An optimal first order method based on optimal quadratic averaging

Dmitriy Drusvyatskiy* Maryam Fazel[†] Scott Roy[‡]

Abstract

In a recent paper, Bubeck, Lee, and Singh introduced a new first order method for minimizing smooth strongly convex functions. Their geometric descent algorithm, largely inspired by the ellipsoid method, enjoys the optimal linear rate of convergence. Motivated by their work, we propose a close variant that iteratively maintains a quadratic global under-estimator of the objective function, whose minimal value approaches the true minimum at an optimal rate. The resulting intuitive scheme comes equipped with a natural stopping criterion and can be numerically accelerated by using accumulated information.

1 Introduction

Consider a function $f: \mathbb{R}^n \to \mathbb{R}$ that is β -smooth and α -strongly convex. Thus each point x yields a quadratic upper estimator and a quadratic lower estimator of the function. Namely, the inequality $q(y;x) \leq f(y) \leq Q(y;x)$ holds for all $x,y \in \mathbb{R}^n$, where we set

$$q(y;x) := f(x) + \langle \nabla f(x), y - x \rangle + \frac{\alpha}{2} \|y - x\|^{2},$$

$$Q(y;x) := f(x) + \langle \nabla f(x), y - x \rangle + \frac{\beta}{2} \|y - x\|^{2}.$$

Classically, one step of the steepest descent algorithm decreases the distance of the iterate to the minimizer of f by the fraction $1 - \alpha/\beta$. This linear convergence rate is suboptimal from a computational complexity viewpoint. Optimal first-order methods, originating in Nesterov's work [8] achieve the superior (and the best possible) linear rate of $1 - \sqrt{\alpha/\beta}$; see also the discussion in [7, Section 2.2]. Such accelerated schemes, on the other hand, are notoriously difficult to analyze. Numerous recent papers (e.g. [1,3,6,9]) have aimed to shed new light on optimal algorithms.

This manuscript is motivated by the novel geometric descent algorithm of Bubeck, Lee, and Singh [3]. Their scheme is highly geometric, sharing some aspects with the ellipsoid method, and it achieves the optimal linear rate of convergence. Moreover, the geometric descent algorithm often has much better practical performance than accelerated gradient

^{*}University of Washington, Department of Mathematics, Seattle, WA 98195; ddrusv@uw.edu. Research of Drusvyatskiy was partially supported by the AFOSR YIP award FA9550-15-1-0237.

[†]University of Washington, Department of Electrical Engineering, Seattle, WA 98195; mfazel@uw.edu. Research partially supported by ONR award N00014-12-1-1002 and NSF award CIF-1409836.

[‡]University of Washington, Department of Mathematics, Seattle, WA 98195; scottroy@uw.edu

methods; see the discussion in [3]. In this paper, we propose an intuitive variant of the geometric descent algorithm that maintains a quadratic lower model of the objective function, whose minimum value converges to the true minimum at an optimal linear rate. The algorithm has a number of virtues. First, it comes equipped with a natural stopping criterion. Second, a formal comparison with the original accelerated gradient method [7,8] is immediate. Finally, one can significantly speed up the method in practice by utilizing accumulated information – a limited memory version of the scheme.

The outline of the paper is as follows. In Section 2, we describe the optimal quadratic averaging framework (Algorithm 1) – the focal point of the manuscript. In Section 3, we propose a limited memory version of Algorithm 1, based on iteratively solving small dimensional quadratic programs. Section 4 discusses the close connection between Algorithm 1 and the geometric descent method of [3]. Section 5 is devoted to numerical illustrations, in particular showing that the optimal quadratic averaging algorithm with memory can be competitive with L-BFGS. We finish the paper within Section 6, where we discuss the challenges that must be overcome in order to derive proximal extensions.

1.1 Notation

We follow the notation of [3] – the motivation for the current work. Given a point $x \in \mathbb{R}^n$, we define a short step $x^+ := x - \frac{1}{\beta} \nabla f(x)$ and a long step $x^{++} := x - \frac{1}{\alpha} \nabla f(x)$. Setting $y = x^+$ in the quadratic bound $f(y) \leq Q(y;x)$ yields the standard inequality

$$f(x^{+}) + \frac{1}{2\beta} \|\nabla f(x)\|^{2} \le f(x).$$
 (1)

We denote the unique minimizer of f by x^* , its minimal value by f^* , and its condition number by $\kappa := \beta/\alpha$. Throughout, the symbol $B(x, R^2)$ stands for the Euclidean ball of radius R around x. For any points $x, y \in \mathbb{R}^n$, we let $\mathtt{line_search}(x, y)$ be the minimizer of f on the line between x and y.

2 Optimal quadratic averaging

The starting point for our development is the elementary observation that every point \bar{x} provides a quadratic under-estimator of the objective function, having a canonical form. Indeed, completing the square in the strong convexity inequality $f(x) \geq q(x; \bar{x})$ yields

$$f(x) \ge \left(f(\bar{x}) - \frac{\|\nabla f(\bar{x})\|^2}{2\alpha} \right) + \frac{\alpha}{2} \|x - \bar{x}^{++}\|^2.$$
 (2)

Suppose we have now available two quadratic lower-estimators:

$$f(x) \ge Q_A(x) := v_A + \frac{\alpha}{2} \|x - x_A\|^2$$
 and $f(x) \ge Q_B(x) := v_B + \frac{\alpha}{2} \|x - x_B\|^2$.

Clearly, the minimal values of Q_A and of Q_B lower-bound the minimal value of f. For any $\lambda \in [0,1]$, the average $Q_{\lambda} := \lambda Q_A + (1-\lambda)Q_B$ is again a quadratic lower-estimator of f. Thus we are led to the question:

What choice of λ yields the tightest lower-bound on the minimal value of f?

To answer this question, observe the equality

$$Q_{\lambda}(x) := \lambda Q_{A}(x) + (1 - \lambda)Q_{B}(x) = v_{\lambda} + \frac{\alpha}{2} \|x - c_{\lambda}\|^{2},$$

where

$$c_{\lambda} = \lambda x_A + (1 - \lambda)x_B$$

and

$$v_{\lambda} = v_B + \left(v_A - v_B + \frac{\alpha}{2} \|x_A - x_B\|^2\right) \lambda - \left(\frac{\alpha}{2} \|x_A - x_B\|^2\right) \lambda^2.$$
 (3)

In particular, the average Q_{λ} has the same canonical form as Q_A and Q_B . A quick computation now shows that v_{λ} (the minimum of Q_{λ}) is maximized by setting

$$\bar{\lambda} := \text{proj}_{[0,1]} \left(\frac{1}{2} + \frac{v_A - v_B}{\alpha \|x_A - x_B\|^2} \right).$$

With this choice of λ , we call the quadratic function $\overline{Q} = \overline{v} + \frac{\alpha}{2} || \cdot -\overline{c} ||^2$ the *optimal averaging* of Q_A and Q_B . See Figure 1 for an illustration.

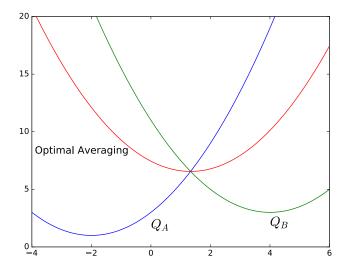


Figure 1: The optimal averaging of $Q_A(x) = 1 + 0.5(x+2)^2$ and $Q_B(x) = 3 + 0.5(x-4)^2$.

An algorithmic idea emerges. Given a current iterate x_k , form the quadratic lower-model $Q(\cdot)$ in (2) with $\bar{x}=x_k$. Then let Q_k be the optimal averaging of Q and the quadratic lower model Q_{k-1} from the previous step. Finally define x_{k+1} to be the minimizer of Q_k , and repeat. Though attractive, the scheme does not converge at an optimal rate. Indeed, this algorithm is closely related to the suboptimal method in [3]; see Section 4.1 for a discussion. The main idea behind acceleration, natural in retrospect, is a separation of roles: one must maintain two sequences of points x_k and c_k . The points x_k will generate quadratic lower models as above, while c_k will be the minimizers of the quadratics. We summarize the proposed method in Algorithm 1. The rule for determining the iterate x_k by a line search is entirely motivated by the geometric descent method in [3].

```
Algorithm 1: Optimal Quadratic Averaging

Input: Starting point x_0 and strong convexity constant \alpha > 0.

Output: Final quadratic Q_K(x) = v_K + \frac{\alpha}{2} \|x - c_K\|^2 and x_K^+.

Set Q_0(x) = v_0 + \frac{\alpha}{2} \|x - c_0\|^2, where v_0 = f(x_0) - \frac{\|\nabla f(x_0)\|^2}{2\alpha} and c_0 = x_0^{++}; for k = 1, \ldots, K do

Set x_k = \text{line\_search}(c_{k-1}, x_{k-1}^+);

Set Q(x) = \left(f(x_k) - \frac{\|\nabla f(x_k)\|^2}{2\alpha}\right) + \frac{\alpha}{2} \|x - x_k^{++}\|^2;

Let Q_k(x) = v_k + \frac{\alpha}{2} \|x - c_k\|^2 be the optimal averaging of Q and Q_{k-1}; end
```

Remark 2.1. When implementing Algorithm 1, we set $x_k^+ = \mathtt{line_search}(x_k, x_k - \nabla f(x_k))$. This does not impact the analysis as x_k^+ still satisfies the key inequality (1). With this modification, the algorithm does require β as part of the input, and we have observed that the algorithm performs better numerically.

To aid in the analysis of the scheme, we record the following easy observation.

Lemma 2.2. Suppose that $\overline{Q} = \overline{v} + \frac{\alpha}{2} \| \cdot -\overline{c} \|^2$ is the optimal averaging of the quadratics $Q_A = v_A + \frac{\alpha}{2} \| \cdot -x_A \|^2$ and $Q_B = v_B + \frac{\alpha}{2} \| \cdot -x_B \|^2$. Then the quantity \overline{v} is nondecreasing in both v_A and v_B . Moreover, whenever the inequality $|v_A - v_B| \leq \frac{\alpha}{2} \|x_A - x_B\|^2$ holds, we have

$$\bar{v} = \frac{\alpha}{8} ||x_A - x_B||^2 + \frac{1}{2} (v_A + v_B) + \frac{1}{2\alpha} \left(\frac{v_A - v_B}{||x_A - x_B||} \right)^2.$$

Proof. Define $\hat{\lambda} := \frac{1}{2} + \frac{v_A - v_B}{\alpha \|x_A - x_B\|^2}$. Notice that we have

$$\hat{\lambda} \in [0,1]$$
 if and only if $|v_A - v_B| \le \frac{\alpha}{2} ||x_A - x_B||^2$.

If $\hat{\lambda}$ lies in [0, 1], equality $\bar{\lambda} = \hat{\lambda}$ holds, and then from (3) we deduce

$$\bar{v} = v_{\bar{\lambda}} = \frac{\alpha}{8} ||x_A - x_B||^2 + \frac{1}{2} (v_A + v_B) + \frac{1}{2\alpha} \left(\frac{v_A - v_B}{||x_A - x_B||} \right)^2.$$

If $\hat{\lambda}$ does not lie in [0, 1], then an easy argument shows that \bar{v} is linear in v_A either with slope one or zero. If $\hat{\lambda}$ lies in (0, 1), then we compute

$$\frac{\partial \bar{v}}{\partial v_A} = \frac{1}{2} + \frac{1}{\alpha \|x_A - x_B\|^2} (v_A - v_B),$$

which is nonnegative because $\frac{|v_A - v_B|}{\alpha ||x_A - x_B||^2} \leq \frac{1}{2}$. Since \bar{v} is clearly continuous, it follows that \bar{v} is nondecreasing in v_A , and by symmetry also in v_B .

We now show that Algorithm 1 achieves the optimal linear rate of convergence.

Theorem 2.3 (Convergence of optimal quadratic averaging). In Algorithm 1, for every index $k \geq 0$, the inequalities $v_k \leq f^* \leq f(x_k^+)$ hold and we have

$$f(x_k^+) - v_k \le \left(1 - \frac{1}{\sqrt{\kappa}}\right)^k (f(x_0^+) - v_0).$$

Proof. Since in each iteration, the algorithm only averages quadratic minorants of f, the inequalities $v_k \leq f^* \leq f(x_k^+)$ hold for every index k. Set $r_0 = \frac{2}{\alpha}(f(x_0^+) - v_0)$ and define the quantities $r_k := \left(1 - \frac{1}{\sqrt{\kappa}}\right)^k r_0$. We will show by induction that the inequality $v_k \geq f(x_k^+) - \frac{\alpha}{2}r_k$ holds for all $k \geq 0$. The base case k = 0 is immediate, and so assume we have

$$v_{k-1} \ge f(x_{k-1}^+) - \frac{\alpha}{2}r_{k-1}$$

for some index k-1. Next set $v_A(x) := f(x_k) - \frac{\|\nabla f(x_k)\|^2}{2\alpha}$ and $v_B := v_{k-1}$. Then the function

$$Q_k(x) = v_k + \frac{\alpha}{2} \|x - c_k\|^2,$$

is the optimal averaging of $Q_A(x) = v_A + \frac{\alpha}{2} \|x - x_k^{++}\|^2$ and $Q_B(x) = v_B + \frac{\alpha}{2} \|x - c_{k-1}\|^2$. An application of (1) yields the lower bound \hat{v}_A on v_A :

$$v_A = f(x_k) - \frac{\|\nabla f(x_k)\|^2}{2\alpha} \ge f(x_k^+) - \frac{\alpha}{2} \frac{\|\nabla f(x_k)\|^2}{\alpha^2} \left(1 - \frac{1}{\kappa}\right) := \hat{v}_A.$$

The induction hypothesis and the choice of x_k yield a lower bound \hat{v}_B on v_B :

$$v_{B} \ge f(x_{k-1}^{+}) - \frac{\alpha}{2} r_{k-1} \ge f(x_{k}) - \frac{\alpha}{2} r_{k-1}$$

$$\ge f(x_{k}^{+}) + \frac{1}{2\beta} \|\nabla f(x_{k})\|^{2} - \frac{\alpha}{2} r_{k-1}$$

$$= f(x_{k}^{+}) - \frac{\alpha}{2} \left(r_{k-1} - \frac{1}{\alpha^{2} \kappa} \|\nabla f(x_{k})\|^{2} \right) := \hat{v}_{B}.$$

Define the quantities $d:=\|x_k^{++}-c_{k-1}\|$ and $h:=\frac{\|\nabla f(x_k)\|}{\alpha}$. We now split the proof into two cases. First assume $h^2\leq \frac{r_{k-1}}{2}$. Then we deduce

$$v_k \ge v_A \ge \hat{v}_A = f(x_k^+) - \frac{\alpha}{2} h^2 \left(1 - \frac{1}{\kappa} \right)$$

$$\ge f(x_k^+) - \frac{\alpha}{2} r_{k-1} \left(\frac{1 - \frac{1}{\kappa}}{2} \right)$$

$$\ge f(x_k^+) - \frac{\alpha}{2} r_{k-1} \left(1 - \frac{1}{\sqrt{\kappa}} \right)$$

$$= f(x_k^+) - \frac{\alpha}{2} r_k.$$

Hence in this case, the proof is complete.

Next suppose $h^2 > \frac{r_{k-1}}{2}$ and let $v + \frac{\alpha}{2} \| \cdot -c \|^2$ be the optimal average of the two quadratics $\hat{v}_A + \frac{\alpha}{2} \| \cdot -x_k^{++} \|^2$ and $\hat{v}_B + \frac{\alpha}{2} \| \cdot -c_{k-1} \|^2$. By Lemma 2.2, the inequality $v_k \geq v$ holds. We claim that equality

$$v = \hat{v}_B + \frac{\alpha}{8} \frac{(d^2 + \frac{2}{\alpha}(\hat{v}_A - \hat{v}_B))^2}{d^2}$$
 holds. (4)

From Lemma 2.2, it suffices to show $\frac{1}{2} \geq \frac{|\hat{v}_A - \hat{v}_B|}{\alpha d^2}$. Note the equality $\frac{|\hat{v}_A - \hat{v}_B|}{\alpha d^2} = \frac{|r_{k-1} - h^2|}{2d^2}$. The choice of x_k ensures the inequality $h^2 \leq d^2$. Thus we have $h^2 - r_{k-1} < h^2 \leq d^2$. Finally, the assumption $h^2 > \frac{r_{k-1}}{2}$ implies

$$r_{k-1} - h^2 < \frac{r_{k-1}}{2} < h^2 \le d^2.$$

Hence we can be sure that (4) holds. Plugging in \hat{v}_A and \hat{v}_B we conclude

$$v = f(x_k^+) - \frac{\alpha}{2} \left(r_{k-1} - \frac{1}{\kappa} h^2 - \frac{(d^2 + r_{k-1} - h^2)^2}{4d^2} \right).$$

Hence the proof is complete once we show the inequality

$$r_{k-1} - \frac{1}{\kappa}h^2 - \frac{(d^2 + r_{k-1} - h^2)^2}{4d^2} \le \left(1 - \frac{1}{\sqrt{\kappa}}\right)r_{k-1}.$$

After rearranging, our task simplifies to showing the inequality

$$\frac{r_{k-1}}{\sqrt{\kappa}} \le \frac{h^2}{\sqrt{\kappa}} + \frac{(d^2 + r_{k-1} - h^2)^2}{4d^2}.$$

Minimizing the right-hand side over d satisfying $h^2 < d^2$, we deduce

$$\frac{h^2}{\sqrt{\kappa}} + \frac{(d^2 + r_{k-1} - h^2)^2}{4d^2} \ge \frac{h^2}{\sqrt{\kappa}} + \frac{r_{k-1}^2}{4h^2}.$$

Minimizing the right-hand side over h satisfying $h^2 \ge \frac{r_{k-1}}{2}$ yields

$$\frac{h^2}{\sqrt{\kappa}} + \frac{r_{k-1}^2}{4h^2} \ge \frac{r_{k-1}}{\sqrt{\kappa}}.$$

The proof is complete.

It is instructive to compare optimal averaging (Algorithm 1) with Nesterov's optimal methods in [7,8]. For convenience, we record the optimal gradient method following [7], in Algorithm 2.

Comparing Algorithms 1 and 2, we see that

- x_k is some point on the line between c_{k-1} and x_{k-1}^+ , and
- Q_k is an average of the previous quadratic Q_{k-1} and the strong convexity quadratic lower bound Q based at x_k .

As we discuss in Appendix A, we can modify Nesterov's method so that like in optimal quadratic averaging, we set $x_k = \mathtt{line_search}\left(c_{k-1}, x_{k-1}^+\right)$ in each iteration. After this change, only two differences remain between the schemes:

```
Algorithm 2: General scheme of an optimal method [Nesterov] Input: Starting points x_0 and c_0, strong convexity constant \alpha>0, smoothness parameter \beta>0, and initial quadratic curvature \gamma_0\geq\alpha. Output: Final quadratic Q_K(x)=v_K+\frac{\gamma_K}{2}\|x-c_K\|^2. Set Q_0(x)=v_0+\frac{\gamma_0}{2}\|x-c_0\|^2, where v_0=f(x_0)-\frac{1}{2\beta}\|\nabla f(x_0)\|^2; for k=1,\ldots,K do | Compute averaging parameter \lambda_k\in(0,1) from \beta\lambda_k^2=(1-\lambda_k)\gamma_{k-1}+\lambda_k\alpha; Set \gamma_k=(1-\lambda_k)\gamma_{k-1}+\lambda_k\alpha.; Set x_k=(1-\theta_k)c_{k-1}+\theta_kx_{k-1}^+ where \theta_k=\frac{\gamma_k}{\gamma_{k-1}+\lambda_k\alpha}; Set Q(x)=\left(f(x_k)-\frac{\|\nabla f(x_k)\|^2}{2\alpha}\right)+\frac{\alpha}{2}\|x-x_k^{++}\|^2; Let c_k be the minimizer of the quadratic Q_k(x)=(1-\lambda_k)Q_{k-1}(x)+\lambda_kQ(x); end /* If we set \gamma_0=\alpha, then we have \gamma_k=\alpha, \lambda_k=\frac{1}{\sqrt{\kappa}}, and \theta_k=\frac{\sqrt{\kappa}}{1+\sqrt{\kappa}}. */
```

- the initial quadratic Q_0 is different, and
- the averaging parameter is computed differently.

These differences, however, are fundamental. In Algorithm 1, the quadratic Q_0 lower bounds f and therefore optimal averaging makes sense; in the accelerated gradient method, Q_0 does not lower bound f, and the idea of optimal averaging does not apply.

3 Optimal quadratic averaging with memory

Each iteration of Algorithm 1 forms an optimal average of the current lower quadratic model with the one from the previous iteration; that is, as stated the scheme has a memory size of one. We next show how the scheme easily adapts to maintaining limited memory, i.e. by averaging multiple quadratics in each iteration. We mention in passing that the authors of [3] left open the question of efficiently speeding up their geometric descent algorithm in practice. One approach of this flavor has recently appeared in [2, Section 4]. The optimal averaging viewpoint, developed here, provides a direct and satisfying alternative. Indeed, computing the optimal average of several quadratics is easy, and amounts to solving a small dimensional quadratic optimization problem.

To see this, fix t quadratics $Q_i(x) := v_i + \frac{\alpha}{2} \|x - c_i\|^2$, with $i \in \{1, \dots, t\}$, and a weight vector λ in the t-dimensional simplex $\Delta_t := \{x \in \mathbb{R}^t : \sum_{i=1}^t x_i = 1, x \geq 0\}$. The average quadratic

$$Q_{\lambda}(x) := \sum_{i=1}^{t} \lambda_{i} Q_{i}(x)$$

maintains the same canonical form as each Q_i .

Proposition 3.1. Define the matrix $C = \begin{bmatrix} c_1 & c_2 & \dots & c_t \end{bmatrix}$ and the vector $v = \begin{bmatrix} v_1 & v_2 & \dots & v_t \end{bmatrix}^T$. Then we have

$$Q_{\lambda}(x) = v_{\lambda} + \frac{\alpha}{2} \|x - c_{\lambda}\|^{2},$$

where

$$c_{\lambda} = C\lambda \quad and \quad v_{\lambda} = \left\langle \frac{\alpha}{2} \operatorname{diag}\left(C^{T}C\right) + v, \lambda \right\rangle - \frac{\alpha}{2} \left\|C\lambda\right\|^{2}.$$

Proof. The Hessian of Q_{λ} is simply $\frac{\alpha}{2}I$, and therefore the quadratic $Q_{\lambda}(x)$ has the form

$$v_{\lambda} + \frac{\alpha}{2} \|x - c_{\lambda}\|^2$$

for some v_{λ} and c_{λ} . Notice that c_{λ} is the minimizer of Q_{λ} , and by differentiating, we determine that $c_{\lambda} = \sum_{i=1}^{t} \lambda_{i} c_{i} = C\lambda$. We then compute

$$\begin{aligned} v_{\lambda} &= Q_{\lambda}(c_{\lambda}) = \sum_{i=1}^{t} \left(\lambda_{i} v_{i} + \frac{\lambda_{i} \alpha}{2} \left\| C \lambda - c_{i} \right\|^{2} \right) \\ &= \langle v, \lambda \rangle + \frac{\alpha}{2} \sum_{i=1}^{t} \lambda_{i} \left(\left\| C \lambda \right\|^{2} - 2 \left\langle C \lambda, c_{i} \right\rangle + \left\| c_{i} \right\|^{2} \right) \\ &= \langle v, \lambda \rangle + \frac{\alpha}{2} \left\| C \lambda \right\|^{2} - \alpha \left\langle C \lambda, \sum_{i=1}^{t} \lambda_{i} c_{i} \right\rangle + \frac{\alpha}{2} \sum_{i=1}^{t} \lambda_{i} \left\| c_{i} \right\|^{2} \\ &= \left\langle \frac{\alpha}{2} \operatorname{diag} \left(C^{T} C \right) + v, \lambda \right\rangle - \frac{\alpha}{2} \left\| C \lambda \right\|^{2}. \end{aligned}$$

The proof is complete.

Naturally, we define the *optimal averaging* of the quadratics Q_i , with $i \in \{1, 2, ..., t\}$, to be $Q_{\bar{\lambda}}$, where $\bar{\lambda}$ is the maximizer of the concave quadratic

$$v_{\lambda} = \left\langle \frac{\alpha}{2} \operatorname{diag}\left(C^{T}C\right) + v, \lambda \right\rangle - \frac{\alpha}{2} \|C\lambda\|^{2}$$

over the simplex Δ_t . There is no closed form expression for $\bar{\lambda}$, but one can quickly find it by solving a quadratic program in t variables, for example by an active set method. Moreover, some thought shows that the matrix C^TC can be efficiently updated if one of the centers changes; we omit the details.

We propose an optimal averaging scheme with memory in Algorithm 3. As we see in Section 5, the method performs well numerically. Moreover, the scheme enjoys the same convergence guarantees as Algorithm 1; that is, Theorem 2.3 applies to Algorithm 3, with nearly the same proof (which we omit).

The reader may notice that Algorithm 3 shows some similarity to the classical Kelley's method for minimizing nonsmooth convex functions [5]. In the simplest case of minimizing a smooth convex function f on \mathbb{R}^n , Kelley's method iterates the following steps

$$x_{k+1} = \underset{x}{\operatorname{argmin}} \ f_k(x)$$

for the functions

$$f_k(x) := \max_{i=1,\dots,k} \{ f(x_i) + \langle \nabla f(x_i), x - x_i \rangle \}.$$

```
Algorithm 3: Optimal Quadratic Averaging with Memory

Input: Starting point x_0, strong convexity constant \alpha > 0, and memory size t \ge 1.

Output: Final quadratic Q_K(x) = v_K + \frac{\alpha}{2} \|x - c_K\|^2 and x_K^+.

Set Q_0(x) = v_0 + \frac{\alpha}{2} \|x - c_0\|^2, where v_0 = f(x_0) - \frac{\|\nabla f(x_0)\|^2}{2\alpha} and c_0 = x_0^{++}; for k = 1, \ldots, K do

Set x_k = \text{line\_search}(c_{k-1}, x_{k-1}^+);

Set M_k(x) = f(x_k) - \frac{\|\nabla f(x_k)\|^2}{2\alpha} + \frac{\alpha}{2} \|x - c_k\|^2;

Let Q_k(x) := v_k + \frac{\alpha}{2} \|x - c_k\|^2 be the optimal averaging of the k + 1 quadratics Q_{k-1}, M_k, M_{k-1}, \ldots, M_1 if k \le t, or of the t + 1 quadratics Q_{k-1}, M_k, M_{k-1}, \ldots, M_{k-t+1} if k \ge t + 1; end
```

In other words, the scheme iteratively minimizes the lower-models f_k of f. Coming back to the optimal averaging viewpoint, suppose that $Q_{\bar{\lambda}}$ is an optimal average of the lower-bounding quadratics Q_i , for i = 1, ..., k. Then we may write

$$v_{\bar{\lambda}} = \max_{\lambda \in \Delta_k} \min_x \sum_i \lambda_i Q_i(x) = \min_x \max_{\lambda \in \Delta_k} \sum_i \lambda_i Q_i(x) = \min_x \left(\max_{i=1,\dots,k} Q_i(x) \right)$$

Thus $v_{\bar{\lambda}}$ is the minimal value of the now different lower-model, $\max_{i=1,\dots,k} Q_i$, of f. Kelly's method is known to have poor numerical performance and convergence guarantees (e.g. [7, Section 3.3.2]), while Algorithm 3 achieves the optimal linear convergence rate. This disparity is of course based on the two key distinctions: (1) using quadratic lower-models coming from strong convexity instead of linear functions, and (2) maintaining two separate sequences c_k (centers) and x_k (sources of lower model updates).

4 Connection to geometric descent

Algorithm 1 is largely motivated by the geometric descent method introduced by Bubeck, Lee, and Singh [3]. In this section, we describe the close connection between the two schemes.

4.1 Suboptimal geometric descent method

The basic idea of geometric descent is that for each point $x \in \mathbb{R}^n$, the strong convexity lower bound $f^* \geq q(x^*; x)$ defines a ball containing x^* :

$$x^* \in B\left(x^{++}, \frac{\|\nabla f(x)\|^2}{\alpha^2} - \frac{2}{\alpha}(f(x) - f^*)\right).$$

In turn, taking into account (1) yields the guarantee

$$x^* \in B\left(x^{++}, \left(1 - \frac{1}{\kappa}\right) \frac{\|\nabla f(x)\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x^+) - f^*\right)\right).$$
 (5)

A crude upper estimate of the radius above is obtained simply by ignoring the nonnegative term $\frac{2}{\alpha}(f(x^+) - f^*)$. The suboptimal geometric descent method proceeds as follows. Suppose we have available some ball $B\left(c_0,R_0^2\right)$ containing x^* . As discussed, the quadratic lower bound at the center c_0 , namely $f^* \geq q(x^*,c_0)$, yields another ball $B\left(c_0^{++},\left(1-\frac{1}{\kappa}\right)\frac{\|\nabla f(c_0)\|^2}{\alpha^2}\right)$ containing x^* . Geometrically it is clear that the intersection of these two balls must be significantly smaller than either of the individual balls. The following lemma from [3] makes this observation precise; see Figure 2 for an illustration.

Lemma 4.1 (Minimal enclosing ball of the intersection). Fix a center $x \in \mathbb{R}^n$, square radius $R^2 > 0$, step $h \in \mathbb{R}^n$, and $\epsilon \in (0,1)$. Then there exists a new center $c \in \mathbb{R}^n$ with

$$B(x, R^2) \cap B(x + h, (1 - \epsilon) ||h||^2) \subset B(c, (1 - \epsilon)R^2).$$

An application of Lemma 4.1 yields a new center c_1 with

$$B\left(c_0, R_0^2\right) \cap B\left(c_0^{++}, \left(1 - \frac{1}{\kappa}\right) \frac{\|\nabla f(c_0)\|^2}{\alpha^2}\right) \subset B\left(c_1, \left(1 - \frac{1}{\kappa}\right) R_0^2\right).$$

Repeating the procedure with the new ball $B\left(c_1,\left(1-\frac{1}{\kappa}\right)R_0^2\right)$ yields a sequence of centers c_k satisfying

$$||c_k - x^*||^2 \le \left(1 - \frac{1}{\kappa}\right)^k R_0^2.$$

We note that the centers c_k and R_0^2 of the minimal enclosing balls in Lemma 4.1 are easy to compute; see Algorithm 1 in [3].

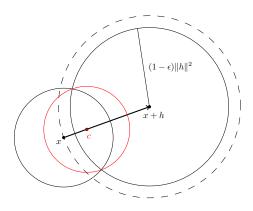


Figure 2: Minimal enclosing ball of the intersection.

There is a very close connection between finding the minimal enclosing ball of the intersection of two balls and of optimally averaging quadratics. To see this, consider again two quadratics

$$f(x) \ge Q_A(x) := v_A + \frac{\alpha}{2} \|x - x_A\|^2$$
 and $f(x) \ge Q_B(x) := v_B + \frac{\alpha}{2} \|x - x_B\|^2$.

Let \overline{Q} be the optimal average of Q_A and Q_B . Notice that since Q_A , Q_B , and \overline{Q} lower bound f, the minimizer x^* of f is guaranteed to lie in the three balls:

$$B\left(x_A, R_A^2\right)$$
 where $R_A^2 = \frac{2}{\alpha} \left(\hat{f} - v_A\right)$,
 $B\left(x_B, R_B^2\right)$ where $R_B^2 = \frac{2}{\alpha} \left(\hat{f} - v_B\right)$,
 $B\left(\bar{c}, R^2\right)$ where $R^2 = \frac{2}{\alpha} \left(\hat{f} - \bar{v}\right)$,

where \hat{f} is any upper bound on f^* . The following elementary fact is true.

Proposition 4.2 (Minimal enclosing ball and optimal averaging). The ball $B(\bar{c}, R^2)$ is precisely the minimal enclosing ball of the intersection $B(x_A, R_A^2) \cap B(x_B, R_B^2)$.

Proof. Define the quantity $\hat{\lambda} = \frac{1}{2} + \frac{v_A - v_B}{\alpha ||x_A - x_B||^2}$. If $\hat{\lambda}$ lies in the unit interval [0, 1], then a quick computation using Lemma 2.2 shows the expressions

$$R^{2} = R_{B}^{2} - \frac{\left(\|x_{A} - x_{B}\|^{2} + R_{B}^{2} - R_{A}^{2}\right)^{2}}{4\|x_{A} - x_{B}\|^{2}}$$

and

$$\bar{c} = \bar{\lambda}x_A + (1 - \bar{\lambda})x_B = \frac{1}{2}(x_A + x_B) - \frac{R_A^2 - R_B^2}{2\|x_A - x_B\|^2}(x_A - x_B).$$

Now observe

$$\hat{\lambda} < 0$$
 if and only if $||x_A - x_B||^2 < R_A^2 - R_B^2$
 $\hat{\lambda} \in [0, 1]$ if and only if $||x_A - x_B||^2 \ge |R_A^2 - R_B^2|$, and $\hat{\lambda} > 1$ if and only if $||x_A - x_B||^2 < R_B^2 - R_A^2$.

Comparing with the recipe [3, Algorithm 1] for computing the minimal enclosing ball, we see that $B(\bar{c}, R^2)$ is the minimal enclosing ball of the intersection $B(x_A, R_A^2) \cap B(x_B, R_B^2)$. \square

4.2 Optimal geometric descent method

To obtain an optimal method, the authors of [3] observe that the term $\frac{2}{\alpha}(f(x^+) - f^*)$ in the inclusion (5) cannot be ignored. Exploiting this term will require maintaining two sequences c_k (the centers of the balls) and x_k (points for generating new balls). Suppose in iteration k, we know that x^* lies in the ball

$$B\left(c_k, R_k^2 - \frac{2}{\alpha}\left(f(x_k^+) - f^*\right)\right).$$

Consider now an arbitrary point, denoted suggestively by x_{k+1} . Then (5) implies the inclusion

$$x^* \in B\left(x_{k+1}^{++}, \left(1 - \frac{1}{\kappa}\right) \frac{\|\nabla f(x_{k+1})\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right). \tag{6}$$

If we choose x_{k+1} to satisfy $f(x_{k+1}) \leq f(x_k^+)$ and apply inequality (1) with $x = x_{k+1}$, we can get a new upper estimate of the initial ball,

$$x^* \in B\left(c_k, R_k^2 - \frac{1}{\kappa} \frac{\|\nabla f(x_{k+1})\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right). \tag{7}$$

It seems clear that if the centers c_k and x_{k+1}^{++} of the two balls in (6) and (7) are "sufficiently far apart", then their intersection is contained in an even smaller ball. This is the content of following lemma from [3].

Lemma 4.3 (Two balls shrinking). Fix centers $x_A, x_B \in \mathbb{R}^n$ and square radii $r_A^2, r_B^2 > 0$. Also fix $\epsilon \in (0,1)$ and suppose $||x_A - x_B||^2 \ge r_B^2$. Then there exists a new center $c \in \mathbb{R}^n$ such that for any $\delta > 0$, we have

$$B(x_A, r_A^2 - \epsilon r_B^2 - \delta) \cap B(x_B, (1 - \epsilon)r_B^2 - \delta) \subset B(c, (1 - \sqrt{\epsilon})r_A^2 - \delta).$$

A quick application of this result shows that provided the estimate

$$\|x_{k+1}^{++} - c_k\|^2 \ge \frac{\|\nabla f(x_{k+1})\|^2}{\alpha^2}$$
 (8)

holds, there exists a new center c_{k+1} with

$$x^* \in B\left(c_{k+1}, \left(1 - \frac{1}{\sqrt{\kappa}}\right) R_k^2 - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right).$$

One way to ensure that x_{k+1} satisfies the two key conditions, $f(x_{k+1}) \leq f(x_k^+)$ and inequality (8), is to simply let x_{k+1} be the minimizer of f along the line between c_k and x_k^+ . Trivially this guarantees the inequality $f(x_{k+1}) \leq f(x_k^+)$, while the univariate optimality condition $\nabla f(x_{k+1}) \perp (c_k - x_{k+1})$ ensures that (8) holds. This is exactly the motivation for the line-search procedure in Algorithm 1. Repeating the process yields iterates c_k that satisfy the optimal linear rate of convergence

$$||c_k - x^*||^2 \le \left(1 - \frac{1}{\sqrt{\kappa}}\right)^k R_0^2.$$

The precise method is described in Algorithm 4.

5 Numerical examples

In this section, we numerically illustrate optimality gap convergence in Algorithm 1, and explore how Algorithm 3, the variant of Algorithm 1 with memory, aids performance. To this end, we focus on minimizing two functions: the regularized logistic loss function

$$L(w) := \frac{1}{N} \sum_{i=1}^{N} \log \left(1 + e^{-y_i w^T x_i} \right) + \frac{\alpha}{2} \|w\|^2,$$

where $x_i \in \mathbb{R}^n$ and $y_i \in \{\pm 1\}$ are labeled training data, and the Rosenbrock function

$$f(x) = \frac{B}{2} \left((1 - x_1)^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2 \right) + \frac{1}{2} \sum_{i=1}^n x_i^2.$$

For the logistic regression examples, we use the LIBSVM [4] data sets a1a (N = 1605, n = 123) and colon-cancer (N = 62, n = 2000).

```
Algorithm 4: Geometric Descent Method [Bubeck, Lee, Singh]

Input: Starting point x_0, strong convexity constant \alpha > 0.

Output: x_K^+

Set c_0 = x_0^{++} and R_0^2 = \frac{\|\nabla f(x_0)\|^2}{\alpha^2} - \frac{2}{\alpha} \left( f(x_0) - f(x_0^+) \right);

for k = 1, \ldots, K do

Set x_k = \text{line\_search} \left( x_{k-1}^+, c_{k-1} \right);

Set x_k = x_k - \alpha^{-1} \nabla f(x_k) and x_k^2 = \frac{\|\nabla f(x_k)\|^2}{\alpha^2} - \frac{2}{\alpha} \left( f(x_k) - f(x_k^+) \right);

Set x_B = c_{k-1} and x_B^2 = x_{k-1}^2 - \frac{2}{\alpha} \left( f(x_{k-1}^+) - f(x_k^+) \right);

Let x_k^2 = x_k^2 - \frac{2}{\alpha} \left( f(x_k^+) - f(x_k^+) \right);

Let x_k^2 = x_k^2 - \frac{2}{\alpha} \left( f(x_k^+) - f(x_k^+) \right);

end
```

5.1 Optimality gap convergence

From inequality (2), we get the well-known optimality gap estimate for strongly convex functions

$$f(x) - f^* \le \frac{\|\nabla f(x)\|^2}{2\alpha}.$$
(9)

How does this estimate compare with the gaps $g_k := f(x_k^+) - v_k$ generated by Algorithm 1? Obviously the answer depends on the point where we evaluate the gap estimate in (9). Nonetheless, we can say that the gaps g_k are tighter than the gaps $G_k := \frac{\|\nabla f(x_k)\|^2}{2\alpha}$. Indeed, by the definition of v_k , we trivially have $v_k \ge f(x_k) - G_k$ and thus

$$g_k = f(x_k^+) - v_k \le f(x_k) - v_k \le G_k.$$

On a relative scale, the difference between g_k and G_k is striking; see Figure 3. Notice that G_k is an optimality gap estimate before averaging, and g_k is an optimality gap estimate after averaging; the plots in Figure 3 show that optimal quadratic averaging makes great relative progress per iteration.

In Figure 4, we plot g_k , the true gaps $f(x_k^+) - f^*$, and the gap estimate in (9) at x_k , x_k^+ , and c_k for the Rosenbrock function and the logistic loss function. The true gaps are the tightest, albeit unknown at runtime. Surprisingly, the gaps $\frac{\|\nabla f(c_k)\|^2}{2\alpha}$ are quite bad: several orders of magnitude larger than g_k . So even though the centers c_k may appear to be the focal points of the algorithm, the points x_k^+ are the ones to monitor in practice. Finally we note that the gaps g_k and $\frac{\|\nabla f(x_k^+)\|^2}{2\alpha}$ are comparable, even though g_k does not rely on gradient information at x_k^+ .

5.2 Optimal quadratic averaging with memory

To demonstrate the effectiveness of optimal quadratic averaging with memory, we use it to minimize the logistic loss (see Figure 5). The speedup over the memoryless method is significant, even when taking into account the extra work per iteration needed to solve the small dimensional quadratic subproblems. In Figure 6, we compare Algorithm 3 with L-BFGS. The two schemes are on par with each other, and neither is better than the other in all cases. L-BFGS with memory size m actually stores m pairs of vectors, whereas Algorithm 3

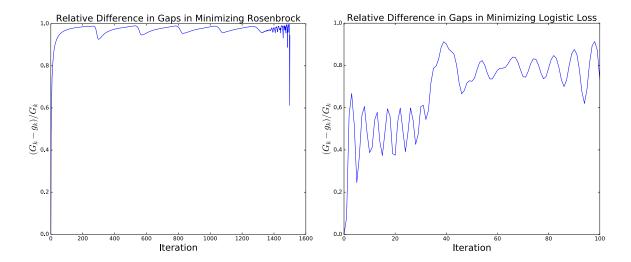


Figure 3: Relative differences in gaps $\frac{G_k - g_k}{G_k}$ on the Rosenbrock function $(B = 10^6, n = 200)$, and on the logistic loss on the colon-cancer data set with regularization $\alpha = 0.0001$.

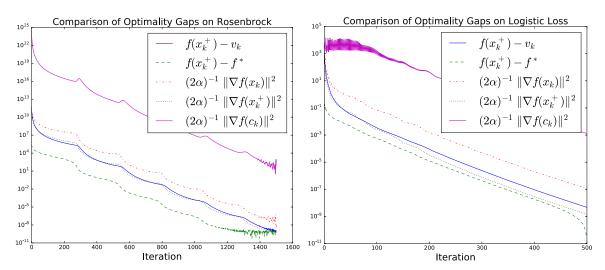


Figure 4: Comparison of various optimality gaps on the Rosenbrock function ($B = 10^6$, n = 200), and on the logistic loss on the a1a data set with regularization $\alpha = 0.0001$.

with memory size t only stores t vectors. Thus it is perhaps fairer to compare L-BFGS with memory size t to Algorithm 3 with memory size t = 2m (see Figure 7).

Empirically, we've noticed that the small dimensional quadratic program in Algorithm 3 must be solved to high accuracy, especially on poorly conditioned problems. In Figure 8, we again compare L-BFGS and Algorithm 3 on logisitic regression, but with less regularization.

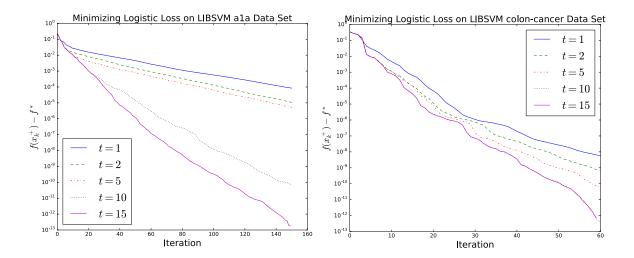


Figure 5: Algorithm 3 with various memory sizes t. The case t=1 corresponds to the memoryless optimal averaging method in Algorithm 1. The task is logistic regression, with regularization $\alpha=0.0001$, on data sets a1a and colon-cancer.

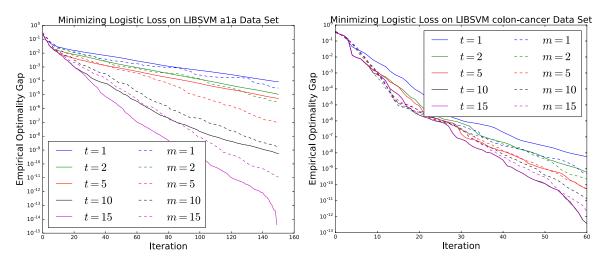


Figure 6: Algorithm 3 with memory size t versus L-BFGS with memory size m. The task is logistic regression, with regularization $\alpha = 0.0001$, on data sets a1a and colon-cancer.

6 Comments on proximal extensions

It is natural to try to extend geometric descent and optimal quadratic averaging to a proximal setting. For the sake of concreteness, let us focus on geometric descent. We can easily extend the suboptimal version of the algorithm to the proximal setting, but some difficulties arise when accelerating the method. Suppose we are interested in solving the problem

$$\min_{x} f(x) := g(x) + h(x),$$

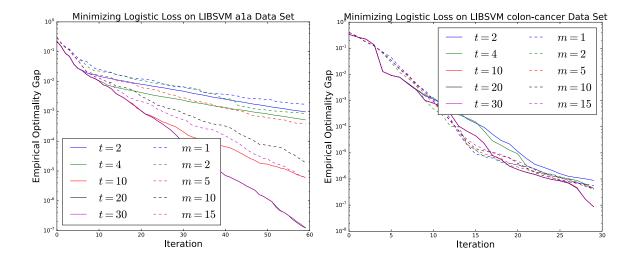


Figure 7: A fairer (equal memory) comparison of Algorithm 3 and L-BFGS. The task is still logistic regression, with regularization $\alpha = 0.0001$, on data sets a1a and colon-cancer. We focus on lower accuracy than we did in Figure 6.

where $g: \mathbb{R}^n \to \mathbb{R}$ is β -smooth and α -strongly convex, and $h: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is closed, convex, and is such that the proximal mapping

$$\operatorname{prox}_{th}(x) := \underset{z}{\operatorname{argmin}} \{ h(z) + \frac{1}{2t} ||z - x||^2 \}$$

is easily computable. In the analysis of first-order methods for such problems, the gradient mapping $G_t(x) := \frac{1}{t} (x - \text{prox}_{th}(x - t\nabla g(x)))$ plays the role of the usual gradient. The following is a standard estimate; see for example [7, Section 2.2.3]. We provide a proof for completeness.

Lemma 6.1. Fix a step length t > 0 and define a proximal gradient step $x^+ := x - tG_t(x)$. Then for every $y \in \mathbb{R}^n$ the inequality holds:

$$f(y) \ge f(x^+) + \langle G_t(x), y - x \rangle + t \left(1 - \frac{\beta t}{2} \right) ||G_t(x)||^2 + \frac{\alpha}{2} ||y - x||^2.$$

Proof. Appealing to β -smoothness of g, we deduce

$$f(x^+) \le g(x) - t \langle \nabla g(x), G_t(x) \rangle + \frac{\beta t^2}{2} ||G_t(x)||^2 + h(x^+).$$

Furthermore, strong convexity of g implies

$$f(x^+) \le g(y) + \langle \nabla g(x), x^+ - y \rangle - \frac{\alpha}{2} \|y - x\|^2 + \frac{\beta t^2}{2} \|G_t(x)\|^2 + h(x^+).$$

Finally, using the observation that $G_t(x) - \nabla g(x)$ belongs to $\partial h(x^+)$, we have

$$f(x^{+}) \le f(y) + \langle G_t(x), x^{+} - y \rangle - \frac{\alpha}{2} \|y - x\|^2 + \frac{\beta t^2}{2} \|G_t(x)\|^2.$$

Rearrangement completes the proof.

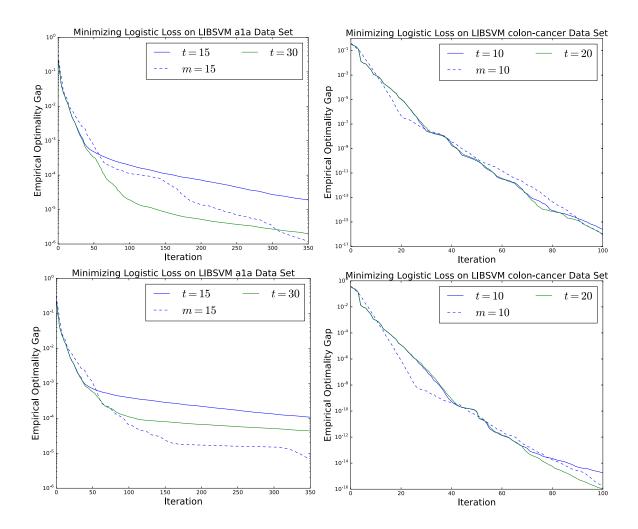


Figure 8: Algorithm 3 with memory size t versus L-BFGS with memory size m. The task is logistic regression on data sets a1a and colon-cancer, with $\alpha = 10^{-6}$ (top row) and $\alpha = 10^{-8}$ (bottom row).

If we let $y = x^*$ in Lemma 6.1 and rearrange we get

$$x^* \in B\left(x - \frac{1}{\alpha}G_t(x), \left(\frac{1}{\alpha^2} - \frac{2}{\alpha}t + \frac{\beta}{\alpha}t^2\right) \|G_t(x)\|^2 - \frac{2}{\alpha}\left(f(x^+) - f^*\right)\right).$$

How should we choose the step length t? A simple approach is to choose t to minimize the quantity $\frac{1}{\alpha^2} - \frac{2}{\alpha}t + \frac{\beta}{\alpha}t^2$, i.e., set $t = \frac{1}{\beta}$. With this choice of t, we deduce the inclusion

$$x^* \in B\left(x^{++}, \left(1 - \frac{1}{\kappa}\right) \frac{\|G_{1/\beta}(x)\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x^+) - f^*\right)\right),$$

where $x^{++} = x - \frac{1}{\alpha}G_{1/\beta}(x)$ is a long step and $x^{+} = x - \frac{1}{\beta}G_{1/\beta}(x)$ is a short step. A proximal version of the suboptimal geometric descent follows easily from Lemma 4.1.

To accelerate the proximal geometric descent algorithm we assume in iteration k that x^* lies in some ball

$$B\left(c_k, R_k^2 - \frac{2}{\alpha}\left(f(y_k) - f^*\right)\right).$$

We then consider a second minimizer enclosing ball derived from information at some point x_{k+1} :

$$x^* \in B\left(x_{k+1}^{++}, \left(1 - \frac{1}{\kappa}\right) \frac{\left\|G_{1/\beta}(x_{k+1})\right\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right).$$

Following the same pattern as in Section 4.2, if we choose x_{k+1} to satisfy $f(x_{k+1}) \leq f(y_k)$ and appeal to the smoothness inequality $f(x_{k+1}^+) \leq f(x_{k+1}) - \frac{1}{2\beta} \|G_{1/\beta}(x_{k+1})\|^2$, we deduce the inclusion

$$x^* \in B\left(c_k, R_k^2 - \frac{1}{\kappa} \frac{\|G_{1/\beta}(x_{k+1})\|^2}{\alpha^2} - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right).$$

By Lemma 4.3 there is a new center c_{k+1} with

$$x^* \in B\left(c_{k+1}, \left(1 - \frac{1}{\sqrt{k}}\right) R_k^2 - \frac{2}{\alpha} \left(f(x_{k+1}^+) - f^*\right)\right),$$

provided the old centers x_{k+1}^{++} and c_k are far apart; specifically, we must be sure that the inequality

$$||x_{k+1}^{++} - c_k||^2 \ge \frac{||G_{1/\beta}(x_{k+1})||^2}{\alpha^2}$$
 holds.

How do we choose x_{k+1} to satisfy both $f(x_{k+1}) \leq f(y_k)$ and $||x_{k+1}^{++} - c_k||^2 \geq \frac{||G_{1/\beta}(x_{k+1})||^2}{\alpha^2}$? The desired x_{k+1} does exist; for example, $x_{k+1} = x^*$ is such a point. In the proximal setting, it is not clear how to choose x_{k+1} to ensure these two inequalities (even for specific problem classes). This is an interesting topic for future research.

References

- [1] H. Attouch, J. Peypouquet, and P. Redont. On the fast convergence of an inertial gradient-like dynamics with vanishing viscosity. *Preprint*, arXiv:1507.04782, 2015.
- [2] S. Bubeck and Y.T. Lee. Black-box optimization with a politician. *Preprint*, arXiv:1602.04847, 2016.
- [3] S. Bubeck, Y.T. Lee, and M. Singh. A geometric alternative to nesterov's accelerated gradient descent. *Preprint*, arXiv:1506.08187, 2015.
- [4] C.-C. Chang and C.-J. Lin. LIBSVM: A library for support vector machines. *ACM Transactions on Intelligent Systems and Technology*, 2:27:1–27:27, 2011.
- [5] J. E. Kelley, Jr. The cutting-plane method for solving convex programs. J. Soc. Indust. Appl. Math., 8:703–712, 1960.

- [6] L. Lessard, B. Recht, and A. Packard. Analysis and Design of Optimization Algorithms via Integral Quadratic Constraints. SIAM J. Optim., 26(1):57–95, 2016.
- [7] Y. Nesterov. Introductory lectures on convex optimization, volume 87 of Applied Optimization. Kluwer Academic Publishers, Boston, MA, 2004. A basic course.
- [8] Yu. E. Nesterov. A method for solving the convex programming problem with convergence rate $O(1/k^2)$. Dokl. Akad. Nauk SSSR, 269(3):543–547, 1983.
- [9] W. Su, S. Boyd, and E. Candes. A differential equation for modeling nesterovs accelerated gradient method: Theory and insights. In Z. Ghahramani, M. Welling, C. Cortes, N.d. Lawrence, and K.q. Weinberger, editors, Advances in Neural Information Processing Systems 27, pages 2510–2518. Curran Associates, Inc., 2014.

A Exact line search in accelerated gradient descent

Nesterov's method is based on an estimate sequence; that is, a sequence of functions Q_k and nonnegative numbers Λ_k with

$$\Lambda_k \to 0$$
 and $Q_k(x) \le (1 - \Lambda_k)f(x) + \Lambda_k Q_0(x)$.

Estimate sequences are useful because if y_k satisfies $f(y_k) \leq v_k := \min_{x \in \mathbb{R}^n} Q_k(x)$, then

$$f(y_k) - f^* \le \Lambda_k (Q_0(x^*) - f^*);$$

that is, $f(y_k)$ approaches f^* with error proportional to Λ_k , see [7].

The quadratics in Algorithm 2 (with appropriately chosen Λ_k) form an estimate sequence. To explain, for $k \geq 1$, pick vectors x_k and numbers $\lambda_k \in (\delta, 1)$ with $\delta > 0$. Next, recursively define

$$Q_0(x) = v_0 + \frac{\gamma_0}{2} \|x - c_0\|^2 \quad \text{and}$$

$$Q_k(x) = (1 - \lambda_k) Q_{k-1}(x) + \lambda_k \left(f(x_k) - \frac{\|\nabla f(x_k)\|^2}{2\alpha} + \frac{\alpha}{2} \|x - x_k^{++}\|^2 \right).$$

Then the quadratics Q_k and numbers $\Lambda_k = \prod_{j=1}^k (1 - \lambda_j)$ are an estimate sequence for f. Nesterov's method is designed to ensure the inequality $f(x_k^+) \leq v_k$ with the added *optimal* rate condition $\lambda_k \geq \sqrt{\frac{\alpha}{\beta}}$.

The scheme in Algorithm 2 with $x_k = \mathtt{line_search}\left(c_{k-1}, x_{k-1}^+\right)$ also guarantees these conditions. Trivially we have $f(x_0^+) \leq v_0$. Assume, for induction, that we have $f(x_{k-1}^+) \leq v_{k-1}$. From [7, Lemma 2.2.3], we know

$$v_{k} = (1 - \lambda_{k})v_{k-1} + \lambda_{k}f(x_{k}) - \frac{\lambda_{k}^{2}}{2\gamma_{k}} \|\nabla f(x_{k})\|^{2} + \frac{\lambda_{k}(1 - \lambda_{k})\gamma_{k-1}}{\gamma_{k}} \left(\frac{\alpha}{2} \|x_{k} - c_{k-1}\|^{2} + \langle \nabla f(x_{k}), c_{k-1} - x_{k} \rangle \right).$$

Since $x_k = \text{line_search}(c_{k-1}, x_{k-1}^+)$, we have $f(x_k) \le f(x_{k-1}^+) \le v_{k-1}$ and $\langle \nabla f(x_k), c_{k-1} - x_k \rangle = 0$, and therefore

$$v_k \ge f(x_k) - \frac{\lambda_k^2}{2\gamma_k} \|\nabla f(x_k)\|^2 = f(x_k) - \frac{1}{2\beta} \|\nabla f(x_k)\|^2 \ge f(x_k^+).$$

Provided we set $\gamma_0 \ge \alpha$, we get the optimal rate condition $\lambda_k = \sqrt{\frac{\gamma_k}{\beta}} \ge \sqrt{\frac{\alpha}{\beta}}$.