Computer-aided analyses for first-order methods
(via semidefinite programming)

Adrien Taylor

SSOPT — June 2019

… great collaborators!

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Bryan Van Scoy
(W-Madison)

Carolina Bergeling
(Lund)

Pontus Giselsson
(Lund)

Topic's genealogy and credits

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All codes used here can be found on github (link at the end).

How do we prove an algorithm works?

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Goal: automate worst-case analyses of optimization algorithms

Take-home messages

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Sometimes, those optimization problems are tractable.

Often tractable for first-order methods in convex optimization!

Toy example

Performance estimation

Further examples

Convex interpolation

Conclusions and discussions

Analysis of a gradient step

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

with $f \in \mathcal{F}_{\mu,L}$: class of μ-strongly convex L-smooth functions.

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

About the assumptions

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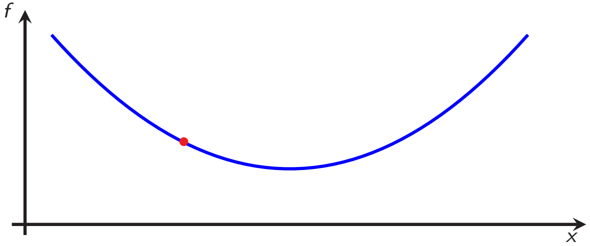

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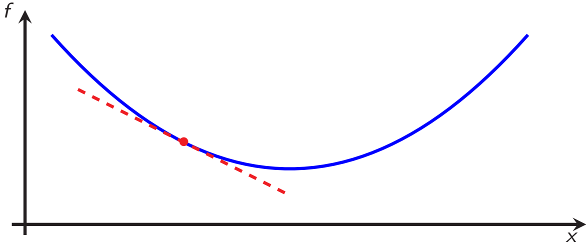

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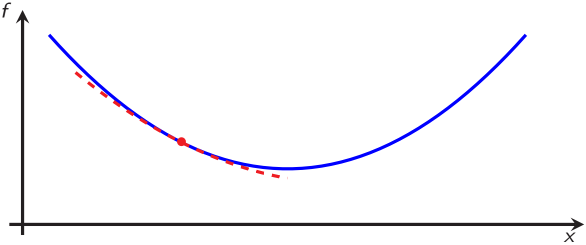

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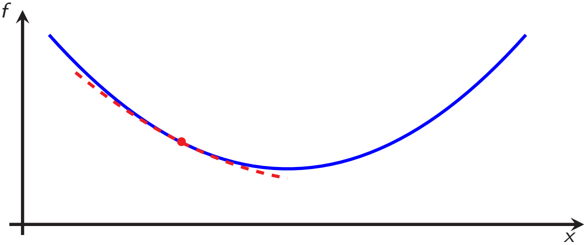

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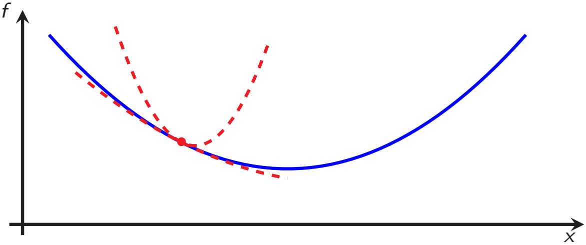

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Performance estimation problem for a gradient step

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Can be solved using semidefinite programming (SDP):

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Matching functions: $f(x) = \frac{\mu}{2}x^2$ and $f(x) = \frac{L}{2}x^2$.

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New variables: x_0, x_1, g_0, g_1, f_0, f_1.

Smooth strongly convex interpolation problem

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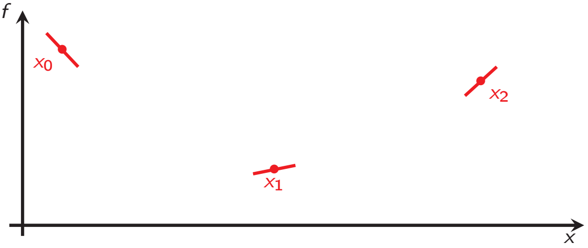

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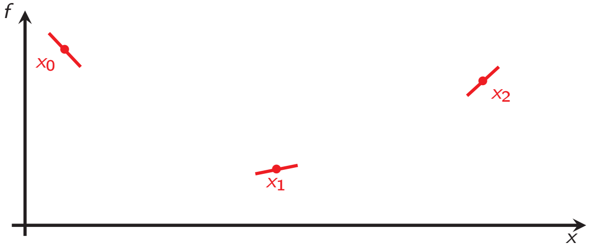

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- Necessary and sufficient condition: $\forall i, j \in S$

$$f_i \geq f_j + \langle g_j, x_i - x_j \rangle + \frac{1}{2L}\|g_i - g_j\|^2 + \frac{\mu}{2(1-\mu/L)}\left\|x_i - x_j - \frac{1}{L}(g_i - g_j)\right\|^2.$$

Solving PEP via Semidefinite Programming

PEP subject to an existence constraint becomes

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Non-convex quadratic program; can be solved using semidefinite programming.

Semidefinite programming: lifting procedure

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Introduces Gram matrix $G \succeq 0$, containing all scalar products:

Semidefinite programming: lifting procedure

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We stack all variables in a matrix $P \in \mathbb{R}^{d \times 4}$:

$$P = [x_0 \ x_1 \ g_0 \ g_1] \updownarrow d,$$

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SDP without rank constraint $\Leftrightarrow$ find smallest dimension-independent guarantee.

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Yes, using Lagrange duality!

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Toy example

Performance estimation

Further examples

Convex interpolation

Conclusions and discussions

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- any dual solution is a worst-case guarantee (i.e., a proof),
- it can be solved using semidefinite programming (SDP).

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Also works for e.g., monotone inclusion problems.

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In some settings, SDPs scale badly with problem parameters (e.g., stochastic settings).

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$$\min_{0\leq i\leq N} f(x_i) - f(x_\star), \quad \min_{0\leq i\leq N} \|x_i - x_\star\|^2, \quad \min_{0\leq i\leq N} \left\|f'(x_i)\right\|^2,$$

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- any concave function of f_i's, $\left\langle x_i, g_j \right\rangle$'s, $\|g_i\|^2$'s and $\|x_i\|^2$'s.

Want to give it a try?

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Performance EStimation TOolbox (PESTO)

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Purpose: automated worst-case analyses of first-order methods without worrying about modelling steps.

PESTO example: inexact fast gradient method

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

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Fast Gradient Method (FGM)

Input: $f \in \mathcal{F}_{0,L}(\mathbb{R}^d)$, $x_0 = y_0 \in \mathbb{R}^d$.

For $i = 0 : N-1$

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

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

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

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

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

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

x    = cell(N+1,1); % we store the iterates in a cell for convenience
x{1} = x0;
y    = x0;
eps  = .1;
for i = 1:N
    d      = inexactsubgradient(y, F, eps);
    x{i+1} = y - 1/param.L * d;
    y      = x{i+1} + (i-1)/(i+2) * (x{i+1} - x{i});
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
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double(f - fs)   % worst-case objective function accuracy
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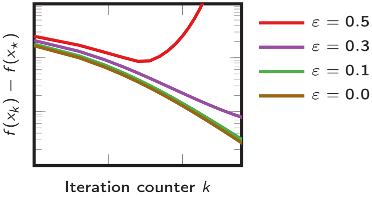

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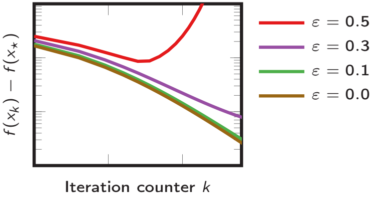

✔ fast prototyping ($\sim$ 20 effective lines)
✔ quick analyses ($\sim$ 10 minutes)
✔ computer-aided proofs (multipliers)

Toy example

Performance estimation

Further examples

Convex interpolation

Conclusions and discussions

Steepest descent with inexact search directions

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

with $f \in \mathcal{F}_{\mu,L}$ (L-smooth μ-strongly convex).

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Noisy gradient descent method with exact line search

Input: $f \in \mathcal{F}_{\mu,L}(\mathbb{R}^n)$, $x_0 \in \mathbb{R}^n$, $0 \leq \varepsilon < 1$.

for $i = 0, 1, \ldots$

Select any seach direction d_i that satisfies (1);

$\gamma = \text{argmin}_{\gamma \in \mathbb{R}} f\left(x_i - \gamma d_i\right)$

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Worst-case behavior: (de Klerk, Glineur, T. 2017)

$$f(x_{i+1}) - f_* \leq \left(\frac{1 - \kappa_\varepsilon}{1 + \kappa_\varepsilon} \right)^2 (f(x_i) - f_*) \quad i = 0, 1, \ldots$$

where $\kappa_\varepsilon = \frac{\mu}{L} \frac{(1-\varepsilon)}{(1+\varepsilon)}$.

Steepest descent with inexact search directions

Quadratic worst-case function:

$$f(\mathbf{x}) = \frac{1}{2}\sum_{i=1}^{n} \lambda_i x_i^2 \quad \text{where} \quad 0 < \mu = \lambda_1 \le \lambda_2 \le \ldots \le \lambda_n = L.$$

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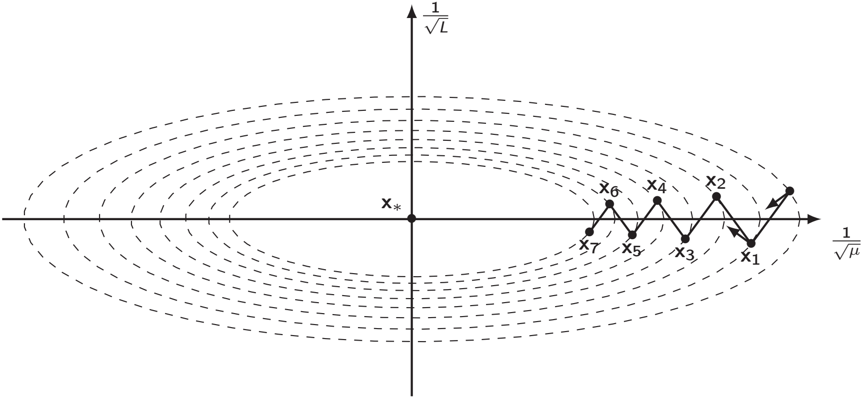

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$$f_0 \geq f_1 + \langle g_1, x_0 - x_1 \rangle + \frac{1}{2L}\|g_0 - g_1\|^2 + \frac{\mu}{2\left(1 - \frac{\mu}{L}\right)}\|x_0 - x_1 - (g_0 - g_1)/L\|^2$$

$$f_\star \geq f_0 + \langle g_0, x_\star - x_0 \rangle + \frac{1}{2L}\|g_\star - g_0\|^2 + \frac{\mu}{2\left(1 - \frac{\mu}{L}\right)}\|x_\star - x_0 - (g_\star - g_0)/L\|^2$$

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$$
y_1 = \frac{L-\mu}{L+\mu}, \quad y_2 = 2\mu\frac{(L-\mu)}{(L+\mu)^2}, \quad y_3 = \frac{2\mu}{L+\mu}, \quad y_4 = \frac{2}{L+\mu}, \quad y_5 = 1.
$$

What does the proof look like?

Resulting inequality:

$$\begin{aligned} f_1 - f_\star \quad \leq \quad & \left(\tfrac{L-\mu}{L+\mu}\right)^2 (f_0 - f_\star) \\ & - \tfrac{\mu L(L+3\mu)}{2(L+\mu)^2} \left\| x_0 - \tfrac{L+\mu}{L+3\mu} x_1 - \tfrac{2\mu}{L+3\mu} x_\star - \tfrac{3L+\mu}{L^2+3\mu L} g_0 - \tfrac{L+\mu}{L^2+3\mu L} g_1 \right\|^2 \\ & - \tfrac{2L\mu^2}{L^2+2L\mu-3\mu^2} \left\| x_1 - x_\star - \tfrac{(L-\mu)^2}{2\mu L(L+\mu)} g_0 - \tfrac{L+\mu}{2\mu L} g_1 \right\|^2. \end{aligned}$$

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Last two terms nonpositive, so

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One actually has equality at optimality, due to the quadratic example.

Optimized gradient methods

Smooth convex minimization setting:

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

with f being L-smooth and convex, with black-box oracle $f'(.)$ available.

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Lower bound for large-scale setting ($d \geq N+2$) by Drori (2017):

$$f(x_N) - f(x_\star) \geq \frac{L\|x_0 - x_\star\|^2}{2\theta_N^2},$$

with $\theta_0 = 1$, and:

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

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Coherent with historical lower bounds (Nemirovski & Yudin 1983) and optimal methods (Nemirovski 1982), (Nesterov 1983).

Optimized gradient methods

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

Greedy First-order Method (GFOM)

Inputs: f, x_0, N.

For $i = 1, 2, \ldots$

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

Worst-case guarantee:

$$f(x_N) - f(x_\star) \le \frac{L\|x_0 - x_\star\|^2}{2\theta_N^2}.$$

See (Drori & T. 2018).

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 $i = 1, \ldots, N$

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

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

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

$$x_i = y_i + \alpha d_i$$

Worst-case guarantee:

$$f(x_N) - f(x_\star) \leq \frac{L\|x_0 - x_\star\|^2}{2\theta_N^2}.$$

See (Drori & T. 2018).

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Optimized gradient method

Inputs: f, x_0, N.

For $i = 1, \ldots, N$

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

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

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

Worst-case guarantee:

$$f(x_N) - f(x_\star) \leq \frac{L\|x_0 - x_\star\|^2}{2\theta_N^2}.$$

See (Drori & Teboulle 2014), (Kim & Fessler 2016), (Drori & T. 2018).

A few more examples

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Intuitions can be developed, but this is another story ☺

Douglas-Rachford Splitting

Let $A : \mathbb{R}^d \to 2^{\mathbb{R}^d}$, $B : \mathbb{R}^d \to 2^{\mathbb{R}^d}$ (point-to-set maps) be maximally monotone;

$$\operatorname*{find}_{x \in \mathbb{R}^d} \; 0 \in A(x) + B(x).$$

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Examples: $A(x) = \partial f(x)$ and $B(x) = \partial h(x)$ for two convex functions f and h.

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amount to iterate:

$$\begin{aligned}
x_{k+1} &= \operatorname{argmin}_{x\in\mathbb{R}^d}\{h(x) + \tfrac{1}{2}\|x - w_k\|^2\}\\
y_{k+1} &= \operatorname{argmin}_{y\in\mathbb{R}^d}\{f(y) + \tfrac{1}{2}\|y - 2x_{k+1} + w_k\|^2\}\\
w_{k+1} &= w_k + \theta(y_{k+1} - x_{k+1})
\end{aligned}$$

Douglas-Rachford Splitting

Question: When is this T a contraction? What is the smallest ρ such that

$$\|Tx - Ty\| \leq \rho \|x - y\|,$$

for all $x, y \in \mathbb{R}^d$?

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Related previous works:

(Douglas & Rachford 1956), (Lions & Mercier 1979), (Giselsson & Boyd 2017), (Giselsson 2017), (Davis & Yin 2017), (Moursi & Vandenberghe 2018), and many others; gentle introduction to monotone operators (Ryu & Boyd 2016).

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Assumptions: A μ-strongly monotone, B β-cocoercive.

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with

$$X = \frac{\sqrt{2-\theta}}{2}\sqrt{\frac{\left((2-\theta)\mu(\beta+1)-\theta\beta(\mu-1)\right)\left((2-\theta)\beta(\mu+1)-\theta\mu(\beta-1)\right)}{(2-\theta)\mu\beta(\mu+1)(\beta+1)-\theta\mu^2\beta^2}}.$$

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$$\rho = \begin{cases} \dfrac{\theta+\sqrt{\frac{(2(\theta-1)\mu+\theta-2)^2+L^2(\theta-2(\mu+1))^2}{L^2+1}}}{2(\mu+1)} & \text{if } (a), \\ \left|1 - \theta\frac{L+\mu}{(\mu+1)(L+1)}\right| & \text{if } (b), \\ \sqrt{\frac{(2-\theta)}{4\mu(L^2+1)}\frac{\left(\theta(L^2+1)-2\mu(\theta+L^2-1)\right)\left(\theta\left(1+2\mu+L^2\right)-2(\mu+1)\left(L^2+1\right)\right)}{2\mu(\theta+L^2-1)-(2-\theta)(1-L^2)}} & \text{otherwise,} \end{cases}$$

with

(a) $\mu\frac{-(2(\theta-1)\mu+\theta-2)+L^2(\theta-2(1+\mu))}{\sqrt{(2(\theta-1)\mu+\theta-2)^2+L^2(\theta-2(\mu+1))^2}} \leq \sqrt{L^2+1}$,

(b) $L < 1$, $\mu > \frac{L^2+1}{(L-1)^2}$, and $\theta \leq \frac{2(\mu+1)(L+1)(\mu+\mu L^2-L^2-2\mu L-1)}{2\mu^2-\mu+\mu L^3-L^3-3\mu L^2-L^2-2\mu^2 L-\mu L-L-1}$.

Toy example

Performance estimation

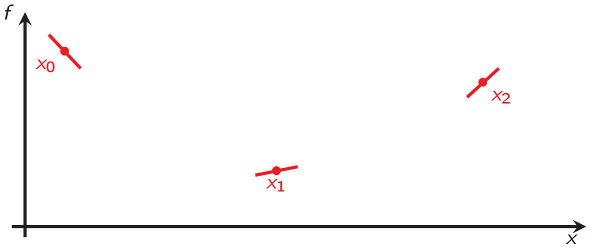
Further examples

Convex interpolation

Conclusions and discussions

Smooth strongly convex interpolation

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

Conditions for $\{(x_i, g_i, f_i)\}_{i\in S}$ to be interpolable by a function $f \in \mathcal{F}_{0,\infty}$ (proper, closed and convex function) ?

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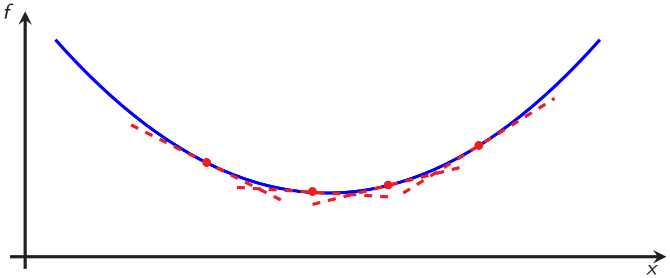

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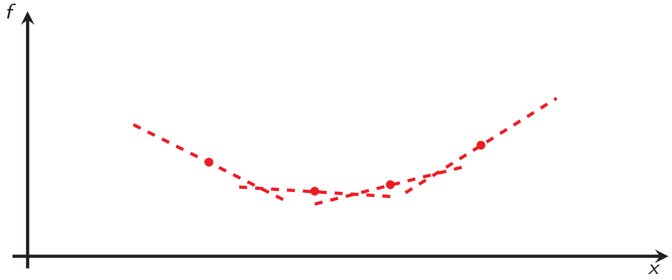

Conditions $f_i \geq f_j + \langle g_j, x_i - x_j \rangle$ is nec.

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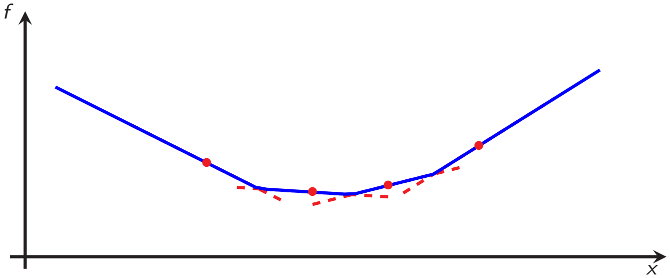

Conditions $f_i \geq f_j + \langle g_j, x_i - x_j \rangle$ is nec. and suff.

Explicit construction:

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

Not unique.

Smooth convex interpolation

Generalization to smooth interpolation ? Interpolation by a function $f \in \mathcal{F}_{0,L}$ (proper, closed and convex function with L-Lipschitz gradient).

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Counter-example 1: what about the conditions:

$$\begin{aligned} & f_i \geq f_j + \langle g_j, x_i - x_j \rangle, && i, j \in S, \\ & \|g_i - g_j\| \leq L \|x_i - x_j\|. && \end{aligned} \tag{C1}$$

Smooth convex interpolation

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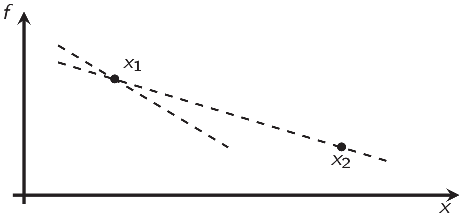
$(x_1, g_1, f_1) = (-1, -2, 1)$
$(x_2, g_2, f_2) = (0, -1, 0)$



satisfies (C1) but cannot be differentiable...

An approach to smooth convex interpolation

Idea: reduce smooth convex interpolation to convex interpolation.

Basic operations needed in order to transform the problem:

- Conjugation: f is closed, proper and convex, then:
  f L-Lipschitz gradient $\Leftrightarrow f^*$ $\frac{1}{L}$-strongly convex.

- Minimal curvature subtraction:
  $f(x)$ μ-strongly convex $\Leftrightarrow f(x) - \frac{\mu}{2}\|x\|^2$ convex.

Conjugation (1): Definition

Consider a proper function $f : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, the (Legendre-Fenchel) conjugate of f is defined as:

$$f^*(y) = \sup_{x \in \mathbb{R}^d} \langle y, x \rangle - f(x),$$

with $f^* \in \mathcal{F}_{\mathbf{0},\infty}$ (proper, closed and convex).

Conjugation (2): Useful properties

For $f \in \mathcal{F}_{0,\infty}$, we have a one-to-one correspondence between f and f^*, and the following propositions are equivalent:

(a) $f(x) + f^*(g) = \langle g, x \rangle$,

(b) $g \in \partial f(x)$,

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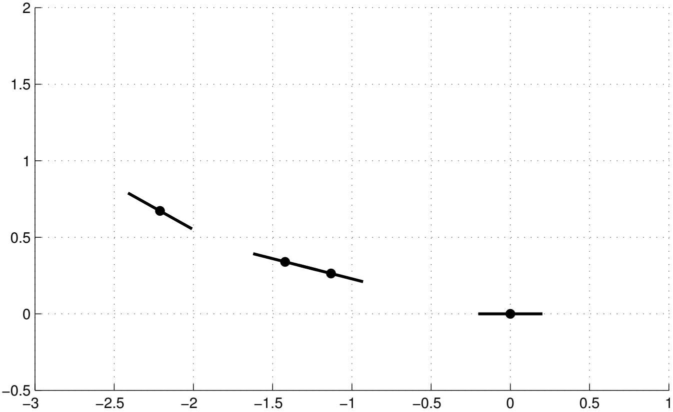
Intuition:

- upper bounds become lower bounds; let $f, u \in \mathcal{F}_{0,\infty}$, we have:

$$f(x) \leq u(x) \text{ for all } x \in \mathbb{R}^d \Leftrightarrow u^*(g) \leq f^*(g) \text{ for all } g \in \mathbb{R}^d.$$

- Conjugate of quadratics are quadratics.

Example: Smooth Convex Interpolation



Interpolate $\{(x_i, g_i, f_i)\}_{i \in S}$ by $f \in \mathcal{F}_{0,L}$

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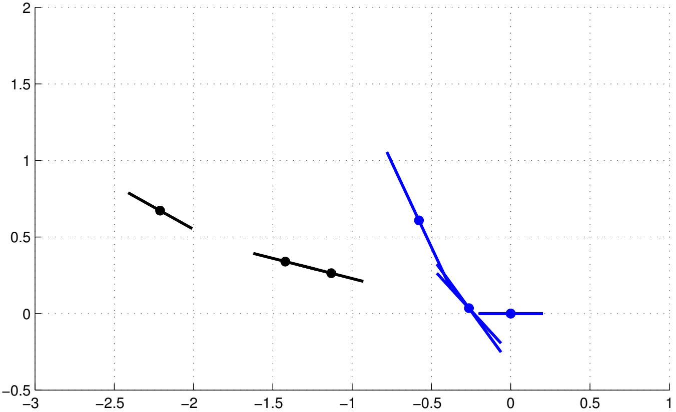

$\Leftrightarrow$ interpolate $\{(g_i, x_i, \langle x_i, g_i\rangle - f_i)\}_{i\in S}$ by $f^* \in \mathcal{F}_{1/L,\infty}$.

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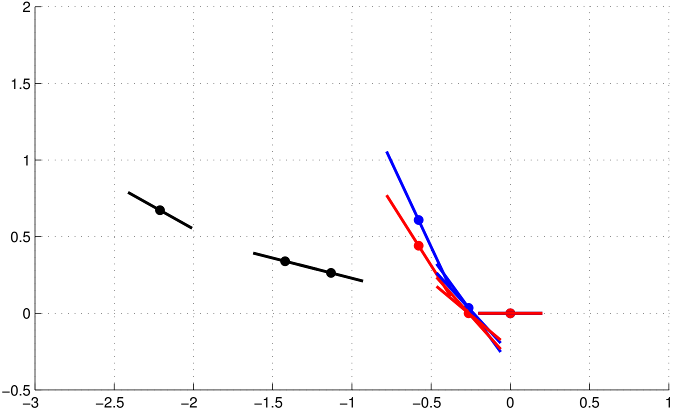

$\Leftrightarrow$ interpolate $\left\{\left(g_i, x_i - \frac{g_i}{L}, \langle x_i, g_i\rangle - f_i - \frac{\|g_i\|^2}{2L}\right)\right\}_{i\in S}$ by $\tilde{f} \in \mathcal{F}_{0,\infty}$.

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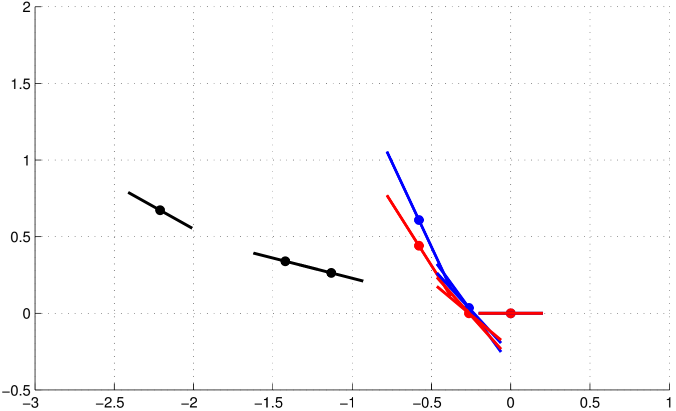

$\Leftrightarrow$ interpolate $\left\{(\tilde{x}_i, \tilde{g}_i, \tilde{f}_i)\right\}_{i\in S}$ by $\tilde{f} \in \mathcal{F}_{0,\infty}$.

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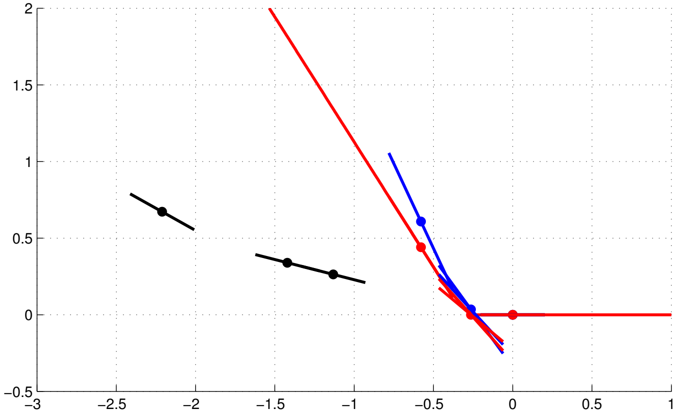
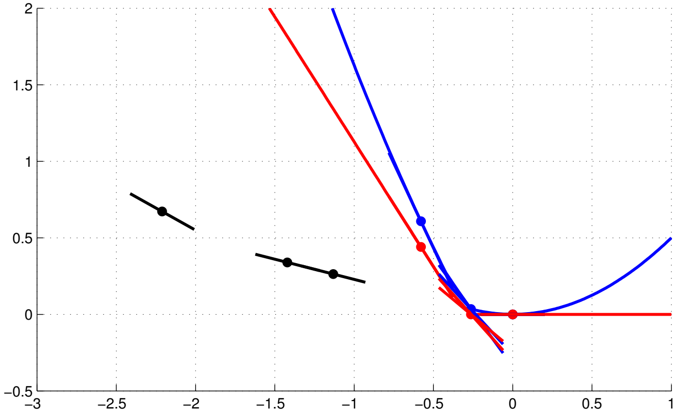


$\tilde{f}(x) = \max_j \left\{ \tilde{f}_j + \langle \tilde{g}_j, x - \tilde{x}_j \rangle \right\}$

Example: Smooth Convex Interpolation



$f^*(x) = \max_j \left\{ \tilde{f}_j + \langle \tilde{g}_j, x - \tilde{x}_j \rangle \right\} + \frac{\|x\|^2}{2L}$

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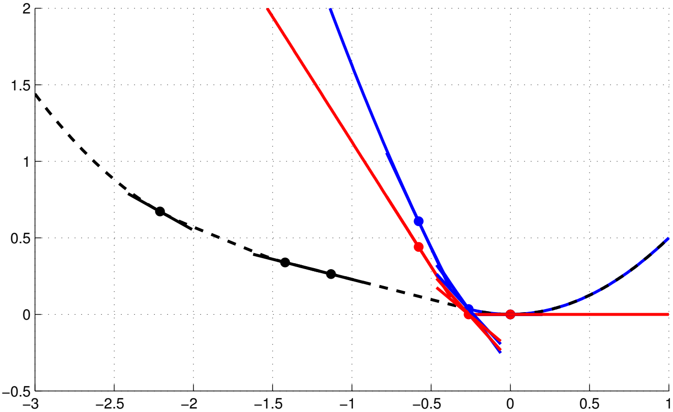

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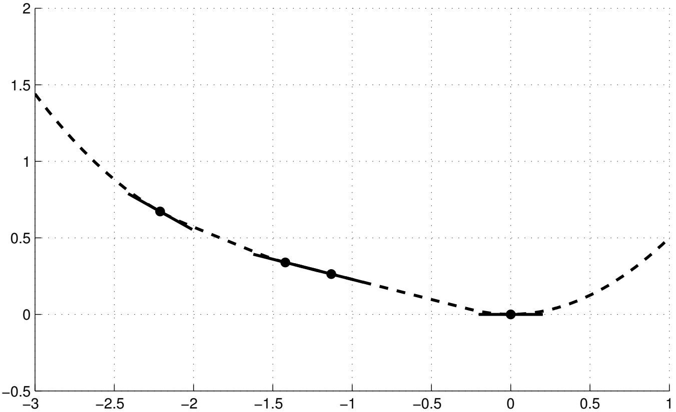

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Conclusion: iff conditions

Using the same reasoning:

The set $\{(x_i, g_i, f_i)\}_{i\in S}$ is interpolable by a function $f \in \mathcal{F}_{\mu,L}$ (proper, closed, μ-strongly convex with L-Lipschitz gradient) iff:

$$f_i - f_j - \langle g_j, x_i - x_j\rangle \geq \frac{1}{2(1-\mu/L)}\left(\frac{1}{L}\|g_i - g_j\|^2 + \mu\|x_i - x_j\|^2 - 2\frac{\mu}{L}\langle g_j - g_i, x_j - x_i\rangle\right).$$

When $\mu = 0$, those conditions transforms to the well-known

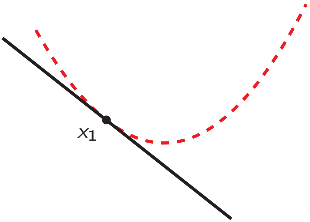
$$f_j \geq f_i + \langle g_i, x_j - x_i\rangle + \frac{1}{2L}\|g_i - g_j\|^2 \qquad \forall i, j \in S.$$

Interpretation: compatible upper and lower bounds

Smooth convex interpolation conditions

$$f_j \geq f_i + \langle g_i, x_j - x_i \rangle + \frac{1}{2L} \| g_i - g_j \|^2 \qquad \forall i, j \in S$$

characterize compatibility between upper and lower bounds.



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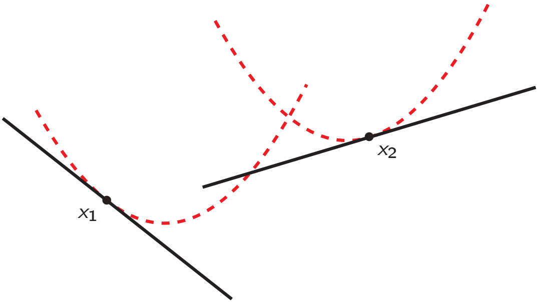

x_1 and x_2 are not compatible.

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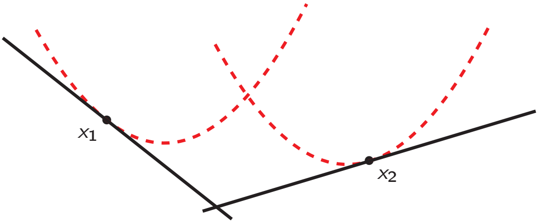

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Interpretation: convex hull of upper bounds

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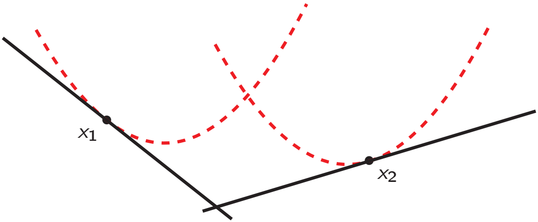
ensure you can perform the following interpolation procedure:



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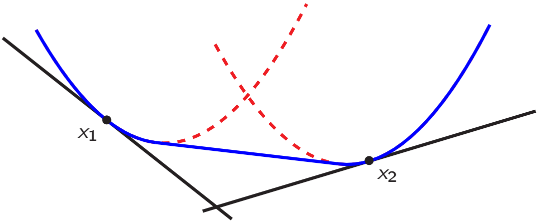

Interpretation: smoothed lower bounds

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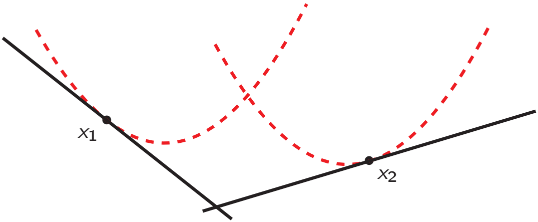

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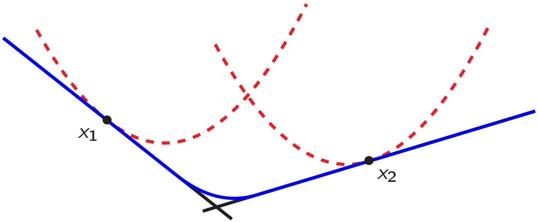

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- And many others...

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Take-home messages

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Often tractable for first-order methods in convex optimization!

Thanks! Questions?

www.di.ens.fr/∼ataylor/

AdrienTaylor/Performance-Estimation-Toolbox on Github

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