to compute stochastic gradient update every 1–2 epochs

**Q:** how to choose step-size  $\eta$ ?

## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

**A:** not obvious even from theory (below). often use  $m \approx n/b_g$  where  $b_g$  is batchsize used to compute stochastic gradient update every 1–2 epochs

**Q:** how to choose step-size  $\eta$ ?

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



## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

**A:** not obvious even from theory (below). often use  $m \approx n/b_g$  where  $b_g$  is batchsize used to compute stochastic gradient update every 1–2 epochs

**Q:** how to choose step-size  $\eta$ ?

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

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

## Using SVRG in practice

**Q:** how to select update frequency  $m$ ?

**A:** not obvious even from theory (below). often use  $m \approx n/b_g$  where  $b_g$  is batchsize used to compute stochastic gradient update every 1–2 epochs

**Q:** how to choose step-size  $\eta$ ?

**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

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

(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

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

## SVRG convergence

### Theorem

Run SVRG with  $S = \mathcal{O}(\log(\frac{1}{\epsilon}))$  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

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

- ▶ 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