Principled approaches and tools for the analysis and design of first-order optimization algorithms

Adrien Taylor
Sierra team, Inria Paris

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François Glineur

Julien Hendrickx

Aymeric Dieuleveut

Baptiste Goujaud

Céline Moucer

Yoel Drori

Francis Bach

Laurent Lessard

Bryan Van Scoy

Pontus Giselsson

Sebastian Banert

Manu Upadhyaya

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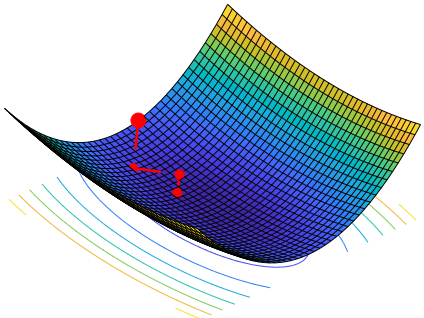

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for $k = 0, 1, \ldots$ **do**

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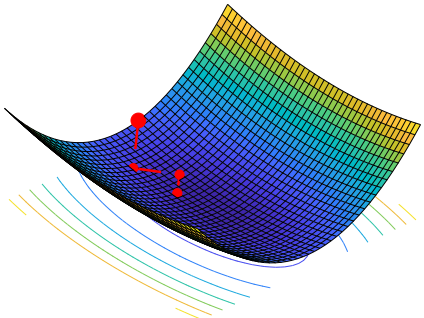

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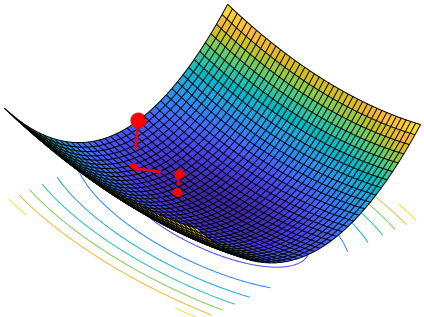

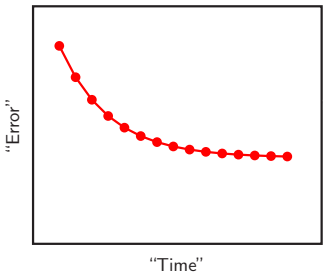

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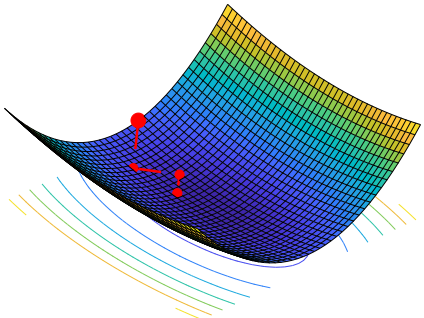

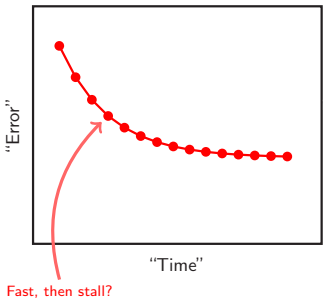

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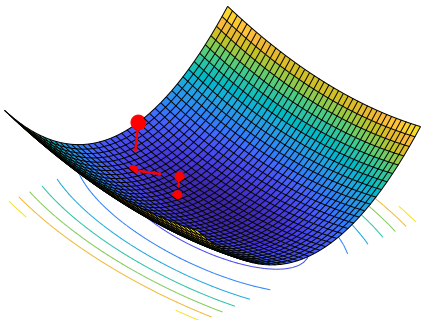

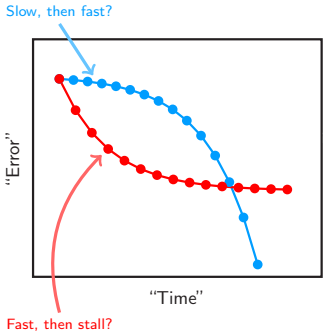

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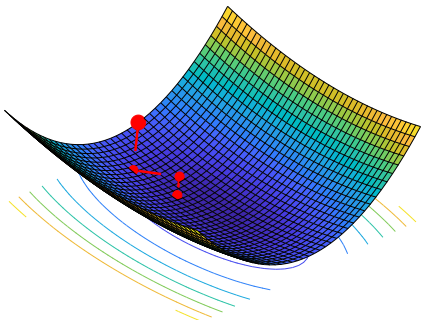

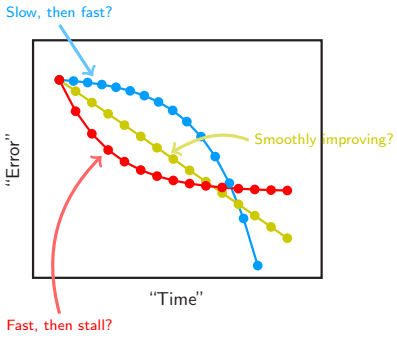

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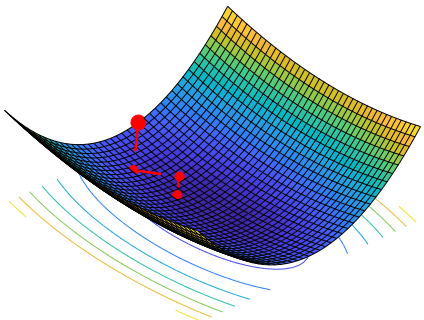

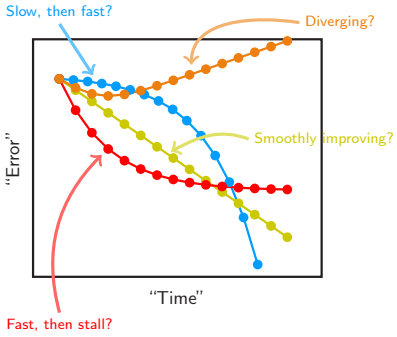

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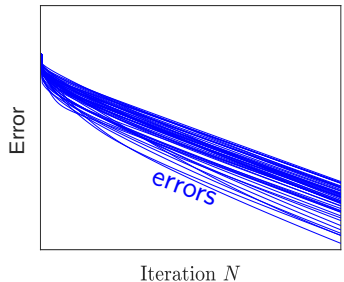

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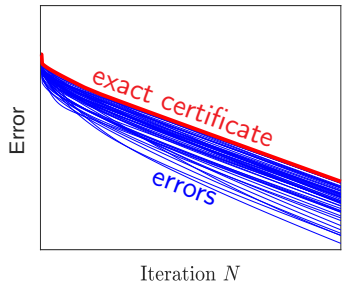

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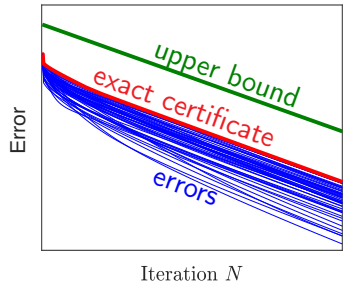

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Structured analyses

Towards optimal algorithms

Concluding remarks

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Example: analysis of a gradient method

Let $f : \mathbb{R}^d \to \mathbb{R}$ (continuously differentiable). Find $x_\star \in \mathbb{R}^d$ such that

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Question: what *a priori* guarantees after n iterations?

Examples: what about $f(x_n) - f(x_\star)$, $\|\nabla f(x_n)\|$, $\|x_n - x_\star\|$?

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Differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex and L-smooth iff $\forall x, y \in \mathbb{R}^d$:

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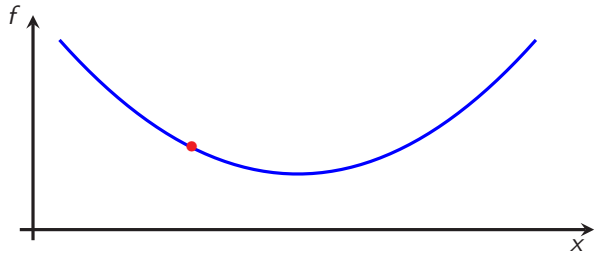

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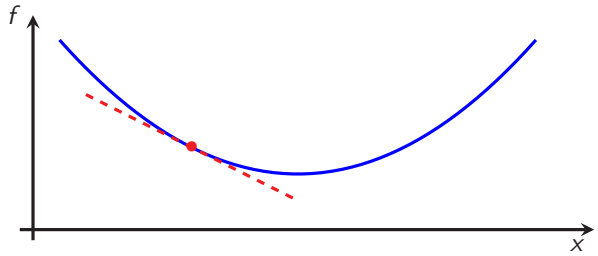

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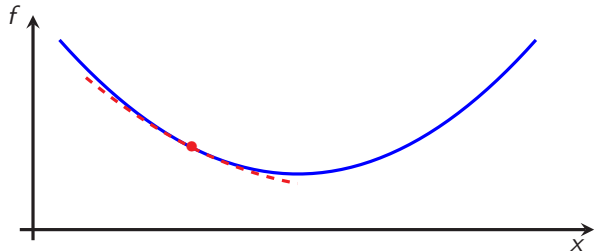

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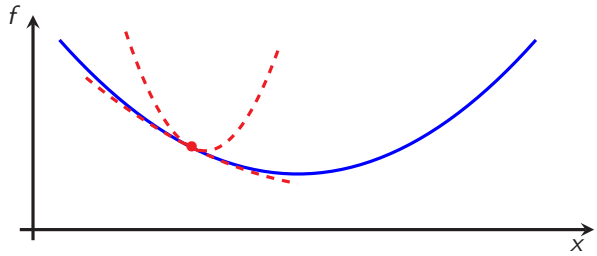

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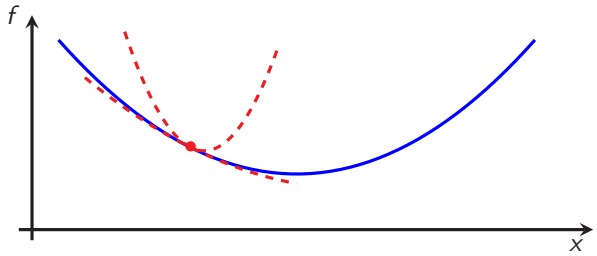

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- ◇ Unique way to arrive to the desired result?
- ◇ How likely are we to find such proofs in more complicated cases?

Legitimate questions about performance analyses?

Lemma 3. *Assume that the function is L-smooth and μ strongly-convex and satisfies the strong-growth condition in Equation 10. Then, using the updates in Equation 3-5 and setting the parameters according to Equations 17-18 if $\eta \leq \frac{1}{\rho L}$, then the following relation holds:*

$$b_{k+1}^2\eta\left[\mathbb{E}f(w_{k+1}) - f^*\right] \leq \frac{\alpha_0^2}{\rho\eta}\left[f(x_0) - f^*\right] + \frac{b_0^2}{2\rho\eta}\left\|x_0 - w^*\right\|^2 + \frac{\alpha^2\eta}{\rho}\sum_{i=0}^{k}\left[\gamma_i^2 b_{i+1}^2\right]$$

Proof.

Let $r_{k+1} = \|w_{k+1} - w^*\|$, then using equation 5

$$\begin{aligned} r_{k+1}^2 &= \|\beta_k v_k + (1-\beta_k)\zeta_k - w^* - \gamma_k\eta\nabla f(\zeta_k, z_k)\|^2 \\ r_{k+1}^2 &= \|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\left\|\nabla f(\zeta_k, z_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k, z_k)\rangle \end{aligned}$$

Taking expectation wrt to z_k,

$$\begin{aligned} \mathbb{E}[r_{k+1}^2] &= \mathbb{E}\|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\mathbb{E}\left\|\nabla f(\zeta_k, z_k)\right\|^2 + 2\gamma_k\eta\mathbb{E}[\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k, z_k)\rangle] \\ &\leq \|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &= \|\beta_k(v_k - w^*) + (1-\beta_k)(\zeta_k - w^*)\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &\leq \beta_k\|v_k - w^*\|^2 + (1-\beta_k)\|\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(By convexity of } \|\cdot\|^2\text{)} \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left\langle\frac{\beta_k(1-\alpha_k)}{\alpha_k}(w_k - \zeta_k) + w^* - \zeta_k, \nabla f(\zeta_k)\right\rangle + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(From equation 4)} \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}\langle\nabla f(\zeta_k), (w_k - \zeta_k)\rangle + \left\langle\nabla f(\zeta_k), w^* - \zeta_k\right\rangle\right] + \gamma_k^2\eta^2\sigma^2 \\ &\leq \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}(f(w_k) - f(\zeta_k)) + \langle\nabla f(\zeta_k), w^* - \zeta_k\rangle\right] + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(By convexity)} \end{aligned}$$

By strong convexity,

$$\begin{aligned} \mathbb{E}[r_{k+1}^2] &\leq \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 \\ &\quad + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}(f(w_k) - f(\zeta_k)) + f^* - f(\zeta_k) - \frac{\mu}{2}\left\|\zeta_k - w^*\right\|^2\right] + \gamma_k^2\eta^2\sigma^2 \end{aligned} \tag{16}$$

By Lipschitz continuity of the gradient,

$$\begin{aligned} f(w_{k+1}) - f(\zeta_k) &\leq \langle\nabla f(\zeta_k), w_{k+1} - \zeta_k\rangle + \frac{L}{2}\left\|w_{k+1} - \zeta_k\right\|^2 \\ &\leq -\eta\langle\nabla f(\zeta_k), \nabla f(\zeta_k, z_k)\rangle + \frac{L\eta^2}{2}\left\|\nabla f(\zeta_k, z_k)\right\|^2 \end{aligned}$$

Taking expectation wrt z_k and using equations 9, 10

$$\begin{aligned} \mathbb{E}\left[f(w_{k+1}) - f(\zeta_k)\right] &\leq -\eta\left\|\nabla f(\zeta_k)\right\|^2 + \frac{L\rho\eta^2}{2}\left\|\nabla f(\zeta_k)\right\|^2 + \frac{L\eta^2\sigma^2}{2} \\ \mathbb{E}\left[f(w_{k+1}) - f(\zeta_k)\right] &\leq \left[-\eta + \frac{L\rho\eta^2}{2}\right]\left\|\nabla f(\zeta_k)\right\|^2 + \frac{L\eta^2\sigma^2}{2} \end{aligned}$$

If $\eta \leq \frac{1}{\rho L}$,

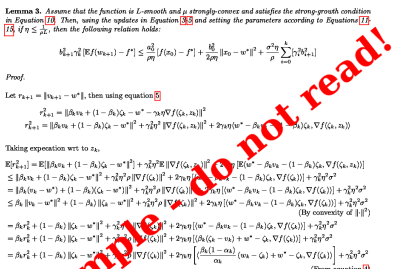
$$\begin{aligned} \mathbb{E}\left[f(w_{k+1}) - f(\zeta_k)\right] &\leq \left(\frac{-\eta}{2}\right)\left\|\nabla f(\zeta_k)\right\|^2 + \frac{L\eta^2\sigma^2}{2} \\ \implies \left\|\nabla f(\zeta_k)\right\|^2 &\leq \left(\frac{2}{\eta}\right)\mathbb{E}[f(\zeta_k) - f(w_{k+1})] + L\eta\sigma^2 \end{aligned} \tag{17}$$

From equations 16 and 17

$$\begin{aligned} \mathbb{E}[r_{k+1}^2] &\leq \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + 2\gamma_k^2\rho\eta\mathbb{E}[f(\zeta_k) - f(w_{k+1})] \\ &\quad + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}(f(w_k) - f(\zeta_k)) + f^* - f(\zeta_k) - \frac{\mu}{2}\left\|\zeta_k - w^*\right\|^2\right] + \gamma_k^2\eta^2\sigma^2 + L\gamma_k^2\eta^2\sigma^2 \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + 2\gamma_k^2\eta\rho\mathbb{E}[f(\zeta_k) - f(w_{k+1})] \\ &\quad + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}(f(w_k) - f(\zeta_k)) + f^* - f(\zeta_k) - \frac{\mu}{2}\left\|\zeta_k - w^*\right\|^2\right] + 2\gamma_k^2\eta^2\sigma^2 \qquad \text{(Since } \eta \leq \tfrac{1}{\rho L}\text{)} \\ &= \beta_k r_k^2 + \left\|\zeta_k - w^*\right\|^2(1-\beta_k) - \gamma_k\mu\eta\right] + f(\zeta_k)\left[2\gamma_k^2\rho - 2\gamma_k\eta\cdot\frac{\beta_k(1-\alpha_k)}{\alpha_k} - 2\gamma_k\eta\right] \\ &\quad - 2\gamma_k^2\eta\mathbb{E}f(w_{k+1}) + 2\gamma_k\eta f^* + \left[2\gamma_k\eta\cdot\frac{\beta_k(1-\alpha_k)}{\alpha_k}\right]f(w_k) + 2\gamma_k^2\eta^2\sigma^2 \end{aligned}$$

Example - do not read!

Legitimate questions about performance analyses?



Lemma 3. *Assume that the function is L-smooth and μ strongly-convex and satisfies the strong-growth condition in Equation 10. Then, using the updates in Equation 3-5 and setting the parameters according to Equations 15-16 if $\eta \leq \frac{1}{\rho L}$, then the following relation holds:*

$$b_{k+1}^2 \eta \mathbb{E}\left[f(w_{k+1}) - f^*\right] \leq \frac{a_k^2}{\rho\eta}\left[f(x_0) - f^*\right] + \frac{b_0^2}{2\rho\eta}\left\|v_0 - w^*\right\|^2 + \frac{\alpha^2\eta}{\rho}\sum_{i=0}^{k}\left[\gamma_i^2 b_{i+1}^2\right]$$

Proof.

Let $r_{k+1} = \|w_{k+1} - w^*\|$, then using equation 5

$$\begin{aligned} r_{k+1}^2 &= \|\beta_k v_k + (1-\beta_k)\zeta_k - w^* - \gamma_k \eta \nabla f(\zeta_k, z_k)\|^2 \\ r_{k+1}^2 &= \|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\left\|\nabla f(\zeta_k, z_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k, z_k)\rangle \end{aligned}$$

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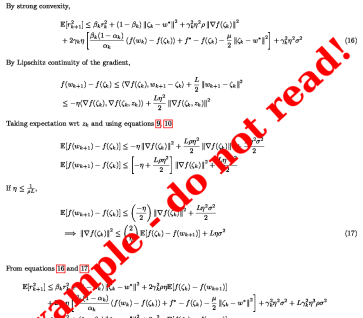
$$\begin{aligned} \mathbb{E}[r_{k+1}^2] &= \mathbb{E}\left[\|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2\right] + \gamma_k^2\eta^2\mathbb{E}\left\|\nabla f(\zeta_k, z_k)\right\|^2 + 2\gamma_k\eta\mathbb{E}[\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k, z_k)\rangle] \\ &\leq \|\beta_k v_k + (1-\beta_k)\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &= \|\beta_k(v_k - w^*) + (1-\beta_k)(\zeta_k - w^*)\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &\leq \beta_k\|v_k - w^*\|^2 + (1-\beta_k)\|\zeta_k - w^*\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(By convexity of } \|\cdot\|^2\text{)} \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\langle w^* - \beta_k v_k - (1-\beta_k)\zeta_k, \nabla f(\zeta_k)\rangle + \gamma_k^2\eta^2\sigma^2 \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}\langle w_k - \zeta_k\rangle + \langle w^* - \zeta_k, \nabla f(\zeta_k)\rangle\right] + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(From equation 4)} \\ &= \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}\langle\nabla f(\zeta_k), (w_k - \zeta_k)\rangle + \langle\nabla f(\zeta_k), w^* - \zeta_k\rangle\right] + \gamma_k^2\eta^2\sigma^2 \\ &\leq \beta_k r_k^2 + (1-\beta_k)\left\|\zeta_k - w^*\right\|^2 + \gamma_k^2\eta^2\rho\left\|\nabla f(\zeta_k)\right\|^2 + 2\gamma_k\eta\left[\frac{\beta_k(1-\alpha_k)}{\alpha_k}(f(w_k) - f(\zeta_k)) + \langle\nabla f(\zeta_k), w^* - \zeta_k\rangle\right] + \gamma_k^2\eta^2\sigma^2 \\ &\qquad \text{(By convexity)} \end{aligned}$$



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- ⚠ Error-prone
- ⚠ Technical, lack global insights.
- ⚠ Few proof patterns.

- ? Easily fixable?
- ? Simple to adapt to variations of target inequality?
- ? Simple to adapt to algorithmic variations?

Convergence rate of a gradient step

Convergence rate of a gradient step

Toy example: What is the smallest τ such that:

$$\|x_1 - x_\star\|^2 \leqslant \tau \|x_0 - x_\star\|^2,$$

for all

- $d \in \mathbb{N}$, L-smooth and μ-strongly convex function f (notation $f \in \mathcal{F}_{\mu,L}$),
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Computing τ?[1]

[1] Original idea from [Drori and Teboulle, 2014]. Developments here from [T, Hendrickx, Glineur, 2017].

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

Functional class

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Variables: f, x_0, x_1, $x_\star$.

Parameters: μ, L, α.

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Sampled version

Sampled version

◇ Performance estimation problem :

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

Sampled version

◇ Performance estimation problem **(Variables:** f**,** x_0**,** x_1**,** $x_\star$**)**:

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Smooth strongly convex interpolation (or extension)

Let I index set, and associated $\{(x_i, g_i, f_i)\}_{i \in I}$: points x_i, (sub)gradients g_i and function values f_i.

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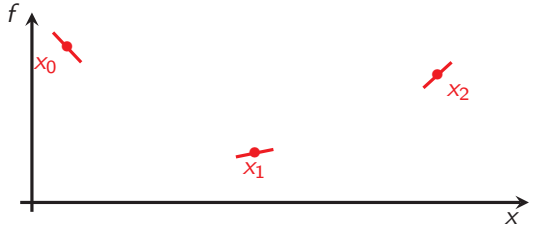

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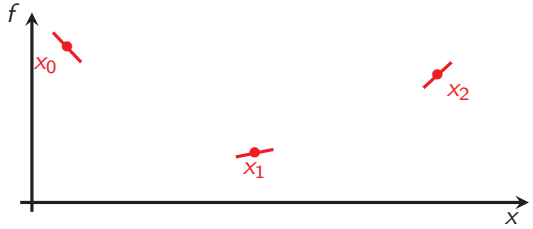

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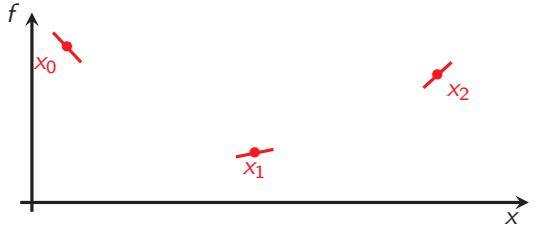

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- Simpler example: pick $\mu = 0$ and $L = \infty$ (just convexity):

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◇ Same optimal value (no relaxation): non-convex quadratic problem.

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

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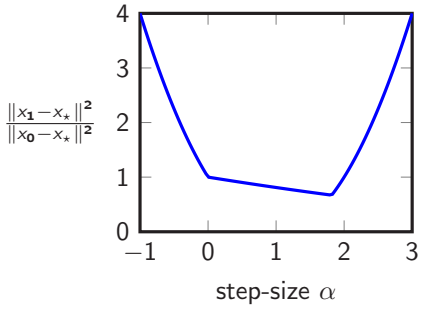

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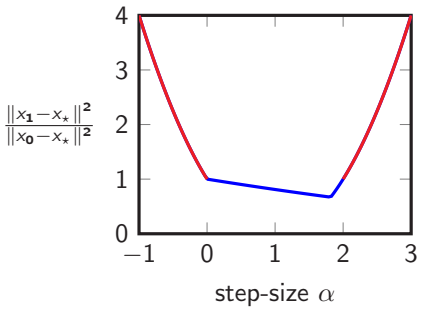

Observations:

- ◇ numerics match the known $\max\{(1-\alpha L)^2, (1-\alpha\mu)^2\}$
- ◇ recovers that gradient descent converges for $\alpha \in (0, 2/L)$ (divergence otherwise).

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- Dual problem is

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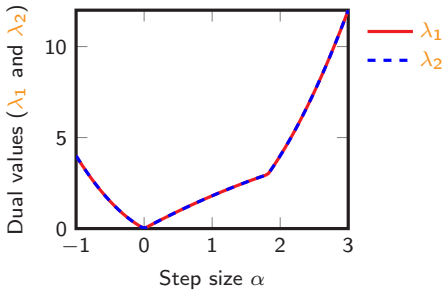

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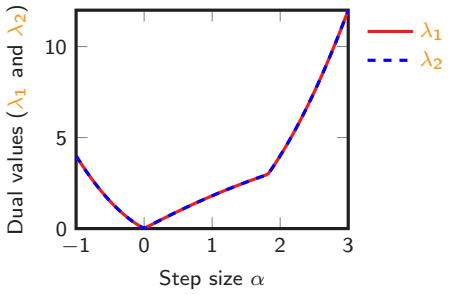

Numerics match $\lambda_1 = \lambda_2 = 2|\alpha|\rho(\alpha)$ with $\rho(\alpha) = \max\{\alpha L - 1, 1 - \alpha\mu\}$.

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- ◇ Feasible points to primal SDP correspond to lower bounds on $\tau(\mu, L, \alpha)$.
- ◇ Feasible points to dual SDP correspond to upper bounds on $\tau(\mu, L, \alpha)$.
  - proof via linear combinations of interpolation inequalities (evaluated at $\{x_k\}_k$ and $x_\star$),
  - proofs can be rewritten as a "sum-of-squares" certificates (sum of squared norms).

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(but other cases are not doomed).

Insight into proof structures?

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Then, proofs of the fact "Perf $\leqslant \tau$Init" can be framed as: $\exists (\lambda_i)_i$, $\lambda_i \geqslant 0$, and $S \succcurlyeq 0$

$$0 \geqslant \sum_i \lambda_i \left(\mathrm{Tr}(G A_i) + b_i^T F \right) = \text{Perf} - \tau \text{Init} + \mathrm{Tr}(GS).$$

Back to legitimate questions

Legitimate questions (gradient descent, one iteration):

- ◇ anything improvable? Realistic analyses?
- ◇ How to choose the right inequalities to combine?
- ◇ Why studying this specific quantity? Possible to adapt to other quantities?
- ◇ Unique way to arrive to the desired result?
- ◇ How likely are we to find such proofs in more complicated cases?

Software: PEPit/PESTO

PEPit

Search docs

CONTENTS:

- Welcome to PEPit's documentation!
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PEPit: Performance Estimation in Python

Tests passing | codecov 89% | docs passing | pypi package 0.3.2 | downloads 29k | 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).
```

Examples: gradient methods and momentum

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What can we guarantee on...

$$\frac{f(x_n) - f(x_\star)}{\|x_0 - x_\star\|^2} \leqslant ? \qquad \frac{\|\nabla f(x_n)\|^2}{\|x_0 - x_\star\|^2} \leqslant ? \qquad \frac{\min\limits_{0 \leqslant k \leqslant n} \|\nabla f(x_k)\|^2}{\|x_0 - x_\star\|^2} \leqslant ?$$

Example: a primal-dual proximal point

Minimize sum of two convex (ccp) functions

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

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Primal-dual proximal point algorithm (see, e.g., [Rockafellar, 1976])

Input: f, h convex (ccp) functions, $(y_0, x_0) \in \mathbb{R}^d \times \mathbb{R}^d$.

For $k = 0, 1, \ldots$

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What guarantees of type (for some elements of ∂f and ∂h^*)

$$\frac{\|\partial f(x_n) + y_n\|^2 + \|x_n - \partial h^*(y_n)\|^2}{\|x_0 - x_\star\|^2 + \|y_0 - y_\star\|^2} \leqslant \tau(n, \alpha)?$$

Recap'

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- ☺ Worst-case guarantees *cannot be improved*, systematic approach,
- ☺ allows reaching analyses that could barely be obtained by hand,
- ☺ fair amount of scenarios/algorithms (e.g., proximal terms, stochastic, etc.),
- ☹ SDPs typically become prohibitively large in a variety of scenarios,
- ☹ transient behavior VS. asymptotic behavior: might be hard to distinguish with small N,
- ☹ proofs (may be) quite involved and hard to intuit,
- ☹ proofs (may be) hard to generalize.

A few research directions

Directions & difficulties to go further?

- ◇ characterization of problem classes (interpolation),
  (account for problem structures)
- ◇ structured proofs,
- ◇ algorithm design,
- ◇ symbolic solves & formalization,
- ◇ packages for ease of use.

Constructive approach to performance analysis

Structured analyses

Towards optimal algorithms

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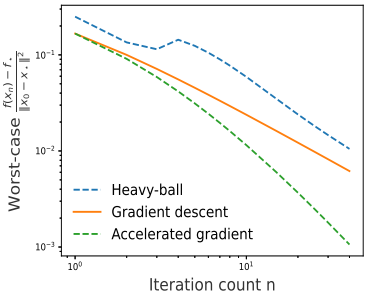

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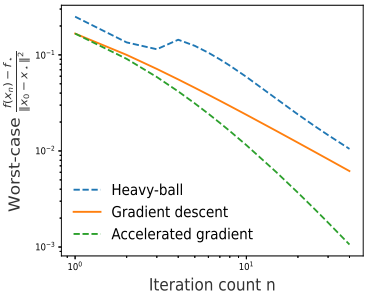

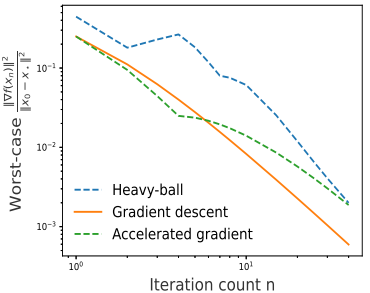

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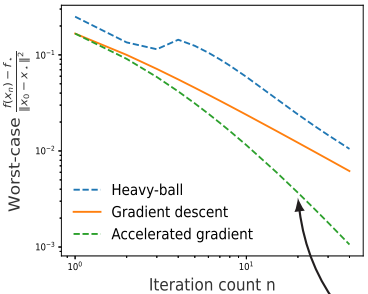

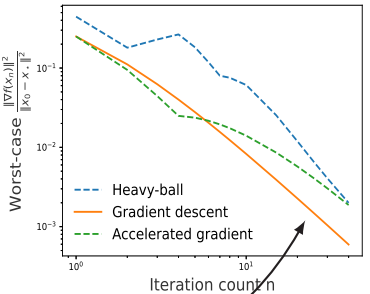

What to expect for larger n?

Structured proofs

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Question: what *a priori* convergence rate?

Examples: we have seen $\frac{\|x_1 - x_\star\|^2}{\|x_0 - x_\star\|^2}$, what about $\frac{\|\nabla f(x_1)\|^2}{\|\nabla f(x_0)\|^2}$, $\frac{f(x_1) - f_\star}{f(x_0) - f_\star}$?

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- ◇ Any of the above is fine: $\frac{\|x_1-x_\star\|^2}{\|x_0-x_\star\|^2}$, $\frac{\|\nabla f(x_1)\|^2}{\|\nabla f(x_0)\|^2}$, $\frac{f(x_1)-f_\star}{f(x_0)-f_\star}$ $\rightarrow$ we could pick the *best*.
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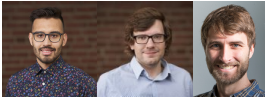
- ◇ What about optimizing over it?

$$\min_{\substack{a,b\geqslant 0\\ a+b=1}} \max_{\substack{f\in\mathcal{F}_{\mu,L}\\ x_0,x_1,x_\star}} \left\{ \frac{a\|x_1-x_\star\|^2+b\|\nabla f(x_1)\|^2}{a\|x_0-x_\star\|^2+b\|\nabla f(x_0)\|^2} : \; x_1 = x_0 - \alpha\nabla f(x_0) \right\}.$$

- ◇ ... yet, one can be smarter (ask Pontus & Manu)



Cycles

Heavy-ball

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Look for non-trivial cycles of length $K \in \mathbb{N}$ by solving:

$$\min_{\substack{f \\ x_0, \ldots, x_{K+1}}} \quad \|x_K - x_0\|^2 + \|x_{K+1} - x_1\|^2$$

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From same steps as before $\rightarrow$ SDP formulation $\rightarrow$ LP (via convexity and symmetries).

Heavy-ball method: Lyapunov vs. cycles

Heavy-ball: $x_{k+1} = x_k - \alpha \nabla f(x_k) + \beta(x_k - x_{k-1})$. Choices of (α, β) for convergence?[2,3,4]

[2] Classical region from [Ghadimi, Feyzmahdavian, Johansson, '15]

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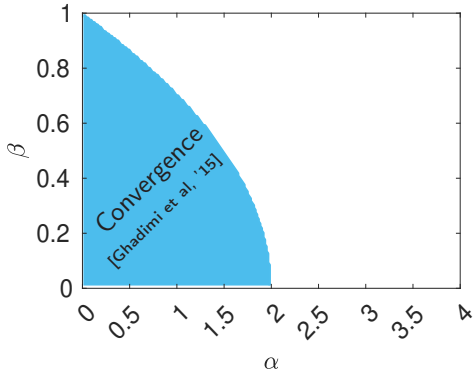

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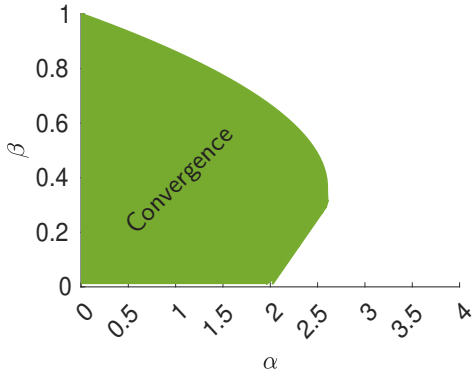

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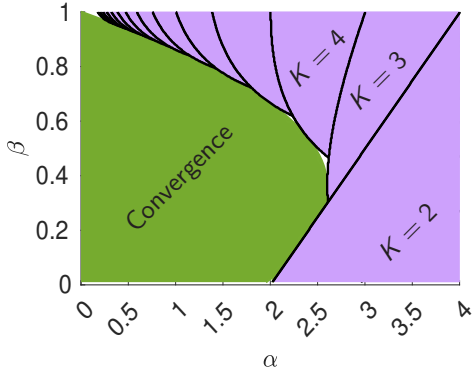

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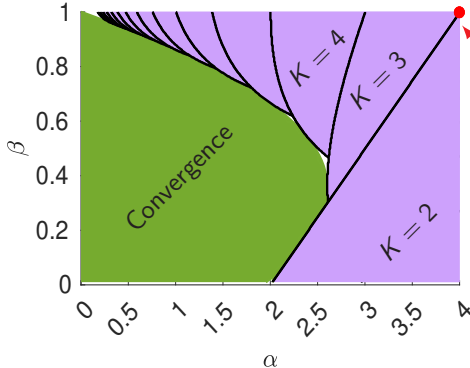

"Optimal tuning" for quadratic optimization[8]

(numerics for $L/\mu = 10^7$)

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Constructive approach to performance analysis

Structured analyses

Towards optimal algorithms

Concluding remarks

Designing algorithms

A "generic" first-order method

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w_1 &= w_0 - \alpha_{1,0}\nabla f(w_0) \\
w_2 &= w_1 - \alpha_{2,0}\nabla f(w_0) - \alpha_{2,1}\nabla f(w_1) \\
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\tag{FOM}
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for some coefficients $\{\alpha_{i,j}\}$. Generic **non-adaptive** first-order method.

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

- ◇ pick a performance criterion, for instance $\frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2}$,
- ◇ solve the minimax (minimize worst-case): $\min_{\{\alpha_{i,j}\}_{i,j}} \max_{f\in\mathcal{F},\{w_i\}} \frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2}$.

Traditional design

Algorithm design (with guarantees):

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- ◇ unconstrained quadratic programming:

  first-order methods $\Leftrightarrow$ polynomials $\rightarrow$ optimal algorithms via optimal polynomials.[5,6,7]

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- ◇ Beyond quadratics: traditionally more "hand-crafted"
  - – Analogy with conjugate gradients.[8,9]
  - – Lyapunov function-type analyses.[10,11]

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[8] Nemirovski (1982). "Orth-method for smooth convex optimization."

[9] Narkiss and Zibulevsky (2005). "Sequential subspace optimization method for large-scale unconstrained problems."

[10] Nesterov (1983). "A method for solving the convex programming problem with convergence rate $O(1/k^2)$."

[11] Beck and Teboulle ('09). "A fast iterative shrinkage-thresholding algorithm for linear inverse problems."

Design problem

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

$$\min_{\{\alpha_{i,j}\}} \max_{f \in \mathcal{F}} \frac{\|w_n - w_\star\|^2}{\|w_0 - w_\star\|^2} ?$$

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- ◇ brutal approaches.

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Fixed stepsize policy from WC analysis of linesearch?

Target convergence rate (example):

$$\rho \overset{\text{(def)}}{=} \max_{w_0, w_1, f \in \mathcal{F}_{\mu,\mathrm{L}}} \frac{f(w_1) - f_\star}{f(w_0) - f_\star} \text{ s.t. } \langle \nabla f(w_1), \nabla f(w_0) \rangle = 0, \ \langle \nabla f(w_1), w_1 - w_0 \rangle = 0,$$

upper bound from a Lagrangian relaxation with $\lambda_1, \lambda_2 \in \mathbb{R}$:

$$\rho \leqslant \bar{\rho}(\lambda_1, \lambda_2) \overset{\text{(def)}}{=} \max_{x_0, x_1, f \in \mathcal{F}_{\mu,\mathrm{L}}} \left\{ \frac{f(w_1) - f_\star}{f(w_0) - f_\star} + \lambda_1 \langle \nabla f(w_1), \nabla f(w_0) \rangle + \lambda_2 \langle \nabla f(w_1), w_1 - w_0 \rangle \right\}.$$

We can also create an intermediary problem

$$\rho \leqslant \max_{w_0, w_1, f \in \mathcal{F}_{\mu,\mathrm{L}}} \left\{ \frac{f(w_1) - f_\star}{f(w_0) - f_\star} \text{ s.t. } \lambda_1 \langle \nabla f(w_1), \nabla f(w_0) \rangle + \lambda_2 \langle \nabla f(w_1), w_1 - w_0 \rangle = 0 \right\} \leqslant \bar{\rho}(\lambda_1, \lambda_2).$$

So, for any pair $\lambda_1, \lambda_2 \in \mathbb{R}$ we get:

- an upper bound $\bar{\rho}(\lambda_1, \lambda_2)$ (possibly $+\infty$) on ρ,
- all methods satisfying $\langle \nabla f(w_1), \lambda_1 \nabla f(w_0) + \lambda_2 (w_1 - w_0) \rangle = 0$ have convergence rate at most $\bar{\rho}(\lambda_1, \lambda_2)$.

Bonus: there exists a choice $\lambda_1^\star, \lambda_2^\star$ such that

$$\rho = \bar{\rho}(\lambda_1^\star, \lambda_2^\star).$$

Design procedure

Algorithm constraints, and associated Lagrange multipliers:

$$\langle \nabla f(w_i), \nabla f(w_j) \rangle = 0, \qquad \text{for all } 0 \leqslant j < i = 1, \dots n \qquad : \beta_{i,j},$$
$$\langle \nabla f(w_i), w_j - w_0 \rangle = 0, \qquad \text{for all } 1 \leqslant j \leqslant i = 1, \dots n \qquad : \gamma_{i,j}.$$

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... replaced by:

$$\langle \nabla f(w_i), \sum_{j=1}^{i} \beta_{i,j}(w_j - w_0) + \sum_{j=0}^{i-1} \gamma_{i,j} \nabla f(w_j) \rangle = 0 \text{ for all } i = 1, \dots, n$$

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1. Choose $n \geqslant 0$, $\mathcal{F}$.

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Subspace-search elimination (abstract)

1. Choose $n \geqslant 0$, $\mathcal{F}$.
2. Find a feasible solution $\{\beta_{i,j}\}, \{\gamma_{i,j}\}$ to (dual) PEP for the greedy method with rate $\bar{\rho}$.
3. Any method satisfying

$$\langle \nabla f(w_i), \sum_{j=1}^{i} \beta_{i,j}(w_j - w_0) + \sum_{j=0}^{i-1} \gamma_{i,j} \nabla f(w_j) \rangle = 0 \text{ for all } i = 1, \dots n$$

benefits from the same worst-case convergence rate $\bar{\rho}$.

Optimized gradient methods

Smooth convex minimization setting:

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

with f being L-smooth and convex.

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Lower bound for large-scale setting ($d \geqslant n+2$) by Drori ('17):

$$f(x_n) - f(x_\star) \geqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2},$$

with $\theta_0 = 1$, and:

$$\theta_{i+1} = \begin{cases} \frac{1+\sqrt{4\theta_i^2+1}}{2} & \text{if } i \leqslant n-2, \\ \frac{1+\sqrt{8\theta_i^2+1}}{2} & \text{if } i = n-1. \end{cases}$$

Greedy First-order Method (GFOM)

Inputs: f, x_0, n.

For $i = 1, 2, \ldots, n$

$$x_i = \operatorname*{argmin}_{x \in \mathbb{R}^d} \{f(x) : \; x \in x_0 + \operatorname{span}\{\nabla f(x_0), \ldots, \nabla f(x_{i-1})\}\}.$$

Worst-case guarantee:

$$f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}.$$

Optimized gradient methods

As a result from subspace-search elimination, all methods satisfying (for $i = 1, \dots, n$)

$$\langle \nabla f(x_i); x_i - \left[\left(1 - \frac{1}{\theta_i}\right) \left(x_{i-1} - \tfrac{1}{L} \nabla f(x_{i-1})\right) + \frac{1}{\theta_i} \left(x_0 - \tfrac{2}{L} \sum_{j=0}^{i-1} \theta_j \nabla f(x_j) \right) \right] \rangle \leqslant 0$$

benefit from the same guarantee:

$$f(x_n) - f(x_\star) \leqslant \frac{L \|x_0 - x_\star\|^2}{2\theta_n^2},$$

Optimized gradient methods

Three methods with the same (optimal) worst-case behavior

Optimized gradient method with exact line-search

Inputs: f, x_0, n.

For $i = 1, \dots, n$

$$y_i = \left(1 - \frac{1}{\theta_i}\right) x_{i-1} + \frac{1}{\theta_i} x_0$$

$$d_i = \left(1 - \frac{1}{\theta_i}\right) \nabla f(x_{i-1}) + \frac{1}{\theta_i} \left(2 \sum_{j=0}^{i-1} \theta_j \nabla f(x_j)\right)$$

$$\alpha = \operatorname*{argmin}_{\alpha \in \mathbb{R}} f(y_i + \alpha d_i)$$

$$x_i = y_i + \alpha d_i$$

Worst-case guarantee: $f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}$

Optimized gradient methods

Three methods with the same (optimal) worst-case behavior

Optimized gradient method

Inputs: f, x_0, n.

For $i = 1, \dots, n$

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

$$z_i = x_0 - \frac{2}{L}\sum_{j=0}^{i-1} \theta_j \nabla f(x_j)$$

$$x_i = \left(1 - \frac{1}{\theta_i}\right) y_i + \frac{1}{\theta_i} z_i$$

Worst-case guarantee: $f(x_n) - f(x_\star) \leqslant \frac{L\|x_0 - x_\star\|^2}{2\theta_n^2}$.

Constructive approach to performance analysis

Structured analyses

Towards optimal algorithms

Concluding remarks

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Performance estimation's philosophy

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- ◇ numerically allows obtaining tight bounds (rigorous baselines),
  - – fast prototyping
  - – worth checking before trying to prove a method works.

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- ◇ numerically allows obtaining tight bounds (rigorous baselines),
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- ◇ algebraic insights into performance analyses: principled approach,
  - – analyses are dual feasible points,
  - – analyses are linear combinations of certain specific inequalities.

Concluding remarks

Performance estimation's philosophy

- ◇ numerically allows obtaining tight bounds (rigorous baselines),
  - – fast prototyping
  - – worth checking before trying to prove a method works.
- ◇ algebraic insights into performance analyses: principled approach,
  - – analyses are dual feasible points,
  - – analyses are linear combinations of certain specific inequalities.

Byproducts:

- ◇ computer-assisted design of analyses,
- ◇ computer-assisted design of numerical methods,
- ◇ step towards reproducible theory
  - – validation & benchmark tool for proofs (also for reviews ☺),
  - – complements existing open-source initiatives.

A few instructive examples

Worst-case analysis for fixed-point iterations:

- ◇ Lieder ('21). "On the convergence of the Halpern-iteration."

Analysis of the proximal-point algorithm for monotone inclusions:

- ◇ Gu, Yang ('19). "Optimal nonergodic sublinear convergence rate of the proximal point algorithm for maximal monotone inclusion problems."

Application to nonconvex optimization:

- ◇ Abbaszadehpeivasti, de Klerk, Zamani ('22). "The exact worst-case convergence rate of the gradient method with fixed step lengths for L-smooth functions."
- ◇ Rotaru, Glineur, Patrinos ('25). "Exact worst-case convergence rates of gradient descent: a complete analysis for all constant stepsizes over nonconvex and convex functions."

Applications to distributed optimization:

- ◇ Sundararajan, Van Scoy, Lessard ('20). "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

Design first-order methods via PEPs:

- Drori, Teboulle ('14). "Performance of first-order methods for smooth convex minimization: a novel approach."
- Kim, Fessler ('16). "Optimized methods for smooth convex optimization."
- Van Scoy, Freeman, Lynch ('17). "The fastest known globally convergent first-order method for minimizing strongly convex functions."
- Kim, Fessler ('21). "Optimizing the efficiency of first-order methods for decreasing the gradient of smooth convex functions." .
- Altschuler, Parrilo ('23). "Acceleration by Stepsize Hedging I: Multi-Step Descent and the Silver Stepsize Schedule."
- Jang, Das Gupta, Ryu ('25). "Computer-assisted design of accelerated composite optimization methods: OptISTA."

Generic approaches:

- Das Gupta, Van Parys, Ryu ('24). "Branch-and-bound performance estimation programming: A unified methodology for constructing optimal optimization methods."
- Kamri, Hendrickx, Glineur ('25). "Numerical Design of Optimized First-Order Algorithms."

A few references

Historical reference:

- Drori, Teboulle ('14). "Performance of first-order methods for smooth convex minimization: a novel approach."

Main messages:

- T, Hendrickx, Glineur ('17). "Smooth strongly convex interpolation and exact worst-case performance of first-order methods."

- Drori, T ('20). "Efficient first-order methods for convex minimization: a constructive approach."

- Goujaud, Dieuleveut, T ('23). "On fundamental proof structures in first-order optimization."

- Goujaud, Moucer, Glineur, Hendrickx, T, Dieuleveut ('24). "PEPit: computer-assisted worst-case analyses of first-order optimization methods in Python."

- Goujaud, T, Dieuleveut ('25). "Provable non-accelerations of the heavy-ball method."

- Upadhyaya, Banert, T, Giselsson ('25). "Automated tight Lyapunov analysis for first-order methods."

Going further — shameless advertisement

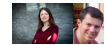
- T, Bach ('19). "Stochastic first-order methods: non-asymptotic and computer-aided analyses via potential functions."

- Dragomir, T, d'Aspremont, Bolte ('22). "Optimal complexity and certification of Bregman first-order methods."

- T, Drori ('23). "An optimal gradient method for smooth strongly convex minimization."

- Berg Thomsen, T, Dieuleveut ('25). "Tight analyses of first-order methods with error feedback."

- Rubbens, Hendrickx, T ('25). "A constructive approach to strengthen algebraic descriptions of function and operator classes."



- Weibel, Gaillard, Koolen, T ('26). "Optimised projection-free algorithms for online learning: construction and worst-case analysis."

Thanks! Questions?

Great PhD students/visiting PhD students/postdocs at Inria Paris:

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Daniel Berg Thomsen

Weijia Wang

Si-Yi Meng

Manu Upadhyaya

Fabian Schaipp

Julien Weibel