Hybrid Stochastic-Deterministic Minibatch Proximal Gradient: Less-Than-Single-Pass Optimization with Nearly Optimal Generalization

Pan Zhou \(^1\)  Xiao-Tong Yuan \(^2\)

Abstract

Stochastic variance-reduced gradient (SVRG) algorithms have been shown to work favorably in solving large-scale learning problems. Despite the remarkable success, the stochastic gradient complexity of SVRG-type algorithms usually scales linearly with data size and thus could still be expensive for huge data. To address this deficiency, we propose a hybrid stochastic-deterministic minibatch proximal gradient (HSDMPG) algorithm for strongly-convex problems that enjoys provably improved data-size-independent complexity guarantees. More precisely, for quadratic loss \(F(\theta)\) of \(n\) components, we prove that HSDMPG can attain an \(\epsilon\)-optimization-error \(\mathbb{E}[F(\theta) - F(\theta^*)] \leq \epsilon\) within \(O\left(\frac{\kappa^{1.5} \epsilon^{0.75} \log^{1.5}(\frac{1}{\epsilon})}{\epsilon} + n \log \left(\frac{1}{\epsilon}\right)\right)\) stochastic gradient evaluations, where \(\kappa\) is condition number. For generic strongly convex loss functions, we prove a nearly identical complexity bound though at the cost of slightly increased logarithmic factors. For large-scale learning problems, our complexity bounds are superior to those of the prior state-of-the-art SVRG algorithms with or without dependence on data size. Particularly, in the case of \(\epsilon = O\left(1/\sqrt{n}\right)\) which is at the order of intrinsic excess error bound of a learning model and thus sufficient for generalization, the stochastic gradient complexity bounds of HSDMPG for quadratic and generic loss functions are respectively \(O(n^{0.875} \log^{1.5}(n))\) and \(O(n^{0.875} \log^{2.25}(n))\), which to our best knowledge, for the first time achieve optimal generalization in less than a single pass over data. Extensive numerical results demonstrate the computational advantages of our algorithm over the prior ones.

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1. Introduction

We consider the following \(\ell_2\)-regularized empirical risk minimization (ERM) problem:

\[
\min_{\theta \in \mathbb{R}^d} F(\theta) := \frac{1}{n} \sum_{i=1}^{n} \ell(\theta^\top x_i, y_i) + \frac{\mu}{2} \|\theta\|_2^2, \tag{1}
\]

where \(\{(x_i, y_i)\}_{i=1}^n\) is a training set; the convex loss function \(\ell(\theta^\top x, y)\) measures the discrepancy between the linear prediction \(\theta^\top x\) and the ground truth \(y\); and the regularization term \(\frac{\mu}{2} \|\theta\|_2^2\) aims at enhancing generalization ability of the linear model. In the field of statistical learning, the formulation (1) encapsulates a vast body of problems including least squares regression, logistic regression and softmax regression, to name a few. In this work, we focus on developing scalable and autonomous first-order optimization methods to solve this fundamental problem, which has been extensively studied with a bunch of efficient algorithms proposed including gradient descent (GD) (Cauchy, 1847), stochastic GD (SGD) (Robbins & Monro, 1951), SDCA (Shalev-Shwartz, 2012), SVRG (Johnson & Zhang, 2013), Catalyst (Lin et al., 2015), SCSG (Lei & Jordan, 2017) and Katyusha (Allen-Zhu, 2017).

Motivation. Despite the remarkable success of the stochastic gradient methods and their variance-reduced extensions, the stochastic gradient evaluation complexity (which usually dominates the computational cost) of these algorithms tends to scale linearly with data size \(n\). Such a linear dependence is not only expensive when data scale is huge but also problematic in online and life-long learning regimes where samples are coming infinitely. As pointed out in (Lei & Jordan, 2017), there are situations in which accurate solutions can be obtained with less than a single pass through the data, e.g. for a large-scale dataset with similar and redundant samples. Therefore, developing data-size-independent learning algorithms is of special importance in big data era.

Particularly, we are interested in efficiently optimizing problem (1) to its intrinsic excess error bound which typically scales as \(O\left(1/\sqrt{n}\right)\). As shown in (Bottou & Bousquet, 2008), the excess error, which measures the expected prediction discrepancy between the optimum model and the learnt model over all possible samples and thus reflects the generalization performance of the model, can be decomposed into model approximation error, estimation error and
The solution $\theta$ with $\epsilon$-optimization-error is measured by sub-optimality $\mathbb{E}[F(\theta) - F(\theta^*)] \leq \epsilon$ with optimum $F(\theta^*)$. Here we define a set of constants for quadratic (generic) loss: $\beta_1 = 1.5$, $\beta_2 = 4$, $\beta_3 = 4.5$, $\beta_4 = 1$, $\beta_5 = 1$, $\gamma = 1.5$, $\mu = 2.25$. These different constants only affects the logarithm factor $\xi = \log(\frac{1}{\epsilon})$. For brevity, we define $\Theta = \frac{\mu^2}{\mu^2 + \frac{1}{2}}$. The third column summarizes the conditions under which HSDMPG has lower IFO complexity than the compared algorithms.

### Table 1: Comparison of IFO complexity for first-order stochastic algorithms on the $\mu$-strongly-convex problem (1) with condition number $\kappa$.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$\epsilon$-Optimization Error for ERM (1)</th>
<th>Better Zoom of HSDMPG</th>
<th>$\frac{1}{\sqrt{n}}$-Optimization Error for ERM (1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SGD</td>
<td>$\mathcal{O}\left(\frac{1}{\mu \epsilon}\right)$</td>
<td>$\Theta \mu \leq 1$ or $n \leq \frac{1}{\mu^2 \epsilon^2}$</td>
<td>$\mathcal{O}(n)$</td>
</tr>
<tr>
<td>SVRG, SAGA, APSDCA</td>
<td>$\mathcal{O}\left((n + \kappa) \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \xi^{-1} \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>APCG</td>
<td>$\mathcal{O}\left(\frac{n}{\mu^2} \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \mu^2 \xi^{-1} \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>SDC, Catalyst, Katyusha</td>
<td>$\mathcal{O}\left((n + \sqrt{n}) \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \xi^{-1} \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>AMSVRG</td>
<td>$\mathcal{O}\left((n + \frac{n \kappa}{n^2}) \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \xi^{-1} \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>Varag</td>
<td>$\mathcal{O}\left(n \log(n) + \frac{1}{\sqrt{n}} + \sqrt{n} \kappa \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \log^{-1}(n) \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>SCSG</td>
<td>$\mathcal{O}\left((n + \frac{1}{\kappa} + \kappa) \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \xi^{-1} \leq \mathcal{O}(n)$</td>
<td>$\mathcal{O}(n \log(n))$</td>
</tr>
<tr>
<td>HSDMPG</td>
<td>$\mathcal{O}\left(\frac{1}{\kappa} + \frac{1}{\mu} n \log \left(\frac{1}{\epsilon}\right)\right) + \frac{1}{\mu} \left(\frac{1}{\kappa} \log \left(\frac{1}{\epsilon}\right) + \frac{1}{\mu} \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \mu \leq 1$ or $n \leq \frac{1}{\mu^2 \epsilon^2}$</td>
<td>$\mathcal{O}(n^{1.875} \log^{1.5}(n))$</td>
</tr>
<tr>
<td>quadratic generic</td>
<td>$\mathcal{O}\left(\frac{1}{\kappa} + \frac{1}{\mu} n \log \left(\frac{1}{\epsilon}\right)\right) + \frac{1}{\mu} \left(\frac{1}{\kappa} \log \left(\frac{1}{\epsilon}\right) + \frac{1}{\mu} \log \left(\frac{1}{\epsilon}\right)\right)$</td>
<td>$\Theta \mu \leq 1$ or $n \leq \frac{1}{\mu^2 \epsilon^2}$</td>
<td>$\mathcal{O}(n^{1.875} \log^{2.25}(n))$</td>
</tr>
</tbody>
</table>

**Optimization error.** Among them, the model approximation error measures how closely the selected prediction model can approximate the optimal model; the estimation error measures the prediction effects of minimizing the empirical risk instead of the population risk; the optimization error denotes the prediction difference between the exact and approximate solutions of ERM. Therefore, to achieve small excess error, one should minimize the three terms jointly. With optimal choice $\mu = \mathcal{O}(1/\sqrt{\kappa})$ to balance empirical risk and generalization gap, the estimation error is known to be at the order of $\mathcal{O}(1/\sqrt{n})$, which implies the excess error is dominated by $\mathcal{O}(1/n)$ (Vapnik, 2006; Shalev-Shwartz et al., 2009; Shalev-Shwartz & Ben-David, 2014). Thus, it is sufficient to optimize the regularized ERM problem (1) to the optimization error $\mathcal{O}(1/\sqrt{n})$ to match the optimal excess error without redundant computation.

**Overview of our contribution.** The main contribution of this paper is a novel Hybrid Stochastic-Deterministic Minibatch Proximal Gradient (HSDMPG) algorithm with substantially improved data-size-independent complexity over existing methods. For quadratic problems, the core idea of our method is to recurrently convert the original large-scale ERM problem into a series of minibatch proximal ERM subproblems for efficient minimization and update. Specifically, as a starting point, we uniformly randomly select a minibatch $S$ of components of the risk function $F$ to form a stochastic approximation $F_S$ that will be fixed throughout the algorithm iteration. Next, at each iteration step, we first construct a stochastic surrogate of $F_S$ by combining the Bregman divergence of $F_S$ at the current iterate and a first-order hybrid stochastic-deterministic approximation of $F$; and then we invoke existing variance-reduced algorithms, such as SVRG, to minimize this surrogate subproblem to desired optimization error. For quadratic loss, we can provably establish sharper bounds of incremental first order oracle (IFO), see Definition 2) for such a hybrid stochastic-deterministic minibatch proximal update procedure in large-scale settings. To extend the strong efficiency guarantee to generic strongly convex losses, we propose to iteratively convert the non-quadratic problem into a sequence of quadratic subproblems such that the aforementioned method can be readily applied for optimization. In this way, up to logarithmic factors, HSDMPG still enjoys a identical sharp bound of IFO for strongly convex problems.

Table 1 summarizes the computational complexity (measured by IFO) of HSDMPG and several representative baselines, including SGD (Robbins & Monro, 1951; Shamir, 2011), SVRG (Johnson & Zhang, 2013), SAGA (Defazio et al., 2014), APSDCA (Shalev-Shwartz & Zhang, 2014), APCG (Lin et al., 2014), SPDC (Zhang & Xiao, 2015), Catalyst (Lin et al., 2015), Varag (Lan et al., 2019), AMSVRG (A. Nitha, 2016), Katyusha (Allen-Zhu, 2017),...
SCSG (Lei & Jordan, 2017). In the following, we highlight the advantages of our method over these prior approaches:

- To achieve $\epsilon$-optimization-error, i.e., $\mathbb{E}[F(\theta) - F(\theta^*)] \leq \epsilon$, the IFO complexity of HSDMPG on problem (1) is
  \[
  \mathcal{O}\left(\frac{\kappa}{\epsilon} \cdot 5\cdot \log(\frac{1}{\epsilon}) + \frac{1}{\epsilon} \cdot \kappa \cdot \sqrt{\kappa} \cdot \log(\frac{1}{\epsilon}) + \frac{1}{\epsilon} \cdot \kappa \cdot \sqrt{\kappa} \cdot \log(\frac{1}{\epsilon})\right),
  \]
  where $\tau_1 = 1.5$, $\tau_2 = 1.5$ and $\tau_3 = 1$ for quadratic loss and $\tau_1 = 2.25$, $\tau_2 = 2.5$ and $\tau_3 = 2$ for generic strongly convex loss. In comparison, the IFO complexity bounds of all the compared algorithms except SGD and SCSG scale linearly w.r.t. the data size $n$. As specified in the third column of Table 1, HSDMPG is superior to these algorithms in large-scale problem settings which are of central interest in big data applications. Compared with SGD, since in most cases, the condition number $\kappa$ is at the order of $\mathcal{O}(1/\mu)$, HSDMPG improves over SGD by a factor at least $\mathcal{O}(\kappa \cdot \sqrt{\kappa} \cdot \log(\frac{1}{\epsilon})$ (up to logarithm factors). For SCSG, HSDMPG also shows higher computational efficiency when (1) the optimization error $\epsilon$ is small which corresponds to conditions $\uplus$ or $\boxplus$ in Table 1; and (2) the data size $n$ is large which corresponds to condition $\boxminus$ in Table 1.

- For the practical setting where $\epsilon = \mathcal{O}(1/\sqrt{n})$ which matches the optimal intrinsic excess error, HSDMPG has the IFO complexity $\mathcal{O}\left(n^{0.875} \log^{1.5}(n)\right)$ for the quadratic loss and $\mathcal{O}\left(n^{0.875} \log^{2.25}(n)\right)$ for the generic strongly convex loss. By ignoring the small logarithmic term $\log(n)$, both complexities of HSDMPG are lower than the complexity bound $\mathcal{O}(n)$ of SGD by a factor $\mathcal{O}(n^{0.125})$. Similarly, HSDMPG respectively improves over APCG and other remaining algorithms, such as SVRG, Katyusha, Varag and SCSG, by factors of $\mathcal{O}(n^{0.375})$ and $\mathcal{O}(n^{0.125})$. These results demonstrate the superior computational efficiency of HSDMPG for attaining near-optimal generalization rate of a statistical learning model.

2. Related Work

Stochastic gradient algorithms. Gradient descent (GD) (Cauchy, 1847) method has long been applied to solve ERM and enjoys linear convergence rate on strongly convex problems. But it needs to compute full gradient per iteration, leading to huge computation cost on large-scale problems. To improve efficiency, incremental gradient algorithms have been developed via leveraging the finite-sum structure and have witnessed tremendous progress recently. For instance, SGD (Robbins & Monro, 1951; Bottou, 1991) only evaluates gradient of one (or a minibatch) randomly selected sample at each iteration, which greatly reduces the cost of each iteration and shows more appealing efficiency than GD on large-scale problems (Shamir, 2011; A. Ntinda, 2016; Hendrikx et al., 2019; Mohammadi et al., 2019). Along this line of research, a variety of variance-reduced variants, such as SVRG (Johnson & Zhang, 2013), SAGA (Defazio et al., 2014), APSDCA (Shamir, 2011), AMSVRG (A. Ntinda, 2016), SCSG (Lei & Jordan, 2017), Catalyst (Lin et al., 2015), Katyusha (Allen-Zhu, 2017), Varag (Lan et al., 2019), are developed and have delivered exciting progress such as linear convergence rates on strongly convex problems as opposed to sublinear rates of vanilla SGD (Shamir, 2011). The hybrid stochastic-deterministic gradient descent method (Friedlander & Schmidt, 2012; Zhou et al., 2018a; b; Mokhtari et al., 2016; Mokhtari & Ribeiro, 2017) iteratively samples an evolving minibatch of samples for gradient estimation or subproblem construction and works favorably in reducing the computational complexity. Our HSDMPG method differs significantly from these prior algorithms. Based on the Bregman-divergence of the minibatch function and a hybrid stochastic-deterministic first-order approximation of the original function, HSDMPG constructs a variance-reduced minibatch proximal function which is provably more efficient. Moreover, HSDMPG can employ any off-the-shelf algorithms to solve the constructed sub-problems in the inner loop and thus is flexible for implementation. HSDMPG shares a similar spirit with the DANE method (Shamir et al., 2014) which also uses a local Bregman-divergence-based function approximation for communication-efficient distributed quadratic loss optimization. The main difference lies in the way of constructing first-order approximation of the risk function: HSDMPG employs a novel hybrid stochastic-deterministic approximation strategy which is substantially more efficient than the deterministic strategy as used by DANE.

Generalization and optimization. In the seminal work of Bottou & Bousquet (2008), it has been demonstrated that the excess error that measures the generalization performance of an ERM model over a function class can be decomposed into three terms in expectation: an approximation error that measures how accurate the function class can approximate the underlying optimum model; an estimation error that measures the effects of minimizing ERM instead of population risk; and an optimization error that represents the difference between the exact solution and the approximate solution of ERM. Particularly, for the $\ell_2$-regularized convex ERM with linear models as in (1), its estimation error (or excess risk) has long been studied with a vast body of deep theoretical results established (Shalev-Shwartz & Ben-David, 2014; Hardt et al., 2016; Bach & Moulines, 2013; Dieuleveut et al., 2017; Zhou & Feng, 2018a; b). A simple yet powerful tool for analyzing estimation error is the stability of an estimator to the changes of training dataset (Bousquet & Elisseeff, 2002). The $\ell_2$-regularized convex ERM has been shown to have uniform stability of order $\mathcal{O}(1/(\mu n))$ (Bousquet & Elisseeff, 2002), which then gives rise to the optimal choice $\mu = \mathcal{O}(1/\sqrt{n})$.
to balance empirical loss and generalization gap to achieve estimation error $O(1/\sqrt{n})$ (Shalev-Shwartz et al., 2009; Feldman & Vondrak, 2019). This implies that the overall excess error is dominated by $O(1/\sqrt{n})$. In this sense, it suffices to solve the $\ell_2$-regularized ERM to optimization error $O(1/\sqrt{n})$ to match the intrinsic excess error.

### 3. Hybrid Stochastic-Deterministic Minibatch Proximal Gradient

In this section, we first introduce the hybrid stochastic-deterministic minibatch proximal gradient (HSDMPG) algorithm for quadratic loss function along with convergence rate and computational complexity analysis. Then, we extend HSDMPG and its theoretical analysis to generic strongly convex loss functions.

#### 3.1. The HSDMPG method for quadratic loss

**3.1.1. ALGORITHM**

The HSDMPG method is outlined in Algorithm 1. The initial step is to randomly sample a minibatch $S$ of data points of size $s$ to construct a stochastic approximation

$$F_S(\theta) = \frac{1}{s} \sum_{i \in S} \ell(\theta^\top x_i, y_i) + \frac{\mu}{2} \|\theta\|_2^2 \tag{2}$$

of the original risk function $F(\theta)$ in problem (1). $F_S(\theta)$ will be fixed throughout the computational procedure to follow. Then in the iteration loop the algorithm iterates between two steps of S1 and S2. In step S1, we uniformly randomly sample a size increasing minibatch $S_t$ of samples to estimate an inexact function $F_{S_t}(\theta) = \frac{1}{|S_t|} \sum_{i \in S_t} \ell(\theta^\top x_i, y_i) + \frac{\mu}{2} \|\theta\|_2^2$. Let $D_\theta(\theta_1, \theta_2) = g(\theta_1) - g(\theta_2) - \langle \nabla g(\theta_2), \theta_1 - \theta_2 \rangle$ denote the Bregman divergence of a function $g$. Based on $F_S(\theta)$ and $F_{S_t}(\theta)$, we construct a variance-reduction minibatch proximal objective $\tilde{P}_{t-1}(\theta)$ to approximate the objective $F(\theta)$ in (1), where $\tilde{P}_{t-1}(\theta) \triangleq F_{S_t}(\theta_{t-1}) + \langle \nabla F_{S_t}(\theta_{t-1}), \theta - \theta_{t-1} \rangle + D_{\theta_{t-1}}(\theta, \theta_{t-1})$.

Here $D_{\theta_{t-1}}(\theta, \theta_{t-1})$ is the Bregman divergence of a regularized loss $\tilde{F}_{S_t}(\theta) = F_{S_t}(\theta) + \frac{\gamma}{2} \|\theta - \theta_{t-1}\|_2^2$ which essentially measures the distance between $\theta_t$ and $\theta_{t-1}$ on the current geometry curve estimated on $F_{S_t}(\theta)$. We define the next iterate as

$$\theta_t = \arg\min_\theta \tilde{P}_{t-1}(\theta) = \arg\min_\theta P_{t-1}(\theta), \tag{3}$$

where $P_{t-1}(\theta) \triangleq F_S(\theta) + \langle \nabla F_S(\theta_{t-1}) - \nabla F_{S_t}(\theta_{t-1}), \theta \rangle + \frac{\gamma}{2} \|\theta - \theta_{t-1}\|_2^2$.

In $P_{t-1}$, its finite-sum structure comes from the initial stochastic approximation $F_S(\theta)$ and its gradient at $\theta_{t-1}$.

**Algorithm 1** Hybrid Stochastic-Deterministic Minibatch Proximal Gradient (HSDMPG) for quadratic loss.

| Input: | initialization $\theta_0$, regularization constant $\gamma$ in (3), optimization error $\varepsilon_t$. |
| Initialization: | Uniformly randomly sample a data batch $S$ of size $s$ to form $F_S(\theta)$ in (2). |
| for $t = 1, 2, \ldots, T$ do | |
| (S1) | Uniformly randomly sample a minibatch $S_t$ to form $F_{S_t}(\theta) = \frac{1}{|S_t|} \sum_{i \in S_t} \ell(\theta^\top x_i, y_i) + \frac{\mu}{2} \|\theta\|_2^2$ and compute $\nabla F_{S_t}(\theta_{t-1})$ to construct loss $P_{t-1}(\theta)$ in (3). |
| (S2) | Optimize the subproblem (3), e.g. via SVRG, to obtain $\theta_t$ that satisfies $\|\nabla P_{t-1}(\theta_t)\|_2 \leq \varepsilon_t$. |
| end for | |
| Output: | $\theta_T$. |

Since along with more iterations, the size of $S_t$ increases which indicates that the loss $P_{t-1}$ is a variance-reduced loss and will converge to the original loss $F(\theta)$ in problem (1). Then in step S2, we approximately solve problem (3) via a stochastic gradient optimization method such as SVRG. The principle behind this strategy is that for the initial optimization progress, inexact gradient already can well decrease the loss since the current solution is far from the optimum, while along more iterations, the current solution becomes closer to optimum, requiring more accurate gradient for further reducing the loss function. In this way, our proposed method can well balance the converge speed and the computational cost at each iteration and thus has the potential to achieve improved overall computational efficiency. Shamir et al. (2014) has proposed the DANE method which uses a similar local Bregman divergence based regularization for distributed quadratic optimization problems. Our method improves upon DANE in two aspects: 1) we use variance-reduction techniques to reduce the overall computational complexity, and 2) HSDMPG is applicable not only to quadratic problems but also to generic strongly convex problems with about the same computational complexity as discussed in Sec. 3.2.

#### 3.1.2. CONVERGENCE AND COMPLEXITY ANALYSIS

We first introduce two necessary definitions, namely strong convexity and Lipschitz smoothness, which are conventionally used in the analysis of convex optimization methods (Shamir, 2011; Johnson & Zhang, 2013).

**Definition 1** (Strong Convexity and Smoothness). A differentiable function $g(\theta)$ is said to be $\mu$-strongly-convex and $L$-smooth if $\forall \theta_1, \theta_2$, it satisfies

$$\frac{\mu}{2} \|\theta_1 - \theta_2\|_2^2 \leq D_\theta(\theta_1, \theta_2) \leq \frac{L}{2} \|\theta_1 - \theta_2\|_2^2,$$

where $D_\theta(\theta_1, \theta_2) = g(\theta_1) - g(\theta_2) - \langle \nabla g(\theta_2), \theta_1 - \theta_2 \rangle$.

For brevity, let $H$ be the Hessian matrix of the quadratic function $F(\theta)$ and $\ell_i(\theta) = \ell(\theta^\top x_i, y_i) + \frac{\mu}{2} \|\theta\|_2^2$. Denote
Algorithm 1 satisfies we only assume each loss when we use evolving size of the minibatch $S$

Theorem 1. Assume each loss $\ell(\theta^T x_i, y_i)$ is quadratic and $L$-smooth w.r.t. $\theta^T x_i$, and suppose $\theta^T \sum_{i=1}^n (H^{-1/2} (\nabla F(\theta) - \nabla \ell_i(\theta))) ||_2 \leq \nu^2$. By setting $\gamma = \sqrt{\log(d)/d}$, $\gamma_i = (\log(d)/\sqrt{d}) L/\|s_i\|_2$, and $\varepsilon_i = \mu^{\gamma} \exp\left(-\frac{\mu(t-1)}{2(\mu+2)}\right)$, the IFO complexity of HSDMPG is at the order of $O\left(\sqrt{\log d} \log \frac{1}{\delta} \right)$, where $\delta = \frac{\|\theta_0 - \theta^*\| \mu}{\mu + 2}$. The main message conveyed by Theorem 1 is that HS-DMPG enjoys linear convergence rate on the quadratic loss when we use evolving size of the minibatch $S$. Note here we only assume each loss $\ell(\theta^T x_i, y_i)$ is $L$-smooth w.r.t. $\theta^T x_i$. This assumption is much milder than the smoothness assumption on the function $F(\theta)$ w.r.t. $\theta$ which is used in other algorithm analysis, such as SGD and SVRG. The assumption that $\sup_{\theta^T x, x, y} \sum_{i=1}^n \|H^{-1/2} (\nabla F(\theta) - \nabla \ell_i(\theta))\|_2^2 \leq \nu^2$ in HS-DMPG is mild, which requires the variance of stochastic gradient under the Hessian matrix is bounded.

Based on this result, we further analyze the computational complexity of HS-DMPG to better understand its overall efficiency in computation. At each iteration, we use the SVRG method solve the inner-loop subproblem (3) because it only accesses the first-order information of the objective function and is efficient. Following Johnson & Zhang, 2015; Zhou et al., 2019; Shen et al., 2019, we employ the incremental first order oracle (IFO) complexity as the computational complexity metric for solving the finite-sum problem (1).

Definition 2. An IFO takes an index $i \in [n]$ and a point $(x, y)$, and returns the pair $(\ell_i(\theta), \nabla \ell_i(\theta))$.

The IFO complexity can accurately reflect the overall computational performance of a first-order algorithm, as objective value and gradient evaluation usually dominate the per-iteration complexity. Based on these preliminaries, we summarize our main result on the computation complexity of HSDMPG in Corollary 1 with proof provided in Appendix B.2.

Corollary 1 (Computation complexity of HSDMPG for quadratic loss). Suppose that the assumptions in Theorem 1 hold and the inner-loop subproblems are solved via SVRG, then the IFO complexity of HSDMPG on the quadratic loss to achieve $\mathbb{E}[F(\theta_t) - F(\theta^*)] \leq \epsilon$ is of the order $O\left(\left(1 + \frac{\kappa^3 \log \frac{1}{\delta}}{\nu^2} \right) \frac{1}{\epsilon} \right)$, where $\kappa = L/\mu$ denotes the conditional number.

According to Corollary 1, by choosing $s$ as $s = \frac{\nu^2}{\epsilon^2 \log(1/\epsilon)}$ and ignoring the logarithm factor $\log(1/\epsilon)$ of the problem dimension $d$, the IFO complexity of HSDMPG is at the order of $O\left(\frac{\nu}{\epsilon} \log \frac{1}{\delta} \log \frac{1}{\epsilon} \right)$.

One may compare such a complexity with the state-of-the-arts listed in Table 1. Compared with those algorithms in the table whose IFO complexity scales linearly with the data size $n$, e.g. SVRG, APCG, Katyusha and AMSVRG, the proposed HSDMPG has data-size-independent IFO complexity and can outperform them for large-scale learning problems where the data size $n$ could be huge. To be more precise, the third column of Table 1 summarizes the conditions under which HS-DMPG outperforms these algorithms in terms of computational complexity. For the algorithms whose IFO complexity does not depend on $n$, namely SGD and SCSG, HSDMPG also enjoys substantially lower complexity in most cases. Concretely, since $\kappa$ is typically at the order of $O(1/\mu)$, when $\kappa \leq \epsilon^{1.5}$ which holds for moderately larger $\kappa$, HSDMPG improves over SGD by a factor at least $O\left(\frac{1}{\epsilon} \log \frac{1}{\delta} \right)$ (up to the logarithmic factor). As for SCSG, HSDMPG also achieves higher efficiency when (1) the optimization error is small which corresponds to condition 1 in the third column of Table 1, (2) the sample size $n$ is large which corresponds to condition 2. These results show that HSDMPG is well suited for solving large-scale learning problems.

From the perspective of generalization, we are particularly interested in the computational complexity of HSDMPG for optimizing the $\ell_2$-ERM model (1) to its intrinsic excess error bound which characterizes the generalization performance of the model. As reviewed in Section 2, the excess error of the considered $\ell_2$-ERM model is typically of order $O(1/\sqrt{n})$. Accordingly, one only needs to solve the optimization problem to the optimization error $\epsilon = O(1/\sqrt{n})$ (Bottou & Bousquet, 2008; Shalev-Shwartz et al., 2009). Moreover, to accord with this intrinsic excess error bound, the regularization constant $\mu$ should also be at the order of $O(1/\sqrt{n})$. In this way, the condition number $\kappa$ could scale as large as $O(\sqrt{n})$. Based on these results and Corollary 1, we can derive the IFO complexity bound of HSDMPG for this case in Corollary 2.

Corollary 2. Suppose that the assumptions in Corol-
Algorithm 2 Hybrid Stochastic-Deterministic Minibatch Proximal Gradient (HSDMPG) on the generic loss.

**Input:** Regularization constant $\gamma$ and initialization $\theta_0$.

for $t = 1, 2, \ldots, T$ do

(S1) Construct a finite-sum quadratic function $Q_{t-1}(\theta)$ in Eqn. (4) to approximate $F(\theta)$ at $\theta_{t-1}$.

(S2) Run Algorithm 1 with regularization constant $\gamma$ and initialization $\theta_{t-1}$ to minimize the finite-sum function $Q_{t-1}(\theta)$ such that $Q_{t-1}(\theta) \leq \min_{\theta} Q_{t-1}(\theta) + \epsilon_t'$.

end for

**Output:** $\theta_T$.

$lary 1$ hold. By setting $s = \mathcal{O}\left(\frac{\nu n^{0.75} \log^5(n)}{\log(n)}\right)$, the IFO complexity of HSDMPG on the quadratic loss to achieve $\mathbb{E}[F(\theta_t) - F(\theta^*)] \leq \frac{1}{\sqrt{n}}$ is at the order of $\mathcal{O}\left(\sqrt{n} 0.875 \log^{0.75}(d) \log^{1.5}(n) + \nu^2 n^{0.5}\right)$.

See its proof in Appendix B.3. From Corollary 2, one can observe that the IFO complexity of HSDMPG for quadratic problems is at the order of $\mathcal{O}\left(n^{0.875} \log^{1.5}(n)\right)$. It means that HSDMPG can reach the intrinsic excess error $\mathcal{O}(1/\sqrt{n})$ with strictly less than a single pass over the entire training dataset. In comparison, we can observe from Table 1 that in the same practical setting, SGD and APCG have IFO complexity $\mathcal{O}(n)$ and $\mathcal{O}(n^{1.25} \log(n))$ respectively. By ignoring the logarithm factor $\log(n)$ which is much smaller than $n$ for large-scale learning problems, HSDMPG improves over these two methods by factors $\mathcal{O}(n^{0.125})$ and $\mathcal{O}(n^{0.375})$, respectively. The IFO complexity of all other algorithms in Table 1, including SVRG, SCSD, SPDC, APSPDCA, AMSVRG, Catalyst, Katyusha and Varag, are all at the order of $\mathcal{O}(n \log(n))$. Similarly, by ignoring the logarithm factors, HSDMPG has lower IFO complexity than these algorithms by a factor $\mathcal{O}(n^{0.125})$. To summarize this group of results comparison, HSDMPG would be significantly superior to all these state-of-the-arts when solving quadratic optimization problems to intrinsic excess error.

3.2. Algorithm for generic convex loss function

The computational complexity guarantees established in the previous section are only applicable to quadratic loss function. In order to extend these results to non-quadratic convex loss function, we apply a quadratic approximation strategy to convert the original non-quadratic problem into a sequence of quadratic optimization sub-problems such that each of the subproblem can be optimized by HSDMPG. More specifically, suppose that the loss function $\ell(\theta^T x, y)$ is twice differentiable w.r.t. $\theta^T x$ and is $L$-smooth w.r.t. $\theta^T x$. Then we can verify that $\nabla^2 F(\theta) = \frac{1}{n} \sum_{i=1}^n \ell''(\theta^T x_i, y_i) x_i x_i^T + \mu I \geq H = \frac{1}{n} \sum_{i=1}^n x_i x_i^T + \mu I$ for all $\theta$. Therefore, at each iteration, we construct an upper bound of the second-order Taylor expansion of $F$ at $\theta_{t-1}$ as expressed by $Q_{t-1}(\theta)$:

$$F(\theta_{t-1}) + \langle \nabla F(\theta_{t-1}), \theta - \theta_{t-1} \rangle + \Delta_{t-1}(\theta),$$

where $\Delta_{t-1}(\theta) = \frac{1}{2}(\theta - \theta_{t-1})^T H(\theta - \theta_{t-1})$. The finite-sum structure in $Q_{t-1}(\theta)$ comes from $\nabla F(\theta_{t-1}) = \frac{1}{n} \sum_{i=1}^n \nabla \ell(\theta^T x_i, y_i) + \mu \theta$ and $H$. Thus we can estimate $\theta_t$ by applying HSDMPG to the quadratic function $Q_{t-1}(\theta)$ with a warm-start initialization $\theta_{t-1}$ such that

$$Q_{t-1}(\theta_t) \leq \min_{\theta} Q_{t-1}(\theta) + \epsilon_t'.$$

The above nested-loop computation procedure is summarized in Algorithm 2. We remark that when computing the gradient of $Q_{t-1}(\theta)$, we can compute the gradient associated with $H$ at the point $\theta$ as $H(\theta - \theta_{t-1}) = \frac{1}{n} \sum_{i=1}^n (x_i^T (\theta - \theta_{t-1})) x_i + \mu (\theta - \theta_{t-1})$ which only computes the inner-product $x_i^T (\theta - \theta_{t-1})$ without explicitly computing $H$. In this way, the computational cost of each stochastic gradient associated with $H$ is actually much cheaper than that of computing stochastic gradient of $\nabla F(\theta_{t-1})$, since the former only involves vector products and the later one is usually complicated, e.g. involving the exponential computation in logistic regression. Then we establish Theorem 2 to guarantee the convergence of Algorithm 2 and analyze its computational complexity. See Appendix C.1 for a proof of this main result.

**Theorem 2** (Convergence rate and computation complexity of HSDMPG for generic loss). Suppose that each loss function $\ell(\theta^T x, y)$ is $L$-smooth and $\sigma$-strongly convex w.r.t. $\theta^T x$. By setting $\epsilon_t' = \frac{\sigma \epsilon}{2L}$, the sequence $\{\theta_t\}$ produced by Algorithm 2 satisfies

$$F(\theta_t) - F(\theta^*) \leq \exp \left( - \frac{\sigma \epsilon}{2L} \right) (1 + F(\theta_0) - F(\theta^*)) .$$

Suppose the assumptions in Corollary 1 hold. Then by setting $\kappa = \frac{\sigma}{L}$ the IFO complexity of Algorithm 2 to achieve $\mathbb{E}[F(\theta_t) - F(\theta^*)] \leq \epsilon$ is at the order of $\mathcal{O}\left(\left(\frac{1}{\kappa^3 \log^5(d)} + \frac{\log^2(\frac{1}{\sqrt{n}})}{\sigma^2} + \frac{\log^2(\frac{1}{\sigma})}{\sigma^2} \right) \left(1 + \frac{\log^{0.875}(d)}{\sigma^{0.875}(d)} \right) \frac{L^2 n}{\sigma^2} \frac{\log^2(\frac{1}{\epsilon})}{\log^3(\frac{1}{\epsilon})} \right)$.

Theorem 2 suggests that the objective $F(\theta_t)$ converges linearly to the optimum $F(\theta^*)$ with rate $\exp(-\frac{\sigma \epsilon}{2L})$. Note that $\sigma$ is the strong convexity parameter of the loss function $\ell(\theta^T x, y)$ w.r.t. $\theta^T x$ instead of $\theta$ which is usually not relying on data scale for widely used loss functions such as the logistic loss (Yuan & Li, 2019) and thus leads to fast outer-loop convergence rate. In contrast, the strong convexity parameter $\mu$ of the risk function $F$ is typically set at the order of $\mathcal{O}(1/\sqrt{n})$ so as to match the intrinsic excess error. In terms of computational complexity, by choosing the proper value of $s$ from $s = \frac{\nu n^{0.75} \log^5(n)}{\log(n)}$ and $s = \ldots$
Finally we consider a realistic case where the optimization error $\epsilon$ is very small or the condition number $\kappa$ is large which corresponds to condition (2) in Table 1, and (2) the sampler number $n$ is sufficiently large which corresponds to condition (3). These results show the advantages of HSDMPG in solving large-scale strongly-convex learning problems.

Corollary 3. Suppose the assumptions in Theorem 2 hold. By setting $s = O\left(\frac{\epsilon n^{0.75} \log^{0.5}(d)}{\log(n)}\right)$, the IFO complexity of HSDMPG on the generic loss to achieve $E[ F(\hat{\theta}_t) - F(\theta^*) ] \leq \frac{1}{\sqrt{t}}$ is of order $O\left(\nu^{0.5} n^{0.875} \log^{0.75}(d) \log^{2.25}(n) + \nu^2 n^{0.5}\right)$.

Corollary 3 shows that for generic convex loss, the IFO complexity of HSDMPG to attain the $O\left(\frac{1}{\sqrt{n}}\right)$ intrinsic excess error is of the order $O\left( n^{0.875} \log^{2.25}(n) \right)$. This shows that HSDMPG is able to achieve nearly optimal generalization with less than a single pass over data. Compared with the complexity bound for the quadratic loss, such a more general IFO complexity bound of HSDMPG only comes at the cost of a slightly increased overhead on the logarithmic factor, i.e., from $\log^{-1.25}(n)$ for the quadratic case to the $\log^{2.25}(n)$ for generic convex loss. Similar to the ob-

Figure 1: Single-epoch processing: stochastic gradient algorithms process data a single pass on quadratic problems.

Figure 2: Multi-epoch processing: stochastic gradient algorithms process data multiple pass on quadratic problems.
4. Experiments

In this section, we carry out experiments to compare the numerical performance of HSDMPG with several representative stochastic gradient optimization algorithms, including SGD (Robbins & Monro, 1951), SVRG (Johnson & Zhang, 2013), APCG (Lin et al., 2014), Katyusha (Allen-Zhu, 2017) and SCSG (Lei & Jordan, 2017). We evaluate all the considered algorithms on two sets of strongly-convex learning tasks. The first set is for ridge regression with least squared loss $\ell(\theta^\top x_i, y_i) = \frac{1}{2}\|\theta^\top x_i - y_i\|_2^2$, where $y_i$ is the target output of sample $x_i$. In the second setting we consider two classification models: logistic regression with loss $\ell(\theta^\top x_i, y_i) = \log(1 + \exp(-y_i\theta^\top x_i))$ and multi-class softmax regression with $k$-classification loss $\ell(\theta^\top x_i, y_i) = \sum_{j=1}^k 1\{y_i = j\} \log \left( \frac{\exp(\theta_j^\top x_i)}{\sum_{j=1}^k \exp(\theta_j^\top x_i)} \right)$.

We run simulations on ten datasets whose details are described in Appendix D.4. For HSDMPG, we set the size $s$ of $S$ around $n^{0.75}$. For the minibatch for inner problems, we set initial minibatch size $|S_0| = 50$ and then follow our theory to exponentially expand size of $S_t$ with proper exponential rate. The regularization constant in the sub-problem (3) is set to be $\gamma = \sqrt{\log(d)}/s$ as suggested by our theory. The optimization error $\varepsilon_t$ in (3) is controlled by respectively allowing SVRG to run 3 epochs and 10 epochs on the two sets of tasks. Similarly, we control the optimization error $\varepsilon_t^k$ in (5) by running SVRG with 3 epochs. Since there is no ground truth on real data, we run FGD sufficiently long until $\|\nabla F(\theta)\|_2 \leq 10^{-10}$ and take $F(\theta)$ as an approximate optimal value $F(\theta^*)$ for sub-optimality estimation.

4.1. Results for the quadratic loss

Single-epoch evaluation results. Here we first evaluate well-conditioned quadratic problems such that moderately accurate solution can be obtained after only one epoch of data pass. Such a one epoch setting usually occurs in online learning. Towards this goal, we set the regularization parameter $\mu = 0.01$ to make the quadratic problems well-conditioned. From Figure 1, one can observe that HSDMPG exhibits much sharper convergence behavior than the considered baselines, though most algorithms can achieve small optimization error after one epoch processing of data. This confirms the theoretical predictions in Corollaries 1 and 2 that HSDMPG is cheaper in IFO complexity than SGD and variance-reduced algorithms, e.g. SVRG and SCSG, when the data scale is large.

Multi-epoch evaluation results. For more challenging problems, an algorithm usually requires multiple cycles of data processing to achieve accurate optimization. Here we reset the regularization strength parameter in quadratic problems as $\mu = 10^{-4}$ for generating more challenging optimization tasks. As shown in Figure 2, one can again observe that HSDMPG converges faster than all the compared algorithms in terms of IFO complexity. Particularly, we compare both IFO complexity and wall-clock running time on the letter and rcv1 datasets. The convergence curves under these two metrics consistently show the superior computational efficiency of HSDMPG to the considered state-of-the-arts on large-scale learning tasks, which well support the theoretical predictions in Corollaries 1 and 2.

4.2. Results for the non-quadratic loss

Finally, we investigate the convergence performance of the proposed HSDMPG on non-quadratic convex loss functions. Specifically, we evaluate all the compared algorithms on logistic regression and its multi-classes version, i.e. softmax regression, in which their regularization modulus parameters are set as $\mu = 0.01$. Figure 3 reports the running time evolving curves which can accurately reflects the efficiency of an algorithm. These results show that HSDMPG converges significantly faster than the baseline.
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for the considered non-quadratic loss functions, which well support the predictions in Theorem 2 and Corollary 3 that HSDMPG has lower IFO complexity than the state-of-the-arts in the regimes where data scale is large. This set of results also demonstrates the effectiveness of our sequential quadratic-approximation approach for extending the attractive computational complexity guarantees on quadratic loss to generic convex loss.

5. Conclusions

We proposed HSDMPG as a hybrid stochastic-deterministic minibatch proximal gradient method for $\ell_2$-regularized ERM problems. For quadratic loss, we showed that HSDMPG enjoys provably lower computational complexity than prior state-of-the-art SVRG algorithms in large-scale settings. Particularly, to attain the optimization error $\epsilon = O(1/\sqrt{n})$ at the order of intrinsic excess error bound of ERM which is sufficient for generalization, the stochastic gradient complexity of HSDMPG is dominated by $O(n^{0.875})$ (up to logarithmic factors). To our best knowledge, HSDMPG for the first time achieves nearly optimal generalization in less than a single pass over data. Almost identical computational complexity guarantees hold for an extension of HSDMPG to generic strongly convex loss functions via sequential quadratic approximation. Extensive numerical results demonstrate the substantially improved computational efficiency of HSDMPG over the prior methods. We expect that the algorithms and computational learning theory developed in this paper for $\ell_2$-regularized ERM can be extended to stochastic convex optimization problems. Also, it is worthwhile to explore the opportunity of using first-order acceleration techniques to further improve the computational complexity guarantees of HSDMPG.

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