Computer-aided analyses of optimization methods via potential functions

Adrien Taylor

CWI-Inria workshop - September 2020

4TUNE

Adaptive, Efficient, Provable and Flexible Tuning for Machine Learning

Joint research team between CWI and Inria.

Team

4TUNE includes 2 research scientists from the Centrum Wiskunde & Informatica (CWI) and 3 researchers from the Sierra project-team of Inria.

CWI researchers


Peter Grünwald


Wouter M. Koolen

INRIA, Sierra project-team researchers


Francis Bach


Pierre Gaillard


Adrien Taylor

Newborn
in the CWI-Inria lab!

Long-term goal: push adaptive machine learning to the next level.

We aim to develop refined methods, going beyond traditional worst-case analysis, for exploiting structure in the learning problem at hand [...]

Francis Bach

“Stochastic first-order methods: non-asymptotic and computer-aided analyses via potential functions” (COLT 2019).

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Focus on *simple* proofs, relying on (quadratic) *potential functions*

(Nesterov 1983), (Beck & Teboulle 2009), (Wilson, Recht & Jordan 2016), (Hu & Lessard 2017), (Bansal & Gupta 2019), and many others.

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Examples: what about $f(x_N) - f(x_\star)$, $\|f'(x_N)\|$, $\|x_N - x_\star\|$?

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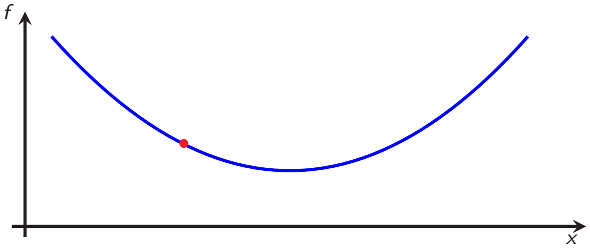

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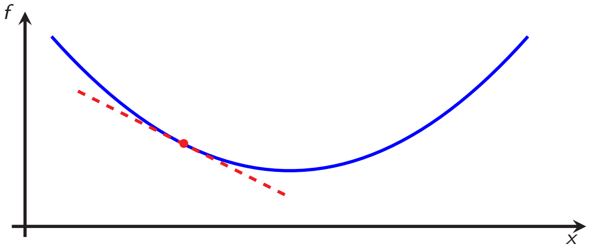

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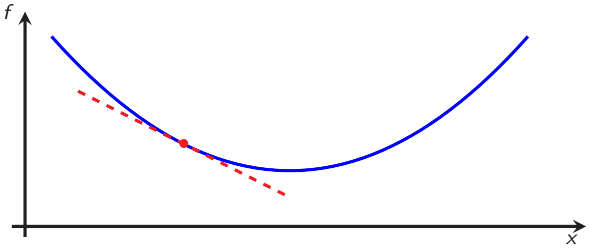

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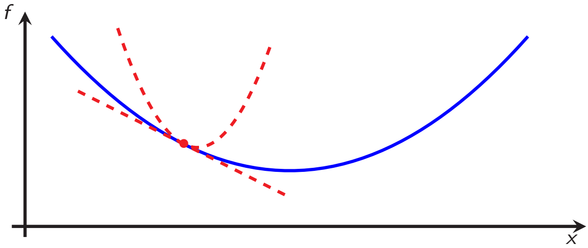

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$$\phi^f_k = k(f(x_k) - f_\star) + \frac{L}{2}\|x_k - x_\star\|^2 \textit{ (potential at iteration } k\textit{)},$$

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

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Starting point: candidate quadratic ϕ_k^f with *all the available information* at iteration k

$$\phi_k^f = a_k \|x_k - x_\star\|^2 + b_k \left\|f'(x_k)\right\|^2 + 2c_k \langle f'(x_k), x_k - x_\star\rangle + d_k \left(f(x_k) - f_\star\right).$$

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How to choose a_k, b_k, c_k, d_k's?

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2. choice should result in bound on $\|f'(x_N)\|^2$.

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In others words: *efficient (convex) representation of $\mathcal{V}_k$ available*!

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4. Prove target result by analytically playing with $\mathcal{V}_k$ (i.e., study single iteration).

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Numerically (live if time allows)

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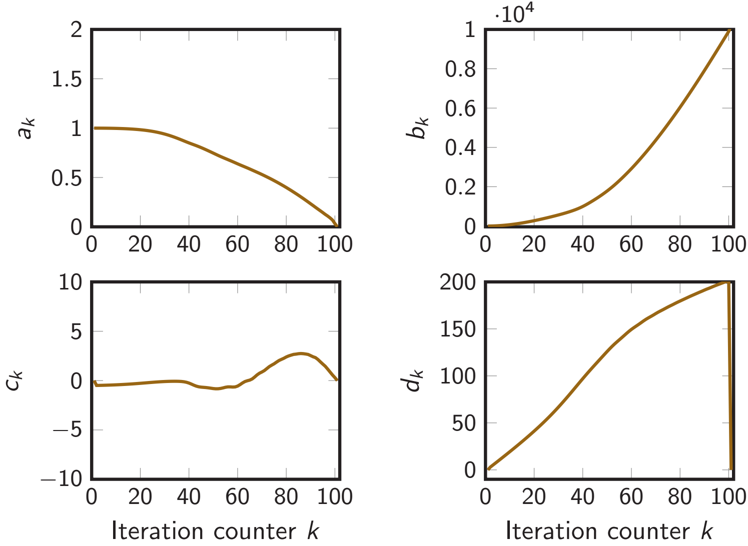

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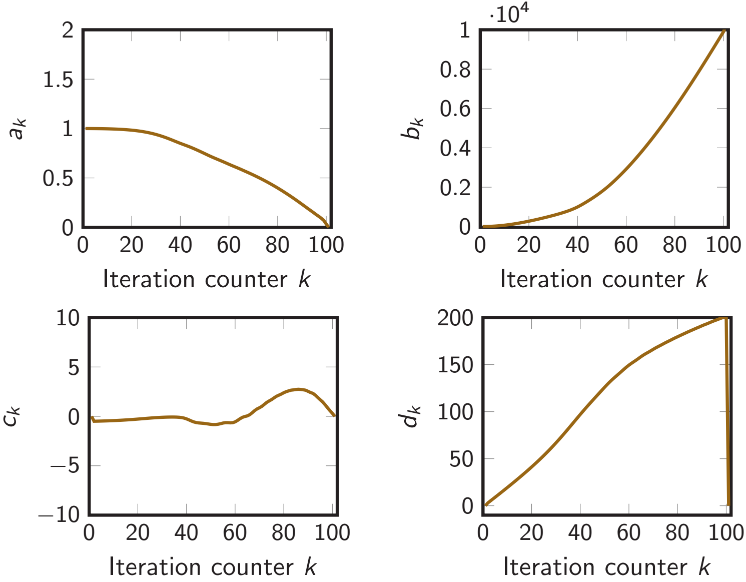

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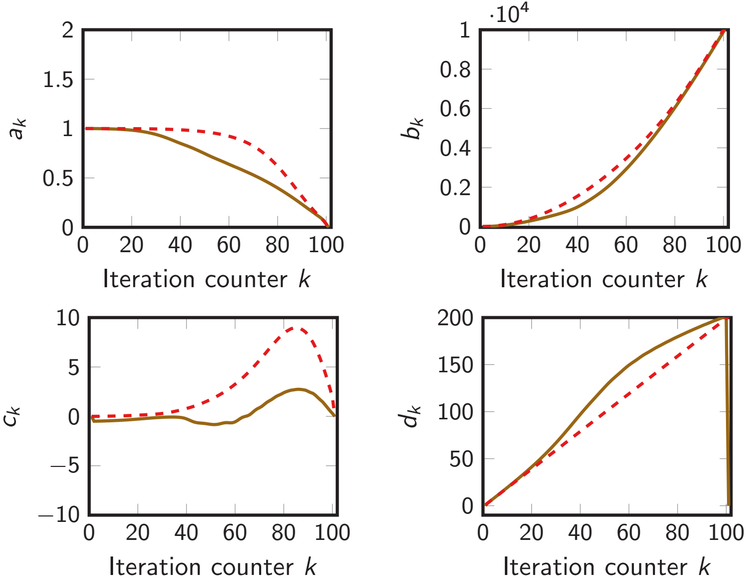

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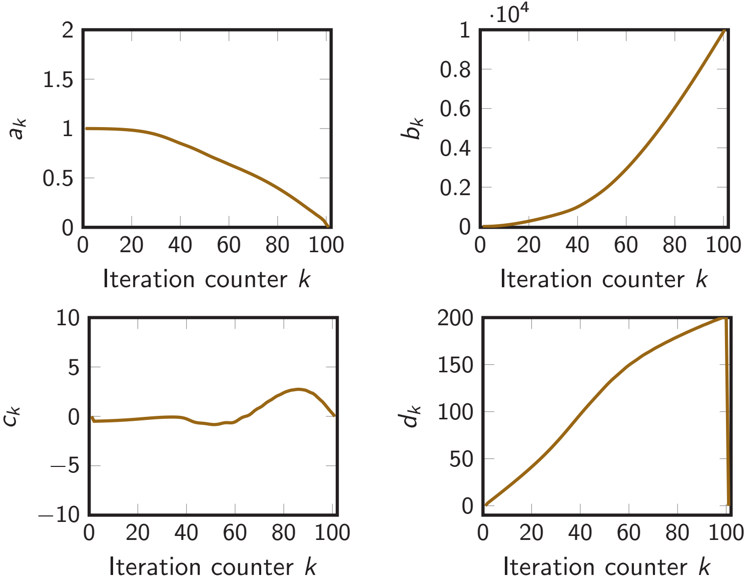

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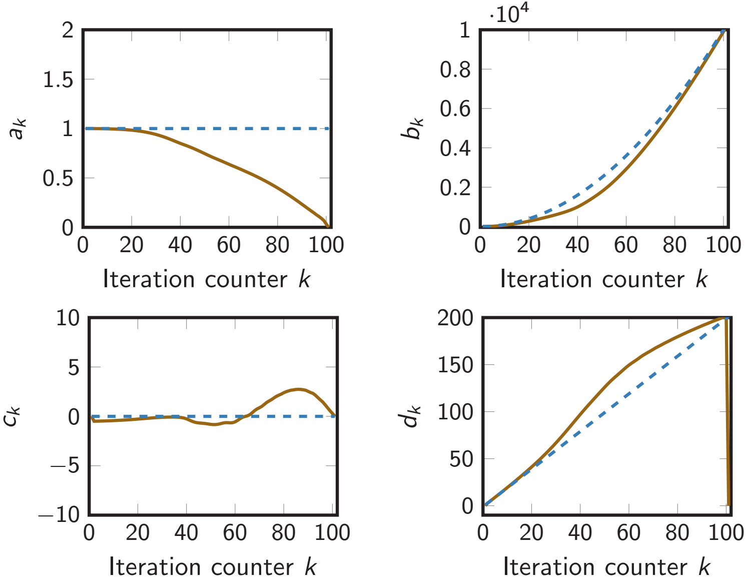

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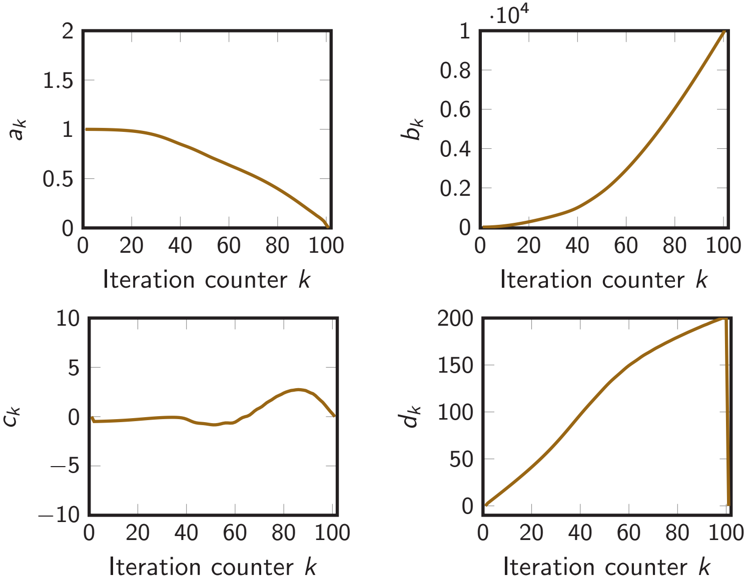

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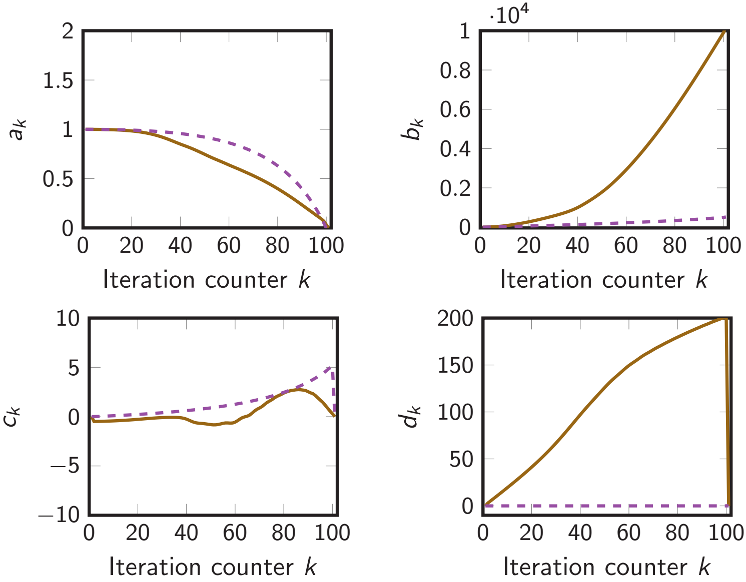

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4. Prove target result by analytically playing with $\mathcal{V}_k$:

$$\phi_k^f(x_k) = (2k+1)L(f(x_k) - f_\star) + k(k+2)\left\|f'(x_k)\right\|^2 + L^2\|x_k - x_\star\|^2,$$

   hence $f(x_N) - f_\star = O(N^{-1})$ and $\|f'(x_N)\|^2 = O(N^{-2})$ using $b_N = N(N+2)$.

Remaining questions

From previous content, we should still answer

- ◇ how to obtain a suitable representation of $\mathcal{V}_k$?
- ◇ How to obtain an analytical potential, rigorously?
- ◇ Does it apply beyond gradient descent?

Toy example: gradient descent

Reformulation as a LMI

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i.e.: replace "for all" by maximization (later formulated as a *semidefinite program*).

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$$0 \geq \max_{x_\star, x_k, g_k, f_\star, f_k} a_{k+1} \|x_k - \gamma_k g_k - x_\star\|^2 - a_k \|x_k - x_\star\|^2$$

$$\text{subject to } \exists f \text{ convex and } L\text{-smooth} : \begin{cases} g_k = f'(x_k), & f_k = f(x_k) \\ 0 = f'(x_\star), & f_\star = f(x_\star). \end{cases}$$

new variables: x_k, $x_\star$, g_k, $f_\star$, f_k. How to handle the existence constraint?

Smooth convex interpolation

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

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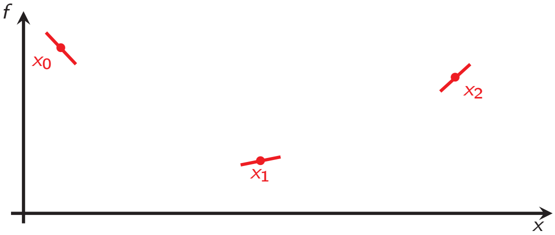

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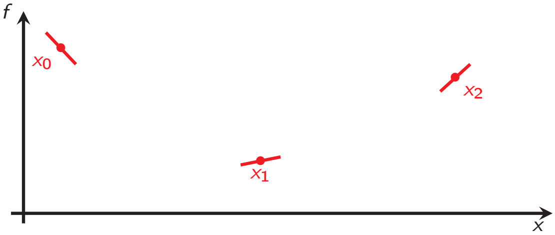

? Possible to find f convex and L-smooth such that

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

- Necessary and sufficient condition: $\forall i, j \in S$

$$f_i \geqslant f_j + \langle g_j, x_i - x_j \rangle + \frac{1}{2L}\|g_i - g_j\|^2.$$

Quadratic reformulation

From sampling, we had "$\phi_{k+1}^f \leq \phi_k^f$" (for all f and x_k) iff

$$0 \geq \max_{x_\star, x_k, g_k, f_\star, f_k} a_{k+1} \left\|x_k - \gamma_k g_k - x_\star\right\|^2 - a_k \left\|x_k - x_\star\right\|^2$$

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and we can replace the *existence constraints* by

$$\begin{aligned} f_k &\geq f_\star + \tfrac{1}{2L}\|g_k\|^2, \\ f_\star &\geq f_k + \langle g_k, x_\star - x_k\rangle + \tfrac{1}{2L}\|g_k\|^2, \end{aligned}$$

reaching a (nonconvex) quadratic problem.

Semidefinite reformulation

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which is linear in terms of

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G = \begin{bmatrix} \|x_k - x_\star\|^2 & \langle x_k - x_\star, g_k \rangle \\ \langle x_k - x_\star, g_k \rangle & \|g_k\|^2 \end{bmatrix}, \quad F = \begin{bmatrix} f_k & f_\star \end{bmatrix},
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where $G \succcurlyeq 0$ by construction.

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\begin{aligned}
0 \geq \max_{G \succcurlyeq 0,\, F} \; & a_{k+1} (G_{1,1} + \gamma_k^2 G_{2,2} - 2\gamma_k G_{1,2}) - a_k \, G_{1,1} \\
\text{subject to } \; & F_1 \geq F_2 + \tfrac{1}{2L} G_{2,2}, \\
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which is a regular *semidefinite program* (SDP).

Verifying a potential

Final step: inequality verified iff *dual SDP is feasible*, that is

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The dual problem has the form (note that no duality gap occurs):

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0 \geq \min_{\lambda_1, \lambda_2 \geq 0} & \; 0 \\
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hence *feasibility problem* equivalent to verification "$\phi_{k+1}^f \leq \phi_k^f$" (for all f and x_k).

Verifying a potential: final formulation

$$a_{k+1}\|x_{k+1}-x_\star\|^2 \leq a_k\|x_k-x_\star\|^2 \text{ with } x_{k+1}=x_k-\gamma_k f'(x_k)\text{, for all } L\text{-smooth convex } f \text{ and } x_k$$

$$\Leftrightarrow$$

$$\exists\lambda\geq 0: \quad \begin{pmatrix} a_k-a_{k+1} & \gamma_k a_{k+1}-\frac{\lambda}{2} \\ \gamma_k a_{k+1}-\frac{\lambda}{2} & \frac{\lambda}{L}-a_{k+1}\gamma_k^2 \end{pmatrix} \succcurlyeq 0.$$

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$a_{k+1}\|x_{k+1}-x_\star\|^2 \leq a_k\|x_k-x_\star\|^2$ with $x_{k+1}=x_k-\gamma_k f'(x_k)$, for all L-smooth convex f and x_k

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How to verify more complicated potential, such as

$$\phi_k^f = a_k\left\|x_k-x_\star\right\|^2 + b_k\left\|f'(x_k)\right\|^2 + 2c_k\left\langle f'(x_k), x_k-x_\star\right\rangle + d_k\left(f(x_k)-f_\star\right)?$$

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Exact *same tricks*, with some adaptations

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How to find a proof for "$\phi_{k+1}^f \leq \phi_k^f$" (for all f and x_k)?

- Exhibit a dual feasible point,
- proof only consists in combining quadratic inequalities.
- If inequality does not hold (for all f and x_k), primal solutions are counter-examples.

Toy example: gradient descent

Reformulation as a LMI

Other examples

Concluding remarks

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y_{k+1} &= (1-\tau_k)x_k + \tau_k z_k, \\
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z_{k+1} &= (1-\delta_k)y_{k+1} + \delta_k z_k - \gamma_k f'(y_{k+1}),
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with carefully chosen values of τ_k and η_k.

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Same as before: pick a family of potentials, such as

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\phi_k^f = \begin{pmatrix} x_k - x_\star \\ f'(x_k) \end{pmatrix}^\top [Q_k \otimes I_d] \begin{pmatrix} x_k - x_\star \\ f'(x_k) \end{pmatrix} + a_k \|z_k - x_\star\|^2 + d_k \left(f(x_k) - f_\star\right),
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\phi_k^f = \begin{pmatrix} x_k - x_\star \\ f'(x_k) \end{pmatrix}^\top [Q_k \otimes I_d] \begin{pmatrix} x_k - x_\star \\ f'(x_k) \end{pmatrix} + a_k \|z_k - x_\star\|^2 + d_k\,(f(x_k) - f_\star),
$$

and solve the corresponding SDP numerically:

$$
\max_{\phi_1^f,\ldots,\phi_{N-1}^f,d_N} d_N \text{ such that } (\phi_0^f,\phi_1^f) \in \mathcal{V}_0, \ldots, (\phi_{N-1}^f,\phi_N^f) \in \mathcal{V}_{N-1}.
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Accelerated/fast gradient method

Consider a fast gradient method for smooth convex minimization:

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\begin{aligned}
y_{k+1} &= (1-\tau_k)x_k + \tau_k z_k, \\
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with carefully chosen values of τ_k and η_k.

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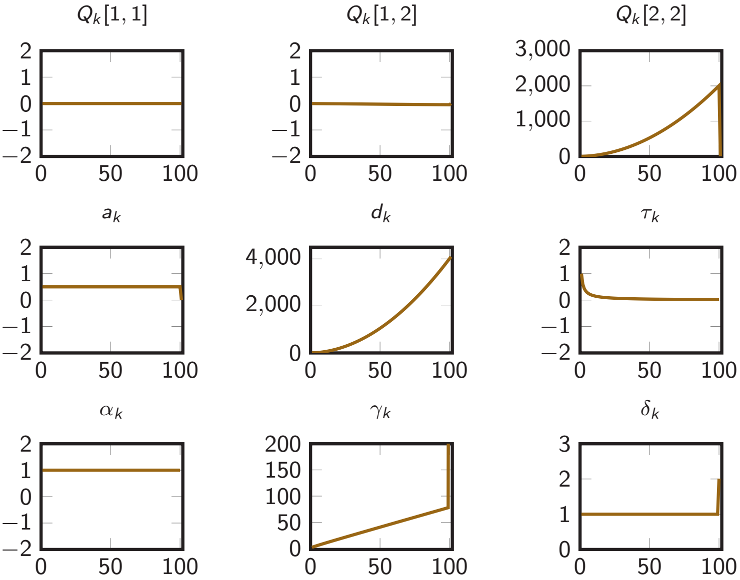
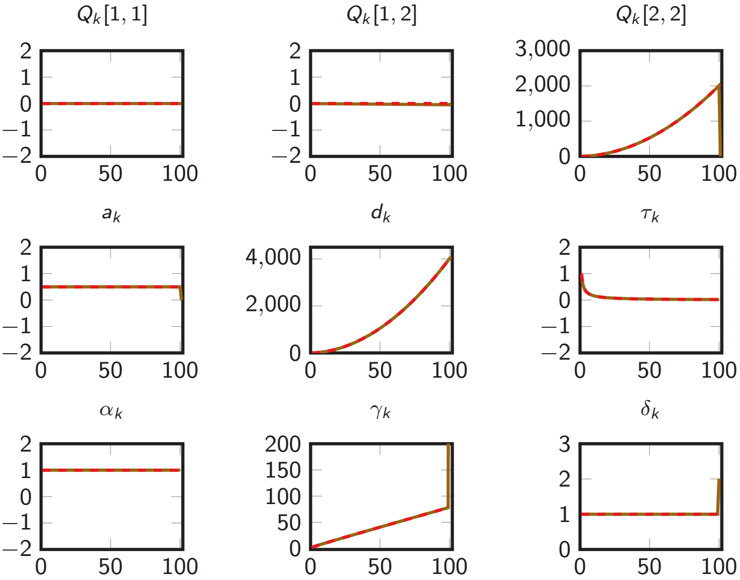
Few additional technical ingredients allow tuning method's parameters simultaneously.

Example for $N = 100$, $L = 1$: numerics (brown),



Example for $N = 100$, $L = 1$: numerics (brown), and analytical solution (red).



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with carefully chosen values of τ_k and η_k.

Recovers standard potential (see e.g.,[Nesterov, 1983] or [Bansal & Gupta 2019]):

$$\phi_k^f = d_k(f(x_k) - f_\star) + \frac{L}{2}\|z_k - x_\star\|^2$$

with $d_k \sim k^2$ (more precisely: $d_{k+1} = 1 + d_k + \sqrt{1+d_k}$).

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From numerical inspirations, alternate ones also possible, such as

$$\phi_k^f = d_k'(f(x_k) - f_\star) + \tfrac{d_k'}{2L}\left\|f'(x_k)\right\|^2 + \tfrac{L}{2}\|z_k - x_\star\|^2$$

with $d_k' \sim k^2$ (more precisely: $d_{k+1}' = 1 + d_k' + \sqrt{1 + \tfrac{3}{2}d_k'}$, *red curves on prev. slide*).

Optimized gradient method

Optimized gradient methods (Kim & Fessler, 2016) can be factorized in a similar form

$$\begin{aligned} y_{k+1} &= (1-\tau_k) y_k + \tau_k z_k - \alpha_k f'(y_k), \\ z_{k+1} &= (1-\delta_k) y_{k+1} + \delta_k z_k - \gamma_k f'(y_k) - \gamma_k' f'(y_{k+1}), \end{aligned}$$

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Starting with, for example,

$$\phi_k^f = \begin{pmatrix} y_k - x_\star \\ f'(y_k) \end{pmatrix}^\top [Q_k \otimes I_d] \begin{pmatrix} y_k - x_\star \\ f'(y_k) \end{pmatrix} + a_k \|z_k - x_\star\|^2 + d_k \left(f(y_k) - f_\star\right),$$

we can perform similar steps.

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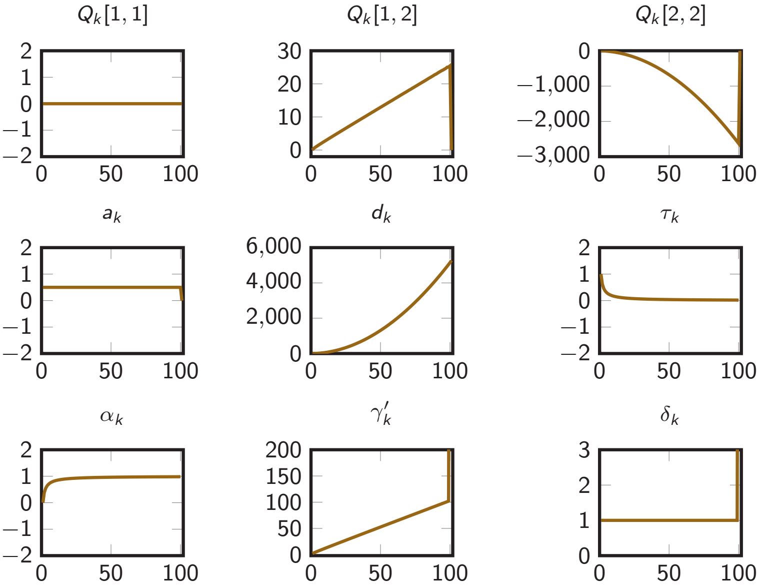

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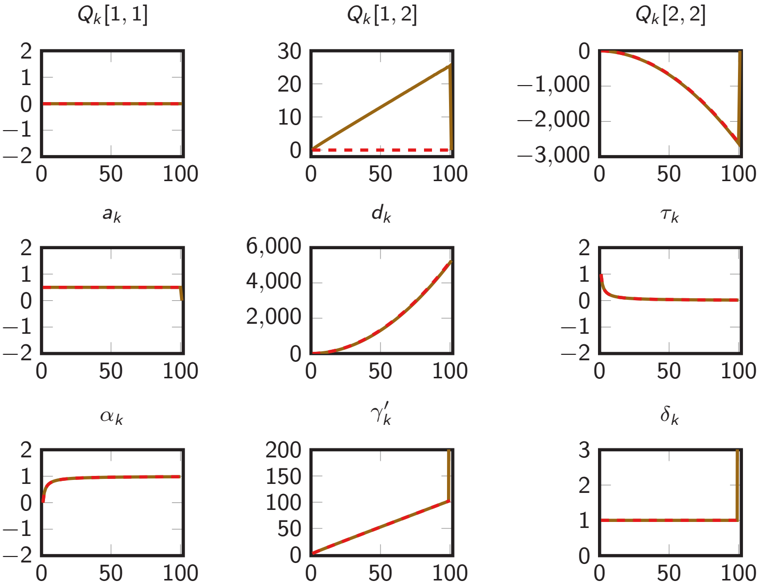

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but current analysis is more involved (not based on potentials).

From numerical inspiration, we get

$$\phi_k^f = d_k''(f(y_k) - f_\star - \tfrac{1}{2L}\left\|f'(y_k)\right\|^2) + \tfrac{L}{2}\|z_k - x_\star\|^2,$$

with $d_k'' \sim k^2$ (more precisely: $d_{k+1}'' = 1 + d_k'' + \sqrt{1 + 2d_k''}$, *red curves on prev. slide*)

Conjugate gradient method

Conjugate gradient method ("ideal version")

$$x_{k+1} = \operatorname{argmin}_x \{f(x) \,:\, x \in x_0 + \operatorname{span}\{f'(x_0), f'(x_1), \ldots, f'(x_k)\}\}.$$

Steps to perform the analysis are slightly trickier (reference at the end), but

- ◇ analysis is exactly the same as that of the optimized gradient method,
- ◇ achieve exactly the lower complexity bound for the class of problems.

Concluding remarks

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- ◇ proximal/projected variants, splitting methods, mirror descent/Bregman gradient, etc.
- ◇ inexact, randomized, and stochastic variants, etc.
- ◇ first attempts on adaptive methods (line searches, Polyak steps),
- ◇ also other classes of functions and problems (nonsmooth, weakly convex, and indicator functions, monotone inclusions, variational inequalities), etc.

… and probably many others!

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... and open questions:

- ◇ beyond Euclidean geometry?
- ◇ Higher-order methods?
- ◇ Adaptive methods (BFGS, nonlinear conjugate gradients)?
- ◇ Beyond worst-case analyses?

A few references

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Shameless advertisement:

- Radu-Alexandru Dragomir, T, Alexandre d'Aspremont, Jérôme Bolte. "Optimal complexity and certification of Bregman first-order methods". Preprint 2019.
- Mathieu Barré, T, Francis Bach. "Principled Analyses and Design of First-Order Methods with Inexact Proximal Operators". Preprint 2020.
- Mathieu Barré, T, Alexandre d'Aspremont. "Complexity Guarantees for Polyak Steps with Momentum". COLT 2020.

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References more thoroughly treated in the papers. Explicitly mentioned in this presentation:

- Yurii Nesterov. A method of solving a convex programming problem with convergence rate $O(1/k^2)$. Soviet Mathematics Doklady, 1983.
- Amir Beck, Marc Teboulle. "A fast iterative shrinkage-thresholding algorithm for linear inverse problems". SIAM Journal on Imaging Sciences, 2009.
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- Nikhil Bansal, Anupam Gupta. "Potential-function proofs for first-order methods". Theory of Computing, 2019.

Thanks! Questions?

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Codes (on Github)

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Presentation mainly based on

- ◇ T., Francis Bach. "Stochastic first-order methods: non-asymptotic and computer-aided analyses via potential functions", 2019.
- ◇ Yoel Drori, T. "Efficient first-order methods for convex minimization: a constructive approach", 2019.
- ◇ T., François Glineur, Julien Hendrickx. "Smooth strongly convex interpolation and exact worst-case performance of first-order methods", 2017.