Stochastic Gauss-Newton Algorithms for Nonconvex Compositional Optimization

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Abstract

We develop two new stochastic Gauss-Newton algorithms for solving a class of non-convex stochastic compositional optimization problems frequently arising in practice. We consider both the expectation and finite-sum settings under standard assumptions, and use both classical stochastic and SARAH estimators for approximating function values and Jacobians. In the expectation case, we establish $O(\varepsilon^{-2})$ iteration-complexity to achieve a stationary point in expectation and estimate the total number of stochastic oracle calls for both function value and its Jacobian, where $\varepsilon$ is a desired accuracy. In the finite sum case, we also estimate $O(\varepsilon^{-2})$ iteration-complexity and the total oracle calls with high probability. To our best knowledge, this is the first time such global stochastic oracle complexity is established for stochastic Gauss-Newton methods. Finally, we illustrate our theoretical results via two numerical examples on both synthetic and real datasets.

1. Introduction

We consider the following nonconvex stochastic compositional nonconvex optimization problem:

$$
\min_{x \in \mathbb{R}^p} \left\{ \Psi(x) := \phi(F(x)) \equiv \mathbb{E}_\xi [F(x, \xi)] \right\}, \quad (1)
$$

where $F : \mathbb{R}^p \times \Omega \to \mathbb{R}^q$ is a stochastic function defined on a probability space $(\Omega, \mathbb{P})$, $\phi : \mathbb{R}^q \to \mathbb{R} \cup \{+\infty\}$ is a proper, closed, and convex, but not necessarily smooth function, and $F$ is the expectation of $F$ w.r.t. to $\xi$.

As a special case, if $\Omega$ is finite, i.e. $\Omega := \{\xi_1, \ldots, \xi_n\}$ and $\mathbb{P}(\xi = \xi_i) = p_i > 0$ for $i \in [n] := \{1, \ldots, n\}$ and $\sum_{i=1}^n p_i = 1$, then by introducing $F_i(x) := n p_i F(x, \xi_i)$, $F(x)$ can be written into a finite-sum $F(x) := \frac{1}{n} \sum_{i=1}^n F_i(x)$, and (1) reduces to

$$
\min_{x \in \mathbb{R}^p} \left\{ \Psi(x) := \phi(F(x)) \equiv \phi\left(\frac{1}{n} \sum_{i=1}^n F_i(x)\right) \right\}, \quad (2)
$$

This expression can also be viewed as a stochastic average approximation of $F(x) := \mathbb{E}_\xi [F(x, \xi)]$ in (1). Note that the setting (1) is completely different from the setting (2) in Davis & Grimmer (2019); Davis & Drusvyatskiy (2019); Duchi & Ruan (2018).

Problem (1) or its special form (2) covers various applications in different domains (both deterministic and stochastic) such as penalized problems for constrained optimization, parameter estimation, nonlinear least-squares, system identification, statistical learning, dynamic programming, and minimax problems (Drusvyatskiy & Paquette, 2019; Duchi & Ruan, 2018; Lewis & Wright, 2016; Nesterov, 2007; Tran-Dinh & Diehl, 2011; Wang et al., 2017a). Note that both (1) and (2) cover the composite form

$$
\min_{x \in \mathbb{R}^p} \left\{ \Psi(x) := \phi(F(x)) + g(x) \right\}, \quad (3)
$$

for a given convex function $g$ if we introduce $\hat{\phi}(\cdot) := \phi(\cdot) + g(\cdot)$ and $\hat{F}(x) := [F(x); x]$ to reformulate it into (1) or (2). This formulation, on the other hand, is an extension of (1). We will also show how to handle (3) in Subsection 4.3.

Our goal in this paper is to develop novel stochastic methods to solve (1) and (2) based on the following assumptions:

Assumption 1.1. The function $\Psi$ of (1) is bounded from below on its domain, i.e. $\Psi^* := \inf_x \Psi(x) > -\infty$. The function $\phi$ is $M_\phi$-Lipschitz continuous, and $F$ is $L_F$-average smooth, i.e., there exist $M_\phi, L_F \in (0, +\infty)$ such that

$$
\begin{align*}
|\phi(u) - \phi(v)| &\leq M_\phi \|u - v\|, \quad \forall u, v \in \mathbb{R}^q, \\
\mathbb{E}_\xi [\|F'(x, \xi) - F'(y, \xi)\|^2] &\leq L_F^2 \|x - y\|^2, \quad \forall x, y.
\end{align*}
$$

(4)

For the finite-sum case (2), we impose a stronger assumption that $\|F_i(x) - F_i(y)\| \leq L_F \|x - y\|$ for all $x, y \in \mathbb{R}^p$ and all $i \in [n]$. Here, we use spectral norm for Jacobian.
Assumption 1.2. There exist $\sigma_F, \sigma_D \in [0, +\infty)$ such that the variance of $F$ and $F'$ is uniformly bounded, i.e., $\mathbb{E}_\xi [||F(x, \xi) - F(x)||^2] \leq \sigma_F^2$ and $\mathbb{E}_\xi [||F'(x, \xi) - F'(x)||^2] \leq \sigma_D^2$, respectively. In the finite sum case (2), we again impose stronger conditions $||F_i(x) - F(x)|| \leq \sigma_F$ and $||F'_i(x) - F'(x)|| \leq \sigma_D$ for all $x \in \mathbb{R}^p$ and for all $i \in [n]$.

Assumptions 1.1 and 1.2 are standard and cover a wide class of models in practice as opposed to existing works. The stronger assumptions imposed on (2) allow us to develop adaptive subsampling schemes later.

Related work. Problem (1) or (2) has been widely studied in the literature under both deterministic (including the finite-sum (2) and $n = 1$) and stochastic settings, see, e.g., (Drusvyatskiy & Paquette, 2019; Duchi & Ruan, 2018; Lewis & Wright, 2016; Nesterov, 2007; Tran-Dinh & Diehl, 2011; Wang et al., 2017a). If $q = 1$ and $\phi(u) = u$, then (1) reduces to the standard stochastic optimization model studied in, e.g., Ghadimi & Lan (2016); Pham et al. (2020).

In the deterministic setting, the common method to solve (1) is the Gauss-Newton (GN) scheme, which is also known as the prox-linear method. This method has been studied in several papers, including Drusvyatskiy & Paquette (2019); Duchi & Ruan (2018); Lewis & Wright (2016); Nesterov (2007); Tran-Dinh & Diehl (2011). In such settings, GN only requires Assumption 1.1 to have global convergence guarantees (Drusvyatskiy & Paquette, 2019; Nesterov, 2007).

In the stochastic setting of the form (1), Wang et al. (2017a;b) proposed stochastic compositional gradient descent methods to solve more general forms than (1), but they required a set of stronger assumptions than Assumptions 1.1 and 1.2, including the smoothness of $\phi$. These methods eventually belong to a gradient-based class. Other works in this direction include Lian et al. (2017); Yu & Huang (2017); Yang et al. (2019); Liu et al. (2017); Xu & Xu (2019), which also rely on a similar approach. Together with algorithms, convergence guarantees and stochastic oracle complexity bounds have also been estimated. For instance, Wang et al. (2017a) estimates $\mathcal{O}(\varepsilon^{-8})$ oracle complexity for solving (1), while it is improved to $\mathcal{O}(\varepsilon^{-4.5})$ in Wang et al. (2017b). Recent works such as Zhang & Xiao (2019a) further improve the complexity to $\mathcal{O}(\varepsilon^{-3})$. However, these methods are completely different from GN and require much stronger assumptions, including the smoothness of $\phi$ and $F$.

One main challenge to design algorithms for solving (1) is the bias of stochastic estimators. Some researchers have tried to remedy this issue by proposing more sophisticated sampling schemes, see, e.g., Blanchet et al. (2017). Other works relies on biased estimators but using variance reduction techniques, e.g., Zhang & Xiao (2019a).

Challenges. The stochastic formulation (1) creates several challenges for developing numerical methods. First, it is often nonconvex. Many papers consider special cases when $\Psi$ is convex. This only holds if $\phi$ is convex and $F$ is linear, or $\phi$ is convex and monotone and $F$ is convex or concave. Clearly, such a setting is almost unrealistic or very limited. One can assume weak convexity of $\Psi$ and add a regularizer to make the resulting problem convex but this completely changes the model. Second, $\phi$ is often non-smooth such as norm, penalty, or gauge functions. This prevents the use of gradient-based methods. Third, even when both $\phi$ and $F$ are smooth, to guarantee Lipschitz continuity of $\nabla \Psi$, it requires simultaneously $F$, $F'$, $\phi$, and $\nabla \phi$ to be Lipschitz continuous. This condition is very restrictive and often requires additional bounded constraints or bounded domain assumption. Otherwise, it fails to hold even for bilinear functions. Finally, in stochastic settings, it is very challenging to form unbiased estimate for gradients or subgradients of $\Psi$, making classical stochastic-based method inapplicable.

Our approach and contribution. Our main motivation is to overcome the above challenges by following a different approach.\(^1\) We extend the GN method from the deterministic setting (Lewis & Wright, 2016; Nesterov, 2007) to the stochastic setting (1). Our methods can be viewed as inexact variants of GN using stochastic estimators for both function values $F(x)$ and its Jacobian $F'(x)$. This approach allows us to cover a wide class of (1), while only requires standard assumptions as Assumptions 1.1 and 1.2. Our contribution can be summarized as follows:

(a) We develop an inexact GN framework to solve (1) and (2) using inexact estimations of $F$ and its Jacobian $F'$. This framework is independent of approximation schemes for generating approximate estimators. We characterize approximate stationary points of (1) and (2) via prox-linear gradient mappings. Then, we prove global convergence guarantee of our method to a stationary point under appropriate inexact computation.

(b) We analyze stochastic oracle complexity of our GN algorithm when mini-batch stochastic estimators are used. We separate our analysis into two cases. The first variant is to solve (1), where we obtain convergence guarantee in expectation. The second variant is to solve (2), where we use adaptive mini-batches and obtain convergence guarantee with high probability.

(c) We also provide oracle complexity of this algorithm when mini-batch SARAH estimators in Nguyen et al. (2017; 2019) are used for both (1) and (2). Under an additional mild assumption, this estimator significantly improves the oracle complexity by an order of $\varepsilon$ compared to the mini-batch stochastic one.

\(^1\)When this paper was under review, Zhang & Xiao (2020) was brought to our attention, which presents similar methods.
for solving (1) and (2) under standard assumptions. It is completely different from existing works such as Wang et al. (2017a; b); Lian et al. (2017); Yu & Huang (2017); Yang et al. (2019); Zhang & Xiao (2019a), where we only use Assumptions 1.1 and 1.2, while not imposing any special structure on Φ and F, including smoothness. When using SARAH estimators, we impose the Lipschitz continuity of F to achieve better oracle complexity. This additional assumption is still much weaker than the ones used in existing works. However, without this assumption, our GN scheme with SARAH estimators still converges (see Remark 4.1).

**Content.** Section 2 recalls some mathematical tools. Section 3 develops an inexact GN framework. Sections 4 analyzes convergence and complexity of the two stochastic GN variants using different stochastic estimators. Numerical examples are given in Section 5. All the proofs and discussion are deferred to Supplementary Document (Supp. Doc.).

## 2. Background and Mathematical Tools

We first characterize the optimality condition of (1). Next, we recall the prox-linear mapping of the compositional function \( \Phi(x) := \phi(F(x)) \) and its properties.

**Basic notation.** We work with Euclidean spaces \( \mathbb{R}^p \) and \( \mathbb{R}^q \). Given a convex set \( \mathcal{A} \), \( \text{dist}(u, \mathcal{A}) := \inf_{x \in \mathcal{A}} \|u - x\| \) denotes the Euclidean distance from \( u \) to \( \mathcal{A} \). For a convex function \( f \), we denote \( \partial f \) its subdifferential, \( \nabla f \) its gradient, and \( f^\ast \) its Fenchel conjugate. For a smooth function \( F : \mathbb{R}^p \to \mathbb{R}^q \), \( F^\ast(\cdot) \) denotes its Jacobian. For vectors, we use Euclidean norms, while for matrices, we use spectral norms, i.e., \( \|X\| := \sigma_{\text{max}}(X) \). \( \lfloor \cdot \rfloor \) stands for number rounding.

### 2.1. Exact and Approximate Stationary Points

The optimality condition of (1) can be written as

\[
0 \in \partial \Phi(x^\ast) \equiv F^\ast(x^\ast)^\top \partial \phi(F(x^\ast)),
\]

or equivalently

\[
\text{dist}(0, \partial \Phi(x^\ast)) = 0. \tag{5}
\]

Any \( x^\ast \) satisfying (5) is called a stationary point of (1) or (2). Since \( \phi \) is convex, let \( \phi^\ast \) be its Fenchel conjugate and \( y^\ast \in \partial \phi(F(x^\ast)) \). Then, (5) can be rewritten as

\[
0 = F^\ast(x^\ast)^\top y^\ast \quad \text{and} \quad 0 \in -F(x^\ast) + \partial \phi^\ast(y^\ast). \tag{6}
\]

Now, if we define

\[
\mathcal{E}(x, y) := \|F^\ast(x)^\top y\| + \text{dist}(0, -F(x) + \partial \phi^\ast(y)), \tag{7}
\]

then the optimality condition (5) of (1) or (2) becomes

\[
\mathcal{E}(x^\ast, y^\ast) = 0. \tag{8}
\]

Note that once a stationary point \( x^\ast \) is available, we can compute \( y^\ast \) as any element \( y^\ast \in \partial \phi(F(x^\ast)) \) of \( \phi \circ F \).

In practice, we can only find an approximate stationary point \( \hat{x} \) and its dual \( \hat{y} \) such that \( (\hat{x}, \hat{y}) \) approximates \( (x^\ast, y^\ast) \) of (1) or (2) up to a given accuracy \( \varepsilon \geq 0 \) as follows:

**Definition 2.1.** Given \( \varepsilon > 0 \), we call \( \hat{x} \in \mathbb{R}^p \) an \( \varepsilon \)-stationary point of (1) if there exists \( \hat{y} \in \mathbb{R}^q \) such that

\[
\mathcal{E}(\hat{x}, \hat{y}) \leq \varepsilon, \tag{9}
\]

where \( \mathcal{E}(\cdot) \) is defined by (7). This condition can be characterized in expectation, where \( \mathbb{E}[\cdot] \) is taken over all the randomness generated by the problem and the corresponding stochastic algorithm, or with high probability \( 1 - \delta \). Such guarantees will be specified in the sequel.

### 2.2. Prox-Linear Operator and Its Properties

(a) **Prox-linear operator.** Since we assume that the Jacobian \( F^\ast(\cdot) \) of \( F \) is Lipschitz continuous with a Lipschitz constant \( L_F \in (0, +\infty) \), and \( \phi \) is \( M_\phi \)-Lipschitz continuous as in Assumption 1.1, we have (see Supp. Doc. A):

\[
\phi(F(z)) \leq \phi(F(x) + F^\ast(x)(z - x)) + \frac{M_\phi L_F}{2} \|z - x\|^2, \tag{10}
\]

for all \( z, x \in \mathbb{R}^p \). Given \( x \in \mathbb{R}^p \), let \( \bar{F}(x) \approx F(x) \) and \( \bar{J}(x) \approx F^\ast(x) \) be a deterministic or stochastic approximation of \( F(x) \) and its Jacobian \( F^\ast(x) \), respectively. We consider the following approximate prox-linear model:

\[
\bar{T}_M(x) := \arg\min_{z \in \mathbb{R}^p} \left\{ \bar{Q}_M(z; x) := \phi(\bar{F}(x) + \bar{J}(z)(z - x)) + \frac{M}{2} \|z - x\|^2 \right\}, \tag{11}
\]

where \( M > 0 \) is a given constant. As usual, if \( \bar{F}(x) = F(x) \) and \( \bar{J}(x) = F^\ast(x) \), then

\[
T_M(x) := \arg\min_{z \in \mathbb{R}^p} \left\{ Q_M(z; x) := \phi(F(x) + F^\ast(x)(z - x)) + \frac{M}{2} \|z - x\|^2 \right\} \tag{12}
\]

is the exact prox-linear operator of \( \Psi \). In this context, we also call \( \bar{T}_M(\cdot) \) an approximate prox-linear operator of \( \Psi \).

(b) **Prox-gradient mapping.** We also define the prox-gradient mapping and its approximation, respectively as

\[
\begin{aligned}
G_M(x) & := M(x - T_M(x)), \\
\bar{G}_M(x) & := M(x - \bar{T}_M(x)).
\end{aligned} \tag{13}
\]

Clearly if \( \|G_M(x)\| = 0 \), then \( x = T_M(x) \) and \( x \) is a stationary point of (1). In our context, we can only compute \( G_M(x) \) as an approximation of \( G_M(x) \).

(c) **Characterizing approximate stationary points.** The following lemma bounds the optimality error \( \mathcal{E}(\cdot) \) defined by (7) via the approximate prox-gradient mapping \( G_M(x) \).
Lemma 2.1. Let \( \tilde{T}_M(x) \) be computed by (11) and \( \tilde{G}_M(x) \) be defined by (13). Then, \( \mathcal{E}(\tilde{T}_M(x), y) \) of (1) defined by (7) with \( y \in \partial \phi(F(\tilde{T}_M(x))) \) is bounded by
\[
\mathcal{E}(\tilde{T}_M(x), y) \leq \left(1 + \frac{M \lambda_F}{M} \right) \| \tilde{G}_M(x) \| + \frac{(1 + L_F)}{2M^2} \| \tilde{G}_M(x) \|^2 \\
+ \| \bar{F}(x) - F(x) \| + \frac{1}{2} \| J(x) - F'(x) \|^2.
\] (14)

Clearly, if we use exact oracles \( \bar{F}(x) = F(x) \) and \( \bar{J}(x) = F'(x) \), then \( \mathcal{E}(\tilde{T}_M(x), y) \) is reduced to
\[
\mathcal{E}(T_M(x), y) \leq \left(1 + \frac{M \lambda_F}{M} \right) \| G_M(x) \| + \frac{(1 + L_F)}{2M^2} \| G_M(x) \|^2.
\]

Alternatively, from (14), if we can guarantee \( \| \bar{F}(x) - F(x) \| \leq O(\varepsilon) \), \( \| \bar{J}(x) - F'(x) \| \leq O(\sqrt{\varepsilon}) \), and \( \| \tilde{G}_M(x) \| \leq O(\varepsilon) \), then
\[
\mathcal{E}(\tilde{T}_M(x), y) \leq O(\varepsilon),
\]
which shows that \( \tilde{T}_M(x) \) is an \( O(\varepsilon) \)-stationary point of (1) in the sense of Definition 2.1. Our goal is to approximate \( F \) and \( F' \) and compute \( \tilde{G}_M(x) \) to guarantee these conditions.

3. Inexact Gauss-Newton Framework

In this section, we develop a conceptual inexact Gauss-Newton (iGN) framework for solving (1) and (2).

3.1. Descent Property and Approximate Conditions

Lemma 3.1 provides a key bound regarding (11), which will be used for convergence analysis of our algorithms.

Lemma 3.1. Let Assumption 1.1 hold and \( \tilde{T}_M(x) \) be computed by (11). Then, for any \( \beta_d > 0 \), we also have
\[
\phi(F(\tilde{T}_M(x))) \leq \phi(F(x)) + 2L_\phi \| F(x) - \bar{F}(x) \| \\
+ \frac{M \lambda_F}{2M^2} \| F'(x) - \bar{J}(x) \|_F^2 \\
\leq \frac{(2M - M_\phi L_F - \beta_d L_o)}{2} \| \tilde{T}_M(x) - x \|^2.
\] (15)

Since we approximate both \( F \) and its Jacobian \( F' \) in our prox-linear model (11), we assume that this approximation satisfies one of the following two conditions:

- **Condition 1:** Given a tolerance \( \varepsilon > 0 \) and \( M > \frac{1}{2} M_\phi (L_F + \beta_d) \), at each iterate \( x_t \in \mathbb{R}^p \), it holds that
\[
\begin{align*}
\| \bar{F}(x_t) - F(x_t) \| &\leq \frac{C_{\varepsilon}^2}{16M^2M^2}, \\
\| \bar{J}(x_t) - F'(x_t) \| &\leq \frac{\sqrt{\beta_d C_{\varepsilon}}}{M^{3/2}M^2}.
\end{align*}
\] (16)

where \( C_{\varepsilon} := 2M - M_\phi (L_F + \beta_d) > 0 \).

- **Condition 2:** Given \( C_f > 0 \), \( C_d > 0 \), and \( \beta_d > 0 \), let \( C_a := 2M - M_\phi (L_F + \beta_d) \) and \( C_a := 2M - M_\phi (L_F + \beta_d) + 2\sqrt{C_f + \frac{1}{M \beta_d}} \) such that \( C_a > 0 \). For any \( x_0 \in \mathbb{R}^p \), we assume that
\[
\begin{align*}
\| \bar{F}(x_0) - F(x_0) \| &\leq \frac{C_f^2}{16M^2}, \\
\| \bar{J}(x_0) - F'(x_0) \| &\leq \frac{\sqrt{M \beta_d C_{\varepsilon}}}{M^{3/2}}.
\end{align*}
\] (17)

while, for any iterate \( x_t \in \mathbb{R}^p \) \((t \geq 1)\), we assume that
\[
\begin{align*}
\| \bar{F}(x_t) - F(x_t) \| &\leq \sqrt{C_f} \| x_t - x_{t-1} \|^2, \\
\| \bar{J}(x_t) - F'(x_t) \| &\leq \sqrt{C_d} \| x_t - x_{t-1} \|^2.
\end{align*}
\] (18)

The condition (16) assumes that both \( \bar{F} \) and \( \bar{J} \) should respectively well approximate \( F \) and \( F' \) up to a given accuracy \( \varepsilon \). Here, the function value \( F \) must have higher accuracy than its Jacobian \( F' \). The condition (18) is adaptive, which depends on the norm \( \| x_t - x_{t-1} \| \) of the iterates \( x_t \) and \( x_{t-1} \). This condition is less conservative than (16).

3.2. The Inexact Gauss-Newton Algorithm

We first present a conceptual stochastic Gauss-Newton method as described in Algorithm 1.

Algorithm 1 (Inexact Gauss-Newton (iGN))

1: **Initialization:** Choose \( x_0 \in \mathbb{R}^p \) and \( M > 0 \).
2: **For** \( t := 0, \ldots, T \) **do**
3: \hspace{1em} Form \( \bar{F}(x_t) \) and \( \bar{J}(x_t) \) satisfying either (16) or (18).
4: \hspace{1em} Update \( x_{t+1} := \tilde{T}_M(x_t) \) based on (11).
5: **End For**

Algorithm 1 remains conceptual since we have not specified how to form \( \bar{F}(x_t) \) and \( \bar{J}(x_t) \).

3.3. Convergence Analysis

Let us first state the convergence of Algorithm 1 under **Condition 1 or Condition 2** in the following theorem.

**Theorem 3.1.** Assume that Assumptions 1.1 and 1.2 are satisfied. Let \( \{x_t\} \) be generated by Algorithm 1 to solve either (1) or (2). Then, the following statements hold:

(a) If (16) holds for some \( \varepsilon \geq 0 \), then
\[
\frac{1}{T+1} \sum_{t=0}^{T} \| \tilde{G}_M(x_t) \|^2 \leq \frac{2M^2 [\Psi(x_0) - \Psi^*]}{C_g(T+1)} + \frac{\varepsilon^2}{2},
\] (19)

where \( C_g := 2M - M_\phi (L_F + \beta_d) \) with \( M > \frac{1}{2} M_\phi (L_F + \beta_d) \).

(b) If (17) and (18) hold for given \( C_a > 0 \), then
\[
\frac{1}{T+1} \sum_{t=0}^{T} \| \tilde{G}_M(x_t) \|^2 \leq \frac{2M^2 [\Psi(x_0) - \Psi^*]}{C_a(T+1)} + \frac{\varepsilon^2}{2}.
\] (20)
Consequently, the total number of iterations $T$ to achieve \( \frac{1}{(T+1)} \sum_{t=0}^{T} \| \tilde{G}_t(x_t) \|^2 \leq \varepsilon^2 \) is at most
\[
T := \left[ \frac{4M^2 \| \Psi(x_0) - \Psi^* \|}{D \varepsilon^2} \right] = O \left( \frac{1}{\varepsilon^2} \right),
\]
where $D := C_g$ for (a) and $D := C_a$ for (b).

**Remark 3.1.** The guarantee \( \frac{1}{(T+1)} \sum_{t=0}^{T} \| \tilde{G}_t(x_t) \|^2 \leq \varepsilon^2 \) implies that \( \lim \inf_{t \to \infty} \| \tilde{G}_t(x_t) \| = 0 \). That is there exists subsequence $x_{t_k}$ of $\{x_t\}$ such that $\| \tilde{G}_t(x_{t_k}) \| \to 0$ as $k \to \infty$ and $\varepsilon \to 0$.

## 4. Stochastic Gauss-Newton Methods

### 4.1. SGN with Mini-Batch Stochastic Estimators

As a natural instance of Algorithm 1, we propose to approximate $F(x_t)$ and $F'(x_t)$ in Algorithm 1 by mini-batch stochastic estimators as:
\[
\begin{align*}
\tilde{F}(x_t) & := \frac{1}{b_t} \sum_{\xi_t \in \mathcal{B}_t} F(x_t, \xi_t), \\
\tilde{J}(x_t) & := \frac{1}{b_t} \sum_{\xi_t \in \mathcal{B}_t} F'(x_t, \xi_t),
\end{align*}
\]
(21)
where the mini-batches $\mathcal{B}_t$ and $\tilde{\mathcal{B}}_t$ are not necessarily independent, $b_t := |\mathcal{B}_t|$, and $\tilde{b}_t := |\tilde{\mathcal{B}}_t|$. Using (21) we prove our first result in expectation on stochastic oracle complexity of Algorithm 1 for solving (1).

In practice, we may not need to explicitly form $\tilde{J}(x_t)$, but its matrix-vector product $\tilde{J}(x_t)d$ for some vector $d$, when evaluating the prox-linear operator $\tilde{T}_M(x_t)$. This requires $F'(x_t, \xi_t)d$, which can be evaluated efficiently by using, e.g., automatic differentiation techniques.

**Theorem 4.1.** Suppose that Assumptions 1.1 and 1.2 hold for (1). Let $F_t$ and $J_t$ defined by (21) be mini-batch stochastic estimators of $F(x_t)$ and $F'(x_t)$, respectively. Let $\{x_t\}$ be generated by Algorithm 1 (called SGN) to solve (1). Assume that $b_t$ and $\tilde{b}_t$ in (21) are chosen as
\[
\begin{align*}
b_t & := \frac{256 M_d^2 \sigma_d^2}{C_g^2 \varepsilon^2} = O \left( \frac{\sigma_d^2}{\varepsilon^2} \right), \\
\tilde{b}_t & := \frac{2 M_d \sigma_d^2}{\beta_d C_a \varepsilon^2} = O \left( \frac{\sigma_d^2}{\varepsilon^2} \right),
\end{align*}
\]
(22)
for some constant $C_f > 0$ and $C_d > 0$. Furthermore, let $\tilde{x}_T$ be chosen uniformly at random in $\{x_t\}_{t=0}^{T}$ as the output of Algorithm 1 after $T$ iterations. Then
\[
\mathbb{E} \left[ \| \tilde{G}_M(\tilde{x}_T) \|^2 \right] \leq \frac{2M^2 \| \Psi(x_0) - \Psi^* \|}{C_g(T+1)} + \varepsilon^2, 
\]
(23)
where $C_g := 2M - M_\phi(L_F + \beta_d) > 0$.

Moreover, the number $T_f$ of function evaluations $F(x_t, \xi)$ and the number $T_d$ of Jacobian evaluations $F'(x_t, \xi)$ to achieve $\mathbb{E} \left[ \| \tilde{G}_M(\tilde{x}_T) \|^2 \right] \leq \varepsilon^2$ do not exceed
\[
\begin{align*}
T_f & := \left[ \frac{1024 M^6 \sigma_d^2 F \| \Psi(x_0) - \Psi^* \|}{C_g^2 \varepsilon^2} \right] = O \left( \frac{\varepsilon^2}{\varepsilon^2} \right), \\
T_d & := \left[ \frac{8M_d \sigma_d^2 \| \Psi(x_0) - \Psi^* \|}{\beta_d C_g \varepsilon^2} \right] = O \left( \frac{\varepsilon^2}{\varepsilon^2} \right).
\end{align*}
\]
(24)

Note that if we replace $b_t$ and $\tilde{b}_t$ in (22) by $\min \{b_t, \tilde{b}_t\}$, respectively, then the result of Theorem 4.1 still holds for (2) since it is a special case of (1).

Now, we derive the convergence result of Algorithm 1 for solving (2) using adaptive mini-batches. However, our convergence guarantee is obtained with high probability.

**Theorem 4.2.** Suppose that Assumptions 1.1 and 1.2 hold for (2). Let $F_t$ and $J_t$ defined by (21) be mini-batch stochastic estimators to approximate $F(x_t)$ and $\tilde{F}(x_t)$, respectively. Let $\{x_t\}$ be generated by Algorithm 1 for solving (2). Assume that $b_t$ and $\tilde{b}_t$ in (21) are chosen such that $b_t := \min \{n_t, \tilde{b}_t\}$ and $\tilde{b}_t := \min \{n_t, \tilde{b}_t\}$ for $t \geq 0$, with
\[
\begin{align*}
\tilde{b}_0 & := \left[ \frac{32M_d M^2 \sigma_d^2 \| \Psi(x_0) - \Psi^* \|}{4 C_g \varepsilon^2} \right], \\
\tilde{b}_t & := \left[ \frac{4M \sqrt{2M_d \sigma_D (3M \sqrt{2M_e \sigma_D + 3\sqrt{2}} \varepsilon)} \cdot \log \left( \frac{p+1}{\delta} \right)}{\beta_d C_g \varepsilon^2} \right], \\
\tilde{b}_t & := \left[ \frac{4M \sqrt{2M_d \sigma_D (3M \sqrt{2M_e \sigma_D + 3\sqrt{2}} \varepsilon)} \cdot \log \left( \frac{p+1}{\delta} \right)}{\beta_d C_g \varepsilon^2} \right], \\
\tilde{b}_t & := \left[ \frac{4M \sqrt{2M_d \sigma_D (3M \sqrt{2M_e \sigma_D + 3\sqrt{2}} \varepsilon)} \cdot \log \left( \frac{p+1}{\delta} \right)}{\beta_d C_g \varepsilon^2} \right],
\end{align*}
\]
(25)
for $\delta \in (0, 1)$, and $C_f$, $C_d$, and $C_\alpha$ given in Condition 2. Then, with probability at least $1 - \delta$, the bound (20) in Theorem 3.1 still holds.

Moreover, the total number $T_f$ of stochastic function evaluations $F(x_t, \xi)$ and the total number $T_d$ of stochastic Jacobian evaluations $F'(x_t, \xi)$ to guarantee $\mathbb{E} \left[ \| \tilde{G}_M(\tilde{x}_T) \|^2 \right] \leq \varepsilon^2$ do not exceed
\[
\begin{align*}
T_f & := O \left( \frac{\varepsilon^2}{\varepsilon^2} \right), \\
T_d & := O \left( \frac{\varepsilon^2}{\varepsilon^2} \right).
\end{align*}
\]
(26)

To the best of our knowledge, the oracle complexity bounds stated in Theorems 4.1 and 4.2 are the first results for the stochastic Gauss-Newton methods described in Algorithm 1 under Assumptions 1.1 and 1.2. Whereas there exist several methods for solving (1), these algorithms are either not in the form of GN schemes as ours or rely on a different set of assumptions. For instance, Duchi & Ruan (2018); Duchi et al. (2011) considers a different model and uses stochastic subgradient methods, while Zhang & Xiao (2019a;b) directly applies a variance reduction gradient descent method and requires a stronger set of assumptions.
4.2. SGN with SARAH Estimators

Algorithm 1 with mini-batch stochastic estimators (21) has high oracle complexity bounds when \( \varepsilon > 0 \) is sufficiently small, especially for function evaluations \( \mathbf{F}(\xi, \xi) \). We attempt to reduce this complexity by exploiting a biased estimator called SARAH in Nguyen et al. (2017) in this subsection.

More concretely, we approximate \( \mathbf{F}(\mathbf{x}_t) \) and \( \mathbf{F}'(\mathbf{x}_t) \) by using the following SARAH estimators, respectively:

\[
\begin{align*}
\tilde{F}_t := & \tilde{F}_{t-1} + \frac{1}{b_t} \sum_{i \in \mathcal{B}_t} (\mathbf{F}(\mathbf{x}_t, \xi_j) - \mathbf{F}(\mathbf{x}_{t-1}, \xi_j)), \\
\tilde{J}_t := & \tilde{J}_{t-1} + \frac{1}{b_t} \sum_{i \in \mathcal{B}_t} (\mathbf{F}'(\mathbf{x}_t, \xi_j) - \mathbf{F}'(\mathbf{x}_{t-1}, \xi_j)),
\end{align*}
\]

where the snapshots \( \tilde{F}_0 \) and \( \tilde{J}_0 \) are given, and \( \mathcal{B}_t \) and \( \tilde{\mathcal{B}}_t \) are two mini-batches of size \( b_t := |\mathcal{B}_t| \) and \( \tilde{b}_t := |\tilde{\mathcal{B}}_t| \).

Using both the standard stochastic estimators (21) and these SARAH estimators (27), we modify Algorithm 1 to obtain the following double-loop variant as in Algorithm 2.

**Algorithm 2** (SGN with SARAH estimators (SNG2))

1. **Initialization:** Choose \( x^0 \in \mathbb{R}^p \) and \( M > 0 \).
2. For \( s = 1, \ldots, S \) do
3. Generate mini-batches \( \mathcal{B}_s \) (size \( b_s \)) and \( \tilde{\mathcal{B}}_s \) (size \( \tilde{b}_s \)).
4. Evaluate \( F_0(s) \) and \( J_0(s) \) at \( x_0(s) := x^s - 1 \) from (21).
5. Update \( x_1(s) := \tilde{T}_M(x_0(s)) \) based on (11).
6. **Inner Loop:** For \( t = 1, \ldots, m \) do
7. Generate mini-batches \( \mathcal{B}_t(s) \) and \( \tilde{\mathcal{B}}_t(s) \).
8. Evaluate \( F_t(s) \) and \( J_t(s) \) from (27).
9. Update \( x_t(s) := \tilde{T}_M(x_t(s)) \) based on (11).
10. **End of Inner Loop**
11. Set \( x^s := x_{m+1} \).
12. **End For**

In Algorithm 2, every outer iteration \( s \), we take a snapshot \( \mathbf{x}^s \) using (21). Then, we run Algorithm 2 up to \( m \) iterations in the inner loop \( t \) but using SARAH estimators (27). Unlike (21), we are unable to exploit matrix-vector products for \( \tilde{J}_t \) in (27) due to its dependence on \( \tilde{J}_{t-1} \).

Let us first prove convergence and oracle complexity estimates in expectation of Algorithm 2 for solving (1). However, we require an additional assumption for this case:

**Assumption 4.1.** \( \mathbf{F} \) is \( M_{F} \)-average Lipschitz continuous, i.e., \( \mathbb{E}[\|\mathbf{F}(\mathbf{x}, \xi) - \mathbf{F}(\mathbf{y}, \xi)\|^2] \leq M_{F}^2 \|\mathbf{x} - \mathbf{y}\|^2 \) for all \( \mathbf{x}, \mathbf{y} \).

Though Assumption 4.1 is relatively strong, it has been used in several models, including neural network training under a bounded weight assumption.

Given a tolerance \( \varepsilon > 0 \) and \( C > 0 \), we first choose \( M > 0 \), \( \delta_d > 0 \), and two constants \( \gamma_1 > 0 \) and \( \gamma_2 > 0 \) such that

\[
\begin{align*}
\theta_F := & 2M_{d}(L_{F} + \delta_d) - \gamma_1 M_{F}^2 - 7\gamma_2 L_{F}^2 > 0, \\
m := & \left\lceil \frac{2}{\theta_F C \varepsilon} \right\rceil.
\end{align*}
\]

Next, we choose the mini-batch sizes of \( b_s, \tilde{b}_s, b_{i(s)}, \) and \( \tilde{b}_{i(s)} \), respectively as follows:

\[
\begin{align*}
b_s := & \frac{2CM_{F}\sigma_d^2}{\theta_F^2 \varepsilon^4}, \\
\tilde{b}_s := & \frac{4CM_{d}\sigma_d^2}{\theta_F \varepsilon^2}, \\
b_{i(s)} := & \frac{8M_{F}(m+1-t)}{\theta_F \varepsilon^2}, \\
\tilde{b}_{i(s)} := & \frac{M_{d}(m+1-t)}{\gamma_2\delta_d}.
\end{align*}
\]

Then, the following theorem states the convergence and oracle complexity bounds of Algorithm 2.

**Theorem 4.3.** Suppose that Assumptions 1.1 and 1.2, and 4.1 are satisfied for (1). Let \( \{x_t(s)\}_{s=1}^{S} \) be generated by Algorithm 2 to solve (1). Let \( \theta_F \) and \( m \) be chosen by (28), and the mini-batches \( b_s, \tilde{b}_s, b_{i(s)}, \) and \( \tilde{b}_{i(s)} \) be set as in (29). Assume that the output \( \tilde{x}_T \) of Algorithm 2 is chosen uniformly at random in \( \{x_t(s)\}_{s=1}^{S} \). Then:

(a) The following bound holds

\[
\frac{1}{S(m+1)} \sum_{s=1}^{S} \sum_{t=0}^{m} \mathbb{E} \left[ \|G_M(x_t)|^2 \right] \leq \varepsilon^2.
\]

(b) The total number of iterations \( T \) to obtain

\[
\mathbb{E} \left[ \|\tilde{G}_M(\tilde{x}_T)|^2 \right] \leq \varepsilon^2
\]

is at most

\[
T := S(m+1) = \left[ \frac{8M_{F}^2 \left(\Psi(\tilde{x}^0) - \Psi^*\right)}{\theta_F \varepsilon^2} \right] = \mathcal{O} \left( \frac{1}{\varepsilon^2} \right).
\]

Moreover, the total stochastic oracle calls \( T_f \) and \( T_d \) for evaluating stochastic estimators of \( \mathbf{F}(\mathbf{x}_t, \xi) \) and its Jacobian \( \mathbf{F}'(\mathbf{x}_t, \xi) \), respectively do not exceed:

\[
\begin{align*}
T_f := & \mathcal{O} \left( \frac{M_{F}^2 \sigma_d^2}{\theta_F^2 \varepsilon^4} + \frac{M_{F}^2 M_{d} \sigma_d^2 \left(\Psi(\tilde{x}^0) - \Psi^*\right)}{\theta_F \varepsilon^2} \right), \\
T_d := & \mathcal{O} \left( \frac{M_{d} \sigma_d^2}{\theta_F \varepsilon^2} + \frac{M_{d}^2 \sigma_d^2 \left(\Psi(\tilde{x}^0) - \Psi^*\right)}{\theta_F \varepsilon^2} \right).
\end{align*}
\]

Finally, we show that \( x_t \) computed by our methods is indeed an approximate stationary point of (1) or (2).

**Corollary 4.1.** If \( x_t \) satisfies \( \|\tilde{G}_M(x_t)\| \leq \varepsilon \) for given \( \varepsilon > 0 \), then under either Condition 1 or Condition 2, and for any \( y_t \in \partial\phi(\mathbf{F}(\mathbf{x}_{t+1})) \), we have \( \mathcal{E}(x_{t+1}, y_t) \leq \mathcal{O}(\varepsilon) \).

Consequently, \( x_{t+1} \) is a \( \mathcal{O}(\varepsilon) \)-stationary point of (1) or (2).

**Proof.** From Lemma 2.1, we have

\[
\begin{align*}
\mathcal{E}(x_{t+1}, y_t) \leq & \left( 1 + \frac{M_{d} \sqrt{L_{d}}}{M_{d}} \right) \|\tilde{G}_M(x_t)\| + \frac{1}{2} \|\tilde{J}_t - \mathbf{F}'(x_t)\|^2 \\
& + \frac{(1+L_{F})}{2M_{F}^2} \|G_M(x_t)\|^2 + M_{d} \|F_t - F(x_t)\|.
\end{align*}
\]
We conduct two numerical experiments to evaluate the performance of Algorithm 1 (SGN) and Algorithm 2 (SGN2). Further details of our experiments are in Supp. Doc. F.

5. Numerical Experiments

As in (3), we can form an average approximation of $F$ as in (21)

$$
\tilde{F}_{M}(x_{t}) := \frac{1}{M} \sum_{i=1}^{M} F(x_{t; i})
$$

where $M$ is the number of samples used in the average approximation of $F$. These functions were used in binary classification involving nonconvex losses, e.g., Zhao et al. (2010). Since they are nonnegative, if we use the $\ell_1$-norm, then (33) can be viewed as a model average of 4 different losses in binary classification (see Supp. Doc. F).

We implement both Algorithms 1 (SGN) and 2 (SGN2) to solve (33). We also compare them with the baseline using the full samples instead of calculating $\tilde{F}$ and $F$ as in (21) and (27). We call it the deterministic GN scheme (GN).

**Experiment setup.** We test three algorithms on four standard datasets: w8a, ijcnn1, covtype, and url_combined from LIBSVM2. Further information about these dataset is described in Supp. Doc. F.

To find appropriate batch sizes for $\tilde{F}$ and $\tilde{F}$, we perform a grid search over different combinations of mini-batch sizes to select the best ones. More information about this process can be found in Supp. Doc. F.

We evaluate these algorithms on instances of (33) using $\phi(\cdot) = \|\cdot\|_2$. We use $M := 1$ and $\rho := 1$ for all datasets. The performance of three algorithms is shown in Figure 1 for the w8a dataset and in Figure 2 for the ijcnn1 dataset. This figure depicts the relative objective residuals $\frac{\Psi(x) - \Psi^*}{\Psi^*}$ over the number of epochs, where $\Psi^*$ is the lowest objective value obtained when running three algorithms until the relative residuals fall below $10^{-6}$. In both cases, SGN2 works best while SGN is still much better than the baseline GN in terms of sample efficiency.

For covtype and url_combined datasets, we observe similar behavior as shown in Figure 2, where SGN2 is more efficient than SGN, and both SGN schemes outperform GN. This experiment shows that both SGN algorithms are indeed much more sample efficient than the baseline GN algorithm.
In order to compare with existing algorithms, we use a smooth objective function in (33) with a Huber loss, \( \phi(u) = \frac{1}{2}u^2 \) for \(|u| \leq \delta\) and \( \phi(u) = \delta(|u| - \frac{1}{2}\delta) \) otherwise, and \( \delta := 1.0 \). We implement the nested SPIDER method in Zhang & Xiao (2019a, Algorithm 3), denoted as N-SPIDER, and the stochastic compositional gradient descent in Wang et al. (2017a, Algorithm 1), denoted as SCGD.

We run 5 algorithms: GN, SGN, SGN2, N-SPIDER, and SCGD on 4 datasets as in the previous test. We choose \( M := 1 \) and \( \rho := 1 \) for all datasets. We tune the learning rate for both N-SPIDER and SCGD and finally obtain \( \eta := 1.0 \) for both algorithms. We also set \( \varepsilon = 10^{-1} \) for N-SPIDER, see Zhang & Xiao (2019a, Algorithm 3). In addition, we conduct similar grid search as before to choose the suitable parameters for these algorithms. The chosen parameters are presented in Supp. Doc. F. The results on these datasets are depicted in Figure 3 and Figure 4.

5.2. Optimization Involving Expectation Constraints

We consider the following optimization problem:

\[
\min_{x \in \mathbb{R}^p} \left\{ g(x) \text{ s.t. } \mathbb{E}_\xi [F(x, \xi)] \leq 0 \right\},
\]

(34)
where \( g : \mathbb{R}^p \rightarrow \mathbb{R} \cup \{+\infty\} \) is a convex function, possibly nonsmooth, and \( F : \mathbb{R}^p \times \Omega \rightarrow \mathbb{R}^q \) is a smooth stochastic function. This problem has various applications such as optimization with conditional value at risk (CVaR) constraints and metric learning (Lan & Zhou, 2016) among others. Let us consider an exact penalty formulation of (34) as

\[
\min_{x \in \mathbb{R}^p} \left\{ \Psi(x) := g(x) + \phi(\mathbb{E}_{\xi} [F(x, \xi)]) \right\}, \tag{35}
\]

where \( \phi(u) := \rho \sum_{i=1}^q [u_i]^+ \) with \([u]_+ := \max\{0, u\}\) and \( \rho > 0 \) is a given penalty parameter. Clearly, (35) coincides with (3), an extension of (1).

We evaluate 3 algorithms on the asset allocation problem (Rockafellar & Uryasev, 2000) as an instance of (34):

\[
\begin{align*}
\min_{\tau \in [\underline{\tau}, \overline{\tau}], \tau \in \mathbb{R}^p} & -c^T z + \phi \left( \tau + \frac{1}{\beta n} \sum_{i=1}^n [ -\xi_i^T z - \tau ]_+ \right) \\
\text{s.t.} & \quad z \in \Delta_p := \{ \hat{z} \in \mathbb{R}^p_+ \mid \sum_{i=1}^p \hat{z}_i = 1 \}. \tag{36}
\end{align*}
\]

To apply our methods, we need to smooth \( [u]_+ \) by \( \frac{1}{2} [u + (u^2 + \gamma^2)^{1/2} - \gamma] \) for a sufficiently small value \( \gamma > 0 \). If we introduce \( x := (z, \tau) \), \( F(x, \xi_i) := \tau + \frac{1}{2} ( [ (\xi_i^T z + \tau)^2 + \gamma^2 )^{1/2} - \xi_i^T z - \tau - \gamma ) \) for \( i = 1, \cdots, n \), and \( g(x) = -c^T z + \delta_{\Delta_p}(x) \), then we can reformulate the smoothed approximation of (36) into (3), where \( \delta_{\Delta_p \times [\underline{\tau}, \overline{\tau}]} \) is the indicator of \( \Delta_p \times [\underline{\tau}, \overline{\tau}] \). Note that \( F'(\cdot, \xi_i) \) is Lipschitz continuous with the Lipschitz constant \( L_i := \frac{\| \xi_i \|^2}{2 \beta n} \). In our experiments, we choose \([\underline{\tau}, \overline{\tau}]\) to be \([0, 1]\), \( \beta := 0.1 \), and \( \gamma := 10^{-3} \). We were experimenting different \( \rho \) and \( M \), and eventually set \( \rho := 5 \) and \( M := 5 \).

We test three algorithms: GN, SGN, and SGN2 on both synthetic and real datasets. We follow the procedures from Lan et al. (2012) to generate synthetic data with \( n = 10^5 \) and \( p \in \{ 300, 500, 700 \} \). We also obtain real datasets of US stock prices for 889, 865, and 500 types of stocks described, e.g., in Sun & Tran-Dinh (2019) then bootstrap them to obtain different datasets of sizes \( n = 10^5 \). The details and additional results are given in Supp. Doc. F.

The performance of 3 algorithms on two datasets is depicted in Figure 5. SGN is still much better than GN in both experiments while SGN2 is the best among three. With the large amount of samples per iteration, GN performs poorly in these experiments.

Numerical results have confirmed the advantages of SGN and SGN2 which well align with our theoretical analysis.

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