

Performance of first-order methods for smooth convex minimization: a novel approach

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Abstract We introduce a novel approach for analyzing the worst-case performance of first-order black-box optimization methods. We focus on smooth unconstrained convex minimization over the Euclidean space. Our approach relies on the observation that by definition, the worst-case behavior of a black-box optimization method is by itself an optimization problem, which we call the performance estimation problem (PEP). We formulate and analyze the PEP for two classes of first-order algorithms. We first apply this approach on the classical gradient method and derive a new and tight analytical bound on its performance. We then consider a broader class of first-order black-box methods, which among others, include the so-called heavy-ball method and the fast gradient schemes. We show that for this broader class, it is possible to derive new bounds on the performance of these methods by solving an adequately relaxed convex semidefinite PEP. Finally, we show an efficient procedure for finding optimal step sizes which results in a first-order black-box method that achieves best worst-case performance.

Keywords Performance of first-order algorithms · Rate of convergence · Complexity · Smooth convex minimization · Duality · Semidefinite relaxations · Fast gradient schemes · Heavy Ball method

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1 Introduction

First-order convex optimization methods have recently gained in popularity both in theoretical optimization and in many scientific applications, such as signal and image processing, communications, machine learning, and many more. These problems are very large scale, and first-order methods, which in general involve very cheap and simple computational iterations, are often the best option to tackle such problems in a reasonable time, when moderate accuracy solutions are sufficient. For convex optimization problems, there exists an extensive literature on the development and analysis of first-order methods, and in recent years, this has been revitalized at a quick pace due to the emergence of many fundamental new applications alluded above. On the theoretical front see e.g., the recent works [9, 12, 19] and for applications see the collections [17, 21] and references therein.

This work is not on the development of new algorithms, rather it focuses on the theoretical performance analysis of first-order methods for unconstrained minimization with an objective function which is known to belong to a given family \mathcal{F} of smooth convex functions over the Euclidean space \mathbb{R}^d .

Following the seminal work of Nemirovsky and Yudin [14] in the complexity analysis of convex optimization methods, we measure the computational cost based on the oracle model of optimization. According to this model, a *first-order black-box* optimization method is an algorithm \mathcal{A} which has knowledge of the underlying space \mathbb{R}^d and the family \mathcal{F} , where the function itself is not known. To gain information on the objective function f to be minimized, the algorithm queries a first-order oracle, that is, a subroutine which given as input a point in \mathbb{R}^d , returns the value of the objective function and its gradient at that point. The algorithm starts with a given point $x_0 \in \mathbb{R}^d$ and generates a finite sequence of points $\{x_i \in \mathbb{R}^d : i = 1, \dots, N\}$, where at each step the algorithm can depend only on the previous steps, their function values and gradients via some rule

$$x_{i+1} = \mathcal{A}(x_0, \dots, x_i; f(x_0), \dots, f(x_i); f'(x_0), \dots, f'(x_i)), \quad i = 0, \dots, N - 1,$$

where $f'(\cdot)$ stands for the gradient of $f(\cdot)$. Note that the algorithm has another implicit knowledge, i.e., that the distance from its initial point x_0 to a minimizer $x_* \in X_*(f)$ of f is bounded by some constant $R > 0$, see more precise definitions in the next section.

Given a desired accuracy $\varepsilon > 0$, applying the given algorithm on the function f in the class \mathcal{F} , the algorithm stops when it produces an approximate solution x_ε which is ε -optimal, that is such that

$$f(x_\varepsilon) - f(x_*) \leq \varepsilon.$$

The worst-case performance (or complexity) of a first-order black-box optimization algorithm is then measured by the number of oracle calls the algorithm needs to find such an approximate solution. Equivalently, we can measure the worst-case performance of an algorithm by looking at the absolute inaccuracy

$$\delta(f, x_N) = f(x_N) - f(x_*),$$

where x_N is the result of the algorithm after making N calls to the oracle. Throughout this paper we will use the latter form to measure the performance of a given algorithm.

Building on this model, in this work we introduce a novel approach for analyzing the performance of a given first-order scheme. Our approach relies on the observation that by definition, the worst-case behavior of a first-order black-box optimization algorithm is by itself an optimization problem which consists of finding the maximal absolute inaccuracy over all possible inputs to the algorithm. Thus, with x_N being the output of the algorithm after making N calls to the oracle, we look at the solution of the following *Performance Estimation Problem* (PEP):

$$\begin{aligned} \max \quad & f(x_N) - f(x_*) & (P) \\ \text{s.t.} \quad & f \in \mathcal{F}, \\ & x_{i+1} = \mathcal{A}(x_0, \dots, x_i; f(x_0), \dots, f(x_i); f'(x_0), \dots, f'(x_i)), \quad i=0, \dots, N-1, \\ & x_* \in X_*(f), \quad \|x_* - x_0\| \leq R, \\ & x_0, \dots, x_N, x_* \in \mathbb{R}^d. \end{aligned}$$

At first glance this problem seems very hard or impossible to solve. We overcome this difficulty through an analysis that relies on various types of relaxations, including duality and semi-definite relaxation techniques. The problem setting and an outline of the underlying idea of the proposed approach for analyzing (P) are described in Sect. 2. In order to develop the basic idea and tools underlying our proposed approach, we first focus on the fundamental gradient method (GM) for smooth convex minimization, and then extend it to a broader class of first-order black-box minimization methods. Obviously, the GM is a particular case of this broader class that will be analyzed below. However, it is quite important to start with the GM for two reasons. First, it allows to acquaint the reader in a more transparent way with the techniques and methodology we need to develop in order to analyze (P), thus paving the way to tackle more general schemes. Secondly, for the GM, we are able to prove a new and tight bound on its performance which is given *analytically*, see Sect. 3. Capitalizing on the methodology and tools developed in the past section, in Sect. 4, we consider a broader class of first-order black-box methods, which among others, is shown to include the so-called heavy-ball [18] and fast gradient schemes [16]. Although an analytical solution is not available for this general case, we show that for this broader class of methods, it is possible to compute *numerical estimates* for an adequate relaxation of the corresponding PEP, allowing to derive new bounds on the performance of these methods. We then derive in Sect. 5 an efficient procedure for finding optimal step sizes which results in a first-order method that achieves best worst-case performance. Our approach and analysis

give rise to some interesting problems leading us to suggest some conjectures. Finally, an “Appendix” includes the proof of a technical result.

Notation For a differentiable function f , its gradient at x is denoted by $f'(x)$. The Euclidean norm of a vector $x \in \mathbb{R}^d$ is denoted as $\|x\|$. The set of symmetric matrices in $\mathbb{R}^{n \times n}$ is denoted by \mathbb{S}^n . For two symmetric matrices A and B , $A \succeq B$, ($A \succ B$) means $A - B \succeq 0$ ($A - B \succ 0$) is positive semidefinite (positive definite). We use e_i for the i th canonical basis vector in \mathbb{R}^N , which consists of all zero components, except for its i th entry which is equal to one, and use v to denote a unit vector in \mathbb{R}^d . For an optimization problem (P), $\text{val}(P)$ stands for its optimal value.

2 The problem and the main approach

2.1 The problem and basic assumptions

Let \mathcal{A} be a first-order algorithm for solving the optimization problem

$$(M) \quad \min\{f(x) : x \in \mathbb{R}^d\}.$$

Throughout the paper we make the following assumptions:

- $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is a convex function of the type $C_L^{1,1}(\mathbb{R}^d)$, i.e., continuously differentiable with Lipschitz continuous gradient:

$$\|f'(x) - f'(y)\| \leq L\|x - y\|, \quad \forall x, y \in \mathbb{R}^d,$$

where $L > 0$ is the Lipschitz constant.

- We assume that (M) is solvable, i.e., the optimal set $X_*(f) := \arg \min f$ is non-empty.
- There exists $R > 0$, such that the distance from the given starting point of the algorithm x_0 to an optimal solution $x_* \in X_*(f)$ is bounded by R .¹

Given a convex function f in the class $C_L^{1,1}(\mathbb{R}^d)$ and any starting point $x_0 \in \mathbb{R}^d$, the algorithm \mathcal{A} is a first-order black-box scheme, i.e., it is allowed to access f only through the sequential calls to the first-order oracle that returns the value and the gradient of f at any input point x . The algorithm \mathcal{A} then generates a sequence of points $x_i \in \mathbb{R}^d$, $i = 0, \dots, N$.

2.2 Basic idea and main approach

We are interested in measuring the worst-case behavior of a given algorithm \mathcal{A} in terms of the absolute inaccuracy $f(x_N) - f(x_*)$, by solving problem (P) defined in the introduction, namely

¹ In general, the terms L and R are unknown or difficult to compute, in which case some upper bound estimates can be used in place. Note that all currently known complexity results for first-order methods depend on L and R .

$$\begin{aligned}
 & \max \quad f(x_N) - f(x_*) & \text{(P)} \\
 & \text{s.t.} \quad f \in C_L^{1,1}(\mathbb{R}^d), f \text{ is convex,} \\
 & \quad x_{i+1} = \mathcal{A}(x_0, \dots, x_i; f(x_0), \dots, f(x_i); f'(x_0), \dots, f'(x_i)), \quad i=0, \dots, N-1, \\
 & \quad x_* \in X_*(f), \|x_* - x_0\| \leq R, \\
 & \quad x_0, \dots, x_N, x_* \in \mathbb{R}^d.
 \end{aligned}$$

To tackle this problem, we suggest to perform a series of relaxations thereby reaching a tractable optimization problem.

A main difficulty in problem (P) lies in the functional constraint (the variable f is a convex function in $C_L^{1,1}(\mathbb{R}^d)$), i.e., we are facing an abstract hard optimization problem in infinite dimensions. To overcome this difficulty, the approach taken in this paper is to *relax* this constraint so that the problem can be reduced and formulated as an explicit finite dimensional problem that can eventually be adequately analyzed.

An informal description of the underlying idea consists of two main steps as follows:

- Given an algorithm \mathcal{A} that generates a finite sequence of points, to build a problem in finite dimensions we replace the functional constraint $f \in C_L^{1,1}$ in (P) by new variables in \mathbb{R}^d . These variables, are the points $\{x_0, x_1, \dots, x_N, x_*\}$ themselves, the function values and their gradients at these points. Roughly speaking, this can be seen as a sort of discretization of f at a selected set of points.
- To define constraints that relate the new variables, we use relevant/useful properties characterizing the family of convex functions in $C_L^{1,1}$, as well as the rule(s) describing the given algorithm \mathcal{A} .

This approach can, in principle, be applied to any optimization algorithm. Note that any relaxation performed on the maximization problem (P) may increase its optimal value, however, the optimal value of the relaxed problem still remains a valid upper bound on $f(x_N) - f(x_*)$. Also note that once a bound on the absolute inaccuracy has been established, it is possible to find a bound that does not depend on the unknown term $f(x_*)$, e.g., from the well-known property $\|f'(x_N)\|^2 \leq f(x_N) - f(x_*)$.

A formal description on how this approach can be applied to the GM is described in the next section, which as we shall see, allows us to derive a new tight bound on the performance of the GM.

3 An analytical bound for the gradient method

To develop the basic idea and tools underlying the proposed approach for analyzing the performance of iterative optimization algorithms, in this section we focus on the simplest fundamental method for smooth convex minimization, the GM. It will also pave the way to tackle more general first-order schemes as developed in the forthcoming sections.

3.1 A performance estimation problem for the gradient method

Consider the gradient algorithm with constant step size, as applied to problem (M) , which generates a sequence of points as follows:

Algorithm GM

0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$ convex, $x_0 \in \mathbb{R}^d$.
1. For $i = 0, \dots, N - 1$, compute $x_{i+1} = x_i - \frac{h}{L} f'(x_i)$.

Here $h > 0$ is fixed. Note that while simple, this algorithm is restricted to problems where the Lipschitz constant L is known or can be efficiently estimated.

At this point, recall that for $h = 1$, the convergence rate of the Algorithm GM can be shown to be (see for example [4, 16]):

$$f(x_N) - f(x_*) \leq \frac{L \|x_0 - x_*\|^2}{2N}, \quad \forall x_* \in X_*(f). \tag{3.1}$$

We begin our analysis with a well-known fundamental property for the class of convex $C_L^{1,1}$ functions, see e.g., [16, Theorem 2.1.5].

Proposition 1 *Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be convex and $C_L^{1,1}$. Then,*

$$\frac{1}{2L} \|f'(x) - f'(y)\|^2 \leq f(x) - f(y) - \langle f'(y), x - y \rangle, \quad \text{for all } x, y \in \mathbb{R}^d. \tag{3.2}$$

Let $x_0 \in \mathbb{R}^d$ be any starting point, let $\{x_1, \dots, x_N\}$ be the points generated by Algorithm GM and let x_* be a minimizer of f . Applying (3.2) on the points $\{x_0, \dots, x_N, x_*\}$, we get:

$$\frac{1}{2L} \|f'(x_i) - f'(x_j)\|^2 \leq f(x_i) - f(x_j) - \langle f'(x_j), x_i - x_j \rangle, \quad i, j = 0, \dots, N, *. \tag{3.3}$$

Now define

$$\begin{aligned} \delta_i &:= \frac{1}{L \|x_* - x_0\|^2} (f(x_i) - f(x_*)), \quad i = 0, \dots, N, * \\ g_i &:= \frac{1}{L \|x_* - x_0\|} f'(x_i), \quad i = 0, \dots, N, * \end{aligned}$$

and note that we always have $\delta_* = 0$ and $g_* = 0$.

In terms of δ_i, g_i , condition (3.3) becomes

$$\frac{1}{2} \|g_i - g_j\|^2 \leq \delta_i - \delta_j - \frac{\langle g_j, x_i - x_j \rangle}{\|x_* - x_0\|}, \quad i, j = 0, \dots, N, *, \tag{3.4}$$

and the recurrence defining Algorithm GM reads:

$$x_{i+1} = x_i - h\|x_* - x_0\|g_i, \quad i = 0, \dots, N - 1.$$

Problem (P) can now be relaxed by *discarding* the underlying function $f \in C_L^{1,1}$ in (P). That is, the constraint in the function space $f \in C_L^{1,1}$ with f convex, is replaced by the inequalities (3.4) characterizing this family of functions and expressed in terms of the variables $x_0, \dots, x_N, x_* \in \mathbb{R}^d, g_0, \dots, g_N \in \mathbb{R}^d$ and $\delta_0, \dots, \delta_N \in \mathbb{R}$ generated by Algorithm GM. Thus, an upper bound on the worst-case behavior of $f(x_N) - f(x_*) = L\|x_* - x_0\|^2\delta_N$ can be obtained by solving the following relaxed PEP:

$$\begin{aligned} & \max_{\substack{x_0, \dots, x_N, x_* \in \mathbb{R}^d, \\ g_0, \dots, g_N \in \mathbb{R}^d, \\ \delta_0, \dots, \delta_N \in \mathbb{R}}} L\|x_* - x_0\|^2\delta_N \\ \text{s.t.} \quad & x_{i+1} = x_i - h\|x_* - x_0\|g_i, \quad i = 0, \dots, N - 1, \\ & \frac{1}{2}\|g_i - g_j\|^2 \leq \delta_i - \delta_j - \frac{\langle g_j, x_i - x_j \rangle}{\|x_* - x_0\|}, \quad i, j = 0, \dots, N, *, \\ & \|x_* - x_0\| \leq R. \end{aligned}$$

Simplifying the PEP The obtained problem remains nontrivial to tackle. We will now perform some simplifications on this problem that will be useful for the forthcoming analysis.

First, we observe that the problem is invariant under the transformation $g'_i \leftarrow Qg_i, x'_i \leftarrow Qx_i$ for any orthogonal transformation Q . We can therefore assume without loss of generality that $x_* - x_0 = \|x_* - x_0\|v$, where v is any given unit vector in \mathbb{R}^d . Therefore, for $i = *$ the inequality constraints reads

$$\frac{1}{2}\|g_* - g_j\|^2 \leq \delta_* - \delta_j - \frac{\langle g_j, \|x_* - x_0\|v + x_0 - x_j \rangle}{\|x_* - x_0\|}, \quad j = 0, \dots, N.$$

Secondly, we consider (3.4) for the four cases $i = *, j = *, i < j$ and $j < i$, and use the equality constraints

$$x_{i+1} = x_i - h\|x_* - x_0\|g_i, \quad i = 0, \dots, N - 1$$

to eliminate the variables x_1, \dots, x_N . After some algebra, we reach the following form for the PEP:

$$\begin{aligned} & \max_{x_0, x_*, g_i \in \mathbb{R}^d, \delta_i \in \mathbb{R}} L\|x_* - x_0\|^2\delta_N \\ \text{s.t.} \quad & \frac{1}{2}\|g_i - g_j\|^2 \leq \delta_i - \delta_j - \left\langle g_j, \sum_{t=i+1}^j hg_{t-1} \right\rangle, \quad i < j = 0, \dots, N, \end{aligned}$$

$$\begin{aligned} \frac{1}{2} \|g_i - g_j\|^2 &\leq \delta_i - \delta_j + \left\langle g_j, \sum_{t=j+1}^i h g_{t-1} \right\rangle, \quad j < i = 0, \dots, N, \\ \frac{1}{2} \|g_i\|^2 &\leq \delta_i, \quad i = 0, \dots, N, \\ \frac{1}{2} \|g_i\|^2 &\leq -\delta_i - \left\langle g_i, v + \sum_{t=1}^i h g_{t-1} \right\rangle, \quad i = 0, \dots, N, \\ \|x_* - x_0\| &\leq R, \end{aligned}$$

where $i < j = 0, \dots, N$ is a shorthand notation for $i = 0, \dots, N - 1, j = i + 1, \dots, N$.

Finally, we note that the optimal solution for this problem is attained when $\|x_* - x_0\| = R$, and hence we can also eliminate the variables x_0 and x_* . This produces the following PEP for the GM, a *nonconvex quadratic* minimization problem:

$$\begin{aligned} \max_{g_i \in \mathbb{R}^d, \delta_i \in \mathbb{R}} \quad &LR^2\delta_N \\ \text{s.t.} \quad &\frac{1}{2} \|g_i - g_j\|^2 \leq \delta_i - \delta_j - \left\langle g_j, \sum_{t=i+1}^j h g_{t-1} \right\rangle, \quad i < j = 0, \dots, N, \\ &\frac{1}{2} \|g_i - g_j\|^2 \leq \delta_i - \delta_j + \left\langle g_j, \sum_{t=j+1}^i h g_{t-1} \right\rangle, \quad j < i = 0, \dots, N, \\ &\frac{1}{2} \|g_i\|^2 \leq \delta_i, \quad i = 0, \dots, N, \\ &\frac{1}{2} \|g_i\|^2 \leq -\delta_i - \left\langle g_i, v + \sum_{t=1}^i h g_{t-1} \right\rangle, \quad i = 0, \dots, N. \end{aligned}$$

This problem can be written in a more compact and useful form. Let G denote the $(N + 1) \times d$ matrix whose rows are g_0^T, \dots, g_N^T , and for notational convenience let $u_i \in \mathbb{R}^{N+1}$ denote the canonical unit vector

$$u_i = e_{i+1}, \quad i = 0, \dots, N.$$

Then for any i, j , we have

$$g_i = G^T u_i, \quad \text{tr}(G^T u_i u_j^T G) = \langle g_i, g_j \rangle, \quad \text{and} \quad \langle G^T u_i, v \rangle = \langle g_i, v \rangle.$$

Therefore, by defining the following $(N + 1) \times (N + 1)$ symmetric matrices

$$A_{i,j} = \frac{1}{2} (u_i - u_j)(u_i - u_j)^T + \frac{1}{2} \sum_{t=i+1}^j h (u_j u_{t-1}^T + u_{t-1} u_j^T),$$

$$\begin{aligned}
 B_{i,j} &= \frac{1}{2}(u_i - u_j)(u_i - u_j)^T - \frac{1}{2} \sum_{t=j+1}^i h \left(u_j u_{t-1}^T + u_{t-1} u_j^T \right), \\
 C_i &= \frac{1}{2} u_i u_i^T, \\
 D_i &= \frac{1}{2} u_i u_i^T + \frac{1}{2} \sum_{t=1}^i h \left(u_i u_{t-1}^T + u_{t-1} u_i^T \right),
 \end{aligned} \tag{3.5}$$

we can express our nonconvex quadratic minimization problem in terms of $\delta := (\delta_0, \dots, \delta_N) \in \mathbb{R}^{N+1}$ and the new matrix variable $G \in \mathbb{R}^{(N+1) \times d}$ as follows

$$\begin{aligned}
 \max_{G \in \mathbb{R}^{(N+1) \times d}, \delta \in \mathbb{R}^{N+1}} & \quad LR^2 \delta_N & \tag{G} \\
 \text{s.t.} & \quad \text{tr}(G^T A_{i,j} G) \leq \delta_i - \delta_j, \quad i < j = 0, \dots, N, \\
 & \quad \text{tr}(G^T B_{i,j} G) \leq \delta_i - \delta_j, \quad j < i = 0, \dots, N, \\
 & \quad \text{tr}(G^T C_i G) \leq \delta_i, \quad i = 0, \dots, N, \\
 & \quad \text{tr}(G^T D_i G + v u_i^T G) \leq -\delta_i, \quad i = 0, \dots, N.
 \end{aligned}$$

Problem (G) is a nonhomogeneous *Quadratic Matrix Program*, a class of problems introduced and studied by Beck [3].

3.2 A tight performance estimate for the gradient method

We now proceed to establish the two main results of this section. First, we derive an upper bound on the performance of the GM, this is accomplished via using duality arguments. Then, we show that this bound can actually be attained by applying the GM on a specific convex function in the class $C_L^{1,1}$.

In order to simplify the following analysis, we will remove some constraints from (G) and consider the bound produced by the following relaxed problem:

$$\begin{aligned}
 \max_{G \in \mathbb{R}^{(N+1) \times d}, \delta \in \mathbb{R}^{N+1}} & \quad LR^2 \delta_N & \tag{G'} \\
 \text{s.t.} & \quad \text{tr}(G^T A_{i-1,i} G) \leq \delta_{i-1} - \delta_i, \quad i = 1, \dots, N, \\
 & \quad \text{tr}(G^T D_i G + v u_i^T G) \leq -\delta_i, \quad i = 0, \dots, N.
 \end{aligned}$$

As we shall show below, it turns out that this additional relaxation has no damaging effects and produces the desired performance bound when $0 < h \leq 1$.

We are interested in deriving a dual problem for (G') which is as simple as possible, especially with respect to its dimension. As noted earlier, problem (G') is a nonhomogeneous quadratic matrix program, and a dual problem for (G') could be directly obtained by applying the results developed by Beck [3]. However, the resulting obtained dual will involve an additional matrix variable $\Phi \in \mathbb{S}^d$, where d can be very large. Instead, here by exploiting the special structure of the second set of

nonhomogeneous inequalities given in (G'), we derive an alternative dual problem, but with only one additional variable $t \in \mathbb{R}$.

To establish our dual result, the next lemma shows that a dimension reduction is possible when minimizing a quadratic matrix function sharing the special form as the one that appears in problem (G').

Lemma 1 *Let $f(X) = \text{tr}(X^T Q X + 2ba^T X)$ be a quadratic function, where $X \in \mathbb{R}^{n \times m}$, $Q \in \mathbb{S}^n$, $a \in \mathbb{R}^n$ and $0 \neq b \in \mathbb{R}^m$. Then*

$$\inf_{X \in \mathbb{R}^{n \times m}} f(X) = \inf_{\xi \in \mathbb{R}^n} f(\xi b^T).$$

Proof First, we recall (this can be easily verified) that $\inf\{f(X) : X \in \mathbb{R}^{n \times m}\} > -\infty$ if and only if $Q \geq 0$, and there exists at least one solution \bar{X} such that

$$Q\bar{X} + ab^T = 0 \Leftrightarrow \bar{X}^T Q + ba^T = 0, \tag{3.6}$$

i.e., the above is just $\nabla f(X) = 0$ and characterizes the minimizers of the convex function $f(X)$. Using (3.6) it follows that $\inf_X f(X) = f(\bar{X}) = \text{tr}(ba^T \bar{X})$. Now, for any $\xi \in \mathbb{R}^n$, we have $f(\xi b^T) = \|b\|^2(\xi^T Q \xi + 2a^T \xi)$. Thus, likewise, $\inf\{f(\xi b^T) : \xi \in \mathbb{R}^n\} > -\infty$ if and only if $Q \geq 0$ and there exists $\bar{\xi} \in \mathbb{R}^n$ such that

$$Q\bar{\xi} + a = 0, \tag{3.7}$$

and using (3.7) it follows $\inf_{\xi} f(\xi b^T) = f(\bar{\xi} b^T) = \|b\|^2 a^T \bar{\xi} = \text{tr}(ba^T \bar{\xi} b^T)$. Now, using (3.6)–(3.7), one obtains $\bar{X}^T Q = -ba^T$ and $Q(\bar{X} - \bar{\xi} b^T) = 0$, and hence it follows that

$$\begin{aligned} f(\bar{X}) - f(\bar{\xi} b^T) &= \text{tr}(ba^T (\bar{X} - \bar{\xi} b^T)) \\ &= \text{tr}(-\bar{X}^T Q (\bar{X} - \bar{\xi} b^T)) = 0. \end{aligned}$$

□

Equipped with Lemma 1, we now derive a Lagrangian dual for problem (G').

Lemma 2 *Consider problem (G') for any fixed $h \in \mathbb{R}$ and $L, R > 0$. A Lagrangian dual of (G') is given by the following convex program:*

$$\min_{\lambda \in \mathbb{R}^N, t \in \mathbb{R}} \left\{ \frac{1}{2} L R^2 t : \lambda \in \Lambda, S(\lambda, t) \geq 0 \right\}, \tag{DG'}$$

where $\Lambda := \{\lambda \in \mathbb{R}^N : \lambda_{i+1} - \lambda_i \geq 0, i = 1, \dots, N - 1, 1 - \lambda_N \geq 0, \lambda_i \geq 0, i = 1, \dots, N\}$, the matrix $S(\cdot, \cdot) \in \mathbb{S}^{N+2}$ is given by

$$S(\lambda, t) = \begin{pmatrix} (1 - h)S_0 + hS_1 & q \\ q^T & t \end{pmatrix},$$

with $q = (\lambda_1, \lambda_2 - \lambda_1, \dots, \lambda_N - \lambda_{N-1}, 1 - \lambda_N)^T$ and where the matrices $S_0, S_1 \in \mathbb{S}^{N+1}$ are defined by:

$$S_0 = \begin{pmatrix} 2\lambda_1 & -\lambda_1 & & & & & \\ -\lambda_1 & 2\lambda_2 & -\lambda_2 & & & & \\ & -\lambda_2 & 2\lambda_3 & -\lambda_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\lambda_{N-1} & 2\lambda_N & -\lambda_N & \\ & & & & -\lambda_N & 1 & \end{pmatrix} \tag{3.8}$$

and

$$S_1 = \begin{pmatrix} 2\lambda_1 & \lambda_2 - \lambda_1 & \dots & \lambda_N - \lambda_{N-1} & 1 - \lambda_N \\ \lambda_2 - \lambda_1 & 2\lambda_2 & & \lambda_N - \lambda_{N-1} & 1 - \lambda_N \\ \vdots & & \ddots & & \vdots \\ \lambda_N - \lambda_{N-1} & \lambda_N - \lambda_{N-1} & & 2\lambda_N & 1 - \lambda_N \\ 1 - \lambda_N & 1 - \lambda_N & \dots & 1 - \lambda_N & 1 \end{pmatrix}. \tag{3.9}$$

Proof For convenience, we recast (G') as a minimization problem, and we also omit the fixed term LR^2 from the objective. That is, we consider the equivalent problem (G'') defined by

$$\begin{aligned} \min_{G \in \mathbb{R}^{(N+1) \times d}, \delta \in \mathbb{R}^{N+1}} & \quad -\delta_N & (G'') \\ \text{s.t. } & \text{tr}(G^T A_{i-1,i} G) \leq \delta_{i-1} - \delta_i, \quad i = 1, \dots, N, \\ & \text{tr}(G^T D_i G + v u_i^T G) \leq -\delta_i, \quad i = 0, \dots, N. \end{aligned}$$

Attaching the dual multipliers $\lambda = (\lambda_1, \dots, \lambda_N) \in \mathbb{R}_+^N$ and $\tau := (\tau_0, \dots, \tau_N)^T \in \mathbb{R}_+^{N+1}$ to the first and second set of inequalities respectively, and using the notation $\delta = (\delta_0, \dots, \delta_N)$, we get that the Lagrangian of this problem is given as a sum of two separable functions in the variables (δ, G) :

$$\begin{aligned} L(G, \delta, \lambda, \tau) &= -\delta_N + \sum_{i=1}^N \lambda_i (\delta_i - \delta_{i-1}) + \sum_{i=0}^N \tau_i \delta_i \\ &\quad + \sum_{i=1}^N \lambda_i \text{tr}(G^T A_{i-1,i} G) + \sum_{i=0}^N \tau_i \text{tr}(G^T D_i G + v u_i^T G) \\ &\equiv L_1(\delta, \lambda, \tau) + L_2(G, \lambda, \tau). \end{aligned}$$

The dual objective function is then defined by

$$H(\lambda, \tau) = \min_{G, \delta} L(G, \delta, \lambda, \tau) = \min_{\delta} L_1(\delta, \lambda, \tau) + \min_G L_2(G, \lambda, \tau),$$

and the dual problem of (G'') is then given by

$$\max \left\{ H(\lambda, \tau) : \lambda \in \mathbb{R}_+^N, \tau \in \mathbb{R}_+^{N+1} \right\}. \tag{DG''}$$

Since $L_1(\cdot, \lambda, \tau)$ is linear in δ , we have $\min_{\delta} L_1(\delta, \lambda, \tau) = 0$ whenever

$$\begin{aligned} -\lambda_1 + \tau_0 &= 0, \\ \lambda_i - \lambda_{i+1} + \tau_i &= 0 \quad (i = 1, \dots, N - 1), \\ -1 + \lambda_N + \tau_N &= 0, \end{aligned} \tag{3.10}$$

and $-\infty$ otherwise. Invoking Lemma 1, we get

$$\min_{G \in \mathbb{R}^{(N+1) \times d}} L_2(G, \lambda, \tau) = \min_{w \in \mathbb{R}^{N+1}} L_2(wv^T, \lambda, \tau).$$

Therefore for any (λ, τ) satisfying (3.10), we have obtained that the dual objective reduces to

$$\begin{aligned} H(\lambda, \tau) &= \min_{w \in \mathbb{R}^{N+1}} \left\{ w^T \left(\sum_{i=1}^N \lambda_i A_{i-1,i} + \sum_{i=0}^N \tau_i D_i \right) w + \tau^T w \right\} \\ &= \max_{t \in \mathbb{R}} \left\{ -\frac{1}{2} t : w^T \left(\sum_{i=1}^N \lambda_i A_{i-1,i} + \sum_{i=0}^N \tau_i D_i \right) w + \tau^T w \leq -\frac{1}{2} t, \forall w \in \mathbb{R}^{N+1} \right\} \\ &= \max_{t \in \mathbb{R}} \left\{ -\frac{1}{2} t : \begin{pmatrix} \sum_{i=1}^N \lambda_i A_{i-1,i} + \sum_{i=0}^N \tau_i D_i & \frac{1}{2} \tau \\ \frac{1}{2} \tau^T & \frac{1}{2} t \end{pmatrix} \succeq 0 \right\}. \end{aligned}$$

where the last equality follows from the well known lemma [6, p. 163].²

Now, recalling the definition of the matrices $A_{i-1,i}, D_i$ (see [3.5]), we obtain

$$\sum_{i=1}^N \lambda_i A_{i-1,i} = \frac{1}{2} \begin{pmatrix} \lambda_1 & (h-1)\lambda_1 & & & & \\ (h-1)\lambda_1 & \lambda_1 + \lambda_2 & (h-1)\lambda_2 & & & \\ & (h-1)\lambda_2 & \lambda_2 + \lambda_3 & (h-1)\lambda_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & (h-1)\lambda_{N-1} & \lambda_{N-1} + \lambda_N & (h-1)\lambda_N \\ & & & & (h-1)\lambda_N & \lambda_N \end{pmatrix}$$

² Let M be a symmetric matrix. Then, $x^T Mx + 2b^T x + c \geq 0, \forall x \in \mathbb{R}^d$ if and only if the matrix $\begin{pmatrix} M & b \\ b^T & c \end{pmatrix}$ is positive semidefinite.

and

$$\sum_{i=0}^N \tau_i D_i = \frac{1}{2} \begin{pmatrix} \tau_0 & h\tau_1 & \dots & h\tau_{N-1} & h\tau_N \\ h\tau_1 & \tau_1 & & h\tau_{N-1} & h\tau_N \\ \vdots & & \ddots & & \vdots \\ h\tau_{N-1} & h\tau_{N-1} & & \tau_{N-1} & h\tau_N \\ h\tau_N & h\tau_N & \dots & h\tau_N & \tau_N \end{pmatrix}.$$

Finally, using the relations (3.10) to eliminate τ_i , and recalling that $\text{val}(G'')$ was defined as $-LR^2\text{val}(G')$, the desired form of the stated dual problem follows. \square

The next lemma will be crucial in invoking duality in the forthcoming theorem. The proof for this lemma is quite technical and appears in the ‘‘Appendix’’.

Lemma 3 *Let*

$$\lambda_i = \frac{i}{2N + 1 - i}, \quad i = 1, \dots, N,$$

then the matrices $S_0, S_1 \in \mathbb{S}^{N+1}$ defined in (3.8)–(3.9) are positive definite for every $N \in \mathbb{N}$.

We are now ready to establish a new upper bound on the complexity of the GM for values of h between 0 and 1. To the best of our knowledge, the tightest bound thus far is given by (3.1).

Theorem 1 *Let $f \in C_L^{1,1}(\mathbb{R}^d)$ and let $x_0, \dots, x_N \in \mathbb{R}^d$ be generated by Algorithm GM with $0 < h \leq 1$. Then*

$$f(x_N) - f(x_*) \leq \frac{LR^2}{4Nh + 2}. \tag{3.11}$$

Proof First note that both (G) and (G') are clearly feasible and $\text{val}(G) \leq \text{val}(G')$. Invoking Lemma 2, by weak duality for the pair of primal-dual problems (G') and (DG') , we thus obtain that $\text{val}(G') \leq \text{val}(DG')$ and hence:

$$f(x_N) - f(x_*) \leq \text{val}(G) \leq \text{val}(G') \leq \text{val}(DG'). \tag{3.12}$$

Now consider the following point (λ, t) for the dual problem (DG') :

$$\lambda_i = \frac{i}{2N + 1 - i}, \quad i = 1, \dots, N, \\ t = \frac{1}{2Nh + 1}.$$

Assuming that this point is (DG') -feasible, it follows from (3.12) that

$$f(x_N) - f(x_*) \leq \text{val}(DG') \leq \frac{LR^2}{4Nh + 2},$$

which proves the desired result. Thus, it remains to show that the above given choice (λ, t) is feasible for (DG') . First, it is easy to see that all the linear constraints of (DG') on the variables $\lambda_i, i = 1, \dots, N$ described through the set Λ hold true. Now we prove that the matrix $S \equiv S(\lambda, t)$ is positive semidefinite. From Lemma 3, with $h \in [0, 1]$, we get that $(1 - h)S_0 + hS_1$ is positive definite, as a convex combination of positive definite matrices. Next, we argue that the determinant of S is zero. Indeed, take $u := (1, \dots, 1, -(2Nh + 1))^T$, then from the definition of S and the choice of λ_i and t it follows by elementary algebra that $Su = 0$. To complete the argument, we note that the determinant of S can also be found via the identity (see, e.g., [7, Section A.5.5]):

$$\det(S) = \left(t - q^T ((1 - h)S_0 + hS_1)^{-1} q \right) \det((1 - h)S_0 + hS_1).$$

Since we have just shown that $(1 - h)S_0 + hS_1 \succ 0$, then $\det((1 - h)S_0 + hS_1) > 0$ and we get from the above identity that the value of $t - q^T ((1 - h)S_0 + hS_1)^{-1} q$, which is the Schur complement of the matrix S , is equal to 0. By a well known lemma on the Schur complement [6, Lemma 4.2.1], we conclude that S is positive semidefinite. \square

The next theorem gives a lower bound on the worst-case complexity of Algorithm GM. In particular, it shows that the bound (3.11) is tight and that it is attained by a specific convex function in $C_L^{1,1}$.

Theorem 2 *Let $L > 0, N \in \mathbb{N}$ and $d \in \mathbb{N}$. Then for every $h > 0$ there exists a convex function $\varphi \in C_L^{1,1}(\mathbb{R}^d)$ and a point $x_0 \in \mathbb{R}^d$ such that after N iterations, Algorithm GM reaches an approximate solution x_N with the following absolute inaccuracy*

$$\varphi(x_N) - \varphi^* = \frac{LR^2}{4Nh + 2}.$$

Proof For the sake of simplicity we will assume that $L = 1$ and $R = \|x_* - x_0\| = 1$. Generalizing this proof to general values of L and R can be done by an appropriate scaling.

Consider the function

$$\varphi(x) = \begin{cases} \frac{1}{2Nh+1} \|x\| - \frac{1}{2(2Nh+1)^2}, & \text{if } \|x\| \geq \frac{1}{2Nh+1}, \\ \frac{1}{2} \|x\|^2, & \text{if } \|x\| < \frac{1}{2Nh+1}. \end{cases}$$

Note that this function is nothing else but the Moreau proximal envelope [13] of the function $x \mapsto \|x\|/(2Nh + 1)$. It is well known that this function is convex, continuously differentiable with Lipschitz constant $L = 1$, and that its minimal value $\varphi(x_*) = 0$, see e.g., [13, 20]. Applying the GM on $\varphi(x)$ with $x_0 = v$ where, as before, v is a unit vector in \mathbb{R}^d (note that only the first part the φ is relevant), we obtain that for $i = 0, \dots, N$:

$$\begin{aligned}
 x_i &= \left(1 - \frac{ih}{2Nh + 1}\right) v, \\
 \varphi'(x_i) &= \frac{1}{2Nh + 1} v, \\
 \text{and } \varphi(x_i) &= \frac{1}{2Nh + 1} \left(1 - \frac{ih}{2Nh + 1}\right) - \frac{1}{2(2Nh + 1)^2} \\
 &= \frac{1}{4Nh + 2} \left(\frac{4Nh + 1 - 2ih}{2Nh + 1}\right).
 \end{aligned}$$

Therefore,

$$\varphi(x_N) - \varphi(x_*) = \varphi(x_N) = \frac{1}{4Nh + 2}$$

and the desired claim is proven. □

We conclude this section by raising a conjecture on the worst-case performance of the GM with a constant step size $0 < h < 2$. Note that when $0 < h \leq 1$ the bound below coincides with (3.11).

Conjecture 1 Suppose the sequence x_0, \dots, x_N is generated by Algorithm GM with $0 < h < 2$, then

$$f(x_N) - f(x_*) \leq \frac{LR^2}{2} \max\left(\frac{1}{2Nh + 1}, (1 - h)^{2N}\right).$$

4 New bounds on a class of first-order methods

The framework developed in the previous sections will now serve as a basis to extend the worst-case performance analysis for a broader class of first-order methods for minimizing a smooth convex function over \mathbb{R}^d . First, we define a general class of first-order algorithms and we show that it encompasses some interesting first-order methods. Then, following our approach, we define the corresponding PEP associated with this class. Although for this more general case, an analytical solution is not available for determining the bound, we establish that given a fixed number of steps N , a bound on the performance of algorithms in this class can be *estimated numerically*. We then illustrate how this result can be applied for deriving new complexity bounds on two first-order methods.

4.1 A general first-order algorithm: definition and examples

As before, our family \mathcal{F} is the class of convex functions in $C_L^{1,1}(\mathbb{R}^d)$, and $\{d, N, L, R\}$ are fixed. Consider the following class of first-order methods:

Algorithm FO

- 0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$, $x_0 \in \mathbb{R}^d$.
- 1. For $i = 0, \dots, N - 1$, compute $x_{i+1} = x_i - \frac{1}{L} \sum_{k=0}^i h_k^{(i+1)} f'(x_k)$.

Here, $h_k^{(i)} \in \mathbb{R}$ play the role of step-sizes, which we assume to be determined by each specific algorithm in this class in a way that is independent of the problem data (i.e., f and x_0).

The interest in the analysis of first-order algorithms of this type is motivated by the fact that it covers some fundamental first-order schemes beyond the GM. In particular, to motivate Algorithm FO, let us consider the following two algorithms which are of particular interest, and as we shall see below can be seen as special cases of Algorithm FO.

We start with the so-called Heavy Ball Method (HBM). For earlier work on this method see Polyak [18], and for some interesting modern developments and applications, we refer the reader to Attouch et al. [1,2] and references therein.

Example 1 **The Heavy Ball Method (HBM)**

Algorithm HBM

- 0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$, $x_0 \in \mathbb{R}^d$,
- 1. $x_1 = x_0 - \frac{\alpha}{L} f'(x_0)$
- 2. For $i = 1, \dots, N - 1$ compute: $x_{i+1} = x_i - \frac{\alpha}{L} f'(x_i) + \beta(x_i - x_{i-1})$

Here the step sizes α and β are chosen such that $0 \leq \beta < 1$ and $0 < \alpha < 2(1 + \beta)$, see [18].

By recursively eliminating the term $x_i - x_{i-1}$ in step 2 of Algorithm HBM, we can rewrite this step as

$$x_{i+1} = x_i - \frac{1}{L} \sum_{k=0}^i \alpha \beta^{i-k} f'(x_k), \quad i = 1, \dots, N - 1.$$

Therefore, the heavy ball method is a special case of Algorithm FO with the choice

$$h_k^{(i+1)} = \alpha \beta^{i-k}, \quad k = 0, \dots, i, \quad i = 0, \dots, N - 1.$$

The next algorithm is Nesterov’s celebrated *Fast Gradient Method* (FGM) [15].

Example 2 The fast gradient method (FGM)

Algorithm FGM

- 0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$, $x_0 \in \mathbb{R}^d$,
- 1. $y_1 = x_0, t_1 = 1$,
- 2. For $i = 1, \dots, N$ compute:
 - (a) $x_i = y_i - \frac{1}{L} f'(y_i)$,
 - (b) $t_{i+1} = \frac{1 + \sqrt{1 + 4t_i^2}}{2}$,
 - (c) $y_{i+1} = x_i + \frac{t_i - 1}{t_{i+1}}(x_i - x_{i-1})$.

A major breakthrough was achieved by Nesterov in [15], where he proved that the FGM, which requires almost no increase in computational effort when compared to the basic gradient scheme, achieves the improved rate of convergence $O(1/N^2)$ for function values. More precisely, one has³

$$f(x_N) - f(x_*) \leq \frac{2L\|x_0 - x_*\|^2}{(N + 1)^2}, \quad \forall x_* \in X_*(f). \tag{4.1}$$

The order of complexity of Nesterov’s algorithm is also *optimal*, as it is possible to show that there exists a convex function $f \in C_L^{1,1}(\mathbb{R}^d)$ such that when $d \geq 2N + 1$, and under some other mild assumptions, *any* first-order algorithm that generates a point x_N by performing N calls to a first-order oracle of f satisfies [16, Theorem 2.1.7]

$$f(x_N) - f(x_*) \geq \frac{3L\|x_0 - x_*\|^2}{32(N + 1)^2}, \quad \forall x_* \in X_*(f).$$

This fundamental algorithm discovered about 30 years ago by Nesterov [15] has been recently revived and is currently subject of intensive research activities. For some of its extensions and many applications, see e.g., the recent survey paper Beck-Teboulle [5] and references therein.

At first glance, Algorithm FGM does not seem to fit the class of algorithms defined above (Algorithm FO). Here two sequences are defined: the main sequence x_0, \dots, x_N and an auxiliary sequence y_1, \dots, y_N . Observing that the gradient of the function is only evaluated on the *auxiliary sequence* of points $\{y_i\}$, we show in the next proposition that Algorithm FGM fits in this class through the following algorithm:

³ See remark following the proof of Theorem 1 in [15].

Algorithm FGM'

- 0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$, $x_0 \in \mathbb{R}^d$,
- 1. $y_1 = x_0, t_1 = 1$,
- 2. For $i = 1, \dots, N - 1$ compute:
 - (a) $t_{i+1} = \frac{1 + \sqrt{1 + 4t_i^2}}{2}$,
 - (b) $y_{i+1} = y_i - \frac{1}{L} \sum_{k=1}^i h_k^{(i+1)} f'(y_k)$,
- 3. $x_N = y_N - \frac{1}{L} f'(y_N)$,

with

$$h_k^{(i+1)} = \begin{cases} \frac{t_i - 1}{t_{i+1}} h_k^{(i)}, & \text{if } k + 2 \leq i, \\ \frac{t_i - 1}{t_{i+1}} (h_{i-1}^{(i)} - 1), & \text{if } k = i - 1, \quad (i = 1, \dots, N - 1, k = 1, \dots, i) \\ 1 + \frac{t_i - 1}{t_{i+1}}, & \text{if } k = i. \end{cases} \tag{4.2}$$

Proposition 2 *The points y_1, \dots, y_N, x_N generated by Algorithm FGM' are identical to the respective points generated by Algorithm FGM.*

Proof We will show by induction that the sequence y_i generated by Algorithm FGM' is identical to the sequence y_i generated by Algorithm FGM, and that the value of x_N generated by Algorithm FGM' is equal to the value of x_N generated by Algorithm FGM.

First note that the sequence t_i is defined by the two algorithms in the same way. Now let $\{x_i, y_i\}$ be the sequences generated by Algorithm FGM and denote by $\{y'_i\}, x'_N$ the sequence generated by Algorithm FGM'. Obviously, $y'_1 = y_1$ and since $t_1 = 1$ we get using the relations 4.2:

$$y'_2 = y'_1 - \frac{1}{L} h_1^{(2)} f'(y'_1) = y_1 - \frac{1}{L} \left(1 + \frac{t_1 - 1}{t_2} \right) f'(y_1) = y_1 - \frac{1}{L} f'(y_1) = x_1 = y_2.$$

Assuming $y'_i = y_i$ for $i = 1, \dots, n$, we then have

$$\begin{aligned} y'_{n+1} &= y'_n - \frac{1}{L} h_n^{(n+1)} f'(y'_n) - \frac{1}{L} h_{n-1}^{(n+1)} f'(y'_{n-1}) - \frac{1}{L} \sum_{k=1}^{n-2} h_k^{(n+1)} f'(y'_k) \\ &= y_n - \frac{1}{L} \left(1 + \frac{t_n - 1}{t_{n+1}} \right) f'(y_n) - \frac{1}{L} \frac{t_n - 1}{t_{n+1}} (h_{n-1}^{(n)} - 1) f'(y_{n-1}) - \frac{1}{L} \sum_{k=1}^{n-2} \frac{t_n - 1}{t_{n+1}} h_k^{(n)} f'(y'_k) \\ &= y_n - \frac{1}{L} f'(y_n) + \frac{t_n - 1}{t_{n+1}} \left(-\frac{1}{L} f'(y_n) + \frac{1}{L} f'(y_{n-1}) - \frac{1}{L} \sum_{k=1}^{n-1} h_k^{(n)} f'(y'_k) \right) \\ &= x_n + \frac{t_n - 1}{t_{n+1}} \left(-\frac{1}{L} f'(y_n) + \frac{1}{L} f'(y_{n-1}) + y'_n - y'_{n-1} \right) \\ &= x_n + \frac{t_n - 1}{t_{n+1}} (x_n - x_{n-1}) = y_{n+1}. \end{aligned}$$

Finally,

$$x'_N = y'_N - \frac{1}{L} f'(y'_N) = y_N - \frac{1}{L} f'(y_N) = x_N.$$

□

4.2 Numerical estimation of a bound on Algorithm FO

To build the PEP for Algorithm FO, from which a complexity bound can be derived, we follow the approach used to derive problem (G) for the GM. The only difference being that here, of course, the relation between the variables x_i is derived from the main iteration of Algorithm FO. After some algebra, the resulting PEP reads

$$\begin{aligned} \max_{G \in \mathbb{R}^{(N+1) \times d}, \delta_i \in \mathbb{R}} \quad & LR^2 \delta_N \tag{Q} \\ \text{s.t.} \quad & \text{tr}(G^T \tilde{A}_{i,j} G) \leq \delta_i - \delta_j, \quad i < j = 0, \dots, N, \\ & \text{tr}(G^T \tilde{B}_{i,j} G) \leq \delta_i - \delta_j, \quad j < i = 0, \dots, N, \\ & \text{tr}(G^T \tilde{C}_i G) \leq \delta_i, \quad i = 0, \dots, N, \\ & \text{tr}(G^T \tilde{D}_i G + \nu u_i^T G) \leq -\delta_i, \quad i = 0, \dots, N, \end{aligned}$$

where $\tilde{A}_{i,j}$, $\tilde{B}_{i,j}$, \tilde{C}_i and \tilde{D}_i are defined, similarly to (3.5), by

$$\begin{aligned} \tilde{A}_{i,j} &= \frac{1}{2}(u_i - u_j)(u_i - u_j)^T + \frac{1}{2} \sum_{t=i+1}^j \sum_{k=0}^{t-1} h_k^{(t)} (u_j u_k^T + u_k u_j^T), \\ \tilde{B}_{i,j} &= \frac{1}{2}(u_i - u_j)(u_i - u_j)^T - \frac{1}{2} \sum_{t=j+1}^i \sum_{k=0}^{t-1} h_k^{(t)} (u_j u_k^T + u_k u_j^T), \\ \tilde{C}_i &= \frac{1}{2} u_i u_i^T, \\ \tilde{D}_i &= \frac{1}{2} u_i u_i^T + \frac{1}{2} \sum_{t=1}^i \sum_{k=0}^{t-1} h_k^{(t)} (u_i u_k^T + u_k u_i^T) \end{aligned} \tag{4.3}$$

and we recall that $\nu \in \mathbb{R}^d$ is a given unit vector, $u_i = e_{i+1} \in \mathbb{R}^{N+1}$ and the notation $i < j = 0, \dots, N$ is a shorthand notation for $i = 0, \dots, N - 1, j = i + 1, \dots, N$.

In view of the difficulties in the analysis required to find the solution of (G), an analytical solution to this more general case seems unlikely. However, as we now proceed to show, we can find an upper bound on the optimal solution of this problem by solving a semidefinite program that can be computed numerically using state of the art SDP software.

Following the analysis of the GM, (cf. (G') in §3.2) we consider the following simpler relaxed problem:

$$\begin{aligned} \max_{G \in \mathbb{R}^{(N+1) \times d}, \delta_i \in \mathbb{R}} \quad & LR^2 \delta_N \tag{Q'} \\ \text{s.t.} \quad & \text{tr}(G^T \tilde{A}_{i-1,i} G) \leq \delta_{i-1} - \delta_i, \quad i = 1, \dots, N, \\ & \text{tr}(G^T \tilde{D}_i G + \nu u_i^T G) \leq -\delta_i, \quad i = 0, \dots, N. \end{aligned}$$

With the same proof as given in Lemma 2 for problem (Q'), we obtain that a dual problem for (Q') is given by the following convex semidefinite optimization problem (as before, we omit the term LR^2):

$$\begin{aligned} \min_{\lambda, \tau, t} \quad & \frac{1}{2} t \tag{DQ'} \\ \text{s.t.} \quad & \left(\begin{array}{c} \sum_{i=1}^N \lambda_i \tilde{A}_{i-1,i} + \sum_{i=0}^N \tau_i \tilde{D}_i \quad \frac{1}{2} \tau \\ \frac{1}{2} \tau^T \end{array} \right) \succeq 0, \\ & (\lambda, \tau) \in \tilde{\Lambda}, \end{aligned}$$

where

$$\begin{aligned} \tilde{\Lambda} = \{(\lambda, \tau) \in \mathbb{R}_+^N \times \mathbb{R}_+^{N+1} : \tau_0 = \lambda_1, \lambda_i - \lambda_{i+1} \\ + \tau_i = 0, i = 1, \dots, N - 1, \lambda_N + \tau_N = 1\}. \end{aligned} \tag{4.4}$$

The structure of problem (DQ') will be very helpful in the analysis of the next section which further addresses the role of the step-sizes. Note that the data matrices of both primal-dual problems (Q') and (DQ') depend on the step-sizes $h_k^{(i)}$.

To avoid a trivial bound on problem (Q'), here we need the following assumption on the dual problem (DQ'):

Assumption 1 Problem (DQ') is solvable, i.e., the minimum is finite and attained for the given step-sizes $h_k^{(i)}$.

Actually, the attainment requirement can be avoided if we can exhibit a feasible point (λ, τ, t) for the problem (DQ'). As noted earlier, given the difficulties already encountered for the simpler GM, finding explicitly such a point for the general Algorithm FO is unlikely.

The promised complexity bound on Algorithm FO now easily follows and is determined by the optimal value of the dual problem (DQ'), which can be efficiently computed by any numerical solvers for SDP [6, 11, 22] for small to medium scale problems.

Proposition 3 Fix any $N, d \in \mathbb{N}$. Let $f \in C_L^{1,1}(\mathbb{R}^d)$ be convex and suppose that $x_0, \dots, x_N \in \mathbb{R}^d$ are generated by Algorithm FO, and that Assumption 1 holds. Then,

$$f(x_N) - f(x_*) \leq LR^2 \text{val}(DQ').$$

Proof Follows from weak duality for the pair of primal-dual problems (Q')–(DQ') \square

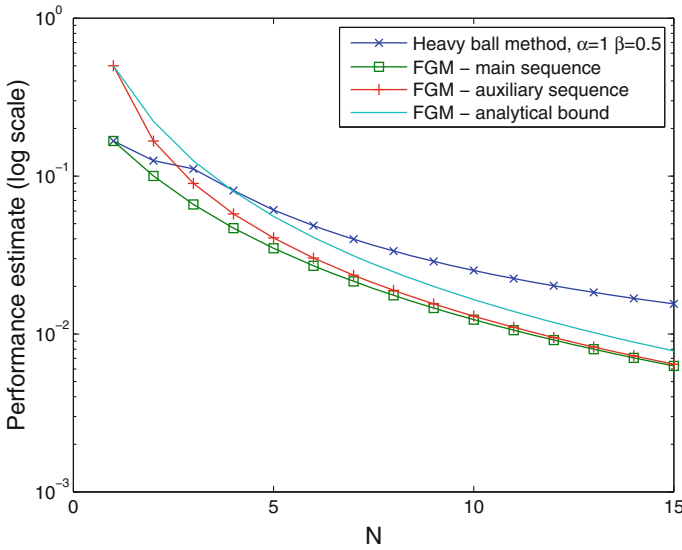


Fig. 1 The computed worst-case bounds on the HBM and FGM versus the classical analytical bound on the FGM (4.1)

4.3 Numerical illustrations

We apply Proposition 3 to find bounds on the complexity of the heavy ball method (HBM) with $\alpha = 1$ and $\beta = \frac{1}{2}$ and on the fast gradient method (FGM) with $h_k^{(i)}$ as given in (4.2), which as shown earlier, can both be viewed as particular realizations of Algorithm FO.

The resulting SDP programs were solved for different values of N using CVX [8, 10]. These results, together with the classical bound on the convergence rate of the main sequence of the fast gradient method (4.1), are summarized in Fig. 1 and Table 1.

Note that as far as the authors are aware, there is no known convergence rate result for the HBM on the class of convex functions in $C_L^{1,1}$. As can be seen from the above results, the numerically estimated bound for the HBM behaves slightly better than the GM (compare with the explicit bound given in Theorem 1), but remains much slower than the fast gradient scheme (FGM).

Considering the results on the FGM, note that the numerically estimated bounds for the main sequence of point x_i and the corresponding values at the auxiliary sequence y_i of FGM are very similar and perform slightly better than predicted by the classical bound (4.1). To the best of our knowledge, the complexity of the auxiliary sequence is yet unknown, thus these results encourage us to raise the following conjecture.

⁴ According to our simulations, this choice for the values of α, β produces results that are typical of the behavior of the algorithm.

Table 1 The computed worst-case bounds on the HBM and FGM versus the classical analytical bound on the FGM (4.1)

N	Heavy Ball	FGM, main	FGM, auxiliary	FGM, analytical bound
1	LR ² /6.00	LR ² /6.00	LR ² /2.00	LR ² /2.0 = 2LR ² /(1 + 1) ²
2	LR ² /7.99	LR ² /10.00	LR ² /6.00	LR ² /4.5 = 2LR ² /(2 + 1) ²
3	LR ² /9.00	LR ² /15.13	LR ² /11.13	LR ² /8.0 = 2LR ² /(3 + 1) ²
4	LR ² /12.35	LR ² /21.35	LR ² /17.35	LR ² /12.5 = 2LR ² /(4 + 1) ²
5	LR ² /16.41	LR ² /28.66	LR ² /24.66	LR ² /18.0 = 2LR ² /(5 + 1) ²
10	LR ² /39.63	LR ² /81.07	LR ² /77.07	LR ² /60.5 = 2LR ² /(10 + 1) ²
20	LR ² /89.45	LR ² /263.65	LR ² /259.65	LR ² /220.5 = 2LR ² /(20 + 1) ²
40	LR ² /188.99	LR ² /934.89	LR ² /930.89	LR ² /840.5 = 2LR ² /(40 + 1) ²
80	LR ² /387.91	LR ² /3490.22	LR ² /3486.22	LR ² /3280.5 = 2LR ² /(80 + 1) ²
160	LR ² /785.68	LR ² /13427.43	LR ² /13423.43	LR ² /12960.5 = 2LR ² /(160 + 1) ²
500	LR ² /2476.11	LR ² /127224.44	LR ² /127220.32	LR ² /125500.5 = 2LR ² /(500 + 1) ²
1,000	LR ² /4962.01	LR ² /504796.99	LR ² /504798.28	LR ² /501000.5 = 2LR ² /(1,000 + 1) ²

Conjecture 2 Let x_0, x_1, \dots and y_1, y_2, \dots be the main and auxiliary sequences defined by FGM (respectively), then $\{f(x_i)\}$ and $\{f(y_i)\}$ converge to the optimal value of the problem with the same rate of convergence.

5 A best performing algorithm: optimal step sizes for Algorithm FO

We now consider the problem of finding the “best” performing algorithm of the form FO with respect to the new bounds. Namely, we consider the problem of minimizing $\text{val}(Q')$, the optimal value of (Q') , with respect to the step sizes $h := (h_k^{(i)})_{0 \leq k < i \leq N}$ defining the Algorithm FO, and which are now considered as unknown variables in FO.

We denote by $\tilde{A}_{i,j}(h)$ and $\tilde{D}_i(h)$, the matrices given in (4.3), which are functions of the algorithm step sizes h . The resulting bound derived in Proposition 3 is thus a function of h , and the problem of minimizing $\text{val}(DQ')$ with respect to the step sizes h thus consists of solving the following bilinear problem:

$$\min_{h, \lambda, \tau, t} \left\{ \frac{1}{2}t : \begin{pmatrix} \sum_{i=1}^N \lambda_i \tilde{A}_{i-1,i}(h) + \sum_{i=0}^N \tau_i \tilde{D}_i(h) & \frac{1}{2}t \\ \frac{1}{2}t^T & \frac{1}{2}t \end{pmatrix} \succeq 0, (\lambda, \tau) \in \tilde{\Lambda} \right\}, \quad (\text{BIL})$$

with $\tilde{\Lambda}$ defined as in (4.4).

Note that the feasibility of (BIL) follows from the proof of Theorem 2, where an explicit feasible point is given to (DG') , which is a special instance of (BIL) when the steps $(h_k^{(i)})$ are chosen as in the GM.

From the definition of the matrices $\tilde{A}_{i,j}(h)$ and $\tilde{D}_i(h)$, we get

$$\sum_{i=1}^N \lambda_i \tilde{A}_{i-1,i}(h) + \sum_{i=0}^N \tau_i \tilde{D}_i(h) = \frac{1}{2} \sum_{i=1}^N \lambda_i (u_{i-1} - u_i)(u_{i-1} - u_i)^T + \frac{1}{2} \sum_{i=0}^N \tau_i u_i u_i^T + \frac{1}{2} \sum_{i=1}^N \sum_{k=0}^{i-1} \left(\lambda_i h_k^{(i)} + \tau_i \sum_{t=k+1}^i h_k^{(t)} \right) (u_i u_k^T + u_k u_i^T).$$

Introducing the new variables:

$$r_{i,k} = \lambda_i h_k^{(i)} + \tau_i \sum_{t=k+1}^i h_k^{(t)}, \quad i = 1, \dots, N, \quad k = 0, \dots, i - 1 \tag{5.1}$$

and denoting $r = (r_{i,k})_{0 \leq k < i \leq N}$, we obtain the following *linear* SDP relaxation of (BIL):

$$\min_{r, \lambda, \tau, t} \left\{ \frac{1}{2} t : \begin{pmatrix} S(r, \lambda, \tau) & \frac{1}{2} t \\ \frac{1}{2} t^T & \frac{1}{2} t \end{pmatrix} \succeq 0, (\lambda, \tau) \in \tilde{\Lambda} \right\}, \tag{LIN}$$

where

$$S(r, \lambda, \tau) = \frac{1}{2} \sum_{i=1}^N \lambda_i (u_{i-1} - u_i)(u_{i-1} - u_i)^T + \frac{1}{2} \sum_{i=0}^N \tau_i u_i u_i^T + \frac{1}{2} \sum_{i=1}^N \sum_{k=0}^{i-1} r_{i,k} (u_i u_k^T + u_k u_i^T).$$

This convex SDP can now be efficiently solved by numerical methods. As the following theorem shows, the optimal solution of (LIN) can then be used to construct an optimal solution for (BIL) and hence recover optimal values for the step sizes h .

Theorem 3 *Suppose $(r^*, \lambda^*, \tau^*, t^*)$ is an optimal solution for (LIN), then $(h, \lambda^*, \tau^*, t^*)$ is an optimal solution for (BIL), where $h = (h_k^{(i)})_{0 \leq k < i \leq N}$ is defined by the following recursive rule*

$$h_k^{(i)} = \begin{cases} \frac{\tau_i^* \sum_{t=k+1}^{i-1} h_k^{(t)} - r_{i,k}^*}{\lambda_i^*} & \text{if } \lambda_i^* \neq 0, \\ 0 & \text{otherwise,} \end{cases} \quad i = 1, \dots, N, \quad k = 0, \dots, i - 1. \tag{5.2}$$

Proof As (LIN) is a relaxation of (BIL), it is enough to show that (BIL) can achieve the same objective value. Let $(r^*, \lambda^*, \tau^*, t^*)$ be an optimal solution for (LIN). If $\lambda_i^* \neq 0$ for all $1 \leq i \leq N$, then (5.2) satisfies all the equations in (5.1) and therefore $(h, \lambda^*, \tau^*, t^*)$ is feasible for (BIL).

Table 2 An approximate solution of $LR^2\text{val}(\text{LIN})$ for various values of N

N	$LR^2\text{val}(\text{LIN})$	N	$LR^2\text{val}(\text{LIN})$
1	$LR^2/8.00$	20	$LR^2/525.09$
2	$LR^2/16.16$	40	$LR^2/1869.22$
3	$LR^2/26.53$	80	$LR^2/6983.13$
4	$LR^2/39.09$	160	$LR^2/26864.04$
5	$LR^2/53.80$	500	$LR^2/254482.61$
10	$LR^2/159.07$	1,000	$LR^2/1009628.17$

Suppose $\lambda_m^* = 0$ for some $1 \leq m \leq N$ and that m is the maximal index with this property. Then by the equality and non-negativity constraints in (LIN), we get that $\lambda_1^* = \lambda_2^* = \dots = \lambda_m^* = 0$ and $\tau_0^* = \tau_1^* = \dots = \tau_{m-1}^* = 0$. Let $S := S(r, \lambda^*, \tau^*)$, then by the positive semidefinite constraint in (LIN), we have $S \succeq 0$. From the linear equalities connecting λ and τ it follows that

$$S_{i,i} = \begin{cases} \frac{1}{2}(\lambda_1^* + \tau_0^*) = \lambda_1^*, & \text{if } i = 1, \\ \frac{1}{2}(\lambda_i^* + \lambda_{i-1}^* + \tau_{i-1}^*) = \lambda_i^*, & \text{if } i = 2, \dots, N, \end{cases}$$

and we get that $S_{1,1} = \dots = S_{m,m} = 0$. By the properties of positive semidefinite matrices we now get that $r_{i,k}^* = 0$ for $i = 1, \dots, m$ and $k = 0, \dots, i - 1$, hence the set of equations (5.1) with the chosen values of $h_k^{(i)}$ is consistent. □

The optimal value of $LR^2\text{val}(\text{LIN})$ for various values of N is summarized in Table 2. As can be seen from these results (compare with Table 1), the worst-case performance of the new algorithm is almost exactly two times better than the worst-case performance of the FGM. Note that the bounds given here are worst-case bounds: the performance of the considered methods on a specific application can be very different.

The resulting first-order algorithm with the computed optimal step sizes $h_k^{(i)}$ for $N = 5$ is illustrated in the example below.

Example 3 Consider the following first-order method, which was constructed by solving (LIN) for $N = 5$.

0. Input: $f \in C_L^{1,1}(\mathbb{R}^d)$, $x_0 \in \mathbb{R}^d$,

1. $x_1 = x_0 - \frac{1.6180}{L} f'(x_0)$,
2. $x_2 = x_1 - \frac{0.1741}{L} f'(x_0) - \frac{2.0194}{L} f'(x_1)$,
3. $x_3 = x_2 - \frac{0.0756}{L} f'(x_0) - \frac{0.4425}{L} f'(x_1) - \frac{2.2317}{L} f'(x_2)$,
4. $x_4 = x_3 - \frac{0.0401}{L} f'(x_0) - \frac{0.2350}{L} f'(x_1) - \frac{0.6541}{L} f'(x_2) - \frac{2.3656}{L} f'(x_3)$,
5. $x_5 = x_4 - \frac{0.0178}{L} f'(x_0) - \frac{0.1040}{L} f'(x_1) - \frac{0.2894}{L} f'(x_2) - \frac{0.6043}{L} f'(x_3) - \frac{2.0778}{L} f'(x_4)$.

A bound on the worst-case performance the algorithm in this example is given by the following inequality (see $N = 5$ in Table 2):

$$f(x_5) - f(x_*) \leq \frac{L\|x_0 - x_*\|^2}{53.80}, \quad \forall x_* \in X_*(f).$$

6 Conclusions

We introduced a novel approach for estimating the worst-case complexity of first-order methods for convex optimization via the PEP problem, its relaxations, and exact or approximate solution using duality. Using this approach we derived a tight bound on the worst-case performance of the fixed-size gradient method and established new bounds that can be numerically estimated for a general class of first-order algorithms, which includes the Heavy Ball method and Nesterov's fast gradient method. We then showed how to construct optimal stepsizes for this first-order class.

While the proposed approach and the PEP problem offer a novel way to measure the complexity of any algorithm, it should be stressed that this approach is of course not without limitations. Indeed, as shown in the paper, finding a bound on the PEP problem is challenging. In the case of the GM with a fixed step size, the derivation of simple closed form expression for the bound required a dedicated analysis. Furthermore, for more general first-order algorithms, we are left with the problem of approximating the solution of the problem using SDP solvers which are often efficient only for small to medium scale problems. Nevertheless, the novelty of the proposed approach offers possible directions for extensions that could be considered in future research by formulating and analyzing the corresponding PEP problem for other first-order algorithms. This includes for example the analysis of GMs with different variable step-size strategies and the analysis of algorithms with different classes \mathcal{F} of input functions, such as for example the class of strongly convex functions.

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7 Appendix: Proof of Lemma 3

We now establish the positive definiteness of the matrices S_0 and S_1 given in (3.8) and (3.9), respectively.

7.1 $S_0 \succ 0$

We begin by showing that S_0 is positive definite. Recall that

$$S_0 = \begin{pmatrix} 2\lambda_1 & -\lambda_1 & & & & & \\ -\lambda_1 & 2\lambda_2 & -\lambda_2 & & & & \\ & -\lambda_2 & 2\lambda_3 & -\lambda_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\lambda_{N-1} & 2\lambda_N & -\lambda_N & \\ & & & & -\lambda_N & 1 & \end{pmatrix}$$

for

$$\lambda_i = \frac{i}{2N + 1 - i}, \quad i = 1, \dots, N.$$

Let us look at $\xi^T S_0 \xi$ for any $\xi = (\xi_0, \dots, \xi_N)^T$:

$$\begin{aligned} \xi^T S_0 \xi &= \sum_{i=0}^{N-1} 2\lambda_{i+1} \xi_i^2 - 2 \sum_{i=0}^{N-1} \lambda_{i+1} \xi_i \xi_{i+1} + \xi_N^2 \\ &= \sum_{i=0}^{N-1} \lambda_{i+1} (\xi_{i+1} - \xi_i)^2 + \lambda_1 \xi_0^2 + \sum_{i=1}^{N-1} (\lambda_{i+1} - \lambda_i) \xi_i^2 + (1 - \lambda_N) \xi_N^2 \end{aligned}$$

which is always positive for $\xi \neq 0$. We conclude that S_0 is positive definite.

7.2 $S_1 \succ 0$

We will show that S_1 is positive definite using Sylvester’s criterion.⁵

Recall that

$$S_1 = \begin{pmatrix} 2\lambda_1 & \lambda_2 - \lambda_1 & \dots & \lambda_N - \lambda_{N-1} & 1 - \lambda_N \\ \lambda_2 - \lambda_1 & 2\lambda_2 & & \lambda_N - \lambda_{N-1} & 1 - \lambda_N \\ \vdots & & \ddots & & \vdots \\ \lambda_N - \lambda_{N-1} & \lambda_N - \lambda_{N-1} & & 2\lambda_N & 1 - \lambda_N \\ 1 - \lambda_N & 1 - \lambda_N & \dots & 1 - \lambda_N & 1 \end{pmatrix}$$

for

$$\lambda_i = \frac{i}{2N + 1 - i}, \quad i = 1, \dots, N.$$

⁵ Despite the interesting structure of the matrix S_1 , this proof is quite involved. A simpler proof would be most welcome!

A recursive expression for the determinants We begin by deriving a recursion rule for the determinant of matrices of the following form:

$$M_k = \begin{pmatrix} d_0 & a_1 & a_2 & \dots & a_{k-1} & a_k \\ a_1 & d_1 & a_2 & & a_{k-1} & a_k \\ a_2 & a_2 & d_2 & & a_{k-1} & a_k \\ \vdots & & & \ddots & & \vdots \\ a_{k-1} & a_{k-1} & a_{k-1} & & d_{k-1} & a_k \\ a_k & a_k & a_k & \dots & a_k & d_k \end{pmatrix}.$$

To find the determinant of M_k , subtract the one before last row multiplied by $\frac{a_k}{a_{k-1}}$ from the last row: the last row becomes

$$\left(0, \dots, 0, a_k - \frac{a_k}{a_{k-1}}d_{k-1}, d_k - \frac{a_k}{a_{k-1}}a_k \right).$$

Expanding the determinant along the last row we get

$$\det M_k = \left(d_k - \frac{a_k}{a_{k-1}}a_k \right) \det M_{k-1} - \left(a_k - \frac{a_k}{a_{k-1}}d_{k-1} \right) \det(M_k)_{k,k-1}$$

where $(M_k)_{k,k-1}$ denotes the $k, k - 1$ minor:

$$(M_k)_{k,k-1} = \begin{pmatrix} d_0 & a_1 & a_2 & \dots & a_{k-2} & a_k \\ a_1 & d_1 & a_2 & & a_{k-2} & a_k \\ a_2 & a_2 & d_2 & & a_{k-2} & a_k \\ \vdots & & & \ddots & & \vdots \\ a_{k-2} & a_{k-2} & a_{k-2} & & d_{k-2} & a_k \\ a_{k-1} & a_{k-1} & a_{k-1} & & a_{k-1} & a_k \end{pmatrix}.$$

If we multiply the last column of $(M_k)_{k,k-1}$ by $\frac{a_{k-1}}{a_k}$ we get a matrix that is different from M_{k-1} by only the corner element. Thus by basic determinant properties we get that

$$\frac{a_{k-1}}{a_k} \det(M_k)_{k,k-1} = \det M_{k-1} + (a_{k-1} - d_{k-1}) \det M_{k-2}.$$

Combining these two results, we have found the following recursion rule for $\det M_k$, $k \geq 2$:

$$\begin{aligned} \det M_k &= \left(d_k - \frac{a_k}{a_{k-1}}a_k\right) \det M_{k-1} \\ &\quad - \left(a_k - \frac{a_k}{a_{k-1}}d_{k-1}\right) \left(\frac{a_k}{a_{k-1}} \det M_{k-1} + \left(a_k - \frac{a_k}{a_{k-1}}d_{k-1}\right) \det M_{k-2}\right) \\ &= \left(\left(d_k - \frac{a_k}{a_{k-1}}a_k\right) - \left(a_k - \frac{a_k}{a_{k-1}}d_{k-1}\right) \frac{a_k}{a_{k-1}}\right) \det M_{k-1} \\ &\quad - \left(a_k - \frac{a_k}{a_{k-1}}d_{k-1}\right)^2 \det M_{k-2} \end{aligned}$$

or

$$\det M_k = \left(d_k - \frac{2a_k^2}{a_{k-1}} + \frac{a_k^2 d_{k-1}}{a_{k-1}^2}\right) \det M_{k-1} - a_k^2 \left(1 - \frac{d_{k-1}}{a_{k-1}}\right)^2 \det M_{k-2}. \tag{7.1}$$

Obviously, the recursion base cases are given by

$$\begin{aligned} \det M_0 &= d_0, \\ \det M_1 &= d_0d_1 - a_1^2. \end{aligned}$$

Closed form expressions for the determinants Going back to our matrix, S_1 , by choosing

$$\begin{aligned} d_i &= 2 \frac{i+1}{2N-i}, \quad i = 0, \dots, N-1 \\ d_N &= 1 \\ a_i &= \frac{i+1}{2N-i} - \frac{i}{2N+1-i}, \quad i = 1, \dots, N-1 \\ a_N &= 1 - \frac{N}{N+1} = \frac{1}{N+1}, \end{aligned}$$

we get that M_k is the $k + 1$ 'th leading principal minor of the matrix S_1 . The recursion rule (7.1) can now be solved for this choice of a_i and d_i . The solution is given by:

$$\det M_k = \frac{(2N+1)^2}{(2N-k)^2} \left(1 + \sum_{i=0}^k \frac{2N-2k-1}{2N+4Ni-2i^2+1}\right) \prod_{i=0}^k \frac{2N+4Ni-2i^2+1}{(2N+1-i)^2}, \tag{7.2}$$

for $k = 0, \dots, N - 1$, and

$$\det M_N = \det L_1 = \frac{(2N + 1)^2}{(N + 1)^2} \prod_{i=0}^{N-1} \frac{2N + 4Ni - 2i^2 + 1}{(2N + 1 - i)^2}. \tag{7.3}$$

Verification We now proceed to verify the expressions (7.2) and (7.3) given above. We will show that these expressions satisfy the recursion rule (7.1) and the base cases of the problem. We begin by verifying the base cases:

$$\det M_0 = \frac{(2N + 1)^2}{(2N)^2} \left(1 + \frac{2N - 1}{2N + 1}\right) \frac{1}{2N + 1} = \frac{1}{N} = d_0,$$

$$\begin{aligned} \det M_1 &= \frac{(2N + 1)^2}{(2N - 1)^2} \left(1 + \frac{2N - 3}{2N + 1} + \frac{2N - 3}{6N - 1}\right) \frac{1}{2N + 1} \frac{6N - 1}{(2N)^2} \\ &= \frac{28N^2 - 20N - 1}{4N^2(2N - 1)^2} = \frac{4}{N(2N - 1)} - \left(\frac{2}{2N - 1} - \frac{1}{2N}\right)^2 = d_0d_1 - a_1^2. \end{aligned}$$

Now suppose $2 \leq k \leq N$. Denote

$$\begin{aligned} \alpha_k &= d_k - \frac{2a_k^2}{a_{k-1}} + \frac{a_k^2d_{k-1}}{a_{k-1}^2} = \begin{cases} 4 \frac{(2N+1)k-k^2-1}{(2N-k)^2}, & \text{if } k < N, \\ 3 \frac{2N^2+2N-1}{(2N+1)^2}, & \text{if } k = N, \end{cases} \\ \beta_k &= a_k^2 \left(1 - \frac{d_{k-1}}{a_{k-1}}\right)^2 = \begin{cases} \frac{(4kN-2N-2k^2+4k-1)^2}{(2N-k)^2(2N-k+1)^2}, & \text{if } k < N, \\ \frac{(2N^2+2N-1)^2}{(N+1)^2(2N+1)^2}, & \text{if } k = N, \end{cases} \end{aligned}$$

then the recursion rule (7.1) can be written as

$$\det M_k = \alpha_k \det M_{k-1} - \beta_k \det M_{k-2}.$$

Further denote

$$\begin{aligned} r_i &= \frac{1}{2N + 4Ni - 2i^2 + 1}, \quad i = 0, \dots, N - 1, \\ s_i &= \frac{(2N + 1)^2}{(2N - i)^2}, \quad i = 0, \dots, N - 1, \\ p_i &= 2N - 2i - 1, \quad i = 0, \dots, N - 1, \\ q_i &= \frac{2N + 4Ni - 2i^2 + 1}{(2N + 1 - i)^2}, \quad i = 0, \dots, N - 1, \end{aligned}$$

then the solution (7.2) becomes

$$\det M_k = s_k \left(1 + p_k \sum_{i=0}^k r_i \right) \prod_{i=0}^k q_i,$$

and (7.3) becomes

$$\det M_N = \frac{(2N + 1)^2}{(N + 1)^2} \prod_{i=0}^{N-1} q_i.$$

Substituting (7.2) in the RHS of (7.1) we get that for $k = 2, \dots, N$

$$\begin{aligned} & \alpha_k \det M_{k-1} - \beta_k \det M_{k-2} \\ &= \alpha_k s_{k-1} \left(1 + p_{k-1} \sum_{i=0}^{k-1} r_i \right) \prod_{i=0}^{k-1} q_i - \beta_k s_{k-2} \left(1 + p_{k-2} \sum_{i=0}^{k-2} r_i \right) \prod_{i=0}^{k-2} q_i \\ &= \left(\alpha_k s_{k-1} \left(1 + p_{k-1} r_{k-1} + p_{k-1} \sum_{i=0}^{k-2} r_i \right) - \frac{\beta_k}{q_{k-1}} s_{k-2} - \frac{\beta_k}{q_{k-1}} s_{k-2} p_{k-2} \sum_{i=0}^{k-2} r_i \right) \prod_{i=0}^{k-1} q_i \\ &= \left(\alpha_k s_{k-1} (1 + p_{k-1} r_{k-1}) - \frac{\beta_k}{q_{k-1}} s_{k-2} + \left(\alpha_k s_{k-1} p_{k-1} - \frac{\beta_k}{q_{k-1}} s_{k-2} p_{k-2} \right) \sum_{i=0}^{k-2} r_i \right) \\ & \quad \times \prod_{i=0}^{k-1} q_i. \end{aligned}$$

It is straightforward (although somewhat involved) to verify that for $k < N$

$$\alpha_k s_{k-1} (1 + p_{k-1} r_{k-1}) - \frac{\beta_k}{q_{k-1}} s_{k-2} = s_k q_k (1 + p_k r_{k-1} + p_k r_k),$$

and

$$\alpha_k s_{k-1} p_{k-1} - \frac{\beta_k}{q_{k-1}} s_{k-2} p_{k-2} = s_k p_k q_k.$$

We therefore get

$$\begin{aligned}
 & \alpha_k \det M_{k-1} - \beta_k \det M_{k-2} \\
 &= \left(s_k q_k (1 + p_k r_{k-1} + p_k r_k) + s_k p_k q_k \sum_{i=0}^{k-2} r_i \right) \prod_{i=0}^{k-1} q_i \\
 &= s_k \left(1 + p_k \sum_{i=0}^k r_i \right) \prod_{i=0}^k q_i \\
 &= \det M_k,
 \end{aligned}$$

and thus (7.2) satisfies (7.1). It is also possible to show that

$$\begin{aligned}
 \alpha_N s_{N-1} (1 + p_{N-1} r_{N-1}) - \frac{\beta_N}{q_{N-1}} s_{N-2} &= \frac{(2N+1)^2}{(N+1)^2}, \\
 \alpha_N s_{N-1} p_{N-1} - \frac{\beta_N}{q_{N-1}} s_{N-2} p_{N-2} &= 0,
 \end{aligned}$$

thus, for $k = N$

$$\begin{aligned}
 & \alpha_N \det M_{N-1} - \beta_N \det M_{N-2} \\
 &= \frac{(2N+1)^2}{(N+1)^2} \prod_{i=0}^{N-1} q_i \\
 &= \det M_N,
 \end{aligned}$$

and the expression (7.3) is also verified.

To complete the proof, note that the closed form expressions for $\det M_k$ consist of sums and products of positive values, hence $\det M_k$ is positive, and thus by Sylvester's criterion S_1 is positive definite.

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