Curvature-aided Incremental Aggregated Gradient Method

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Abstract

We propose a new algorithm for finite sum optimization which we call the curvature-aided incremental aggregated gradient (CIAG) method. Motivated by the problem of training a classifier for a $d$-dimensional problem, where the number of training data is $m$ and $m \gg d \gg 1$, the CIAG method seeks to accelerate incremental aggregated gradient (IAG) methods using aids from the curvature (or Hessian) information, while avoiding the evaluation of matrix inverses required by the incremental Newton (IN) method. Specifically, our idea is to exploit the incrementally aggregated Hessian matrix to trace the full gradient vector at every incremental step, therefore achieving an improved linear convergence rate over the state-of-the-art IAG methods.

For strongly convex problems, the fast linear convergence rate requires the objective function to be close to quadratic, or the initial point to be close to optimal solution. Importantly, we show that running one iteration of the CIAG method yields the same improvement to the optimality gap as running one iteration of the full gradient method, while the complexity is $\mathcal{O}(d^2)$ for CIAG and $\mathcal{O}(md)$ for the full gradient. Overall, the CIAG method strikes a balance between the high computation complexity incremental Newton-type methods and the slow IAG method. Our numerical results support the theoretical findings and show that the CIAG method often converges with much fewer iterations than IAG, and requires much shorter running time than IN when the problem dimension is high.

1 Introduction

In this paper we consider the unconstrained optimization problem whose objective is a finite sum of functions, i.e.,

$$\min_{\theta \in \mathbb{R}^d} F(\theta) := \sum_{i=1}^{m} f_i(\theta),$$  \hspace{1cm} (1)

where each $f_i : \mathbb{R}^d \to \mathbb{R}$ is a convex and twice continuously differentiable function and $\theta \in \mathbb{R}^d$ is the parameter variable. We shall refer to each $f_i(\theta)$ as a component function and $F(\theta)$ as the sum objective function. The problem above is motivated by many practical machine learning applications. For instance, consider training a support vector machine (SVM) system with the data set $\{(x_i, y_i)\}_{i=1}^{m}$. To cast the training problem in the form of (1), each of the function $f_i(\theta)$ can be set as a loss function $\ell(\theta; x_i, y_i)$ which measures the statistical mismatch between the parameter $\theta$ and the data tuple $(x_i, y_i)$.

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We focus on a large-scale optimization setting where \( m \gg d \gg 1 \), considering the prototypical situation of the so called “big data” challenge in machine learning. In fact, in the SVM classifier case this situation arises when we use a large amount of training data (\( m \gg 1 \)) on a problem with a large number of features (\( d \gg 1 \)). To cope with these challenges, a popular approach is to apply incremental methods \([1]\) to Problem \((1)\). Compared to conventional methods, such as gradient or Newton methods, which require accessing to all \( m \) component functions at every iteration, incremental methods access to only one of the component functions at each iteration and, therefore, the complexity per iteration is independent of \( m \). The prior art on incremental methods have focused on the gradient-type methods which approximate the gradient method. Related work include the celebrated stochastic gradient descent method \([2]\) and its accelerated variants \([3–5]\). The deterministic counterpart of these methods have been studied, e.g., in \([6–9]\), while incremental subgradient methods for nonsmooth problems have been investigated in \([10–12]\). Even though the gradient algorithms are shown to converge linearly for strongly convex problems, the convergence rate is typically slow. In fact, it was shown in \([7]\) that the linear convergence rate of the incremental aggregated gradient (IAG) method is \( 1 - O(1/Qm) \) where \( Q \) is the condition number of the objective function \( F \) in \((1)\), and an improved IAG method was studied in \([9]\). To accelerate the convergence, there has been recently renewed interest in studying incremental Newton(-type) methods. For example, the incremental Newton (IN) method in \([13]\) and the incremental quasi Newton method (IQN) in \([14]\). While these algorithms are shown to achieve superlinear local convergence for strongly convex problems, the computational complexity is usually high, the algorithm involves computing the Hessian inverses.

This paper proposes a new algorithm called curvature-aided incremental aggregated gradient (CIAG) method which is a first order method based on gradient descent. To accelerate convergence, the method exploits curvature information (Hessian) to aid in tracing the full gradient at every iteration using only incremental information. We first show that the CIAG is globally convergent with a sufficiently small step size when the objective function is strongly convex. Furthermore, when the objective function \( F(\theta) \) is quadratic-like or when the CIAG method is initialized at a point close to the optimal solution, we show that each incremental step of the CIAG method can asymptotically achieve a similar linear rate as applying an iteration of the full gradient step. In other words, the method converges to an optimal solution of \((1)\) at an equivalent rate of running \( m \) gradient steps after one cycle of accessing the component functions. We also suggest an adaptive step size rule that can conceptually attain the accelerated convergence rate. This results in an efficient algorithm with fast convergence at a low complexity. We show a comparison of CIAG to the state-of-the-art methods in Table \([1]\).

### 1.1 Notations and Preliminaries

For any \( d \in \mathbb{N} \), we use the notation \([d]\) to refer to the set \( \{1,\ldots,d\} \). We use boldfaced lower-case letters to denote vectors and boldfaced upper-case letters to denote matrices. The positive operator \((x)_+\) denotes \( \max\{0,x\} \). For a vector \( \mathbf{x} \) (or a matrix \( \mathbf{X} \)), the notation \([\mathbf{x}]_i\) (or \([\mathbf{X}]_{i,j}\)) denotes its \( i \)th element (or \((i,j)\)th element). For some positive finite constants \( C_1, C_2, C_3, C_4 \) where \( C_3 \leq C_4 \), and non-negative functions \( f(t), g(t) \), the notations \( f(t) = \mathcal{O}(g(t)) \), \( f(t) = \Omega(g(t)) \), \( f(t) = \Theta(g(t)) \) indicate \( f(t) \leq C_1 g(t), f(t) \geq C_2 g(t), C_3 g(t) \leq f(t) \leq C_4 g(t) \), respectively. Unless otherwise specified, \( \| \cdot \| \) denotes the standard Euclidean norm.
The computation complexity is stated in the per iteration sense, which refers to the computational cost of the full gradient for FG, and the incremental gradient/Hessian for the incremental methods. The last column is the local linear convergence rate and \( Q = L / \mu \) is the condition number of \( \Omega \).

Note that [7] analyzed the convergence rate of IAG in terms of the optimality gap of objective value, showing that \( F(\theta^k) - F(\theta^*) \leq (1 - 1/(4Qm))(F(\theta^0) - F(\theta^*)) \), where \( \theta^* \) is an optimal solution.

The (1 – 4Q/(Q + 1)^2) rate of CIAG is achieved using an adaptive step size described in Section 3.2.

### 2 The CIAG Method

We develop the CIAG method starting from the classical gradient method. We shall call the latter as full gradient method (FG) from now on to distinguish it from incremental gradient methods. The FG method applied to (1) can be described by the recursion: at iteration \( k \in \mathbb{N} \),

\[
\theta^{k+1} = \theta^k - \gamma \nabla F(\theta^k) = \theta^k - \gamma \sum_{i=1}^{m} \nabla f_i(\theta^k),
\]

where \( \gamma > 0 \) is a step size. Notice that evaluating the update above requires accessing the gradients of all component functions at every iteration. This is expensive in terms of the computation cost as \( m \gg 1 \).

The CIAG method adopts the incremental update paradigm to address the complexity issue above, i.e., at the \( k \)th iteration, we restrict the algorithm’s access to only one component function, say the \( i_k \)th function \( f_{i_k}(\theta) \). As desired, the per-iteration computation cost will become independent of \( m \). However, this also implies that the exact gradient vector \( \nabla F(\theta^k) \) is no longer available since the rest of the component functions are not accessible. Our idea is to apply the following Taylor’s approximation:

\[
\nabla f_j(\theta^k) \approx \nabla f_j(\theta^0) + \nabla^2 f_j(\theta^0)(\theta^k - \theta^0).
\]

It suggests that even when the \( j \)th function is not available at the current iteration \( k \), its gradient \( \nabla f_j(\theta^k) \) can still be approximated using the historical gradients/Hessians. To this end, let us model the CIAG method using a delayed gradient/Hessian setting similar to [S]. Let us define \( \tau_{j_k} \in \mathbb{N} \) as the iteration number in which the CIAG method has last accessed to \( f_j(\cdot) \) prior to iteration \( k \), i.e.,

\[
\tau_{j_k} := \max\{k' : i_{k'} = j, \, k' \leq k\}.
\]

Note that \( \tau_{ik_k} = k \). We assume \( m \leq K < \infty \) such that

\[
\max\{0, k - K\} \leq \tau_{j_k} \leq k, \, j = 1, ..., m,
\]

Table 1: Comparison of the storage & computation complexities, convergence speed of different methods.

| Method  | Storage | Computation | \( \lim_{k \to \infty} \frac{\|	heta^{k+1} - \theta^*\|^2}{\|	heta^k - \theta^*\|^2} \) |
|---------|---------|-------------|--------------------------------------------------------------------------------|
| FG      | \( \mathcal{O}(d) \) | \( \mathcal{O}(nd) \) | 1 - 4Q/(Q + 1)^2 |
| IG [1]  | \( \mathcal{O}(d) \) | \( \mathcal{O}(d) \) | 1, i.e., sub-linear |
| IAG [7] | \( \mathcal{O}(md) \) | \( \mathcal{O}(d) \) | 1 - \( \mathcal{O}(1/Qm) \) |
| IQN [14] | \( \mathcal{O}(md^2) \) | \( \mathcal{O}(d^2) \) | 0, i.e., super-linear |
| IN [13] | \( \mathcal{O}(md) \) | \( \mathcal{O}(d^3) \) | 0, i.e., super-linear |
| CIAG (Proposed) | \( \mathcal{O}(md) \) | \( \mathcal{O}(d^2) \) | 1 - 4Q/(Q + 1)^2 |

Note that [7] analyzed the convergence rate of IAG in terms of the optimality gap of objective value, showing that \( F(\theta^k) - F(\theta^*) \leq (1 - 1/(4Qm))(F(\theta^0) - F(\theta^*)) \), where \( \theta^* \) is an optimal solution.

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\[
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Note that \( \tau_{ik_k} = k \). We assume \( m \leq K < \infty \) such that

\[
\max\{0, k - K\} \leq \tau_{j_k} \leq k, \, j = 1, ..., m,
\]
Algorithm 1 CIAG Method.

1: **Input**: Initial point $\theta^1 \in \mathbb{R}^d$.
2: Initialize the vectors/matrices:
   \[
   \theta_i \leftarrow \theta^1, \ i = 1, \ldots, m, \ b^0 \leftarrow 0, \ H^0 \leftarrow mI .
   \]  
   
3: **for** $k = 1, 2, \ldots$ **do**
4: \ Select $i_k \in \{1, \ldots, m\}$, e.g., $i_k = (k \mod m) + 1$.
5: \ Update the vector and matrix $b^k, H^k$ as:
   \[
   b^k = b^{k-1} - \nabla f_{i_k}(\theta_{i_k}) + \nabla f_{i_k}(\theta^k) \\
   + \nabla^2 f_{i_k}(\theta_{i_k}) \theta_{i_k} - \nabla^2 f_{i_k}(\theta^k) \theta^k , \ \\
   H^k = H^{k-1} - \nabla^2 f_{i_k}(\theta_{i_k}) + \nabla^2 f_{i_k}(\theta^k) .
   \]  
   
6: \ Compute the CIAG update:
   \[
   \theta^{k+1} = \theta^k - \gamma (b^k + H^k \theta^k) .
   \]  
   
7: \ Update the parameter stored in memory $\theta_{i_k} \leftarrow \theta^k$.
8: **end for**
9: **Return**: an approximate solution to (1), $\theta^{k+1}$.

and at iteration $k$, the vectors of the following historical iterates are available:

\[
\{\theta_{i_k}^j\}_{j=1}^m .
\]  

The exact gradient can then be approximated by the following Taylor’s approximation:

\[
\tilde{g}^k := \sum_{i=1}^m \left( \nabla f_i(\theta_{i_k}^k) + \nabla^2 f_i(\theta_{i_k}^k)(\theta^k - \theta_{i_k}^k) \right) ,
\]  

where $\tilde{g}^k \approx \sum_{i=1}^m \nabla f_i(\theta^k)$. We remark that the *incremental aggregated gradient* (IAG) method takes almost the same form of update as CIAG, i.e., the IAG method uses

\[
\sum_{i=1}^m \nabla f_i(\theta^k) \approx \sum_{i=1}^m \nabla f_i(\theta_{i_k}^k) .
\]  

From (10), we note that one needs to aggregate (i) the incremental gradient $\nabla f_i(\theta_{i_k}^k)$, (ii) the incremental Hessian-iterate product $\nabla^2 f_i(\theta_{i_k}^k) \theta_{i_k}^k$ and (iii) the incremental Hessian $\nabla^2 f_i(\theta_{i_k}^k)$, in order to compute an CIAG update. These can be achieved efficiently using the procedure outlined in Algorithm 1. In particular, the updates in line 5 essentially swap out the previously aggregated gradient/Hessian information and replace them with the ones computed at the current iterate for the $i_k$th component function; and line 7 keeps track of the historical iterates to ensure that $\theta_{i_k}^k$ is

\[1\text{In the pseudo code, we use } \theta_i, \ i = 1, \ldots, m \text{ to denote the variable that we use to store } \theta_{i_k}^k, \ i.e., \text{the historical parameter at the iteration when the } i \text{th component function is last accessed.} \]
stored. It can be verified that the term, \( b^k + H^k \theta^k \), inside the bracket of (11) is equivalent to the right hand side of (7). Both forms of the CIAG update are presented as the form in (11) gives a more efficient implementation, while (7) is more tamable for analysis. Furthermore, for the special case with a cyclic selection rule for the component functions, the sequence of \( \tau^k \) satisfies (5) with \( K = m \).

Lastly, we comment on the complexity of the CIAG method. First let us focus on the computation complexity — from Line 5 to 6 in Algorithm 1, we observe that the CIAG method requires a computation complexity of \( O(d^2) \) (due to the matrix-vector multiplication) per iteration; meanwhile, the IAG method requires \( O(d) \), the IQN method requires \( O(md^2) \) and the IN method requires \( O(d^3) \) per iteration. Secondly, the storage requirement for CIAG, IAG and IN methods are the same, i.e., \( O(md) \) is needed in storing (6), while the IQN method requires \( O(md^2) \) to store the historical quasi-Hessians. The above analysis shows that the CIAG method provides a tradeoff between the slow convergence in IAG method and the high complexity of IN or IQN method. These comparisons are summarized in Table 1.

### 3 Convergence Analysis

In this section we analyze the convergence of the CIAG method. We focus on strongly convex problems, where the CIAG method is shown to converge linearly. To proceed with our analysis, we state a few required assumptions on the component functions \( f_i(\theta) \) and sum function \( F(\theta) \).

**Assumption 1** The Hessian of each of the component function \( f_i(\theta) \) is \( L_{H,i} \)-Lipschitz. In other words, for all \( \theta', \theta \in \mathbb{R}^d \),

\[
\|\nabla^2 f_i(\theta) - \nabla^2 f_i(\theta')\| \leq L_{H,i} \|\theta - \theta'\| .
\]  

(12)

Note that if \( f_i(\theta) \) is a quadratic function, then \( L_{H,i} = 0 \). Furthermore, we define \( L_H := \sum_{i=1}^{m} L_{H,i} \) as the Hessian Lipschitz constant for \( F(\theta) \).

**Assumption 2** The gradient of the sum function \( F(\theta) \) is \( L \)-Lipschitz. In other words, for all \( \theta', \theta \in \mathbb{R}^d \),

\[
\|\nabla F(\theta) - \nabla F(\theta')\| \leq L \|\theta - \theta'\| .
\]  

(13)

We remark that, if the \( i \)th component function has a \( L_i \)-Lipschitz gradient, then the Lipschitz constant for the gradient of \( F(\theta) \) can be bounded as \( L \leq \sum_{i=1}^{m} L_i \).

**Assumption 3** The sum function \( F(\theta) \) is \( \mu \)-strongly convex, \( \mu > 0 \), i.e., for all \( \theta', \theta \in \mathbb{R}^d \),

\[
F(\theta') \geq F(\theta) + \langle \nabla F(\theta), \theta' - \theta \rangle + \frac{\mu}{2} \|\theta' - \theta\|^2 .
\]  

(14)

Under Assumption 3 a unique optimal solution to problem (1) exists and it is denoted by \( \theta^* \).

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\(^2\)We have neglected the computation complexity of evaluating \( \nabla f_i(\theta^k) \) and \( \nabla^2 f_i(\theta^k) \) as they are often problem dependent. The difference that it makes is minimal as long as the algorithms are incremental, i.e., does not require accessing a large number of these gradient/Hessian.
As a matter of fact, objective functions satisfying the above assumptions are common in machine learning. For example, consider the logistic loss function corresponding to a data tuple \((y_i, x_i)\), where \(y_i \in \{\pm 1\}\) is the data label and \(x_i \in \mathbb{R}^d\) is the associated feature vector, the loss function is given as:

\[
\ell(\theta; (y_i, x_i)) = \frac{1}{\rho} \log(1 + e^{-y_i \langle x_i, \theta \rangle}) + \frac{1}{2} \|\theta\|^2,
\]

where the latter term is a standard \(\ell_2\) regularizer and \(\rho > 0\) controls the strength of regularization.

Taking \(f_i(\theta) = \ell(\theta; (y_i, x_i))\) in problem (1), it can be verified that problem (1) satisfies Assumption 1 to 3 with the following Lipschitz constants:

\[
L = \frac{1}{\rho} \|\sum_{i=1}^m x_i x_i^\top\|_2 + m, \quad L_{H,i} = \frac{1}{\rho} \|x_i x_i^\top\|_2,
\]

and the strongly convex constant of \(\mu = m\). We observe that if \(\rho\) is large, then the Hessian’s Lipschitz constant \(L_{H,i}\) is small.

We next show that the CIAG method converges linearly for strongly convex problems. The following holds:

**Theorem 1** Under Assumption 1, 2 and 3. Let \(V(k) := \|\theta^k - \theta^*\|^2\) where \(\theta^k\) is the \(k\)th iterate generated by CIAG and \(\theta^*\) is the optimal solution to (1). Fix \(s \in \mathbb{N}\) as an arbitrary integer and \(\epsilon > 0\), if the step size \(\gamma\) satisfies:

\[
\gamma \leq \epsilon + \min\left\{\frac{2}{\mu + L}, \frac{\mu L}{2K \sqrt{L_H (L^2 V(s)^{1/2} + 16L_H^2 V(s)^{3/2}) (\mu + L)}}, \left(1 - \frac{\mu L}{8K^4 L_H^2 L^4 V(s) + 256L_H V(s)^3 (\mu + L)}\right)^{1/5}\right\},
\]

then the sequence \(\{V(k)\}_{k \geq s}\) converges linearly as:

\[
V(k) \leq (1 - \epsilon)^{(k-s)/(2K+1)} V(s), \quad \forall k \geq s.
\]

Moreover, asymptotically the linear rate can be improved to:

\[
\lim_{k \to \infty} \frac{V(k+1)}{V(k)} \leq 1 - 2\gamma \frac{\mu L}{L + \mu},
\]

i.e., as \(k \to \infty\), the CIAG method converges linearly at the same rate of FG using the step size \(\gamma\).

The next subsection provides a proof sketch of Theorem 1.

We observe that the convergence rate of CIAG in (19) is equivalent to that of FG with the same step size \(\gamma\). Importantly, to achieve the same worst-case decrement of the distance to the optimal solution, the CIAG method only requires access to one component function at each iteration, while the FG method requires access to all the \(m\) component functions. Furthermore, if the objective function is ‘quadratic’-like, i.e., when \(L_H\) is small, then one can take \(\gamma \approx 2/(\mu + L)\), which is the
same maximum allowable step size for the FG method [15]. In the above case, the CIAG method has a linear convergence rate of

\[ 1 - \frac{4\mu L}{(\mu + L)^2} = 1 - \frac{4Q}{(Q + 1)^2}, \tag{20} \]

where \( Q = L/\mu \) is the condition number of \( \Pi \).

Theorem 1 shows that the CIAG method is globally convergent when an appropriate, fixed step size is chosen. This is in contrast to other curvature information based methods such as IQN, which only have local convergence guarantee. One of the main reasons is that the CIAG method is developed as an approximation to the classical FG method, whose global convergence is established with less restrictions.

3.1 Proof Sketch of Theorem 1

As opposed to the IAG method, the CIAG method applies a first-order Taylor’s approximation to the gradient vector. By utilizing Assumption 1 (Lipschitz smoothness of the Hessian), it can be shown that the gradient error is bounded by:

\[ \| \nabla F(\theta^k) - \tilde{g}^k \| = O(\gamma^2 m^2 \max_{k^i \in [(k-K)+,k]} \| \theta^{k^i} - \theta^* \|^2) . \tag{21} \]

We observe that the norm of the error is bounded by a squared norm of the optimality gap \( \| \theta^{k^i} - \theta^* \|^2 \). The latter decays quickly when the optimality gap is close to zero. Consequently, studying the iteration of the optimality gap leads us to the following inequality:

\[ \| \theta^{k+1} - \theta^* \|^2 \leq \left( 1 - 2\gamma \frac{\mu L}{L + \mu} \right) \| \theta^k - \theta^* \|^2 
+ O\left( \gamma^3 m^2 \max_{k^i \in [(k-2K)+,k]} \| \theta^{k^i} - \theta^* \|^3 \right) , \tag{22} \]

notice that difference in the power of the term \( \| \theta^k - \theta^* \| \) on the right hand side and the fact that the expression \( \left( 1 - 2\gamma \mu L/(\mu + L) \right) \) is the linear rate obtained for the FG method [16]. In other words, the optimality gap at the \((k+1)\)th iteration is bounded by the sum of a term that decays with a linear rate of \( \left( 1 - 2\gamma \mu L/(\mu + L) \right) \) and delayed error terms of higher order.

The observation above prompts us to study the following general inequality system with the non-negative sequence: consider \( \{ R(k) \}_{k \geq 0} \) satisfying the inequality:

\[ R(k+1) \leq p R(k) + \sum_{j=1}^{J} q_j \max_{k^i \in S_j^k} R(k^i)^{\eta_j} , \tag{23} \]

where \( 0 \leq p < 1, q_j \geq 0, \eta_j > 1 \) and \( S_j^k \subseteq [(k-M+1)_,k] \) for all \( j \) with some \( J,M < \infty \). We have

**Lemma 1** For some \( p \leq \delta < 1, \)

\[ p + \sum_{j=1}^{J} q_j R(0)^{\eta_j-1} \leq \delta < 1 , \tag{24} \]

then (a) \( \{ R(k) \}_k \) converges linearly for all \( k \) as

\[ R(k) \leq \delta^{[k/M]} \cdot R(0), \forall k \geq 0 , \tag{25} \]

and (b) the rate is accelerated to \( p \) asymptotically,

\[ \lim_{k \to \infty} R(k+1)/R(k) \leq p . \tag{26} \]
Observe that (22) fits into the requirement of (23) with \( R(k) = \| \theta^k - \theta^* \|^2 \), \( M = 2K \) and \( p = 1 - 2\gamma \mu L/(L + \mu) \). The claims in Theorem 1 thus follow by applying Lemma 1 and carefully characterizing the constants.

### 3.2 Linear Convergence Rate of CIAG Method

We note that the linear convergence rate of CIAG hinges on the choice of step size \( \gamma \) as specified in (17), where the latter depends on the number of parameters in the optimization problem. This section discusses the relationship between the convergence rate and the choice of step size \( \gamma \) under different settings.

**Worst-case convergence rate with a constant step size** — We now compare the (worst-case) convergence rate of the CIAG method with other incremental methods when using a constant step size. To proceed, let us define the following constants:

\[
Q := \frac{L}{\mu}, \quad Q_H := \frac{L}{L_H} = \frac{\mu}{L_H} Q,
\]

which correspond to the condition number of (1) and the ratio between the gradient’s and Hessian’s Lipschitz constant. Substituting the constants above into the expression in (17) of the CIAG’s step size and that the second term inside \( \min \{ \cdot \} \) is dominant when \( K \) is large, the step size has to satisfy:

\[
\gamma = \frac{1}{2K} \sqrt{\frac{Q_H}{(L^2 V(0)^{1/2} + 16L_H^2 V(0)^{3/2})(Q + 1)}} - \epsilon,
\]

The linear convergence rate achieved at \( k \to \infty \) is \( 1 - p \), where \( p \) is approximately:

\[
p \approx \frac{L}{K(Q + 1)} \sqrt{\frac{Q_H}{(L^2 V(0)^{1/2} + 16L_H^2 V(0)^{3/2})(Q + 1)}}
= \frac{1}{K(Q + 1)} \sqrt{\frac{Q_H}{Q + 1} \frac{1}{V(0)^{1/2} + 16V(0)^{3/2}/Q_H^2}}.
\]

It is instructive to compare the rate rate to the best known rate of the IAG method from [7]. In particular, [7, Theorem 3.4] shows that the linear convergence rate of IAG is given by \( 1 - p' \), with

\[
p' = \frac{1}{K(Q + 1)} \frac{1}{49}.
\]

The comparison above shows that the CIAG method has at least the same scaling as the IAG method, as well as the SAG method, i.e., the stochastic counterpart of the IAG method.

Moreover, we observe that when

\[
\sqrt{\frac{Q_H}{Q + 1}} \sqrt{\frac{1}{V(0)^{1/2} + 16V(0)^{3/2}/Q_H^2}} > \frac{1}{49},
\]

then the CIAG method enjoys a faster convergence rate than the IAG method. Notice that this depends on the ratio \( Q_H/Q = \mu/L_H \) and the initial distance to optimal solution \( V(0) \) such that
holds when \( L_H \) is small or when \( V(0) \) is small. We remark that the analysis above is a representative of a worst case scenario for the CIAG method. In practice, we find that CIAG method is convergent for most cases when the largest possible step size \( 2/(\mu + L) \) is chosen. Furthermore, in the following, we argue that the CIAG algorithm can be accelerated significantly using an adaptive step size rule.

**Achieving FG’s rate with one incremental step** — An important insight from Theorem 1 is that the maximum allowable step size \( \gamma \) is inversely proportional to the initial distance to optimal solution, \( V(s) \). In particular, it is possible to set the step size to the maximum allowable value \( \gamma = 2/(\mu + L) \) when the initial point is sufficiently close to the optimum. In fact, for large \( K \), whenever the optimality gap \( V(s) \) satisfies

\[
V(s) + 16 \frac{V(s)^{\frac{3}{2}}}{Q_H} < \frac{1}{16K^2} Q_H < \left( \frac{Q + 1}{Q} \right)^2,
\]

then the CIAG method is allowed to take the maximum allowable step size \( 2/(\mu + L) \) at the iteration numbers \( k \geq s \).

For the given condition numbers \( Q, Q_H \) and an initial step size choice that satisfies (17) at \( s = 0 \), Theorem 1 shows that Eq. (32) can be satisfied when \( s \) is large, since the optimality gap \( V(s) \) also decreases to zero linearly with the iteration number \( s \). This suggests that the step size \( 2/(\mu + L) \) is allowable once we run the CIAG method for long enough time. Note that this holds regardless of the ‘quadratic’-ness, \( L_H \), of the objective function. As an heuristic, we may apply a time-varying step size that increases to \( 2/(\mu + L) \). Designing a globally converging step size scheme and analyzing its property are left as future work topics.

### 4 Numerical Experiments

In this section, we compare the performance of several incremental methods. For a fair comparison, in the following we shall concentrate on testing the incremental methods with the deterministic, cyclic component selection rule similar to Line 4 of Algorithm 1, i.e., we shall not test the stochastic variants of the incremental methods, e.g., SAG [3] or SAGA [5]. We focus on the problem of training an SVM using the logistic loss function given in (15). For the logistic loss function (15), we set \( \rho = 1/m \). Note that as analyzed in (16), the condition number \( Q \) increases with \( m \) in general.

Our first set of experiments considers training an SVM with synthetic data — we first generate \( \theta_{true} \in \mathbb{R}^d \) as a random vector with each element distributed independently as \( U[-1, 1] \); then each of the feature vector \( x_i \in \mathbb{R}^d \) is generated as \( x_i = [\tilde{x}_i; 1] \) where \( \tilde{x}_i \sim U[-1, 1]^{d-1} \) and the label \( y_i \) is computed as \( y_i = \text{sign}(\langle x_i, \theta_{true} \rangle) \). We remark that the set up described is equivalent to an SVM with bias term, which is given by the last element of \( \theta_{true} \).

To set up the benchmark algorithms, the step sizes for both IN and IQN are both set as \( \gamma = 1 \) to attain the fastest convergence (at superlinear rate) even though it may not guarantee global convergence. For the IAG method, we have optimized the step size and we set \( \gamma = 50/(mL) \), where \( L \) is the Lipschitz constant for \( \nabla F(\theta) \) that is computed as \( m + m \| \sum_{i=1}^m x_i x_i^\top \|_2 \). We also test the incremental gradient (IG) method using a vanishing step size \( \gamma_k = 1/(\lfloor k/m \rfloor L) \). For the CIAG method, we set \( \gamma = 1/L \).
Fig. 1: Convergence of the incremental methods for logistic regression problem of dimension $m = 1000$, $d = 51$. The $y$-axis denotes the optimality gap plotted in log-scale and the $x$-axis shows the number of effective passes (defined as $k/m$), i.e., number of completed cycles through the $m$ component functions.

Fig. 1 compares the primal optimality gap $F(\theta^k) - F(\theta^\star)$, against the iteration number $k$ (notice that $k/m$ is the effective number of passes through the component functions) for a logistic regression problem instance of dimensions $d = 51$ and $m = 1000$. Observe that all the incremental methods tested except IG converge at least linearly, and both the IN and IQN methods appear to converge at a superlinear rate, since the slope increases as the iteration number grows. This corroborates with the claims in [13,14]. We also see that the curvature information aided methods outperform the others, with the IN method being the fastest. Even though the CIAG method converges only linearly, it reaches the same level of optimality ($\approx 10^{-13}$) as the superlinearly converging IQN method using the same number of iterations.

Fig. 2 considers an instance of a similar problem with larger dimensions of $d = 501$ and $m = 2000$. We observe that the IN method is not converging in this problem instance. In fact, in our experiments, the IN method using a step size of $\gamma = 1$ is often not converging on random problem instances with large $d$ and $m$. On the other hand, both the CIAG and IQN methods appear to have significantly better numerical stability. Moreover, the CIAG method has the fastest convergence among the incremental methods tested, even though its theoretical convergence rate is at most linear, as opposed to the superlinear convergence rate of the IQN method.

Our second set of experiments focuses on training an SVM from real training data. The incremental methods are implemented in c++. We use the implementations of IAG and IN from [13] with the IN method set to compute the inverse of the aggregated Hessian in an exact fashion. The training datasets used are mushrooms ($m = 8124$, $d = 112$), w8a ($m = 49749$, $d = 300$) and alpha ($m = 500000$, $d = 500$) from libsvm [17]. Notice that as both $m$ and $d$ are large in these cases, the IQN method run out of memory while initializing its working variables. We use a minibatch setting such that 5 samples are selected for every iteration of the incremental methods. Lastly, we choose the step sizes for CIAG as $\gamma = 0.001/L$ for mushrooms, w8a and $\gamma = 10^{-5}/L$ for alpha; for IAG as $\gamma = 0.1/(mL)$ for mushrooms, $\gamma = 0.05/(mL)$ for w8a and $\gamma = 10^{-5}/(mL)$ for alpha.

The optimal objective value $F(\theta^\star)$ is found by applying the full Newton method on (1) until the latter converges, i.e., when $\|\nabla F(\theta^k)\| \leq 10^{-13}$.
Figure 2: Convergence of the incremental methods for logistic regression problem of dimension \( m = 2000, \) \( d = 501 \). Note that the IN method is not converging in this example.

| Dataset      | CIAG method                  | IN method \cite{13} | IAG method \cite{8} |
|--------------|------------------------------|---------------------|---------------------|
| mushrooms    | 43.5 eff. pass               | 4.8 eff. pass       | 1920 eff. pass      |
|              | 2.256 sec.                   | 1.002 sec.          | 6.848 sec.          |
| w8a          | 7.2 eff. pass                | 5.3 eff. pass       | \( \geq 10^3 \) eff. pass |
|              | 16.38 sec.                   | 64.62 sec.          | \( \geq 75.83 \) sec.\(^\dagger\) |
| alpha        | 7.6 eff. pass                | 2.3 eff. pass       | \( \geq 10^3 \) eff. pass |
|              | 463.08 sec.                  | 1130.7 sec.         | \( \geq 1353.8 \) sec.\(^\dagger\) |

Table 2: Performance of the incremental methods on different training datasets. We show the number of effective passes (defined as \( k/m \)) and the corresponding running time required to reach convergence such that \( \| \nabla F(\theta^k) \| \leq 10^{-10} \). \(^\dagger\)the IAG method only converges to a solution with \( \| \nabla F(\theta^k) \| \approx 10^{-6} \) [for w8a] and \( \| \nabla F(\theta^k) \| \approx 10^{-4} \) [for alpha] after 1000 effective passes.

In Table 2 we compare the performance in terms of the running time and number of required iterations to reach convergence, \( i.e., \) when \( \| \nabla F(\theta^k) \| \leq 10^{-10} \). We observe that the IN method has the fastest convergence rate, \( i.e., \) requiring the least number of iterations (or effective passes), for all the problem instances. However, except for the low-dimension problem case (\( e.g., \) mushrooms) where \( d \approx 100 \), the IN method requires a much longer running time than the proposed CIAG method to reach convergence. This is due to the added complexity required for computing the \( d \times d \) Hessian inverse. These experimental findings corroborate our claim that the CIAG method achieves a desirable tradeoff between complexity and convergence speed.

5 Conclusions

In this paper, we have proposed a new incremental gradient-type method that uses curvature information to accelerate convergence. We show that the proposed CIAG method converges linearly with a rate comparable to that of the FG method, while requiring a single incremental step only.
Numerical results are presented to support our theoretical claims. Future work includes incorporating the Nesterov’s acceleration into the CIAG update, analyzing the convergence speed for CIAG with randomized component selection scheme, relaxing the strong convexity assumption, etc. The recently developed double IAG technique developed in [9] may also be adopted into the CIAG method for further acceleration.

6 Acknowledgement

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7 Proof of Theorem 1

Our idea is to analyze the CIAG method as a noisy gradient descent method. In particular, let us define

\[ \tilde{g}^k := \sum_{i=1}^{m} \left( \nabla f_i(\theta^i_k) + \nabla^2 f_i(\theta^i_k)(\theta^k - \theta^i_k) \right) \]  

(33)
as the gradient surrogate employed in CIAG. Define \( e^k := \tilde{g}^k - \nabla F(\theta^k) \) as the error between the exact gradient and the gradient surrogate used by CIAG. We define the following as our optimality measure:

\[ V(k) := \| \theta^k - \theta^* \|^2 . \]  

(34)

Recall that \( \tilde{g}^k = \nabla F(\theta^k) + e^k \) and let us define:

\[ E(k) := \gamma^2 \| e^k \|^2 - 2\gamma \langle \theta^k - \theta^* - \gamma \nabla F(\theta^k), e^k \rangle . \]  

(35)

We observe the following chain\(^4\):

\[
V(k+1) = V(k) - 2\gamma \langle \nabla F(\theta^k), \theta^k - \theta^* \rangle \\
+ \gamma^2 \| \nabla F(\theta^k) \|^2 + E(k) \\
\leq V(k) - 2\gamma \left( \frac{\mu L}{\mu + L} V(k) + \frac{1}{\mu + L} \| \nabla F(\theta^k) \|^2 \right) \\
+ \gamma^2 \| \nabla F(\theta^k) \|^2 + E(k) \\
= \left( 1 - 2\gamma \frac{\mu L}{\mu + L} \right) V(k) + E(k) \\
+ \left( \gamma^2 - \frac{2\gamma}{\mu + L} \right) \| \nabla F(\theta^k) \|^2 \]  

(36)

where the first inequality is due to Assumption 2 and 3 and the last inequality is due to the choice of step size that \( \gamma < 2/(\mu + L) \) [cf. (17)].

The next step is to bound the error term \( E(k) \). We observe that:

\[ |E(k)| \leq \gamma^2 \| e^k \|^2 + 2\gamma \| e^k \| \| \theta^k - \gamma \nabla F(\theta^k) - \theta^* \| \]  

\[ \leq \gamma^2 \| e^k \|^2 + 2\gamma \sqrt{V(k)} \| e^k \| , \]  

(37)

where the last inequality is due to the fact that the term \( \theta^k - \gamma \nabla F(\theta^k) \) is equivalent to applying an exact gradient descent step to \( \theta^k \). It follows that the conclusion in (36) holds with \( E(k) = 0 \), therefore the difference between the term and \( \theta^* \) cannot be greater than \( V(k) \) due to the choice of our step size. Moreover, we observe that

\[ \| e^k \| \leq \sum_{i=1}^{m} L_{H,i} \| \theta^i_k - \theta^k \|^2 , \]  

(38)

\(^4\)This chain of analysis follows from [8, Section 3.3] and is repeated here merely for the sake of self-containedness.
where the inequality is due to Assumption 1. Importantly, we observe that the error’s norm is bounded by a squared norm of the difference $\theta^{i,k} - \theta^k$. Proceeding from (38), we can bound $|E(k)|$ as:

$$|E(k)| \leq \gamma^6 8K^4 L_H^2 \left( \max_{k' \in [k-2K,k]} (L^4 V(k')^2 + 256 L_H^4 V(k')^4) \right)$$

$$+ \gamma^3 4K^2 L_H \left( \max_{k' \in [k-2K,k]} (L^2 V(k')^{3/2} + 16 L_H^2 V(k')^{3/2}) \right),$$

the derivation of the above can be found in Section 7.1.

We can now conclude the proof by substituting $V(k) = R(k)$ in Lemma 1, where the proof of the latter can be found in Section 7.2. Our sequence $\{V(k)\}_k$ is non-negative and it satisfies (23) with:

$$p = 1 - 2\gamma \mu L/(\mu + L),$$

$$q_1 = \gamma^6 \cdot 8K^4 L_H^2 L^4,$$

$$q_2 = \gamma^6 \cdot 2048K^4 L_H^6,$$

$$q_3 = \gamma^3 \cdot 4K^2 L_H L^2,$$

$$q_4 = \gamma^3 \cdot 64K^2 L_H^3,$$

and $\eta_1 = 2$, $\eta_2 = 4$, $\eta_3 = 3/2$, $\eta_4 = 5/2$, $M = 2K + 1$. To satisfy (24), we require the following on the step size $\gamma$:

$$p + \sum_{j=1}^4 q_j V(0)^{\eta_j-1} < 1$$

$$\iff \sum_{j=1}^4 q_j V(0)^{\eta_j-1} < 2\gamma \mu L/(\mu + L)$$

$$\iff \gamma^5 \cdot 8K^4 L_H^2 \left( L^4 V(0) + 256 L_H^4 V(0)^3 \right)$$

$$+ \gamma^2 \cdot 4K^2 L_H \left( L^2 V(0)^{1/2} + 16 L_H^2 V(0)^{3/2} \right)$$

$$< 2\mu L/(\mu + L),$$

which can be satisfied by having:

$$\gamma^5 \cdot 8K^4 L_H^2 \left( L^4 V(0) + 256 L_H^4 V(0)^3 \right) < \frac{\mu L}{\mu + L}$$

and

$$\gamma^2 \cdot 4K^2 L_H \left( L^2 V(0)^{1/2} + 16 L_H^2 V(0)^{3/2} \right) < \frac{\mu L}{\mu + L}.$$

The above can be satisfied by the step size choice in (17). As such, the conclusions in the lemma hold and the conclusions of Theorem 1 follow.
7.1 Derivation of Eq. (39)

We observe that:

\[
\|e^k\| \leq \sum_{i=1}^{m} L_{H,i} \|\theta^{r_i^k} - \theta^k\|^2 \\
\leq \sum_{i=1}^{m} L_{H,i} \sum_{j=r_i^k}^{k-1} \|\theta^{j+1} - \theta^j\|^2 \\
\leq KL_H \sum_{j=(k-K)_+}^{k-1} \|\theta^{j+1} - \theta^j\|^2 \\
\leq KL_H \gamma^2 \sum_{j=(k-K)_+}^{k-1} \|e^j + \nabla F(\theta^j)\|^2 \\
\leq 2\gamma^2 KL_H \sum_{j=(k-K)_+}^{k-1} (\|e^j\|^2 + \|\nabla F(\theta^j)\|^2)
\]

We have

\[
\|\nabla F(\theta^j)\|^2 = \|\nabla F(\theta^j) - \nabla F(\theta^*)\|^2 \leq L^2 V(j),
\]

and

\[
\|e^j\| \leq \sum_{i=1}^{m} L_{H,i} \|\theta^i - \theta^{\tau_i^j}\|^2 \\
\leq 2 \sum_{i=1}^{m} L_{H,i} \cdot (V(j) + V(\tau_i^j)) \\
\leq 4L_H \max_{\ell \in \{\tau_i^j\}_{i=1}^{m} \cup \{j\}} V(\ell)
\]

Plugging these back into (42) gives:

\[
\|e^k\| \\
\leq 2\gamma^2 KL_H \sum_{j=(k-K)_+}^{k-1} \left(L^2 V(j) + 4L_H \max_{\ell \in \{\tau_i^j\}_{i=1}^{m} \cup \{j\}} V(\ell)^2\right) \\
\leq 2\gamma^2 K^2 L_H \left(L^2 \max_{(k-K)_+ \leq \ell \leq k-1} V(\ell) \\
+ 16L_H^2 \max_{(k-2K)_+ \leq \ell \leq k-1} V(\ell)^2\right),
\]

where we have used the fact that \(\tau_i^{k-K} \geq k-2K\) in the last inequality. Consequently, we can upper bound \(E(k)\) as

\[
|E(k)| \leq 4\gamma^6 K^4 L_H^2 \left(L^2 \max_{(k-K)_+ \leq \ell \leq k-1} V(\ell) \\
+ 16L^2_H \max_{(k-2K)_+ \leq \ell \leq k-1} V(\ell)^2\right) \\
+ 4\gamma^3 K^2 L_H \cdot \sqrt{V(k)} \cdot \left(L^2 \max_{(k-K)_+ \leq \ell \leq k-1} V(\ell) \\
+ 16L^2_H \max_{(k-2K)_+ \leq \ell \leq k-1} V(\ell)^2\right),
\]
which can be further bounded as (39).

7.2 Proof of Lemma 1

The proof of Lemma 1 is divided into two parts. We first show that under (24), the sequence \( R(k) \) converges linearly as in (25); then we show that the rate of convergence can be improved to \( p \) as in (26).

The first part of the proof is achieved using induction on all \( \ell \geq 1 \) with the following statement:

\[
R(k) \leq \delta^\ell \cdot R(0), \quad \forall \; k = (\ell - 1)M + 1, \ldots, \ell M.
\]

(46)

The base case when \( \ell = 1 \) can be straightforwardly established:

\[
R(1) \leq pR(0) + \sum_{j=1}^{J} q_j R(0)^{\eta_j} \leq \delta R(0),
\]

\[
R(2) \leq pR(1) + \sum_{j=1}^{J} q_j R(0)^{\eta_j} \leq \delta R(0),
\]

\[
\vdots
\]

\[
R(M) \leq pR(M - 1) \sum_{j=1}^{J} q_j R(0)^{\eta_j} \leq \delta R(0).
\]

(47)

Now suppose that the statement (46) is true up to \( \ell = c \), for \( \ell = c + 1 \), we have:

\[
R(cM + 1) \leq pR(cM) + \sum_{j=1}^{J} q_j \max_{k' \in [(c-1)M+1,cM]} R(k'^{\eta_j})
\]

\[
\leq p(\delta^c R(0)) + \sum_{j=1}^{J} q_j (\delta^c R(0))^{\eta_j}
\]

\[
\leq \delta^c \cdot (pR(0) + \sum_{j=1}^{J} q_j R(0)^{\eta_j}) \leq \delta^{c+1} R(0).
\]

(48)

Similar statement also holds for \( R(k) \) with \( k = cM + 2, \ldots, (c + 1)M \). We thus conclude that:

\[
R(k) \leq \delta^{\lceil k/M \rceil} \cdot R(0), \quad \forall \; k \geq 0,
\]

(49)

which proves (25).

The second part of the proof establishes the linear rate of convergence of \( p \). We observe that

\[
\frac{R(k + 1)}{R(k)} \leq p + \sum_{j=1}^{J} q_j \max_{k' \in [(k-M+1)+,k]} R(k'^{\eta_j})
\]

\[
\leq \frac{R(k')^{\eta}}{R(k)} \leq \frac{R(k')}{R(k)} R(0)^{\eta-1} \delta^{(\lceil k'/M \rceil)(\eta-1)}
\]

(50)

For any \( k' \in [k - M + 1, k] \) and any \( \eta > 1 \), we have:

As \( \eta > 1 \), we observe that \( \delta^{(\lceil k'/M \rceil)(\eta-1)} \to 0 \) when \( k \to \infty \). We have two cases to be analyzed — the first case is

\[
\lim_{k \to \infty} \frac{R(k')}{R(k)} = \infty \iff \lim_{k \to \infty} \frac{R(k)}{R(k')} = 0,
\]

(52)
Assume that $\lim_{k \to \infty} R(k)/R(k-1)$ is well defined, for $k' \neq k$, we observe that:

$$\lim_{k \to \infty} \frac{R(k)}{R(k-1)} \frac{R(k-1)}{R(k-2)} \cdots \frac{R(k'+1)}{R(k')} = 0$$

$$\implies \left( \lim_{k \to \infty} \frac{R(k+1)}{R(k)} \right)^{k-k'} = 0$$

$$\implies \lim_{k \to \infty} \frac{R(k+1)}{R(k)} = 0 \ ,$$

where we have used the property for the limit of products. On the other hand, when $k' = k$ it leads to a contradiction to (52) since $\lim_{k \to \infty} R(k)/R(k) = 1$.

The second case is that

$$\lim_{k \to \infty} R(k')\eta/R(k) = 0 \ .$$

(54)

Notice that if (52) happens for some $k' \in [k-M+1, k]$, then the derivation in (53) implies that $\lim_{k \to \infty} R(k+1)/R(k) = 0 \leq p$. Alternatively, if (54) happens for all $k' \in [k-M+1, k]$, then (50) implies that

$$\lim_{k \to \infty} R(k+1)/R(k) \leq p ,$$

this concludes our proof.