Glocal Smoothness: Line Search can really help!

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Abstract

Iteration complexities are bounds on the number of iterations of an algorithm. Iteration complexities for first-order numerical optimization algorithms are typically stated in terms of a global Lipschitz constant of the gradient, and near-optimal results are achieved using fixed step sizes. But many objective functions that arise in practice have regions with small Lipschitz constants where larger step sizes can be used. Many local Lipschitz assumptions have thus been proposed, which lead to results showing that adaptive step sizes and/or line searches yield improved convergence rates over fixed step sizes. However, these faster rates tend to depend on the iterates of the algorithm, which makes it difficult to compare the iteration complexities of different methods. We consider a simple characterization of global and local smoothness that only depends on properties of the function. This allows upper bounds on iteration complexities in terms of problem-dependent constants, which allows us to compare iteration complexities between algorithms. Under this assumption it is straightforward to show the advantages of line searches over fixed step sizes, and that in some settings gradient descent with line search has a better iteration complexity than accelerated gradient methods with fixed step sizes.

1. Setting the Step Size: Theory vs. Practice

Machine learning models are typically trained using numerical optimization algorithms. The simplest algorithm used is gradient descent [5], which on iteration t takes steps of the form

$$w_{t+1} = w_t - \eta_t \nabla f(w_t), \tag{1}$$

for some positive step size η_t . The simplest way to set the step size η_t is to use a constant value throughout training. Other methods have also been proposed in order to give faster convergence in practice, including line searches [1] or adaptive step sizes such as the Polyak step size [24]. To prove theoretical guarantees on the convergence of gradient descent using different step sizes, the function being optimized is often assumed to have a globally Lipschitz continuous gradient (also known as being L-smooth).

Definition 1 A function f has an L-Lipschitz continuous gradient (for L > 0) if $\forall x, y \in \mathbb{R}^d$, then:

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|.$$

Unfortunately, there is often a disconnect between the step sizes that work in theory and those that work well in practical applications. To illustrate the disconnect between theory and practice, contrast using a fixed step size of $\eta_t = \frac{1}{L}$ with choosing the step using line optimization (LO) to minimize the function.

$$\eta_t \in \operatorname*{arg\,min}_{\eta} f(w_t - \eta \nabla f(w_t)).$$
(2)

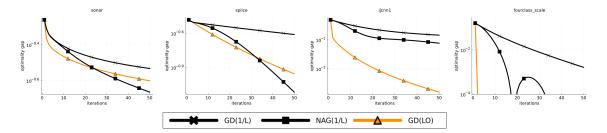


Figure 1: Logistic regression on 4 different datasets showing the optimality gap throughout training for gradient descent (GD) and Nesterov's accelerated gradient (NAG) method with a fixed step size of $\frac{1}{L}$, along with gradient descent with line optimization (LO). From left to right, we have a problem where GD(LO) has a similar rate to GD(1/L), a problem where GD(LO) is converging faster than GD(1/L), and two problems where GD(LO) is also converging faster than NAG(1/L). We refer the reader to Shea & Schmidt [27] for the experimental details.

We refer to gradient descent with $\eta_t = \frac{1}{L}$ as GD(1/L) and gradient descent with η_t set using (2) as GD(LO). Standard analyses of GD(1/L) and GD(LO) give nearly-identical theoretical convergence rates [10], but GD(LO) typically converges faster in practice. Further, GD(LO) has a worse theoretical convergence rate than Nesterov's accelerated gradient (NAG) method using a step size of $\frac{1}{L}$ [18]. But experimentally, GD(LO) converges faster than NAG(1/L) on many problems (see Figure 1).

One reason GD(LO) can converge faster than GD(1/L) and NAG(1/L) is that it can use much larger step sizes than $\frac{1}{L}$. These larger step sizes are possible because, in a region around each w_t , the Lipschitz smoothness assumption (1) may hold with a smaller value of the constant L. Many works have analyzed first-order methods under local measures of L (see Section 2). However, these analyses generally depend on the iterates w_t of the algorithm, making it difficult to compare convergence rates between algorithms; different algorithms will take differing paths during training so have different local L values. Thus, it is hard to use these assumptions to explain why GD(LO) can outperform NAG(1/L).

In Section 3, we introduce a "glocal" smoothness assumption that augments global smoothness with a measure of local smoothness near the solution. In particular, a function is (L, L^*, δ) -glocal smooth if it is globally L-smooth and locally L_* -smooth when the sub-optimality is at most δ . This characterization of global and local smoothness leads to iteration complexities that only depend on the properties of the function being optimized, and not on the precise path taken by the algorithm. Similar to previous local smoothness assumptions, we show under glocal smoothness that GD(LO) has an improved iteration complexity over GD(1/L). But under the glocal assumption, we also give conditions under which GD(LO) has a better iteration complexity than NAG(1/L). While using LO is not always practical, in Section 4 we consider practical step sizes under the glocal assumption. Finally, in Section 5 we discuss related research directions.

2. Related Work: how much does line search and local smoothness help?

It may seem possible that the performance of GD(LO) may be explained by a better analysis under global smoothness. Indeed, recent work by de Klerk et al. [7] gives tight rates for GD(LO) that are faster than for GD(1/L). However, these rates do not explain why GD(LO) can converge much faster than NAG(1/L).

Many works define a notion of local smoothness based on the iterates w_t [3, 12–15, 21, 25, 30]. These local smoothness conditions depend on the lines between successive iterations w_{t-1} and w_t , balls around the w_t , the convex hull of the w_t , or sub-level sets of the $f(w_t)$. Under these assumptions we can show that GD(LO) converges faster than GD(1/L). The reason for GD(LO)'s faster convergence is that it can use larger step sizes that exploit the local smoothness, while the step sizes of GD(1/L) are based on the global smoothness constant. However, we cannot easily compare GD(LO) and NAG(1/L) using these measures. Different algorithms will have different iterates w_t , so the particular local smoothness constants cannot be compared between algorithms.

Many algorithms use estimates of local smoothness to speed convergence [8, 11, 13, 19, 22, 23, 26, 28, 29, 31]. We can use the assumptions of the previous paragraph to show that such methods can converge faster than methods that do not exploit local smoothness. However, existing assumptions do not allow us to compare between different algorithms exploiting local smoothness.

The most-closely related works to our glocal-smoothness assumption are works that assume local smoothness but do not assume global smoothness [12, 22, 23, 31]. These works tend to focus on achieving global convergence despite the lack of global smoothness. In contrast, our focus is on exploring assumptions under which it is easy to compare the iteration complexities of different algorithms.

Finally, we note that glocal-smoothness is a special case of the general framework of Curtis and Robinson [6]. They propose partitioning the search space of an algorithm into different regions that satisfy different assumptions, and analyzing the progress an algorithm makes in each region. Our work considers the simpler case where we consider just two regions: the whole space and a sublevel set. We believe that this is an important special case as it leads to simple analyses that better reflect practical performance. Further, we expect that algorithms that perform well under glocal smoothness should have good performance under other measures of local smoothness.

3. Glocal Smoothness

In order to more easily compare optimization algorithms that may exploit local smoothness, we propose a notion of global-local smoothness, which we call "glocal smoothness":

Definition 2 A function f is glocally (L, L_*, δ) -smooth if f is globally L-smooth, and locally L_* -smooth for all $x \in \mathbb{R}^d$ such that $f(x) - f_* \le \delta$ for some $\delta > 0$.

Assumptions of this type have been explored for speeding convergence [29] and analyzing the quality of local optima [16]. Note that $L_* \leq L$ since L^* is measured over a subset of the space, but that for some problems we have $L_* << L$. For example, the standard bound for binary logistic regression with a data matrix X is $(1/4)\|X\|^2$ [4]. The 1/4 factor is the upper bound on $p(y_i = +1)p(y_i = -1)$ for labels y_i . However, if near solutions we have $p(y_i = +1) > 0.99$ or $p(y_i = -1) > .99$ for all i, then L_* is around $(1/100)\|X\|^2$. This allows GD(LO) to eventually take steps that are 25-times larger than those used by GD(1/L) yet still decrease the function.

3.1. Iteration Complexity under Glocal Smoothness

To illustrate how glocal smoothness allows comparisons between algorithms, we consider the case of strongly-convex functions:

Definition 3 A function f is μ -strongly convex for some $\mu > 0$ if $\forall x, y \in \mathbb{R}^d$,

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} ||y - x||^2.$$

Under strong convexity and global smoothness assumptions, GD(1/L) reaches an accuracy of ϵ after $(L/\mu)\log((f(w_0)-f_*)/\epsilon)$ iterations. This is worse than the $O(\sqrt{L/\mu}\log((f(w_0)-f_*)/\epsilon))$ iteration complexity of NAG(1/L) with appropriate algorithm parameter settings [see 17]. Under strong convexity and glocal smoothness, we have the following iteration complexity for GD(LO):

Theorem 4 Assume that f is glocally (L, L_*, δ) -smooth and μ -strongly convex. For all $t \geq 0$, let w_t be the iterates of gradient descent as defined in (1) with step-size η_t given by (2). Then for $\delta > \epsilon$,

$$f(w_T) - f_* \le \epsilon \quad \text{for all} \quad T \ge \frac{L}{\mu} \log \left(\frac{f(w_0) - f_*}{\delta} \right) + \frac{L_*}{\mu} \log \left(\frac{\delta}{\epsilon} \right).$$

The proof is given in Appendix A.1. The rate of GD(LO) under glocal smoothness is faster than the rate of GD(1/L) whenever we have $L_* < L$. Indeed, the analysis proceeds by arguing that GD(LO) makes at least as much progress as GD(1/L) globally and makes at least as much progress as GD(1/L*) locally (without needing to know any of L, L^* , or δ).

It is notable that the rate of GD(LO) under glocal smoothness is faster than NAG(1/L) if

$$\frac{L_*}{L} \le \frac{(\sqrt{\kappa})^{-1} \log(1/\epsilon) - \log(1/\delta)}{\log(1/\epsilon) - \log(1/\delta)}.$$

This is possible when $L_* < L$, $\delta > \epsilon$, and the condition number $\kappa = \frac{L}{\mu}$ is not too large. In words, we expect line search to outperform acceleration if the problem is not too badly conditioned and there is a large region around the minimizers with a smaller local smoothness constant than the global smoothness constant.

4. Practical Algorithms

Unfortunately, neither GD(1/L) or GD(LO) are practical algorithms in general as it may not be possible in practice to compute the Lipschitz constant L or perform LO. Under global smoothness, we can achieve the rate of GD(1/L) using a backtracking line search procedure [2]. This method starts with an initial guess L_0 of L, and doubles the value whenever a sufficient decrease condition is not satisfied. If $L_0 \leq L$, it achieves the GD(1/L) rate of $O((L/\mu)\log((f(w_0)-f_*)/\epsilon))$. Unfortunately, this backtracking method does not achieve a faster rate under glocal smoothness since it never decreases its guess of L (and thus does not increase the step size in the local region).

It is possible to obtain an improved iteration complexity over GD(1/L) in practice under glocal smoothness using a backtracking procedure with resets [25]. When the guess of L is reset to L_0 on each iteration, the rate of gradient descent is improved to $O((L/\mu)\log((f(w_0)-f_*)/\delta)+$ $(\max\{L_*,L_0\}/\mu)\log(\delta/\epsilon))$ under the glocal framework. This backtracking-with-resets method achieves the fast rate of GD(LO) if $L_0 \le L_*$. However, this method may require significant backtracking on each iteration while it has a worse complexity than GD(LO) if $L_0 > L^*$.

We can achieve the rate of GD(LO) under glocal smoothness using a procedure that includes both a forwardtracking and a backtracking procedure [8]. Unfortunately, the iterations of such methods can be expensive since the step size could be increased or decreased many times within each iteration of the algorithm. Fortunately, many practical heuristics exist to reduce the cost of this type of algorithm [see 20].

Finally, we note that it is possible to achieve a rate similar to GD(LO) under glocal smoothness without increasing the iteration cost if we know f_* and use the Polyak step size [24],

$$\eta_t = \frac{f(w_t) - f_*}{\|\nabla f(w_t)\|^2}.$$
(3)

Theorem 5 Assume that f is glocally (L, L_*, δ) -smooth and μ -strongly convex. For all $t \geq 0$, let w_t be the iterates of gradient descent as defined in (1) with step-size η_t given by (3). Then for $\delta > \epsilon$,

$$f(w_T) - f_* \le \epsilon \quad \text{for all} \quad T \ge 4 \left(\frac{L}{\mu} \log \left(\frac{L}{2} \frac{\|w_0 - w_*\|^2}{\delta} \right) + \frac{L_*}{\mu} \log \left(\frac{\delta}{\epsilon} \right) \right).$$

See Appendix A.2 for the proof of this result. This result is similar to GD(LO), with a worse dependence inside the first logarithmic factor since the non-monotonicity of the Polyak step size means we may take more iterations to guarantee that we stay within the δ region.

5. Discussion

We focus on glocal smoothness and global strong convexity, but other global-local assumptions could be explored. For example, we could obtain faster rates if we allowed a larger local μ_* within the δ region. We could also relax strong-convexity to consider functions satisfying the Polyak-Łojasiewicz condition [see 10]. An alternate relaxation is to consider functions that are strongly-convex in the local region but only convex globally. However, it is less clear how to exploit a condition like glocal smoothness for non-convex functions.

Our analysis focuses on variants of GD, but glocal smoothness can be used to analyze other algorithms. For example, it can be inserted into existing analyses of coordinate descent and proximal-gradient methods to obtain better rates for those methods under LO. It would be interesting to explore accelerated and stochastic methods that adapt to glocal smoothness. A challenge with analyzing some stochastic methods is that they may leave the local δ region infinitely often.

Compared to popular global smoothness assumptions, we believe that performance under glocal smoothness better reflects the performance of numerical optimization algorithms in practice. Thus, we encourage theoreticians to adopt assumptions like glocal smoothness in order for their theoretical results to better reflect empirical performance. Further, a key advantage of glocal smoothness compared to many previous local smoothness assumptions is that glocal smoothness allows comparisons between algorithms. Indeed, we have given a precise condition under which "line search can really help" in the sense that using line search with the basic GD method leads to a faster convergence rate than using acceleration.

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Appendix A. Convergence Proofs

A.1. Glocally Smooth, Strongly Convex Convergence Proof

In this section we give the proof of Theorem 4. This proof exploits a classic result regarding the convergence rate of GD(1/L) and GD(LO) as for example stated in Karimi et al. [10, Theorem 1].

Lemma 6 Assume that f is glocally \bar{L} -smooth and μ -strongly convex. For all t the iterates of gradient descent as defined in (1) with step-size η_t given by $1/\bar{L}$ or exact line optimization (2) satisfy

$$f(w_t) - f_* \le \left(1 - \frac{\mu}{\bar{L}}\right) (f(w_{t-1}) - f_*)$$

Note that this implies the following two properties:

- 1. Since $\mu/\bar{L} \leq 1$ the function values decrease monotonically, $f(w_t) \leq f(w_{t-1})$.
- 2. By applying the lemma recursively, if we initialize at \bar{w}_0 and apply t iterations we have

$$f(w_t) - f_* \le \left(1 - \frac{\mu}{\bar{L}}\right)^t (f(\bar{w}_0) - f_*).$$

By using that $(1 - \mu/\bar{L}) \le \exp(-\bar{L}/\mu)$, we have that $f(w_t) - f_*$ is less than a value $\bar{\epsilon} > 0$ beginning from \bar{w}_0 for all t satisfying

$$t \ge \frac{\bar{L}}{\mu} \log \left(\frac{f(\bar{w}_0) - f_*}{\bar{\epsilon}} \right). \tag{4}$$

We also note that any sub-level set $f(w) - f_* \le \delta$ of a convex function is convex. Thus, given any w_t and w_{t-1} in the sub-level set, the line segment between w_t and w_{t-1} remains in the set.

Proof [Theorem 4]

We break the proof into two parts. The first part gives the number of iterations of gradient descent required to reach an accuracy of δ for an L-smooth function starting from w_0 . The second part gives the number of iterations to reach an accuracy of ϵ for an L_* -smooth function starting from the first iteration t_{δ} that is within the δ region (recall that we assume $\epsilon < \delta$).

Part 1: Since f is glocally $\{L, L_* \delta\}$ -smooth, f is globally L-smooth. Using Lemma 6 with $\bar{L} = L$, GD(LO) starting from $\bar{w}_0 = w_0$ satisfies $f(w_t) - f_* \leq \delta$ for all t satisfying

$$t \ge \frac{L}{\mu} \log \left(\frac{f(w_0) - f_*)}{\delta} \right),$$

by using $\bar{\epsilon} = \delta$ in (4). Let t_{δ} be the first iteration satisfying the above inequality, i.e.,

$$t_{\delta} \triangleq \left\lceil \frac{L}{\mu} \log \left(\frac{f(w_0) - f_*}{\delta} \right) \right\rceil.$$

Part 2: By monotonicity, we have that $f(w_t) - f_* \le \delta$ for all $t \ge t_\delta$. Further, by convexity the lines between all such w_t remaining in the δ sublevel set where f is L_* smooth. Thus, we can treat the function as if it is L_* -smooth on these iterations. Using Lemma 6 with $\bar{L} = L_*$, GD(LO) starting from $\bar{w}_0 = w_{t_\delta}$ satisfies $f(w_t) - f_* \le \epsilon$ for all t satisfying

$$t \ge \frac{L_*}{\mu} \log \left(\frac{\delta}{\epsilon} \right) \ge \frac{L_*}{\mu} \log \left(\frac{f(w_{t_\delta}) - f_*}{\epsilon} \right)$$

by using $\bar{\epsilon} = \epsilon$ in (4). Adding this t to t_{δ} gives the result.

A.2. Polyak Convergence Proof

In this section we give the proof of Theorem 5. This proof exploits results used in Hazan and Kakade [9, Lemma 1, Lemma 2] and uses the classic Polyak step size [24].

Lemma 7 Assume that f is glocally \bar{L} -smooth and μ -strongly convex. For all t the iterates of gradient descent as defined in (1) with step-size η_t given by (3) satisfy

$$||w_t - w_*||^2 \le (1 - \frac{\mu}{4\bar{L}})||w_{t-1} - w_*||^2$$

Note that this implies the following two properties:

- 1. Since $\mu/\bar{L} \leq 1$ the iterate distances decrease monotonically, $\|w_t w_*\|^2 \leq \|w_{t-1} w_*\|^2$. Note that unlike Lemma 6, there is no guarantee that the function values decrease monotonically when using the Polyak step size.
- 2. By applying the lemma recursively, if we initialize at \bar{w}_0 and apply t iterations we have

$$\|w_t - w_*\|^2 \le \left(1 - \frac{\mu}{4\bar{L}}\right)^t \|\bar{w}_0 - w_*\|^2.$$
 (5)

Note that if f is globally L-smooth, and w_* is a minimizer of f, then:

$$f(w) - f_* \le \frac{L}{2} ||w - w_*||^2$$

Combining the above inequality with (5), we have

$$f(w_t) - f_* \le \frac{L}{2} \left(1 - \frac{\mu}{4\bar{L}} \right)^t \|\bar{w}_0 - w_*\|^2.$$

By using that $(1 - \mu/4\bar{L}) \le \exp(-4\bar{L}/\mu)$, we have that $f(w_t) - f_*$ is less than a value $\bar{\epsilon} > 0$ beginning from \bar{w}_0 for all t satisfying

$$t \ge \frac{4\bar{L}}{\mu} \log \left(\frac{L}{2} \frac{\|\bar{w}_0 - w_*\|^2}{\bar{\epsilon}} \right). \tag{6}$$

We also note that any sub-level set $f(w) - f_* \le \delta$ of a convex function is convex. Thus, given any w_t and w_{t-1} in the sub-level set, the line segment between w_t and w_{t-1} remains in the set.

Proof [Theorem 5]

We break the proof into two parts. The first part gives the number of iterations of gradient descent required to reach an accuracy of δ for an L-smooth function starting from w_0 . The second part gives the number of iterations to reach an accuracy of ϵ for an L_* -smooth function starting from the first iteration t_{δ} that is within the δ region (recall that we assume $\epsilon < \delta$).

Part 1: Since f is glocally $\{L, L_* \delta\}$ -smooth, f is globally L-smooth. Using Lemma 7 with L = L, GD with the Polyak step size (3) starting from $\bar{w}_0 = w_0$ satisfies $f(w_t) - f_* \le \delta$ for all t satisfying

$$t \ge \frac{4L}{\mu} \log \left(\frac{L}{2} \frac{\|w_0 - w_*\|^2}{\delta} \right),$$

by using $\bar{\epsilon} = \delta$ in (6). Let t_{δ} be the first iteration satisfying the above inequality, i.e.,

$$t_{\delta} \triangleq \left\lceil \frac{4L}{\mu} \log \left(\frac{L}{2} \frac{\|w_0 - w_*\|^2}{\delta} \right) \right\rceil.$$

One immediate consequence of this definition is that

$$\frac{L}{2}||w_{t_{\delta}} - w_*||^2 \le \delta,\tag{7}$$

which we will use in Part 2 of this proof.

Part 2: By monotonicity, we have that $f(w_t) - f_* \le \delta$ for all $t \ge t_\delta$. Further, by convexity the lines between all such w_t remaining in the δ sublevel set where f is L_* smooth. Thus, we can treat the function as if it is L_* -smooth on these iterations. Using Lemma 7 with $\bar{L} = L_*$, GD with the Polyak step size (3) starting from $\bar{w}_0 = w_{t_\delta}$ satisfies $f(w_t) - f_* \le \epsilon$ for all t satisfying

$$t \ge \frac{4L_*}{\mu} \log\left(\frac{\delta}{\epsilon}\right) \ge \frac{4L_*}{\mu} \log\left(\frac{L}{2} \frac{\|w_{t\delta} - w_*\|^2}{\epsilon}\right)$$

by using (7) and $\bar{\epsilon} = \epsilon$ in (6). Adding this t to t_{δ} gives the result.