Polyhedral Newton-min algorithms for complementarity problems [28]

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June 7, 2023

Outline

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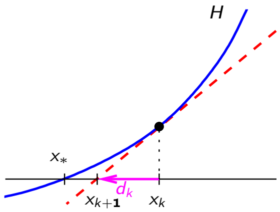
Local Newton's method for a smooth function

- Let $H : \mathbb{E} \to \mathbb{F}$ be a smooth function ($\mathbb{E}$ a vector space).
- Find $x_* \in \mathbb{E}$ such that $H(x_*) = 0$?
- Local Newton's algorithm:

$$\begin{cases} H(x_k) + H'(x_k)d_k = 0 \\ x_{k+1} := x_k + d_k. \end{cases}$$



- 3 conditions for quadratic convergence
  - x_0 close to x_*,
  - $H \in \mathcal{C}^{1,1}$,
  - $H'(x_*)$ nonsingular.

Globalization of Newton's method for a smooth function: miracle or mirage?

- Let $(\mathbb{F}, \langle\cdot,\cdot\rangle)$ be a Euclidean space; associated norm $\|\cdot\| = \langle\cdot,\cdot\rangle^{1/2}$.
- Consider the least-square merit function: $\theta : \mathbb{E} \to \mathbb{R}$ defined at $x \in \mathbb{E}$ by

$$\theta(x) := \frac{1}{2}\|H(x)\|^2.$$

- Miracle: the Newton's direction $d := -H'(x)^{-1}H(x)$ is a descent direction of θ:

$$\theta'(x)d = \langle H(x), H'(x)d\rangle = -\|H(x)\|^2 = -2\theta(x) < 0 \qquad [\text{if } d \text{ exists and } H(x) \neq 0]$$

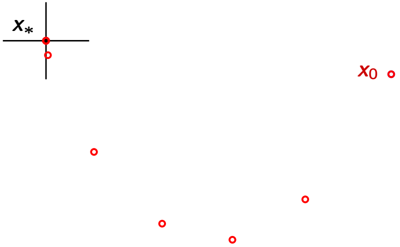
- Globalization by linesearch: $x_{k+1} := x_k + \alpha_k d_k$ with $\alpha_k > 0$ *not too small* such that

$$\theta(x_k + \alpha_k d_k) \leqslant \theta(x_k) + \omega\alpha_k\theta'(x_k)d_k \qquad [\omega \simeq 10^{-4}].$$

- Mirage: If $\bar{x}$ is a limit point of $\{x_k\}$, that is regular ($F'(\bar{x})$ nonsingular), then $F(\bar{x}) = 0$.

But there may be no such limit point!

Success of the globalization of Newton's algorithm with LS



$$F(x) = \begin{pmatrix} x_1 \\ -(x_1-2)^2 + x_2 + 4 \end{pmatrix}$$

$$F'(x) = \begin{pmatrix} 1 & 0 \\ -2(x_1-2) & 1 \end{pmatrix}.$$

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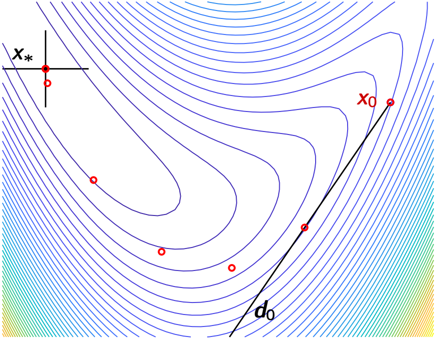

Failure of the globalization of Newton's algorithm with LS I

$$F(x) = \begin{pmatrix} x_1 \\ -(x_1-2)^2 + (x_2-1)^2 + 3 \end{pmatrix},$$

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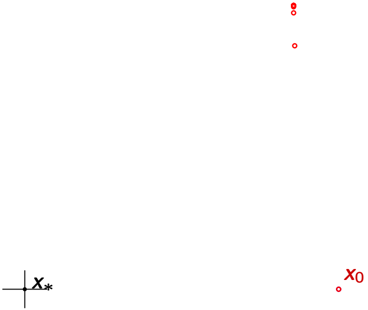

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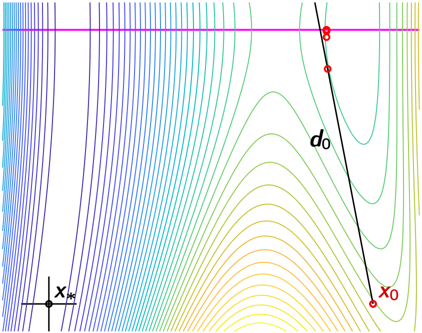

Failure of the globalization of Newton's algorithm with LS II

$$F(x) = \begin{pmatrix} x_1 \\ -(x_1 - 2)^2 + e^{x_2} + 3 \end{pmatrix},$$

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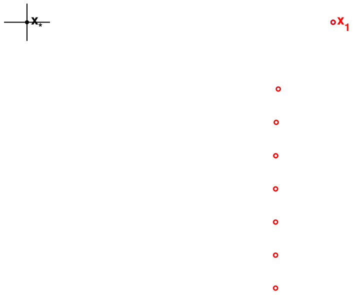

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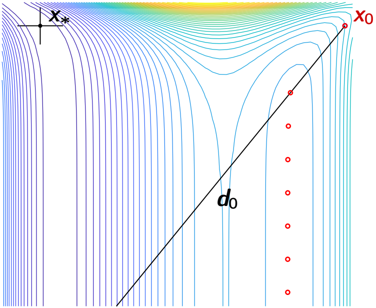


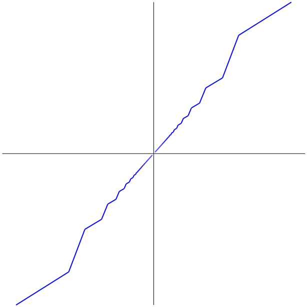
Failure of the globalization of Newton's algorithm with LS III

Conclusion

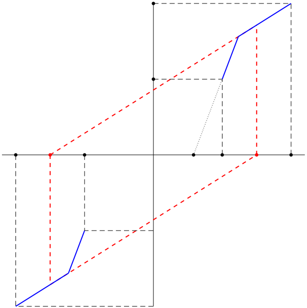
- A "global" convergence result of the kind "any regular limit point of the generated sequence is a solution" must be taken with caution, since the generated sequence may have no regular limit point.
- Such a "global" convergence result is just a means to improve algorithms.

Local Newton's method for a nonsmooth function may fail

Newton's method may cycle, regardless of the proximity of x_0 and x_*.
Example, Kummer's function [49; 1988] (differentiable at 0, $\partial_C H(0) = [1/2, 2] \not\ni 0$)



Kummer's function



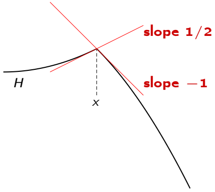
Cycling of Newton's algorithm

B-differential and C-differential

- Let $\mathbb{E}$ and $\mathbb{F}$ be two vector spaces of finite dimensions $n := \dim \mathbb{E}$ and $m := \dim \mathbb{F}$.
- Let $H : \mathbb{E} \to \mathbb{F}$ be a function.
- The B-differential (B for Bouligand) of H at $x \in \mathbb{E}$ is denoted and defined by

$$\partial_B H(x) := \{J \in \mathcal{L}(\mathbb{E}, \mathbb{F}) : H'(x_k) \to J \text{ for a sequence } \{x_k\} \subseteq \mathcal{D}_H \text{ converging to } x\},$$

where $\mathcal{L}(\mathbb{E}, \mathbb{F})$ is the set of linear (continuous) maps from $\mathbb{E}$ to $\mathbb{F}$ and $\mathcal{D}_H$ is the set of points at which H is differentiable.



$\partial_B H(x) = \{-1, 1/2\}$
$\partial_C H(x) = [-1, 1/2]$

- The C-differential (C for Clarke [19]) of H at $x \in \mathbb{E}$ is denoted and defined by

$$\partial_C H(x) := \operatorname{co} \partial_B H(x),$$

where $\operatorname{co} S$ denotes the convex hull of a set S.

- H locally Lipschitz near $x \implies \partial_B H(x)$ and $\partial_C H(x)$ nonempty and bounded.

Semismoothness definition [61, 60; 1993]

- Let $\mathbb{E}$ and $\mathbb{F}$ be two normed spaces and Ω be an open set of $\mathbb{E}$.
- Let $H : \Omega \to \mathbb{F}$ be a function and $x \in \Omega$.
- The function H is said to be semismooth at x if the following three conditions hold:

  (SS1) H is Lipschitz near x,
  (SS2) H has directional derivatives at x in all directions,
  (SS3) when $h \to 0$ in $\mathbb{E}$, one has

$$\sup_{J \in \partial_C H(x+h)} \|H(x+h) - H(x) - Jh\| = o(\|h\|). \tag{1a}$$

- The function H is said to be strongly semismooth at x if it is semismooth at x with (SS3) strengthened into

  (SS3') for h near 0, one has

$$\sup_{J \in \partial_C H(x+h)} \|H(x+h) - H(x) - Jh\| = O(\|h\|^2). \tag{1b}$$

- The function $H : \Omega \to \mathbb{F}$ is said to be semismooth (resp. strongly semismooth) on a part P of Ω if it is semismooth (resp. strongly semismooth) at all points of P.

Semismoothness properties

- Semismooth Newton's method [61, 60; 1993]
  - Choose some nonsingular $J_k \in \partial_B H(x_k)$, if any,
  - $x_{k+1} := x_k - J_k^{-1} H(x_k)$.
- Local quadratic convergence of semismooth Newton's method if
  - x_0 is close to x_*,
  - H is strongly semismooth,
  - all $J \in \partial_B H(x_*)$ is nonsingular.
- Nice properties
  - H continuously differentiable at $x \Rightarrow H$ semismooth at x.
  - H_1 semismooth at x, H_2 semismooth at $H_1(x) \Rightarrow H_2 \circ H_1$ semismooth at x.
    - H_1, H_2 semismooth at $x \Rightarrow H_1 + H_2$ semismooth at x.
    - H_1, H_2 semismooth at $x \Leftrightarrow (H_1, H_2)$ semismooth at x.
    - H_1, H_2 semismooth at $x \Rightarrow \langle H_1, H_2 \rangle$ semismooth at x.
  - H_1, H_2 semismooth at $x \Rightarrow \min(H_1, H_2)$ semismooth at x.

Globalization of Newton's method for a nonsmooth function

No general technique.

Reason: $d_k = -J_k^{-1} H(x_k)$ may not be a descent direction of $\theta : x \mapsto \frac{1}{2}\|H(x)\|^2$. Often, it depends on the choice of $J_k \in \partial_B H(x_k)$.

Outline

Nonlinear complementarity problem

A complementarity problem consists in finding $x \in \Omega$ (open subset of $\mathbb{R}^n$) such that

$$F(x) \geqslant 0, \qquad G(x) \geqslant 0, \qquad \text{and} \qquad F(x)^{\mathsf{T}} G(x) = 0, \tag{2a}$$

where $F : \Omega \to \mathbb{R}^n$ and $G : \Omega \to \mathbb{R}^n$ are smooth. This is written compactly as follows:

$$\text{(NLCP)} \qquad 0 \leqslant F(x) \perp G(x) \geqslant 0. \tag{2b}$$

Linear complementarity problem

Sometimes, we shall refer to the *linear* complementarity problem [22]: this is (2) with $F(x) = Mx + q$ and $G(x) = x$:

$$\text{(LCP)} \qquad 0 \leqslant (Mx + q) \perp x \geqslant 0, \tag{3}$$

where $M \in \mathbb{R}^{n \times n}$ and $q \in \mathbb{R}^n$.

P-matrix

$$M \in \mathbf{P} \iff \det M_{I,I} > 0 \text{ for all } I \subseteq [1:n]$$
$$\iff \text{(3) has a unique solution for all } q \in \mathbb{R}^n.$$

We are interested in *linearization numerical methods* to solve these problems.

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Comments on the problem

- It is a set of nonlinear inequalities and one equation, so it may look like an easy problem to solve.

- Mangasarian-Fromovitz does not hold $\Longrightarrow$ instability for small perturbations.

- By the inequalities $F(x) \geqslant 0$ and $G(x) \geqslant 0$, the equation $F(x)^{\mathsf{T}} G(x) = 0$ also reads

$$\forall\, i \in [1:n]: \quad F_i(x) G_i(x) = 0.$$

  There are 2^n ways of realizing these complementarity conditions. Hence a huge combinatorial aspect.

- Even the LCP (3) is NP-hard in general [18, 47]. Depends on M:
  - at most n iterations if M is an **M**-matrix (Newton-min) [2],
  - ??? if M is a **P**-matrix (Lemke exponential [54], Newton-min cycles [9, 10, 11]),
  - ??? if M is a nondegenerate matrix,
  - NP-hard if M is a $\mathbf{P}_0$-matrix [47],
  - $O((1+\kappa)n^\alpha \log \varepsilon^{-1})$ iterations if M is a $\mathbf{P}_*(\kappa)$-matrix (interior points) [47, 59], but κ may be exponential in the length L of the data [24].

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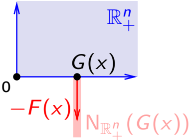
Link with other problems

- It is a particular case of functional inclusion problem

$$F(x) + (\mathrm{N}_{\mathbb{R}^n_+} \circ G)(x) \ni 0.$$



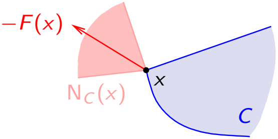
- First order optimality conditions of the optimization problem "$\min\{f(x) : c(x) \leqslant 0\}$":

$$\text{Find } (x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^m \text{ s.t. } \left\{ \begin{array}{ll} \nabla f(x) + c'(x)^{\mathsf{T}} \lambda = 0 & (n \text{ equations}) \\ 0 \leqslant \lambda \perp -c(x) \geqslant 0 & (m \text{ "conditions"}). \end{array} \right. \quad (4)$$

- The LCP was introduced and analyzed in the linear case by Cottle in his PhD thesis [20, 21; 1964], as an extension of the linear optimization problem.

- The related variational inequality problem

$$\left\{ \begin{array}{l} x \in C \text{ (a convex set)} \\ \langle F(x), y - x \rangle \geqslant 0, \quad \forall y \in C. \end{array} \right.$$



was introduced by Hartman and Stampacchia [44; 1966] for an EDP.

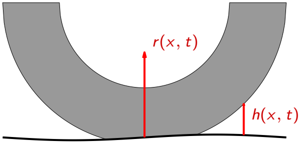
Examples of use

- **General principle**. Useful for systems in competition with threshold effects:

$$\text{If the threshold } F_i(x) \text{ is inactive } (> 0) \quad \Longrightarrow \quad G_i(x) = 0.$$

- Examples in
  - nonsmooth mechanics and dynamics, contact problems [1, 14, 3],

Tire/road contact
in (space,time)



$$\begin{cases} r(x,t) \geqslant 0 \\ h(x,t) \geqslant 0 \\ r(x,t)h(x,t) = 0. \end{cases}$$

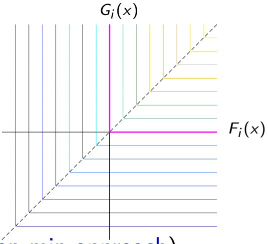
  - phase transition problem in multiphase flows [52, 53, 7, 4, 6, 5, 16, 23],
  - precipitation-dissolution problems in chemistry [15, 48],
  - portfolio management in finance [41],
  - computer graphics [31],
  - free boundary problems, meteorology simulation, economic equilibrium, ...

- More examples of applications in [42, 45, 57, 37, 32].

- Pivoting (Lemke) for LCP.
- Interior points.
- Nonsmooth equation reformulation and pseudo-linearization. $\longleftarrow$
- Smoothing nonsmooth reformulations.
- Other methods . . .

Outline

Equation reformulation of NLCP (I)



Solve the following nonsmooth reformulation of (NLCP):

$$H(x) = 0, \qquad (5a)$$

where $H : \Omega \to \mathbb{R}^n$ is the function defined at $x \in \Omega$ by

$$H(x) := \min(F(x), G(x)). \qquad (5b)$$

Compute a direction d by a pseudo-linearization of H ($\equiv$ Newton-min approach).

- (5) is equivalent to (NLCP) since $\min(a, b) = 0$ iff $a \geqslant 0$, $b \geqslant 0$ and $ab = 0$.
- H has directional derivatives and is semismooth (if F and G are smooth).
- There are other equation reformulations, like the one using the Fischer function $\varphi_{\mathrm{F}}(a, b) = \sqrt{a^2 + b^2} - (a + b)$ [38, 34, 51, 25, 58].
- The function "min" reformulation is a choice guided by
  - scientific curiosity (there are still possibilities of improvement),
  - efficiency of the approach ("min" is more linear, although less differentiable than φ_{F}),
  - can give better local convergence result than with φ_{F} [32],
  - can give finite termination for LCP [39].

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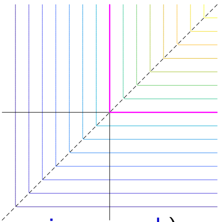

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Equation reformulation of NLCP (II): globalization [12, 13]

The quadratic merit function associated with (5) is defined at $x \in \mathbb{R}^n$ by

$$\theta(x) := \frac{1}{2}\|H(x)\|^2 = \frac{1}{2}\|\min(F(x), G(x))\|^2. \tag{6}$$

- θ has directional derivatives and is semismooth.
- Algorithmic goal

Algorithm

- *Compute $d \in \mathbb{R}^n$ such that*
  - *it is a descent direction of θ, i.e., $\theta'(x; d) < 0$,*
  - *it is efficient locally (quadratic or finite convergence).*
- *Do a standard Armijo line-search on θ: find a not too small $\alpha > 0$ such that ($\omega \in (0, 1)$)*

$$\theta(x + \alpha d) \leqslant \theta(x) + \omega\alpha\theta'(x; d).$$

- *Update $x_+ = x + \alpha d$.*

- Certify the algorithm by some kind of global convergence.

Josephy-Newton (JN) method

For a function Φ and a multifunction N, the JN algorithm [46] aims at solving

$$\Phi(x) + N(x) \ni 0,$$

by linearizing Φ, while keeping N unchanged. Hence $x_+ = x + d$, where d solves

$$\Phi(x) + \Phi'(x)d + N(x+d) \ni 0.$$

Applied to the NLCP "$0 \leqslant F(x) \perp G(x) \geqslant 0$" $\iff$ "$F(x) + (\mathrm{N}_{\mathbb{R}^n_+} \circ G)(x) \ni 0$", it computes $x_+ = x + d$ where d solves

$$\text{(JN)} \qquad 0 \leqslant \Big(F(x) + F'(x)d\Big) \perp \Big(G(x) + G'(x)d\Big) \geqslant 0.$$

Properties (similar to those of the SQP algorithm in constrained optimization):

- ⊕ fast local convergence (quadratic) with realistic assumptions,
- ⊕ yields descent directions of the quadratic merit function θ,
- ⊕ global convergence,
- ⊖ expensive iteration (one LCP to solve),
- ⊖ makes no sense for solving the LCP, since (JN) $\equiv$ (LCP).

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$$\text{(JN)} \qquad 0 \leqslant \Big(F(x) + F'(x)d\Big) \perp \Big(G(x) + G'(x)d\Big) \geqslant 0.$$

Properties (similar to those of the SQP algorithm in constrained optimization):

- $\oplus$ fast local convergence (quadratic) with realistic assumptions,
- $\oplus$ yields descent directions of the quadratic merit function θ,
- $\oplus$ global convergence,
- $\ominus$ expensive iteration (one LCP to solve),
- $\ominus$ makes no sense for solving the LCP, since (JN) $\equiv$ (LCP).

B-Newton method

For a locally Lipschitz function H, the B-Newton algorithm [55] aims at solving $H(x) = 0$ by taking $x_+ = x + d$, where d solves

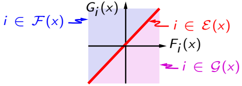
$$H(x) + H'(x; d) = 0.$$

Applied to the NLCP [55, 56] and $H = \min(F, G)$, it computes $x_+ = x + d$ where d solves

$$\text{(BN)} \qquad \begin{cases} (F(x) + F'(x)d)_{\mathcal{F}(x)} = 0, \\ (G(x) + G'(x)d)_{\mathcal{G}(x)} = 0, \\ 0 \leqslant (F(x) + F'(x)d)_{\mathcal{E}(x)} \perp (G(x) + G'(x)d)_{\mathcal{E}(x)} \geqslant 0, \end{cases}$$

where

$$\begin{aligned} \mathcal{E}(x) &:= \{i \in [1:n] : F_i(x) = G_i(x)\}, \\ \mathcal{F}(x) &:= \{i \in [1:n] : F_i(x) < G_i(x)\}, \\ \mathcal{G}(x) &:= \{i \in [1:n] : F_i(x) > G_i(x)\}. \end{aligned}$$



Properties:

- ⊕ yields descent directions of the quadratic merit function θ,
- ⊕ global convergence,
- ⊖ a limit point $\bar{x}$ is a solution if it is "regular" and satisfies $F_i(\bar{x}) = G_i(\bar{x}) = 0$ for $i \in \mathcal{E}(\bar{x})$,
- ⊖ much less expensive iteration than JN ($|\mathcal{E}(x)|$ small), but still one LCP to solve,
- ⊖ makes no sense for solving the LCP, since (BN) ≡ (JN) when $\mathcal{E}(x) = [1:n]$.

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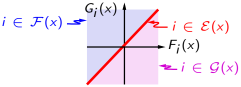

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Semismooth Newton method

- Algorithm for solving $H(x) := \min(F(x), G(x)) = 0$
  - Choose a nonsingular Jacobian

$$J \in \partial_B H(x) \subseteq \partial_B H_1(x) \times \cdots \times \partial_B H_n(x) =: \partial_B^{\times} H(x) \quad \text{or}$$
$$J \in \partial_C H(x) \subseteq \partial_C H_1(x) \times \cdots \times \partial_C H_n(x) =: \partial_C^{\times} H(x).$$

  - Determine d by $H(x) + Jd = 0$.
  - If d is descent direction of θ, do a LS along d to get $x_+ := x + \alpha d$.
- Discussion
  - Define the piecewise affine model $\mathcal{L}_x H$ of H at $x \in \mathbb{R}^n$ by

$$y \in \mathbb{R}^n \mapsto (\mathcal{L}_x H)(y) := \min\big(F(x) + F'(x)(y-x), G(x) + G'(x)(y-x)\big).$$

    Then,

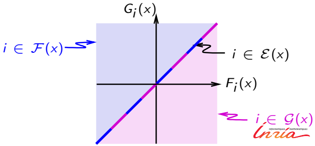
$$\partial_B(\mathcal{L}_x H)(x) \subseteq \partial_B H(x) \qquad \text{and} \qquad \partial_C(\mathcal{L}_x H)(x) \subseteq \partial_C H(x).$$

  - Computing a single Jacobian J of $\partial_B(\mathcal{L}_x H)(x)$, hence of $\partial_B H(x)$, is easy (all the Jacobians is difficult) [29]. Same observation for ∂_C.
  - Having J nonsingular is a matter of assumption (not guaranteed in general).
  - But d is not necessarily a descent direction of θ (a counter-example in a while).

Plain Newton-min method

- Algorithm for solving $H(x) := \min(F(x), G(x)) = 0$
  - Choose a nonsingular Jacobian
$$J \in \partial_B H_1(x) \times \cdots \times \partial_B H_n(x) =: \partial_B^{\times} H(x) \quad \text{or}$$
$$J \in \partial_C H_1(x) \times \cdots \times \partial_C H_n(x) =: \partial_C^{\times} H(x).$$
  - Determine d by $H(x) + Jd = 0$.
  - If d is descent direction of θ, do a LS along d to get $x_+ := x + \alpha d$.

- Discussion
  - For $i \in [1:n]$, one has
$$\partial_B H_i(x) = \begin{cases} \{F_i'(x)\} & \text{if } F_i(x) < G_i(x) \;\Leftrightarrow\; i \in \mathcal{F}(x), \\ \{F_i'(x), G_i'(x)\} & \text{if } F_i(x) = G_i(x) \;\Leftrightarrow\; i \in \mathcal{E}(x), \\ \{G_i'(x)\} & \text{if } F_i(x) > G_i(x) \;\Leftrightarrow\; i \in \mathcal{G}(x). \end{cases}$$
  - Hence d with $J \in \partial_B^{\times} H(x)$ is defined by
$$\begin{cases} F_i(x) + F_i'(x)d = 0 & \text{if } i \in \tilde{\mathcal{F}}(x) \\ G_i(x) + G_i'(x)d = 0 & \text{if } i \in \tilde{\mathcal{G}}(x), \end{cases} \qquad (7)$$
    where $(\tilde{\mathcal{F}}(x), \tilde{\mathcal{G}}(x))$ forms a partition of $[1:n]$ with $\tilde{\mathcal{F}}(x) \supseteq \mathcal{F}(x)$ and $\tilde{\mathcal{G}}(x) \supseteq \mathcal{G}(x)$.



The (semismooth Newton/Newton-min) direction can be an ascent direction for θ

Consider the LCP (3), which is $0 \leqslant x \perp (Mx + q) \geqslant 0$, with

$$M = \begin{pmatrix} 1 & 4 \\ 0 & 1 \end{pmatrix}, \qquad q = \begin{pmatrix} -4 \\ -2 \end{pmatrix}, \quad x = \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \quad \text{so that} \quad Mx + q = \begin{pmatrix} -2 \\ -1 \end{pmatrix}. \qquad (8)$$

One has $\mathcal{E}(x) = \{1\}$, $\mathcal{F}(x) = \{2\}$, $\mathcal{G}(x) = \varnothing$.

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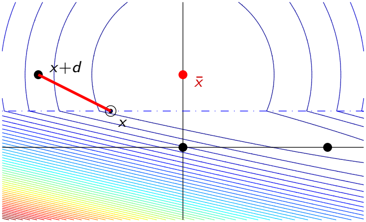
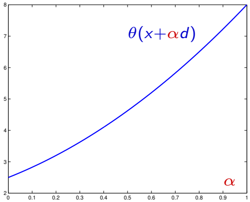
Take $\tilde{\mathcal{F}}(x) = \{1, 2\}$ and $\tilde{\mathcal{G}}(x) = \varnothing$ in (7), then d is an ascent direction of θ at x:





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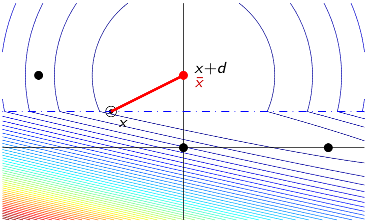
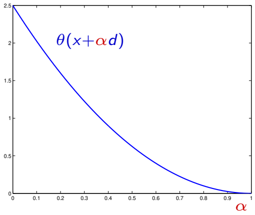
One has $\mathcal{E}(x) = \{1\}$, $\mathcal{F}(x) = \{2\}$, $\mathcal{G}(x) = \varnothing$.

Take $\tilde{\mathcal{F}}(x) = \{2\}$ and $\tilde{\mathcal{G}}(x) = \{1\}$ in (7), then d is a descent direction of θ at x:





Outline

Orientation

Slightly modify the plain Newton-min direction such that:

- ⊕⊖ it computes a point in a convex polyhedron (harder than a LS, easier than an LCP):
  - ⊕ very few inequalities define the convex polyhedron,
  - ⊖ the computation of d is more expensive, but polynomial,
  - ⊕ there is a bypass that accepts the plain NM direction most of the iterations,
- ⊕ it becomes a descent direction of θ,
- ⊕ it yields some global convergence.

Ensuring descent

For the quadratic merit function $\theta(x) = \frac{1}{2}\|H(x)\|^2 = \frac{1}{2}\|\min(F(x), G(x))\|^2$, one has

$$\begin{aligned}\theta'(x;d) &= H(x)^\mathsf{T} H'(x;d)\\ &= F_{\mathcal{F}(x)}(x)^\mathsf{T} F'_{\mathcal{F}(x)}(x)d + G_{\mathcal{G}(x)}(x)^\mathsf{T} G'_{\mathcal{G}(x)}(x)d + F_{\mathcal{E}(x)}(x)^\mathsf{T} \min(F'_{\mathcal{E}(x)}(x)d, G'_{\mathcal{E}(x)}(x)d).\end{aligned}$$

If $(F(x) + F'(x)d)_{\mathcal{F}(x)} = 0$ and $(G(x) + G'(x)d)_{\mathcal{G}(x)} = 0$, it follows

$$\begin{aligned}\theta'(x;d) =& -\|F_{\mathcal{F}(x)}(x)\|^2 - \|G_{\mathcal{G}(x)}(x)\|^2 - \|F_{\mathcal{E}(x)}(x)\|^2\\ &+ F_{\mathcal{E}(x)}(x)^\mathsf{T} \min(F_{\mathcal{E}(x)}(x) + F'_{\mathcal{E}(x)}(x)d, G_{\mathcal{E}(x)}(x) + G'_{\mathcal{E}(x)}(x)d)\\ =& -2\,\theta(x) + F_{\mathcal{E}(x)}(x)^\mathsf{T} \min(F_{\mathcal{E}(x)}(x) + F'_{\mathcal{E}(x)}(x)d, G_{\mathcal{E}(x)}(x) + G'_{\mathcal{E}(x)}(x)d).\end{aligned}$$

How can we get $\theta'(x;d) < 0$ when $\theta(x) \neq 0$?

- If $F_i(x) = G_i(x) \geqslant 0$, the last term is $\leqslant 0$ when
  $$F_i(x) + F_i'(x)d = 0 \quad \text{or} \quad G_i(x) + G_i'(x)d = 0.$$
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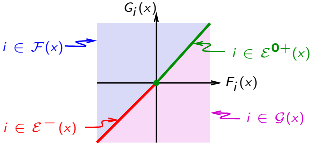
This leads to the following direction definition.

Plain polyhedral Newton-min direction

A *plain polyhedral Newton-min* (plain PNM) *direction* is a direction d that satisfies

$$\begin{cases} F_i(x) + F_i'(x)d = 0 & \text{if } i \in \mathcal{F}(x) \cup \mathcal{E}_{\mathcal{F}}^{0+}(x) \\ G_i(x) + G_i'(x)d = 0 & \text{if } i \in \mathcal{G}(x) \cup \mathcal{E}_{\mathcal{G}}^{0+}(x) \\ F_i(x) + F_i'(x)d \geqslant 0 & \text{if } i \in \mathcal{E}^{-}(x) \\ G_i(x) + G_i'(x)d \geqslant 0 & \text{if } i \in \mathcal{E}^{-}(x), \end{cases}$$



where $(\mathcal{E}_{\mathcal{F}}^{0+}(x), \mathcal{E}_{\mathcal{G}}^{0+}(x))$ is a partition of

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and

$$\mathcal{E}^{-}(x) := \{i \in [1:n] : F_i(x) = G_i(x) < 0\}.$$

Features of the algorithm:

- ⊖ d must be found in a convex polyhedron (instead of the solution to a LS),
- ⊕ the number of inequalities $2|\mathcal{E}^{-}(x)|$ should be very small (in exact arithmetic!),
- ⊕ can be computed in polynomial time (by LO or QO),
- ⊕ there is a bypass to avoid this computation most of the time (see below),
- ⊕ d is a descent direction of θ,
- ⊖ we were not able to prove global convergence with that d.

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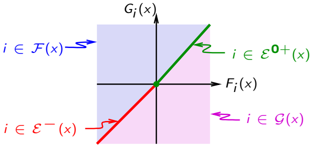

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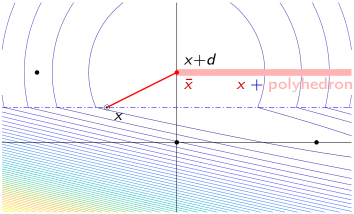
- ⊖ we were not able to prove global convergence with that d.

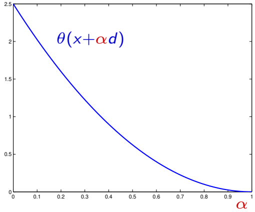
Behavior on the baby problem (8)

Since $\mathcal{E}(x) = \{1\}$, $\mathcal{F}(x) = \{2\}$, $\mathcal{G}(x) = \varnothing$, the algorithm computes the solution to

$$\begin{cases} \min \ \frac{1}{2}\,\|d\|_2^2 \\ M_{2:}\,d + y_2 = 0 \\ M_{1:}\,d + y_1 \geqslant 0 \\ d_1 + x_1 \geqslant 0 \end{cases} \qquad \text{or} \qquad \begin{cases} \min \ \frac{1}{2}\,(d_1^2 + 1) \\ d_1 \geqslant 2, \end{cases} \quad d_2 = 1.$$

A little by chance, it is the right direction $d = (2, 1)$.





Difficulty with global convergence

Let $\bar{x}$ be an accumulation point of the sequence $\{x_k\}_{k\geqslant 1}$ (it may not exist) generated by

$$x_{k+1} := x_k + \alpha_k d_k$$

where $\alpha_k > 0$ is the largest stepsize of the form 2^{-i} for $i \in \mathbb{N}$ such that

$$\theta(x_k + \alpha_k d_k) \leqslant \theta(x_k) + 10^{-4}\alpha_k(\text{"sth negative"}). \tag{9a}$$

We want to show that $\bar{x}$ is a solution of the NLCP (with a regularity assumption).

- If $\limsup_k \alpha_k > 0$, it is easy to show that $\theta(x_k) \downarrow 0$ and that $\bar{x}$ is a solution.
- If $\limsup_k \alpha_k = 0$, it is more difficult.

  Necessarily (9a) is not satisfied for $\check{\alpha}_k = 2\alpha_k$:

$$\theta(x_k + \check{\alpha}_k d_k) > \theta(x_k) + 10^{-4}\check{\alpha}_k(\text{"sth negative"}). \tag{9b}$$

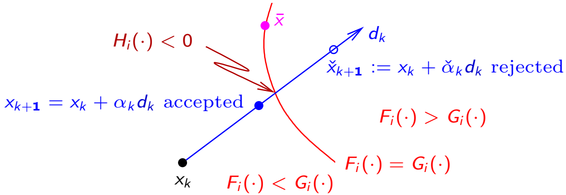
  To get convergence, it is necessary to get information from both (9a) and (9b).

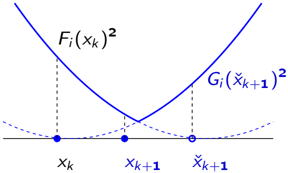
Difficulty with global convergence (negative kink)

- Near a negative kink, one can have with $\check{x}_{k+1} := x_k + \check{\alpha}_k d_k$:

$$F_i(x_{k+1}) < G_i(x_{k+1}) < 0, \qquad 0 > F_i(\check{x}_{k+1}) > G_i(\check{x}_{k+1}),$$

$$0 < H_i(x_{k+1})^2 = F_i(x_{k+1})^2, \qquad 0 < H_i(\check{x}_{k+1})^2 = G_i(\check{x}_{k+1})^2 > F_i(\check{x}_{k+1})^2.$$





- Hence $\check{x}_{k+1}$ is rejected because of $G_i(\check{x}_{k+1})^2$, but one has no information on $G_i(x_k) + G_i'(x_k)d_k$.

- Remedy: for x_k near a <u>negative</u> kink of H,

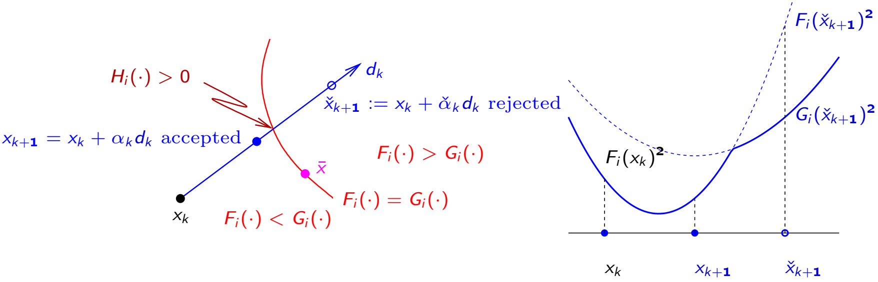
$$F_i(x_k) + F_i'(x_k)d_k = 0 \quad \curvearrowright \quad \begin{cases} F_i(x_k) + F_i'(x_k)d_k \geqslant 0 \\ G_i(x_k) + G_i'(x_k)d_k \geqslant 0. \end{cases}$$

Difficulty with global convergence (positive kink)

- Near a positive kink, one can have with $\check{x}_{k+1} := x_k + \check{\alpha}_k d_k$:

$$0 < F_i(x_{k+1}) < G_i(x_{k+1}), \qquad F_i(\check{x}_{k+1}) > G_i(\check{x}_{k+1}) > 0,$$

$$0 < H_i(x_{k+1})^2 = F_i(x_{k+1})^2, \qquad 0 < H_i(\check{x}_{k+1})^2 = G_i(\check{x}_{k+1})^2 < F_i(\check{x}_{k+1})^2.$$



- Hence $\check{x}_{k+1}$ is rejected because of $G_i(\check{x}_{k+1})^2$ and would also be rejected because of $F_i(\check{x}_{k+1})^2$.

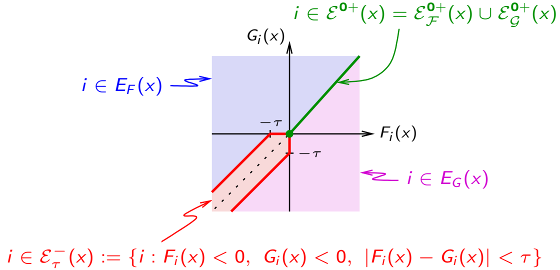
- Since we have information on $F_i(x_k) + F_i'(x_k)d_k = 0$, there's no need for a remedy.

Secure polyhedral Newton-min algorithm

A *secure polyhedral Newton-min* (PNM) *direction* is a direction d satisfying

$$\left\{\begin{array}{ll} F_i(x)+F_i'(x)d=0 & \text{if } i\in E_F(x):=\left[\mathcal{F}(x)\setminus\mathcal{E}_\tau^-(x)\right]\cup\mathcal{E}_{\mathcal{F}}^{\mathbf{0}+}(x)\\ G_i(x)+G_i'(x)d=0 & \text{if } i\in E_G(x):=\left[\mathcal{G}(x)\setminus\mathcal{E}_\tau^-(x)\right]\cup\mathcal{E}_{\mathcal{G}}^{\mathbf{0}+}(x)\\ F_i(x)+F_i'(x)d\geqslant 0 & \text{if } i\in I(x):=\mathcal{E}_\tau^-(x)\\ G_i(x)+G_i'(x)d\geqslant 0 & \text{if } i\in I(x):=\mathcal{E}_\tau^-(x), \end{array}\right. \tag{10}$$

where, for some kink tolerance parameter $\tau\in(0,\infty)$,



PNM regularity condition

- The usual regularity at a limit point $\bar{x}$ assumes that the system to solve has a solution, whatever the vectors defining it are.
- Here, there must be a d satisfying the system below, whatever $F_i(\bar{x})$, $G_i(\bar{x})$, $F_i(\bar{x})$, $G_i(\bar{x})$ are:

$$\begin{cases} F_i(\bar{x}) + F_i'(\bar{x})d = 0 & \text{if } i \in E_F(\bar{x}) \\ G_i(\bar{x}) + G_i'(\bar{x})d = 0 & \text{if } i \in E_G(\bar{x}) \\ F_i(\bar{x}) + F_i'(\bar{x})d \geqslant 0 & \text{if } i \in I(\bar{x}) \\ G_i(\bar{x}) + G_i'(\bar{x})d \geqslant 0 & \text{if } i \in I(\bar{x}). \end{cases}$$

- This is guaranteed by the Mangasarian-Fromovitz "constraint qualification" (MFCQ):

$$\textstyle\sum_{i\in E_F(\bar{x})} \alpha_i \nabla F_i(\bar{x}) + \sum_{i\in E_G(\bar{x})} \beta_i \nabla G_i(\bar{x}) + \sum_{i\in I(\bar{x})} \big[\alpha_i \nabla F_i(\bar{x}) + \beta_i \nabla G_i(\bar{x})\big] = 0$$

and $(\alpha_{I(\bar{x})}, \beta_{I(\bar{x})}) \geqslant 0$ imply that $(\alpha, \beta) = 0$.

- Must be reinforced to have a "diffusion property" near $\bar{x}$ (difficulty with the index sets that change with $\bar{x}$). This yields the PNM regularity. Ensures
  - existence of a d satisfying (10) for x near $\bar{x}$,
  - boundedness of the d's.

Features of the PNM algorithm:

- $\ominus$ d must be found in a convex polyhedron (instead of the solution to a LS),
- $\oplus$ the number of inequalities $2|\mathcal{E}_\tau^-(x)|$ should be very small ($\tau > 0$ can be very small),
- $\oplus$ can be computed in polynomial time (by LO or QO),
- $\oplus$ there is a bypass to avoid this computation most of the time (see below),
- $\oplus$ d is a descent direction of θ,
- $\oplus$ global convergence.

Theorem (global convergence of the PNM algorithm)

If
- *F and $G : \Omega \to \mathbb{R}^n$ are differentiable,*
- *the PNM algorithm generates a sequence $\{x_k\} \subseteq \Omega$,*
- *$\bar{x} \in \Omega$ is an accumulation point of $\{x_k\}$ that is PNM regular,*
- *F' and G' are continuous at $\bar{x}$,*

then, $\{\theta(x_k)\}_{k \geqslant 1} \downarrow 0$ and $\bar{x}$ is a solution to the NLCP (2).

Acceptation criterion (sufficient decrease condition)

One Looks for a criterion for accepting the cheap plain Newton-min direction (7).

- Newton direction for smooth H satisfies $\theta'(x;d) = -2\theta(x)$, hence requiring for some $\eta \in (0,1)$:

  $\theta'(x;d) \leqslant -2(1-\eta)\theta(x) \qquad \longrightarrow \qquad$ not strong enough to get global convergence.

- One requires instead, for some $\eta \in (0,1)$, close to 1:

$$\underbrace{-\sum_{i\in[1:n]} (1-\rho_i(x,d))\, H_i(x)^2}_{\text{upper bound on } \theta'(x;d)} \leqslant -2(1-\eta)\,\theta(x), \tag{11}$$

where

$$\rho_i(x,d) := \begin{cases} \frac{F_i(x)+F_i'(x)d}{F_i(x)} & \text{if } i \in E_F(x) \text{ and } F_i(x) \neq 0 \\ 0 & \text{if } i \in E_F(x) \text{ and } F_i(x) = 0 \\ \frac{G_i(x)+G_i'(x)d}{G_i(x)} & \text{if } i \in E_G(x) \text{ and } G_i(x) \neq 0 \\ 0 & \text{if } i \in E_G(x) \text{ and } G_i(x) = 0 \\ \max\left(\frac{F_i(x)+F_i'(x)d}{F_i(x)}, \frac{G_i(x)+G_i'(x)d}{G_i(x)}\right) & \text{if } i \in I(x), \end{cases}$$

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where

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Hybrid polyhedral Newton-min algorithm

Hybrid Polyhedral NM algorithm (HPNM)

- If the plain Newton-min direction d in (7) satisfies (11), take it (very cheap),
- Else take the secure polyhedral Newton-min direction d (more expensive).

Features of the HPNM algorithm:

- ⊕ in most iterations, a plain NM direction (7) is computed (a single LS to solve),
- ⊕ the number of inequalities $2|\mathcal{E}_\tau^-(x)|$ should be very small ($\tau > 0$ can be very small),
- ⊕ can be computed in polynomial time (by LO or QO),
- ⊕ d is a decrease direction of θ,
- ⊕ global convergence.

Theorem (global convergence of the HPNM algorithm)

If
- *F and $G : \Omega \to \mathbb{R}^n$ are differentiable,*
- *the HPNM algorithm generates a sequence $\{x_k\} \subseteq \Omega$,*
- *$\bar{x} \in \Omega$ is an accumulation point of $\{x_k\}$ that is NM and PNM regular,*
- *F' and G' are continuous at $\bar{x}$,*

then, $\{\theta(x_k)\}_{k \geqslant 1} \downarrow 0$ and $\bar{x}$ is a solution to the NLCP (2).

Outline

Comparison of 3 solvers [40]

- PNM (Polyhedral Newton-Min algorithm [26, 17])
  - Direction determined by solving the quadratic optimization problem (QP)

$$\min \frac{1}{2}\|d\|_2^2 \text{ s.t. } \begin{cases} F_i(x) + F_i'(x)d = 0 & \text{if } i \in E_F(x) \\ G_i(x) + G_i'(x)d = 0 & \text{if } i \in E_G(x) \\ F_i(x) + F_i'(x)d \geqslant 0 & \text{if } i \in I(x) \\ G_i(x) + G_i'(x)d \geqslant 0 & \text{if } i \in I(x). \end{cases} \tag{12}$$

  - Kink tolerance τ determined to try to have $|\mathrm{qp}| \leqslant 10$.

- HPNM (Hybrid Polyhedral Newton-Min algorithm [26, 17])
  - Take the plain Newton-min direction if it satisfies the sufficient decrease criterion (11).
  - Otherwise, take the minimum-norm PNM direction (12).
  - Kink tolerance τ determined to try to have $|\mathrm{qp}| \leqslant 10$.

- PATH (pathlcp)
  - The reference CP solver by Dirkse, Ferris, Li, Munson [27, 35, 36, 50].
  - Uses the normal map reformulation [62]: x solves (2) if and only if (x, z) solves

$$F(x) = z^+ \quad \text{and} \quad G(x) = z^-.$$

Dense random problems

Dense random problems of Harker and Pang [43]

- $M = A^{\mathsf{T}}A + \mathrm{Diag}(d) + Z \in \mathbf{P}$, with random $A \in \mathbb{R}^{n\times n}$, $d \in \mathbb{R}^n_{++}$, and $Z \in \mathcal{Z}^n$.
- q such that $0 = x_A < y_A$, $x_I > y_I = 0$, $x_E = y_E = 0$ where na $:= |A|$, ni $:= |I|$, ne $:= |E|$ are given.

			PNM					HPNM					PATH
n	na	ni	iter	#qp	|qp|	α	sec	iter	#qp	|qp|	α	sec	sec
512	128	256	29	27	7.8	$3\,10^{-1}$	0.81	6	4	8.5	$1\,10^{-0}$	0.61	0.21
1024	256	512	47	45	7.9	$2\,10^{-1}$	1.46	7	5	9.0	$1\,10^{-0}$	0.61	1.55
2048	512	1024	62	60	9.6	$1\,10^{-1}$	5.17	7	4	10.0	$1\,10^{-0}$	1.04	7.26
4096	1024	2048	134	132	8.8	$4\,10^{-2}$	57.30	8	1	10.0	$1\,10^{-0}$	3.14	45.10
8192	2048	4096	223	221	9.4	$3\,10^{-2}$	700.14	7	0	–	$1\,10^{-0}$	14.96	233.10
16384	4096	8192	425	423	9.9	$1\,10^{-2}$	9516.20	7	0	–	$1\,10^{-0}$	100.08	stuck!
$O(n^p)$ with $p =$			0.78				2.79	0.04				1.49	2.51

#qp = number of QP's, |qp| = mean size of the QP's, α = $\log_{10}$-mean stepsize, sec = tic-toc time

Academic difficult problems (Murty [54])

Problem yielding exponential complexity of the Lemke algorithms for an LCP with a **P**-matrix:

$$M = L_M := \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 2 & 1 & 0 & \ddots \\ 2 & 2 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} \in \mathbf{P}, \qquad q = -e, \qquad \text{and} \qquad x_1 = 0. \tag{13}$$

Murty problem (S2)

		PNM					HPNM					PATH
n	sec	iter	#qp	|qp|	α	sec	iter	#qp	|qp|	α	sec	sec
512	0.00	396	394	9.8	$1\,10^{-2}$	2.65	480	49	9.7	$1\,10^{-2}$	1.66	0.03
1024	0.02	1094	1092	9.9	$3\,10^{-3}$	8.07	1061	142	10.0	$4\,10^{-3}$	5.03	0.13
2048	0.08	1850	1848	9.9	$2\,10^{-3}$	27.88	2421	412	10.0	$1\,10^{-3}$	32.98	0.63
4096	0.55	3951	3949	10.0	$1\,10^{-3}$	224.11	5821	1494	10.0	$4\,10^{-4}$	340.30	2.44
8192	2.67	7756	7754	10.0	$5\,10^{-4}$	2864.29	12880	4032	10.0	$1\,10^{-4}$	5905.34	13.10
$O(n^p)$, $p =$		1.04				2.50	1.19				2.97	2.18

#qp = number of QP's, |qp| = mean size of the QP's, α = $\log_{10}$-mean stepsize, sec = tic-toc time

Academic difficult problems (Fathi [33, 30])

Problem yielding exponential complexity of the Lemke algorithms for an LCP with a **PD**-matrix:

$$M = L_M L_M^{\mathsf{T}} \in \mathbf{PD}, \qquad q = -e, \qquad \text{and} \qquad x_1 = 0, \tag{14}$$

Fathi problem (S2)

		PNM					HPNM					PATH
n	sec	iter	#qp	|qp|	α	sec	iter	#qp	|qp|	α	sec	sec
512	0.00	255	214	5.9	$2\,10^{-2}$	2.07	248	18	10.0	$2\,10^{-2}$	1.57	2.08
1024	0.02	468	318	5.9	$1\,10^{-2}$	4.98	430	12	10.0	$2\,10^{-2}$	5.08	24.86
2048	0.09	1005	686	5.7	$4\,10^{-3}$	35.67	883	20	10.0	$4\,10^{-3}$	50.71	370.13
4096	0.55	2220	1563	5.5	$1\,10^{-3}$	525.28	1488	42	10.0	$6\,10^{-3}$	340.88	2726.22
8192	2.98	5145	3369	4.4	$7\,10^{-4}$	4574.70	2844	36	10.0	$2\,10^{-3}$	4350.27	
$O(n^p)$, $p =$		1.09				2.89	0.88				2.89	3.50

#qp = number of QP's, |qp| = mean size of the QP's, α = $\log_{10}$-mean stepsize, sec = `tic-toc` time

Diphasic flow in a porous media [8]

	PNM					HPNM					PATH
n	iter	#qp	|qp|	α	sec	iter	#qp	|qp|	α	sec	sec
201	4	0	–	$1\,10^{-0}$	0.25	4	0	–	$1\,10^{-0}$	0.27	0.04
501	4	0	–	$1\,10^{-0}$	0.26	4	0	–	$1\,10^{-0}$	0.26	0.22

#qp = number of QP's, |qp| = mean size of the QP's, α = $\log_{10}$-mean stepsize, sec = tic-toc time

Outline

Conclusion

- We have proposed a means to globalize the NM/SSN algorithm for complementarity problems.
- Sometimes spectacularly efficient (random, diphasic flow, many practical applications), but not on particular problems (Murty).
- There is still much to understand and to do, but it seems worth the effort.
  - Baptiste Plaquevent-Jourdain (PhD) works on the Levenberg-Marquardt globalization (to avoid convergence to meaningless points and weaken the regularity condition).
  - A thorough experiment campaign on LCP is programmed (with Mathieu Frappier).
  - To do: asymptotic analysis of the algorithm (admissibility of the unit stepsize, quadratic convergence, finite termination on LCP(**P**)).
  - To do: robustness of the algorithm away from a regular solution (i.e., deal with the possible infeasibility of the linearized system (10)).
  - To do: application of the same solution principle to optimization.
  - To do: application of the same solution principle to other nonsmooth systems, if any.

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