Perspective on the analysis and design of optimization algorithms

Adrien Taylor

AGIMUS Winter School — December 2023

Sierra team at Inria Paris

Main research themes: optimization, statistical learning, and interactions.

- ◇ Team leader: Francis Bach,
- ◇ Assistant: Marina Kovacic,
- ◇ 5 permanent researchers,
- ◇ 4 postdocs,
- ◇ 15 PhD students.

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Etienne de Klerk


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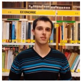
Laurent Lessard


Aymeric Dieuleveut


Céline Moucer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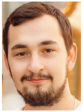
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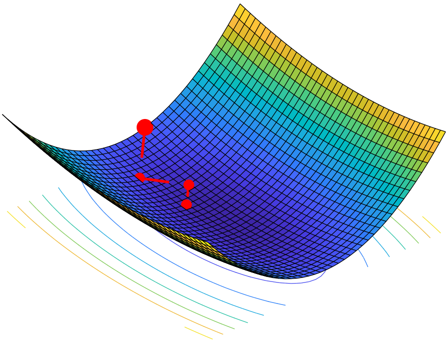

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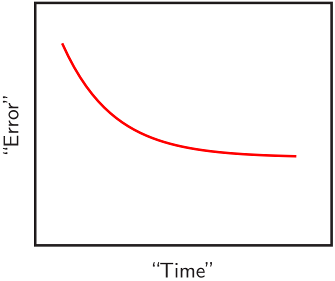

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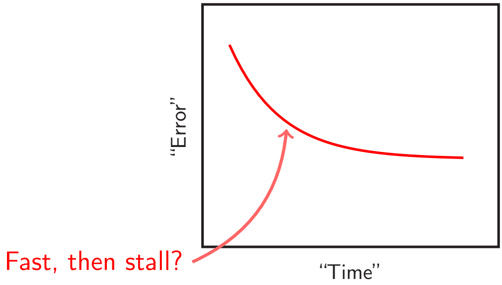

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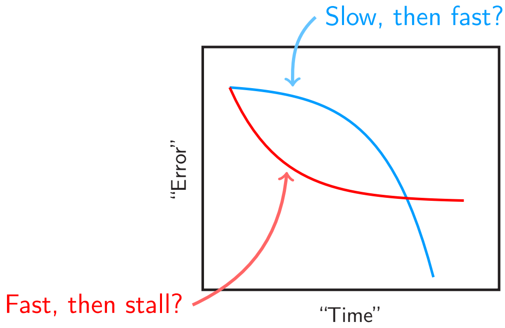

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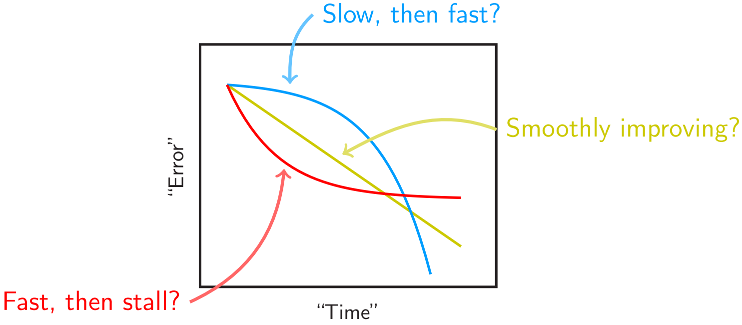

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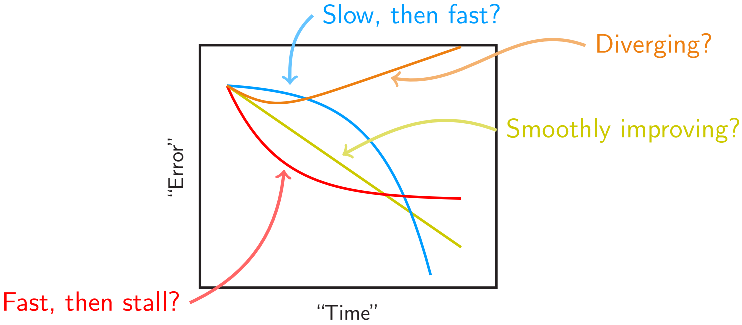

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- ◇ smoothed analyses.

A few elements of convex analysis

Extended-valued functions

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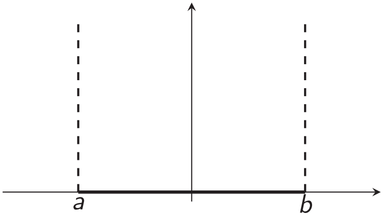

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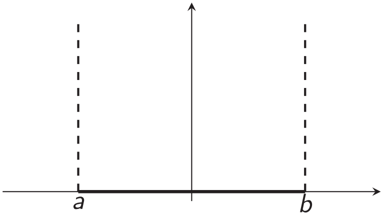

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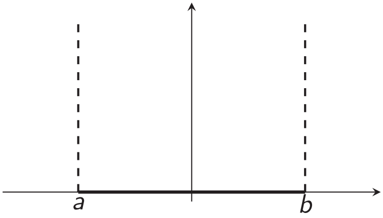

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Note: so f might encode *implicit constraints*.

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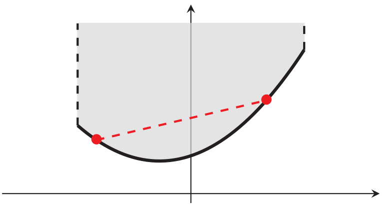

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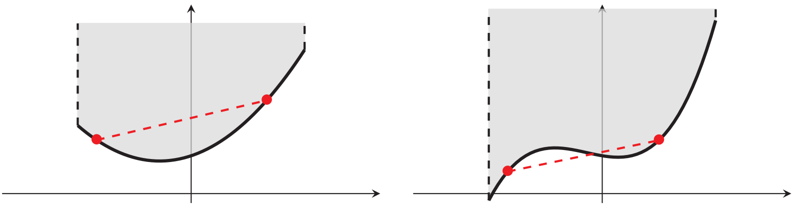

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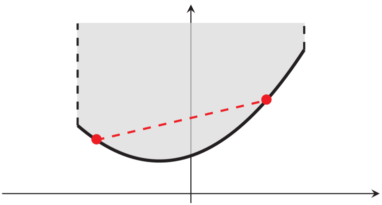

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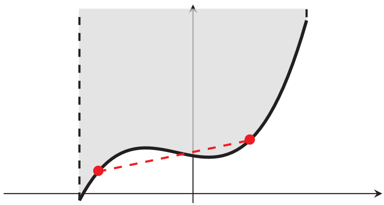

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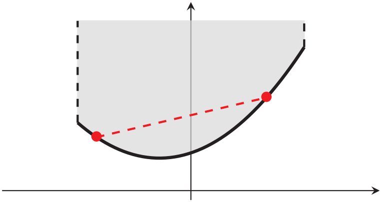

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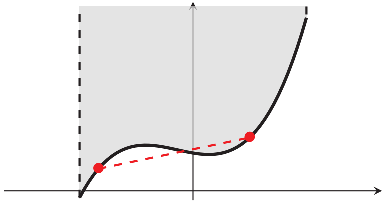
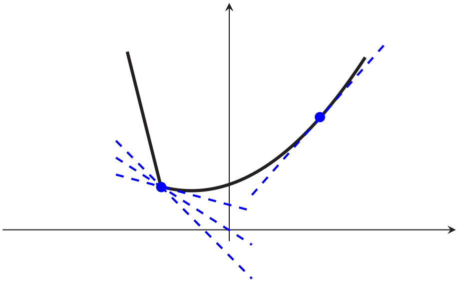


non-convex function.

Subgradients and subdifferentials



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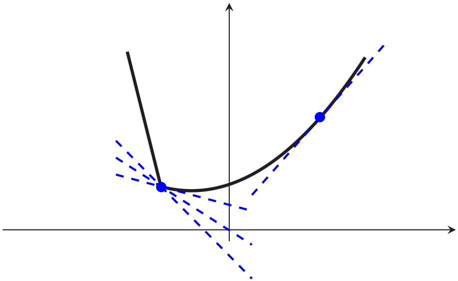

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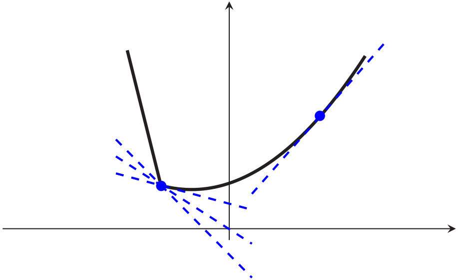

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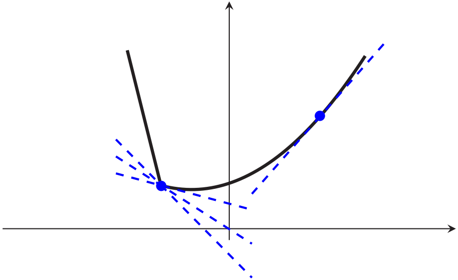

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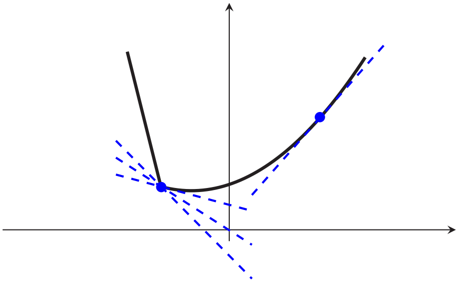

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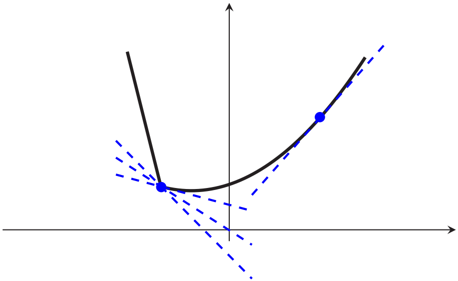

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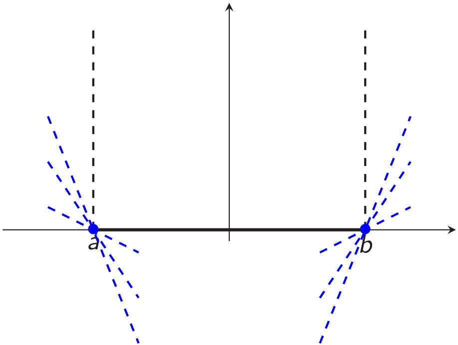

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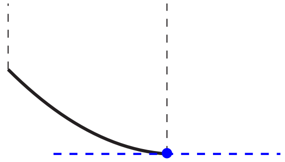
- Example: several subgradients at solution, including 0:



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- ◇ allows for simple manipulations.

A few approaches to constrained (convex) optimization

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- ◇ still, a few key “algorithmic templates” emerged.

Splitting methods: a few examples

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(choices also depends on the targets, e.g., accuracy).

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Equivalently:

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so $x_{k+1} = \mathrm{Proj}_{\mathcal{D}}(x_k - \gamma\nabla f(x_k))$.

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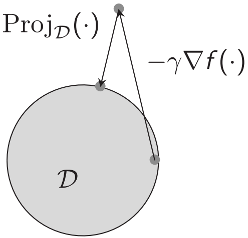

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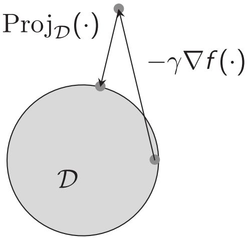

Guarantees when f convex with L-Lipschitz gradient and $\gamma \in (0, 2/L)$.
For instance, when $\gamma = 1/L$:

$$f(x_N) - f_\star \leqslant \frac{L\|x_0 - x_\star\|_2^2}{2N}.$$

Example: Projected gradient descent (III)

Smooth convex function f and (closed) convex set $\mathcal{D}$:

$$\min_{x \in \mathbb{R}^n} f(x) + i_{\mathcal{D}}(x),$$

with (convex) indicator function of set $\mathcal{D}$: $i_{\mathcal{D}}(x) = \begin{cases} 0 & \text{if } x \in \mathcal{D} \\ +\infty & \text{otherwise.} \end{cases}$.

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Typical choice for $\lambda_k = \frac{2}{k+1}$.

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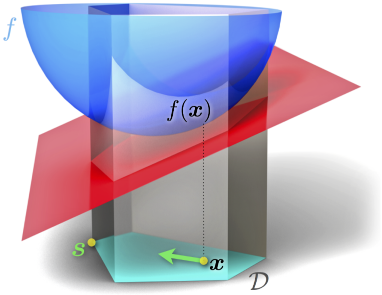

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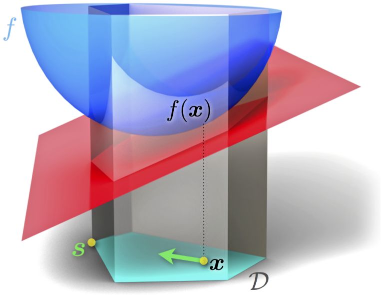

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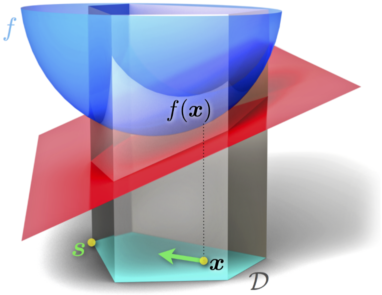

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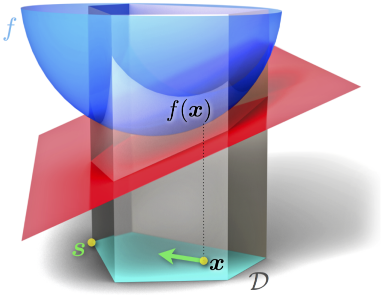

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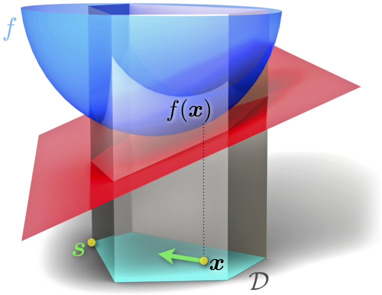

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- ◇ most of those strategies apply to more general situations
  - that include primal-dual optimality conditions.

The proximal-point method

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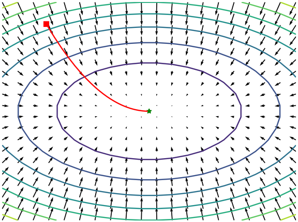

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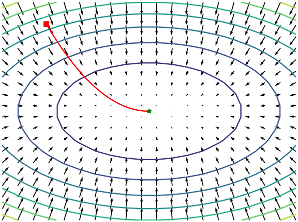

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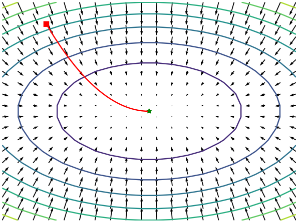

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Proximal-point splittings

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- ◇ many results on "approximated" proximal-point too.

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Proximal-point for convex QPs (I)

Minimize a quadratic function (with $Q \succcurlyeq 0$) under linear constraints:

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is just as hard as the original problem.

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Explicitly max. over λ (not over x) yields the **method of mulipliers**:

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$$\lambda_{k+1} = [\lambda_k - \gamma_k (Ax_{k+1} - b)]_+$$

(problem in x is piecewise quadratic, but convex and unconstrained).

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Proximal-point also applies to the saddle-point formulation:

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- ◇ choose appropriate step size policies (β_k and γ_k) trading-off:
  - – large values: less iterations,
  - – small values: inner problem is simpler.

Antoine Bambade

Sarah Kazdadi

Fabian Schramm

Justin Carpentier

ProxSuite

THE ADVANCED PROXIMAL OPTIMIZATION TOOLBOX

License BSD 2-Clause | docs online | CI - Linux/OSX/Windows - Conda passing | pypi package 0.3.6 | Anaconda.org 0.3.6

ProxSuite is a collection of open-source, numerically robust, precise and efficient numerical solvers (e.g., LPs, QPs, etc.) rooted in revisited primal-dual proximal algorithms. Through **ProxSuite**, we aim to offer the community scalable optimizers that can deal with dense, sparse or matrix-free problems. While the first targeted application is Robotics, **ProxSuite** can be used in other contexts without limits.

ProxSuite is actively developped and supported by the Willow and Sierra research groups, joint research teams between Inria, École Normale Supérieure de Paris and Centre National de la Recherche Scientifique localized in France.

ProxSuite is already integrated into:

- CVXPY modeling language for convex optimization problems,
- CasADi's symbolic framework for numerical optimization in general and optimal control. ProxQP is available in CasADi as plugin to solve quadratic programs,
- TSID: robotic software for efficient robot inverse dynamics with contacts and based on Pinocchio.

We are ready to integrate **ProxSuite** within other optimization ecosystems.

About

The Advanced Proximal Optimization Toolbox

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Releases 35

ProxSuite 0.6.1 Latest

last month

+ 34 releases

A priori working guarantees?

for numerical optimization algorithms

Convergence of an algorithm? (if it works)

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Here: classical worst-case framework

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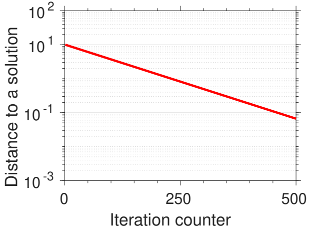

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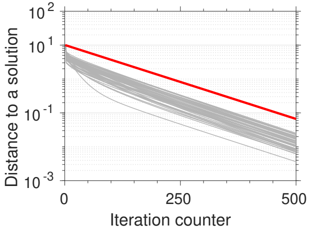

— Worst-case guarantee — Experiments

(Here: convex quadratic min., gradient descent with random init.)

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Global insight of worst-case analyses?

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Such guarantees reachable only by assuming something on f.

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Among many others: diff. function f is commonly assumed to be (for all $x, y \in \mathbb{R}^d$):

- ◇ L-smooth: $f(x) \leqslant f(y) + \langle \nabla f(y), x - y \rangle + \frac{L}{2}\|x - y\|^2$,
- ◇ convex: $f(x) \geqslant f(y) + \langle \nabla f(y), x - y \rangle$,
- ◇ μ-strongly convex: $f(x) \geqslant f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2}\|x - y\|^2$.

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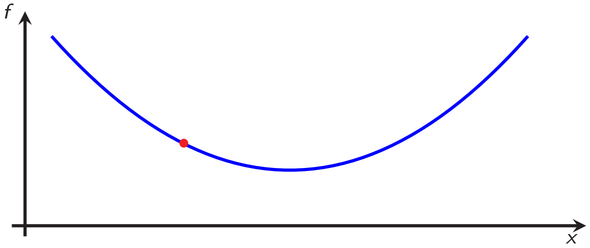

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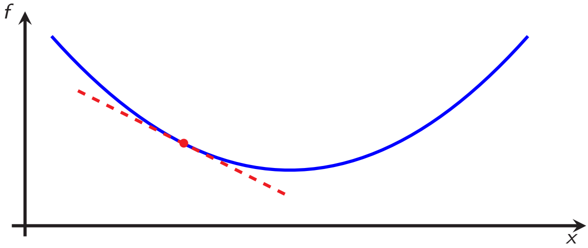

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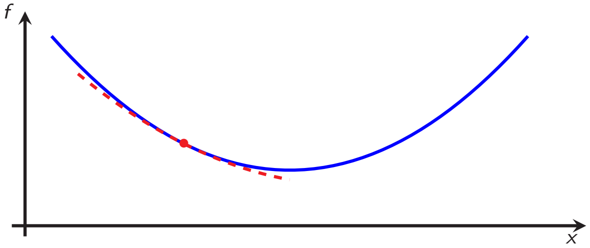

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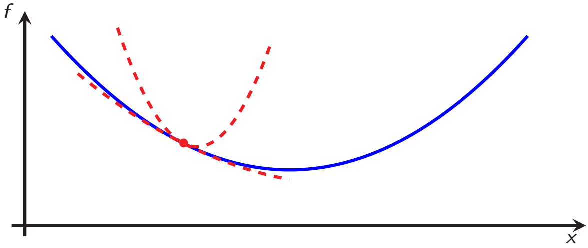

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$$\begin{aligned} \tau = \max_{f, x_0, x_1, x_\star} \; & \frac{\|x_1 - x_\star\|^2}{\|x_0 - x_\star\|^2} & \\ \text{s.t.} \; & f \in \mathcal{F}_{\mu,L} & \text{Functional class} \\ & x_1 = x_0 - \gamma_0 \nabla f(x_0) & \text{Algorithm} \\ & \nabla f(x_\star) = 0 & \text{Optimality of } x_\star \end{aligned}$$

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Toy example: What is the smallest τ such that:

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for all

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Variables: f, x_0, x_1, $x_\star$; parameters: μ, L, γ_0.

Problem can be reformulated as semidefinite program (SDP).

Sampled version

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$$\begin{array}{rl}\displaystyle\max_{f, x_0, x_1, x_\star} & \dfrac{\|x_1 - x_0\|^2}{\|x_0 - x_\star\|^2} \\ \text{subject to} & f \text{ is } L\text{-smooth and } \mu\text{-strongly convex,} \\ & x_1 = x_0 - \gamma_0 \nabla f(x_0) \\ & \nabla f(x_\star) = 0. \end{array}$$

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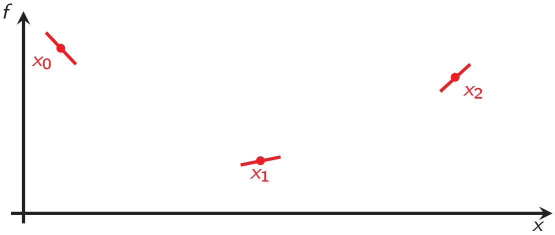

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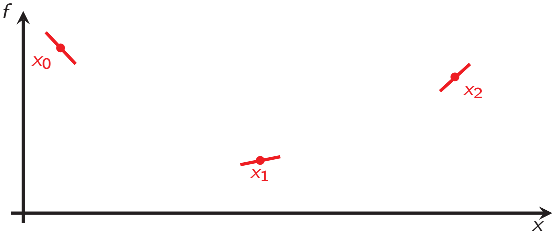

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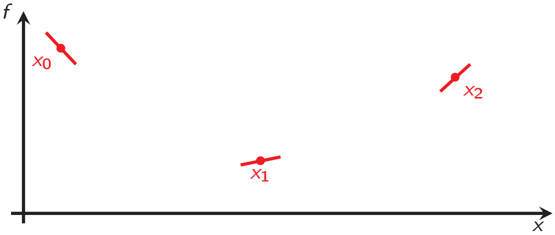

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- Simpler example: pick $\mu = 0$ and $L = \infty$ (just convexity):

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

Replace constraints

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◇ Interpolation conditions allow removing red constraints

$$\max_{\substack{x_0, x_1, x_\star \\ g_0, g_\star \\ f_0, f_\star}} \quad \frac{\|x_1 - x_\star\|^2}{\|x_0 - x_\star\|^2}$$

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◇ Same optimal value (no relaxation); but still non-convex quadratic problem.

Semidefinite lifting

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- Using the new variables $G \succcurlyeq 0$ and F

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$$\begin{aligned} \max_{G,\,F} \quad & G_{1,1} + \gamma_0^2 G_{2,2} - 2\gamma_0 G_{1,2} \\ \text{subject to} \quad & F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{L}{L-\mu} G_{1,2} \leqslant 0 \\ & -F + \tfrac{L\mu}{2(L-\mu)} G_{1,1} + \tfrac{1}{2(L-\mu)} G_{2,2} - \tfrac{\mu}{L-\mu} G_{1,2} \leqslant 0 \\ & G_{1,1} = 1 \\ & G \succcurlyeq 0 \end{aligned}$$

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(using an an homogeneity argument and substituting x_1 and $g_\star$).

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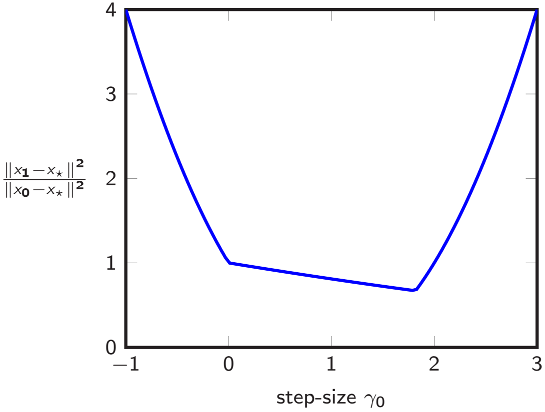

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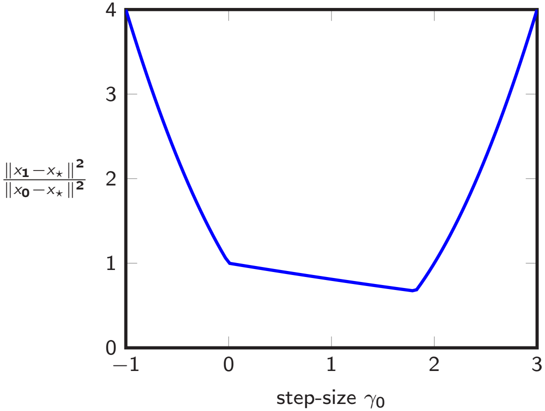

⋄ Observation: numerics match $\max\{(1-\gamma_0 L)^2, (1-\gamma_0\mu)^2\}$.

Performance estimation & gradient descent

- ⋄ We can compute for the smallest $\tau(\gamma_0)$ such that

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is satisfied for all $x_0 \in \mathbb{R}^d$, $d \in \mathbb{N}$, $f \in \mathcal{F}_{\mu,L}$, and $x_1 = x_0 - \gamma_0 \nabla f(x_0)$.

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◇ Want to know more?

- `https://francisbach.com/computer-aided-analyses/`
- Toolboxes (next slides).

Software


François


Julien


Céline

Baptiste


Aymeric

- ◇ Performance Estimation Toolbox (PESTO) in Matlab, 2017.
- ◇ Performance Estimation in Python (PEPit), 2022.

PESTO example: an inexact accelerated gradient method

Minimize L-smooth convex function $f(x)$:

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For $i = 0 : N - 1$

$$x_{i+1} = y_i - \frac{1}{L} \nabla f(y_i)$$

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What guarantees of type

$$\frac{f(x_N) - f_\star}{\|x_0 - x_\star\|^2} \leqslant \tau(N, L)?$$

Next slide: compute $\tau(N, L)$ numerically using SDP.

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% (0) Initialize an empty PEP
P = pep();

% (1) Set up the objective function
param.mu = 0;      % strong convexity parameter
param.L  = 1;      % Smoothness parameter

F=P.DeclareFunction('SmoothStronglyConvex',param); % F is the objective function

% (2) Set up the starting point and initial condition
x0       = P.StartingPoint();        % x0 is some starting point
[xs, fs] = F.OptimalPoint();         % xs is an optimal point, and fs=F(xs)
P.InitialCondition((x0-xs)^2 <= 1);  % Add an initial condition ||x0-xs||^2<= 1

% (3) Algorithm
N = 7; % number of iterations

x    = cell(N+1,1); % we store the iterates in a cell for convenience
x{1} = x0;
y    = x0;
eps  = .1;
for i = 1:N
    d      = inexactsubgradient(y, F, eps);
    x{i+1} = y - 1/param.L * d;
    y      = x{i+1} + (i-1)/(i+2) * (x{i+1} - x{i});
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% (4) Set up the performance measure
[g, f] = F.oracle(x{N+1});    % g=grad F(x), f=F(x)
P.PerformanceMetric(f - fs); % Worst-case evaluated as F(x)-F(xs)

% (5) Solve the PEP
P.solve()

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    y       = x{i+1} + (i-1)/(i+2) * (x{i+1} - x{i});
end
```

```
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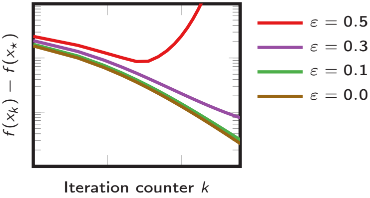
end

% (4) Set up the performance measure
[g, f] = F.oracle(x{N+1});    % g=grad F(x), f=F(x)
P.PerformanceMetric(f - fs); % Worst-case evaluated as F(x)-F(xs)

% (5) Solve the PEP
P.solve()

% (6) Evaluate the output
double(f - fs)   % worst-case objective function accuracy
```



PESTO example: Douglas-Rachford splitting

Minimize sum of two convex (cpp) functions

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

Douglas-Rachford Splitting

Input: f, h convex (cpp) functions, $w_0 \in \mathbb{R}^d$.

For $i = 0 : N-1$

$$\begin{aligned}
x_{i+1} &= \mathrm{argmin}_{x \in \mathbb{R}^d} \{\gamma h(x) + \tfrac{1}{2}\|x - w_i\|^2\} \\
y_{i+1} &= \mathrm{argmin}_{y \in \mathbb{R}^d} \{\gamma f(y) + \tfrac{1}{2}\|y - 2x_{i+1} + w_i\|^2\} \\
w_{i+1} &= w_i + \tfrac{1}{2}(y_{i+1} - x_{i+1}).
\end{aligned}$$

Next slide: compute convergence rates when f is strongly convex and h is smooth.

PESTO example: Douglas-Rachford splitting

```matlab
% (0) Initialize an empty PEP
P=pep();

N = 1;
% (1) Set up the class of monotone inclusions
paramA.L  =  1; paramA.mu = 0; % A is 1-Lipschitz and 0-strongly monotone
paramB.mu = .1;                % B is .1-strongly monotone

A = P.DeclareFunction('LipschitzStronglyMonotone',paramA);
B = P.DeclareFunction('StronglyMonotone',paramB);

w  = cell(N+1,1);   wp = cell(N+1,1);
x  = cell(N,1);     xp = cell(N,1);
y  = cell(N,1);     yp = cell(N,1);

% (2) Set up the starting points
w{1}    = P.StartingPoint(); wp{1}    = P.StartingPoint();
P.InitialCondition((w{1}-wp{1})^2<=1);

% (3) Algorithm
lambda = 1.3;       % step size (in the resolvents)
theta  = .9;         % overrelaxation

for k = 1 : N
    x{k}    = proximal_step(w{k},B,lambda);
    y{k}    = proximal_step(2*x{k}-w{k},A,lambda);
    w{k+1}  = w{k}-theta*(x{k}-y{k});

    xp{k}   = proximal_step(wp{k},B,lambda);
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end

% (4) Set up the performance measure: ||z0-z1||^2
P.PerformanceMetric((w{k+1}-wp{k+1})^2);

% (5) Solve the PEP
P.solve()

% (6) Evaluate the output
double((w{k+1}-wp{k+1})^2)   % worst-case contraction factor
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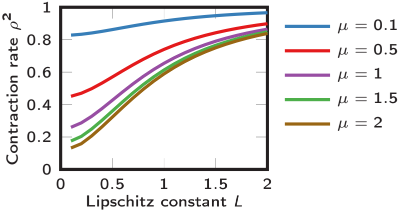

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First ideas in this line of research coined by Drori and Teboulle (2014).

PEPit: Performance Estimation in Python

Tests passing | codecov 90% | docs passing | pypi package 0.2.1 | downloads 12k | license MIT

This open source Python library provides a generic way to use PEP framework in Python. Performance estimation problems were introduced in 2014 by **Yoel Drori** and **Marc Teboulle**, see [1]. PEPit is mainly based on the formalism and developments from [2, 3] by a subset of the authors of this toolbox. A friendly informal introduction to this formalism is available in this blog post and a corresponding Matlab library is presented in [4] (PESTO).

Website and documentation of PEPit: https://pepit.readthedocs.io/

Source Code (MIT): https://github.com/PerformanceEstimation/PEPit

Using and citing the toolbox

This code comes jointly with the following `reference`:

```
B. Goujaud, C. Moucer, F. Glineur, J. Hendrickx, A. Taylor, A. Dieuleveut (2022).
"PEPit: computer-assisted worst-case analyses of first-order optimization methods in Python."
```

When using the toolbox in a project, please refer to this note via this Bibtex entry:

```
@article{pepit2022,
  title={{PEPit}: computer-assisted worst-case analyses of first-order optimization methods in {P}yt
  author={Goujaud, Baptiste and Moucer, C\'eline and Glineur, Fran\c{c}ois and Hendrickx, Julien and
  journal={arXiv preprint arXiv:2201.04040},
  year={2022}
}
```

About

PEPit is a package enabling computer-assisted worst-case analyses of first-order optimization methods.

pepit.readthedocs.io/en/latest/

python | optimization | semidefinite-programming | worst-case-analyses | first-order-methods | performance-estimation-problems

Readme

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Activity

68 stars

4 watching

6 forks

Report repository

Releases 5

0.2.1 Latest
on Dec 17, 2022

+ 4 releases

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◇ T., Hendrickx, Glineur ('17). "Exact worst-case performance of first-order methods for composite convex optimization."

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Designing algorithms with PEPs:

- ⋄ Drori, T ('20). "Efficient first-order methods for convex minimization: a constructive approach."
- ⋄ Drori, T ('22). "On the oracle complexity of smooth strongly convex minimization."
- ⋄ T, Drori ('23). "An optimal gradient method for smooth strongly convex minimization."

Informal introduction: `https://francisbach.com/computer-aided-analyses/`.

Concluding remarks

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- ◇ validation & benchmark tool for proofs (also for reviews ☺).

Thanks! Questions?

PerformanceEstimation/Performance-Estimation-Toolbox on Github

PerformanceEstimation/PEPit on Github