A few constructive approaches to optimal first-order optimization methods for convex optimization

Adrien Taylor

All Russian optimization seminar – May 2021

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

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More examples in toolbox' manual

`https://github.com/AdrienTaylor/Performance-Estimation-Toolbox`

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But also:

- ◇ Fair amount of algorithmic analyses (and design) originated from SDPs (from different authors, examples below), in different settings.
- ◇ We try keeping track of related works in the toolbox' manual (see later), incomplete references in this presentation.

François Glineur

Julien Hendrickx

Etienne de Klerk

Ernest Ryu

Yoel Drori

Francis Bach

Jérôme Bolte

Alexandre d'Aspremont

Mathieu Barré

Radu-Alexandru Dragomir

Bryan Van Scoy

Laurent Lessard

Carolina Bergeling

Pontus Giselsson

Take-home messages

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When it does: principled approach to worst-case analyses.

Performance estimation problems

Designing methods using PEPs

Conclusions

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Analysis of a gradient method

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Examples: how small should $f(x_N) - f(x_\star)$, $\|f'(x_N)\|$, $\|x_N - x_\star\|$ be?

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By definition, the "best" such guarantee is

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In other words:

$$\begin{aligned} \left\|f'(x_N)\right\| \leqslant \sup_{F, y_0, \ldots, y_N} \quad & \left\|F'(y_N)\right\| \\ \text{subject to} \quad & y_1, \ldots, y_N \text{ generated by gradient method from } y_0 \\ & F \text{ satisfies the assumptions on } f \end{aligned}$$

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Standard workaround: assume something on the starting point,
for example: assume bounded $\|x_0 - x_\star\|^2$, $\|f'(x_0)\|^2$ or $f(x_0) - f(x_\star)$.

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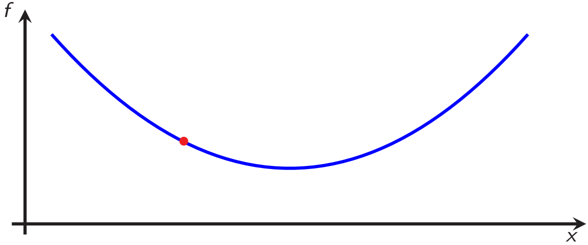

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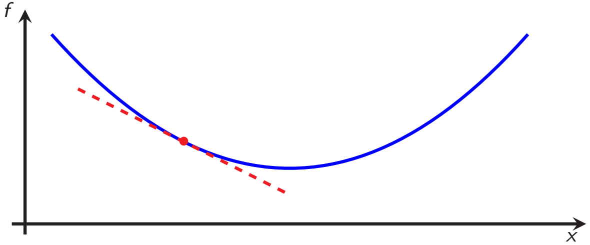

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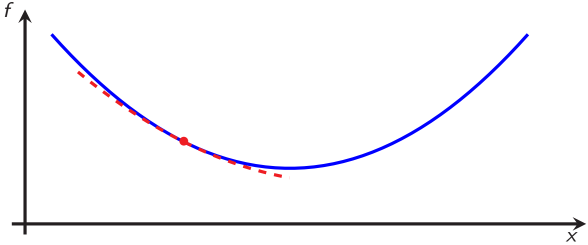

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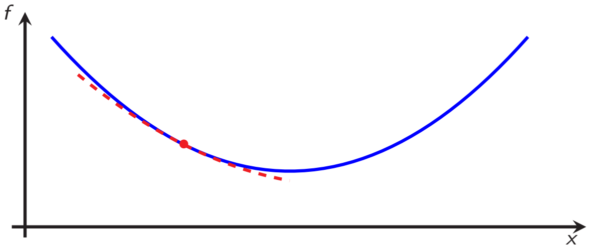

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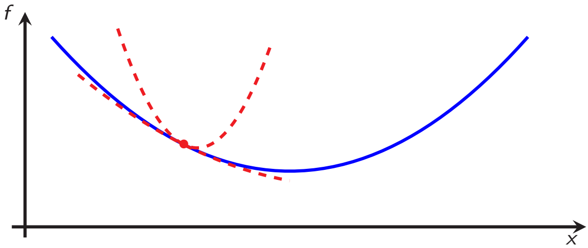

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Toy example: What can we guarantee on $\|f'(x_1)\|$ given that:

- f is L-smooth and μ-strongly convex (notation $f \in \mathcal{F}_{\mu,\mathsf{L}}$),
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$$\max_{f, x_0, x_1} \left\|f'(x_1)\right\|^2$$

$$\text{s.t. } f \in \mathcal{F}_{\mu,L} \qquad\qquad \text{Functional class}$$

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- Variables: x_0, x_1, g_0, g_1, f_0, f_1.

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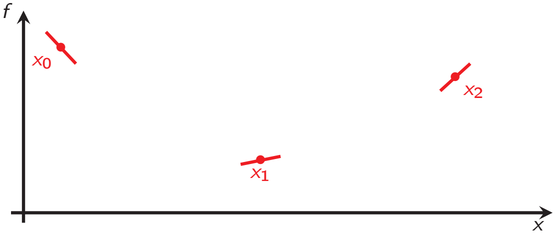

? Possible to find $f \in \mathcal{F}_{\mu,L}$ such that

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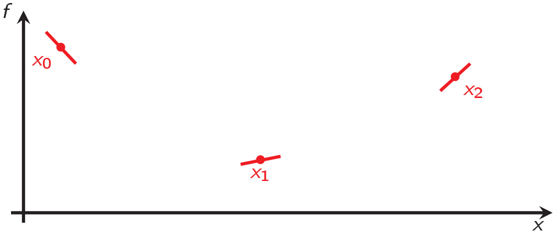

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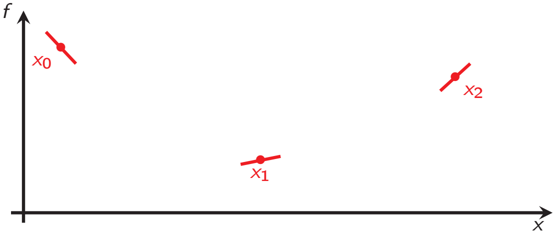

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- Simpler example: pick $\mu = 0$ and $L = \infty$ (just convexity):

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

Replace constraints

Replace constraints

◇ Interpolation conditions allow removing red constraints

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\max_{\substack{x_0, x_1, g_0, g_1 \\ f_0, f_1}} \quad & \|g_1\|^2 \\
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- Same optimal value (no relaxation); but still non-convex quadratic problem.

Semidefinite lifting

Semidefinite lifting

◇ Using $x_1 = x_0 - \gamma g_0$, all elements are quadratic in (g_0, g_1), and linear in (f_0, f_1):

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- They are therefore linear in terms of a Gram matrix G and a vector F, with

$$G = \begin{bmatrix} \|g_0\|^2 & \langle g_0, g_1\rangle \\ \langle g_0, g_1\rangle & \|g_1\|^2 \end{bmatrix} = \begin{bmatrix} g_0 & g_1 \end{bmatrix}^\top \begin{bmatrix} g_0 & g_1 \end{bmatrix}, \quad F = \begin{bmatrix} f_0 & f_1 \end{bmatrix},$$

where $G \succcurlyeq 0$ by construction.

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

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- For $d = 1$ same optimal value by adding $\mathrm{rank}(G) \leqslant 1$.

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Fix $L = 1$, $\mu = .1$ and solve the SDP for a few values of γ.

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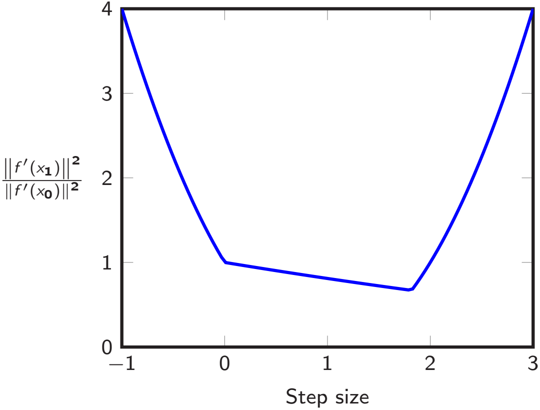

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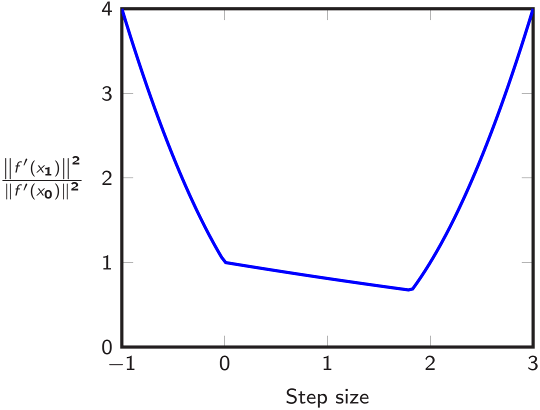

Observation: numerics match the (expected) $\max\{(1-\gamma L)^2, (1-\gamma\mu)^2\}$.

Translation to worst-case guarantees

- Let us rephrase our target: we look for $\rho(\gamma)$ (hopefully small) such that

$$\|f'(x_1)\| \leq \rho(\gamma)\|f'(x_0)\|$$

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

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- Any such $\rho(\gamma)$ that is valid for all $x_0 \in \mathbb{R}^d$, $d \in \mathbb{N}$, $f \in \mathcal{F}_{\mu,L}$ is a feasible point to the dual SDP.

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Fix $L = 1$, $\mu = .1$ and solve the dual SDP for a few values of γ.

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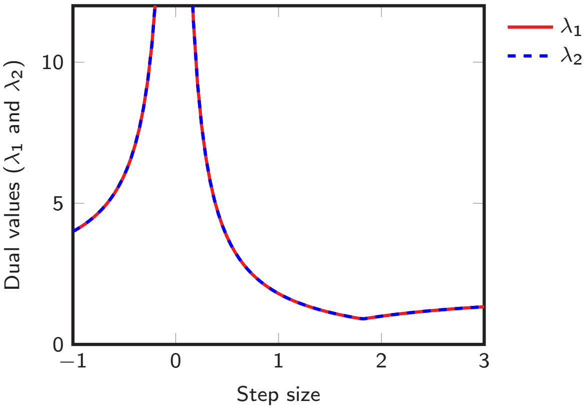

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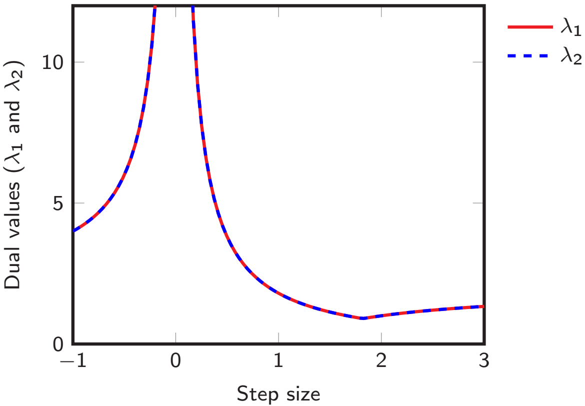

Note: numerics match $\lambda_1 = \lambda_2 = \frac{2}{|\gamma|}\rho(\gamma)$ with $\rho(\gamma) = \max\{|1 - \gamma L|, |1 - \gamma\mu|\}$.

Recovering a "standard" proof

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  - play with primal (e.g., worst-case functions might be easy to identify),
  - play with dual (e.g., dual variables might be easy to identify).
- ◇ Standard tricks apply, e.g., trace norm minimization for promoting low-rank solutions (on primal or dual).

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Problem setting:

- ◇ pick a method
- ◇ pick a class of functions
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In other situations, one might want to relax the PEP for obtaining upper-bounds.

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- Optimizing/designing methods? upcoming!

Avoiding semidefinite programming modeling steps?

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François Glineur
(UCLouvain)

Julien Hendrickx
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"Performance Estimation Toolbox (PESTO): automated worst-case analysis of first-order optimization methods" (CDC 2017)

PESTO example: inexact fast gradient method

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

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

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Fast Gradient Method (FGM)

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For $i = 0 : N-1$

$$x_{i+1} = y_i - \frac{1}{L} f'(y_i)$$
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PESTO example: an inexact fast gradient method

```matlab
% (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});
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: an inexact fast gradient method

```
% (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
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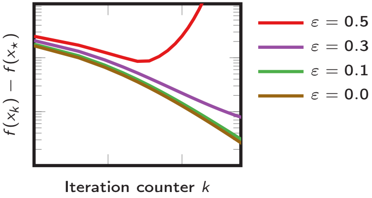

PESTO example: Douglas-Rachford splitting

```
% (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});

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% (4) Set up the performance measure: ||z0-z1||^2
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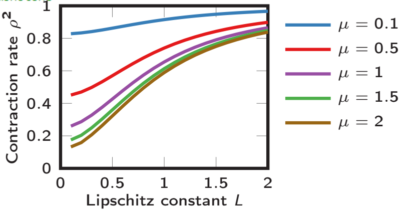

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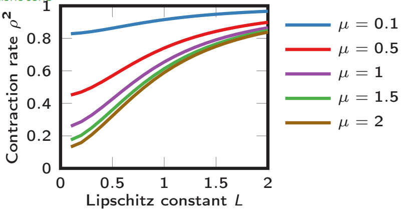

✔ fast prototyping ($\sim$ 20 effective lines)
✔ quick analyses ($\sim$ 10 minutes)
✔ computer-aided proofs (multipliers)

Current library of examples within PESTO

Includes... but not limited to

- ◇ subgradient, gradient, heavy-ball, fast gradient, optimized gradient methods,
- ◇ proximal point algorithm,
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Currently in Matlab, soon in Python.

Performance estimation problems

Designing methods using PEPs

Conclusions

Main inspiration

Great inspiration from previous works.

- B. Polyak. "Introduction to optimization" (1964)
- Y. Nesterov. "A method of solving a convex programming problem with convergence rate $O(1/k^2)$". (1983)
- A. Nemirovsky, and B. Polyak. "Iterative methods for solving linear ill-posed problems under precise information." (1984)
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In next couple of slides:

- ◇ goal: principled way towards optimal methods.
- ◇ in some sense, *generalization* of Chebyshev methods (tailored for quadratic minimization) to non-quadratic smooth strongly convex setup.

Main references

Yoel Drori

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Main references for the following slides (sloppy references throughout):

- ◇ Y. Drori, T., "On the oracle complexity of smooth strongly convex minimization". (2021)
- ◇ T., Y. Drori, "An optimal gradient method for smooth strongly convex minimization". (2021)
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- ⋄ Y. Drori, "The exact information-based complexity of smooth convex minimization". (2017)
- ⋄ D. Kim, J.F. Fessler, "Optimized first-order methods for smooth convex minimization". (2016)
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Also closely related:

- ⋄ B. Van Scoy, R.A. Freeman, K.M. Lynch, "The fastest known globally convergent first-order method for minimizing strongly convex functions". (2017)
- ⋄ D. Kim, J.F. Fessler, "Optimizing the efficiency of first-order methods for decreasing the gradient of smooth convex functions". (2021)

Designing methods using PEPs

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How could we use PEPs for designing methods, and lower complexity bounds?

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  - can be used for designing "worst functions in the world".

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w_1 &= w_0 - h_{1,0} f'(w_0),\\
w_2 &= w_1 - h_{2,0} f'(w_0) - h_{2,1} f'(w_1),\\
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$\Rightarrow$ Resulting design problem, for example

$$\min_{\{h_{i,j}\}} \max_{f\in\mathcal{F}_{0,L}} \left\{ \frac{f(w_N)-f_\star}{\|w_0-w_\star\|^2} \,:\, w_N \text{ obtained from (FOM) and } w_0 \right\}.$$

(i.e., "minimize worst-case")

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- ◇ The situation actually quite similar beyond quadratics.

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  - – those methods are incredibly close to Nesterov's method!
- ⋄ Beyond that, a few criterion/settings/methods for which "perfectly optimal" algorithms might be known, but matching lower bounds are still missing.
  - – $\frac{\|f'(w_N)\|^2}{f(w_0) - f_\star}$,
  - – a few numerically-generated methods.

Optimized gradient method (OGM)

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which rely on some exotic sequence

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\theta_{k+1,N} = \begin{cases} \frac{1+\sqrt{4\theta_{k,N}^2+1}}{2} & \text{if } k \leqslant N-2 \\ \frac{1+\sqrt{8\theta_{k,N}^2+1}}{2} & \text{if } k = N-1, \end{cases}
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The (tight) worst-case guarantee is

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\frac{f(y_N) - f_\star}{L\|y_0 - y_\star\|^2} \leqslant \frac{1}{2\theta_{N,N}^2} \approx \frac{2}{N^2},
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which matches exactly the corresponding lower complexity bound (Drori, 2017).

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- ◇ Nesterov's method: can be obtained as an optimized gradient method whose proof relies only on more convenient inequalities.

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Let us pick $L = 1$, $\mu = .1$. The best method we could reach (through numerical optimization) for $N = 5$ satisfies

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with step sizes

$$[h^\star_{i,j}] = \begin{bmatrix} 1.9060 & & & & \\ 0.3879 & 2.1439 & & & \\ 0.1585 & 0.4673 & 2.1227 & & \\ 0.0660 & 0.1945 & 0.4673 & 2.1439 & \\ 0.0224 & 0.0660 & 0.1585 & 0.3879 & 1.9060 \end{bmatrix}.$$

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- For $N = 3$, we obtain $\frac{f(w_3)-f_\star}{f(w_0)-f_\star} \leq 0.1698$ with
$$[h^\star_{i,j}] = \begin{bmatrix}1.9470 & & \\ 0.4599 & 2.2406 & \\ 0.1705 & 0.4599 & 1.9470\end{bmatrix}.$$

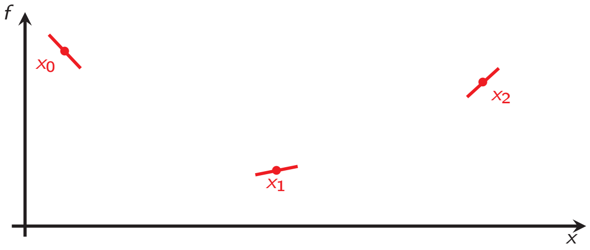
Shape of lower complexity bounds

Role of extension/interpolation results, so far?

- For obtaining *tight* SDP representation of the worst-case computation problem.
- We can infer shapes for the worst-case functions!
  - Why? Let's flashback into the interpolation/extension problem!

Reminder: smooth strongly convex interpolation/extension

Consider a set S, and its associated values $\{(x_i, g_i, f_i)\}_{i\in S}$ with coordinates x_i, subgradients g_i and function values f_i.



? Possible to find a $f \in \mathcal{F}_{\mu,L}$ s.t.

$$f(x_i) = f_i, \quad \text{and} \quad g_i \in \partial f(x_i), \qquad \forall i \in S.$$

Special case: convex interpolation problem

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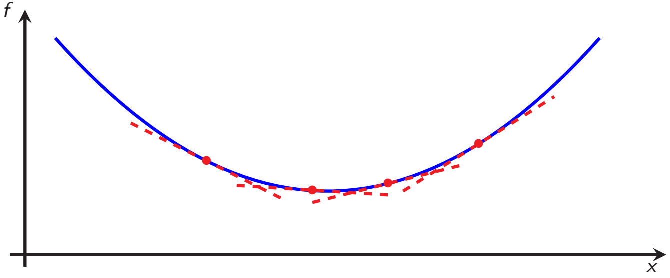

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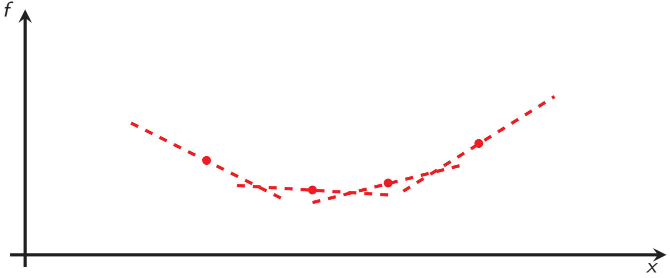

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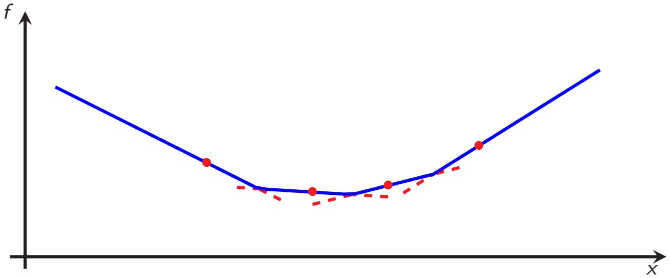

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Explicit construction:

$$f(x) = \max_j \left\{ f_j + \langle g_j, x - x_j \rangle \right\},$$

Not unique.

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- ◇ Similar constructions for smooth (possibly) strongly convex functions.
- ◇ We can use that for generating algorithm-independent lower bounds numerically (with a few additional ingredients)

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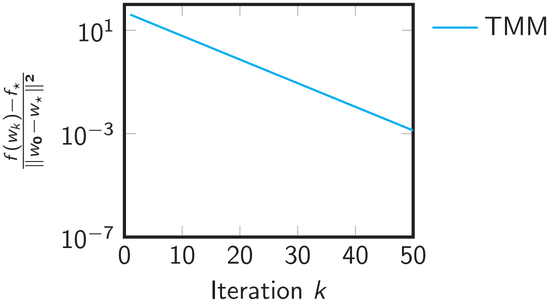

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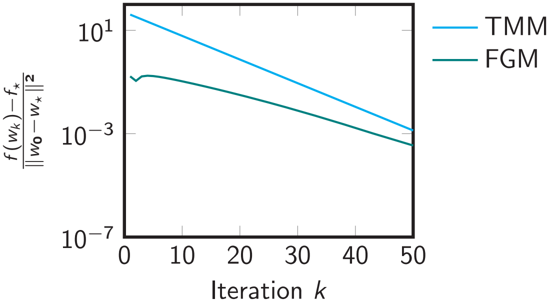

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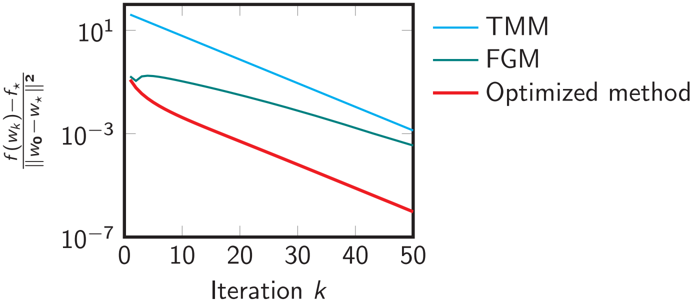

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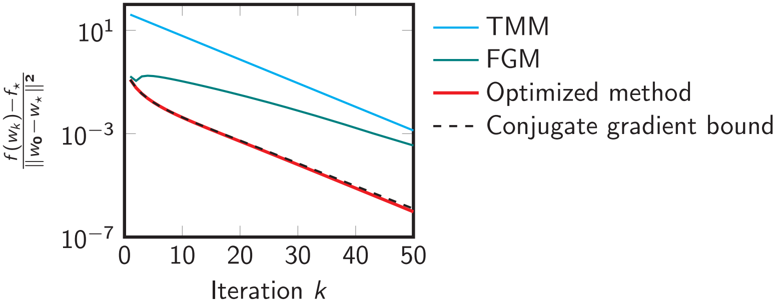

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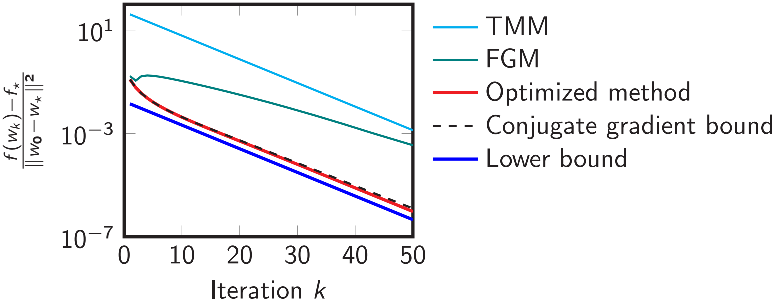

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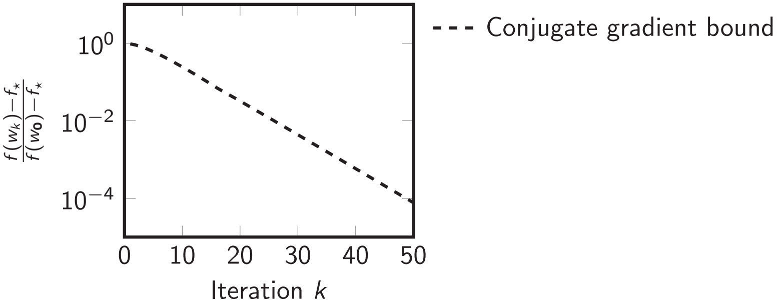

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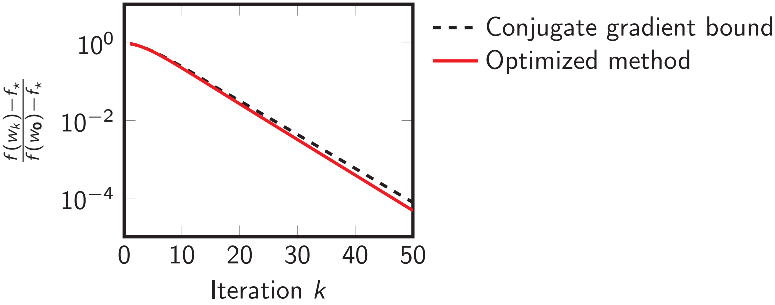

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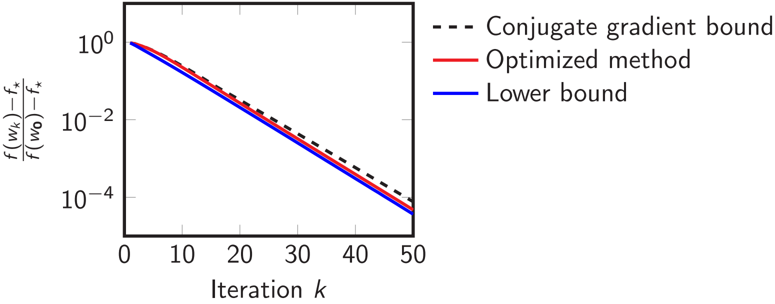

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When it does: principled approach to worst-case analyses.

Thanks! Questions?

www.di.ens.fr/~ataylor/

AdrienTaylor/Performance-Estimation-Toolbox on Github