Nonconvex Variance Reduced Optimization with Arbitrary Sampling

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The Problem

$$\min_{x\in\mathbb{R}^d} \quad f(x) := \frac{1}{n}\sum_{i=1}^{n} f_i(x) \qquad (1)$$

- f_i is L_i-smooth but **non-convex**
- n **is big**

Arbitrary Sampling

- Sampling: a random set-valued mapping S with values being subsets of $[n] := \{1, 2, \ldots, n\}$. A sampling is used to generate minibatches in each iteration.
- Probability matrix associated with sampling S :

$$\mathbf{P}_{ij} \overset{\text{def}}{=} \text{Prob}(\{i, j\} \subseteq S)$$

- Probability vector associated with sampling S :

$$p = (p_1, \ldots, p_n), \quad p_i \overset{\text{def}}{=} \text{Prob}(i \in S)$$

- Minibatch size: $b = \mathrm{E}[|S|]$ (expected size of S)
- Proper sampling: Sampling for which $p_i > 0$ for all $i \in [n]$
- "Arbitrary sampling" = any proper sampling

Main Contributions

- We develop arbitrary sampling variants of 3 popular variance-reduced methods for solving the non-convex problem (1): `SVRG` [1], `SAGA` [2], `SARAH` [3].
- Our rates for $b = 1$: up to $n\times$ better (depending on $\{L_i\}$). Improvements even in the case when $L_i = L_j$ for all i, j (for `SVRG` & `SAGA`).
- Our rates for $b \geq 1$: Linear or superlinear speedup in minibatch size b. That is, # of iterations needed to output a solution of a given accuracy drops by a factor equal or greater to b.
- We design importance sampling & approximate importance sampling for minibatches, which vastly outperform standard uniform minibatch strategies in practice.

Key Lemma

Let $\zeta_1, \zeta_2, \ldots, \zeta_n$ be vectors in $\mathbb{R}^d$ and let $\bar{\zeta} \overset{\text{def}}{=} \frac{1}{n}\sum_{i=1}^n \zeta_i$ be their average. Let S be a proper sampling. Let $v = (v_1, \ldots, v_n) > 0$ be such that

$$\mathbf{P} - pp^\top \preceq \mathbf{Diag}(p_1 v_1, p_2 v_2, \ldots, p_n v_n). \qquad (2)$$

Then

$$\mathrm{E}\left[\left\|\sum_{i\in S}\frac{\zeta_i}{np_i} - \bar{\zeta}\right\|^2\right] \leq \frac{1}{n^2}\sum_{i=1}^n \frac{v_i}{p_i}\|\zeta_i\|^2.$$

Whenever (2) holds, it must be the case that

$$v_i \geq 1 - p_i.$$

Optimal Sampling & Superlinear Speedup

- Under our analysis, the independent sampling S^* defined by

$$p_i \overset{\text{def}}{=} \begin{cases} (b + k - n)\frac{L_i}{\sum_{j=1}^k L_j}, & \text{if } i \leq k \\ 1, & \text{if } i > k \end{cases},$$

is optimal, where k is the largest integer satisfying $0 < b + k - n \leq \frac{\sum_{i=1}^k L_i}{L_k}$.
- All 3 methods enjoy superlinear speed in b up to the minibatch size $b_{\max} := \max\{b \mid bL_n \leq \sum_{i=1}^n L_i\}$.

Stochastic Gradient Evaluations to Achieve $\mathrm{E}[\|\nabla f(x)\|^2] \leq \epsilon$

Alg	Uniform sampling	Arbitrary sampling [NEW]	S^* [NEW]
`SVRG`	$\max\left\{n, \frac{(1+4/3)L_{\max}c_1 n^{2/3}}{\epsilon}\right\}$ [1]	$\max\left\{n, \frac{(1+4\alpha/3)\bar{L}c_1 n^{2/3}}{\epsilon}\right\}$	$\max\left\{n, \frac{\left(1+\frac{4(n-b)}{3n}\right)\bar{L}c_1 n^{2/3}}{\epsilon}\right\}$
`SAGA`	$n + \frac{2L_{\max}c_2 n^{2/3}}{\epsilon}$ [2]	$n + \frac{(1+\alpha)\bar{L}c_2 n^{2/3}}{\epsilon}$	$n + \frac{(1+\frac{n-b}{n})\bar{L}c_2 n^{2/3}}{\epsilon}$
`SARAH`	$n + \frac{\frac{n-b}{n-1}L_{\max}^2 c_3}{\epsilon^2}$ [3]	$n + \frac{\alpha\bar{L}^2 c_3}{\epsilon^2}$	$n + \frac{\frac{n-b}{n}\bar{L}^2 c_3}{\epsilon^2}$

Constants: $L_{\max} = \max_i L_i$ $\quad \bar{L} = \frac{1}{n}\sum_i L_i$ $\quad c_1, c_2, c_3 =$ universal constants $\quad \alpha := \frac{b}{\bar{L}^2 n^2}\sum_{i=1}^n \frac{v_i L_i^2}{p_i}$

Samplings

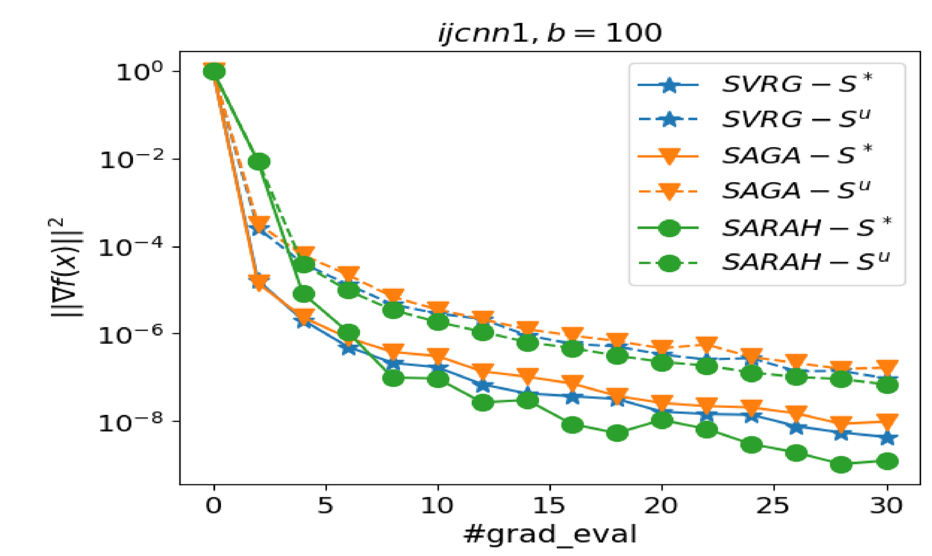
- **Uniform** S^u: Every subset of $[n]$ of size b (minibatch size) is chosen with the same probability: $1/\binom{n}{b}$
- **Independent** S^*: For each $i \in [n]$ we independently flip a coin, and with probability p_i include element i into S.
- **Approximate Independent** S^a: Fix some $k \in [n]$ and let $a = \lceil k \max_{i\leq k} p_i \rceil$. We now sample a single set S' of cardinality a using the uniform minibatch sampling S^u. Subsequently, we apply an independent sampling S^* to select elements of S', with selection probabilities $p'_i = kp_i/a$. The resulting random set is S^a.

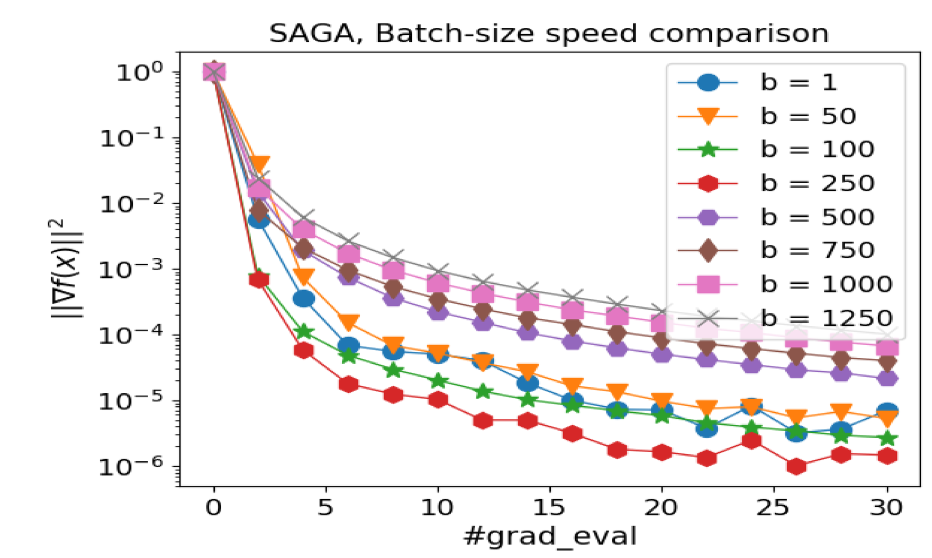
SVRG with Arbitrary Sampling

Algorithm 1: `SVRG` (x^0, m, T, η, S)

$\tilde{x}^0 = x_m^0 = x^0$, $M = \lceil T/m \rceil$;
for $s = 0$ ***to*** $M - 1$ **do**
  $x_0^{s+1} = x_m^s$; $g^{s+1} = \frac{1}{n}\sum_{i=1}^n \nabla f_i(\tilde{x}^s)$
  for $t = 0$ ***to*** $m - 1$ **do**
    Draw a random subset (minibatch) $S_t \sim S$
    $v_t^{s+1} = \sum_{i_t\in S_t} \frac{1}{np_{i_t}}(\nabla f_{i_t}(x_t^{s+1}) - \nabla f_{i_t}(\tilde{x}^s)) + g^{s+1}$
    $x_{t+1}^{s+1} = x_t^{s+1} - \eta v_t^{s+1}$
  end
  $\tilde{x}^{s+1} = x_m^{s+1}$
end
Output: Iterate x_a chosen uniformly random from $\{\{x_t^{s+1}\}_{t=0}^m\}_{s=0}^M$

Numerical Results





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