

PEPit: a Python package for worst-case analysis of first-order optimization methods and their continuous versions

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Joint work with



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Outline

- ① Introduction
- ② Example: analysis of the gradient flow
- ③ Package

Motivations

- A principled approach to worst-case analysis of optimization methods and their continuous-time limit
- Quick numerical evaluation of (new) first-order methods
- Reproducible research

PEPit:

- **A python package**¹ for worst-scale analyses of a large family of first-order methods (so-called Performance Estimation Problems - PEPs, see PESTO for the matlab version [9])
- Technique based on semidefinite programming (SDP)
- An example: **gradient flow originating from strongly convex functions**².

¹[3] **B. Goujaud et al.** PEPit: computer-assisted worst-case analyses of first-order optimization methods in Python

²[5] **M., A. Taylor, and F. Bach.** A systematic approach to Lyapunov analyses of continuous-time models in convex optimization

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First-order methods in convex optimization

A very popular setting:

$$f(x_\star) = \min_{x \in \mathbf{R}^d} f(x),$$

where f is convex, differentiable, and $x_\star \in \mathbf{R}^d$ an optimal point.

- **First-order methods:** low-cost per iteration, accuracy is not critical (machine learning, signal processing, etc.)

$$x_{k+1} \in \mathbf{Span}(x_0, \nabla f(x_0), \dots, \nabla f(x_{k+1}))$$

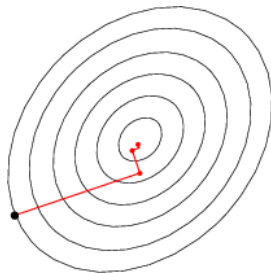


Figure: Convex function and optimization algorithm

First-order methods in convex optimization

Gradient descent with fixed step size $\gamma > 0$:

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

First-order methods in convex optimization

Gradient descent with fixed step size $\gamma > 0$:

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

- **Ordinary differential equations (ODEs):** When taking the step size γ to 0, it is directly related to the gradient flow,

$$\dot{X}_t = -\nabla f(X_t), \quad X_0 = x_0 \in \mathbf{R}^d,$$

where X_t verifies $X_{t_k} \approx x_k$ with the identification $t_k = \gamma k$.

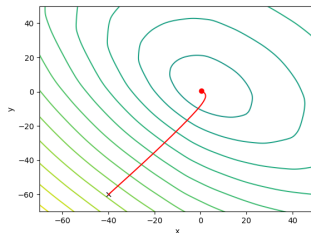


Figure: Integration of the gradient flow for a logistic regression problem.

Optimization methods and ODEs: convergence guarantees

- **First-order methods:** given a class of functions \mathcal{F} , a starting point $x_0 \in \mathbf{R}^d$, and given gradient descent with step size $\gamma > 0$

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

the goal is to quantify the convergence speed to an optimum x_\star in a small number of steps k ,

$$\|x_k - x_\star\|^2 \leq \tau(k, \mathcal{F}, \gamma) \|x_0 - x_\star\|^2.$$

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- **ODEs :** given a class of function \mathcal{F} , a starting point $x_0 \in \mathbf{R}^d$, the gradient flow starting is given by,

$$\frac{d}{dt} X_t = -\nabla f(X_t),$$

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the goal is to quantify the convergence speed to an x_\star ,

$$f(X_t) - f_\star \leq \tilde{\tau}(t, \mathcal{F}) (f(x_0) - f(x_\star)).$$

Convex optimization setting

Common assumptions:

- f is convex and differentiable,
- A differentiable function f is **L -smooth** if and only if it satisfies

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

- A convex differentiable function f is **μ -strongly convex** if and only if it satisfies

$$\|\nabla f(x) - \nabla f(y)\| \geq \mu\|x - y\|.$$

$\mathcal{F}_{\mu,L}$ is the family of a L -smooth μ -strongly convex functions, with $0 \leq \mu \leq L \leq +\infty$.

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Performance estimation problems (PEPs)

Main ideas:

- ① Optimization methods and associated ODEs are usually studied via worst-case analyses.
- ② Convergence proofs are combinations of inequalities (from methods and problem class).
- ③ Automated search for combinations of inequalities.

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- ③ Automated search for combinations of inequalities.

References:

- Initiated by Drori and Teboulle (2012) [2]
- Analyses of first-order methods and design of proofs by Taylor et al. (2017) [8]

An example: the gradient flow

We consider the **gradient flow** starting from $x_0 \in \mathbf{R}^d$, and originating from differentiable functions f :

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Lyapunov functions: given a trajectory X_t , many proofs construct a Lyapunov function $\mathcal{V} : x, t \in \mathbf{R}^d, \mathbf{R}^+ \rightarrow \mathbf{R}$, such that,

- ① $\mathcal{V}(x, t) = 0 \iff x = x_\star,$
- ② $\mathcal{V}(X_t, t) \geq 0,$
- ③ $\frac{d}{dt}\mathcal{V}(X_t, t) \leq 0.$

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For example, let us consider the function $\mathcal{V}(X_t, t) = f(X_t)$:

$$\frac{d}{dt}\mathcal{V}(X_t, t) = \dot{X}_t^T \nabla f(X_t) = -\|\nabla f(X_t)\|^2 \leq 0.$$

Worst-case guarantee using Lyapunov functions

We consider the **gradient flow** starting from $x_0 \in \mathbf{R}^d$, and originating from **strongly convex functions** $f \in \mathcal{F}_{\mu, \infty}$:

$$\frac{d}{dt}X_t = -\nabla f(X_t).$$

Worst-case guarantee: given a Lyapunov function \mathcal{V} , we look for (the largest) values $\tau(\mu) \geq 0$ such that

$$\frac{d}{dt}\mathcal{V}(X_t) \leq -\tau(\mu)\mathcal{V}(X_t),$$

is true for all functions $f \in \mathcal{F}_{\mu, \infty}$, and all trajectories X_t .

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Reformulation as an optimization problem:

$$\begin{aligned} -\tau(\mu) &= \max_{X_t \in \mathbf{R}^d, f \in \mathcal{F}_{\mu,\infty}} \frac{d}{dt}\mathcal{V}(X_t), \\ &\text{subject to } \mathcal{V}(X_t) = 1, \\ &\quad \dot{X}_t = -\nabla f(X_t). \end{aligned}$$

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Given the Lyapunov function $\mathcal{V}(X_t) = f(X_t) - f_\star$,

$$\begin{aligned} -\tau(\mu) &= \max_{X_t, f \in \mathcal{F}_{\mu, \infty}} \dot{X}_t^T \nabla f(X_t), \\ &\text{subject to } f(X_t) - f_\star = 1, \\ &\quad \dot{X}_t = -\nabla f(X_t). \end{aligned}$$

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This infinite dimensional problem can be reformulated as an SDP.

A reformulation using sampling

Reformulation as a feasibility condition over the class of functions,

$$\begin{aligned}
 & \max_{(X_i, g_i, f_i)_{t, \star}} -\|g_t\|^2, \\
 & \text{subject to } f_t - f_\star = 1, \\
 & \exists f \in \mathcal{F}_{\mu, \infty} : \begin{cases} g_t = \nabla f(X_t) & f_t = f(X_t), \\ g_\star = \nabla f(x_\star) = 0 & f_\star = f(x_\star). \end{cases}
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 \end{aligned}$$

Theorem [8, Theorem 4]

Set $\{(X_i, g_i, f_i)\}_{i \in I}$ if $\mathcal{F}_{\mu, \infty}$ interpolable if and only if the following set of conditions holds for every pair of indices $i \in I$ and $j \in J$

$$f_i - f_j - g_j^T(X_i - X_j) \geq \frac{\mu}{2} \|X_i - X_j\|^2.$$

A reformulation as a finite-dimensional quadratic problem

Reformulation as a nonconvex QCQP (quadratically constrained quadratic program):

$$\max_{(X_i, g_i, f_i)_{t, \star}, g_\star=0} -\|g_t\|^2,$$

$$\text{subject to } (f_t - f_\star) = 1,$$

$$f_i - f_j - g_j^T (X_i - X_j) \geq \frac{\mu}{2} \|X_i - X_j\|^2, \quad \forall i, j = t, \star.$$

Linear in (f_t, f_\star) and quadratic in (X_t, X_\star, g_t) .

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Linear in (f_t, f_\star) and quadratic in (X_t, X_\star, g_t) .

A finite-dimensional problem that is still nonconvex.

A reformulation into an SDP

Let us introduce:

- G be a Gram matrix defined by $G = \begin{pmatrix} \|X_t - x_\star\|^2 & \langle X_t - x_\star, g_t \rangle \\ \langle X_t - x_\star, g_t \rangle & \|g_t\|^2 \end{pmatrix} \succeq 0$
- the vector $F = f_t - f_\star$

Formulation into an SDP,

$$\begin{aligned} & \max_{G \succeq 0, F} \text{Tr}(A_0 G), \\ & \text{subject to } b_0^T F = 1, \\ & \quad b_1^T F + \text{Tr}(A_1 G) \geq 0, \\ & \quad b_2^T F + \text{Tr}(A_2 G) \geq 0, \end{aligned}$$

where $A_0 = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$, $A_1 = \begin{pmatrix} -\mu/2 & 1/2 \\ 1/2 & 0 \end{pmatrix}$, $A_2 = \begin{pmatrix} -\mu/2 & 0 \\ 0 & 0 \end{pmatrix}$, $b_1 = -1$ and $b_2 = b_0 = 1$.

Linear SDP \rightarrow can be solved numerically.

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Automated SDP modeling using PEPit

Goals of the toolbox:

- Performing numerical worst-case analyses
- Avoiding the SDP modeling part
- Avoiding some potential mistakes in the SDP formulation / numerous interpolation inequalities involved
- Describing the method / ODE as the user would have implemented it

See this colab notebook.

PEPit VS known bounds: gradient flow

A closed-form upper bound in the worst-case is given by the lemma.

Lemma

Let f be a μ -strongly convex function, $x_0 \in \mathbf{R}^d$, and x_\star the minimizer of f . The solution X_t to the gradient flow verifies

$$\frac{d}{dt} (f(X_t) - f(x_\star)) \leq -2\mu (f(X_t) - f(x_\star)),$$

and after integrating between 0 and t , $f(X_t) - f(x_\star) \leq e^{-2\mu t}(f(x_0) - f(x_\star))$.

Proof: Let us define $\mathcal{V}(X_t) = f(X_t) - f_\star$. Then, deriving and using strong convexity,

$$\frac{d}{dt} \mathcal{V}(X_t) = \dot{X}_t^T \nabla f(X_t) = -\|\nabla f(X_t)\|^2 \leq -2\mu(f(X_t) - f_\star) \leq -2\mu \mathcal{V}(X_t).$$

PEPit VS known upper bound: gradient flow

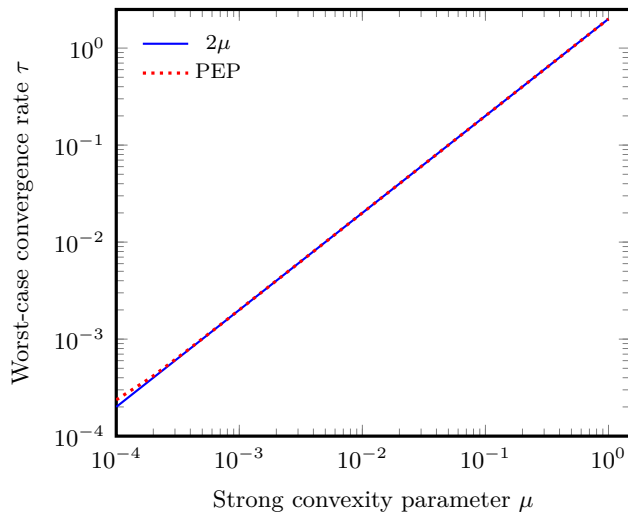


Figure: Worst-case rate τ on the class of quadratic Lyapunov functions for the gradient flow [5].

Important ingredients for the SDP reformulations

Given the gradient flow $\frac{d}{dt}X_t = -\nabla f(X_t)$ originating from strongly convex functions f , we look for the convergence guarantee,

$$\frac{d}{dt}\mathcal{V}(X_t) \leq -\tau(\mu)\mathcal{V}(X_t).$$

4 main ingredients:

- **A class of functions** with interpolating conditions linear in G and F
 $\rightarrow \mathcal{F}_{\mu,\infty}$
- **An ODE / first-order method:** linear in G and F
 \rightarrow *Gradient flow*
- **A performance measure:** linear in G and F
 \rightarrow *Derivative $\frac{d}{dt}\mathcal{V}(X_t)$ of Lyapunov functions given by $\mathcal{V}(X_t) = f(X_t) - f_\star$*
- **An initial condition:** linear in G and F
 \rightarrow *Lyapunov function $\mathcal{V}(X_t) = 1$*

Important ingredients for the SDP reformulations

Given $f \in \mathcal{F}_{\mu,L}$, and an accelerated gradient method starting from $x_0 \in \mathbf{R}^d$, with $\kappa = \frac{\mu}{L}$

$$y_{n+1} = x_{n+1} - \frac{1 - \sqrt{\kappa}}{1 + \sqrt{\kappa}}(x_{n+1} - x_n), \quad x_{n+1} = y_n - \frac{1}{L} \nabla f(x_n),$$

An upper bound guarantee is given in [1],

$$f(x_k) - f_\star \leq (1 - \sqrt{\kappa})^k \left(f(x_0) - f_\star + \frac{\mu}{2} \|x_0 - x_\star\|^2 \right).$$

4 main ingredients:

- **A class of functions** with interpolating conditions linear in G and F
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- **An ODE / first-order method:** linear in G and F
 \rightarrow *An accelerated gradient descent*
- **A performance measure:** linear in G and F
 $\rightarrow f(x_k) - f_\star$
- **An initial condition:** linear in G and F
 $\rightarrow f(x_0) - f_\star + \frac{\mu}{2} \|x_0 - x_\star\|^2$

PEPit VS known upper bound : an accelerated gradient method

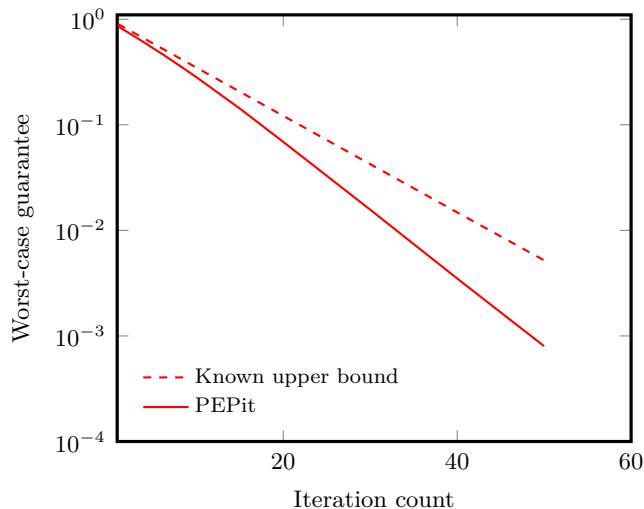


Figure: Accelerated gradient method (with constant momentum): strong convexity parameter fixed to $\mu = 0.1$. Worst-case guarantee on $f(x_n) - f_\star$ as a function of n .

Overview and contents of the toolbox

- **Black-box oracles** include (sub)-gradient steps, proximal steps, linear optimization steps, and their approximate / inexact and Bregman versions.
- **Problem classes** include convex functions (with Lipschitz functions, bounded domains, smoothness, strong-convexity), convex indicator functions, smooth nonconvex functions, monotone operators.
- **Performance measure and initial conditions** include everything that has a convex representation in terms of a Gram matrix:
 - linear in function values
 - quadratic in gradient / iterates

Already about 50 examples in the toolbox:

<https://pepit.readthedocs.io/en/latest/examples.html>

Concluding remarks

Future work:

- Automated export of numerical proofs
- Implementing the automated search for Lyapunov functions [7, 6, 4]
- Additional oracles / class of functions

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Conclusion:

- A tool for validating proofs and worst-case guarantees
- Flexible criterion, initial conditions, oracles, methods, ...
- Easy to implement for the user
- Intuition on methods behaviors
- Possibly a great help in the review process! :)

PEPit: a Python package for worst-case analysis of first-order optimization methods and their continuous versions

Céline Mouter

ICCOPT, July 2022

Thanks!
Any question?



Dual formulation

- A numerical proof assistant:

Let us recall the PEP for gradient flow in its SDP reformulation

$$\begin{aligned} & \max_{G \succeq 0, F \in \mathbf{R}^2} \operatorname{Tr}(A_0 G), \\ & \text{subject to } b_0^T F = 1, (\tau) \\ & \qquad b_1^T F + \operatorname{Tr}(A_1 G) \geq 0, (\lambda_1 \geq 0) \\ & \qquad b_2^T F + \operatorname{Tr}(A_2 G) \geq 0, (\lambda_2 \geq 0) \end{aligned}$$

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 \end{aligned}$$

Thanks to strong duality (Slater point), it is possible to select the inequalities (dual variables) involves at the optimum,

$$\begin{aligned}
 & \min_{\tau} \tau, \\
 & \quad \lambda_1 b_1 + \lambda_2 b_1 - \tau b_0 \leq 0, \\
 & \quad \lambda_1 A_1 + \lambda_2 A_2 + A_0 \preceq 0, \\
 & \quad \lambda_1, \lambda_2 \geq 0.
 \end{aligned} \tag{1}$$

Optimizing over classes of Lyapunov functions

- A numerical proof assistant
- Searching for Lyapunov functions :

For the gradient flow, what is the best choice of Lyapunov function minimizing worst-case convergence guarantee?

$$\mathcal{V}_{a,c}(X_t) = a(f(X_t) - f_\star) + c\|X_t - x_\star\|^2.$$

Then the maximization problem for the gradient flow becomes,

$$\begin{aligned} -\tau &= \min_{a,c \geq 0} \max_{X_t \in \mathbf{R}^d, f \in \mathcal{F}_{\mu,\infty}} \frac{d}{dt} \mathcal{V}(X_t), \\ &\text{subject to } \mathcal{V}(X_t) = 1, \\ &\dot{X}_t = -\nabla f(X_t). \end{aligned} \tag{2}$$

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