Nonsmooth Semi-Newton Method in Difference Programming

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Joint work with

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Mathematical model: Nonsmooth difference programming

We consider general optimization problems of the form

$$\min_{x\in\mathbb{R}^n} \varphi(x) := g(x) - h(x),$$

where $g : \mathbb{R}^n \to \mathbb{R}$ is of class $\mathcal{C}^{1,1}$ (i.e., $\mathcal{C}^1$-smooth with locally Lipschitz derivatives), and $h : \mathbb{R}^n \to \mathbb{R}$ is a locally Lipschitzian and prox-regular function.

Definition (Poliquin–Rockafellar '96)

A function $f : \mathbb{R}^n \to \overline{\mathbb{R}}$ is prox-regular at $\bar{x} \in \mathbb{R}^n$ for $\bar{v} \in \partial f(\bar{x})$ if it is l.s.c. around $\bar{x}$ and there exist $\varepsilon > 0$ and $r \geq 0$ such that

$$f(x') \geq f(x) + \langle v, x' - x\rangle - \frac{r}{2}\|x' - x\|^2$$

whenever $x, x' \in \mathbb{B}_\varepsilon(\bar{x})$ with $f(x) \leq f(\bar{x}) + \varepsilon$ and $v \in \partial f(x) \cap \mathbb{B}_\varepsilon(\bar{v})$. If this holds for all $\bar{v} \in \partial f(\bar{x})$, f is said to be prox-regular at $\bar{x}$.

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- Every convex function is prox-regular
- Every $\mathcal{C}^2$ function is prox-regular.

Tools of Variational Analysis and Generalized Differentiation

- The limiting (Mordukhovich) subdifferential of f is denoted by $\partial f(\bar{x})$.

$$\partial f(\bar{x}) := \left\{u \in \mathbb{R}^n \;\middle|\; \exists\, x_k \to \bar{x}, f(x_k) \to f(x)\; u_k \to u,\; u_k \in \widehat{\partial} f(x_k) \text{ as } k \in \mathbb{N}\right\},$$

where

$$\widehat{\partial} f(\bar{x}) := \left\{x^* \in \mathbb{R}^n \;\middle|\; f(\bar{x}) + \langle x^*, x - \bar{x}\rangle \le f(x) + o(\|x - \bar{x}\|)\right\}.$$

Tools of Variational Analysis and Generalized Differentiation

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- Let $\varphi = g - h$ be the cost function of our problem, where g is of class $\mathcal{C}^{1,1}$ around $\bar{x} \in \mathbb{R}^n$ and h is locally Lipschitzian around $\bar{x}$ and prox-regular at $\bar{x}$. We say that $\bar{x}$ is a stationary point if $0 \in \partial\varphi(\bar{x})$.

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- We make use of the second-order subdifferential/generalized Hessian of the function $g : \mathbb{R}^n \to \mathbb{R}$ (of class $\mathcal{C}^{1,1}$) at $x \in \mathbb{R}^n$ defined by

$$\partial^2 g(x)(d) = \partial\langle d, \nabla g(\cdot)\rangle(x), \quad d \in \mathbb{R}^n.$$

If f is $\mathcal{C}^2$-smooth around x, then $\partial^2 f(x)(d) = \{\nabla^2 f(x)d\}$.

We introduce the following extension of the notion of positive-definiteness.

Definition

Let $F : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ be a set-valued mapping and $\xi \in \mathbb{R}$. Then F is ξ-lower-definite if

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- If $g : \mathbb{R}^n \to \mathbb{R}$ is strongly convex with modulus $\rho > 0$, (i.e., $g - \frac{\rho}{2}\|\cdot\|^2$ is convex), then $\partial^2 g(x)$ is ρ-lower-definite for all $x \in \mathbb{R}^n$.

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- If $F_1, F_2 : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ are ξ_1 and ξ_2-lower-definite, then the sum $F_1 + F_2$ is $(\xi_1 + \xi_2)$-lower-definite.

The algorithm...

Newton-type algorithm

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Newton's method

$$x_{k+1} = x_k + d_k, \text{ where } \nabla^2\varphi(x_k)d_k = -\nabla\varphi(x_k)$$

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Regularized coderivative-based damped semi-Newton algorithm

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Input: $x_0 \in \mathbb{R}^n$, $\beta \in (0,1)$, $\zeta > 0$, $t_{\min} > 0$, $\rho_{\max} > 0$ and $\sigma \in (0,1)$.

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

2: Take $w_k \in \partial\varphi(x_k)$. If $w_k = 0$, STOP and **return** x_k.

3: Choose $\rho_k \in [0, \rho_{\max}]$ and $d_k \in \mathbb{R}^n \backslash \{0\}$ such that

$$-w_k \in \partial^2 g(x_k)(d_k) + \rho_k d_k \quad \text{and} \quad \langle w_k, d_k \rangle \leq -\zeta \|d_k\|^2.$$

4: Choose any $\overline{\tau}_k \geq t_{\min}$. Set $\tau_k := \overline{\tau}_k$.

5: **while** $\varphi(x_k + \tau_k d_k) > \varphi(x_k) + \sigma\tau_k\langle w_k, d_k\rangle$ **do**

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Convergence to stationary points vs. critical points

Our algorithm uses $w_k \in \partial\varphi(x_k) = \nabla g(x_k) + \partial(-h)(x_k) \iff v_k := w_k - \nabla g(x_k) \in \partial(-h)(x_k)$.
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DC ALGORITHM (DCA): Let x_0 be any initial point and set $k := 0$.

1. Choose $u_k \in \partial h(x_k)$ and find a solution y_k of
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2. If $y_k = x_k \Rightarrow$ **stop** (x_k is a critical point, since $\nabla g(x_k) = \nabla g(y_k) = u_k \in \partial h(x_k)$).
Otherwise, set $x_{k+1} := y_k$, $k := k+1$ and **go to** Step 1.

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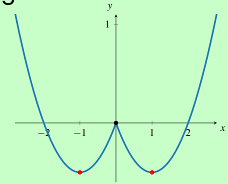
Example

Consider $\varphi = g - h$ with $g(x) := \frac{1}{2}x^2$ and $h(x) := |x|$. If an algorithm was run by using $x_0 = 0$ as the initial point but choosing $w_0 = \nabla g(x_0) - v_0$ with $v_0 = 0 \in \partial h(0)$ (instead of $w_0 \in \partial\varphi(x_0)$), it would stop and return $x = 0$, which is a critical point, but not a stationary one. On the other hand, for any $w_0 \in \partial\varphi(0) = \{-1, 1\}$ we get $w_0 \neq 0$, and so our algorithm will continue iterating until it converges to one of the two stationary points $-1/2$ and $1/2$.



Lemma (Our algorithm is well-defined)

Let $\varphi = g - h$, with $g \in \mathcal{C}^{1,1}$ and h being locally Lipschitz around $\bar{x}$ and prox-regular at this point. Assume that $\partial^2 g(\bar{x})$ is ξ-lower-definite for some $\xi \in \mathbb{R}$ and consider a nonzero subgradient $w \in \partial\varphi(\bar{x})$. Then for any $\zeta > 0$ and any $\rho \geq \zeta - \xi$, there exists a nonzero direction $d \in \mathbb{R}^n$ satisfying the inclusion

$$-w \in \partial^2 g(\bar{x})(d) + \rho d. \tag{1}$$

Moreover, any nonzero direction from (1) *obeys the conditions:*

(i) $\varphi'(\bar{x}; d) = \limsup_{t \to 0^+} \frac{\varphi(\bar{x}+td) - \varphi(\bar{x})}{t} \leq \langle w, d \rangle \leq -\zeta \|d\|^2$.

(ii) *Whenever $\sigma \in (0, 1)$, there exists $\eta > 0$ such that*

$$\varphi(\bar{x} + \tau d) < \varphi(\bar{x}) + \sigma\tau\langle w, d \rangle \leq \varphi(\bar{x}) - \sigma\zeta\tau\|d\|^2 \;\; \textit{when} \;\; \tau \in (0, \eta).$$

Example (Necessity of prox-regularity)

Let us consider the problem

$$\min_{x\in\mathbb{R}^2} \varphi(x) := \underbrace{\frac{1}{2}(Ax-b)^2}_{g(x)} - (\underbrace{\|x\|_2 - \|x\|_1}_{h(x)}), \quad x \in \mathbb{R}^2, \text{ with } A := [1,0] \text{ y } b := 1.$$

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- Let $\bar{x} := (1,0)^\top$

$$\partial\varphi(\bar{x}) = \left\{ \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}.$$

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- Take $w := (0,1)^\top \in \partial\varphi(\bar{x})$
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- Take $w := (0,1)^\top \in \partial\varphi(\bar{x})$
- Then for every $\rho > 0$, the system $-w = \nabla^2 g(\bar{x})(d) + \rho d$ has the solution $d = (0, -1/\rho)^\top$.
- Nevertheless, d is not a descend direction for $\varphi(x) = g(x) - h(x)$ at $\bar{x}$. Indeed,

$$\varphi(\bar{x} + \tau d) = 1 + \frac{\tau}{\rho} - \sqrt{1 + (\tau/\rho)^2} > \varphi(\bar{x}) = 0 \text{ for all } \tau > 0,$$

Convergence of the algorithm

Theorem 1

Let $\varphi : \mathbb{R}^n \to \mathbb{R}$ be given by $\varphi = g - h$ with $\inf \varphi > -\infty$. Pick an initial point $x_0 \in \mathbb{R}^n$ and suppose that the sublevel set $\Omega := \{x \in \mathbb{R}^n \mid \varphi(x) \leq \varphi(x_0)\}$ is closed, that g is $\mathcal{C}^{1,1}$ around every $x \in \Omega$ and $\partial^2 g(x)$ is ξ-lower-definite for all $x \in \Omega$ with some $\xi \in \mathbb{R}$, and h is locally Lipschitzian and prox-regular on Ω. Then our algorithm either stops at a stationary point, or produces sequences $\{x_k\} \subseteq \Omega$, $\{\varphi(x_k)\}$, $\{w_k\}$, $\{d_k\}$, and $\{\tau_k\}$ such that:

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Let $\varphi : \mathbb{R}^n \to \mathbb{R}$ be given by $\varphi = g - h$ with $\inf \varphi > -\infty$. Pick an initial point $x_0 \in \mathbb{R}^n$ and suppose that the sublevel set $\Omega := \{x \in \mathbb{R}^n \mid \varphi(x) \leq \varphi(x_0)\}$ is closed, that g is $\mathcal{C}^{1,1}$ around every $x \in \Omega$ and $\partial^2 g(x)$ is ξ-lower-definite for all $x \in \Omega$ with some $\xi \in \mathbb{R}$, and h is locally Lipschitzian and prox-regular on Ω. Then our algorithm either stops at a stationary point, or produces sequences $\{x_k\} \subseteq \Omega$, $\{\varphi(x_k)\}$, $\{w_k\}$, $\{d_k\}$, and $\{\tau_k\}$ such that:

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(i) The sequence $\{\varphi(x_k)\}$ monotonically decreases and converges.

(ii) If $\{x_{k_j}\}$ as $j \in \mathbb{N}$ is any bounded subsequence of $\{x_k\}$, then $\inf_{j \in \mathbb{N}} \tau_{k_j} > 0$,

$$\sum_{j \in \mathbb{N}} \|d_{k_j}\|^2 < \infty, \quad \sum_{j \in \mathbb{N}} \|x_{k_j+1} - x_{k_j}\|^2 < \infty, \quad \text{and} \quad \sum_{j \in \mathbb{N}} \|w_{k_j}\|^2 < \infty.$$

Then, boundedness of the entire sequence $\{x_k\}$ ensures that the set of accumulation points of $\{x_k\}$ is nonempty, closed and connected.

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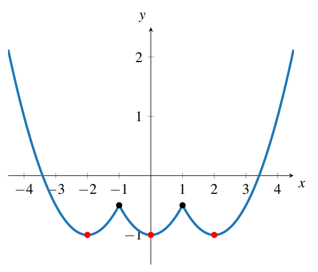
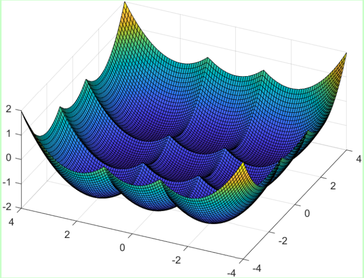
(iv) If $\{x_k\}$ has an isolated accumulation point $\bar{x}$, then the entire sequence $\{x_k\}$ converges to $\bar{x}$ as $k \to \infty$, where $\bar{x}$ is a stationary point.

Example (An illustrative example)

$$\varphi(x) := \sum_{i=1}^{n} \varphi_i(x_i), \text{ where } \varphi_i(x_i) := g_i(x_i) - h_i(x_i) \text{ with } g_i(x_i) := \frac{1}{2}x_i^2 \text{ and } h_i(x_i) := |x_i| + |1 - |x_i||$$

Then, φ satisfies the assumptions of the previous theorem with $g(x) := \sum_{i=1}^{n} g_i(x_i)$, $h(x) := \sum_{i=1}^{n} h_i(x_i)$ and $\xi = 1$. The points $\{-2,-1,0,1,2\}^n$ are critical points, but the stationary points, which are also the global minima, are only the points in the set $\{-2,0,2\}^n$. Therefore, our algorithm will return a global minimum starting from any initial point.





Example

Consider the function $\varphi : \mathbb{R} \to \mathbb{R}$ given by

$$\varphi(x) := \int_0^x t^4 \sin\left(\frac{\pi}{t}\right) dt.$$

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- Observe furthermore that φ is a DC function because it is $\mathcal{C}^2$.
- However, it is not possible to write its DC decomposition with $g(x) = \varphi(x) + ax^2$ and $h(x) = ax^2$ for $a > 0$, since there exists no scalar $a > 0$ such that the function $g(x) = \varphi(x) + ax^2$ is convex on the entire real line.
- Therefore, we cannot apply DCA with the decomposition $g(x) = \varphi(x) + ax^2$ and $h(x) = ax^2$ for $a > 0$.

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Consider the function $\varphi : \mathbb{R} \to \mathbb{R}$ given by

$$\varphi(x) := \int_0^x t^4 \sin\left(\frac{\pi}{t}\right) dt.$$

- φ is coercive, and satisfies the assumption of Theorem 1 over the level set $\Omega = \{x \mid \varphi(x) \le \varphi(x_0)\}$ with $g(x) := \varphi(x)$ and $h(x) := 0$.
- The stationary points of φ are described by $S := \left\{\frac{1}{n} \;\middle|\; n \in \mathbb{Z}\backslash\{0\}\right\} \cup \{0\}$.
- If Algorithm 1 generates an iterative sequence $\{x_k\}$ starting from x_0, then the accumulation points form by Theorem 1 a nonempty, closed, and connected set $A \subseteq S$
- If $A = \{0\}$, the sequence $\{x_k\}$ converges to $\bar{x} = 0$. If A contains any point of the form $\bar{x} = \frac{1}{n}$, then it is an isolated point, and Theorem 1 tells us that the entire sequence $\{x_k\}$ converges to that point, and consequently we have $A = \{\bar{x}\}$.

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Regularized coderivative-based damped semi-Newton algorithm

What about the rate of convergence?

$$\min_{x\in\mathbb{R}^n} \varphi(x) := g(x) - h(x)$$

Input: $x_0 \in \mathbb{R}^n$, $\beta \in (0,1)$, $\zeta > 0$, $t_{\min} > 0$, $\rho_{\max} > 0$ and $\sigma \in (0,1)$.

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

  Take $w_k \in \partial\varphi(x_k)$. If $w_k = 0$, STOP and **return** x_k.

  Choose $\rho_k \in [0, \rho_{\max}]$ and $d_k \in \mathbb{R}^n \setminus \{0\}$ such that

$$-w_k \in \partial^2 g(x_k)(d_k) + \rho_k d_k \quad \text{and} \quad \langle w_k, d_k \rangle \leq -\zeta \|d_k\|^2.$$

  Choose any $\overline{\tau}_k \geq t_{\min}$. Set $\tau_k := \overline{\tau}_k$.

  while $\varphi(x_k + \tau_k d_k) > \varphi(x_k) + \sigma\tau_k \langle w_k, d_k \rangle$ **do**

    $\tau_k = \beta\tau_k$.

  end while

  Set $x_{k+1} := x_k + \tau_k d_k$.

end for

Definition

Let $\{x_k\}$ be a sequence in $\mathbb{R}^n$ converging to $\bar{x}$ as $k \to \infty$. The convergence rate is said to be:

(i) *R-linear* if there exist $\mu \in (0,1), c > 0$, and $k_0 \in \mathbb{N}$ such that

$$\|x_k - \bar{x}\| \leq c\mu^k \text{ for all } k \geq k_0.$$

(ii) *Q-linear* if there exists $\mu \in (0,1)$ such that

$$\limsup_{k\to\infty} \frac{\|x_{k+1} - \bar{x}\|}{\|x_k - \bar{x}\|} = \mu.$$

(iii) *Q-superlinear* if it is Q-linear for all $\mu \in (0,1)$, i.e., if

$$\lim_{k\to\infty} \frac{\|x_{k+1} - \bar{x}\|}{\|x_k - \bar{x}\|} = 0.$$

(iv) *Q-quadratic* if we have

$$\limsup_{k\to\infty} \frac{\|x_{k+1} - \bar{x}\|}{\|x_k - \bar{x}\|^2} < \infty.$$

Linear and superlinear convergence under additional assumptions

Corollary 1

In addition, suppose that $\{x_k\}$ has an accumulation point $\bar{x}$ such that $\partial\varphi$ is strongly metrically subregular at $(\bar{x}, 0)$. Then the entire sequence converges to $\bar{x}$, with Q-linear convergence rate for $\{\varphi(x_k)\}$ and R-linear convergence rate for $\{x_k\}$ and $\{w_k\}$.

- A set-valued mapping $F : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ is said to be strongly metrically subregular at $(\bar{x}, \bar{y}) \in \operatorname{gph} F$ if there are $\kappa > 0$ and $\varepsilon > 0$ such that
$$\|x - \bar{x}\| \leq \kappa\|y - \bar{y}\|, \text{ for all } (x, y) \in \mathbb{B}_\varepsilon(\bar{x}, \bar{y}) \cap \operatorname{gph} F.$$

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$$\|x - \bar{x}\| \leq \kappa\|y - \bar{y}\|, \text{ for all } (x, y) \in \mathbb{B}_\varepsilon(\bar{x}, \bar{y}) \cap \operatorname{gph} F.$$
- A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is calm at $\bar{x} \in \mathbb{R}^n$ with modulus $\kappa \geq 0$ if there is $\varepsilon > 0$ s.t.
$$\|f(x) - f(\bar{x})\| \leq \kappa\|x - \bar{x}\|, \text{ for all } x \in \mathbb{B}_\varepsilon(\bar{x}).$$
- A function $g : \mathbb{R}^n \to \mathbb{R}$ is semismoothly differentiable at $\bar{x}$ if it is $\mathcal{C}^{1,1}$ around $\bar{x}$, its gradient mapping ∇g is directionally differentiable at this point, and
$$\lim_{\substack{\bar{x} \neq x \to \bar{x} \\ w \in \partial^2 g(x)(\bar{x} - x)}} \frac{\nabla g(x) - \nabla g(\bar{x}) + w}{\|x - \bar{x}\|} = 0.$$

Superlinear and quadratic convergence for pointwise maximum of affine functions

Corollary 2

In addition to the assumptions of Theorem 1, assume that $\xi > 0$, $0 < \zeta \leq \xi$, $\sigma \in (0, \frac{1}{2})$, $t_{\min} = 1$, and $\rho_k = 0$ for all $k \in \mathbb{N}$. Suppose also that the sequence $\{x_k\}$ generated has an accumulation point $\bar{x}$ at which g is semismoothly differentiable and h can be represented as

$$h(x) = \max_{i=1,\ldots,p} \{\langle x_i^*, x\rangle + \alpha_i\} \quad \text{for all } x \in \mathbb{B}_\varepsilon(\bar{x}),$$

for some $(x_i^*, \alpha_i)_{i=1}^p \subseteq \mathbb{R}^n \times \mathbb{R}$ and $\varepsilon > 0$. Then $x_k \to \bar{x}$, $\varphi(x_k) \to \varphi(\bar{x})$, $w_k \to 0$, and $\nabla g(x_k) \to \nabla g(\bar{x})$ as $k \to \infty$ with at least Q-superlinear rate. If in addition g is of class $\mathcal{C}^{2,1}$ around $\bar{x}$, then the rate of convergence is at least quadratic.

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Example

These assumptions do not imply the smoothness of φ at stationary points. For instance, consider the nonconvex function $\varphi : \mathbb{R}^n \to \mathbb{R}$ defined as in our previous example but letting now $h_i(x_i) := |x_i| + |1 - x_i|$. The function φ satisfies the assumptions of Corollary 2 at any of its stationary points $\{-2, 0, 2\}^n$, but φ is not differentiable at $\bar{x} = 0$.

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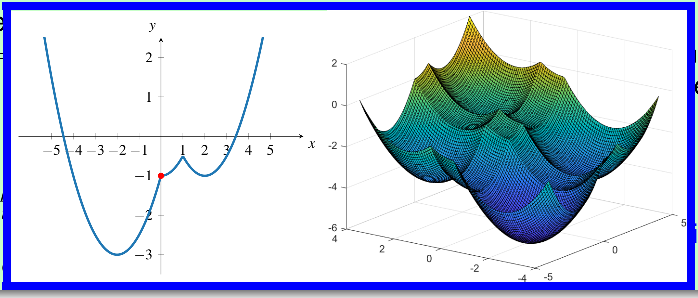

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Convergence rates under the Kurdyka–Łojasiewicz property

Kurdyka–Łojasiewicz property

The Kurdyka–Łojasiewicz property holds for φ at $\bar{x}$ if there exist $\eta > 0$ and a continuous concave function $\psi : [0, \eta] \to [0, \infty)$ with $\psi(0) = 0$ such that ψ is $\mathcal{C}^1$-smooth on $(0, \eta)$ with the strictly positive derivative ψ' and that

$$\psi'\big(\varphi(x) - \varphi(\bar{x})\big)\,\text{dist}\big(0; \partial\varphi(x)\big) \geq 1$$

for all $x \in \mathbb{B}_\eta(\bar{x})$ with $\varphi(\bar{x}) < \varphi(x) < \varphi(\bar{x}) + \eta$.

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Remark

- Every analytic function satisfies this property. More precisely, $\psi(t) = Mt^{1-\theta}$ with $M > 0$ and $\theta \in [0, 1)$. [Łojasiewicz, '65].

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- Extension to nonsmooth functions[Bolte–Daniilidis–Lewis '06].

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In addition to the assumptions of Theorem 1, suppose that the sequence $\{x_k\}$ has an accumulation point $\bar{x}$ at which the Kurdyka–Łojasiewicz property is satisfied. Then $\{x_k\}$ converges $\bar{x}$ as $k \to \infty$, which is a stationary point.

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Corollary 3

In addition, suppose that the Kurdyka–Łojasiewicz property holds at $\bar{x}$ with $\psi(t) := Mt^{1-\theta}$ for some $M > 0$ and $\theta \in [0, 1)$. The following holds:

(i) If $\theta = 0$, then the sequence $\{x_k\}$ converges in a finite number of steps.

(ii) If $\theta \in (0, 1/2]$, then the sequence $\{x_k\}$ converges at least linearly.

(iii) If $\theta \in (1/2, 1)$, then there exist $\mu > 0$ and $k_0 \in \mathbb{N}$ s.t. $\|x_k - \bar{x}\| \leq \mu k^{-\frac{1-\theta}{2\theta-1}}$ for all $k \geq k_0$.

A problem in biochemistry...

Consider a biochemical network with m molecular species and n reversible elementary reactions. Let $u \in (0, +\infty)^n$ be the vector of concentrations of molecular species, and the (deterministic) dynamic equation for the time evolution of the concentration of molecular species is given by:

$$\frac{du}{dt} = (R - F)\left[\exp(\ln(k_f) + F^\top \ln(u)) - \exp(\ln(k_r) + R^\top \ln(u))\right]$$

where

- $F, R \in \mathbb{N}^{m \times n}$ represent the direct and inverse reaction matrices.
- k_f y k_r elementary kinetic parameters.
- $\exp(\cdot)$ y $\ln(\cdot)$ denote the component-by-component functions, i.e, $\exp(u) := (\exp(u_i))_{i=1}^n$ y $\ln(u) := (\ln(u_i))_{i=1}^n$.

The investigation of stationary states plays a crucial role in the modeling of biochemical reaction systems.

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Taking $x := \ln(u)$, $w := [\ln(k_f)^\top, \ln(k_r)^\top]^\top$, $A = [F, R]$ and $B = [F, R]$

$$f(x) = (A - B)\exp\left(w + A^\top x\right)$$

Mathematical Problem

Find $x \in \mathbb{R}^n$ such that

$$\boxed{f(x) = 0}$$

Numerical experiments: Smooth DC models in biochemistry

We are interested in finding a zero of the function

$$f(x) := ([F,R] - [R,F]) \exp\left(w + [F,R]^T x\right),$$

where $F, R \in \mathbb{Z}_{\geq 0}^{m \times n}$ denote the forward and reverse stoichiometric matrices, respectively, where $w \in \mathbb{R}^{2n}$ is the componentwise logarithm of the kinetic parameters, and $\exp(\cdot)$ is the componentwise exponential function.

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$$g(x) := 2\left(\|p(x)\|^2 + \|c(x)\|^2\right) \quad \text{and} \quad h(x) := \|p(x)+c(x)\|^2,$$

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We can also decompose $\varphi(x)$ as the difference of the functions

$$g(x) := \|p(x)\|^2 + \|c(x)\|^2 \quad \text{and} \quad h(x) = 2\langle p(x), c(x)\rangle$$

with g being convex (thus, $\nabla^2 g(x)$ is 0-lower definite).

Regularized coderivative-based damped semi-Newton algorithm

$$\min_{x\in\mathbb{R}^n} \varphi(x) := g(x) - h(x)$$

Input: $x_0 \in \mathbb{R}^n$, $\beta \in (0,1)$, $\zeta > 0$, $t_{\min} > 0$, $\rho_{\max} > 0$ and $\sigma \in (0,1)$.

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

2: Take $w_k \in \partial\varphi(x_k)$. If $w_k = 0$, STOP and **return** x_k.

3: Choose $\rho_k \in [0, \rho_{\max}]$ and $d_k \in \mathbb{R}^n \backslash \{0\}$ such that

$$-w_k \in \partial^2 g(x_k)(d_k) + \rho_k d_k \quad \text{and} \quad \langle w_k, d_k\rangle \leq -\zeta \|d_k\|^2.$$

4: Choose any $\overline{\tau}_k \geq t_{\min}$. Set $\tau_k := \overline{\tau}_k$.

5: **while** $\varphi(x_k + \tau_k d_k) > \varphi(x_k) + \sigma\tau_k\langle w_k, d_k\rangle$ **do**

6: $\tau_k = \beta\tau_k$.

7: **end while**

8: Set $x_{k+1} := x_k + \tau_k d_k$.

9: **end for**

The effect of the regularization parameter ρ_k

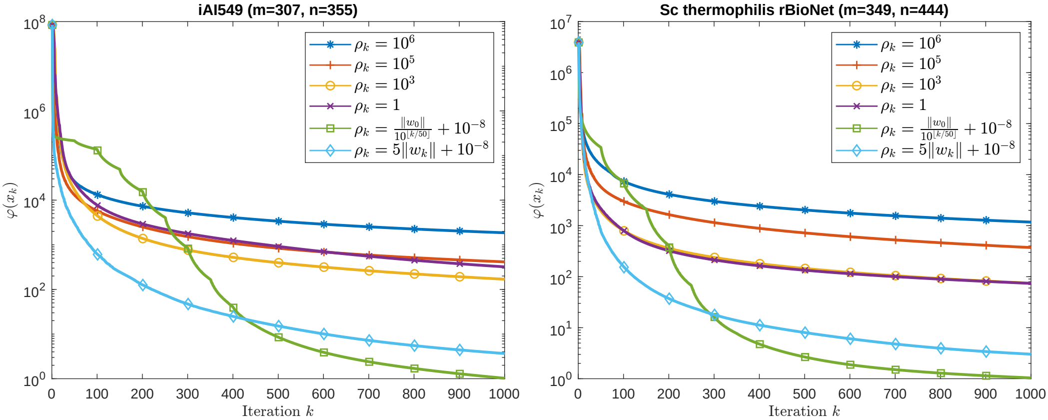

Figure: Comparison of the objective values for three strategies for setting the regularization parameter ρ_k: constant (with values 10^6, 10^5, 10^3 and 1), decreasing, and adaptive with respect to the value of $\|w_k\|$.

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  end while

  Set $x_{k+1} := x_k + \tau_k d_k$.

end for

Choosing the trial stepsize $\overline{\tau}_k$

Self-adaptive trial stepsize

Input: $\gamma > 1, \overline{\tau}_0 > 0$.

Obtain τ_0 by Steps 5-7 of the algorithms.
Set $\overline{\tau}_1 := \max\{\tau_0, t_{\min}\}$ and obtain τ_1 by Steps 5-7 of the algorithms.
for $k = 2, 3, \dots$ **do**
    if $\tau_{k-2} = \overline{\tau}_{k-2}$ **and** $\tau_{k-1} = \overline{\tau}_{k-1}$ **then**
        $\overline{\tau}_k := \gamma \tau_{k-1}$;
    else
        $\overline{\tau}_k := \max\{\tau_{k-1}, t_{\min}\}$.
    end if
    Obtain τ_k by Steps 5-7 of the algorithms.
end for

Constant vs. self-adaptive trial stepsize

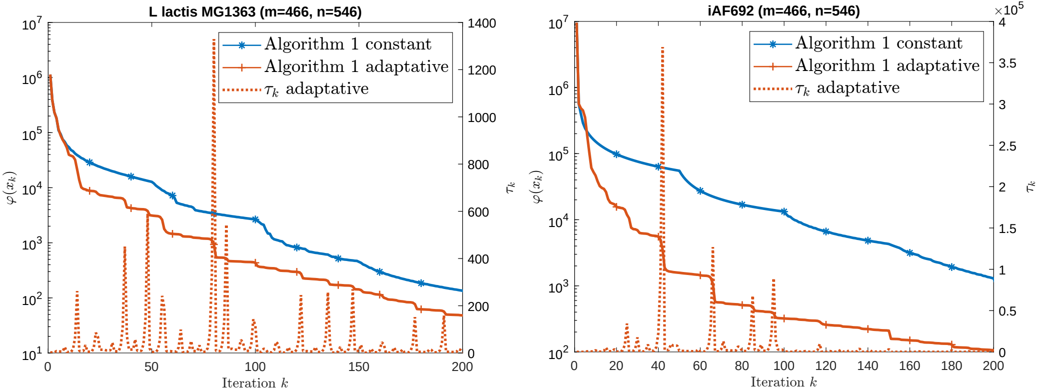


Figure: Comparison of the self-adaptive and the constant (with $\overline{\tau}_k = 50$) choices for the trial stepsizes for two biochemical models. The plots include two scales, a logarithmic one for the objective function values and a linear one for the stepsizes (which are represented with discontinuous lines).

Our algorithm vs. DCA & BDCA

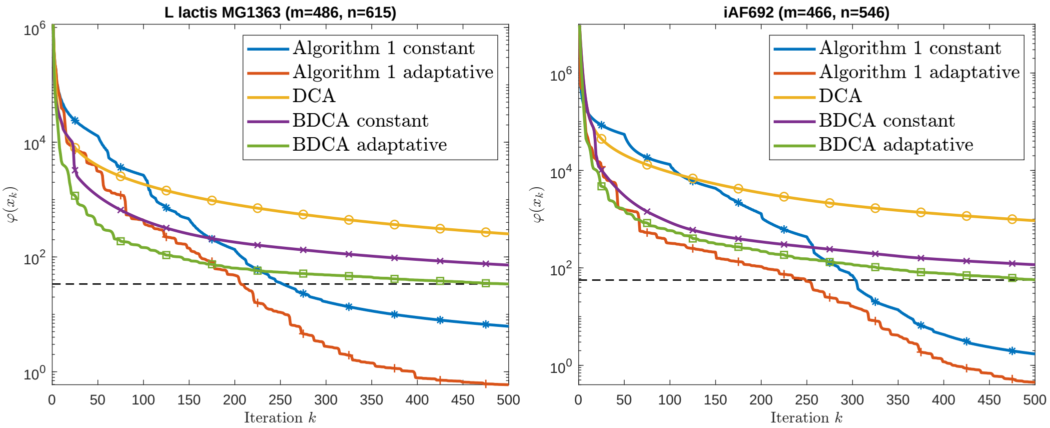
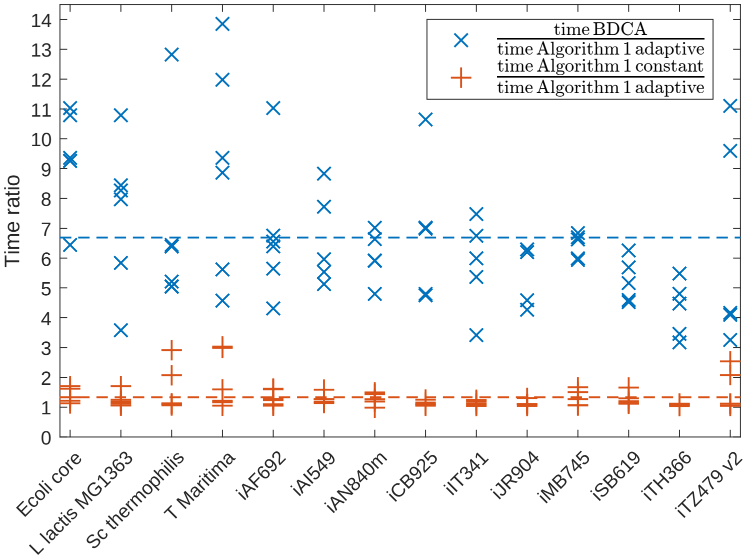
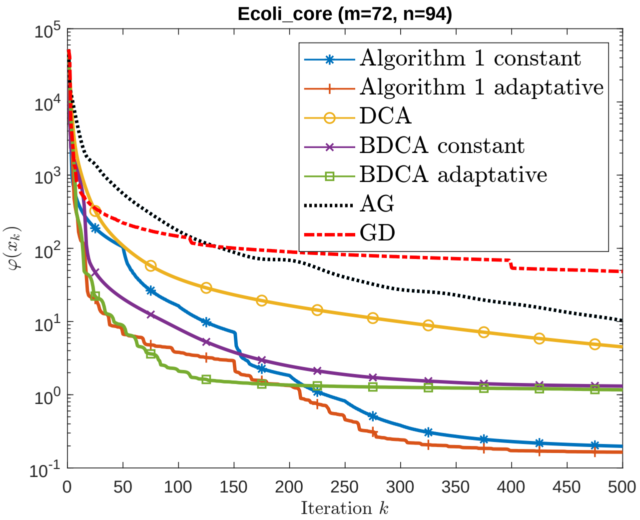


Figure: Value of the objective function (with logarithmic scale) of our algorithm, DCA and BDCA for two biochemical models. The value attained after 500 iterations of BDCA with self-adaptive stepsize is shown by a dashed line.

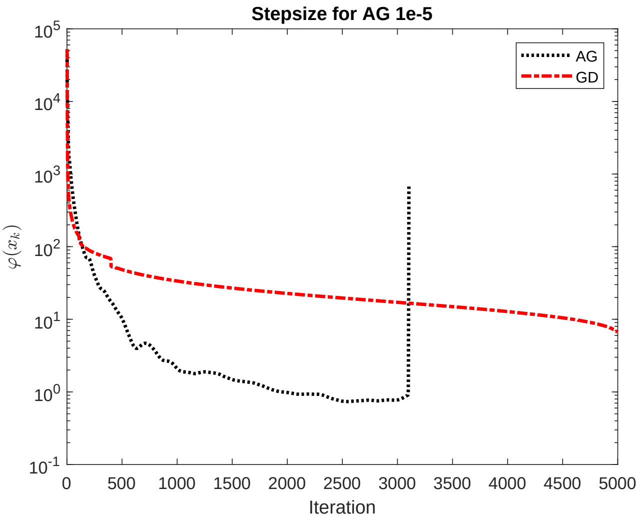
Our algorithm vs. BDCA on 14 biochemical models



Our algorithm vs. AG and GD



Our algorithm vs. AG and GD



Minimization of Piecewise Nonconvex Loss Functions

We consider the optimization problem

$$\min_{x\in\mathbb{R}^n} \varphi(x) := \frac{1}{m}\sum_{j=1}^{m} v(c_j^\top x) + \lambda\|x\|^2, \tag{2}$$

where v is a $\mathcal{C}^{1,1}$ real-valued function formed by twice differentiable pieces, where $c_j \in \mathbb{R}^n$ and $\lambda > 0$. Specifically, we consider a $\mathcal{C}^{1,1}$-smooth function $v : \mathbb{R} \to \mathbb{R}$ given by the expression

$$v(t) := v_i(t) \text{ if } t \in (t_{i-1}, t_i] \text{ and } i = 1, \ldots, p,$$

Example: binary classification

Consider the nonconvex loss function proposed in *Zhao-Mammadov-Yearwood 2010* for binary classification that is defined by

$$v(t) := \begin{cases} 1 & t < -1, \\ \frac{1}{4}t^3 - \frac{3}{4}t + \frac{1}{2} & -1 \le t \le 1, \\ 0 & t > 1. \end{cases} \tag{3}$$

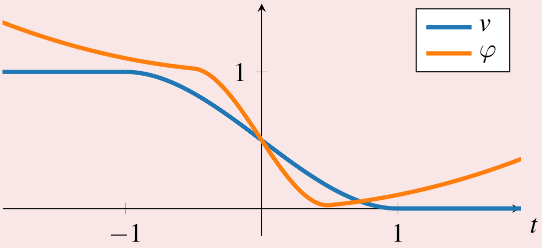


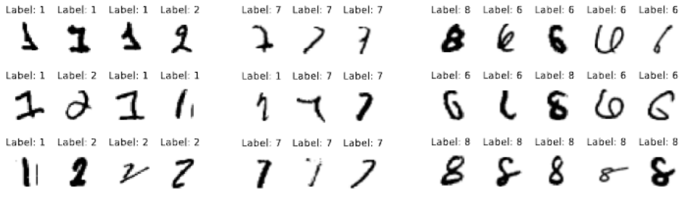
Figure: Plot of the loss function v in (3) and the objective function φ in (2) for $n = m = 1$, $c = 2$ and $\lambda = 0.1$

Experiment

The MNIST database consists of 70 000 grayscale labeled images of handwritten digits from 0 to 9 with a resolution of 28×28 pixels. The dataset is split into a training and a test set of 60 000 and 10 000 sample images, respectively. Given a pair digits d_1 and d_2, we consider problem (2) with the piecewise loss function (3) and vectors $c_j \in \mathbb{R}^{785}$ are taken as:

$$c_j := \begin{cases} \begin{bmatrix} -1 \\ -z_j \end{bmatrix} & \text{if the label of image } j \text{ is } d_1, \\ \begin{bmatrix} 1 \\ z_j \end{bmatrix} & \text{if the label of image } j \text{ is } d_2, \end{cases}$$

where z_j denotes grayscale values of the flattened images whose labels are d_1 or d_2.



(a) Digits 1 and 2 (b) Digits 1 and 7 (c) Digits 6 and 8

Results

		Success training		Success test		Time (sec.)		Iterations	
Digits	Noise	RCSN	GD	RCSN	GD	RCSN	GD	RCSN	GD
1, 2	0.01	99.72%	99.73%	99.26%	99.28%	67.7	158.2	857.9	4148.5
1, 2	0	99.71%	99.71%	99.29%	99.27%	64.3	155.2	851.9	4166.0
1, 7	0.01	99.85%	99.86%	99.36%	99.39%	51.9	149.5	673.3	3939.3
1, 7	0	99.84%	99.87%	99.40%	99.39%	46.6	162.1	591.7	4176.9
5, 6	0.01	99.27%	99.27%	98.03%	97.98%	111.8	215.4	1623.5	6404.5
5, 6	0	99.24%	99.26%	97.98%	97.99%	122.2	237.0	1732.2	6689.3
6, 8	0.01	99.70%	99.72%	99.03%	99.12%	86.9	192.1	1205.1	5452.1
6, 8	0	99.68%	99.71%	99.05%	99.04%	88.0	185.0	1243.4	5353.4

Table 1: Results of Experiment 2 for the binary classification problem on the MNIST dataset for various pairs of similar digits. We present the average values of Algorithm 1 (RCSN) and the gradient descent algorithm (GD) for 10 random starting points.

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Thank you for listening