Introduction to stochastic optimization

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Part 1: General stochastic optimization

Stochastic optimization

Problem: $\min_{x \in \mathbb{R}^n} f(x)$, where f is a differentiable function.

Main assumption: cannot compute $f(x)$, $\nabla f(x)$ etc. exactly, but we have a stochastic oracle.

Stochastic oracle (SO):

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Stochastic oracle (SO): Given $x \in \mathbb{R}^n$, it returns a stochastic gradient (SG) $g(x)$:

- $g(x)$ is a random vector in $\mathbb{R}^n$ such that $\mathbb{E}g(x) = \nabla f(x)$ (plus some assumptions on the fluctuations).

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Goal: A method for solving the problem given the SO.

Example 1: Stochastic programming

Let ξ be a random variable supported on $\Omega \subseteq \mathbb{R}^d$ and distributed according to a probability measure P. For each $\omega \in \Omega$, let $f_\omega : \mathbb{R}^n \to \mathbb{R}$ be a simple differentiable function, and let

$$f(x) := \mathbb{E} f_\xi(x) = \int_\Omega f_\omega(x) dP(\omega).$$

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Let $f_1, \ldots, f_m : \mathbb{R}^n \to \mathbb{R}$ be simple differentiable functions, and let

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SO: Given $x \in \mathbb{R}^n$, generate $i_0 \sim \mathrm{Unif}\{1, \ldots, m\}$, and return $g(x) := \nabla f_{i_0}(x)$.

Complexity: $O(1)$, not depending on m.

Stochastic optimization: goals and complexity

Problem: $f^* := \min_{x \in \mathbb{R}^n} f(x)$, where f is given by an SO.

Goal: Given $\varepsilon > 0$, find a random $\bar{x} \in \mathbb{R}^n$:

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NB 2: $O(\varepsilon^{-2})$ is the complexity of Monte-Carlo ε-approximation of $f(x)$ for a <u>single</u> x.
The above $O(\varepsilon^{-2})$ is the complexity of the whole optimization process!

Remark: Same results with high probability under some regularity assumptions.

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Example: Empirical risk minimization (ERM)

Let $\phi_1, \ldots, \phi_m : \mathbb{R} \to \mathbb{R}$ be convex functions, $a_1, \ldots, a_m \in \mathbb{R}^n$, and let

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Main result: $\frac{1}{T}\sum_{k=0}^{T-1}(\mathbb{E}f(x_k) - f^*) + \frac{\mathbb{E}\|x_T - x^*\|^2}{2\alpha T} \leq \frac{\mathbb{E}\|x_0 - x^*\|^2}{2\alpha T} + \frac{\alpha}{2T}\sum_{k=0}^{T-1}\mathbb{E}\|g_k\|^2.$

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\begin{aligned}
\mathbb{E}\|x_{k+1} - x^*\|^2 &= \mathbb{E}\|x_k - x^* - \alpha g_k\|^2 = \mathbb{E}(\|x_k - x^*\|^2 - 2\alpha\langle g_k, x_k - x^*\rangle + \alpha^2\|g_k\|^2) \\
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Main result: $\frac{1}{T}\sum_{k=0}^{T-1}(\mathbb{E}f(x_k) - f^*) + \frac{\mathbb{E}\|x_T - x^*\|^2}{2\alpha T} \leq \frac{\mathbb{E}\|x_0 - x^*\|^2}{2\alpha T} + \frac{\alpha}{2T}\sum_{k=0}^{T-1}\mathbb{E}\|g_k\|^2.$

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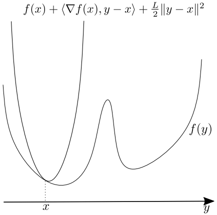
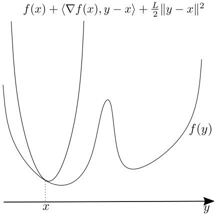
Smooth functions in optimization

Smooth functions in optimization

Def: A differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is called <u>L-smooth</u> if $f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2}\|y - x\|^2$ for all $x, y \in \mathbb{R}^n$.



Smooth functions in optimization



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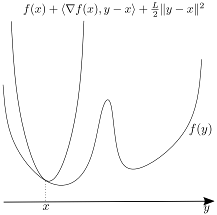

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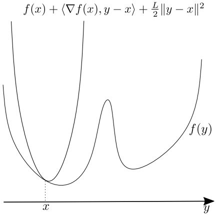

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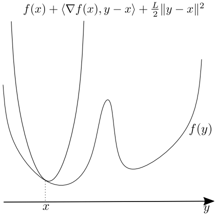

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where $H := \sup_{t\in\mathbb{R}} \phi''(t)$, $B := \|a\|$. Hence, $L = HB^2$.

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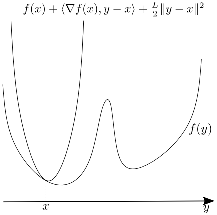

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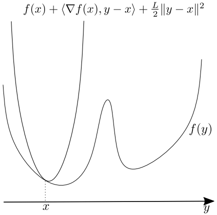

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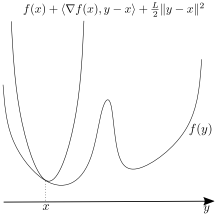

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- (Least squares) $\phi(t) := \frac{1}{2}t^2$. Here $\phi''(t) = 1$ and hence $H = 1$.
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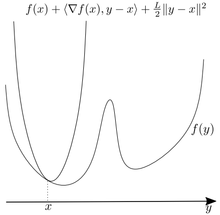

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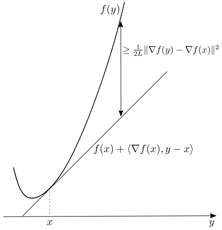
Smooth functions in optimization



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Important fact: If f is convex and L-smooth, then for all $x, y \in \mathbb{R}^n$, we have

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Variance of stochastic gradients

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Previous assumption: $\mathbb{E}\|g(x)\|^2 \leq M^2$ (bounded second moment).

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NB: Since $\mathbb{E}\|g(x) - \nabla f(x)\|^2 = \mathbb{E}\|g(x)\|^2 - \|\nabla f(x)\|^2$, we always have $\sigma \leq M$. However, sometimes σ can be much smaller than M.

Example 1: Let $g(x) := \nabla f(x) + \xi(x)$, where $\mathbb{E}\xi(x) = 0$, $\mathbb{E}\|\xi(x)\|^2 \leq \sigma^2$. Then $\mathbb{E}\|g(x) - \nabla f(x)\|^2 \leq \sigma^2$, while $\mathbb{E}\|g(x)\|^2 = \|\nabla f(x)\|^2 + \mathbb{E}\|\xi(x)\|^2 \leq \|\nabla f(x)\|^2 + \sigma^2$.

Example 2: Mini-batching (in a couple of slides).

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Problem: $\min_{x \in \mathbb{R}^n} f(x)$, where f is convex L-smooth and given by an SO.

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NB: For $\sigma = 0$, we recover the $\frac{LD^2}{T}$ convergence rate of the gradient descent (GD).

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Complexity:

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Complexity: Still $O(\varepsilon^{-2})$.

SGD in the smooth convex optimization: Proof

Let $\delta_k := g_k - \nabla f(x_k)$. Using $\|\nabla f(x_k)\|^2 \le L\langle \nabla f(x_k), x_k - x^*\rangle$, we have

$$
\begin{aligned}
\mathbb{E}\|x_{k+1} - x^*\|^2 - \mathbb{E}\|x_k - x^*\|^2 &\le -2\alpha\mathbb{E}\langle \nabla f(x_k), x_k - x^*\rangle + \alpha^2\mathbb{E}\|g_k\|^2 \\
&= -2\alpha\mathbb{E}\langle \nabla f(x_k), x_k - x^*\rangle + \alpha^2\mathbb{E}(\|\nabla f(x_k)\|^2 + 2\langle \nabla f(x_k), \delta_k\rangle + \|\delta_k\|^2) \\
&\le -\alpha(2 - L\alpha)\mathbb{E}\langle \nabla f(x_k), x_k - x^*\rangle + \alpha^2\sigma^2 \le -\alpha(2 - L\alpha)(\mathbb{E}f(x_k) - f^*) + \alpha^2\sigma^2
\end{aligned}
$$

Hence, using $\alpha = \frac{1}{L + \frac{\sigma\sqrt{T}}{D}} \le \frac{1}{L}$, we obtain

$$
\begin{aligned}
\mathbb{E}f(\bar{x}_T) - f^* &\le \frac{1}{T}\sum_{k=0}^{T-1}(\mathbb{E}f(x_k) - f^*) \le \frac{\sum_{k=0}^{T-1}(\mathbb{E}\|x_k - x^*\|^2 - \mathbb{E}\|x_{k+1} - x^*\|^2)}{\alpha(2 - L\alpha)T} + \frac{\alpha\sigma^2}{2 - L\alpha} \\
&\le \frac{D^2}{\alpha(2 - L\alpha)T} + \frac{\alpha\sigma^2}{2 - L\alpha} \le \frac{D^2(L + \frac{\sigma\sqrt{T}}{D})}{T} + \frac{\sigma D}{2\sqrt{T}} = \frac{LD^2}{T} + \frac{3\sigma D}{2\sqrt{T}}. \quad \square
\end{aligned}
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Result: Instead of $\mathbb{E}f(\bar{x}_T) - f^* \le \frac{LD^2}{T} + \frac{3\sigma D}{2\sqrt{T}}$, we get $\mathbb{E}f(\bar{x}_T) - f^* \le \frac{LD^2}{T} + \frac{3\sigma D}{2\sqrt{N}\sqrt{T}}$.

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NB: When $\sigma = 0$, we recover the $O(\frac{1}{T})$ convergence rate of the standard GD.

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Remark: If f is convex, then for $\alpha:=\frac{1}{L+\frac{\sigma\sqrt{T}}{D}}$, we have $\mathbb{E}f(y_T)-f^*\leq\frac{LD^2}{T}+\frac{3\sigma D}{2\sqrt{T}}$, where $D^2:=\mathbb{E}\|x_0-x^*\|^2$.

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&= \mathbb{E}f(x_k) - \frac{\alpha(2 - L\alpha)}{2}\mathbb{E}\|\nabla f(x_k)\|^2 + \frac{L\alpha^2\sigma^2}{2}.
\end{aligned}$$

Hence,

$$\frac{1}{L}\mathbb{E}\|\nabla f(y_T)\|^2 = \frac{1}{LT}\sum_{k=0}^{T-1}\mathbb{E}\|\nabla f(x_k)\|^2 \le$$

SGD for smooth non-convex optimization: Proof

Let $\delta_k := g_k - \nabla f(x_k)$. By L-smoothness, we have

$$
\begin{aligned}
\mathbb{E} f(x_{k+1}) &\le \mathbb{E}\left(f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2 \right) \\
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Part 2: Noise reduction for finite sums

Overview

Problem: $\min_{x\in\mathbb{R}^n} f(x)$, where $f(x) := \frac{1}{m}\sum_{i=1}^m f_i(x)$ with smooth $f_1,\ldots,f_m$.

Goal: Given $\varepsilon > 0$, find $\bar{x} \in \mathbb{R}^n$:

- $\mathbb{E}f(\bar{x}) - f^* \leq \varepsilon$ (convex optimization).
- $\mathbb{E}\|\nabla f(\bar{x})\|^2 \leq \varepsilon$ (non-convex optimization).

Complexity measure:

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Special algorithm:

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Special algorithm: SVRG (Stochastic Variance Reduced Gradient method).

	Convex	Non-convex
GD		

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	Convex	Non-convex
GD	$O(m\varepsilon^{-1})$	$O(m\varepsilon^{-1})$
SGD		

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GD	$O(m\varepsilon^{-1})$	$O(m\varepsilon^{-1})$
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SVRG		

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	Convex	Non-convex
GD	$O(m\varepsilon^{-1})$	$O(m\varepsilon^{-1})$
SGD	$O(\varepsilon^{-2})$	$O(\varepsilon^{-2})$
SVRG	$O(\varepsilon^{-1} + m\log\varepsilon^{-1})$	$O(m + m^{\frac{2}{3}}\varepsilon^{-1})$.

Noise reduction for convex optimization

Recall the convergence rate of SGD:

$$\mathbb{E} f(\bar{x}_T) - f^* \leq \frac{D^2}{2\alpha T} + \frac{\alpha M^2}{2},$$

where $\mathbb{E}\|g_k\|^2 \leq M^2$.

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This gives $O(\frac{1}{\sqrt{T}})$ convergence rate for $\alpha = \Theta(\frac{1}{\sqrt{T}})$.

NB:

Noise reduction for convex optimization

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Example:

Noise reduction for convex optimization

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Example: For $g_k := \nabla f(x_k)$, we have $\mathbb{E}\|g_k\|^2 = \|\nabla f(x_k)\|^2 \to 0$.

Main question:

Noise reduction for convex optimization

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Example: For $g_k := \nabla f(x_k)$, we have $\mathbb{E}\|g_k\|^2 = \|\nabla f(x_k)\|^2 \to 0$.

Main question: How to ensure $\mathbb{E}\|g_k\|^2 \to 0$ in the presence of noise?

Key idea of SVRG

Let $f := \frac{1}{m}\sum_{i=1}^m f_i$. Let $x, \tilde{x} \in \mathbb{R}^n$, $i_0 \sim \mathrm{Unif}\{1, \ldots, m\}$,

$$g(x) := \underbrace{\nabla f_{i_0}(x)}_{\mathbb{E}=\nabla f(x)} +$$

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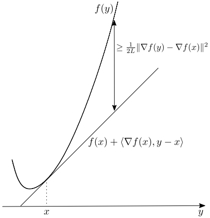
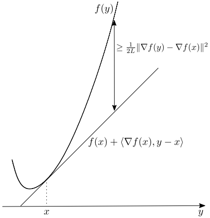


Key lemma:

Key idea of SVRG



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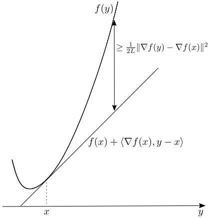
$$\mathbb{E}\|g(x)\|^2 \leq 4L(\mathbb{E}f(x) - f^* + \mathbb{E}f(\tilde{x}) - f^*)$$

Key idea of SVRG



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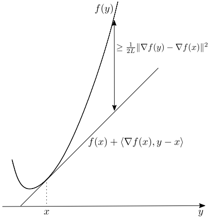
Proof:

Key idea of SVRG



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Proof: Using the inequalities $\|u + v\|^2 \leq 2\|u\|^2 + 2\|v\|^2$, $\mathbb{E}\|\xi - \mathbb{E}\xi\|^2 \leq \mathbb{E}\|\xi\|^2$ and the important fact about convex L-smooth functions, we obtain

$$\mathbb{E}\|g(x)\|^2 = \mathbb{E}\|\nabla f_{i_0}(x) + (\nabla f(\tilde{x}) - \nabla f_{i_0}(\tilde{x}))\|^2$$

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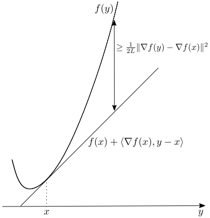
Key idea of SVRG



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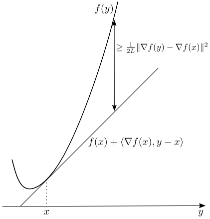

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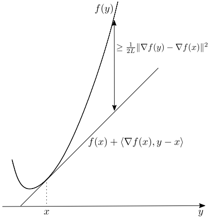

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&\leq 4L\mathbb{E}(f_{i_0}(x) - f_{i_0}(x^*) - \langle \underbrace{\nabla f_{i_0}(x^*)}_{\mathbb{E}=0}, x - x^*\rangle) +
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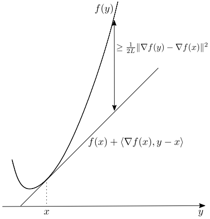
Key idea of SVRG



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$$\mathbb{E}\|g(x)\|^2 \leq 4L(\mathbb{E}f(x) - f^* + \mathbb{E}f(\tilde{x}) - f^*) \to 0 \text{ when } f(x),\ f(\tilde{x}) \to f^*.$$

Proof: Using the inequalities $\|u + v\|^2 \leq 2\|u\|^2 + 2\|v\|^2$, $\mathbb{E}\|\xi - \mathbb{E}\xi\|^2 \leq \mathbb{E}\|\xi\|^2$ and the important fact about convex L-smooth functions, we obtain

$$\begin{aligned}
\mathbb{E}\|g(x)\|^2 &= \mathbb{E}\|\nabla f_{i_0}(x) + (\nabla f(\tilde{x}) - \nabla f_{i_0}(\tilde{x}))\|^2 \\
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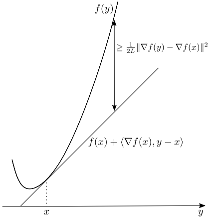
&\leq 4L\mathbb{E}(f_{i_0}(x) - f_{i_0}(x^*) - \langle \underbrace{\nabla f_{i_0}(x^*)}_{\mathbb{E}=0}, x - x^*\rangle) + 4L\mathbb{E}(f_{i_0}(\tilde{x}) - f_{i_0}(x^*) - \langle \underbrace{\nabla f_{i_0}(x^*)}_{\mathbb{E}=0}, \tilde{x} - x^*\rangle) \\
&=
\end{aligned}$$

Key idea of SVRG



Let $f := \frac{1}{m}\sum_{i=1}^m f_i$. Let $x, \tilde{x} \in \mathbb{R}^n$, $i_0 \sim \mathrm{Unif}\{1,\dots,m\}$,

$$g(x) := \underbrace{\nabla f_{i_0}(x)}_{\mathbb{E}=\nabla f(x)} + \underbrace{(\nabla f(\tilde{x}) - \nabla f_{i_0}(\tilde{x}))}_{\mathbb{E}=\nabla f(\tilde{x})-\nabla f(\tilde{x})=0}.$$

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&\leq 2\mathbb{E}\|\nabla f_{i_0}(x) - \nabla f_{i_0}(x^*)\|^2 + 2\mathbb{E}\|\nabla f_{i_0}(x^*) - \nabla f_{i_0}(\tilde{x}) - (\nabla f(x^*) - \nabla f(\tilde{x}))\|^2 \\
&\leq 2\mathbb{E}\|\nabla f_{i_0}(x) - \nabla f_{i_0}(x^*)\|^2 + 2\mathbb{E}\|\nabla f_{i_0}(\tilde{x}) - \nabla f_{i_0}(x^*)\|^2 \\
&\leq 4L\mathbb{E}(f_{i_0}(x) - f_{i_0}(x^*) - \langle \underbrace{\nabla f_{i_0}(x^*)}_{\mathbb{E}=0}, x - x^*\rangle) + 4L\mathbb{E}(f_{i_0}(\tilde{x}) - f_{i_0}(x^*) - \langle \underbrace{\nabla f_{i_0}(x^*)}_{\mathbb{E}=0}, \tilde{x} - x^*\rangle) \\
&= 4L(\mathbb{E}f(x) - f^*) + 4L(\mathbb{E}f(\tilde{x}) - f^*). \quad \square
\end{aligned}$$

SVRG for convex optimization [cf. Allen-Zhu and Yuan, 2016]

Problem: $\min_{x \in \mathbb{R}^n} f(x)$, where $f(x) := \frac{1}{m}\sum_{i=1}^m f_i(x)$ and f_i are convex.

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Output: $\tilde{x}_S$.

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Complexity: $O(\sum_{s=0}^{S-1} K_s + mS)$.

Theorem:

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Theorem: Let $\Delta := \mathbb{E} f(x_0) - f^*$, $D^2 := \mathbb{E}\|x_0 - x^*\|^2$. For $\alpha := \frac{1}{6L}$, $K_s := 2^s K_0$, $K_0 := \frac{9LD^2}{\Delta}$, $S := \log_2 \frac{2\Delta}{\varepsilon}$, we have $\mathbb{E} f(\tilde{x}_S) - f^* \le \varepsilon$. Complexity: $O(\frac{LD^2}{\varepsilon} + m \log \frac{\Delta}{\varepsilon})$.

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Gain: $O(\varepsilon^{-1})$ instead of the $O(\varepsilon^{-2})$ of SGD.

SVRG for convex optimization: Proof

It suffices to prove that $\mathbb{E}f(\tilde{x}_S) - f^* \leq \frac{\Delta + \frac{9LD^2}{K_0}}{2^S}$ (*), and then plug in K_0 and S.

By the main result of SGD and the key lemma of SVRG, we have

$$\begin{aligned}
\frac{1}{K_s}\sum_{k=0}^{K_s-1}(\mathbb{E}f(x_k^s) - f^*) + \frac{1}{2\alpha K_s}\mathbb{E}\|x_{K_s}^s - x^*\|^2 &\leq \frac{1}{2\alpha K_s}\mathbb{E}\|x_0^s - x^*\|^2 + \frac{\alpha}{2K_s}\sum_{k=0}^{K_s-1}\mathbb{E}\|g_k^s\|^2 \\
&\leq \frac{1}{2\alpha K_s}\mathbb{E}\|x_0^s - x^*\|^2 + 2L\alpha(\mathbb{E}f(\tilde{x}_s) - f^*) + \frac{2L\alpha}{K_s}\sum_{k=0}^{K_s-1}(\mathbb{E}f(x_k^s) - f^*).
\end{aligned}$$

Hence,

$$\frac{1}{K_s}\sum_{k=0}^{K_s-1}(\mathbb{E}f(x_k^s) - f^*) + \frac{\mathbb{E}\|x_{K_s}^s - x^*\|^2}{2\alpha K_s(1-2L\alpha)} \leq \frac{1}{2}\left(\frac{4L\alpha}{1-2L\alpha}(\mathbb{E}f(\tilde{x}_s) - f^*) + \frac{\mathbb{E}\|x_0^s - x^*\|^2}{\alpha K_s(1-2L\alpha)}\right)$$

Using $\alpha := \frac{1}{6L}$, $K_{s+1} := 2K_s$, $\tilde{x}_{s+1} := \frac{1}{K_s}\sum_{k=0}^{K_s-1} x_k$ and $x_0^{s+1} := x_{K_s}^s$, we obtain

$$\mathbb{E}f(\tilde{x}_{s+1}) - f^* + \frac{\mathbb{E}\|x_0^{s+1} - x^*\|^2}{\alpha K_{s+1}(1-2L\alpha)} \leq \frac{1}{2}\left(\mathbb{E}f(\tilde{x}_s) - f^* + \frac{\mathbb{E}\|x_0^s - x^*\|^2}{\alpha K_s(1-2L\alpha)}\right).$$

Now (*) follows by induction. □

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Complexity of SGD: $O(\varepsilon^{-2})$. **Complexity of GD:** $O(m\varepsilon^{-1})$.

Practical performance [Reddi et al., 2016]

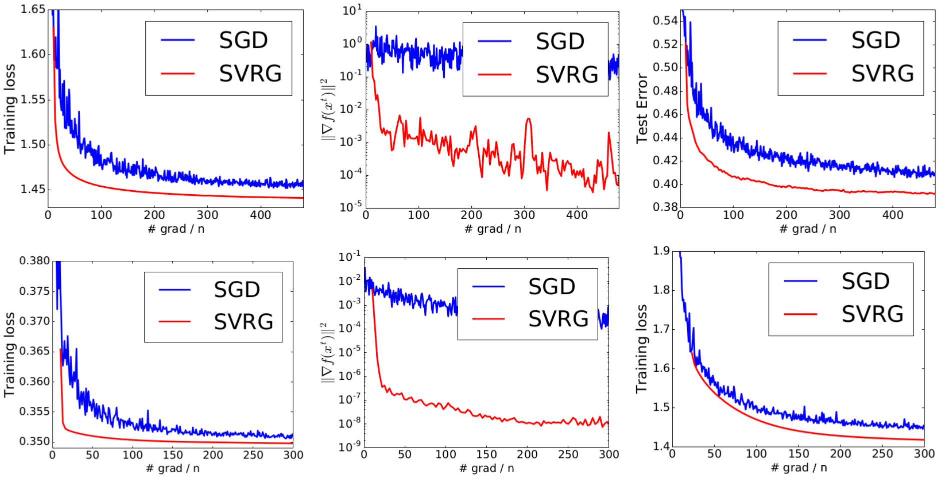

Figure: Neural network results for CIFAR-10, MNIST and STL-10 datasets.

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