CMPT 409/981: Optimization for Machine Learning

Lecture 12

Sharan Vaswani

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Recap

- Interpolation: Over-parameterized models (such as deep neural networks) are capable of exactly fitting the training dataset.
- When minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$, if $\|\nabla f(w)\| = 0$, then $\|\nabla f_i(w)\| = 0$ for all $i \in [n]$ i.e. the variance in the stochastic gradients becomes zero at a stationary point.
- Under interpolation, since the noise is zero at the optimum, SGD does not need to decrease the step-size and can converge to the minimizer by using a *constant* step-size.
- If f is strongly-convex and interpolation is satisfied (e.g. when using kernels or least squares with d > n), constant step-size SGD can converge to the minimizer at an $O(\exp(-T/\kappa))$ rate. Hence, SGD matches the rate of deterministic GD, but compared to GD, each iteration is cheap.

Claim: When minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ such that (i) f is μ -strongly convex, (ii) each f_i is convex and L-smooth, (iii) interpolation is exactly satisfied i.e. $\|\nabla f_i(w^*)\| = 0$, T iterations of SGD with $\eta_k = \eta = \frac{1}{L}$ returns iterate w_T such that,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \exp\left(\frac{-T}{\kappa}\right) \|w_0 - w^*\|^2$$
.

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Proof: Following the same proof as before, we get that,

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E} \left[\|\nabla f_{ik}(w_k)\|^2 \right]$$

$$\leq \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + \eta_k^2 \mathbb{E}_i \left[2L \left[f_{ik}(w_k) - f_{ik}(w^*) \right] \right]$$
(Using *L*-smoothness, convexity of f_i and $\nabla f_i(w^*) = 0$)
$$= \|w_k - w^*\|^2 - 2\eta_k \langle \nabla f(w_k), w_k - w^* \rangle + 2L \eta_k^2 \mathbb{E} \left[f(w_k) - f(w^*) \right]$$
(Unbiasedness)
$$= \|w_k - w^*\|^2 \left(1 - \mu \eta_k \right) - 2\eta_k \left[f(w_k) - f(w^*) \right] + 2L \eta_k^2 \mathbb{E} \left[f(w_k) - f(w^*) \right]$$
(Strong-convexity)
$$= \left(1 - \frac{\mu}{L} \right) \|w_k - w^*\|^2$$
(Since $\eta_k = \eta = \frac{1}{L}$)

Taking expectation w.r.t the randomness from iterations k=0 to $\mathcal{T}-1$ and recursing,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \left(1 - \frac{\mu}{L}\right)^T \|w_0 - w^*\|^2 \le \exp\left(\frac{-T}{\kappa}\right) \|w_0 - w^*\|^2$$

- We can modify the proof in order to get an $O\left(\exp\left(\frac{-T}{\kappa}\right) + \zeta^2\right)$ where $\zeta^2 \propto \mathbb{E}_i \left\|\nabla f_i(w^*)\right\|^2$.
- Moreover, as before, if we use a mini-batch of size b, the effective noise is $\zeta_b^2 \propto \frac{\mathbb{E}_i \|\nabla f_i(w^*)\|^2}{b}$. Hence, if the model is sufficiently over-parameterized so that it *almost* interpolates the data, and we are using a large batch-size, then ζ_b^2 is small, and constant step-size works well.
- When minimizing convex functions under (exact) interpolation, constant step-size SGD results in O(1/T) convergence, matching deterministic GD, but with much smaller per-iteration cost (Need to prove this in Assignment 3!)



- When minimizing non-convex functions, interpolation is not enough to guarantee a fast (matching the deterministic) O(1/T) rate for SGD.
- Can achieve this rate under the strong growth condition (SGC) on the stochastic gradients. Formally, there exists a constant $\rho > 1$ such that for all w,

$$\mathbb{E}_{i} \left\| \nabla f_{i}(w) \right\|^{2} \leq \rho \left\| \nabla f(w) \right\|^{2}$$

Hence, SGC implies that $\|\nabla f_i(w^*)\|^2 = 0$ for all i and hence interpolation.

• As before, let us study the effect of SGC on the variance $\sigma^2(w)$.

$$\sigma^{2}(w) := \mathbb{E}_{i} \left\| \nabla f_{i}(w) - \nabla f(w) \right\|^{2} = \mathbb{E}_{i} \left\| \nabla f_{i}(w) \right\|^{2} - \left\| \nabla f(w) \right\|^{2}$$
 (Unbiasedness)
$$\Rightarrow \sigma^{2}(w) \leq (\rho - 1) \left\| \nabla f(w) \right\|^{2}$$
 (SGC)

Hence, SGC implies that as w gets closer to a stationary point (in terms of the gradient norm), the variance decreases and constant step-size SGD converges to a stationary point.

Claim: For (i) *L*-smooth functions lower-bounded by f^* , (ii) under ρ -SGC, T iterations of SGD with $\eta_k = \frac{1}{aL}$ returns an iterate \hat{w} such that,

$$\mathbb{E}[\|\nabla f(\hat{w})\|^2] \leq \frac{2\rho L\left[f(w_0) - f^*\right]}{T}$$

Proof: Similar to the proof in Lecture 8, using the *L*-smoothness of *f* with $x = w_k$ and $y = w_{k+1} = w_k - \eta_k \nabla f_{ik}(w_k)$,

$$f(w_{k+1}) \leq f(w_k) + \langle \nabla f(w_k), -\eta_k \nabla f_{ik}(w_k) \rangle + \frac{L}{2} \eta_k^2 \| \nabla f_{ik}(w_k) \|^2$$

Taking expectation w.r.t i_k on both sides and using that η_k is independent of i_k

$$\mathbb{E}[f(w_{k+1})] \leq f(w_k) - \eta_k \mathbb{E}\left[\langle \nabla f(w_k), \nabla f_{ik}(w_k) \rangle\right] + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$

$$\mathbb{E}[f(w_{k+1})] \leq f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right] \qquad \text{(Unbiasedness)}$$

Recall
$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\eta_k^2}{2} \mathbb{E}\left[\|\nabla f_{ik}(w_k)\|^2\right]$$
. Using ρ -SGC,
$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \eta_k \|\nabla f(w_k)\|^2 + \frac{L\rho\eta_k^2}{2} \|\nabla f(w_k)\|^2$$

$$\mathbb{E}[f(w_{k+1})] \le f(w_k) - \frac{1}{2\rho L} \|\nabla f(w_k)\|^2 \qquad \qquad \text{(Using } \eta_k = \eta = \frac{1}{\rho L}\text{)}$$

Taking expectation w.r.t the randomness from iterations i = 0 to k - 1, and summing

$$\sum_{k=0}^{T-1} \mathbb{E}[\|\nabla f(w_k)\|^2] \le 2\rho L \sum_{k=0}^{T-1} \mathbb{E}[f(w_k) - f(w_{k+1})] \implies \frac{\sum_{k=0}^{T-1} \mathbb{E}[\|\nabla f(w_k)\|^2]}{T} \le \frac{2\rho L \mathbb{E}[f(w_0) - f^*]}{T}$$
(Dividing by T)

Defining $\hat{w} := \arg\min_{k \in \{0,1,\dots,T-1\}} \mathbb{E}[\|\nabla f(w_k)\|^2]$,

$$\mathbb{E}[\|\nabla f(\hat{w})\|^2] \leq \frac{2\rho L\left[f(w_0) - f^*\right]}{T}$$



Stochastic Line-Search

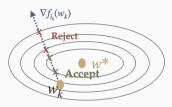
• Algorithmically, convergence under interpolation requires knowledge of *L*. We will use a *stochastic line-search* (SLS) procedure [VML⁺19] to estimate *L*. SLS is similar to the deterministic variant in Lecture 3, but uses only stochastic function/gradient evaluations.

Algorithm SGD with Stochastic Line-search

- 1: function SGD with Stochastic Line-search $(f, w_0, \eta_{\text{max}}, c \in (0, 1), \beta \in (0, 1))$
- 2: **for** k = 0, ..., T 1 **do**
- 3: $\tilde{\eta}_k \leftarrow \eta_{\text{max}}$
- 4: while $f_{ik}(w_k \tilde{\eta}_k \nabla f_{ik}(w_k)) > f_{ik}(w_k) c \cdot \tilde{\eta}_k \|\nabla f_{ik}(w_k)\|^2$ do
- 5: $\tilde{\eta}_k \leftarrow \tilde{\eta}_k \beta$
- 6: end while
- 7: $\eta_k \leftarrow \tilde{\eta}_k$
- 8: $w_{k+1} = w_k \eta_k \nabla f_{ik}(w_k)$
- 9: end for
- 10: **return** w_T

Stochastic Line-Search

- SLS searches for a good step-size in the wrong direction.
- ullet Since all f_i have zero gradient at w^* and the noise decreases as we get closer to the solution (because of interpolation), SGD with SLS converges to the minimizer.



Claim: If each f_i is L-smooth, then the (exact) backtracking procedure for SLS terminates and returns $\eta_k \in \left[\min\left\{\frac{2(1-c)}{L}, \eta_{\max}\right\}, \eta_{\max}\right]$.

Proof: Similar to the deterministic case (Lecture 3), but requires that each f_i is L-smooth.

Claim: When minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ such that (i) f is μ -strongly convex, (ii) each f_i is convex and L-smooth, (iii) interpolation is exactly satisfied i.e. $\|\nabla f_i(w^*)\| = 0$, T iterations of SGD with SLS (with c = 1/2) returns iterate w_T such that,

$$\mathbb{E}[\|w_T - w^*\|^2] \le \exp\left(-\mu T \min\left\{\frac{1}{L}, \eta_{\text{max}}\right\}\right) \|w_0 - w^*\|^2$$

Proof: Similar to the previous proof, we get that,

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\mathbb{E}\left[\eta_k \langle \nabla f_{ik}(w_k), w_k - w^* \rangle\right] + \mathbb{E}\left[\eta_k^2 \|\nabla f_{ik}(w_k)\|^2\right] \quad (1)$$

Since η_k depends on i_k , we can not push the expectation in. η_k is set by SLS, it satisfies the stochastic Armijo condition. Simplifying the third term and denoting $f_{ik}^* := \min f_{ik}(w)$,

$$\mathbb{E}\left[\eta_k^2 \left\|\nabla f_{ik}(w_k)\right\|^2\right] \leq \mathbb{E}\left[\eta_k \frac{f_{ik}(w_k) - f_{ik}(w_{k+1})}{c}\right] \leq \mathbb{E}\left[\eta_k \frac{f_{ik}(w_k) - f_{ik}^*}{c}\right] \tag{2}$$

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Using eq. (1) + eq. (2),

$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\mathbb{E}\left[\eta_k \langle \nabla f_{ik}(w_k), w_k - w^* \rangle\right] + \mathbb{E}\left[\eta_k \frac{f_{ik}(w_k) - f_{ik}^*}{c}\right]$$
(3)
$$\mathbb{E}\left[\eta_k \frac{f_{ik}(w_k) - f_{ik}^*}{c}\right] = \mathbb{E}\left[2\eta_k \left(f_{ik}(w_k) - f_{ik}(w^*) + f_{ik}(w^*) - f_{ik}^*\right)\right]$$
(Setting $c = 1/2$)
$$= \mathbb{E}\left[2\eta_k \left(f_{ik}(w_k) - f_{ik}(w^*)\right)\right] + \mathbb{E}\left[2\eta_k \underbrace{\left(f_{ik}(w^*) - f_{ik}^*\right)\right)}_{\text{Positive}}\right]$$

$$\leq \mathbb{E}\left[2\eta_k \left(f_{ik}(w_k) - f_{ik}(w^*)\right)\right] + 2\eta_{\text{max}} \mathbb{E}\left[f_{ik}(w^*) - f_{ik}^*\right]$$
(Since $\eta_k \leq \eta_{\text{max}}$)

Since f_{ik} is convex and $\nabla f_{ik}(w^*) = 0$, $f_{ik}(w^*) = f_{ik}^*$.

$$\mathbb{E}\left[\eta_k \frac{f_{ik}(w_k) - f_{ik}^*}{c}\right] \le \mathbb{E}\left[2\eta_k \left(f_{ik}(w_k) - f_{ik}(w^*)\right)\right] \tag{4}$$

Using eq. (3) + eq. (4),
$$\mathbb{E}[\|w_{k+1} - w^*\|^2] = \|w_k - w^*\|^2 - 2\mathbb{E}\left[\eta_k \langle \nabla f_{ik}(w_k), w_k - w^* \rangle\right] + \mathbb{E}\left[2\eta_k \left(f_{ik}(w_k) - f_{ik}(w^*)\right)\right]$$

$$= \|w_k - w^*\|^2 + 2\mathbb{E}\left[\eta_k (f_{ik}(w_k) - f_{ik}(w^*) + \langle \nabla f_{ik}(w_k), w^* - w_k \rangle\right]$$
Since f_{ik} is convex, $f_{ik}(w_k) - f_{ik}(w^*) + \langle \nabla f_{ik}(w_k), w^* - w_k \rangle \leq 0$

$$\leq \|w_k - w^*\|^2 + 2\eta_{\min} \mathbb{E}\left[f_{ik}(w_k) - f_{ik}(w^*) + \langle \nabla f_{ik}(w_k), w^* - w_k \rangle\right]$$
(Lower-bounding η_k . $\eta_{\min} := \min\left\{\frac{1}{L}, \eta_{\max}\right\}$)
$$= \|w_k - w^*\|^2 + 2\eta_{\min} \mathbb{E}\left[f(w_k) - f(w^*) + \langle \nabla f(w_k), w^* - w_k \rangle\right]$$
(Unbiasedness)
$$\leq \|w_k - w^*\|^2 + 2\eta_{\min} \left[\frac{-\mu}{2} \|w_k - w^*\|^2\right] \qquad (f \text{ is } \mu\text{-strongly convex})$$

$$\implies \mathbb{E}[\|w_{k+1} - w^*\|^2] \leq (1 - \mu \eta_{\min}) \|w_k - w^*\|^2$$

Recall that $\mathbb{E}[\|w_{k+1} - w^*\|^2] \le (1 - \mu \eta_{\min}) \|w_k - w^*\|^2$. Taking expectation w.r.t the randomness from iterations k = 0 to T - 1 and recursing,

$$\mathbb{E}[\|w_{T} - w^{*}\|^{2}] \leq (1 - \mu \eta_{\min})^{T} \|w_{0} - w^{*}\|^{2} \leq \exp(-\mu T \eta_{\min}) \|w_{0} - w^{*}\|^{2}$$

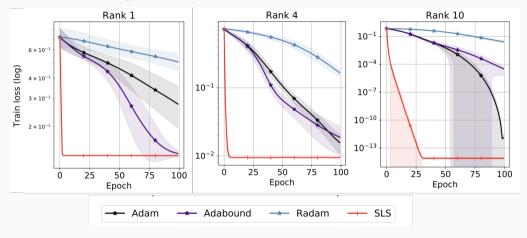
$$\implies \mathbb{E}[\|w_{T} - w^{*}\|^{2}] \leq \exp\left(-\mu T \min\left\{\frac{1}{L}, \eta_{\max}\right\}\right) \|w_{0} - w^{*}\|^{2}$$

Hence, when minimizing smooth, strongly-convex functions under interpolation, SGD + SLS will will converge to the minimizer at an exponential rate.

- If interpolation is not exactly satisfied, we can modify the proof to get an $O\left(\exp\left(\frac{-T}{\kappa}\right) + \zeta^2\right)$ rate, where $\zeta^2 := \mathbb{E}\left[f_{ik}(w^*) f_{ik}^*\right]$.
- When minimizing convex functions under (exact) interpolation, SGD + SLS results in an O(1/T) rate without requiring knowledge of L. (Need to prove this in Assignment 3!)
- Do not have strong theoretical results for SGD + SLS on smooth, non-convex problems.

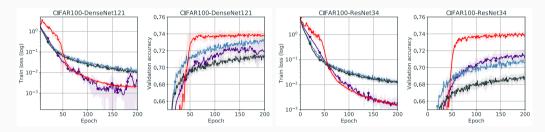
Stochastic Line-Search and Effect of Over-parametrization

Objective: $\min_{\theta_1,\theta_2} \frac{1}{2n} \sum_{i=1}^n \|\theta_2 \theta_1 x_i - y_i\|^2$; **Parameterization**: $\theta_1 \in \mathbb{R}^{k \times 6}$, $\theta_2 \in \mathbb{R}^{10 \times k}$.



Stochastic Line-Search - Experimental Results

Task: Multi-class classification with logistic loss.



Stochastic Polyak Step-size

• When interpolation is (approximately) satisfied, we can use SGD with the *stochastic Polyak* step-size (SPS) [LVLLJ21]: At iteration k, for hyper-parameter $c \in (0,1)$ and $f_{ik}^* := \min_w f_{ik}(w)$,

$$\eta_k = \frac{f_{ik}(w_k) - f_{ik}^*}{c \left\| \nabla f_{ik}(w_k) \right\|^2}.$$

Common machine learning losses (squared loss, logistic loss, exponential loss) are lower-bounded by zero. Algorithmically, we can set $f_{ik}^* = 0$.

- SPS matches the SLS rates on smooth, (strongly) convex functions. E.g. SPS with c=1/2 achieves the $O\left(\exp\left(\frac{-T}{\kappa}\right)+\zeta^2\right)$ rate for smooth, strongly-convex functions.
- Much simpler and computationally inexpensive to implement compared to SLS.
- Unlike SLS, SPS can be used for minimizing non-smooth, convex functions.
- Results in large step-sizes and requires some additional heuristics for stabilizing the method.
- ullet For neural networks, generalization for SGD + SPS was typically worse than for SGD + SLS.
- \bullet Requires access to f_{ik}^* which might be difficult to compute for more general problems.

Adaptivity for SGD

Noise-adaptivity: When minimizing smooth, strongly-convex functions, with T iterations of SGD with $\eta_k := \frac{1}{L} \left(\frac{1}{T}\right)^{\frac{k}{T}}$, we can obtain an $O\left(\exp\left(\frac{-T}{\kappa}\right) + \frac{\zeta^2}{T}\right)$ rate, where $\zeta^2 := \mathbb{E}_i[f_i(w^*) - f_i^*]$. Adaptive to the extent of interpolation, but requires L to set the step-size.

Problem-adaptivity: SGD with the step-size set according to SLS/SPS is adaptive to L, but results in an $O\left(\exp\left(\frac{-T}{\kappa}\right) + \zeta^2\right)$ rate.

- [VDTB21] attempts to combine the above ideas to obtain both noise and problem adaptivity i.e. use SLS to set $\gamma_k \approx \frac{1}{L}$ and use $\eta_k = \gamma_k \left(\frac{1}{T}\right)^{\frac{k}{T}}$. Either not guaranteed to converge to the minimizer or will converge to the minimizer at a slower (than optimal) rate.
- For smooth, strongly-convex problems, we do not (yet) know how to make SGD problem and noise-adaptive, and achieve the optimal rate.
- For smooth, convex problems, AdaGrad is both problem and noise-adaptive.



Minimizing smooth, strongly-convex functions

For minimizing smooth, strongly-convex functions $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ to an ϵ -suboptimality,

- Deterministic GD requires $O(\kappa \log(1/\epsilon))$ iterations, and $O(n \kappa \log(1/\epsilon))$ gradient evaluations.
- SGD with a decreasing step-size requires $O(1/\epsilon)$ iterations, and $O(1/\epsilon)$ gradient evaluations.
- Under exact interpolation, SGD with a constant step-size requires $O(\kappa \log(1/\epsilon))$ iterations, and $O(\kappa \log(1/\epsilon))$ gradient evaluations.
- For finite-sum problems of the form $\frac{1}{n}\sum_{i=1}^{n}f_{i}(w)$, variance reduced methods require $O((n+\kappa)\log(1/\epsilon))$ gradient evaluations.

Variance Reduced Methods

- Recall that under exact interpolation, the variance decreases as we approach the minimizer.
- On the other hand, variance reduced methods explicitly reduce the variance by either storing the past stochastic gradients to approximate the full gradient [SLRB17] or by computing the full gradient every "few" iterations [JZ13].
- With variance reduction, we can use acceleration techniques to improve the dependence on the condition number, and require $O((n+\sqrt{\kappa})\log(1/\epsilon))$ gradient evaluations [AZ17].
- For smooth, convex finite-sum problems, variance reduced techniques require $O\left((n+\frac{1}{\epsilon})\log(1/\epsilon)\right)$ gradient evaluations [NLST17], compared to deterministic GD that requires $O(\frac{n}{\epsilon})$ gradient evaluations and SGD that requires $O(\frac{1}{\epsilon^2})$ gradient evaluations.
- We will use SVRG (Stochastic Variance Reduced Gradient) [JZ13] for smooth, strongly-convex finite-sum problems, and prove that it requires $O((n + \kappa) \log(1/\epsilon))$ gradient evaluations.

SVRG

For simplicity, we will use Loopless SVRG [KHR20] that has a simpler implementation and analysis compared to the original paper [JZ13].

Algorithm SVRG

- 1: function SVRG $(f, w_0, \eta, p \in (0, 1])$
- 2: $v_0 = w_0$
- 3: **for** k = 0, ..., T 1 **do**
- 4: $g_k = \nabla f_{ik}(w_k) \nabla f_{ik}(v_k) + \nabla f(v_k)$
- 5: $w_{k+1} = w_k \eta g_k$
- 6: $v_{k+1} = \begin{cases} v_k \text{ with probability } 1 p \\ w_k \text{ with probability } p \end{cases}$
- 7: end for
- 8: **return** w_T

Minimizing smooth, strongly-convex functions using SVRG

Claim: When minimizing $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ such that (i) f is μ -strongly convex, (ii) each f_i is convex and L-smooth, T iterations of SVRG with $\eta = \frac{1}{6L}$ and $p = \frac{1}{n}$ returns iterate w_T ,

$$\mathbb{E}[\left\|w_T - w^*\right\|^2] \leq \left(\max\left\{\left(1 - \frac{\mu}{6L}\right), \left(1 - \frac{1}{2n}\right)\right\}\right)^T \left[2n \left\|w_0 - w^*\right\|^2\right].$$

Case 1: $\left(1-\frac{\mu}{6L}\right) \leq \left(1-\frac{1}{2n}\right) \implies n \geq 3\kappa$. In this case, for achieving an ϵ -suboptimality, we need T iterations such that $T \geq 2n\log\left(\frac{2n\|w_0-w^*\|^2}{\epsilon}\right)$.

Case 2: $\left(1-\frac{\mu}{6L}\right)>\left(1-\frac{1}{2n}\right) \implies n \leq 3\kappa$. In this case, for achieving an ϵ -suboptimality, we need T iterations such that $T\geq 6\kappa\,\log\left(\frac{2n\,\|w_0-w^*\|^2}{\epsilon}\right)$.

- Putting the cases together, for achieving an ϵ -suboptimality, we need $T = O((n + \kappa) \log(1/\epsilon))$.
- In each iteration, the number of expected gradient evaluations is (1-p)(2)+(p)(n+2)=pn+2=3. Hence, in expectation, SVRG requires $O\left((n+\kappa)\log(1/\epsilon)\right)$ gradient evaluations to achieve an ϵ -suboptimality.

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