Worst-case analyses for first-order optimization methods

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Foreword & Acknowledgements

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1 Introduction

This document provides a series of exercises for getting familiar with "performance estimation problems" and the use of semidefinite programming for analyzing the worst-case behaviors of first-order optimization methods. An informal introduction can be found in this blog post.

In short, considering problems of the form $\min_x F(x)$ (we generally denote an optimal solution by $x_\star \in \operatorname{argmin}_x F(x)$), our goal is to access "a priori" the quality of the output (denoted by x_k) of some iterative algorithm. There are typically different ways of doing so, which might or might not be relevent depending on the target applications. In first-order optimization, we often want to upper bound the quality of x_k in one of the following terms (which we all ideally would like to be as small as possible): $\|x_k - x_\star\|^2$, $\|\nabla f(x_k)\|^2$, or $f(x_k) - f(x_\star)$. There are of course other possibilities.

So, our goal is to assess the quality of x_k by providing hopefully meaningfull upper bounds on (one of) those quantities. 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).

After studying the performance estimation framework for optimization methods, one can realize that it has a broader applicability for performing worst-case studies in numerical analysis (see exercises in Section 3 and suggested readings in Section 5 for further information).

Notation and necessary background material is provided in Section 4.

2 Getting familiar with performance estimation problems

Exercise 1 (Gradient method) *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 step sizes $\{\gamma_k\}_k$; 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

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

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 $x_\star = \operatorname{argmin}_x f(x)$.

1. *Show that*

$$\begin{aligned} \tau(\mu, L, \gamma_k) = \sup_{\substack{d, f \\ x_k, x_{k+1}, x_\star}} \; & \frac{\|x_{k+1} - x_\star\|^2}{\|x_k - x_\star\|^2} \\ \text{s.t. } & f \in \mathcal{F}_{\mu,L} \\ & x_{k+1} = x_k - \gamma_k \nabla f(x_k) \\ & \nabla f(x_\star) = 0, \end{aligned}$$

   where f, x_k, x_{k+1}, $x_\star$, and d are the variables and μ, L, γ are parameters.

   Note that we will (sometimes abusively) use max *instead of* sup *in the sequel as the optimum is usually attained for such problems (for this exercise, this is actually easy to show as the optimization problem is over a compact set).*

2. *Show that*

$$\begin{aligned}\tau(\mu, L, \gamma_k) = \max_{\substack{x_k, x_{k+1}, x_\star\\ g_k, g_\star\\ f_k, f_\star}} \quad & \frac{\|x_{k+1}-x_\star\|^2}{\|x_k-x_\star\|^2}\\ \text{s.t. } \exists f \in \mathcal{F}_{\mu,L} \text{ such that } & \begin{cases} f_i = f(x_i) & i = k, \star\\ g_i = f'(x_i) & i = k, \star \end{cases}\\ & x_{k+1} = x_k - \gamma_k g_k\\ & g_\star = 0.\end{aligned}$$

3. *Using Theorem 2, show that*

$$\begin{aligned}\tau(\mu, L, \gamma_k) = \max_{\substack{x_k, x_{k+1}, x_\star\\ g_k, g_\star\\ f_k, f_\star}} \quad & \frac{\|x_{k+1}-x_\star\|^2}{\|x_k-x_\star\|^2}\\ \text{s.t. } \quad & f_\star \geqslant f_k + \langle g_k, x_\star - x_k\rangle + \tfrac{1}{2L}\|g_\star - g_k\|^2 + \tfrac{\mu}{2(1-\mu/L)}\left\|x_\star - x_k - \tfrac{1}{L}(g_\star - g_k)\right\|^2\\ & f_k \geqslant f_\star + \langle g_\star, x_k - x_\star\rangle + \tfrac{1}{2L}\|g_k - g_\star\|^2 + \tfrac{\mu}{2(1-\mu/L)}\left\|x_k - x_\star - \tfrac{1}{L}(g_k - g_\star)\right\|^2\\ & x_{k+1} = x_k - \gamma_k g_k\\ & g_\star = 0.\end{aligned}$$

4. *Show that*

$$\begin{aligned}\tau(\mu, L, \gamma_k) = \max_{\substack{x_k, x_{k+1}, x_\star\\ g_k, g_\star\\ f_k, f_\star}} \quad & \|x_{k+1}-x_\star\|^2\\ \text{s.t. } \quad & f_\star \geqslant f_k + \langle g_k, x_\star - x_k\rangle + \tfrac{1}{2L}\|g_\star - g_k\|^2 + \tfrac{\mu}{2(1-\mu/L)}\left\|x_\star - x_k - \tfrac{1}{L}(g_\star - g_k)\right\|^2\\ & f_k \geqslant f_\star + \langle g_\star, x_k - x_\star\rangle + \tfrac{1}{2L}\|g_k - g_\star\|^2 + \tfrac{\mu}{2(1-\mu/L)}\left\|x_k - x_\star - \tfrac{1}{L}(g_k - g_\star)\right\|^2\\ & \|x_k - x_\star\|^2 = 1\\ & x_{k+1} = x_k - \gamma_k g_k\\ & g_\star = 0.\end{aligned}$$

5. *Define G and F*

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

(note that $G = [x_k - x_\star \quad g_k]^\top [x_k - x_\star \quad g_k] \succcurlyeq 0$). Show that $\tau(\mu, L, \gamma_k)$ can be computed using the following 2×2 semidefinite program (SDP):

$$\begin{aligned}\tau(\mu, L, \gamma_k) = \max_{G, F} \quad & G_{1,1} + \gamma_k^2 G_{2,2} - 2\gamma_k G_{1,2}\\ \text{s.t.} \quad & F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{L}{L-\mu} G_{1,2} \leqslant 0\\ & -F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{\mu}{L-\mu} G_{1,2} \leqslant 0\\ & G_{1,1} = 1\\ & G \succcurlyeq 0,\end{aligned} \tag{2}$$

6. *Define $h_k \triangleq \gamma_k L$ and $\kappa = L/\mu$. 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. *Using Lagrangian duality with the following primal-dual pairing ($\tau, \lambda_1, \lambda_2$ are dual variables):*

$$\begin{aligned}
&F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{L}{L-\mu} G_{1,2} \leqslant 0 && : \lambda_1\\
&-F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{\mu}{L-\mu} G_{1,2} \leqslant 0 && : \lambda_2\\
&G_{1,1} = 1 && : \tau
\end{aligned}$$

one can show that

$$\begin{aligned}
\tau(\mu, L, \gamma_k) = \min_{\tau, \lambda_1, \lambda_2 \geqslant 0}\ & \tau\\
\text{s.t. } S = & \begin{bmatrix} \tau - 1 + \frac{\lambda_1 L\mu}{L-\mu} & \gamma_k - \frac{\lambda_1(\mu+L)}{2(L-\mu)} \\ \gamma_k - \frac{\lambda_1(\mu+L)}{2(L-\mu)} & \frac{\lambda_1}{L-\mu} - \gamma_k^2 \end{bmatrix} \succcurlyeq 0\\
0 = & \lambda_1 - \lambda_2.
\end{aligned} \tag{3}$$

Note that equility holds due to strong duality (for going further: obtain this dual formulation and prove strong duality using a Slater condition).

Show that any feasible point ($\tau, \lambda_1, \lambda_2$) to (3) corresponds to an upper bound on $\tau(\mu, L, \gamma_k)$ (i.e., $\tau(\mu, L, \gamma_k) \leqslant \tau$).

9. *Is there a simple closed-form expression for $\tau(\mu, L, \gamma_k)$? Hint #1: can we solve (3) in closed-form? Hint #2: the objective is linear in τ; the optimal solution (if it exists) is therefore necessarily on the boundary of the PSD cone; hence τ must be such that at least one eigenvalue of S is zero.*

   Does it match the numerical values obtained using the previous codes for computing $\tau(\mu, L, \gamma_k)$ numerically?

10. *How can we adapt the SDP formulation (2) for computing the smallest possible τ such that the inequality*

$$\|\nabla f(x_{k+1})\|^2 \leqslant \tau \|\nabla f(x_k)\|^2$$

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 $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$? Modify your previous code for computing such a bound. Can you guess a closed-form expression for it?

For going further: a dual problem is given by

$$\begin{aligned}
\min_{\tau, \lambda_1, \lambda_2 \geqslant 0}\ & \tau\\
\text{s.t. } S = & \begin{bmatrix} \tau + \lambda_1 \frac{(1-\gamma_k L)(1-\gamma_k \mu)}{L-\mu} & -\lambda_1 \frac{2-\gamma_k(L+\mu)}{2(L-\mu)} \\ -\lambda_1 \frac{2-\gamma_k(L+\mu)}{2(L-\mu)} & \frac{\lambda_1}{L-\mu} - 1 \end{bmatrix} \succcurlyeq 0\\
0 = & \lambda_1 - \lambda_2.
\end{aligned} \tag{4}$$

Is there a simple closed-form solution for this problem?

11. *How can we adapt the SDP formulation (2) for computing the smallest possible τ such that the inequality*

$$f(x_{k+1}) - f(x_\star) \leqslant \tau (f(x_k) - f(x_\star))$$

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 $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$? Modify your previous code for computing such a bound. Can you guess a closed-form expression for it?

For going further: using the following primal-dual pairing

$$\begin{array}{ll}
f(x_0) \geqslant f(x_\star) + \frac{1}{2L}\|\nabla f(x_0)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_0 - x_\star - \frac{1}{L}\nabla f(x_0)\|^2 & : \lambda_1 \\
f(x_\star) \geqslant f(x_0) + \langle \nabla f(x_0), x_\star - x_0\rangle + \frac{1}{2L}\|\nabla f(x_0)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_0 - x_\star - \frac{1}{L}\nabla f(x_0)\|^2 & : \lambda_2 \\
f(x_1) \geqslant f(x_\star) + \frac{1}{2L}\|\nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_1 - x_\star - \frac{1}{L}\nabla f(x_1)\|^2 & : \lambda_3 \\
f(x_\star) \geqslant f(x_1) + \langle \nabla f(x_1), x_\star - x_1\rangle + \frac{1}{2L}\|\nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_1 - x_\star - \frac{1}{L}\nabla f(x_1)\|^2 & : \lambda_4 \\
f(x_0) \geqslant f(x_1) + \langle \nabla f(x_1), x_0 - x_1\rangle + \frac{1}{2L}\|\nabla f(x_0) - \nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_1 - x_0 - \frac{1}{L}(\nabla f(x_1) - \nabla f(x_0))\|^2 & : \lambda_5 \\
f(x_1) \geqslant f(x_0) + \langle \nabla f(x_0), x_1 - x_0\rangle + \frac{1}{2L}\|\nabla f(x_0) - \nabla f(x_1)\|^2 + \frac{\mu}{2(1-\mu/L)}\|x_1 - x_0 - \frac{1}{L}(\nabla f(x_1) - \nabla f(x_0))\|^2 & : \lambda_6 \\
f(x_0) - f(x_\star) = 1 & : \tau
\end{array}$$

a dual problem is given by

$$\begin{aligned}
\min_{\tau,\lambda_1,\lambda_2 \geqslant 0} \ & \tau \\
s.t. \ & \begin{bmatrix} \frac{\mu L(\lambda_1+\lambda_2+\lambda_3+\lambda_4)}{L-\mu} & -\frac{L(\lambda_2+\gamma\mu(\lambda_3+\lambda_4))+\mu\lambda_1}{L-\mu} & -\frac{L\lambda_4+\mu\lambda_3}{L-\mu} \\ * & \frac{\gamma\mu(\gamma L(\lambda_3+\lambda_4+\lambda_5+\lambda_6)-2\lambda_5)-2\gamma L\lambda_6+\lambda_1+\lambda_2+\lambda_5+\lambda_6}{L-\mu} & \frac{\gamma L\lambda_4+\lambda_5(\gamma L-1)+\gamma\mu(\lambda_3+\lambda_6)-\lambda_6}{L-\mu} \\ * & * & \frac{\lambda_3+\lambda_4+\lambda_5+\lambda_6}{L-\mu} \end{bmatrix} \succcurlyeq 0 \\
& 0 = \tau - \lambda_1 + \lambda_2 - \lambda_5 + \lambda_6 \\
& 1 = -\lambda_3 + \lambda_4 + \lambda_5 - \lambda_6,
\end{aligned} \tag{5}$$

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)

Hint #1: plot some values for the multipliers; hint #2: pick $\lambda_1 = \lambda_3 = \lambda_6 = 0$; does the problem simplify?

12. *Can we use this formalism for computing worst-case guarantees for a few iterations simultaneously? That is, to compute $\tau(\mu, L, \{\gamma_k\}_{k=0,\ldots,N-1})$ the smallest value such that the inequality*

$$\|x_N - x_\star\|^2 \leqslant \tau(\mu, L, \{\gamma_k\}_{k=0,\ldots,N-1})\|x_0 - x_\star\|^2$$

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 $x_0, x_1, \ldots, x_N \in \mathbb{R}^d$ such that $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$ ($k = 0, \ldots, N-1$), and $x_\star = \operatorname{argmin}_x f(x)$.

13. *What happens if $\mu = 0$? Can you isolate the problem on a simple counter example? You can, for example, use this PEPit code (alternative in Matlab: PESTO code). Can you imagine a solution for avoiding such pathological behaviors in the analyses? What about studying guarantees of type*

$$f(x_N) - f_\star \leqslant \tau(\mu, L, \{\gamma_k\}_{k=0,\ldots,N-1})\|x_0 - x_\star\|^2$$

instead? Modify your code for studying such worst-case bounds, and try it numerically for the choice $\gamma_k = 1/L$, $L = 1$ and $\mu = 0$. Guess the depence on N based on a few numerical trials.

14. *Based on your current experience, what are, according to you, the key elements which allowed casting the worst-case analysis as an SDP?*

15. *Given the optimal value of the multipliers $\tau, \lambda_1, \lambda_2$ in (3), can you write a "direct" proof for the linear convergence in terms of distance to an optimal point without resorting on any SDP formulation?*

3 Further exercises

Exercise 2 (Sublinear convergence of gradient descent and acceleration) *Show that the smallest τ such that the inequality*

$$\ldots$$

1. *show that it can be formulated as an SDP.*

2. *numerical trials (code: XXX).*

3. *Can we compute guarantees of type*

$$\min_{0\leqslant i\leqslant N} \|\nabla f(x_i)\|^2 \leqslant \tau \|x_0 - x_\star\|^2$$

   using semidefinite programming?

4. *Modify your code for computing the worst-case ratios* $\frac{\min_{0\leqslant i\leqslant N}\|\nabla f(x_i)\|^2}{\|x_0-x_\star\|^2}$ *and* $\frac{\|\nabla f(x_N)\|^2}{\|x_0-x_\star\|^2}$ *as functions of* N*. What can you conclude?*

5. *Modify your code for computing worst-case guarantees for the following variant of Nesterov's accelerated gradient method:*

$$XXX$$

   in terms of the same ratios, and compare them to those of gradient descent (as functions of N*). What can you conclude?*

Exercise 3 (Subgradient method) *Show that the smallest* τ *such that the inequality*

...

1. *show that it can be formulated as ...*

2. *show that the previous problem can be framed using a discrete version...*

3. *numerical trials (code: XXX). Ex: modify the code to compute worst gradient norm, and worst best gradient norm among iterates*

Exercise 4 (Acceleration and Lyapunov analyses) *Show that the smallest* τ *such that the inequality*

...

1. *show that it can be formulated as ...*

2. *show that the previous problem can be framed using a discrete version...*

3. *numerical trials*

Exercise 5 (Fixed-point iterations) *Show that the smallest* τ *such that the inequality*

...

1. *two methods: Halpern and Kras...*

2. *show that it can be formulated as ...*

3. *show that the previous problem can be framed using a discrete version...*

4. *show that it is equivalent to the SDP XXXX*

5. *using duality show that ... (dual SDP)*

6. *numerical trials*

Exercise 6 (Stochastic gradient descent) *Show that the smallest* τ *such that the inequality*

...

1. *show that it can be formulated as ...*

2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *using duality show that ... (dual SDP)*
5. *numerical trials*

Exercise 7 (Proximal point method) *Show that the smallest τ such that the inequality*

$$...$$

1. *show that it can be formulated as ...*
2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *numerical trials*

Exercise 8 (Proximal gradient method) *Show that the smallest τ such that the inequality*

$$...$$

1. *show that it can be formulated as ...*
2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *numerical trials*

Exercise 9 (Douglas-Rachford splitting) *Show that the smallest τ such that the inequality*

$$...$$

1. *show that it can be formulated as ...*
2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *numerical trials*

Exercise 10 (Frank-Wolfe) *Show that the smallest τ such that the inequality*

$$...$$

1. *show that it can be formulated as ...*
2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *numerical trials*

Exercise 11 (Alternate projections & Dykstra) *Show that the smallest τ such that the inequality*

$$...$$

1. *show that it can be formulated as ...*
2. *show that the previous problem can be framed using a discrete version...*
3. *show that it is equivalent to the SDP XXXX*
4. *numerical trials*

4 Background material and useful facts

4.1 Standard definitions

smoothness, strong convexity...

Definition 1 *cpp*

Definition 2 *sm str cvx (notation...)*

Definition 3 *lip cvx*

Definition 4 *smooth nonconvex?*

Definition 5 *convex indicator*

4.2 Interpolation/extension theorems

This section gathers useful elements allowing to answer certain questions ...

Theorem 1 *interpolation ... (ccp)*

Theorem 2 *interpolation ... (smooth str convex)*

Theorem 3 *nonsmooth*

Theorem 4 *interpolation ... (smooth nonconvex)*

Theorem 5 *indicator*

4.3 SDP duality

Useful?

++primal and dual SDP formulations

Theorem 6 *slater*

5 Going further - suggested readings

Lyapunov analyses.

Designing methods.

Adaptive methods.

Primal-dual methods. Ernest'

Mirror descent. Radu's

Identifying lower complexity bounds. QG, Radu's

Continuous-time analyses.

Identifying counter-examples

Other analyses.