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Nonconvex Variance Reduced Optimization with Arbitrary Sampling

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Empirical Risk Minimization

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

n is big

non-convex, L_i-smooth

$$\|\nabla f_i(x) - \nabla f_i(y)\| \le L_i \|x - y\|$$

Baseline Variance Reduced SGD Methods

Expected mini-batch size:
$b = \mathrm{E}|S|$

SVRG
Johnson & Zhang
NIPS 2013

$$x^+ = x - \eta \left(\frac{1}{b} \sum_{i \in \mathbb{S}} (\nabla f_i(x) - \nabla f_i(\hat{x})) + \nabla f(\hat{x}) \right)$$

Uniform sampling

SAGA
Defazio, Bach & Lacoste-Julien
NIPS 2014

$$x^+ = x - \eta \left(\frac{1}{b} \sum_{i \in \mathbb{S}} (\nabla f_i(x) - g_i) + \frac{1}{n} \sum_{j=1}^{n} g_j \right)$$

Uniform sampling

SARAH
Nguyen, Liu, Scheinberg & Takáč
ICML 2017

$$x^+ = x - \eta \left(\frac{1}{b} \sum_{i \in \mathbb{S}} (\nabla f_i(x) - \nabla f_i(x^-)) + \nabla f(x^-) \right)$$

Uniform sampling

Contributions

Richtárik & Takáč (OL 2016; arXiv 2013)
Qu, Richtárik & Zhang (NIPS 2015)
Qu & Richtárik (COAP 2016)
Chambolle, Ehrhardt, Richtárik & Schoenlieb (SIOPT 2018)
Hanzely & Richtárik (AISTATS 2019)
Qian, Qu & Richtárik (ICML 2019)
Gower, Loizou, Qian, Sailanbayev, Shulgin & Richtárik (ICML 2019)

- Analysis of SVRG, SAGA and SARAH in the arbitrary sampling paradigm

- Construction of optimal minibatch sampling

First optimal/importance sampling for minibatches!

Data Sampling (i.e., Mini-batching) Mechanisms

A **sampling** is uniquely defined by assigning probabilities to all 2^n subsets of {1, 2, … , *n*}

Sampling: a random subset of {1, 2, … , *n*}

Probability matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$ associated with sampling S

$$\mathbf{P}_{ij} := \mathrm{Prob}(\{i, j\} \subseteq S)$$

Probability vector $p \in \mathbb{R}^n$ associated with sampling S

$$p_i := \mathrm{Prob}(\{i\} \subseteq S) = \mathbf{P}_{ii}$$

Proper sampling: $p_i > 0$ for all $i = 1, 2, \dots, n$

Examples

Standard sampling:

$S = \{i\}$ with probability $\frac{1}{n}$ for all $i = 1, 2, \dots, n$

Standard mini-batch sampling:

$S = C$ with probability $\frac{1}{\binom{n}{b}}$
for all $C \subset \{1, 2, \dots, n\}$
such that $|C| = b$

Arbitrary sampling paradigm = perform iteration complexity analysis for **any proper sampling**

From Standard Sampling to Arbitrary Sampling

SVRG with
Arbitrary Sampling

Unbiased estimator of
the gradient

$$x^+ = x - \eta \left(\sum_{i \in S} \frac{1}{np_i} (\nabla f_i(x) - \nabla f_i(\hat{x})) + \nabla f(\hat{x}) \right)$$

Arbitrary
sampling

Standard sampling:

$p_i = \frac{1}{n}$ for all i

Convergence Rate I

data points

$$\mathcal{O}\left(n + \alpha \frac{n^{2/3}}{\epsilon}\right)$$

$\mathrm{E}\|\nabla f(x)\|^2 \leq \epsilon$

KEY QUANTITY: DEPENDS ON THE SAMPLING

Convergence Rate II

Constants satisfying:

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

$\mathbf{P}_{ij} := \mathrm{Prob}(\{i,j\} \subseteq S)$

$\|\nabla f_i(x) - \nabla f_i(y)\| \le L_i \|x - y\|$

Expected mini-batch size:

$b = \mathrm{E}|S|$

$$\alpha := \frac{b}{\bar{L} n^2} \sum_{i=1}^{n} \frac{v_i L_i^2}{p_i}$$

$\bar{L} = \frac{1}{n} \sum_{i=1}^{n} L_i$

data points

$p_i := \mathrm{Prob}(\{i\} \subseteq S) = \mathbf{P}_{ii}$

Optimal rate: minimize α over $\{(v_i, p_i)\}_{i=1}^{n}$

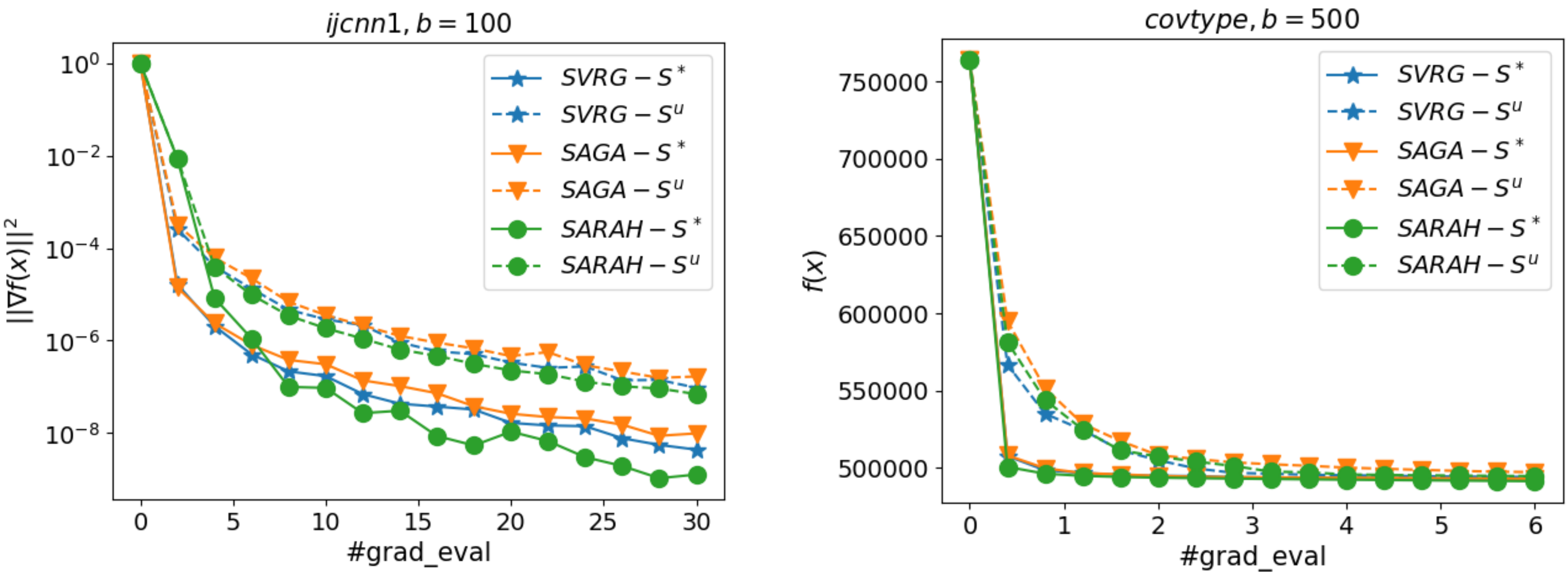
Complexity Results

$$\#\ \textbf{Stochastic Gradient Evaluations to Achieve}\ \mathrm{E}\left[\|\nabla f(x)\|^2\right] \le \epsilon$$

Alg	Uniform sampling	Arbitrary sampling [NEW]	S^* (Best Sampling) [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: $L_{\max} = \max_i L_i$ $\bar{L} = \frac{1}{n}\sum_i L_i$ $c_1, c_2, c_3 =$ universal constants $\alpha := \frac{b}{\bar{L}^2 n^2}\sum_{i=1}^n \frac{v_i L_i^2}{p_i}$

Experiments



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].
- We are able calculate the optimal sampling out of all samplings of a given minibatch size. This is the first time an optimal minibatch sampling was computed (from the class of all samplings).
- 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

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

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

$$v_i \ge 1 - p_i.$$

Optimal Sampling & Superlinear Speedup

- Under our analysis, the independent sampling S^* defined by
  $$p_i \overset{\text{def}}{=} \begin{cases} (b + k - n)\frac{L_i}{\sum_{j=1}^k L_j}, & \text{if } i \le k \\ 1, & \text{if } i > k \end{cases},$$
  is optimal, where k is the largest integer satisfying $0 < b + k - n \le \frac{\sum_{i=1}^k L_i}{L_k}$.
- All 3 methods enjoy superlinear speed in b up to the minibatch size $b_{\max} := \max\{b \mid bL_n \le \sum_{i=1}^n L_i\}$.

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

Alg	Uniform sampling	Arbitrary sampling [NEW]	S^* (Best Sampling) [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

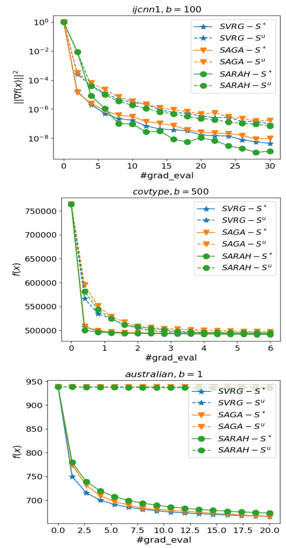
- **Uniform** S^u: Every subset of $[n]$ of size b (minibatch size) is chosen with the same probability: $1/\binom{n}{b}$
- **Independent** S^*: For each $i \in [n]$ we independently flip a coin, and with probability p_i include element i into S.
- **Approximate Independent** S^a: Fix some $k \in [n]$ and let $a = \lceil k \max_{i \le k} p_i \rceil$. 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

$\tilde{x}^0 = x_m^0 = x^0$, $M = \lceil T/m \rceil$;
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) $S_t \sim S$
    $v_t^{s+1} = \sum_{i_t \in S_t} \frac{1}{n p_{i_t}} (\nabla f_{i_t}(x_t^{s+1}) - \nabla f_{i_t}(\tilde{x}^s)) + g^{s+1}$
    $x_{t+1}^{s+1} = x_t^{s+1} - \eta v_t^{s+1}$
  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



References

[1] Sashank J Reddi, Ahmed Hefny, Suvrit Sra, Barnabás Póczos, and Alex Smola. Stochastic variance reduction for nonconvex optimization. In *The 33th International Conference on Machine Learning*, pages 314–323, 2016.

[2] Sashank J Reddi, Suvrit Sra, Barnabás Póczos, and Alex Smola. Fast incremental method for smooth nonconvex optimization. In *Decision and Control (CDC), 2016 IEEE 55th Conference on*, pages 1971–1977. IEEE, 2016.

[3] Lam M Nguyen, Jie Liu, Katya Scheinberg, and Martin Takáč. Stochastic recursive gradient algorithm for nonconvex optimization. *arXiv:1705.07261*, 2017.

Poster: Pacific Ballroom #95 (Today 6:30–9:00 PM)

Thank you!