Constructive approaches to the analysis and design of first-order methods for optimization

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DIPopt workshop – November 2023

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Bryan Van Scoy

Laurent Lessard

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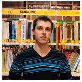
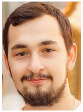
Céline Moucer



Baptiste Goujaud

Sebastian Banert

Manu Uphadyaya



Eduard Gorbunov

Gauthier Gidel

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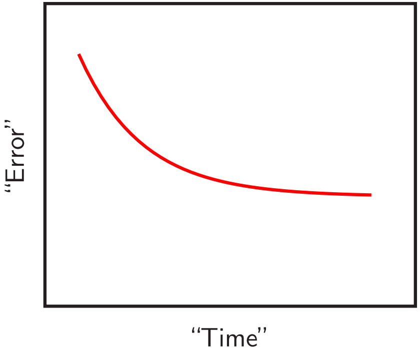

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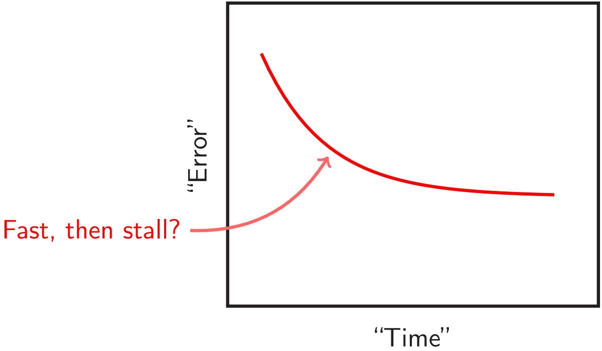

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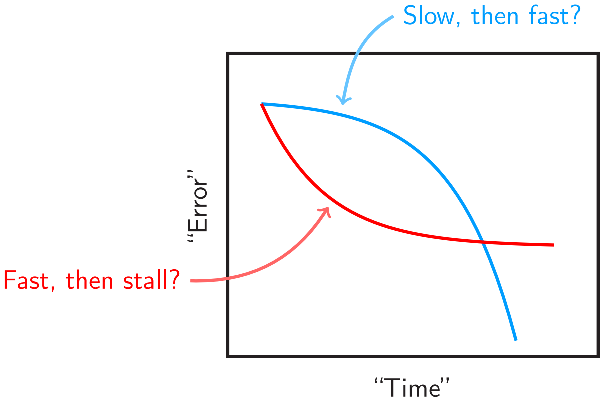

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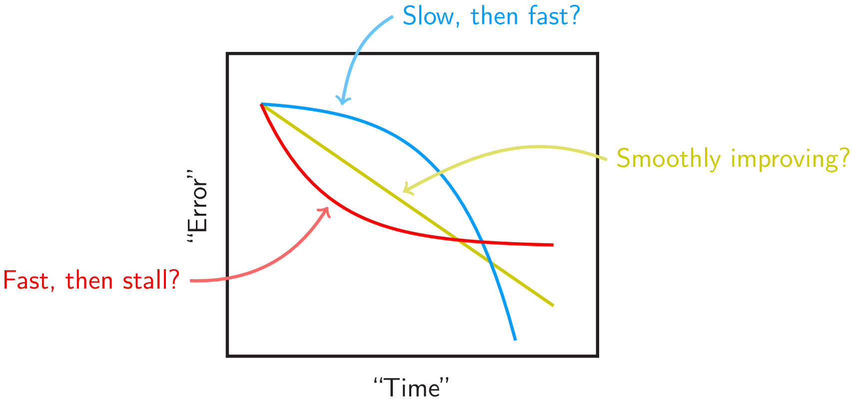

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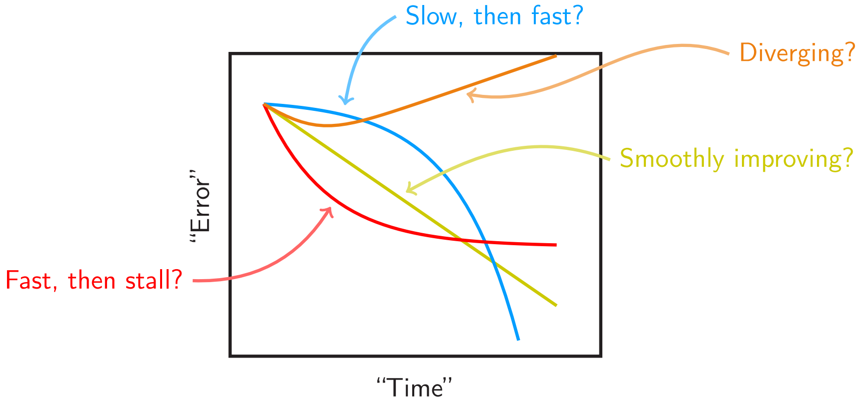

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Here: principled approach to worst-case analysis.

Important inspiration & reference:

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First part of the presentation:

- ◇ T., Hendrickx, Glineur ('17). "Smooth strongly convex interpolation and exact worst-case performance of first-order methods."
- ◇ T., Hendrickx, Glineur ('17). "Exact worst-case performance of first-order methods for composite convex optimization."
- ◇ T., Hendrickx, Glineur ('17). "Performance estimation toolbox (PESTO): Automated worst-case analysis of first-order optimization methods."
- ◇ Goujaud, Moucer, et al. ('22). "PEPit: computer-assisted worst-case analyses of first-order optimization methods in Python."

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Second part

- ◇ 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/`.

Example: minimize differentiable $f : \mathbb{R}^d \to \mathbb{R}$:

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

where f is L-smooth and μ-strongly convex ($0 \leqslant \mu \leqslant L < \infty$).

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

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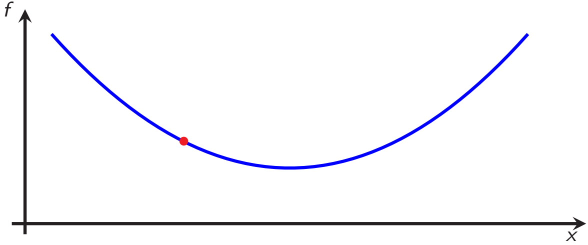

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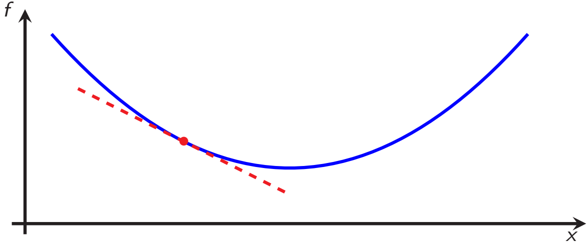

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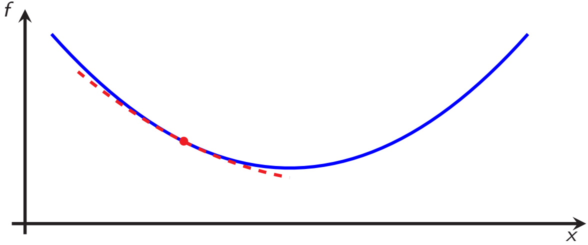

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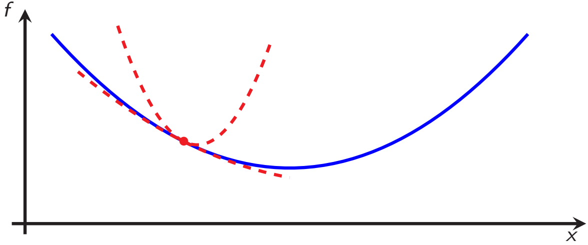

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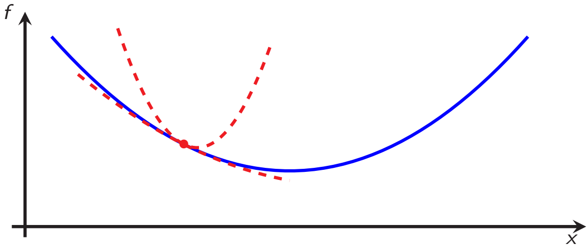

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(1&2) $\langle \nabla f(x) - \nabla f(y); x - y \rangle \geqslant \frac{1}{L+\mu} \|\nabla f(x) - \nabla f(y)\|^2 + \frac{\mu L}{L+\mu} \|x - y\|^2$.

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- $\diamond$ Unique way to arrive to the desired result?
- $\diamond$ How likely are we to find such proofs in more complicated cases?

Take-home messages

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Acceleration/optimal methods by optimizing worst-cases.

Example

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Step-size optimization

Concluding remarks

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$$x_1 = x_0 - hg_0$$

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Sampled version

- Performance estimation problem:

$$\begin{aligned} \max_{f, x_0, x_1, x_\star} \quad & \frac{\|x_1 - x_0\|^2}{\|x_0 - x_\star\|^2} \\ \text{subject to} \quad & f \text{ is } L\text{-smooth and } \mu\text{-strongly convex,} \\ & x_1 = x_0 - h\nabla f(x_0) \\ & \nabla f(x_\star) = 0. \end{aligned}$$

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Smooth strongly convex interpolation (or extension)

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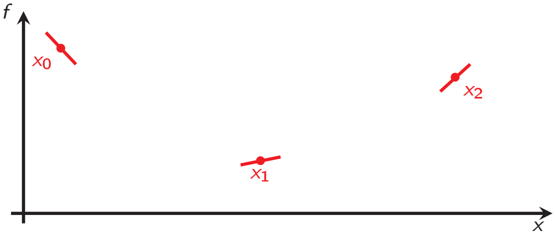

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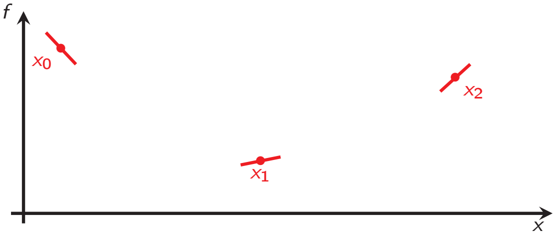

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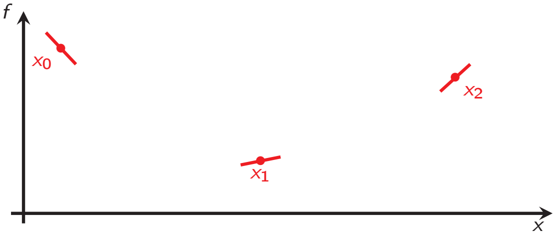

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- Simpler example: pick $\mu = 0$ and $L = \infty$ (just convexity):

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- Interpolation conditions allow removing red constraints

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

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

$$G = \begin{bmatrix} \|x_0 - x_\star\|^2 & \langle g_0, x_0 - x_\star\rangle \\ \langle g_0, x_0 - x_\star\rangle & \|g_0\|^2 \end{bmatrix}, \quad F = f_0 - f_\star,$$

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- For $d = 1$ same as original problem by adding $\text{rank}(G) \leqslant 1$.

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

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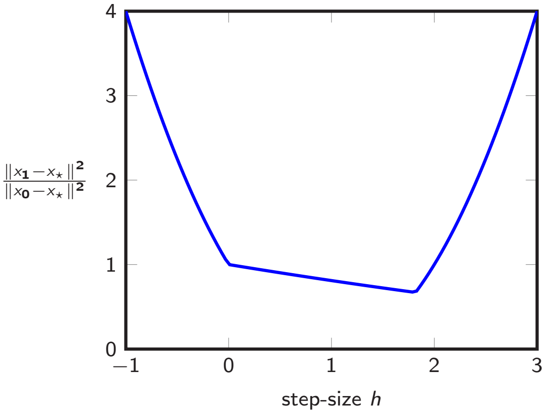

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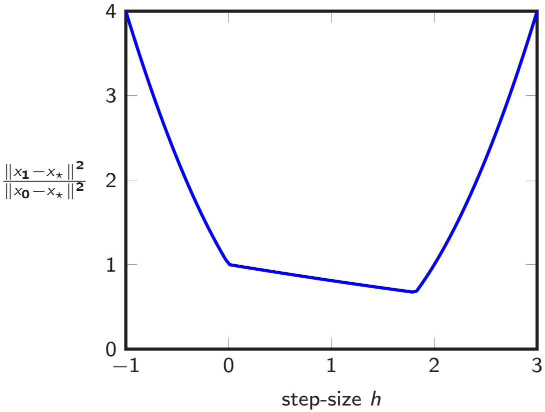

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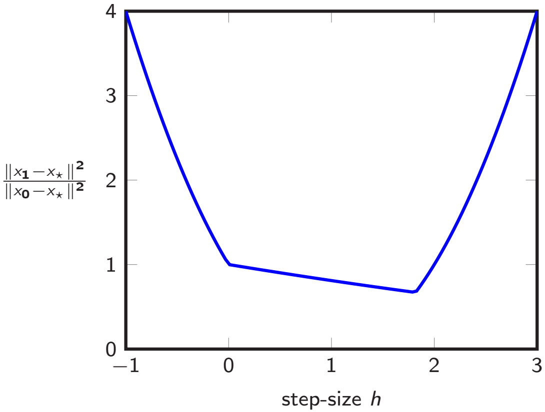

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◇ We recover the celebrated $\frac{2}{L+\mu}$ as the optimal step-size.

Dual problem

◇ Dual problem is

$$\min_{\tau,\lambda_1,\lambda_2\geqslant 0} \tau$$

$$\text{subject to } S = \begin{bmatrix} \tau - 1 + \frac{\lambda_1 L\mu}{L-\mu} & h - \frac{\lambda_1(\mu+L)}{2(L-\mu)} \\ h - \frac{\lambda_1(\mu+L)}{2(L-\mu)} & \frac{\lambda_1}{L-\mu} - h^2 \end{bmatrix} \succcurlyeq 0$$

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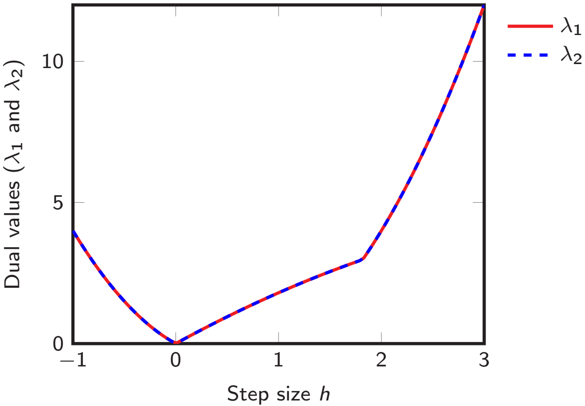

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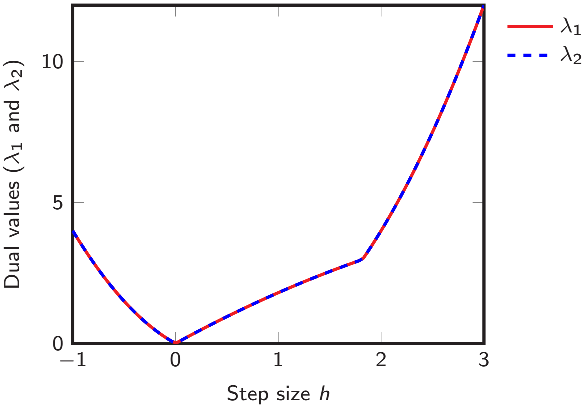

Numerics match $\lambda_1 = \lambda_2 = 2|h|\rho(h)$ with $\rho(h) = \max\{hL - 1, 1 - h\mu\}$.

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Gradient with $h = \frac{1}{L}$. Perform weighted sum of two inequalities

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... what happens beyond gradient descent for smooth strongly convex minimization?

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- Step-size optimization?

  Optimize worst-case performance.

Example

Software

Step-size optimization

Concluding remarks

Avoiding semidefinite programming modeling steps?

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Baptiste Goujaud

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Aymeric Dieuleveut

Julien Hendrickx

François Glineur

- ◇ Matlab version: Performance Estimation Toolbox (PESTO) available at

  github.com/PerformanceEstimation/Performance-Estimation-Toolbox

- ◇ Python version: PEPit available at

  github.com/PerformanceEstimation/PEPit/

Packages contain more than 75 examples!

A few examples

Algorithms for solving:

$$\min_x f(x)$$

with f convex and L-smooth.

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Proximal point algorithm for (maximal) monotone inclusion:

$$\text{find } x : \; 0 \in A(x)$$

with $A : \mathbb{R}^d \to 2^{\mathbb{R}^d}$ maximal monotone.

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What is the worst-case $\frac{\|x_{k+1}-x_k\|^2}{\|x_0-x_\star\|^2}$ when $x_{i+1} = J_A(x_i)$?

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Among others, see works by Drori, Teboulle, Kim, Fessler, Ryu, Lieder, Lessard, Recht, Packard, Van Scoy, Cyrus, Gu, Yang, etc.

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A few instructive examples

Worst-case analysis for fixed-point iterations:

- ◇ Lieder ('20). "On the convergence of the Halpern-iteration".

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Application to nonconvex optimization:

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Applications to distributed optimization:

- ⋄ Sundararajan, Van Scoy, Lessard ('19). "Analysis and design of first-order distributed optimization algorithms over time-varying graphs."
- ⋄ Colla, Hendrickx ('23). "Automatic performance estimation for decentralized optimization."

A few instructive examples—shameless advertisement

Applications to mirror descent + lower complexity bound

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Lyapunov functions (compact proofs) & counter-examples

- ◇ Lessard, Recht, Packard ('16). "Analysis and design of optimization algorithms via integral quadratic constraints."
- ◇ T, Bach ('19). "Stochastic first-order methods: non-asymptotic and computer-aided analyses via potential functions."
- ◇ Upadhyaya, Banert, T, Giselsson ('23). "Automated tight Lyapunov analysis for first-order methods."
- ◇ Goujaud, Dieuleveut, T ('23). "Counter-examples in first-order optimization: a constructive approach."

Poster

Nizar
Bousselmi

Julien
Hendrickx

François
Glineur

→ Bousselmi, Hendrickx, Glineur ('23). "Interpolation Conditions for Linear Operators and applications to Performance Estimation Problems."

Example

Software

Step-size optimization

Concluding remarks

Creating new algorithms

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How to choose $\{h_{i,j}\}$?

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x_N &= x_{N-1} - h_{N,0}\nabla f(x_0) - \ldots - h_{N,N-1}\nabla f(x_{N-1})
\end{aligned}
$$

How to choose $\{h_{i,j}\}$?

- pick a performance criterion, for instance

$$
\frac{\|x_N - x_\star\|^2}{\|x_0 - x_\star\|^2},
$$

Creating new algorithms

Smooth (strongly) convex minimization with more than gradient descent?

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$$
\frac{\|x_N - x_\star\|^2}{\|x_0 - x_\star\|^2},
$$

- ⋄ solve the minimax:

$$
\min_{\{h_{i,j}\}_{i,j}} \max_{f\in\mathcal{F},\{x_i\}} \frac{\|x_N - x_\star\|^2}{\|x_0 - x_\star\|^2}.
$$

Solution to inner maximization via $N \times N$ SDP.

Design problem

How to solve the design problem (or proxy of it)?

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Recall primal problem, with step-size optimization

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\min_{h_{1,0}} \; \max_{G,\,F} \quad & G_{1,1} + h_{1,0}^2 G_{2,2} - 2h_{1,0} 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 \\
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"Simple" minimization problem by dualizing inner maximization.

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"Simple" minimization problem by dualizing inner maximization.

Dualize inner maximization $\rightarrow \min\min$.

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Optimize $h_{1,0}$ "for free" (linear SDP via Schur complement):

$$\begin{aligned} \min_{\tau,\lambda\geqslant 0,h_{1,0}} \quad & \tau \\ \text{subject to} \quad & \begin{bmatrix} \tau - 1 + \frac{\lambda L\mu}{L-\mu} & -\frac{\lambda(\mu+L)}{2(L-\mu)} & 1 \\ -\frac{\lambda(\mu+L)}{2(L-\mu)} & \frac{\lambda}{L-\mu} & -h_{1,0} \\ 1 & -h_{1,0} & 1 \end{bmatrix} \succcurlyeq 0. \end{aligned}$$

Optimizing the step-sizes ($N = 2$)

When $N = 2$, the problem becomes

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In particular

$$S_{1,2} = -\frac{L\lambda_3 - 2(L-\mu)h_{2,0} + \mu\lambda_1 + L\mu(\lambda_2+\lambda_5)h_{1,0}}{L-\mu}$$

$$S_{2,2} = \frac{-2(\mu\lambda_6 + L\lambda_4)h_{1,0} - 2(L-\mu)h_{2,0}^2 + L\mu(\lambda_2+\lambda_4+\lambda_5+\lambda_6)h_{1,0}^2 + \lambda_1+\lambda_3+\lambda_4+\lambda_6}{L-\mu}$$

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LMI convex in some step-sizes ($h_{2,0}$ and $h_{2,1}$) but not in the others.

Numerical examples I

Example for $L = 1$ and $\mu = .1$

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- ◇ For $N = 1$, we reach $\frac{\|x_1 - x_\star\|^2}{\|x_0 - x_\star\|^2} \leqslant 0.6694$ with step-sizes

$$[h^\star_{i,j}] = \begin{bmatrix} 1.8182 \end{bmatrix}.$$

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- For $N = 2$, we reach $\frac{\|x_2 - x_\star\|^2}{\|x_0 - x_\star\|^2} \leqslant 0.3769$ with

$$[h^\star_{i,j}] = \begin{bmatrix} 1.5466 & \\ 0.2038 & 2.4961 \end{bmatrix}.$$

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- For $N = 4$, we reach $\frac{\|x_4 - x_\star\|^2}{\|x_0 - x_\star\|^2} \leqslant 0.0944$ with

$$[h^\star_{i,j}] = \begin{bmatrix}1.5466 & & & \\ 0.1142 & 1.8380 & & \\ 0.0331 & 0.2432 & 1.9501 & \\ 0.0217 & 0.1593 & 0.6224 & 3.0093\end{bmatrix}.$$

Numerical examples II

What about different performance measure? Example $\frac{f(x_N)-f_\star}{f(x_0)-f_\star}$ and $L=1$, $\mu=.1$.

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- For $N=4$, we obtain $\frac{f(x_4)-f_\star}{f(x_0)-f_\star} \leqslant 0.0789$ with
$$[h_{i,j}] = \begin{bmatrix} 1.9187 & & & \\ 0.4098 & 2.1746 & & \\ 0.1796 & 0.5147 & 2.1746 & \\ 0.0627 & 0.1796 & 0.4098 & 1.9187 \end{bmatrix}.$$

Numerical examples III

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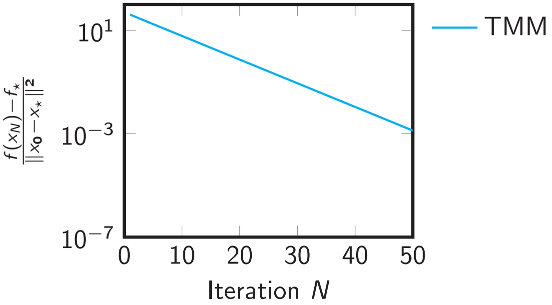

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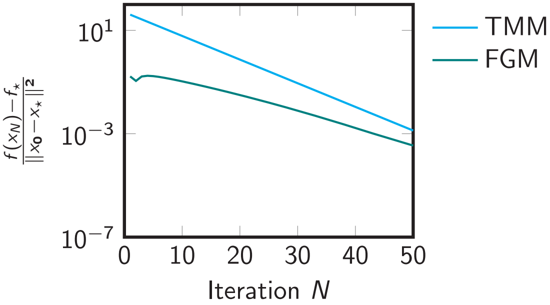

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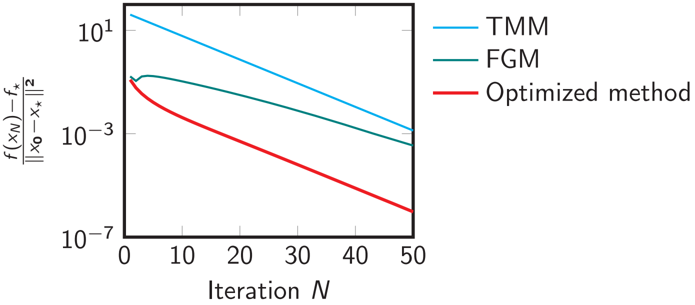

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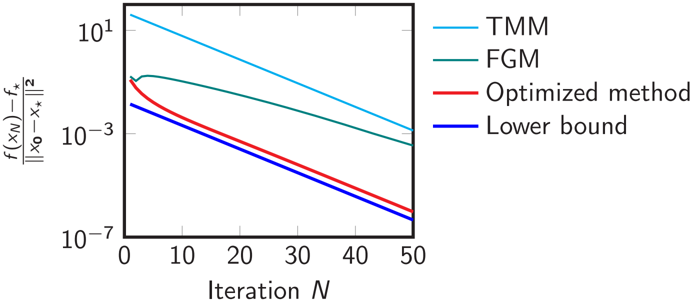

Analytical solutions

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$$y_k = (1-\beta_k)z_k + \beta_k\left(y_{k-1} - \frac{1}{L}\nabla f(y_{k-1})\right)$$
$$z_{k+1} = (1 - \tfrac{\mu}{L}\delta_k)z_k + \tfrac{\mu}{L}\delta_k\left(y_k - \frac{1}{\mu}\nabla f(y_k)\right),$$

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- ◇ Worst-case guarantee of order

$$\frac{\|z_N - z_\star\|^2}{\|z_0 - z_\star\|^2} = O\left(\left(1 - \sqrt{\tfrac{\mu}{L}}\right)^{2N} \right).$$

Analytical solutions

- It turns out that for $\frac{\|x_N - x_\star\|^2}{\|x_0 - x_\star\|^2}$, we can also solve the minimax in closed-form.
- The method referred to as "Information-Theoretic Exact Method" (ITEM)

$$y_k = (1 - \beta_k) z_k + \beta_k \left(y_{k-1} - \frac{1}{L} \nabla f(y_{k-1}) \right)$$
$$z_{k+1} = (1 - \tfrac{\mu}{L} \delta_k) z_k + \tfrac{\mu}{L} \delta_k \left(y_k - \frac{1}{\mu} \nabla f(y_k) \right),$$

  for some sequences $\{\beta_k\}$, $\{\delta_k\}$ (depending on μ, L, and k).
- The worst-case guarantee matches exactly a lower complexity bound.
- Worst-case guarantee of order

$$\frac{\|z_N - z_\star\|^2}{\|z_0 - z_\star\|^2} = O\left(\left(1 - \sqrt{\tfrac{\mu}{L}} \right)^{2N} \right).$$

- The proof is "simple"!

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- ◇ see e.g.: A. Nemirovsky's "Information-based complexity of convex programming." (lecture notes, 1995)

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- ◇ Grimmer ('23). "Provably faster gradient descent via long steps."
- ◇ Altschuler, Parrilo ('23). "Acceleration by Stepsize Hedging I: Multi-Step Descent and the Silver Stepsize Schedule."

Example

Software

Step-size optimization

Concluding remarks

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  - fast prototyping
  - worth checking before trying to prove a method works.

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  - proofs are linear combinations of certain specific inequalities.

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  - proofs are linear combinations of certain specific inequalities.

Byproducts:

- ◇ computer-assisted design of proofs,
- ◇ computer-assisted design of numerical methods,
- ◇ step towards reproducible theory
  - validation & benchmark tool for proofs (also for reviews ☺).

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- ◇ non-Euclidean algorithms (mirror descent-type), what
- ◇ adaptative algorithms, high-order, beyond worst-cases,
- ◇ many open setups: bi-level optimization, multi-objective optimization, etc.

Take-home messages

Optimization can be seen as the science of proving inequalities

...including complexity bounds for numerical methods.

Powerful framework for designing methods and guarantees.

Thanks! Questions?

PerformanceEstimation/Performance-Estimation-Toolbox on Github

PerformanceEstimation/PEPit on Github