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

# Acceleration, Stochastic Gradient Descent, and Variance Reduction

Professor Udell

Management Science and Engineering
Stanford

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slides developed with Zachary Frangella

## **Convergence of gradient descent**

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

minimize 
$$f(x)$$
 (1)

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

we analyzed gradient descent (GD) on this problem:

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

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

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

#### **Acceleration: motivation**

#### Definition

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

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

**Q:** Is GD the best first-order method to optimize a L-smooth,  $\mu$ -strongly convex function? **A:** Not Nemirovski and Yudin showed a *lower-bound* of

$$\mathcal{T}_{\mathrm{opt}} = \Omega\left(\sqrt{\kappa}\log\left(rac{1}{\epsilon}
ight)
ight)$$
 iterations

to find an  $\epsilon$ -suboptimal point of any L-smooth,  $\mu$ -strongly convex function **notice:** same rate as CG if f is quadratic

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Let's work in the infinite dimensional-space  $\ell^2(\mathbf{R})$ : vectors x of infinite length satisfying

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

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

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How would you find the minimum? How would a first-order method find the minimum? source: Section 2.1, Nesterov, 2018

#### The lower bound

The functions on the preceding slide yield the following bound:

# Theorem (Theorem 2.1.12, Nesterov, 2018)

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

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

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

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

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

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Q: Does gradient descent satisfy the conditions of this bound? Newton's method? BFGS?

#### **Accelerated Gradient Descent**

Nesterov's accelerated gradient method (AGD) is

- 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  $x_0, y_0 \in \mathbb{R}^n$
- 2. for k = 0, 1, ..., T,

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

3. Return  $x_{k+1}$ 

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

source: Section 2.2, Nesterov, 2018

## GD vs. AGD: numerical example

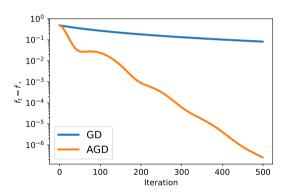
goal is to solve the logistic regression problem

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

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

- ▶ GD and AGD both use theoretically-chosen stepsizes:
  - ▶ GD is run with stepsize  $\frac{1}{I}$ , 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

- ightharpoonup AGD is theoretically optimal among first-order methods for *L*-smooth and  $\mu$ -strongly convex functions
- ightharpoonup converges to  $\epsilon$ -suboptimality in at most

$$\mathcal{O}\left(\sqrt{\kappa}\log\left(\frac{1}{\epsilon}\right)\right)$$
 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
- closely related: momentum methods like heavy-ball and Adam, which get same fast convergence rate on quadratic functions. This distill.pub tutorial gives more intuition.

## **Outline**

Stochastic optimization

Finite sum minimization

finite sum minimization: solve

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

finite sum minimization: solve

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

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:

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idea: throw away data! (cleverly)

# Minimizing an expectation

Stochastic optimization: solve

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

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

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

# Minimizing an expectation

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- random loss function f
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examples:  $data \omega = (a, b)$  is random

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

minimize expected loss on data from same distribution, 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
  - $\triangleright$  flying an airplane:  $\omega$  represents wind and other weather conditions
  - ightharpoonup trading a large portfolio slowly to reduce market impact:  $\omega$  represents exogenous moves of asset prices

## Stochastic optimization: what distribution?

stochastic optimization problem

minimize 
$$\mathbb{E}_{\omega \sim \mu_{\Omega}}[f(\omega, x)]$$
 variable  $x \in \mathbf{R}^n$  (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  $\omega$ :

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

1. 
$$n=1, \Omega=\mathbf{R}$$
, and  $f(\omega,x)=(x-ga)^2$ . minimize  $\mathbb{E}_{\omega\sim\mu_{\mathbf{R}}}\left[(x-\omega)^2\right]$ 

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

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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  $\omega_1,\ldots,\omega_m$ ) results in the finite sum minimization problem

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

#### Definition

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

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

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

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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 a stochastic gradient at x

## Stochastic gradient method

#### Stochastic gradient method:

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

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

- Generally called stochastic gradient descent (SGD) although it is not a descent method!
- ▶ SGD uses a stochastic gradient  $g(\omega_k, x_k)$  rather than the true gradient
- ▶ how to select stepsize  $\eta_k$ ?

## 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  $\eta_k = O(1)$ ,

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

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

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

## SGD convergence: discussion

- $\blacktriangleright$  with fixed stepsize, the algorithm converges to  $\epsilon$ -sublevel set
- ► convergence to optimum requires a decreasing stepsize ⇒ slow!

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- convergence to optimum requires a decreasing stepsize has spawned industry of "stepsize schedules"
  - Cosine schedule
  - The road less scheduled

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

analysis is tight: there is a matching lower bound.

## Theorem (Agarwal et al., 2012)

For strongly convex objectives, any algorithm using a stochastic gradient oracle must make at least  $\Omega(1/\epsilon)$  queries to obtain an  $\epsilon$ -suboptimal point.

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don't despair: add more assumptions!

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Finite sum minimization

#### Finite-sum minimization

return to finite sum problem:

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

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

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prove SGD minimizes finite sum (3):

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=  $||x_{k} - x_{\star}||^{2} - 2\eta \langle x_{k} - x_{\star}, \widehat{\nabla} f(x_{k}) \rangle + \eta^{2} ||\widehat{\nabla} f(x_{k})||^{2}.$ 

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

$$\mathbb{E}_{k} \|x_{k+1} - x_{\star}\|^{2} = \|x_{k} - x_{\star}\|^{2} - 2\eta \langle x_{k} - x_{\star}, \nabla f(x_{k}) \rangle + \eta^{2} \mathbb{E}_{k} \|\widehat{\nabla} f(x_{k})\|^{2}$$

$$\leq (1 - \eta \mu) \|x_{k} - x_{\star}\|^{2} - 2\eta \left(f(x_{k}) - f(x_{\star})\right)$$

$$+ \eta^{2} \mathbb{E}_{k} \|\widehat{\nabla} f(x_{k})\|^{2}$$

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,

$$\mathbb{E}_{k} \|x_{k+1} - x_{\star}\|^{2} \leq (1 - \eta \mu) \|x_{k} - x_{\star}\|^{2}$$
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how to show convergence? ideas:

- ightharpoonup small/decreasing stepsize  $\eta$  e.g., Statistical Adaptive Stochastic Gradient Methods
- **b** bound variance  $\mathbb{E}_k \|\widehat{\nabla} f(x_k)\|^2$ , 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

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

reduces to *L*-smoothness if we replace  $\widehat{\nabla}$  by  $\nabla$ :

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## Corollary

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

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

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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  $\widehat{\nabla} f = \frac{1}{|S|} \sum_{i \in S} f_i(x)$  with batch-size  $b_g = |S|$ . Then

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

with

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

and

$$\sigma^{2} = \frac{m - b_{g}}{b_{g}(m - 1)} \frac{1}{m} \sum_{i=1}^{m} \|\nabla f_{i}(x_{\star})\|^{2}$$

#### 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  $\widehat{\nabla} f = \frac{1}{|S|} \sum_{i \in S} f_i(x)$  with batch-size  $b_g = |S|$ . Then

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

with

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

and

$$\sigma^{2} = \frac{m - b_{g}}{b_{g}(m - 1)} \frac{1}{m} \sum_{i=1}^{m} \|\nabla f_{i}(x_{\star})\|^{2}$$

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

## Back to SGD convergence

using the one-step lemma with  $\mu$ -strong convexity and L-ES, we find

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

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

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

## **SGD** convergence contd

apply induction + take total expectation to get

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

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

$$\mathbb{E}||x_{k+1} - x_{\star}||^{2} \le (1 - \eta\mu)^{k+1}||x_{0} - x_{\star}||^{2} + \frac{\epsilon}{2}$$

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

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

## SGD convergence with fixed stepsize

we have shown

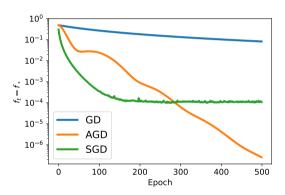
#### **Theorem**

Suppose  $f: \mathbf{R}^n \to \mathbf{R}$  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  $k \geq (\eta \mu)^{-1} \log\left(\frac{2(f(x_0) - f(x_\star))}{\epsilon}\right)$  iterations,

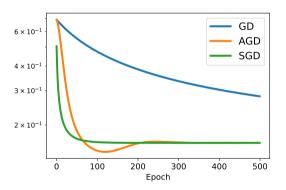
$$\mathbb{E}||x_k - x_\star||^2 \le \epsilon$$

- lacktriangle 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, even at  $x_{\star}$ :

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

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

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

#### **Stochastic Variance Reduced Gradient**

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

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

#### where

- $ightharpoonup \widehat{\nabla}$  still denotes the minibatch gradient
- $\triangleright x_s \in \mathbf{R}^n$  is a reference point
- $ightharpoonup 
  abla f(x_s) \widehat{\nabla} f(x_s)$  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, ..., S
  - 2.1 compute and store  $\nabla f(x_s)$
  - 2.2 for k = 0, ..., m-1

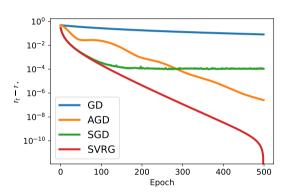
$$x_{k+1}^{(s)} = x_k^{(s)} - \eta \left( \widehat{\nabla} f(x_k^{(s)}) - \widehat{\nabla} f(x_s) + \nabla f(x_s) \right)$$

- 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  $\mathbb{E}f(x_0^{(s+1)}) = \frac{1}{m} \sum_{k=1}^m f(x_i^{(s)})$  (needed for proof)
- ightharpoonup in practice, fine to choose last iterate  $x_0^{(s+1)}=x_m^{(s)}$  instead of sampling

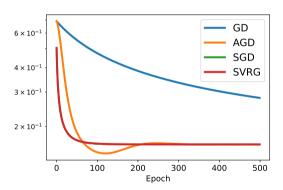
## **SVRG** numerical performance

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

## **Results: Optimization error**



## **Results: Test loss**



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

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

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

#### Some useful identities

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

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

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  $x_s$ 

$$\mathbb{E}\|g(x)\|^{2} = \mathbb{E}\|g(x) - \widehat{\nabla}f(x_{\star}) + \widehat{\nabla}f(x_{\star})\|^{2}$$

$$= \mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_{\star}) + \widehat{\nabla}f(x_{\star}) - \widehat{\nabla}f(x_{s}) + \nabla f(x_{s})\|^{2}$$

$$\leq 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_{\star})\|^{2}$$

$$+2\mathbb{E}\|\widehat{\nabla}f(x_{s}) - \widehat{\nabla}f(x_{\star}) - \nabla f(x_{s})\|^{2}$$

$$= 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_{\star})\|^{2}$$

$$+2\mathbb{E}\|\widehat{\nabla}f(x_{s}) - \widehat{\nabla}f(x_{\star}) - \mathbb{E}[\widehat{\nabla}f(x_{s}) - \widehat{\nabla}f(x_{\star})]\|^{2}$$

$$= 2\mathbb{E}\|\widehat{\nabla}f(x) - \widehat{\nabla}f(x_{\star})\|^{2} + 2\mathbb{E}\|\widehat{\nabla}f(x_{s}) - \widehat{\nabla}f(x_{\star})\|^{2}$$

$$= 4L[f(x) - f(x_{\star}) + f(x_{s}) - f(x_{\star})]$$

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

### How to select $x_s$ ?

to ensure x,  $x_s o x_\star$  (and so  ${\sf Var}(g(x)) o 0)$ 

- ▶ update  $x_s$  as we make progress (so  $f(x_s) \rightarrow f(x_\star)$ )
- 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,  $m=O(\kappa)$  inner iterations, and fixed stepsize  $\eta=O(1/L)$ . Then

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

The number of gradient oracle calls is bounded by

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

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

### **Proof of SVRG convergence**

We will prove convergence with two lemmas. First, we prove a one-step progress bound for outer-iteration s:

## Lemma (One-step lemma)

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

$$\mathbb{E}_{k} \|x_{k+1}^{(s)} - x_{\star}\|^{2} \leq \|x_{k}^{(s)} - x_{\star}\|^{2} + 2\eta (2\eta L - 1) [f(x_{k}^{(s)}) - f(x_{\star})] + 4\eta^{2} L[f(x_{s}) - f(x_{\star})]$$

## **Proof of One-step lemma**

$$\begin{split} \mathbb{E}_{k} \| x_{k+1}^{(s)} - x_{\star} \|^{2} &= \\ \| x_{k}^{(s)} - x_{\star} \|^{2} - 2\eta \langle \nabla f(x_{k}), x_{k} - x_{\star} \rangle + \eta^{2} \mathbb{E}_{k} \| g(x_{k}) \|^{2} \\ &\leq \| x_{k}^{(s)} - x_{\star} \|^{2} - 2\eta \left( f(x_{k}) - f(x_{\star}) \right) + \eta^{2} \mathbb{E}_{k} \| g(x_{k}) \|^{2} \\ &\leq \| x_{k}^{(s)} - x_{\star} \|^{2} - 2\eta \left( f(x_{k}) - f(x_{\star}) \right) + \\ &4\eta^{2} \mathcal{L}[f(x) - f(x_{\star}) + f(x_{s}) - f(x_{\star}), ] \end{split}$$

where the first inequality uses convexity

$$f(x_k) - f(x_k) \le \langle \nabla f(x_k), x_k - x_k \rangle$$

so, after rearranging

$$\mathbb{E}_{k} \|x_{k+1}^{(s)} - x_{\star}\|^{2} \leq \|x_{k}^{(s)} - x_{\star}\|^{2} + 2\eta (2\eta L - 1) [f(x_{k}^{(s)}) - f(x_{\star})] + 4\eta^{2} L[f(x_{s}) - f(x_{\star})]$$

#### **Outer iteration contraction**

Next, we show the outer iteration produces a contraction:

# Lemma (Outer iteration contraction)

Suppose we are in outer iteration s. Then

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

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, ..., m - 1,

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

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

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

### Proof contd.

rearranging gives

$$\mathbb{E}_{0:s-1} \|x_s - x_\star\|^2 + 2\eta m (1 - 2\eta L) (\mathbb{E}_{0:s-1} [f(x_s)] - f(x_\star))$$

$$\leq 2 \left(\frac{1}{\mu} + 2m\eta^2 L\right) [f(x_{s-1}) - f(x_\star)],$$

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

$$2\eta m (1 - 2\eta L) (\mathbb{E}_{0:s-1} [f(x_s)] - f(x_{\star}))$$

$$\leq 2 \left(\frac{1}{\mu} + 2m\eta^2 L\right) [f(x_{s-1}) - f(x_{\star})],$$

and so the claim follows by rearrangement

# Finishing the proof

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

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

$$\mathbb{E}_{0:s-1}[f(x_s)] - f(x_\star) \le \frac{1}{2} \left( f(x_{s-1}) - f(x_\star) \right)$$

now taking expectations over all outer iterations and recursing,

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

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

#### **SVRG:** Final comments

- ▶ variance reduction delivers linear convergence for convex finite-sum optimization.
- ► SVRG has motivated the development of better (usually) variance reduced algorithms such as SAGA and Katyusha.
- ▶ alas, variance reduction has so far proved useful only in finite-sum convex optimization.