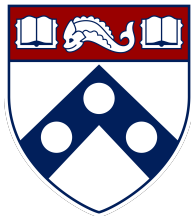


# Variance reduction for stochastic gradient methods



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# Outline

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- Stochastic variance reduced gradient (SVRG)
  - Convergence analysis for strongly convex problems
- Stochastic recursive gradient algorithm (SARAH)
  - Convergence analysis for nonconvex problems
- Other variance reduced stochastic methods
  - Stochastic dual coordinate ascent (SDCA)

# Finite-sum optimization

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$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^d} \quad F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n \underbrace{f_i(\mathbf{x})}_{\substack{\text{loss for } i\text{th sample} \\ (\mathbf{a}_i, y_i)}} + \underbrace{\psi(\mathbf{x})}_{\text{regularizer}}$$

common task in machine learning

- linear regression:  $f_i(\mathbf{x}) = \frac{1}{2}(\mathbf{a}_i^\top \mathbf{x} - y_i)^2$ ,  $\psi(\mathbf{x}) = 0$
- logistic regression:  $f_i(\mathbf{x}) = \log(1 + e^{-y_i \mathbf{a}_i^\top \mathbf{x}})$ ,  $\psi(\mathbf{x}) = 0$
- Lasso:  $f_i(\mathbf{x}) = \frac{1}{2}(\mathbf{a}_i^\top \mathbf{x} - y_i)^2$ ,  $\psi(\mathbf{x}) = \lambda \|\mathbf{x}\|_1$
- SVM:  $f_i(\mathbf{x}) = \max\{0, 1 - y_i \mathbf{a}_i^\top \mathbf{x}\}$ ,  $\psi(\mathbf{x}) = \frac{\lambda}{2} \|\mathbf{x}\|_2^2$
- ...

# Stochastic gradient descent (SGD)

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## Algorithm 12.1 Stochastic gradient descent (SGD)

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- 1: **for**  $t = 1, 2, \dots$  **do**
  - 2:   pick  $i_t \sim \text{Unif}(1, \dots, n)$
  - 3:    $\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t \nabla f_{i_t}(\mathbf{x}^t)$
- 

As we have shown in the last lecture

- large stepsizes poorly suppress variability of stochastic gradients  
 $\implies$  SGD with  $\eta_t \asymp 1$  tends to oscillate around global mins
- choosing  $\eta_t \asymp 1/t$  mitigates oscillation, but is too conservative

## Recall: SGD theory with fixed stepsizes

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$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta_t \mathbf{g}^t$$

- $\mathbf{g}^t$ : an unbiased estimate of  $F(\mathbf{x}^t)$
- $\mathbb{E}[\|\mathbf{g}^t\|_2^2] \leq \sigma_g^2 + c_g \|\nabla F(\mathbf{x}^t)\|_2^2$
- $F(\cdot)$ :  $\mu$ -strongly convex;  $L$ -smooth

From the last lecture, we know

$$\mathbb{E}[F(\mathbf{x}^t) - F(\mathbf{x}^*)] \leq \frac{\eta L \sigma_g^2}{2\mu} + (1 - \eta\mu)^t (F(\mathbf{x}^0) - F(\mathbf{x}^*))$$

## Recall: SGD theory with fixed stepsizes

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$$\mathbb{E}[F(\mathbf{x}^t) - F(\mathbf{x}^*)] \leq \frac{\eta L \sigma_g^2}{2\mu} + (1 - \eta\mu)^t (F(\mathbf{x}^0) - F(\mathbf{x}^*))$$

- vanilla SGD:  $\mathbf{g}^t = \nabla f_{i_t}(\mathbf{x}^t)$ 
  - **issue:**  $\sigma_g^2$  is non-negligible even when  $\mathbf{x}^t = \mathbf{x}^*$
- **question:** it is possible to design  $\mathbf{g}^t$  with reduced variability  $\sigma_g^2$ ?

# A simple idea

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Imagine we take some  $\mathbf{v}^t$  with  $\mathbb{E}[\mathbf{v}^t] = \mathbf{0}$  and set

$$\mathbf{g}^t = \nabla f_{i_t}(\mathbf{x}^t) - \mathbf{v}^t$$

— so  $\mathbf{g}^t$  is still an unbiased estimate of  $\nabla F(\mathbf{x}^t)$

**question:** how to reduce variability (i.e.  $\mathbb{E}[\|\mathbf{g}^t\|_2^2] < \mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}^t)\|_2^2]$ )?

**answer:** find some zero-mean  $\mathbf{v}^t$  that is positively correlated with  $\nabla f_{i_t}(\mathbf{x}^t)$  (i.e.  $\langle \mathbf{v}^t, \nabla f_{i_t}(\mathbf{x}^t) \rangle > 0$ ) ([why?](#))

# Reducing variance via gradient aggregation

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If the current iterate is not too far away from previous iterates, then historical gradient info might be useful in producing such a  $v^t$  to reduce variance

**main idea of this lecture:** aggregate previous gradient info to help improve the convergence rate



**Stochastic variance reduced gradient (SVRG)**

# Strongly convex and smooth problems (no regularization)

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$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^d} \quad F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})$$

- $f_i$ : convex and  $L$ -smooth
- $F$ :  $\mu$ -strongly convex
- $\kappa := L/\mu$ : condition number

# Stochastic variance reduced gradient (SVRG)

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— Johnson, Zhang '13

**key idea:** if we have access to a history point  $\mathbf{x}^{\text{old}}$  and  $\nabla F(\mathbf{x}^{\text{old}})$ , then

$$\underbrace{\nabla f_{i_t}(\mathbf{x}^t) - \nabla f_{i_t}(\mathbf{x}^{\text{old}})}_{\rightarrow \mathbf{0} \text{ if } \mathbf{x}^t \approx \mathbf{x}^{\text{old}}} + \underbrace{\nabla F(\mathbf{x}^{\text{old}})}_{\rightarrow \mathbf{0} \text{ if } \mathbf{x}^{\text{old}} \approx \mathbf{x}^*} \quad \text{with } i_t \sim \text{Unif}(1, \dots, n)$$

- is an unbiased estimate of  $\nabla F(\mathbf{x}^t)$
- converges to  $\mathbf{0}$  if  $\mathbf{x}^t \approx \mathbf{x}^{\text{old}} \approx \mathbf{x}^*$   
variability is reduced!

# Stochastic variance reduced gradient (SVRG)

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- operate in epochs
- in the  $s^{\text{th}}$  epoch
  - **very beginning**: take a snapshot  $\mathbf{x}_s^{\text{old}}$  of the current iterate, and compute the *batch gradient*  $\nabla F(\mathbf{x}_s^{\text{old}})$
  - **inner loop**: use the snapshot point to help reduce variance

$$\mathbf{x}_s^{t+1} = \mathbf{x}_s^t - \eta \{ \nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) + \nabla F(\mathbf{x}_s^{\text{old}}) \}$$

**a hybrid approach**: the batch gradient is computed only once per epoch

# SVRG algorithm (Johnson, Zhang '13)

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## Algorithm 12.2 SVRG for finite-sum optimization

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- 1: **for**  $s = 1, 2, \dots$  **do**
- 2:  $\mathbf{x}_s^{\text{old}} \leftarrow \mathbf{x}_{s-1}^m$ , and compute  $\underbrace{\nabla F(\mathbf{x}_s^{\text{old}})}_{\text{batch gradient}}$  // update snapshot
- 3: initialize  $\mathbf{x}_s^0 \leftarrow \mathbf{x}_s^{\text{old}}$
- 4: **for**  $\underbrace{t = 0, \dots, m-1}_{\text{each epoch contains } m \text{ iterations}}$  **do**
- 5: choose  $i_t$  uniformly from  $\{1, \dots, n\}$ , and

$$\mathbf{x}_s^{t+1} = \mathbf{x}_s^t - \eta \left\{ \underbrace{\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{\text{old}})}_{\text{stochastic gradient}} + \nabla F(\mathbf{x}_s^{\text{old}}) \right\}$$

# Remark

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- constant stepsize  $\eta$
- each epoch contains  $2m + n$  gradient computations
  - the batch gradient is computed only once every  $m$  iterations
  - the average per-iteration cost of SVRG is comparable to that of SGD if  $m \gtrsim n$

# Convergence analysis of SVRG

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## Theorem 12.1

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

$$\mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \leq \rho^s [F(\mathbf{x}_0^{\text{old}}) - F(\mathbf{x}^*)]$$

- **linear convergence:** choosing  $m \gtrsim L/\mu = \kappa$  and constant stepsizes  $\eta \asymp 1/L$  yields  $0 < \rho < 1/2$   
 $\implies O(\log \frac{1}{\varepsilon})$  epochs to attain  $\varepsilon$  accuracy

# Convergence analysis of SVRG

## Theorem 12.1

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

$$\mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \leq \rho^s [F(\mathbf{x}_0^{\text{old}}) - F(\mathbf{x}^*)]$$

- total computational cost:

$$\underbrace{(m+n)}_{\text{\# grad computation per epoch}} \log \frac{1}{\varepsilon} \asymp \underbrace{(n+\kappa)}_{\text{if } m \asymp \max\{n, \kappa\}} \log \frac{1}{\varepsilon}$$



# Proof of Theorem 12.1

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Here, we provide the proof for an alternative version, where in each epoch,

$$\mathbf{x}_{s+1}^{\text{old}} = \mathbf{x}_s^j \quad \underbrace{\text{with } j \sim \text{Unif}(0, \dots, m-1)}_{\text{rather than } j=m} \quad (12.1)$$

The interested reader is referred to Tan et al. '16 for the proof of the original version

# Proof of Theorem 12.1

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Let  $\mathbf{g}_s^t := \nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) + \nabla F(\mathbf{x}_s^{\text{old}})$  for simplicity. As usual, conditional on everything prior to  $\mathbf{x}_s^{t+1}$ , one has

$$\begin{aligned}\mathbb{E}[\|\mathbf{x}_s^{t+1} - \mathbf{x}^*\|_2^2] &= \mathbb{E}[\|\mathbf{x}_s^t - \eta \mathbf{g}_s^t - \mathbf{x}^*\|_2^2] \\ &= \|\mathbf{x}_s^t - \mathbf{x}^*\|_2^2 - 2\eta(\mathbf{x}_s^t - \mathbf{x}^*)^\top \mathbb{E}[\mathbf{g}_s^t] + \eta^2 \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \\ &\leq \|\mathbf{x}_s^t - \mathbf{x}^*\|_2^2 - 2\eta(\mathbf{x}_s^t - \mathbf{x}^*)^\top \underbrace{\nabla F(\mathbf{x}_s^t)}_{\text{since } \mathbf{g}_s^t \text{ is an unbiased estimate of } \nabla F(\mathbf{x}_s^t)} + \eta^2 \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \\ &\leq \|\mathbf{x}_s^t - \mathbf{x}^*\|_2^2 - \underbrace{2\eta(F(\mathbf{x}_s^t) - F(\mathbf{x}^*))}_{\text{by convexity}} + \eta^2 \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \quad (12.2)\end{aligned}$$

- **key step:** control  $\mathbb{E}[\|\mathbf{g}_s^t\|_2^2]$ 
  - we'd like to upper bound it via the (relative) objective value

# Proof of Theorem 12.1

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**main pillar:** control  $\mathbb{E}[\|\mathbf{g}_s^t\|_2^2]$  via ...

## Lemma 12.2

$$\mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \leq 4L[F(\mathbf{x}_s^t) - F(\mathbf{x}^*) + F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)]$$

this means if  $\mathbf{x}_s^t \approx \mathbf{x}_s^{\text{old}} \approx \mathbf{x}^*$ , then  $\mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \approx 0$  (reduced variance)

# Proof of Theorem 12.1

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main pillar: control  $\mathbb{E}[\|\mathbf{g}_s^t\|_2^2]$  via ...

## Lemma 12.2

$$\mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \leq 4L[F(\mathbf{x}_s^t) - F(\mathbf{x}^*) + F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)]$$

this allows one to obtain: conditional on everything prior to  $\mathbf{x}_s^{t+1}$ ,

$$\begin{aligned} \mathbb{E}[\|\mathbf{x}_s^{t+1} - \mathbf{x}^*\|_2^2] &\leq (12.2) \\ &\leq \|\mathbf{x}_s^t - \mathbf{x}^*\|_2^2 - 2\eta[F(\mathbf{x}_s^t) - F(\mathbf{x}^*)] \\ &\quad + 4L\eta^2[F(\mathbf{x}_s^t) - F(\mathbf{x}^*) + F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \\ &= \|\mathbf{x}_s^t - \mathbf{x}^*\|_2^2 - 2\eta(1 - 2L\eta)[F(\mathbf{x}_s^t) - F(\mathbf{x}^*)] \\ &\quad + 4L\eta^2[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \quad (12.3) \end{aligned}$$

## Proof of Theorem 12.1 (cont.)

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Taking expectation w.r.t. all history, we have

$$\begin{aligned} & 2\eta(1 - 2L\eta)m \mathbb{E}[F(\mathbf{x}_{s+1}^{\text{old}}) - F(\mathbf{x}^*)] \\ &= 2\eta(1 - 2L\eta) \sum_{t=0}^{m-1} \mathbb{E}[F(\mathbf{x}_s^t) - F(\mathbf{x}^*)] && \text{by (12.1)} \\ &\leq \underbrace{\mathbb{E}[\|\mathbf{x}_{s+1}^m - \mathbf{x}^*\|_2^2]}_{\geq 0} + 2\eta(1 - 2L\eta) \sum_{t=0}^{m-1} \mathbb{E}[F(\mathbf{x}_s^t) - F(\mathbf{x}^*)] \\ &\leq \mathbb{E}[\|\mathbf{x}_{s+1}^0 - \mathbf{x}^*\|_2^2] + 4Lm\eta^2[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] && \text{(apply (12.3) recursively)} \\ &= \mathbb{E}[\|\mathbf{x}_s^{\text{old}} - \mathbf{x}^*\|_2^2] + 4Lm\eta^2\mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \\ &\leq \frac{2}{\mu}\mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] + 4Lm\eta^2\mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] && \text{(strong convexity)} \\ &= \left(\frac{2}{\mu} + 4Lm\eta^2\right) \mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \end{aligned}$$

## Proof of Theorem 12.1 (cont.)

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Consequently,

$$\begin{aligned} & \mathbb{E}[F(\mathbf{x}_{s+1}^{\text{old}}) - F(\mathbf{x}^*)] \\ & \leq \frac{\frac{2}{\mu} + 4Lm\eta^2}{2\eta(1 - 2L\eta)m} \mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \\ & = \underbrace{\left( \frac{1}{\mu\eta(1 - 2L\eta)m} + \frac{2L\eta}{1 - 2L\eta} \right)}_{=\rho} \mathbb{E}[F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \end{aligned}$$

Applying this bound recursively establishes the theorem.

## Proof of Lemma 12.2

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$$\begin{aligned} & \mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) + \nabla F(\mathbf{x}_s^{\text{old}})\|_2^2] \\ &= \mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}^*) - (\nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) - \nabla f_{i_t}(\mathbf{x}^*) - \nabla F(\mathbf{x}_s^{\text{old}}))\|_2^2] \\ &\leq 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}^*)\|_2^2] + 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) - \nabla f_{i_t}(\mathbf{x}^*) - \nabla F(\mathbf{x}_s^{\text{old}})\|_2^2] \\ &= 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}^*)\|_2^2] \\ &\quad + 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) - \nabla f_{i_t}(\mathbf{x}^*) - \underbrace{\mathbb{E}[\nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) - \nabla f_{i_t}(\mathbf{x}^*)]}_{\text{since } \mathbb{E}[\nabla f_{i_t}(\mathbf{x}^*)] = \nabla F(\mathbf{x}^*) = \mathbf{0}}\|_2^2] \\ &\leq 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}^*)\|_2^2] + 2\mathbb{E}[\|\nabla f_{i_t}(\mathbf{x}_s^{\text{old}}) - \nabla f_{i_t}(\mathbf{x}^*)\|_2^2] \\ &\leq 4L[F(\mathbf{x}_s^t) - F(\mathbf{x}^*) + F(\mathbf{x}_s^{\text{old}}) - F(\mathbf{x}^*)] \end{aligned}$$

where the last inequality would hold if we could justify

$$\underbrace{\frac{1}{n} \sum_{i=1}^n \|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{x}^*)\|_2^2}_{\text{relies on both smoothness and convexity of } f_i} \leq 2L[F(\mathbf{x}) - F(\mathbf{x}^*)] \quad (12.4)$$

## Proof of Lemma 12.2 (cont.)

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To establish (12.4), observe from smoothness and convexity of  $f_i$  that

$$\underbrace{\frac{1}{2L} \|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{x}^*)\|_2^2 \leq f_i(\mathbf{x}) - f_i(\mathbf{x}^*) - \nabla f_i(\mathbf{x}^*)^\top (\mathbf{x} - \mathbf{x}^*)}_{\text{an equivalent characterization of } L\text{-smoothness}}$$

Summing over all  $i$  and recognizing that  $\nabla F(\mathbf{x}^*) = \mathbf{0}$  yield

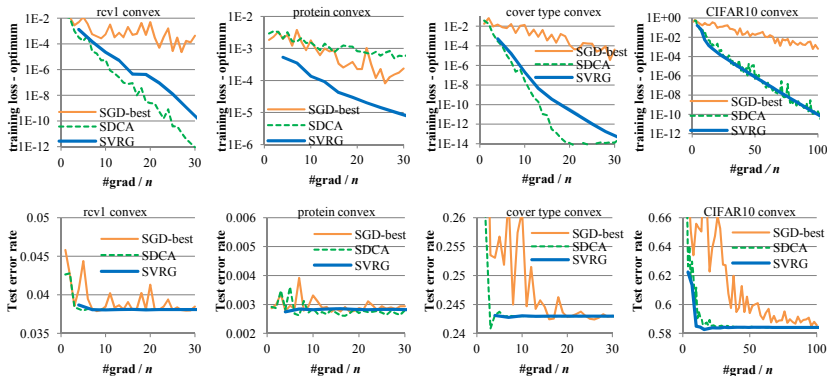
$$\begin{aligned} \frac{1}{2L} \sum_{i=1}^n \|\nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{x}^*)\|_2^2 &\leq nF(\mathbf{x}) - nF(\mathbf{x}^*) - n(\nabla F(\mathbf{x}^*))^\top (\mathbf{x} - \mathbf{x}^*) \\ &= nF(\mathbf{x}) - nF(\mathbf{x}^*) \end{aligned}$$

as claimed



# Numerical example: logistic regression

— Johnson, Zhang '13



$\ell_2$ -regularized logistic regression on CIFAR-10

# Comparisons with GD and SGD

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	SVRG	GD	SGD
comp. cost	$(n + \kappa) \log \frac{1}{\epsilon}$	$n\kappa \log \frac{1}{\epsilon}$	$\frac{\kappa^2}{\epsilon}$ (practically often $\frac{\kappa}{\epsilon}$ )

# Proximal extension

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$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})}_{=: F(\mathbf{x})} + \psi(\mathbf{x})$$

- $f_i$ : convex and  $L$ -smooth
- $F$ :  $\mu$ -strongly convex
- $\kappa := L/\mu$ : condition number
- $\psi$ : potentially non-smooth

# Proximal extension (Xiao, Zhang '14)

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## Algorithm 12.3 Prox-SVRG for finite-sum optimization

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- 1: **for**  $s = 1, 2, \dots$  **do**
- 2:  $\mathbf{x}_s^{\text{old}} \leftarrow \mathbf{x}_{s-1}^m$ , and compute  $\underbrace{\nabla F(\mathbf{x}_s^{\text{old}})}_{\text{batch gradient}}$  // update snapshot
- 3: initialize  $\mathbf{x}_s^0 \leftarrow \mathbf{x}_s^{\text{old}}$
- 4: **for**  $\underbrace{t = 0, \dots, m-1}_{\text{each epoch contains } m \text{ iterations}}$  **do**
- 5: choose  $i_t$  uniformly from  $\{1, \dots, n\}$ , and

$$\mathbf{x}_s^{t+1} = \text{prox}_{\eta\psi} \left( \mathbf{x}_s^t - \eta \left\{ \underbrace{\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{\text{old}})}_{\text{stochastic gradient}} + \nabla F(\mathbf{x}_s^{\text{old}}) \right\} \right)$$

# **Stochastic recursive gradient algorithm (SARAH)**

# Nonconvex and smooth problems

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$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^d} \quad F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})$$

- $f_i$ :  $L$ -smooth, potentially nonconvex

# Recursive stochastic gradient estimates

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— Nguyen, Liu, Scheinberg, Takac '17

**key idea:** recursive / adaptive updates of gradient estimates  
stochastic

$$\begin{aligned} \mathbf{g}^t &= \nabla f_{i_t}(\mathbf{x}^t) - \nabla f_{i_t}(\mathbf{x}^{t-1}) + \mathbf{g}^{t-1} \\ \mathbf{x}^{t+1} &= \mathbf{x}^t - \eta \mathbf{g}^t \end{aligned} \quad (12.5)$$

**comparison to SVRG** (use a **fixed** snapshot point for the entire epoch)

$$(\text{SVRG}) \quad \mathbf{g}^t = \nabla f_{i_t}(\mathbf{x}^t) - \nabla f_{i_t}(\mathbf{x}^{\text{old}}) + \nabla F(\mathbf{x}^{\text{old}})$$

# Restarting gradient estimate every epoch

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For many (e.g. strongly convex) problems, recursive gradient estimate  $\mathbf{g}^t$  may decay fast (variance  $\downarrow$ ; bias (relative to  $\nabla F(\mathbf{x}^t)$ )  $\uparrow$ )

- $\mathbf{g}^t$  may quickly deviate from the target gradient  $\nabla F(\mathbf{x}^t)$
- progress stalls as  $\mathbf{g}^t$  cannot guarantee sufficient descent

**solution:** reset  $\mathbf{g}^t$  every few iterations to calibrate with the true batch gradient



# Bias of gradient estimates

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Unlike SVRG,  $\mathbf{g}^t$  is NOT an unbiased estimate of  $\nabla F(\mathbf{x}^t)$

$$\mathbb{E}[\mathbf{g}^t \mid \text{everything prior to } \mathbf{x}_s^t] = \nabla F(\mathbf{x}^t) \underbrace{-\nabla F(\mathbf{x}^{t-1}) + \mathbf{g}^{t-1}}_{\neq 0}$$

But if we average out all randomness, we have (exercise!)

$$\mathbb{E}[\mathbf{g}^t] = \mathbb{E}[\nabla F(\mathbf{x}^t)]$$

# StochAstic Recursive grAdient algorithM

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## Algorithm 12.4 SARAH (Nguyen et al. '17)

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- 1: **for**  $s = 1, 2, \dots, S$  **do**
  - 2:  $\mathbf{x}_s^0 \leftarrow \mathbf{x}_{s-1}^{m+1}$ , and compute  $\underbrace{\mathbf{g}_s^0 = \nabla F(\mathbf{x}_s^0)}_{\text{batch gradient}}$  // restart  $\mathbf{g}$  anew
  - 3:  $\mathbf{x}_s^1 = \mathbf{x}_s^0 - \eta \mathbf{g}_s^0$
  - 4: **for**  $t = 1, \dots, m$  **do**
  - 5: choose  $i_t$  uniformly from  $\{1, \dots, n\}$
  - 6:  $\mathbf{g}_s^t = \underbrace{\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{t-1})}_{\text{stochastic gradient}} + \mathbf{g}_s^{t-1}$
  - 7:  $\mathbf{x}_s^{t+1} = \mathbf{x}_s^t - \eta \mathbf{g}_s^t$
-

# Convergence analysis of SARAH (nonconvex)

## Theorem 12.3 (Nguyen et al. '19)

Suppose each  $f_i$  is  $L$ -smooth. Then SARAH with  $\eta \lesssim \frac{1}{L\sqrt{m}}$  obeys

$$\frac{1}{(m+1)S} \sum_{s=1}^S \sum_{t=0}^m \mathbb{E} \left[ \|\nabla F(\mathbf{x}_s^t)\|_2^2 \right] \leq \frac{2}{\eta(m+1)S} [F(\mathbf{x}_0^0) - F(\mathbf{x}^*)]$$

- iteration complexity for finding  $\varepsilon$ -approximate stationary point (i.e.  $\|\nabla F(\mathbf{x})\|_2 \leq \varepsilon$ ):

$$O \left( n + \frac{L\sqrt{n}}{\varepsilon^2} \right) \quad \left( \text{setting } m \asymp n, \eta \asymp \frac{1}{L\sqrt{m}} \right)$$

# Convergence analysis of SARAH (nonconvex)

## Theorem 12.3 (Nguyen et al. '19)

Suppose each  $f_i$  is  $L$ -smooth. Then SARAH with  $\eta \lesssim \frac{1}{L\sqrt{m}}$  obeys

$$\frac{1}{(m+1)S} \sum_{s=1}^S \sum_{t=0}^m \mathbb{E} \left[ \|\nabla F(\mathbf{x}_s^t)\|_2^2 \right] \leq \frac{2}{\eta(m+1)S} [F(\mathbf{x}_0^0) - F(\mathbf{x}^*)]$$

- also derived by Fang et al. '18 (for a SARAH-like algorithm “Spider”) and improved by Wang et al. '19 (for “SpiderBoost”)

## Proof of Theorem 12.3

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Theorem 12.3 follows immediately from the following claim on the total objective improvement in one epoch (why?)

$$\mathbb{E}[F(\mathbf{x}_s^{m+1})] \leq \mathbb{E}[F(\mathbf{x}_s^0)] - \frac{\eta}{2} \sum_{t=0}^m \mathbb{E}[\|\nabla F(\mathbf{x}_s^t)\|_2^2] \quad (12.6)$$

We will then focus on establishing (12.6)

## Proof of Theorem 12.3 (cont.)

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To establish (12.6), recall that the smoothness assumption gives

$$\mathbb{E}[F(\mathbf{x}_s^{t+1})] \leq \mathbb{E}[F(\mathbf{x}_s^t)] - \eta \mathbb{E}[\nabla F(\mathbf{x}_s^t)^\top \mathbf{g}_s^t] + \frac{L\eta^2}{2} \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \quad (12.7)$$

Since  $\mathbf{g}_s^t$  is not an unbiased estimate of  $\nabla F(\mathbf{x}_s^t)$ , we first decouple

$$2\mathbb{E}[\nabla F(\mathbf{x}_s^t)^\top \mathbf{g}_s^t] = \underbrace{\mathbb{E}[\|\nabla F(\mathbf{x}_s^t)\|_2^2]}_{\text{desired gradient estimate}} + \underbrace{\mathbb{E}[\|\mathbf{g}_s^t\|_2^2]}_{\text{variance}} - \underbrace{\mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2]}_{\text{squared bias of gradient estimate}}$$

Substitution into (12.7) with straightforward algebra gives

$$\begin{aligned} \mathbb{E}[F(\mathbf{x}_s^{t+1})] &\leq \mathbb{E}[F(\mathbf{x}_s^t)] - \frac{\eta}{2} \mathbb{E}[\|\nabla F(\mathbf{x}_s^t)\|_2^2] + \frac{\eta}{2} \mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2] \\ &\quad - \left(\frac{\eta}{2} - \frac{L\eta^2}{2}\right) \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \end{aligned}$$

## Proof of Theorem 12.3 (cont.)

Sum over  $t = 0, \dots, m$  to arrive at

$$\begin{aligned} \mathbb{E}[F(\mathbf{x}_s^{m+1})] &\leq \mathbb{E}[F(\mathbf{x}_s^0)] - \frac{\eta}{2} \sum_{t=0}^m \mathbb{E}[\|\nabla F(\mathbf{x}_s^t)\|_2^2] \\ &\quad + \frac{\eta}{2} \left\{ \sum_{t=0}^m \mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2] - \underbrace{(1 - L\eta)}_{\geq 1/2} \sum_{t=0}^m \mathbb{E}[\|\mathbf{g}_s^t\|_2^2] \right\} \end{aligned}$$

The proof of (12.6) is thus complete if we can justify

### Lemma 12.4

If  $\eta \leq \frac{1}{L\sqrt{m}}$ , then (for fixed  $\eta$ , the epoch length  $m$  cannot be too large)

$$\sum_{t=0}^m \underbrace{\mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2]}_{\text{squared bias of gradient estimate}} \leq \frac{1}{2} \sum_{t=0}^m \underbrace{\mathbb{E}[\|\mathbf{g}_s^t\|_2^2]}_{\text{variance}}$$

- informally, this says the accumulated squared bias of gradient estimates (w.r.t. batch gradients) can be controlled by the accumulated variance

# Proof of Lemma 12.4

---

Key step:

## Lemma 12.5

$$\mathbb{E} \left[ \|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2 \right] \leq \sum_{k=1}^t \mathbb{E} \left[ \|\mathbf{g}_s^k - \mathbf{g}_s^{k-1}\|_2^2 \right]$$

- convert the bias of gradient estimates to the differences of consecutive gradient estimates (a consequence of the smoothness and the recursive formula of  $\mathbf{g}_s^t$ )



## Proof of Lemma 12.4 (cont.)

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From Lemma 12.5, it suffices to connect  $\{\|\mathbf{g}_s^t - \mathbf{g}_s^{t-1}\|_2\}$  with  $\{\|\mathbf{g}_s^t\|_2\}$ :

$$\begin{aligned}\|\mathbf{g}_s^t - \mathbf{g}_s^{t-1}\|_2^2 &\stackrel{(12.5)}{=} \|\nabla f_{i_t}(\mathbf{x}_s^t) - \nabla f_{i_t}(\mathbf{x}_s^{t-1})\|_2^2 \stackrel{\text{smoothness}}{\leq} L^2 \|\mathbf{x}_s^t - \mathbf{x}_s^{t-1}\|_2^2 \\ &= \eta^2 L^2 \|\mathbf{g}_s^{t-1}\|_2^2\end{aligned}$$

Invoking Lemma 12.5 then gives

$$\mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2] \leq \sum_{k=1}^t \mathbb{E}[\|\mathbf{g}_s^k - \mathbf{g}_s^{k-1}\|_2^2] \leq \eta^2 L^2 \sum_{k=1}^t \mathbb{E}[\|\mathbf{g}_s^{k-1}\|_2^2]$$

Summing over  $t = 0, \dots, m$ , we obtain

$$\sum_{t=0}^m \mathbb{E}[\|\nabla F(\mathbf{x}_s^t) - \mathbf{g}_s^t\|_2^2] \leq \eta^2 L^2 m \sum_{t=0}^{m-1} \mathbb{E}[\|\mathbf{g}_s^t\|_2^2]$$

which establishes Lemma 12.4 if  $\eta \lesssim \frac{1}{L\sqrt{m}}$

## Proof of Lemma 12.5

Since this lemma only concerns a single epoch, we shall drop the dependency on  $s$  for simplicity. Let  $\mathcal{F}_k$  contain all info up to  $\mathbf{x}^k$  and  $\mathbf{g}^{k-1}$ , then

$$\begin{aligned} & \mathbb{E} \left[ \left\| \nabla F(\mathbf{x}^k) - \mathbf{g}^k \right\|_2^2 \mid \mathcal{F}_k \right] \\ &= \mathbb{E} \left[ \left\| \nabla F(\mathbf{x}^{k-1}) - \mathbf{g}^{k-1} + (\nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1})) - (\mathbf{g}^k - \mathbf{g}^{k-1}) \right\|_2^2 \mid \mathcal{F}_k \right] \\ &= \left\| \nabla F(\mathbf{x}^{k-1}) - \mathbf{g}^{k-1} \right\|_2^2 + \left\| \nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1}) \right\|_2^2 + \mathbb{E} \left[ \left\| \mathbf{g}^k - \mathbf{g}^{k-1} \right\|_2^2 \mid \mathcal{F}_k \right] \\ &\quad + 2 \langle \nabla F(\mathbf{x}^{k-1}) - \mathbf{g}^{k-1}, \nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1}) \rangle \\ &\quad - 2 \langle \nabla F(\mathbf{x}^{k-1}) - \mathbf{g}^{k-1}, \mathbb{E}[\mathbf{g}^k - \mathbf{g}^{k-1} \mid \mathcal{F}_k] \rangle \\ &\quad - 2 \langle \nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1}), \mathbb{E}[\mathbf{g}^k - \mathbf{g}^{k-1} \mid \mathcal{F}_k] \rangle \\ &\stackrel{\text{(exercise)}}{=} \left\| \nabla F(\mathbf{x}^{k-1}) - \mathbf{g}^{k-1} \right\|_2^2 - \left\| \nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1}) \right\|_2^2 + \mathbb{E} \left[ \left\| \mathbf{g}^k - \mathbf{g}^{k-1} \right\|_2^2 \mid \mathcal{F}_k \right] \end{aligned}$$

Since  $\nabla F(\mathbf{x}^0) = \mathbf{g}^0$ . Sum over  $k = 1, \dots, t$  to obtain

$$\mathbb{E} \left[ \left\| \nabla F(\mathbf{x}^k) - \mathbf{g}^k \right\|_2^2 \right] = \sum_{k=1}^t \mathbb{E} \left[ \left\| \mathbf{g}^k - \mathbf{g}^{k-1} \right\|_2^2 \right] - \underbrace{\sum_{k=1}^t \left\| \nabla F(\mathbf{x}^k) - \nabla F(\mathbf{x}^{k-1}) \right\|_2^2}_{\leq 0; \text{ done!}}$$

# Stochastic dual coordinate ascent (SDCA)

— *a dual perspective*

# A class of finite-sum optimization

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$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^d} \quad F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) + \frac{\mu}{2} \|\mathbf{x}\|_2^2 \quad (12.8)$$

- $f_i$ : convex and  $L$ -smooth

# Dual formulation

---

The dual problem of (12.8)

$$\text{maximize}_{\boldsymbol{\nu}} \quad D(\boldsymbol{\nu}) = \frac{1}{n} \sum_{i=1}^n -f_i^*(-\mathbf{v}_i) - \frac{\mu}{2} \left\| \frac{1}{\mu n} \sum_{i=1}^n \boldsymbol{\nu}_i \right\|_2^2 \quad (12.9)$$

- a primal-dual relation

$$\mathbf{x}(\boldsymbol{\nu}) = \frac{1}{\mu n} \sum_{i=1}^n \boldsymbol{\nu}_i \quad (12.10)$$

# Derivation of the dual formulation

---

$$\min_{\mathbf{x}} \quad \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) + \frac{\mu}{2} \|\mathbf{x}\|_2^2$$

$$\iff \min_{\mathbf{x}, \{\mathbf{z}_i\}} \quad \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{z}_i) + \frac{\mu}{2} \|\mathbf{x}\|_2^2 \quad \text{s.t. } \mathbf{z}_i = \mathbf{x}$$

$$\iff \max_{\{\boldsymbol{\nu}_i\}} \min_{\mathbf{x}, \{\mathbf{z}_i\}} \quad \underbrace{\frac{1}{n} \sum_{i=1}^n f_i(\mathbf{z}_i) + \frac{\mu}{2} \|\mathbf{x}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \langle \boldsymbol{\nu}_i, \mathbf{z}_i - \mathbf{x} \rangle}_{\text{Lagrangian}}$$

$$\iff \max_{\{\boldsymbol{\nu}_i\}} \min_{\mathbf{x}} \quad \underbrace{\frac{1}{n} \sum_{i=1}^n -f_i^*(-\boldsymbol{\nu}_i)}_{\text{conjugate: } f_i^*(\boldsymbol{\nu}) := \max_{\mathbf{z}} \{\langle \boldsymbol{\nu}, \mathbf{z} \rangle - f_i(\mathbf{z})\}} + \frac{\mu}{2} \|\mathbf{x}\|_2^2 - \frac{1}{n} \sum_{i=1}^n \langle \boldsymbol{\nu}_i, \mathbf{x} \rangle$$

$$\iff \max_{\{\boldsymbol{\nu}_i\}} \quad \frac{1}{n} \sum_{i=1}^n -f_i^*(-\boldsymbol{\nu}_i) - \frac{\mu}{2} \left\| \underbrace{\frac{1}{\mu n} \sum_{i=1}^n \boldsymbol{\nu}_i}_{\text{optimal } \mathbf{x} = \frac{1}{\mu n} \sum_i \boldsymbol{\nu}_i} \right\|_2^2$$

# Randomized coordinate ascent on dual problem

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— Shalev-Shwartz, Zhang '13

- **randomized coordinate ascent:** at each iteration, randomly pick one **dual** (block) coordinate  $\nu_{i_t}$  of (12.9) to optimize
- **maintain the primal-dual relation** (12.10)

$$\mathbf{x}^t = \frac{1}{\mu n} \sum_{i=1}^n \nu_i^t \quad (12.11)$$





## A variant of SDCA without duality

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SDCA might not be applicable if the conjugate functions are difficult to evaluate

This calls for a dual-free version of SDCA



# A variant of SDCA without duality

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A little intuition

- the optimality condition requires (check!)

$$\boldsymbol{\nu}_i^* = -\nabla f_i(\mathbf{x}^*), \quad \forall i \quad (12.12)$$

- with a modified update rule, one has

$$\boldsymbol{\nu}_{i_t}^{t+1} \leftarrow \underbrace{(1 - \eta\mu n)\boldsymbol{\nu}_{i_t}^t + \eta\mu n(-\nabla f_{i_t}(\mathbf{x}^t))}_{\text{cvx combination of current dual iterate and gradient component}}$$

— when it converges, it will satisfy (12.12)

# SDCA as SGD

---

The SDCA (without duality) update rule reads:

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta \underbrace{(\nabla f_{i_t}(\mathbf{x}^t) + \boldsymbol{\nu}_{i_t}^t)}_{:=\mathbf{g}^t}$$

It is straightforward to verify that  $\mathbf{g}^t$  is an **unbiased gradient estimate**

$$\mathbb{E}[\mathbf{g}^t] = \mathbb{E}[\nabla f_{i_t}(\mathbf{x}^t)] + \mathbb{E}[\boldsymbol{\nu}_{i_t}^t] = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\mathbf{x}^t) + \underbrace{\frac{1}{n} \sum_{i=1}^n \boldsymbol{\nu}_i^t}_{=\boldsymbol{\mu}\mathbf{x}^t} = \nabla F(\mathbf{x}^t)$$

# SDCA as variance-reduced SGD

---

The SDCA (without duality) update rule reads:

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta \underbrace{(\nabla f_{i_t}(\mathbf{x}^t) + \boldsymbol{\nu}_{i_t}^t)}_{:= \mathbf{g}^t}$$

The variance of  $\|\mathbf{g}^t\|_2$  goes to 0 as we converge to the optimizer

$$\begin{aligned} \mathbb{E}[\|\mathbf{g}^t\|_2^2] &= \mathbb{E}[\|\boldsymbol{\nu}_{i_t}^t - \boldsymbol{\nu}_{i_t}^* + \boldsymbol{\nu}_{i_t}^* + \nabla f_{i_t}(\mathbf{x}^t)\|_2^2] \\ &\leq 2 \underbrace{\mathbb{E}[\|\boldsymbol{\nu}_{i_t}^t - \boldsymbol{\nu}_{i_t}^*\|_2^2]}_{\rightarrow 0 \text{ as } t \rightarrow \infty} + 2 \underbrace{\mathbb{E}[\|\boldsymbol{\nu}_{i_t}^* + \nabla f_{i_t}(\mathbf{x}^t)\|_2^2]}_{\leq \|\mathbf{w}^t - \mathbf{w}^*\|_2^2 \text{ (Shalev-Shwartz '16)}} \end{aligned}$$

# Convergence guarantees of SDCA

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## Theorem 12.6 (informal, Shalev-Shwartz '16)

Assume each  $f_i$  is convex and  $L$ -smooth, and set  $\eta = \frac{1}{L+\mu n}$ . Then it takes SDCA (without duality)  $O\left((n + \frac{L}{\mu}) \log \frac{1}{\varepsilon}\right)$  iterations to yield  $\varepsilon$  accuracy

- the same computational complexity as SVRG
- storage complexity:  $O(nd)$  (needs to store  $\{\nu_i\}_{1 \leq i \leq n}$ )

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