Worst-case analyses for first-order optimization methods

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1	Introduction	2
2	Getting familiar with base performance estimation problems	2
3	Further exercises	7
4	Slightly more advanced techniques	12
5	Background material and useful facts 5.1 Standard definitions	12 12 13
	0.2 Interpolation/extension theorems	Т,

Foreword & Acknowledgements

This document provides a series of exercises for getting familiar with "performance estimation problems" and the use of semidefinite programming for analyzing worst-case behaviors of optimization methods. An informal introduction can be found in this blog post. Exercises summarizing the main ingredients of the approach are provided in Section 2 (Exercise 1 focuses on the primal PEP formulation—i.e., on finding worst-case scenarios—, whereas Exercise 2 focuses on the dual formulation—i.e., on finding rigorous worst-case guarantees). Section 3 contains exercises for going further. Background material that might be used for the exercises is provided in Section 5.

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1 Introduction

In short, considering problems of the form

$$\min_{x \in \mathbb{R}^d} F(x),$$

where we denote an optimal solution by $x_{\star} \in \operatorname{argmin}_{x \in \mathbb{R}^d} F(x)$, our goal here is to assess "a priori" the quality of the output of some "black-box" iterative algorithm, whose iterates are denoted by x_0, x_1, \ldots, x_N . There are typically different ways of doing so, which might or might not be relevent depending on the target applications of a particular optimization method. In first-order optimization, we often want to upper bound the quality of an iterate x_k in one of the following terms (which we all ideally would like to be as small as possible, and decreasing functions of $k \in \mathbb{N}$): $||x_k - x_{\star}||^2$, $||\nabla f(x_k)||^2$, or $f(x_k) - f(x_{\star})$. There are of course other possibilities, including combinations of them (see examples below).

So, our goal is to assess the quality of x_k by providing hopefully meaningfull upper bounds on at least one such quantity. For doing so, we consider classes of problems (i.e., sets of assumptions on F), and perform worst-case analyses (i.e., we want the bound to be valid for all F satisfying the set of assumptions at hand). The following exercises try to shed a bit of light on this topic, by examplifying a principled approach to construct such worst-case convergence bounds using the so-called "performance estimation framework", introduced by Drori and Teboulle in [1]. This document presents the performance estimation problem using the formalism from Taylor, Hendrickx, and Glineur [2, 3].

Notations. We denote by $\langle \cdot, \cdot \rangle : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ the standard Euclidean inner product, and by $\|\cdot\|^2 : \mathbb{R}^d \to \mathbb{R}$ the standard Euclidean norm, that is, the induced norm: for any $x \in \mathbb{R}^d : \|x\|^2 = \langle x, x \rangle$ (the results and techniques below apply more broadly (see, e.g., [2, 4]), but it is not needed for understanding the exercises below). Other notations are defined throughout the text.

Packages The numerical parts of the exercises were mostly done for using Python (or alternatively Matlab), but the reader can use other languages if he is proficient with semidefinite programming with it (although there is currently no interface for easing the access to performance estimation beyond Python and Matlab). A few exercises were designed for using the PEPit package [5] (alternatively, for Matlab, PESTO [6]). For users planning to keep using performance estimation, we advise to install a good SDP solver such as MOSEK [7]. In any case, the Python package relies on CVXPY [8] (see PEPit installation) and the Matlab one relies on YALMIP [9] (see PESTO installation). Some exercises might be simpler to approach using some symbolic computations, such as Sympy [10] (which is used in some of the Python notebooks).

Getting corrected exercises? Just recompile this latex file after setting the second line of the document to \def\includeCorrections{1} (\def\includeCorrections{0} to remove corrections).

2 Getting familiar with base performance estimation problems

In this section, we introduce the main base ingredients underlying the performance estimation technique. Those ingredients are all examplified for the analysis of gradient descent.

The goal of this first exercise is to (i) get familiar with the concept of performance estimation problem, that is, how can we cast, and solve, the problem of looking for worst-case scenarios in the context of first-order optimization; and (ii) get an idea on the applicability of the methodology for standard settings.

Exercise 1 (Gradient method—"primal performance estimation") For this exercise, consider the problem of "black-box" minimization of a smooth strongly convex function:

$$f_{\star} \triangleq \min_{x \in \mathbb{R}^d} f(x), \tag{1}$$

where f is L-smooth and μ -strongly convex (see Definition 2), and where $x_{\star} \triangleq \operatorname{argmin}_{x} f(x)$ and $f_{\star} \triangleq f(x_{\star})$ its optimal value. For minimizing (1) we use gradient descent with a pre-determined sequence of stepsizes $\{\gamma_{k}\}_{k}$; that is, we iterate $x_{k+1} = x_{k} - \gamma_{k} \nabla f(x_{k})$. The goal of this exercise is to compute $\tau(\mu, L, \gamma_{k})$, a.k.a. a convergence rate, the smallest value such that the inequality

$$||x_{k+1} - x_{\star}||^2 \leqslant \tau(\mu, L, \gamma_k) ||x_k - x_{\star}||^2 \tag{2}$$

is valid for any $d \in \mathbb{N}$, for any L-smooth μ -strongly convex function f (notation $f \in \mathcal{F}_{\mu,L}$) and for all $x_k, x_{k+1} \in \mathbb{R}^d$ such that $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$, and any $x_* \in \operatorname{argmin}_x f(x)$.

1. Assuming $x_{\star} \neq x_k$ (without loss of generality), show that

$$\tau(\mu, L, \gamma_k) = \sup_{\substack{d, f \\ x_k, x_{k+1}, x_{\star}}} \frac{\|x_{k+1} - x_{\star}\|^2}{\|x_k - x_{\star}\|^2}$$

$$s.t. \ f \in \mathcal{F}_{\mu, L}$$

$$x_{k+1} = x_k - \gamma_k \nabla f(x_k)$$

$$\nabla f(x_{\star}) = 0,$$
(3)

where f, x_k , x_{k+1} , x_{\star} , and d are the variables of the optimization problem.

2. Show that

$$\tau(\mu, L, \gamma_{k}) = \sup_{\substack{d \\ x_{k}, x_{k+1}, x_{\star} \\ g_{k}, g_{\star} \\ f_{k}, f_{\star}}} \frac{\|x_{k+1} - x_{\star}\|^{2}}{\|x_{k} - x_{\star}\|^{2}}$$

$$s.t. \ \exists f \in \mathcal{F}_{\mu, L} \ such \ that \ \begin{cases} f_{i} = f(x_{i}) & i = k, \star \\ g_{i} = \nabla f(x_{i}) & i = k, \star \end{cases}$$

$$x_{k+1} = x_{k} - \gamma_{k} g_{k}$$

$$q_{\star} = 0.$$
(4)

3. Using Theorem 2, show that $\tau(\mu, L, \gamma_k)$ is also equal to

$$\sup_{\substack{d \\ x_{k}, x_{k+1}, x_{\star} \\ g_{k}, g_{\star} \\ f_{k}, f_{\star}}} \frac{\|x_{k+1} - x_{\star}\|^{2}}{\|x_{k} - x_{\star}\|^{2}}$$

$$s.t. \quad f_{\star} \geqslant f_{k} + \langle g_{k}, x_{\star} - x_{k} \rangle + \frac{1}{2L} \|g_{\star} - g_{k}\|^{2} + \frac{\mu}{2(1 - \mu/L)} \|x_{\star} - x_{k} - \frac{1}{L} (g_{\star} - g_{k})\|^{2}$$

$$f_{k} \geqslant f_{\star} + \langle g_{\star}, x_{k} - x_{\star} \rangle + \frac{1}{2L} \|g_{k} - g_{\star}\|^{2} + \frac{\mu}{2(1 - \mu/L)} \|x_{k} - x_{\star} - \frac{1}{L} (g_{k} - g_{\star})\|^{2}$$

$$x_{k+1} = x_{k} - \gamma_{k} g_{k}$$

$$g_{\star} = 0.$$

$$(5)$$

4. Using the change of variables

$$G \triangleq \begin{bmatrix} \|x_k - x_\star\|^2 & \langle g_k, x_k - x_\star \rangle \\ \langle g_k, x_k - x_\star \rangle & \|g_k\|^2 \end{bmatrix}, \quad F \triangleq f_k - f_\star, \tag{6}$$

(note that $G = [x_k - x_\star \quad g_k]^\top [x_k - x_\star \quad g_k] \geq 0$), show that $\tau(\mu, L, \gamma_k)$ can be computed as

$$\sup_{G,F} \frac{G_{1,1} + \gamma_k^2 G_{2,2} - 2\gamma_k G_{1,2}}{G_{1,1}}$$
s.t.
$$F + \frac{L\mu}{2(L-\mu)} G_{1,1} + \frac{1}{2(L-\mu)} G_{2,2} - \frac{L}{L-\mu} G_{1,2} \leqslant 0$$

$$- F + \frac{L\mu}{2(L-\mu)} G_{1,1} + \frac{1}{2(L-\mu)} G_{2,2} - \frac{\mu}{L-\mu} G_{1,2} \leqslant 0$$

$$G \geqslant 0.$$
(7)

Hint: you can use the following fact ("Cholesky factorization"). Let $X \in \mathbb{S}^n$ (symmetric matrix of size $n \times n$), we have:

$$X \succcurlyeq 0$$
 with $\operatorname{rank}(X) \leqslant d \Leftrightarrow \exists P \in \mathbb{R}^{d \times n}$ such that $X = P^{\top}P$.

5. Show that $\tau(\mu, L, \gamma_k)$ can also be computed as a semidefinite program (SDP):

$$\sup_{G,F} G_{1,1} + \gamma_k^2 G_{2,2} - 2\gamma_k G_{1,2}
s.t. \quad F + \frac{L\mu}{2(L-\mu)} G_{1,1} + \frac{1}{2(L-\mu)} G_{2,2} - \frac{L}{L-\mu} G_{1,2} \leqslant 0
- F + \frac{L\mu}{2(L-\mu)} G_{1,1} + \frac{1}{2(L-\mu)} G_{2,2} - \frac{\mu}{L-\mu} G_{1,2} \leqslant 0
G_{1,1} = 1
G \succcurlyeq 0$$
(8)

(note that at this stage, it is actually simpler to show that the supremum is attained and that we can write max instead of sup.)

- 6. Let $L \geqslant \mu > 0$ and define $h_k \triangleq \gamma_k L$ and $\kappa \triangleq L/\mu$. Show that $\tau(\mu, L, \gamma_k) = \tau(1/\kappa, 1, h_k)$ (in other words: we can study the case L = 1 only and deduce the dependence of τ on L afterwards).
- 7. Complete the PEPit code (alternative in Matlab: PESTO code) for computing $\tau(\mu, L, \gamma_k)$ and compute its value for a few numerical values of μ and γ_k .
- 8. Set L=1 and compute the optimal value of γ_k numerically for a few values of μ . Similarly, compute the range of γ_k for which the ratios is smaller than 1 in the worst-case.
- 9. Update your code for computing (numerically) the worst-case ratio $\frac{\|\nabla f(x_{k+1})\|^2}{\|\nabla f(x_k)\|^2}$ as a function of L, μ , and γ_k . For what values of γ_k do you observe that this ratio is smaller than 1? How would you update the SDP formulation for taking this change into account?
- 10. Update your code for computing (numerically) the worst-case ratio $\frac{f(x_{k+1})-f(x_{\star})}{f(x_k)-f(x_{\star})}$ as a function of L, μ , and γ_k . For what values of γ_k do you observe that this ratio is smaller than 1? How would you update the SDP formulation for taking this change into account?
- 11. Update your code for computing (numerically) the worst-case ratio $\frac{\|x_N x_\star\|^2}{\|x_0 x_\star\|^2}$ as a function of L, μ , and a sequence $\{\gamma_k\}_{0 \leqslant k \leqslant N-1}$. How would you update the SDP formulation for taking this change into account?
- 12. Using previous points: assume you computed an optimal solution to the SDP formulation for the ratio $\frac{\|x_N x_\star\|^2}{\|x_0 x_\star\|^2}$ what is the link between the rank of the Gram matrix G and the dimension d in which this counter-example lives?
- 13. For obtaining "low-dimensional" worst-case instances, it is often useful to use heuristics. One of them is known as the "trace heuristic" (alternatively, the "logdet heuristic" is sometimes more efficient; see Exercise 7), which consists in solving a second optimization problem, whose solution hopefully forces G to have a lower rank. The trace heuristic for (8) consists in solving

$$\min_{G,F} \operatorname{Trace}(G)
s.t. \quad F + \frac{L\mu}{2(L-\mu)}G_{1,1} + \frac{1}{2(L-\mu)}G_{2,2} - \frac{L}{L-\mu}G_{1,2} \leq 0
\quad - F + \frac{L\mu}{2(L-\mu)}G_{1,1} + \frac{1}{2(L-\mu)}G_{2,2} - \frac{\mu}{L-\mu}G_{1,2} \leq 0
G_{1,1} = 1
G_{1,1} + \gamma_k^2 G_{2,2} - 2\gamma_k G_{1,2} = \tau(\mu, L, \gamma_k)
G \geq 0,$$
(9)

for which one first needs to obtain a precise approximation of $\tau(\mu, L, \gamma_k)$.

The trace heuristic is already implemented within PEPit and PESTO; see this PEPit code (alternative in Matlab: PESTO code). Can you plot the resulting worst-case function(s) for a few different values of N (e.g., N=1,2,5,10) with $\gamma_k=\frac{1}{L}$. Does it correspond to a simple function? (Hint: two extremely simple examples of L-smooth μ -strongly convex functions are $\frac{\mu}{2}x^2$ and $\frac{L}{2}x^2$). Can you use this conclusion for "guessing" an expression for $\tau(\mu, L, 1/L)$ based on the behavior of gradient descent on the worst-case function that you identified?

- 14. Set $\gamma_k = \frac{1}{L}$ and $\mu = 0$. What worst-case ratio $\frac{\|x_N x_\star\|^2}{\|x_0 x_\star\|^2}$ do you observe numerically? A classical way to avoid such a pathological behavior (in the analyses) is to study different types of ratios. Modify your code for studying the ratio $\frac{f(x_N) f_\star}{\|x_0 x_\star\|^2}$. Can you guess the dependence of the worst-case ratio on N based on a few numerical trials? and the dependence on L?
- 15. Same question with $\gamma_k = \frac{1}{L}$, $\mu = 0$, and the ratio $\frac{\|\nabla f(x_N)\|^2}{\|x_0 x_\star\|^2}$.
- 16. Same question with $\gamma_k = \frac{1}{L}$, $\mu = 0$, and the ratio $\frac{\|x_N x_\star\|^2}{\|\nabla f(x_0)\|^2}$.
- 17. Based on your current experience, what are, according to you, the key elements which allowed casting the worst-case analysis as an SDP?

At this stage, the reader is familiar with necessary ingredients for attacking most exercises from Section 3. Before going further, we advise the reader to go through Exercise 3.

The goal of the next exercise is to link what we have seen so far with "classical convergence proofs". That is, we want to illustrate how to create rigorous worst-case convergence bounds using the previous concept together with SDP duality. Once such a proof is found, one can convert it to a certificate that is easy to verify without resorting on any semidefinite programming.

Exercise 2 (Gradient method—"dual performance estimation") This exercise uses the same problem formulations and notation as Exercise 1.

1. Using Lagrangian duality with the following primal-dual pairing $(\tau, \lambda_1, \lambda_2)$ are dual variables)

$$F + \frac{L\mu}{2(L-\mu)}G_{1,1} + \frac{1}{2(L-\mu)}G_{2,2} - \frac{L}{L-\mu}G_{1,2} \leqslant 0 \qquad : \lambda_1$$

$$-F + \frac{L\mu}{2(L-\mu)}G_{1,1} + \frac{1}{2(L-\mu)}G_{2,2} - \frac{\mu}{L-\mu}G_{1,2} \leqslant 0 \qquad : \lambda_2$$

$$G_{1,1} = 1 \qquad : \rho,$$
(10)

one can show that (we will do it in the sequel):

$$\min_{\substack{\rho,\lambda_1,\lambda_2\geqslant 0}} \rho$$

$$s.t. S = \begin{bmatrix} \rho - 1 + \frac{\lambda_1 L \mu}{L - \mu} & \gamma_k - \frac{\lambda_1 (\mu + L)}{2(L - \mu)} \\ \gamma_k - \frac{\lambda_1 (\mu + L)}{2(L - \mu)} & \frac{\lambda_1}{L - \mu} - \gamma_k^2 \end{bmatrix} \succcurlyeq 0$$

$$0 = \lambda_1 - \lambda_2,$$
(11)

is a standard Lagrangian dual for the problem of computing $\tau(\mu, L, \gamma_k)$. Note that equality holds due to strong duality (for going further: prove strong duality using a Slater condition).

What is the relationship between feasible points to (11) and $\tau(\mu, L, \gamma_k)$?

2. (Lagrangian dual) Show that (11) is a dual for (8) using the primal-dual pairing (10).

3. (Trick) The intent of this second point is to provide a shortcut to obtain a symbolical formulation of the dual problem. In short, consider the following variation of (5) with d = 1:

$$\sup_{\substack{x_{k}, x_{k+1}, x_{\star} \in \mathbb{R} \\ g_{k}, g_{\star} \in \mathbb{R} \\ f_{k}, f_{\star} \in \mathbb{R}}} \|x_{k+1} - x_{\star}\|^{2}$$

$$s.t. \ f_{\star} \geqslant f_{k} + \langle g_{k}, x_{\star} - x_{k} \rangle + \frac{1}{2L} \|g_{\star} - g_{k}\|^{2} + \frac{\mu}{2(1 - \mu/L)} \|x_{\star} - x_{k} - \frac{1}{L} (g_{\star} - g_{k})\|^{2}$$

$$f_{k} \geqslant f_{\star} + \langle g_{\star}, x_{k} - x_{\star} \rangle + \frac{1}{2L} \|g_{k} - g_{\star}\|^{2} + \frac{\mu}{2(1 - \mu/L)} \|x_{k} - x_{\star} - \frac{1}{L} (g_{k} - g_{\star})\|^{2}$$

$$x_{k+1} = x_{k} - \gamma_{k} g_{k}$$

$$\|x_{k} - x_{\star}\|^{2} = 1$$

$$g_{\star} = 0.$$
(12)

After substitution of x_{k+1} and g_{\star} (one can also set $x_{\star} = f_{\star} = 0$ wlog) in the objective and the constraints, write the Lagrangian $\mathcal{L}(x_k, g_k, f_k, x_{\star}, f_{\star}; \lambda_1, \lambda_2, \rho)$ (where $\lambda_1, \lambda_2, \rho \geqslant 0$ are associated as in (10)). Then, show that the expression of S in (11) (i.e., the LMI in (11)) corresponds to $S = -\frac{1}{2}\nabla^2_{x_k,g_k}\mathcal{L}(x_k, g_k, f_k, x_{\star}, f_{\star}; \lambda_1, \lambda_2, \rho)$ and that the linear constraint in (11) corresponds to requiring $S = \nabla_{f_k}\mathcal{L}(x_k, g_k, f_k, x_{\star}, f_{\star}; \lambda_1, \lambda_2, \rho)$ to be zero.

An advantage of this approach is that it allows to easily obtain the dual formulations using symbolic computation (see, e.g., Python this notebook, or this Matlab file).

- 4. Solve (11) numerically. Do those values match those obtained in the first exercise?

 For doing that, you can complete the following Python code (alternative: Matlab code).
- 5. Is there a simple closed-form expression for $\tau(\mu, L, \gamma_k)$? Does it match the numerical values obtained using the previous codes for computing $\tau(\mu, L, \gamma_k)$ numerically?

Hint: can you solve (11) in closed-form? Some help relying on symbolic computations is provided in the same notebook as in the previous exercise (alternative: Matlab code).

- 6. Consider $\gamma_k = \frac{1}{L}$ for simplicity. Given the optimal value of the multipliers ρ , λ_1 , λ_2 in (11), can you write a "direct" proof for the linear convergence in terms of distance to an optimal point without resorting on any SDP formulation?
- 7. A corresponding dual problem for the worst-case ratio $\frac{\|\nabla f(x_{k+1})\|^2}{\|\nabla f(x_k)\|^2}$ given by

$$\min_{\rho,\lambda_{1},\lambda_{2}\geqslant 0} \rho$$

$$s.t. \ S = \begin{bmatrix} \rho + \lambda_{1} \frac{(1-\gamma_{k}L)(1-\gamma_{k}\mu)}{L-\mu} & -\lambda_{1} \frac{2-\gamma_{k}(L+\mu)}{2(L-\mu)} \\ -\lambda_{1} \frac{2-\gamma_{k}(L+\mu)}{2(L-\mu)} & \frac{\lambda_{1}}{L-\mu} - 1 \end{bmatrix} \geqslant 0$$

$$0 = \lambda_{1} - \lambda_{2}.$$
(13)

Is there a simple closed-form solution for this problem? Alternatively: solve this problem numerically and try to guess a solution.

8. Using the following primal-dual pairing

$$\begin{split} f(x_0) &\geqslant f(x_\star) + \frac{1}{2L} \|\nabla f(x_0)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_0 - x_\star - \frac{1}{L} \nabla f(x_0)\|^2 \\ f(x_\star) &\geqslant f(x_0) + \langle \nabla f(x_0), x_\star - x_0 \rangle + \frac{1}{2L} \|\nabla f(x_0)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_0 - x_\star - \frac{1}{L} \nabla f(x_0)\|^2 \\ f(x_1) &\geqslant f(x_\star) + \frac{1}{2L} \|\nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_1 - x_\star - \frac{1}{L} \nabla f(x_1)\|^2 \\ f(x_\star) &\geqslant f(x_1) + \langle \nabla f(x_1), x_\star - x_1 \rangle + \frac{1}{2L} \|\nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_1 - x_\star - \frac{1}{L} \nabla f(x_1)\|^2 \\ f(x_0) &\geqslant f(x_1) + \langle \nabla f(x_1), x_0 - x_1 \rangle + \frac{1}{2L} \|\nabla f(x_0) - \nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_1 - x_0 - \frac{1}{L} (\nabla f(x_1) - \nabla f(x_0))\|^2 \\ f(x_1) &\geqslant f(x_0) + \langle \nabla f(x_0), x_1 - x_0 \rangle + \frac{1}{2L} \|\nabla f(x_0) - \nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)} \|x_1 - x_0 - \frac{1}{L} (\nabla f(x_1) - \nabla f(x_0))\|^2 \\ f(x_0) - f(x_\star) &= 1 \\ &: \rho \end{split}$$

a corresponding dual problem for the worst-case ratio $\frac{f(x_{k+1})-f_{\star}}{f(x_k)-f_{\star}}$ is given by

$$\min_{\rho,\lambda_1,\lambda_2\geqslant 0}\rho \\ s.t. \begin{bmatrix} \frac{\mu L(\lambda_1+\lambda_2+\lambda_3+\lambda_4)}{L-\mu} & -\frac{L(\lambda_2+\gamma\mu(\lambda_3+\lambda_4))+\mu\lambda_1}{L-\mu} & -\frac{L\lambda_4+\mu\lambda_3}{L-\mu} \\ * & \frac{\gamma\mu(\gamma L(\lambda_3+\lambda_4+\lambda_5+\lambda_6)-2\lambda_5)-2\gamma L\lambda_6+\lambda_1+\lambda_2+\lambda_5+\lambda_6}{L-\mu} & \frac{\gamma L\lambda_4+\lambda_5(\gamma L-1)+\gamma\mu(\lambda_3+\lambda_6)-\lambda_6}{L-\mu} \\ * & * & \frac{\lambda_3+\lambda_4+\lambda_5+\lambda_6}{L-\mu} \end{bmatrix} \succcurlyeq 0 \\ 0 = \rho - \lambda_1 + \lambda_2 - \lambda_5 + \lambda_6 \\ 1 = -\lambda_3 + \lambda_4 + \lambda_5 - \lambda_6,$$

where "*" denotes symmetrical elements in the PSD matrix. Is there a simple closed-form solution for this problem? Note that this SDP is already coded here (alternative in Matlab: here)

Trick #1: solve the problem numerically and plot some values for the multipliers; trick #2: pick $\lambda_1 = \lambda_3 = \lambda_6 = 0$; does the problem simplify?

Trick #3: one can use trace norm of logdet minimization (on S), or $\|.\|_1$ norm minimization on λ 's on the dual side for trying to get simpler/sparser proofs. That being said, when there are only few inequalities involved, it is often easier to simply greedily try different combinations of λ_i 's to be set to 0.

9. Obtain the dual formulations for the problems of computing the worst-case ratios $\frac{\|\nabla f(x_{k+1})\|^2}{\|\nabla f(x_k)\|^2}$ and $\frac{f(x_{k+1})-f_{\star}}{f(x_k)-f_{\star}}$, either using symbolic computations or by hand.

3 Further exercises

The goal of this second set of exercises is to get familiar with the approach and to understand to what extend it applies beyond a single iteration of gradient descent. There main points of attention below can be categorized within three types:

- what type of algorithms can it study?
- What classes of problems can it study?
- What types of guarantees can it study?

The corrections are much lighter and are mostly contained in a few notebooks.

Exercise 3 (Sublinear convergence of gradient descent and acceleration) For this exercise, we consider the problem of minimizing

$$\min_{x} f(x),$$

where f is an L-smooth convex function (see Definition 1). We consider three algorithms, which respectively iterate:

• a gradient method:

$$x_{k+1} = x_k - \frac{1}{L}\nabla f(x_k),$$

• an heavy-ball method:

$$x_{k+1} = x_k + \frac{k}{k+2}(x_k - x_{k-1}) - \frac{1}{k+2}\frac{1}{L}\nabla f(x_k),$$

• an accelerated (or fast) gradient method:

$$x_{k+1} = y_k - \frac{1}{L}\nabla f(y_k)$$

$$y_{k+1} = x_{k+1} + \frac{k-1}{k+2}(x_{k+1} - x_k)$$

1. Consider the following ratios:

(a)
$$\frac{f(x_N) - f_{\star}}{\|x_0 - x_{\star}\|^2}$$
 and $\frac{\min_{0 \le i \le N} \{f(x_i) - f_{\star}\}}{\|x_0 - x_{\star}\|^2}$

(a)
$$\frac{f(x_N) - f_{\star}}{\|x_0 - x_{\star}\|^2}$$
 and $\frac{\min_{0 \le i \le N} \{f(x_i) - f_{\star}\}}{\|x_0 - x_{\star}\|^2}$,
(b) $\frac{\|\nabla f(x_N)\|^2}{\|x_0 - x_{\star}\|^2}$ and $\frac{\min_{0 \le i \le N} \{\|\nabla f(x_i)\|^2\}}{\|x_0 - x_{\star}\|^2}$.

Can we formulate the worst-case analyses for those methods and those ratios as SDPs? What is the influence of N on its size and on the number of inequalities under consideration?

2. Using PEPit or PESTO compare those methods in terms of those ratios (for L=1 and as a function of N few values of N = 0, 1, ..., 30).

Exercise 4 (Primal proximal point method) Consider the problem of minimizing a (closed, proper) convex function

$$\min_{x \in \mathbb{P}^d} f(x),$$

with the proximal-point method (with stepsize γ):

$$x_{k+1} = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \{ f(x) + \frac{1}{2\gamma} ||x - x_k||^2 \}.$$

1. Note that using optimality conditions on the definition of the proximal-point iteration, one can rewrite the iteration as

$$x_{k+1} = x_k - \gamma g_{k+1},$$

with $g_{k+1} \in \partial f(x_{k+1})$ (the subdifferential of f at x_{k+1} ; i.e., g_{k+1} is a subgradient at x_{k+1}). Can you reformulate the problem of finding a worst-case example for the ratio $\frac{f(x_N)-f_{\star}}{\|x_0-x_{\star}\|^2}$ as an SDP? What are the key ingredients for arriving to it?

- 2. Provide a PEPit or PESTO code for computing the worst-case value for this ratio, and experiment with it.
- 3. Guess the dependence of the worst-case ratio on γ and on N; confirm your findings using numerics.
- 4. Can you guess the shape of a worst-case function? You may want to use an heuristic for finding lower rank worst-case examples.

Exercise 5 (Projected gradient and Frank-Wolfe) We consider the minimization problem

$$\min_{x \in Q} f(x),$$

where f is an L-smooth convex function and Q is a non-empty convex set with finite diameter (i.e., $||x-y|| \le D$ for all $x,y \in Q$ for some D > 0). Given some $x_0 \in Q$, we consider two possible first-order methods:

• projected gradient:

$$x_{k+1} = \operatorname{Proj}_{Q} \left[x_k - \frac{1}{L} \nabla f(x_k) \right]$$

• conditional gradient (a.k.a., Frank-Wolfe):

$$y_k = \underset{y \in Q}{\operatorname{argmin}} \langle \nabla f(x_k), y \rangle$$
$$x_{k+1} = \frac{k}{k+2} x_k + \frac{1}{k+2} y_k.$$

- 1. For each method, how can you write the problem of computing the worst-case for the value of $f(x_N) - f_{\star}$? (note that we do not need a denominator as the diameter $D < \infty$ is bounded).
- 2. For each method, how can we sample the problem? (at which points do we need to sample each function?)

3. Write a PEPit or PESTO code and guess the dependence on the iteration counter N of the worst-case $f(x_N) - f_{\star}$ for each of those methods. What are the dependences on D and L?

Exercise 6 (Proximal point method for monotone inclusions) For this exercise, we consider the problem of solving a monotone inclusion problem:

find
$$x \in \mathbb{R}^d$$
 such that $0 \in M(x)$,

where $M: \mathbb{R}^d \to \mathbb{R}^d$ (point to set mapping) is a (maximal) mononotone operator (see Definition 5). In this context, the proximal point method consists in iterating

$$x_{k+1} = \operatorname{prox}_{\alpha M}(x_k) = (I + \alpha M)^{-1} x_k,$$

(where I is the identity operator) or equivalently

$$x_{k+1} = x_k - \alpha M(x_{k+1}).$$

- 1. Consider the ratio $\frac{\|x_N x_{N+1}\|^2}{\|x_0 x_{\star}\|^2}$, where x_{\star} is such that $0 \in M(x_{\star})$. Can you compute this worst-case ratio using an SDP? Hint: you can use Theorem 5.
- 2. Write a PEPit or PESTO code for studying this ratio as a function of N and α .
- 3. Using dimension reduction, there should exist a low-dimensional worst-case example. Find it (numerically) and plot it.

Hint: more information about the worst-case guarantee and a low-dimensional worst-case example can be found in [14] (see pdf). Are your observations compatible with the fact that M might encode a rotation matrix?

Exercise 7 (Fixed-point iterations) For this exercise, we consider the fixed point problem

find
$$x \in \mathbb{R}^d$$
 such that $x = F(x)$,

where $F: \mathbb{R}^d \to \mathbb{R}^d$ is a nonexpansive mapping (i.e., it is 1-Lipschitz; that is, for all $x, y \in \mathbb{R}^d$, $||F(x) - F(y)|| \leq ||x - y||$).

1. The Halpern iteration is given by

$$x_{k+1} = \left(1 - \frac{1}{k+2}\right)F(x_k) + \frac{1}{k+2}x_0$$

Can you write an SDP formulation for computing the worst-case ratio $\frac{\|x_N - F(x_N)\|^2}{\|x_0 - x_\star\|^2}$ (for some $x_\star = F(x_\star)$)?

Hint: Theorem 6 with L = 1.

- 2. Write a PEPit or PESTO code for computing the worst-case value of this ratio. Can you guess the dependence in N of the worst-case behavior of the previous ratio?
- 3. Can you find low-dimensional worst-case examples for this method? (Hint: use a few iterations of the logdet heuristic (implemented within PEPit and described in [11] (see pdf)).
- 4. An alternative is the so-called Krasnolselskii-Mann iteration, which can be instantiated as

$$x_{k+1} = \left(1 - \frac{1}{k+2}\right)F(x_k) + \frac{1}{k+2}x_k$$

How does it compare to Halpern in terms of worst-case ratios?

Exercise 8 (Subgradient methods) For this exercise, we consider the problem of minimizing an M-Lipschitz convex function (which is possibly nonsmooth; see Definition 4)

$$\min_{x} f(x),$$

using a subgradient method $x_{k+1} = x_k - \gamma_k s_k$ with $s_k \in \partial f(x_k)$. We aim to compute worst-case bounds on $\min_{0 \le i \le N} \{ f(x_i) - f_{\star} \}$ for certain values of N under the condition that $||x_0 - x_{\star}||^2 \le R^2$ for some $x_{\star} \in \operatorname{argmin}_x f(x)$ and when $f \in \mathcal{C}_M$ (notation for closed, proper, convex, and M-Lipschitz).

- 1. Write a code for computing a worst-case bound on $\min_{0 \le i \le N} \{f(x_i) f_{\star}\}$.
- 2. How does your bound compare to the known

$$\min_{0 \le i \le N} \{ f(x_i) - f_{\star} \} \le \frac{R^2 + M^2 \sum_{k=0}^{N-1} \gamma_k^2}{\sum_{k=0}^{N-1} \gamma_k}$$

for a few stepsize policies, including:

- fixed stepsize policy $\gamma_k = 1$,
- fixed stepsize policy depending on the horizon $\gamma_k = \frac{R}{M\sqrt{N+1}}$,
- decreasing stepsize policy $\gamma_k = \frac{R}{M\sqrt{k+1}}$,
- decreasing stepsize policy $\gamma_k = \frac{R}{M(k+1)}$.
- 3. Adapt your code for computing a worst-case bound on the last iterate $f(x_N) f_{\star}$. Does the worst-case deteriorate?
- 4. Evaluate the same two worst-case guarantees (best function value accuracy among the iterates and last one) for the quasi-monotone subgradient method: (from [16], or [17]):

$$s_k \in \partial f(x_k)$$

$$d_k = \frac{1}{k+2} \sum_{i=0}^k s_i$$

$$y_{k+1} = \frac{k+1}{k+2} x_k + \frac{1}{k+2} x_0$$

$$x_{k+1} = y_{k+1} - \frac{R}{M\sqrt{N+1}} d_k.$$

Exercise 9 (Proximal gradient method) We consider the composite convex minimization problem of the form

$$\min_{x \in \mathbb{R}^d} \{ F(x) \triangleq f(x) + h(x) \},$$

where f is L-smooth and μ -strongly convex and h is ccp (closed, convex, proper) so that its proximal operation is well-defined. We want to use the proximal gradient method

$$x_{k+1} = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \{ h(x) + \langle \nabla f(x_k), x - x_k \rangle + \frac{L}{2} ||x - x_k||^2 \}$$

for solving the problem.

- 1. Can we formulate the problem of computing the worst-case ratio $\frac{\|x_{k+1}-x_{\star}\|^2}{\|x_k-x_{\star}\|^2}$ as an SDP? Describe at which points each function needs to be sampled.
- 2. Write a code for computing it, and compare the numerical values with those of Exercise 1.
- 3. Can you find low-dimensional worst-case instances?

Exercise 10 (Douglas-Rachford) Consider a composite convex minimization problem of the form

$$\min_{x \in \mathbb{R}^d} \{ F(x) \triangleq f(x) + h(x) \},\$$

where f is L-smooth and μ -strongly convex and h is ccp (closed, convex, proper) so that both proximal operations are well-defined. We want to use the Douglas-Rachford (DR) method

$$x_k = \operatorname{prox}_{\alpha h}(w_k),$$

$$y_k = \operatorname{prox}_{\alpha f}(2x_k - w_k),$$

$$w_{k+1} = w_k + \theta(y_k - x_k),$$

for solving the problem.

- 1. Let w_0 and w'_0 be two different starting points. Formulate the problem of computing the worst-case ratio $\frac{\|w_1-w'_1\|^2}{\|w_0-w'_0\|^2}$ where w_1 and w'_1 are the outputs of a DR iteration from respectively w_0 and w'_0 . Where should the two functions be sampled?
- 2. Write a code for computing it. As a reference when $\theta = 1$: how do the numerics compare to the bound $\|w_1 w_1'\|^2 \leqslant \left(\max\left\{\frac{1}{1+\alpha\mu}, \frac{\alpha L}{1+\alpha L}\right\}\right)^2 \|w_0 w_0'\|^2$ (see, e.g., [18, Theorem 2]).
- 3. Can you find low-dimensional worst-case instances?

Exercise 11 (Alternate projections) We consider the problem of finding a point in the intersection of two closed convex sets:

find
$$x \in Q_1 \cap Q_2$$
,

where $Q_1, Q_2 \subseteq \mathbb{R}^d$ are two closed convex sets. We will compare, in terms of their worst-case behaviors, a few methods for solving this problem.

Write PEPit (or PESTO) codes for computing the worst-case ratios $\frac{\|\operatorname{Proj}_{Q_1}(x_N)-\operatorname{Proj}_{Q_2}(x_N)\|^2}{\|x_0-x_\star\|^2}$ (where $\operatorname{Proj}_Q(\cdot)$ denotes the projections onto a set Q, some $x_\star \in Q_1 \cap Q_2$, and x_k denotes the iterate of the following methods; N denotes the "final" iteration count); you may experiment with other types of ratios. Can you guess the dependence on k of the worst-case value for this ratio?

1. Alternate projections: set $y_0 = x_0$ and iterate

$$x_{k+1} = \operatorname{Proj}_{Q_1}(y_k),$$

$$y_{k+1} = \operatorname{Proj}_{Q_2}(x_k),$$

2. averaged projections: iterate

$$x_{k+1} = \frac{1}{2} \left(\operatorname{Proj}_{Q_1}(x_k) + \operatorname{Proj}_{Q_2}(x_k) \right),\,$$

3. Dykstra: initialize $p_0 = q_0 = 0$ and iterate

$$y_k = \operatorname{Proj}_{Q_1}(x_k + p_k),$$

$$p_{k+1} = x_k + p_k - y_k,$$

$$x_{k+1} = \operatorname{Proj}_{Q_2}(y_k + q_k),$$

$$q_{k+1} = y_k + q_k - x_{k+1}.$$

Credits Detailed results for Exercise 2 (closed-form worst-case convergence rates for gradient descent in different performance measures) can be found in [2]; the analyses from Exercise 7 can be found in [15]; the closed-form worst-case analysis of the proximal minimization algorithm from Exercise 9 can be found in [19]; the worst-case analysis for the proximal point method in the context of monotone inclusions can be found in [14]; the analysis from Exercise 10 can be found in [18].

4 Slightly more advanced techniques

This section will be completed shortly. We currently only provide a few pointers to some relevant literature. The corresponding exercises will be provided in an upcoming version of this document.

Exercise 12 (Lyapunov analyses—linear convergence) How to search for Lyapunov functions guaranteeing linear convergence? See, e.g., [20, 21].

Exercise 13 (Lyapunov analyses—sublinear convergence) How to verify Lyapunov functions guaranteeing sublinear convergence? See, e.g., [22].

Exercise 14 (Designing methods—via line-searches) How to design new methods using "idealistic methods" involving line-searches or span-searches? See, e.g., [17] or [23] for a simple example.

Exercise 15 (Designing methods—by optimizing stepsizes) How to design new methods by optimizing their stepsize coefficients? See, e.g., [24, 25, 26, 27, 28] (using convex relaxations), or the more recent [29] (using a more "to-the-point" approach, i.e., more heavy-duty nonlinear optimization).

Exercise 16 (Relaxations and upper bounds) How to study algorithms on problem classes for which we don't have "interpolation/extensions" theorems? See, e.g., [30] for a setting where no known interpolation theorem holds.

Further pointers Mirror descent [4], decentralized/distributed optimization [31, 32, 33, 34], continuous-time approaches [35, 36], approximate first-order information [2, 37, 38], stochasticity [39, 22, 40] and adaptivity [37, 41] will also be part of future versions.

5 Background material and useful facts

5.1 Standard definitions

All convex functions under consideration in this exercise statements are closed and proper per assumption (i.e., they have a closed and non-empty epigraph).

Definition 1 A differentiable convex function $f : \mathbb{R}^d \to \mathbb{R}$ is L-smooth (with $L \in [0, \infty)$; we denote $f \in \mathcal{F}_{0,L}$) if it satisfies $\forall x, y \in \mathbb{R}^d : \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$.

Definition 2 A convex differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is L-smooth and μ -strongly convex $(0 \le \mu < L < \infty)$; we denote $f \in \mathcal{F}_{\mu,L}$ if it satisfies $\forall x, y \in \mathbb{R}^d : \|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|$ and $\|\nabla f(x) - \nabla f(y)\| \ge \mu \|x - y\|$.

Definition 3 Let $Q \subseteq \mathbb{R}^d$ be a non-empty closed convex set. The convex indicator function for Q is defined as

$$i_Q(x) \triangleq \begin{cases} 0 & \text{if } x \in Q, \\ +\infty & \text{otherwise.} \end{cases}$$

Definition 4 A closed proper convex function $f : \mathbb{R}^d \to \mathbb{R}$ is M-Lipschitz (with $M \in [0, \infty)$; notation $f \in \mathcal{C}_M$) if it satisfies $\forall x \in \mathbb{R}^d$ and $s_x \in \partial f(x) : ||s_x|| \leq M$.

Definition 5 A point to set operator M (notation: $M : \mathbb{R}^d \rightrightarrows \mathbb{R}^d$) is monotone if for all $x, y \in \mathbb{R}^d$ and all $m_x \in M(x)$, $m_y \in M(y)$ it holds that

$$\langle x - y, m_x - m_y \rangle \geqslant 0.$$

In addition, M is maximal if there is no monotone operator M' such that for all $x: M(x) \subset M'(x)$.

Definition 6 A mapping $F: \mathbb{R}^d \to \mathbb{R}^d$ is L-Lipschitz if for all $x, y \in \mathbb{R}^d$

$$||F(x) - F(y)|| \le L||x - y||.$$

5.2 Interpolation/extension theorems

This section gathers useful elements allowing to answer certain questions. Those results (or references to them) can be found in, e.g., [2, 42].

Theorem 1 Let I be an index set and $S = \{(x_i, g_i, f_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$ be a set of triplets. There exists $f \in \mathcal{F}_{0,\infty}$ (a closed, proper and convex function) satisfying $f(x_i) = f_i$ and $g_i \in \partial f(x_i)$ for all $i \in I$ if and only if

$$f_i \geqslant f_j + \langle g_j; x_i - x_j \rangle$$

holds for all $i, j \in I$.

Theorem 2 ($\mathcal{F}_{\mu,L}$ -interpolation) Let I be an index set and $S = \{(x_i, g_i, f_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$ be a set of triplets. There exists $f \in \mathcal{F}_{\mu,L}$ satisfying $f(x_i) = f_i$ and $g_i \in \partial f(x_i)$ for all $i \in I$ if and only if

$$f_i \geqslant f_j + \langle g_j; x_i - x_j \rangle + \frac{1}{2L} \|g_i - g_j\|^2 + \frac{\mu}{2(1 - \mu/L)} \|x_i - x_j - \frac{1}{L} (g_i - g_j)\|^2$$

holds for all $i, j \in I$.

Theorem 3 (Indicator-interpolation) Let I be an index set and $S = \{(x_i, s_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d$ be a set of pairs. There exists a (closed proper convex) indicator function $i_Q : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ (for a non-empty closed domain $Q \subseteq \mathbb{R}^d$ of diameter D) satisfying $s_i \in \partial i_Q(x_i)$ for all $i \in I$ if and only if

$$\langle s_j; x_i - x_j \rangle \leqslant 0$$

 $||x_i - x_j||^2 \leqslant D^2,$

holds for all $i, j \in I$.

Theorem 4 (\mathcal{C}_M -interpolation) Let I be an index set and $S = \{(x_i, g_i, f_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$ be a set of triplets. There exists $f \in \mathcal{C}_M$ (a closed, proper, convex, and M-Lipschitz function) satisfying $f(x_i) = f_i$ and $g_i \in \partial f(x_i)$ for all $i \in I$ if and only if

$$f_i \geqslant f_j + \langle g_j; x_i - x_j \rangle$$
$$M^2 \geqslant ||g_i||^2$$

holds for all $i, j \in I$.

Theorem 5 (Monotone-interpolation) Let I be an index set and $S = \{(x_i, s_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d$ be a set of pairs. There exists a maximal monotone operator $M : \mathbb{R}^d \rightrightarrows \mathbb{R}^d$ satisfying $s_i \in M(x_i)$ for all $i \in I$ if and only if

$$\langle s_i - s_i; x_i - x_i \rangle \geqslant 0$$

holds for all $i, j \in I$.

Theorem 6 (Lipschitz-interpolation) Let I be an index set and $S = \{(x_i, s_i)\}_{i \in I} \subseteq \mathbb{R}^d \times \mathbb{R}^d$ be a set of pairs. There exists an L-Lipschitz mapping $F : \mathbb{R}^d \to \mathbb{R}^d$ satisfying $s_i = F(x_i)$ for all $i \in I$ if and only if

$$||s_i - s_j||^2 \leqslant L^2 ||x_i - x_j||^2$$

holds for all $i, j \in I$.

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