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On complexity and convergence of high-order coordinate descent algorithms for smooth nonconvex box-constrained minimization

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Abstract
Coordinate descent methods have considerable impact in global optimization because global (or, at least, almost global) minimization is affordable for low-dimensional problems. Coordinate descent methods with high-order regularized models for smooth nonconvex box-constrained minimization are introduced in this work. High-order stationarity asymptotic convergence and first-order stationarity worst-case evaluation complexity bounds are established. The computer work that is necessary for obtaining first-order ε-stationarity with respect to the variables of each coordinate-descent block is $O(\varepsilon^{-(p+1)/p})$ whereas the computer work for getting first-order ε-stationarity with respect to all the variables simultaneously is $O(\varepsilon^{-(p+1)})$. Numerical examples involving multidimensional scaling problems are presented. The numerical performance of the methods is enhanced by means of coordinate-descent strategies for choosing initial points.

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1 Introduction

In order to minimize a multivariate function it is natural to keep fixed some of the variables and to modify the remaining ones trying to decrease the objective function value. Coordinate descent (CD) methods proceed systematically in this way and, many times, obtain nice approximations to minimizers of practical optimization problems. Wright [51] surveyed traditional approaches and modern advances on the introduction and analysis of CD methods. Although the CD idea is perhaps the most natural one to optimize functions, it received little attention from researchers due to poor performance in many cases and lack of challenges in terms of convergence theory [49]. The situation changed dramatically in the last decades. CD methods proved to be useful for solving machine learning, deep learning and statistical learning problems in which the number of variables is big and the accuracy required at the solution is moderate [17, 46]. Many applications arose and, in present days, efficient implementations and insightful theory for understanding the CD properties are the subject of intense research. See, for example, [2, 3, 14–16, 19, 27, 31, 41, 53, 54] among many others.

In this paper we are concerned with complexity issues of CD methods that employ high-order models to approximate the subproblems that arise at each iteration. The use of high-order models for unconstrained optimization was defined and analyzed from the point of view of worst-case complexity in [5] and subsequent papers [4, 23, 34, 35, 42, 55]. In [4] numerical implementations with quartic regularization were introduced. In [23], [34], [35], and [42], new high-order regularization methods were introduced with Hölder, instead of Lipschitz, conditions on the highest-order derivatives employed. In [40], high-order methods were studied as discretizations of ordinary differential equations. These methods generalize the methods based on third-order models introduced in [37] and later developed in [21, 22, 29, 30, 47] among many others. Griewank [37] introduced third-order regularization having in mind affine scaling properties. Nesterov and Polyak [47] introduced the first cubic regularized Newton methods with better complexity results than the ones that were known for gradient-like algorithms [36]. In [20], a multilevel strategy that exploits a hierarchy of problems of decreasing dimension was introduced in order to reduce the global cost of the step computation. However, high-order methods remain difficult to implement in the many-variables case due to the necessity of computing high-order derivatives and solving nontrivial model-based subproblems. Nevertheless, if the number of variables is small, high-order model-based methods are reliable alternatives to classical methods. This feature can be exploited in the CD framework.

High-order models are interesting from the point of view of global optimization because, many times, local algorithms get stuck at points that satisfy low-order optimality conditions from which one is able to escape using high-order resources. The escaping procedure is affordable if one restricts the search to low-dimensional subspaces, which suggests the employment of CD procedures.

This paper is organized as follows. In Sect. 2, we present some background on optimality conditions, while in Sect. 3 we survey a high-order algorithmic framework that provides a basis for the development of CD algorithms. In Sect. 4, we present block CD methods that,

for each approximate minimization on a group of variables, employ high-order regularized subproblems and we prove asymptotic convergence. In Sect. 5 we prove worst-case complexity results. In Sect. 6 the obtained theoretical results are discussed. In Sect. 7, we study a family of problems for which CD is suitable and we include a CD-strategy that improves convergence to global solutions. Conclusions are given in Sect. 8.
Notation. The symbol $\|\cdot\|$ denotes the Euclidean norm.

2 Background on high-order optimality conditions

In order to understand the main results of this paper we need to visit the topic of necessary optimality conditions of high order. The main question is: What is the relation between minimizers of a function and minimizers of its Taylor polynomials? Firstly, we show that, in one variable, the two concepts are closely related in the sense that local minimizers of a function are local minimizers of all its Taylor polynomials. Immediately, we show with a simple counterexample that this property is not true if the number of variables is greater than 1. The third step is to show that, for an arbitrary number of variables, every minimizer of f is a minimizer of its Taylor polynomials regularized by a suitable Lipschitz constant. This definition leads us to distinguish between exclusive and inclusive optimality conditions. Exclusive conditions are the ones that can be expressed exclusively in terms of the function derivatives. Inclusive ones are related with a slightly more global behavior and include Lipschitz bounds. Inclusive conditions are stronger than exclusive ones. In this paper, we show that algorithmic limit points are more related to inclusive conditions than to exclusive ones.

As it is well known from elementary calculus, if a function $\underline{f} : \mathbb{R} \to \mathbb{R}$ possesses derivatives up to order p at $\bar{x} \in \mathbb{R}$, denoted by $\underline{f}^{(j)}$ for $j = 1, \ldots, p$, its Taylor polynomial of order p around $\bar{x}$ is given by

$$\underline{T}_p(\bar{x}, x) = \underline{f}(\bar{x}) + \sum_{j=1}^{p} \frac{1}{j!} \underline{f}^{(j)}(\bar{x})(x - \bar{x})^j.$$

If $\underline{f}$ and its derivatives up to order p are continuous and $\underline{f}^{(p)}$ satisfies a Lipschitz condition defined by $\gamma_1 > 0$ in a neighborhood of $\bar{x}$, we know that

$$|\underline{f}(x) - \underline{T}_p(\bar{x}, x)| \leq \frac{\gamma_1}{(p+1)!} |x - \bar{x}|^{p+1} \tag{1}$$

for all x in a neighborhood of $\bar{x}$. This fact allows one to prove the necessary optimality condition given in Theorems 2.1 and 2.2.

Theorem 2.1 *Assume that $\underline{f} : \mathbb{R} \to \mathbb{R}$, its derivatives up to order p are continuous, and $\underline{f}^{(p)}$ satisfies a Lipschitz condition defined by $\gamma_1 > 0$ in a neighborhood of x^*. Assume, moreover, that $a < b$, x^* is a local minimizer of $\underline{f}$ subject to $x \in [a, b]$, and there exists $q \leq p$ such that $\underline{f}^{(j)}(x^*) = 0$ for $j = 1, \ldots, q-1$ and $\underline{f}^{(q)}(x^*) \neq 0$. Then,*

1. *if q is even, then we have that $\underline{f}^{(q)}(x^*) > 0$;*
2. *if $a < x < b$, then q is even;*
3. *if $x = a$ and q is odd, then $\underline{f}^{(q)}(x^*) > 0$;*
4. *if $x = b$ and q is odd, then $\underline{f}^{(q)}(x^*) < 0$.*

Proof Suppose that $q \leq p$ is such that all the derivatives of order $j < q \leq p$ are null and $\underline{f}^{(q)}(x^*) \neq 0$. Then, by (1),

$$\left|\underline{f}(x) - \underline{f}(x^*) - \left[\frac{1}{q!}\underline{f}^{(q)}(x^*)(x-x^*)^q + \cdots + \frac{1}{p!}\underline{f}^{(p)}(x^*)(x-x^*)^p\right]\right| \leq \frac{\gamma_1}{(p+1)!}|x-x^*|^{p+1}.$$

Then,

$$\left|\underline{f}(x) - \underline{f}(x^*) - \frac{1}{q!}\underline{f}^{(q)}(x^*)(x-x^*)^q\right| - \left|\frac{1}{(q+1)!}\underline{f}^{(q+1)}(x^*)(x-x^*)^{q+1} \cdots + \frac{1}{p!}\underline{f}^{(p)}(x^*)(x-x^*)^p\right|$$
$$\leq \frac{\gamma_1}{(p+1)!}|x-x^*|^{p+1}.$$

Thus, if $p = q$, it follows trivially that

$$\left|\underline{f}(x) - \underline{f}(x^*) - \frac{1}{q!}\underline{f}^{(q)}(x^*)(x-x^*)^q\right| \leq c|x-x^*|^{q+1}. \tag{2}$$

If $p > q$, for all $j = q+1, \ldots, p$, the quantities $|\frac{1}{j!}f^{(j)}(x^*)|$ are bounded by the same constant. By the boundedness of $|x-x^*|$ in a neighborhood of x^* and the fact that $p+1 > q+1$, (2) follows as well. Assume firstly that q is even. Then, dividing (2) by $(x-x^*)^q > 0$, we have that

$$\left|\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-x^*)^q} - \frac{1}{q!}\underline{f}^{(q)}(x^*)\right| \leq c|x-x^*|. \tag{3}$$

Taking limits for $x \to x^*$ we deduce that

$$\lim_{x\to x^*}\left|\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-x^*)^q} - \frac{1}{q!}\underline{f}^{(q)}(x^*)\right| = 0. \tag{4}$$

Thus,

$$\lim_{x\to x^*}\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-x^*)^q} = \frac{1}{q!}\underline{f}^{(q)}(x^*). \tag{5}$$

Since $\underline{f}(x) \geq \underline{f}(x^*)$ for all x sufficiently close to x^* and the right-hand side of (5) is different from zero, we deduce that $\underline{f}^{(q)}(x^*) > 0$. Therefore, we proved that if not all the derivatives are null, the first statement in the thesis is true.

Now consider the case in which all the derivatives of order $j < q \leq p$ are null, $a < x^* < b$, and $f^{(q)}(x^*) \neq 0$. Suppose, by contradiction that q is odd. Assume, firstly, that $x > x^*$. Dividing (2) by $(x-x^*)^q > 0$, we have that

$$\left|\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-x^*)^q} - \frac{1}{q!}\underline{f}^{(q)}(x^*)\right| \leq c|x-x^*|. \tag{6}$$

Taking lateral limits for $x > x^*$ and $x \to x^*$ we deduce that

$$\lim_{x\to x^*,\ x>x^*}\left|\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-x^*)^q} - \frac{1}{q!}\underline{f}^{(q)}(x^*)\right| = 0. \tag{7}$$

Thus,

$$\lim_{x\to x^*,\ x>x^*}\frac{\underline{f}(x) - \underline{f}(x^*)}{(x-\bar{x})^q} = \frac{1}{q!}\underline{f}^{(q)}(x^*). \tag{8}$$

Since $f(x) \geq f(x^*)$ for all x sufficiently close to x^*, we deduce that $\underline{f}^{(q)}(x^*) \geq 0$. A similar reasoning for $x < x^*$ leads to $\underline{f}^{(q)}(x^*) \leq 0$. Therefore, $\underline{f}^{(q)}(x^*) = 0$. Therefore, we proved

that if all the derivatives of order $j < q \leq p$ are null, $a < x < b$, and $\underline{f}^{(q)}(x^*) \neq 0$, then q is even.

Let us prove now that, if all the derivatives of order $j < q \leq p$ are null, $\underline{f}^{(q)}(x^*) \neq 0$, $x^* = a$ and q is odd, we have that $\underline{f}^{(q)}(x^*) > 0$. Dividing (2) by $(x - x^*)^q > 0$, we obtain (6), (7), and (8) with $x^* = a$. Since $\underline{f}(x) \geq \underline{f}(x^*)$ for all x sufficiently close to x^* and, by assumption, $\underline{f}^{(q)}(x^*) \neq 0$, we have that $\underline{f}^{(q)}(x^*) \geq 0$. The last part of the thesis follows exactly in the same way.

Theorem 2.2 *Assume that $\underline{f} : \mathbb{R} \to \mathbb{R}$ and its derivatives up to order p are continuous and $\underline{f}^{(p)}$ satisfies a Lipschitz condition defined by $\gamma_1 > 0$ in a neighborhood of x^*. Assume, moreover, that x^* is a local minimizer of $\underline{f}$. Then, x^* is a local minimizer of the Taylor polynomial $\underline{T}_p(x^*, x)$.*

Proof By Theorem 2.1 we have four alternatives for the coefficients of the Taylor polynomial of order p. The first one is that all its coefficients are null. In this case, x^* is, trivially, a minimizer of the polynomial and there is nothing to prove.

In the second case the first nonnull coefficient of the polynomial is positive and its order is even. Therefore, the Taylor polynomial can be written as

$$\underline{T}_p(x^*, x) = \underline{f}(x^*) + \sum_{j=q}^{p} \frac{1}{j!} \underline{f}^{(j)}(x^*)(x - x^*)^j$$

for some even $q \leq p$ and $\frac{1}{q!}\underline{f}^{(j)}(x^*) > 0$. Then,

$$\frac{\underline{T}_p(x^*, x) - \underline{f}(x^*)}{(x - x^*)^q} = \frac{1}{q!}\underline{f}^{(q)}(x^*) + \sum_{j=q+1}^{p} \frac{1}{j!}\underline{f}^{(j)}(x^*)(x - x^*)^{j-q}. \tag{9}$$

This implies that x^* is a local minimizer of $\underline{T}_p(x^*, x)$ as we wanted to prove.

In the third case $x^* = a$, q is odd and $\frac{1}{q!}\underline{f}^{(j)}(x^*) > 0$. Then, (9) takes place and a is a local minimizer. The fourth case, in which $x^* = b$ and $\frac{1}{q!}\underline{f}^{(j)}(x^*) < 0$, follows in a similar way.

We now consider the $\underline{n}$-dimensional case. If $\underline{f} : \mathbb{R}^{\underline{n}} \to \mathbb{R}$ admits continuous derivatives up to order $p \in \{1, 2, 3, \dots\}$, then the Taylor polynomial of order p of $\underline{f}$ around x^* is defined as

$$\underline{T}_p(x^*, x) = \underline{f}(x^*) + \sum_{j=1}^{p} \underline{P}_j(x^*, x), \tag{10}$$

where $\underline{P}_j(x^*, x)$ is an homogeneous polynomial of degree j given by

$$\underline{P}_j(x^*, x) = \frac{1}{j!}\left((x_1 - x_1^*)\frac{\partial}{\partial x_1} + \cdots + (x_n - x_n^*)\frac{\partial}{\partial x_n}\right)^j \underline{f}(x). \tag{11}$$

For completeness we define $\underline{P}_0(x^*, x) = \underline{f}(x^*)$.

Let us define $\varphi(t) = \underline{f}(x^* + t(x - x^*))$. Obviously, if x^* is a local minimizer of $\underline{f}$ over a nonempty closed and convex set $C \subset \mathbb{R}^{\underline{n}}$, it turns out that 0 is a local minimizer of $\varphi(t)$ for every choice of $x \in C$. Thus, by Theorem 2.2, 0 is a local minimizer of the Taylor polynomial associated with φ subject to the interval defined by the boundary of C. But, by the construction of (10), this implies that x^* is a minimizer of $\underline{T}_p(x^*, x)$ along any line

that passes through x^* over the interval defined by the boundary of C. This fact is stated in Theorem 2.3.

Theorem 2.3 *Assume that $\underline{f} : \mathbb{R}^{\underline{n}} \to \mathbb{R}$ and its derivatives up to order p are continuous and satisfy a Lipschitz condition in a neighborhood of x^*. Assume, moreover, that x^* is a local minimizer of $\underline{f}$. Let $\mathcal{L}$ be a line that passes through x^*. Then, x^* is a local minimizer of the Taylor polynomial $\underline{T}_p(x^*, x)$ subject to $\mathcal{L} \cap C$.*

Proof Observe that the fact that the derivatives of order p satisfy a Lipschitz condition imply that the p-th derivative of φ exhibits the same property. Then, apply Theorem 2.2.

Definition 2.1 We say that x^* is pth-order stationary of $\underline{f}$ over the closed and convex set C if, for all $x \in C$, 0 is a local minimizer of the Taylor polynomial of order p that corresponds to the univariate function $\varphi(t) = \underline{f}(x^* + t(x - x^*))$ restricted to the constraint $x^* + t(x - x^*) \in C$.

Counterexample Unfortunately, it is not true that, when x^* is a local minimizer of $\underline{f}$, it is also a local minimizer of the associated Taylor polynomial. (As we saw in Theorem 2.2, this property is indeed true when $\underline{n} = 1$.) For example, if $\underline{f}(x_1, x_2) = x_2^2 - x_1^2 x_2 + x_1^4$, we have that $(0, 0)$ is a global minimizer of $\underline{f}$, but it is not a local minimizer of its Taylor polynomial of order $p = 3$.

In the following theorem we prove that, although according to the counterexample above, a minimizer does not need to minimize the Taylor polynomial, such property is true if the Taylor polynomial is regularized with a Lipschitz term.

Theorem 2.4 *Assume that $\mathcal{D} \subset \mathbb{R}^{\underline{n}}$, $\underline{f} : \mathcal{D} \to \mathbb{R}$, and x^* is a local minimizer of $\underline{f}(x)$ over $\mathcal{D}$ such that, for all $x \in \mathcal{D}$,*

$$\underline{f}(x) \leq \underline{T}_p(x^*, x) + \gamma \|x - x^*\|^{p+1}, \tag{12}$$

where $\underline{T}_p$ is, as defined in (10), the Taylor polynomial of order p of $\underline{f}$ around x^*. Then, for all $\sigma \geq \gamma$, x^* is a local minimizer of $\underline{T}_p(x^*, x) + \sigma \|x - x^*\|^{p+1}$ over $\mathcal{D}$.

Proof Suppose that the thesis is not true. Then, x^* is not a local minimizer of $\underline{T}_p(x^*, x) + \gamma \|x - x^*\|^{p+1}$ over $\mathcal{D}$. Thus, there exists $\{x^k\} \subset \mathcal{D}$ such that $\lim_{k\to\infty} x^k = x^*$ and

$$\underline{T}_p(x^*, x^k) + \gamma \|x^k - x^*\|^{p+1} < \underline{T}_p(x^*, x^*) = \underline{f}(x^*).$$

Thus, by (12),

$$\underline{f}(x^k) < \underline{f}(x^*)$$

for all $k = 0, 1, 2, \ldots$ This contradicts the fact that x^* is a local minimizer of $\underline{f}$ over $\mathcal{D}$.

The following definition is motivated by Theorem 2.4.

Definition 2.2 Assume that $\mathcal{D} \subset \mathbb{R}^{\underline{n}}$, $\underline{f} : \mathcal{D} \to \mathbb{R}$, x^* is such that (12) holds for all $x \in \mathcal{D}$, and that $\sigma \geq \gamma$. Then $x^* \in \mathcal{D}$ is said to be pth-order σ-stationary of $\underline{f}$ over $\mathcal{D}$ if x^* is a local minimizer of $\underline{T}_p(x^*, x) + \sigma \|x - x^*\|^{p+1}$ over $\mathcal{D}$.

It is trivial to see that, if $\mathcal{D}$ is convex and x^* is pth-order σ-stationary of $\underline{f}$ over $\mathcal{D}$ according to Definition 2.2, then it is pth-order $\tilde{\sigma}$-stationary for every $\tilde{\sigma} \geq \sigma$ and it is also pth-order stationary according to Definition 2.1. However, pth-order σ-stationarity is strictly stronger than pth-order stationarity. Consider the function $\underline{f}(x_1, x_2) = x_2^2 - x_1^2 x_2$ and $p = 3$. Note that $x^* = (0, 0)$ satisfies (12) with $\gamma = 0$. Straightforward calculations show that the point

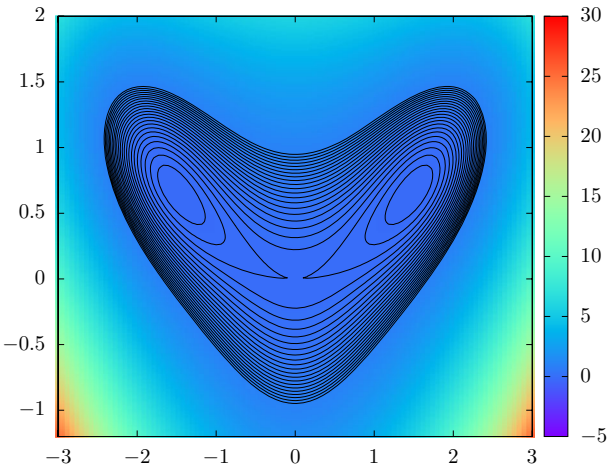

Fig. 1 Level sets of $\underline{T}_p((0,0),(x_1,x_2)) + \sigma\|(x_1,x_2)-(0,0)\|^{p+1}$ with $p=3$ and $\sigma = 0.125$, where $\underline{T}_p((0,0),(x_1,x_2))$ is the pth-order Taylor polynomial of $\underline{f}(x_1,x_2) = x_2^2 - x_1^2 x_2$ (that coincides with $\underline{f}$). The graphic shows that Condition **C5** with $p=3$ and $\sigma = 0.125$ does not hold at $(0,0)$, since it is *not* a local minimizer of the regularized pth-order Taylor polynomial. There are two local minimizers at "the eyes of the cat"

$(0,0)$, that is not a local minimizer of $\underline{f}$, is pth-order stationary according to Definition 2.1. On the other hand, $(0,0)$ is not pth-order σ-stationarity if $\sigma < 1/4$. See Fig. 1.

At this point it is convenient to summarize the properties of candidates to solutions of Minimize $\underline{f}(x)$ subject to $x \in C$, where C is closed and convex. Let us consider the following conditions with respect to $x^* \in C$:

- **C1:** x^* is a local minimizer.
- **C2:** x^* is a local minimizer of the Taylor polynomial over every feasible segment that passes through x^*.
- **C3:** x^* is a local minimizer of the Taylor polynomial around x^*.
- **C4:** x^* is a local minimizer of $\underline{T}_p(x^*,x) + \gamma\|x-x^*\|^{p+1}$, where γ is a Lipschitz constant.
- **C5:** x^* is a local minimizer of $\underline{T}_p(x^*,x) + \sigma\|x-x^*\|^{p+1}$, where $\sigma > \gamma$ and γ is a Lipschitz constant.
- **C6:** x^* is a local minimizer of $\underline{T}_p(x^*,x) + \sigma\|x-x^*\|^{p+1}$, where $0 < \sigma < \gamma$ and γ is a Lipschitz constant.

We proved that **C1**, **C2**, **C4** and **C5** are necessary optimality conditions, while **C3** and **C6** are not. We also showed that **C1** $\Rightarrow$ **C4** $\Rightarrow$ **C5**, and **C3** $\Rightarrow$ **C6** $\Rightarrow$ **C4** $\Rightarrow$ **C5**. However, **C1** does not imply neither **C3** nor **C6**.

Definition 2.3 We say that an optimality condition is *exclusive* if it can be verified using only values of the derivatives up to order p at the point under consideration.

Optimality conditions that are not exclusive are said to be *inclusive*. Only condition **C2** above is exclusive. **C4** and **C5** are inclusive necessary optimality conditions because they use information on the Lipschitz constant in a neighborhood of x^*. Thus, the information that they require is not restricted to derivatives of order at most p at a single point. The annihilation of the gradient at x^* and the positive semidefiniteness of the Hessian are exclusive first-order

and second-order necessary optimality conditions for unconstrained optimization. The most natural high-order exclusive optimality condition for convex constrained optimization is **C2**. In [24], an exclusive optimality condition based on curves was presented. However, exclusive necessary optimality conditions are essentially weaker than inclusive ones. In fact, assume that x^* satisfies **C5** and that **C** is an arbitrary exclusive necessary optimality condition. Then, x^* is a local minimizer of $\underline{T}_p(x^*, x) + \sigma\|x - x^*\|^{p+1}$, where $\sigma > \gamma$ and γ is a Lipschitz constant. Then, x^* satisfies the exclusive condition **C** for the minimization of $\underline{T}_p(x^*, x) + \sigma\|x - x^*\|^{p+1}$. Then, since **C** is a necessary optimality condition, it is satisfied by x^* for the local minimization of $\underline{T}_p(x^*, x) + \sigma\|x - x^*\|^{p+1}$. But all the derivatives up to order p of $\underline{T}_p(x^*, x) + \sigma\|x - x^*\|^{p+1}$ exist at x^* and coincide with the derivatives up to order p of $\underline{f}$. So, x^* satisfies **C** for the minimization of $\underline{f}$.

In order to see that **C5** is strictly stronger than **C** (for every exclusive necessary optimality condition **C**), consider the functions $\underline{f}(x_1, x_2) = x_2^2 - x_1^2 x_2$ and $F(x_1, x_2) = x_2^2 - x_1^2 x_2 + x_1^4$. The origin $x^* = (0, 0)$ is a local (and global) minimizer of F, therefore, it must satisfy the necessary exclusive optimality condition **C** of order $p = 3$. Since, up to order $p = 3$, the derivatives of $\underline{f}$ and F are the same, it turns out that x^* satisfies the necessary optimality condition **C** of order $p = 3$, applied to the minimization of $\underline{f}$. (Note that x^* is not a local minimizer of $\underline{f}$.) However, x^* does not satisfy condition **C5** if $\sigma < 1/4$. In this case, every $\sigma > 0$ is bigger than the Lipschitz constant of $\underline{f}$ associated with third-order derivatives, thus, we found an example in which the exclusive condition **C** holds but the inclusive condition **C5** does not.

3 Regularized high-order minimization with box constraints

In this section, we consider the problem

$$\text{Minimize } \underline{f}(x) \text{ subject to } x \in \underline{\Omega}, \tag{13}$$

where $\underline{\Omega} \subset \mathbb{R}^{\underline{n}}$ is given by

$$\underline{\Omega} = \{x \in \mathbb{R}^{\underline{n}} \mid \underline{\ell} \leq x \leq \underline{u}\} \tag{14}$$

and $\underline{\ell}, \underline{u} \in \mathbb{R}^{\underline{n}}$ are such that $\underline{\ell} < \underline{u}$. We assume that $\underline{f}$ has continuous first derivatives into $\underline{\Omega}$. We denote $\underline{g}(x) = \nabla \underline{f}(x)$ and $\underline{g}_P(x) = P_{\underline{\Omega}}(x - \underline{g}(x)) - x$, for all $x \in \underline{\Omega}$, where $P_{\underline{\Omega}}$ is the Euclidean projection operator onto $\underline{\Omega}$. In the remaining of this section, the results from [7] that are relevant to the present work are surveyed and a natural extension of the main algorithm in [7], that makes it possible to consider a wider class of models, is introduced.

Each iteration k of Algorithm 2.1 introduced in [7] computes a new iterate x^{k+1} satisfying $(p + 1)$th-order descent with respect to $\underline{f}(x^k)$ through the approximate minimization of a $(p + 1)$th-regularized model of the function $\underline{f}$ around the iterate x^k. For all $\bar{x} \in \mathbb{R}^n$, let $\underline{M}_{\bar{x}} : \mathbb{R}^n \to \mathbb{R}$ be a "model" of $\underline{f}(x)$ around $\bar{x}$; and assume that $\nabla \underline{M}_{\bar{x}}(x)$ exists for all $x \in \underline{\Omega}$. We now present an algorithm that corresponds to a single iteration of the algorithm introduced in [7].

Algorithm 3.1 Assume that $p \in \{1, 2, 3, \dots\}$, $\alpha > 0$, $\sigma_{\min} > 0$, $\tau_2 \geq \tau_1 > 1$, $\theta > 0$, and $\bar{x} \in \underline{\Omega}$ are given.

Step 1. Set $\sigma \leftarrow 0$.

Step 2. Compute $x^{\text{trial}} \in \underline{\Omega}$ such that

$$\underline{M}_{\bar{x}}(x^{\text{trial}}) + \sigma\|x^{\text{trial}} - \bar{x}\|^{p+1} \leq \underline{M}_{\bar{x}}(\bar{x}) \tag{15}$$

and

$$\left\| P_{\underline{\Omega}}\left[x^{\text{trial}} - \nabla\left(\underline{M}_{\bar{x}}(x) + \sigma\|x - \bar{x}\|^{p+1}\right)\big|_{x=x^{\text{trial}}}\right] - x^{\text{trial}}\right\| \leq \theta\|x^{\text{trial}} - \bar{x}\|^{p}. \quad (16)$$

Step 3. If

$$\underline{f}(x^{\text{trial}}) \leq \underline{f}(\bar{x}) - \alpha\|x^{\text{trial}} - \bar{x}\|^{p+1}, \quad (17)$$

then define $x^+ = x^{\text{trial}}$ and stop returning x^+ and σ. Otherwise, update $\sigma \leftarrow \max\{\sigma_{\min}, \tau\sigma\}$ with $\tau \in [\tau_1, \tau_2]$ and go to Step 2.

Remark The trial point x^{trial} computed at Step 2 is intended to be an approximate solution to the subproblem

$$\text{Minimize } \underline{M}_{\bar{x}}(x) + \sigma\|x - \bar{x}\|^{p+1} \text{ subject to } x \in \underline{\Omega}. \quad (18)$$

Note that conditions (15) and (16) can always be achieved. In fact, by the compactness of $\underline{\Omega}$, if x^{trial} is a global minimizer of (18), then it satisfies the condition

$$\left\| P_{\underline{\Omega}}[x^{\text{trial}} - \nabla(\underline{M}_{\bar{x}}(x) + \sigma\|x - \bar{x}\|^{p+1})\big|_{x=x^{\text{trial}}}] - x^{\text{trial}}\right\| = 0;$$

and so (16) takes place. In addition, if x^{trial} is a global minimizer, since $\bar{x}$ is a feasible point, (15) must hold as well.

Assumption A1 There exists $L > 0$ such that, for all x^{trial} computed by Algorithm 3.1, $x = x^{\text{trial}}$ satisfies

$$\left\|\underline{g}(x) - \nabla\underline{M}_{\bar{x}}(x)\right\| \leq L\|x - \bar{x}\|^{p}, \quad (19)$$

$$\underline{M}_{\bar{x}}(\bar{x}) = \underline{f}(\bar{x}) \text{ and } \underline{f}(x) \leq \underline{M}_{\bar{x}}(x) + L\|x - \bar{x}\|^{p+1}. \quad (20)$$

If $\underline{M}_{\bar{x}}(x)$ is the Taylor polynomial of order p of $\underline{f}$ around $\bar{x}$ and the pth-order derivatives of $\underline{f}$ satisfy a Lipschitz condition with Lipschitz constant L, then Assumption A1 is satisfied. However, the situations in which Assumption A1 holds are not restricted to the case in which $\underline{M}_{\bar{x}}(x) = \underline{T}_p(\bar{x}, x)$. For example, we may choose $\underline{M}_{\bar{x}}(x) = \underline{f}(x)$. (Note that, in this case, p may be arbitrarily large but only first derivatives of $\underline{f}(x)$ need to exist.) Although the results in [7] only mention the choice $\underline{M}_{\bar{x}}(x) = \underline{T}_p(\bar{x}, x)$, these results only depend on Assumption A1. Thus, they can be trivially extended to the general choice of $\underline{M}_{\bar{x}}(x)$.

Theorem 3.1 *Suppose that Assumption A1 holds. If the regularization parameter σ in (15) satisfies $\sigma \geq L + \alpha$, then the trial point x^{trial} satisfies the sufficient descent condition (17). Moreover,*

$$\left\|\underline{g}_P(x^+)\right\| \leq (L + \tau_2(L + \alpha)(p + 1) + \theta)\|x^+ - \bar{x}\|^{p} \quad (21)$$

and

$$\underline{f}(x^+) \leq \underline{f}(\bar{x}) - \alpha\left(\frac{\|\underline{g}_P(x^+)\|}{L + \tau_2(L + \alpha)(p + 1) + \theta}\right)^{(p+1)/p}. \quad (22)$$

Proof This theorem condensates the results in [7, Lemmas 3.2–3.4].

Theorem 3.1 justifies the definition of an algorithm for solving (13) based on repetitive application of Algorithm 3.1 and shows that such algorithm enjoys good properties in terms of convergence and complexity. On the one hand, each iteration of the algorithm requires

$O(1)$ functional evaluations and finishes satisfying a suitable sufficient descent condition. On the other hand, that condition implies that infinitely many iterations with gradient-norm bounded away from zero are not possible if the function is bounded below. Moreover, (22) leads to a complexity bound on the number of iterations based on the norm of the projected gradient. In the following sections, we prove that, thanks to Theorem 3.1, similar convergence and evaluation complexity properties hold for a coordinate descent algorithm.

4 High-order coordinate descent algorithm

In this section, we consider the problem

$$\text{Minimize } f(x) \text{ subject to } x \in \Omega, \tag{23}$$

where $\Omega \subset \mathbb{R}^n$ is given by

$$\Omega = \{x \in \mathbb{R}^n \mid \ell \leq x \leq u\} \tag{24}$$

and $\ell, u \in \mathbb{R}^n$ are such that $\ell < u$. We assume that f has continuous first derivatives over Ω.

At each iteration of the coordinate descent method introduced in this section for solving (23), (i) a nonempty set of indices $I_k \subseteq \{1, \ldots, n\}$ is selected, (ii) coordinates corresponding to indices that are not in I_k remain fixed, and (iii) Algorithm 3.1 is applied to the minimization of f over Ω with respect to the free variables, i.e. variables with indices in I_k. From now on, given $v \in \mathbb{R}^n$, we denote by $v_I \in \mathbb{R}^{|I|}$ the vector whose components are the components of v whose indices belong to $I \subseteq \{1, \ldots, n\}$. For all $x \in \Omega$, we define $g_{P,I}(x) \in \mathbb{R}^n$ by

$$[g_{P,I}(x)]_i = \begin{cases} [g_P(x)]_i, & \text{if } i \in I, \\ 0, & \text{if } i \notin I. \end{cases}$$

Since Ω is a box, this definition is equivalent to $g_{P,I}(x) = P_\Omega(x - g_I(x)) - x$, where

$$[g_I(x)]_i = \begin{cases} [g(x)]_i, & \text{if } i \in I, \\ 0, & \text{if } i \notin I. \end{cases}$$

This equivalence, that will be used in the theoretical convergence results below, is not true if Ω is an arbitrary closed and convex set. This is the reason for which we consider CD algorithms only with box constraints.

Algorithm 4.1 Assume that $p \in \{1, 2, 3, \ldots\}$, $\alpha > 0$, $\sigma_{\min} > 0$, $\tau_2 \geq \tau_1 > 1$, $\theta > 0$, and $x^0 \in \Omega$ are given. Initialize $k \leftarrow 0$.

Step 1. Choose a nonempty set $I_k \subseteq \{1, \ldots, n\}$.

Step 2. Consider the problem

$$\text{Minimize } f(x) \text{ subject to } x \in \Omega \text{ and } x_i = x_i^k \text{ for all } i \notin I_k. \tag{25}$$

Let $\bar{x} = x^k_{I_k}$. Setting $\underline{f}$, $\underline{\Omega}$, and $\underline{M}_{\bar{x}}$ properly, apply Algorithm 3.1 to obtain x^+ and σ_k. **Step 3.** Define x^{k+1} as $x^{k+1}_{I_k} = x^+$ and $x_i^{k+1} = x_i^k$ for all $i \notin I_k$, set $k \leftarrow k + 1$, and go to Step 1.

Assumption A2 There exists $L > 0$ such that for all k, $\bar{x}$, $\underline{f}$, and $\underline{M}_{\bar{x}}$ set at the kth iteration of Algorithm 4.1 and for all x^{trial} computed by Algorithm 3.1 when called at the kth iteration of Algorithm 4.1, (19) and (20) take place with $x = x^{\text{trial}}$.

If $\underline{M}_{\bar{x}}(x)$ is the Taylor polynomial of order p of $\underline{f}$ around $\bar{x}$ and the pth-order derivatives of f satisfy a Lipschitz condition with Lipschitz constant L, then Assumption A2 is satisfied.

Theorem 4.1 *Suppose that Assumption A2 holds. Then, there exists $c > 0$, which only depends on L, τ_2, α, p, and θ such that, for all $k = 0, 1, 2, \ldots$, the point x^{k+1} computed by Algorithm 4.1 is well defined and satisfies*

$$f(x^{k+1}) \leq f(x^k) - \alpha \|x^{k+1} - x^k\|^{p+1} \tag{26}$$

and

$$\left\| g_{P,I_k}(x^{k+1}) \right\| \leq c \|x^{k+1} - x^k\|^p. \tag{27}$$

Proof (26) follows from (17), while (27) follows from the application of Theorem 3.1.

Theorem 4.2 *Suppose that Assumption A2 holds. Let $\{x^k\}$ be the sequence generated by Algorithm 4.1. Then,*

$$\lim_{k\to\infty} \|x^{k+1} - x^k\| = 0, \tag{28}$$

$$\lim_{k\to\infty} \left\| g_{P,I_k}(x^{k+1}) \right\| = 0, \tag{29}$$

and

$$\lim_{k\to\infty} \left\| g_{P,I_k}(x^k) \right\| = 0. \tag{30}$$

Proof Since Ω is compact, we have that f is bounded below onto Ω. Thus, (28) follows from (26) and, in consequence, (29) follows from (28) and (27). Let us prove (30). Assume that $I \subseteq \{1, \ldots, n\}$ is nonempty and arbitrary. By the continuity of the gradient, the function $\|g_{P,I}(x)\|$ is continuous for all $x \in \Omega$ and, since Ω is compact, it is uniformly continuous. Then, given $\varepsilon > 0$, there exists $\delta_I > 0$ such that, whenever $\|x - y\| \leq \delta_I$, we have that $\|g_{P,I}(x) - g_{P,I}(y)\| \leq \varepsilon/2$. Since the number of different subsets of $\{1, \ldots, n\}$ is finite, we have that $\delta \equiv \min\{\delta_I \mid \emptyset \neq I \subseteq \{1, \ldots, n\}\} > 0$. Thus, for all $I \subseteq \{1, \ldots, n\}$, if $\|x - y\| \leq \delta$, we have that $\|g_{P,I}(x) - g_{P,I}(y)\| \leq \varepsilon/2$. Now, by (28), there exists k_0 such that, whenever $k \geq k_0$, we have that $\|x^{k+1} - x^k\| \leq \delta$. Then, by the definition of δ, if $k \geq k_0$, $\|g_{P,I}(x^{k+1}) - g_{P,I}(x^k)\| \leq \varepsilon/2$ for all nonempty $I \subseteq \{1, \ldots, n\}$. In particular, taking $I = I_k$, if $k \geq k_0$, we have that $\|g_{P,I_k}(x^{k+1}) - g_{P,I_k}(x^k)\| \leq \varepsilon/2$. Finally, by (29), there exists $k_1 \geq k_0$ such that, for all $k \geq k_1$, $\|g_{P,I_k}(x^{k+1})\| \leq \varepsilon/2$. By the triangular inequality, adding the last two inequalities we have that $\|g_{P,I_k}(x^k)\| \leq \varepsilon$. Since $\varepsilon > 0$ was arbitrary, this completes the proof of (30).

The following assumption guarantees that all the indices $i \in \{1, \ldots, n\}$ belong to some I_k at least every $\bar{m}$ iterations. This guarantees that the CD method tries to reduce the function with respect to each variable x_i infinitely many times.

Assumption A3 There exists $\bar{m} < +\infty$ such that, for all $i \in \{1, \ldots, n\}$:

1. There exists $k \leq \bar{m}$ such that $i \in I_k$;
2. For any $k \in \mathbb{N}$, if $i \in I_k$, then there exists $m \leq \bar{m}$ such that $i \in I_{k+m}$.

Note that Assumption A3 allows us to use not only cyclic versions, but also random versions of the CD method. In particular, the block of coordinates chosen at each iteration can be chosen at random, with the condition that, every $\bar{m}$ iterations, all blocks are chosen at least once.

Theorem 4.3 *Suppose Assumptions A2 and A3 hold. Let $\{x^k\}$ be the sequence generated by Algorithm 4.1. Then,*

$$\lim_{k\to\infty} \|g_P(x^k)\| = 0. \tag{31}$$

Moreover, if $x^* \in \Omega$ is a limit point of $\{x^k\}$, then we have that $\|g_P(x^*)\| = 0$.

Proof Let $i \in \{1, \ldots, n\}$. By Assumption A3, there exists an infinite set of increasing indices $K = \{k_1, k_2, k_3, \ldots\}$ such that $i \in I_{k_\ell}$ and $k_{\ell+1} \leq k_\ell + \bar{m}$ for all $\ell = 1, 2, 3, \ldots$ Then, by (30) in Theorem 4.2, since, by definition, given $I \subseteq \{1, \ldots, n\}$, $[g_{P,I}(x)]_i = [g_P(x)]_i$ for any $i \in I$,

$$\lim_{k\in K} [g_P(x^k)]_i = 0. \tag{32}$$

Let $j \in \{1, 2, \ldots\}$ be arbitrary. By (28), the triangular inequality, and the uniform continuity of g_P, we have that

$$\lim_{k\in K} |[g_P(x^{k+j})]_i - [g_P(x^k)]_i| = 0.$$

Therefore, by (32),

$$\lim_{k\in K} [g_P(x^{k+j})]_i = 0. \tag{33}$$

In particular, (33) holds for all $j = 1, \ldots, \bar{m}$. This implies that

$$\lim_{k\to\infty} [g_P(x^k)]_i = 0. \tag{34}$$

Thus, the thesis is proved.

Theorem 4.3 shows that limit points of sequences generated by Algorithm 4.1 are first-order stationary. The rest of this section is dedicated to prove that, under suitable conditions, pth-order stationarity with respect to each variable also holds. More precisely, if the same nonempty set I_k is repeated infinitely many times, p-stationarity holds in the limit for the variables x_i with $i \in I_k$. For this purpose, we need to define different notions of stationarity.

In Theorem 4.3 we proved that Algorithm 4.1 is satisfactory from the point of view of first-order stationarity. In the CD approach we cannot advocate for full stationarity of high order because cross derivatives that involve variables that are never optimized together are not computed at all. However, if optimization with respect to the same group of variables occurs at infinitely many iterations, it is reasonable to conjecture that high-order optimality with respect to those variables would, in the limit, take place. For obtaining such result, it is not enough to satisfy criteria (15) and (16) when solving subproblems. The reason is that condition (16) is based on a first-order optimality criterion for problem (18). A stronger assumption on the subproblem solution is made in the following theorem. Namely, it is assumed that, instead of requesting (15) and (16), a global solution to subproblem (18) is computed. This assumption could be rather mild in the case that all the subproblems are chosen to be small dimensional. In this case, it is possible to prove that, in the limit, suitable pth-order optimality conditions are satisfied. Observe that partial derivatives that are not necessary for computing Taylor approximations are not assumed to exist at all, let alone to be continuous.

Theorem 4.4 *Suppose that Assumption A2 holds and the sequence $\{x^k\}$ is generated by Algorithm 4.1. Suppose that, at iteration k, the function $\underline{f}$ has as variables x_i with $i \in I_k$,*

$\underline{\Omega}$ is the box Ω restricted to the variables $i \in I_k$, $\underline{M}_{\bar{x}}(x)$ is chosen as the pth-order Taylor polynomial of $\underline{f}$ defined in (10), the derivatives involved in (10) exist and are continuous for all $x \in \Omega$, and Algorithm 3.1 computes x^+ as a global minimizer of (18). Let K be an infinite set of indices such that $I = I_k$ for all $k \in K$. Let x^* be a limit point of the sequence $\{x^k\}_{k\in K}$. Then, for all $j \leq p$, x^* is jth-order stationary of problem (13) according to Definition 2.1 and it is also jth-order σ-stationary for some $\sigma \leq \tau_2(L+\alpha)$ according to Definition 2.2 of problem (13).

Proof Consider the problem

$$\text{Minimize } T_p(x^*, x) + \sigma\|x - x^*\|^{p+1} \text{ subject to } x \in \Omega \text{ and } x_i = x_i^* \text{ for all } i \notin I. \quad (35)$$

By the hypothesis, for all $k \in K$, x^+ is obtained as a global minimizer of

$$\text{Minimize } T_p(x^k, x) + \sigma\|x - x^k\|^{p+1} \text{ subject to } x \in \Omega \text{ and } x_i = x_i^k \text{ for all } i \notin I, \quad (36)$$

for some $\sigma > 0$. Then, by Theorem 3.1, x^{k+1} is a global minimizer of (36) with $\sigma = \sigma_k \leq \tau_2(L+\alpha)$. By (28), $\lim_{k\in K} x^{k+1} = \lim_{k\in K} x^k = x^*$. Taking a convenient subsequence, assume, without loss of generality, that $\lim_{k\in K} \sigma_k = \sigma_* \leq \tau_2(L+\alpha)$. Let $x \in \Omega$ be such that $x_i = x_i^*$ for all $i \notin I$. Let $z^k \in \Omega$ be such that $z_i^k = x_i$ for all $i \in I$ and $z_i^k = x_i^k$ for all $i \notin I$. Then, by the definition of x^{k+1}, for all $k \in K$,

$$T_p(x^k, x^{k+1}) + \sigma_k\|x^{k+1} - x^k\|^{p+1} \leq T_p(x^k, z^k) + \sigma_k\|z^k - x^k\|^{p+1}. \quad (37)$$

Taking limits for $k \in K$, by the definition of z^k, we have that

$$T_p(x^*, x^*) + \sigma_*\|x^* - x^*\|^{p+1} \leq T_p(x^*, x) + \sigma_*\|x - x^*\|^{p+1}. \quad (38)$$

Since x was arbitrary, this implies that x^* is a global solution of (35). Consequently, x^* is also a local solution of (35). Since the Taylor polynomial of order p of $T_p(x^*, x) + \sigma_*\|x - x^*\|^{p+1}$ coincides with the Taylor polynomial of order p of $\underline{f}$, the thesis is proved.

Remark 1 Theorem 4.4 shows that the convergence of our CD method is related to the inclusive optimality condition given in Definition 2.2, which, as stated in the last two paragraphs of Sect. 2, is stronger than every possible exclusive optimality condition.

Remark 2 Note that the hypothesis of Theorem 4.4 implies a stronger thesis than the one stated. In fact, we proved that, in the limit, each partial Taylor polynomial has a global minimizer. This is interesting because that fact is not a necessary optimality condition, as it has been shown in the counterexample exhibited in Sect. 2. However, since **C3** implies **C4** and **C5**, it turns out that x^* certainly satisfies the inclusive optimality condition **C5** according to Definition 2.3.

Corollary 4.1 *Consider the assumptions of Theorem 4.4 and assume that, for all k,*

$$I_k = \{\text{mod}(k, n) + 1\}.$$

If x^* is a limit point of the sequence generated by Algorithm 4.1, then for all $i = 1, \ldots, n$, x_i^* is a jth-order stationary point of the problem

$$\text{Minimize } f(x_1^*, \ldots, x_{i-1}^*, x_i, x_{i+1}^*, \ldots, x_n^*) \text{ subject to } \ell_i \leq x_i \leq u_i \quad (39)$$

for all $j \leq p$.

Proof The proof is a direct application of Theorem 4.4.

5 Complexity

Given a tolerance $\varepsilon > 0$, we wish to know the worst possible computer effort that we need to obtain an iterate x at which the objective function is smaller than a given target or the projected gradient norm $\|g_P(x)\|$ is smaller than ε. We show that the number of iterations that are needed to obtain $|[g_P(x^{k+1})]_i| \leq \varepsilon$ for all $i \in I_k$ is, at most, a constant times $\varepsilon^{-(p+1)/p}$ as in typical high-order methods. However, obtaining $|[g_P(x^{k+1})]_i| \leq \varepsilon$ for all $i \notin I_k$ is harder as, for this purpose, we need that consecutive iterations be close enough. This difficulty is intrinsic to coordinate descent methods. Powell's example of non-convergence of CD methods [49] satisfies the requirement $|[g_P(x^{k+1})]_i| \leq \varepsilon$ for all $i \in I_k$ at every iteration but never satisfies $|[g_P(x^{k+1})]_i| \leq \varepsilon$ for $i \notin I_k$. Our method converges even in Powell's example because we require sufficient descent based on regularization but it is affected by Powell's effect because the number of iterations at which the distance between consecutive iterates is bigger than a fixed distance grows with the order p. Then, it is not surprising that our worst-case complexity bound is significantly worse than $O(\varepsilon^{-(p+1)/p})$. These results are rigorously proved in this section and discussed in Sect. 6.

Theorem 5.1 *Suppose that Assumption A2 holds. Let $f_{\text{target}} \leq f(x^0)$ and $\varepsilon > 0$ be given. Then, the quantity of iterations k such that*

(i) $f(x^{k+1}) > f_{\text{target}}$ *and*
(ii) $|[g_P(x^{k+1})]_i| > \varepsilon$ *for some* $i \in I_k$

is bounded by

$$\frac{f(x^0) - f_{\text{target}}}{c\,\varepsilon^{(p+1)/p}}, \tag{40}$$

where c only depends on α, τ_2, L, p, and θ.

Proof By (22) in Theorem 3.1,

$$f(x^{k+1}) \leq f(x^k) - c\|g_{P,I_k}(x^{k+1})\|^{(p+1)/p},$$

where $c = (\alpha/(L + \tau_2(L + \alpha)(p + 1) + \theta))^{(p+1)/p}$. Therefore, if $i \in I_k$,

$$f(x^{k+1}) \leq f(x^k) - c\left|[g_P(x^{k+1})]_i\right|^{(p+1)/p}.$$

So, if $\left|[g_P(x^{k+1})]_i\right| > \varepsilon$,

$$f(x^{k+1}) \leq f(x^k) - c\varepsilon^{(p+1)/p}. \tag{41}$$

Since the sequence $\{f(x^k)\}$ decreases monotonically, the number of iterations at which (41) occurs together with $f(x^{k+1}) > f_{\text{target}}$ cannot exceed $(f(x^0) - f_{\text{target}})/(c\varepsilon^{(p+1)/p})$. This completes the proof.

Theorem 5.2 *Suppose that Assumption A2 holds. Let $f_{\text{target}} \leq f(x^0)$ and $\delta > 0$ be given. Then, the quantity of iterations k such that $f(x^k) > f_{\text{target}}$ and $\|x^{k+1} - x^k\| > \delta$ is bounded by*

$$\frac{f(x^0) - f_{\text{target}}}{\alpha\,\delta^{p+1}}. \tag{42}$$

Proof The proof follows directly from (26) in Theorem 4.1.

Theorem 5.3 *Suppose that Assumption A2 holds. Let $f_{\text{target}} \leq f(x^0)$, $\varepsilon > 0$, and $\delta > 0$ be given. Then, the quantity of iterations k such that*

(i) $f(x^{k+1}) > f_{\text{target}}$ *and*
(ii) $\|x^{k+1} - x^k\| > \delta$ *or* $|[g_P(x^{k+1})]_i| > \varepsilon$ *for some* $i \in I_k$

is bounded by

$$\frac{f(x^0) - f_{\text{target}}}{c\,\varepsilon^{(p+1)/p}} + \frac{f(x^0) - f_{\text{target}}}{\alpha\,\delta^{p+1}}, \tag{43}$$

where c only depends on α, τ_2, L, p, and θ.

Proof The proof follows directly from Theorems 5.1 and 5.2.

We now divide the iterations of Algorithm 4.1 in *cycles*. Each cycle is composed by $\bar{m}$ iterations, where $\bar{m}$ is the one assumed to exist in Assumption A3. Therefore, the successive cycles start at iterations $x^0, x^{\bar{m}}, x^{2\bar{m}}, \ldots, x^{\ell\bar{m}}, \ldots$ The iterates $x^{\ell\bar{m}+1}, \ldots, x^{\ell\bar{m}+\bar{m}}$ are said to be *produced* at cycle ℓ. Iterations $k = \ell\bar{m}, \ldots, \ell\bar{m} + \bar{m} - 1$, at which these iterates were produced, are said to be *internal* iterations of cycle ℓ. Each iteration k is associated with a set of indices I_k. Due to Assumption A3, for every coordinate $i = 1, \ldots, n$ and every cycle $\ell \geq 0$, there is at least an iteration k internal to cycle ℓ such that $i \in I_k$. In other words, all coordinates are considered in at least an iteration of every cycle. With the notion of cycle at hand, we can now restate Theorems 5.1, 5.2, and 5.3 as follows.

Theorem 5.4 *Suppose that Assumptions A2 and A3 hold. Let $f_{\text{target}} \leq f(x^0)$ and $\varepsilon > 0$ be given. Then, the quantity of cycles ℓ that contain an internal iteration k such that*

(i) $f(x^{k+1}) > f_{\text{target}}$ *and*
(ii) $|[g_P(x^{k+1})]_i| > \varepsilon$ *for some* $i \in I_k$

is not bigger than

$$\frac{f(x^0) - f_{\text{target}}}{c\,\varepsilon^{(p+1)/p}}, \tag{44}$$

where c only depends on α, τ_2, L, p, and θ.

Proof Let ℓ be a cycle that contains an internal iteration k satisfying (i) and (ii). By Theorem 5.1, the quantity of this type of iteration is bounded by (44); and so the same bound applies to the quantity of cycles containing an iteration with these properties. This completes the proof.

Theorem 5.5 *Suppose that Assumptions A2 and A3 hold. Let $f_{\text{target}} \leq f(x^0)$ and $\varepsilon > 0$ be given. Then, the quantity of cycles ℓ that contain an internal iteration k such that $f(x^k) > f_{\text{target}}$ and $\|x^{k+1} - x^k\| > \delta$ is bounded by*

$$\frac{f(x^0) - f_{\text{target}}}{\alpha\,\delta^{p+1}}. \tag{45}$$

Proof Let ℓ be a cycle that contains an internal iteration k such that $f(x^k) > f_{\text{target}}$ and $\|x^{k+1} - x^k\| > \delta$. By Theorem 5.2, the quantity of this type of iteration is bounded by (45); and so the same bound applies to the quantity of cycles containing an iteration with these properties. This completes the proof.

Theorem 5.6 *Suppose that Assumptions A2 and A3 hold. Let* $f_{\text{target}} \leq f(x^0)$, $\varepsilon > 0$, *and* $\delta > 0$ *be given. Then, the quantity of cycles* ℓ *that contain an internal iteration* k *such that*

(i) $f(x^{k+1}) > f_{\text{target}}$ *and*
(ii) $\|x^{k+1} - x^k\| > \delta$ *or* $|[g_P(x^{k+1})]_i| > \varepsilon$ *for some* $i \in I_k$

is bounded by

$$\frac{f(x^0) - f_{\text{target}}}{c\,\varepsilon^{(p+1)/p}} + \frac{f(x^0) - f_{\text{target}}}{\alpha\,\delta^{p+1}}, \tag{46}$$

where c *only depends on* α, τ_2, L, p, *and* θ.

Proof The proof follows directly from Theorems 5.4 and 5.5.

The following assumption guarantees that small increments cause small differences on the projected gradients.

Assumption A4 There exists $L_g > 0$ such that for all $i = 1, \ldots, n$ and $x, z \in \Omega$,

$$|[g_P(x)]_i - [g_P(z)]_i| \leq L_g \|x - z\|. \tag{47}$$

By the non-expansiveness property of projections, Assumption A4 is satisfied if the gradient of f satisfies a Lipschitz condition with constant L_g.

With the tools given by Assumption A4 and Theorem 5.6, we are now able to establish a bound on the number of cycles at which the whole projected gradient is bigger than a given tolerance.

Theorem 5.7 *Suppose that Assumptions A2, A3, and A4 hold. Let* $f_{\text{target}} \leq f(x^0)$, $\varepsilon > 0$, *and* $\delta > 0$ *be given. Then, there exists a cycle* ℓ, *with* ℓ *exceeding* (46) *by one in the worst case, such that either*

(i) *for some iteration* k *internal to cycle* ℓ, *we have that* $f(x^k) \leq f_{\text{target}}$ *or*
(ii) *for all the iterations* k *internal to cycle* ℓ *we have that*

$$\left|[g_P(x^{k+1})]_i\right| \leq \varepsilon + \bar{m} L_g \delta \text{ for all } i = 1, \ldots, n. \tag{48}$$

Proof By Theorem 5.6, there exists a cycle ℓ that does not exceeds (46) by more than one such that, for each iterations k internal to cycle ℓ, either $f(x^{k+1}) \leq f_{\text{target}}$ or

$$\|x^{k+1} - x^k\| \leq \delta \text{ and } |[g_P(x^{k+1})]_i| \leq \varepsilon \text{ for all } i \in I_k. \tag{49}$$

If there exists an iteration k internal to cycle ℓ such that $f(x^{k+1}) \leq f_{\text{target}}$, then we are done. So, we assume that, for all iterations k internal to cycle ℓ, (49) holds. Let $i \in \{1, \ldots, n\}$ be arbitrary. Assumption A3 implies that there is an iteration k internal to cycle ℓ such that $i \in I_k$ and, thus, by (49), $|[g_P(x^{k+1})]_i| \leq \varepsilon$. For any other iterate z produced at cycle ℓ, by Assumption A4, the triangle inequality, and the first inequality in (49), we have that

$$|[g_P(z)]_i - [g_P(x^{k+1})]_i| \leq L_g \|z - x^{k+1}\| \leq \bar{m} L_g \delta.$$

Thus,

$$|[g_P(z)]_i| \leq \varepsilon + \bar{m} L_g \delta,$$

as we wanted to prove.

Theorem 5.8 *Suppose that Assumptions A2, A3, and A4 hold. Let* $f_{\text{target}} \leq f(x^0)$, $\varepsilon > 0$, *and* $\delta > 0$ *be given. Then, there exists a cycle* ℓ *of index not larger than*

$$\frac{f(x^0) - f_{\text{target}}}{c\,(\varepsilon/2)^{(p+1)/p}} + \frac{f(x^0) - f_{\text{target}}}{\alpha\,(\varepsilon/(2\bar{m}L_g))^{p+1}} + 1, \tag{50}$$

where c *only depends on* α, τ_2, L, p, *and* θ, *such that, in its first internal iteration* k, *either* $f(x^k) \leq f_{\text{target}}$ *or*

$$\left|[g_P(x^{k+1})]_i\right| \leq \varepsilon \text{ for all } i = 1, \ldots, n. \tag{51}$$

Proof The proof follows from Theorem 5.7 replacing ε with $\varepsilon/2$ and defining $\delta = \varepsilon/(2\bar{m}L_g)$. Note that the thesis holds for the first iteration of the cycle because, in fact, due to Theorem 5.7, it holds for all its iterations.

The impact of $\bar{m}$ on the complexity limit is expressed in formula (50). Note that the second term of (50) grows proportionally to $\bar{m}^{p+1}$. If n increases and the size of the subproblems remains bounded, then $\bar{m}$ grows proportionately to n. Under these conditions, an increase in the number of iterations proportional to n^{p+1} is expected. Theorems 5.1–5.8 give upper bounds on the number of iterations of Algorithm 4.1. (Bounds on the number of cycles translate into bounds on the number of iterations if multiplied by $\bar{m}$.) The first term of the sequence of regularization parameters used in Algorithm 3.1 is 0. If the corresponding trial point is rejected, the second term is $\sigma_{\min}$. Then, each time that σ needs to be increased, it is multiplied by a number larger than or equal to τ_1. Therefore, by definition, the sequence of σ's generated by Algorithm 3.1 is bounded from below by the sequence $0,\ \tau_1^0\sigma_{\min},\ \tau_1^1\sigma_{\min},\ \tau_1^2\sigma_{\min},\ \tau_1^3\sigma_{\min},\ \ldots$ Thus, by Theorem 3.1, the number of functional evaluations per call to Algorithm 3.1 at Step 2 of Algorithm 4.1 is bounded by

$$\log_{\tau_1}((L+\alpha)/\sigma_{\min}) + 2.$$

This establishes analogous bounds on the number of functional evaluations of Algorithm 4.1.

6 Discussion

Theorems 5.4 and 5.5 are complementary for showing that, eventually, Algorithm 4.1 computes an iterate x^k such that $\|\underline{g}_P(x^k)\|$ is smaller than a given tolerance; and that this task employs an amount of computer time that depends on tolerances and problem parameters. In Theorem 5.4, we proved that within $O(\varepsilon^{-(p+1)/p})$ iterations Algorithm 4.1 computes a sequence (cycle) of $\bar{m}$ iterates such that, for each $i = 1, \ldots, n$, there is at least one k such that $|[g_P(x^{k+1})]_i| \leq \varepsilon$. The number of required iterations for this purpose decreases with p and tends to $O(1/\varepsilon)$ when p tends to infinity. However, this result does not guarantee that the projected gradient norm is smaller than ε at a single iterate. For this purpose, we need the different iterates within a cycle to be clustered in a ball of small size. Unfortunately, in order to guarantee that this happens with tolerance δ, we need, according to Theorem 5.5, $O(1/\delta^{p+1})$ iterations. This quantity increases with p, which seems to indicate that, in the worst case, high-order coordinate descent is less efficient than low-order coordinate descent.

Examples given by Powell in [49] indicate that, in fact, this may be the case. In these examples, if coordinate descent is employed with exact coordinate minimization and cyclic coordinate descent, the generated sequence has more than one limit point. So, the distance

between consecutive iterations does not tend to zero. This behavior is not observed if Algorithm 4.1 is applied because the descent condition (17) implies that $\lim \|x^{k+1} - x^k\| = 0$. However, exact minimization at each iteration evokes the case $p = \infty$ of Algorithm 4.1 in the sense that the trial point computed as an exact minimizer satisfies the conditions for accepting the trial steps for any p. So, the conjecture arises that if one applies Algorithm 4.1 to Powell's examples with different values of p, the resulting sequence, although convergent to a solution, stays an increasing number of iterations oscillating around Powell's limiting cycle.

This conjecture is not easy to verify because, except one, Powell's examples are unstable in the sense that small perturbations cause convergence to the true minimizers far from the limit spurious cycle. In any case, we can emulate the application of Algorithm 4.1 to the most famous of Powell's examples (slightly modified here):

$$\text{Minimize } f(x_1, x_2, x_3) \equiv -(x_1x_2 + x_1x_3 + x_2x_3) + \sum_{i=1}^{3}(|x_i| - 0.1)_+^2. \tag{52}$$

If coordinate descent method employing exact coordinate minimization and cyclic coordinate descent is applied to problem (52) starting from

$$x^0 = (-0.1 - \epsilon, 0.1 + \epsilon/2, -0.1 - \epsilon/4),$$

it generates, after six iterations, an iterate x^6 that corresponds to x^0 with ϵ substituted with $\epsilon/64$, i.e.

$$x^6 = (-0.1 - \epsilon/64, 0.1 + \epsilon/128, -0.1 - \epsilon/256);$$

and, in general, for all k,

$$x^{6k} = (-0.1 - \epsilon/64^k, 0.1 + \epsilon/(2 \times 64^k), -0.1 - \epsilon/(4 \times 64^k)).$$

In the intermediate iterations, that are not multiples of 6, one has that

$$x^{6k+j} = (\pm 0.1 \pm \epsilon/\nu_{k,j}, \pm 0.1 \pm \epsilon/ \times \nu_{k,j}, \pm 0.1 \pm \epsilon/\nu_{k,j})$$

where $\nu_{k,j} \leq 4 \times 64^{k+1}$ for all k, j.

Now, we wish to show that this sequence could be generated by Algorithm 4.1. Moreover, for any given p, we wish to know how many iterations are necessary to obtain consecutive iterations such that $\|x^{k+1} - x^k\| \leq 0.01$. Let

$$x^0 = (-0.1 - \epsilon, 0.1 + \epsilon/2, -0.1 - \epsilon/4).$$

The global minimizer of $f(x_1, x_2, x_3)$ subject to $x_2 = x_2^0$ and $x_3 = x_3^0$ is

$$z^0 = (0.1 + \epsilon/8, 0.1 + \epsilon/2, -0.1 - \epsilon/4).$$

(The iterate x^1 in the Powell's sequence is given by $x^1 = z^0$, but we preserve the notation z^0 for the sake of simplicity.) On the one hand,

$$f(x^0) = -(x_1^0x_2^0 + x_1^0x_3^0 + x_2^0x_3^0) + \sum_{i=1}^{3}(|x_i^0| - 0.1)_+^2.$$

On the other hand, since $z_2^0 = x_2^0$ and $z_3^0 = x_3^0$,

$$f(z^0) = -(z_1^0x_2^0 + z_1^0x_3^0 + x_2^0x_3^0) + (|z_1^0| - 0.1)_+^2 + \sum_{i=2}^{3}(|x_i^0| - 0.1)_+^2.$$

Therefore,

$$f(x^0) - f(z^0) = (z_1^0 - x_1^0)(x_0^2 + x_0^3) + (|x_1^0| - 0.1)_+^2 - (|z_1^0| - 0.1)_+^2.$$

Thus,

$$\begin{aligned} f(x^0) - f(z^0) &= ((0.1 + \epsilon/8) - (-0.1 - \epsilon))(\epsilon/2 - \epsilon/4) + (|-0.1 - \epsilon| - 0.1)_+^2 \\ -(|0.1 + \epsilon/8| - 0.1)_+^2 & \\ &= (0.2 + 9\epsilon/8)\epsilon/4 + \epsilon^2 - \epsilon^2/64 = 0.2\epsilon/4 + 9\epsilon^2/32 + \epsilon^2 - \epsilon^2/64 \\ &= 0.2\epsilon/4 + 9\epsilon^2/32 + \epsilon^2 - \epsilon^2/64 = 0.2\epsilon/4 + 81\epsilon^2/64 \geq \epsilon/20. \end{aligned}$$

Consider Algorithm 4.1 using $f(x)$ as the model of the objective function. We must verify whether (15), (16), and (17) are satisfied with $x^{\text{trial}} = z^0$. Trivially, for $\sigma = 0$, (15) and (16) hold by the definition of the model and the fact that z^0 is a global minimizer. In order to show that (17) also holds, let as assume that $\epsilon < 0.1$ and $2^{p+1} \geq 20\alpha/\epsilon$, i.e. $\alpha/2^{p+1} \leq \epsilon/20$. So, by the calculations above,

$$f(x^0) - f(x^{\text{trial}}) \geq \alpha/2^{p+1}.$$

Since $\epsilon < 0.1$, we have that $\|x^{\text{trial}} - x^0\| \leq 0.5$. Thus,

$$f(x^0) - f(x^{\text{trial}}) \geq \alpha\|x^{\text{trial}} - x^0\|^{p+1}.$$

This implies (17). Therefore, a sufficient condition for the acceptance of $x^1 = z^0$ as an iterate of Algorithm 4.1 is

$$\alpha/2^{p+1} \leq \frac{\epsilon}{20 \times 4 \times 64^k}.$$

In other words,

$$20 \times 4 \times 64^k \alpha \leq \epsilon 2^{p+1}.$$

Taking logarithms, this condition is

$$\log_2 80 + 6k + \log_2 \alpha \leq p + 1.$$

That is, if

$$k_0 \leq (p + 1 - \log_2 80 - \log_2 \alpha)/6,$$

the first k_0 iterations of Algorithm 4.1 will reproduce the cycling example of Powell. In all these iterations we have that $\|x^{k+1} - x^k\| \geq 0.1$. Note that k_0 tends to infinity as p tends to infinite, as we wanted to show. In addition, note also that k_0 tends to infinity as α tends to zero, which reflects the obvious fact that, if we are more tolerant with the acceptance of the trial point, the probability of staying around Powell's six-points cycle increases.

It is not sensible to decide about usefulness of algorithms based only on theoretical convergence or complexity results. Since these results deal with worst-case behavior the possibility exists that a class of problems in which practitioners are interested always exhibit characteristics that exclude extreme unfortunate cases. However, it is pertinent to examine pure mathematical properties in order to foster unexpected good or bad computer behaviors.

1. Many optimization users believe that if a smooth function has a minimizer at a point x^*, then this point is a local minimizer of all its Taylor polynomials. This is true only if the dimension n is equal to 1. For arbitrary n, it is true only up to second order polynomials. Examples that illustrates this phenomenon have been given in this paper with the purpose of justifying adequate high-order optimality conditions (for example, $f(x_1, x_2) = x_2^2 -$

$x_1^2 x_2 + x_1^4$). This fact implies that, in the vicinity of a global minimizer, a high-order algorithm may try to find improvements far from the current point, being subject to a painful sequence of "backtrackings" before obtaining descent. Does this imply that only quadratic approximations are useful in the minimization context? It is too soon to give a definite response to this question.

2. Our regularization approach for CD-algorithms makes it impossible to exhibit the cyclic behavior of Powell's examples [49]. The reason is that, under regularization descent algorithms, the difference between consecutive iterates tends to zero. However, it seems to be possible that convergence to zero of consecutive iterates could be very slow, as predicted by complexity results. Is this an argument for discarding high-order CD algorithms? We believe that the answer is no, as far as the use of CD algorithms is, in general, motivated by the structure of the problems, which in some sense should evoke some degree of separability. Moreover, since high-order models are also low-order models one can use high-order associated with a small p in (15), (16), and (17). In other words, if $1 \leq q < p$, then the conditions that define a model of order q are satisfied by models of order p. Therefore, we may use models of order p associated with the regularization required by models of order q. For example, we may use a second-order model associated to quadratic regularization preserving first-order convergence results and the corresponding complexity.
3. It is interesting to consider the case in which we use $f(x)$ as a model for $f(x)$. In this case, high-order analysis makes a lot of sense. In fact, efficient algorithms for finding global minimizers of functions of one variable exist, a possibility that decreases very fast as the number of variables grow. Moreover high-order one-dimensional models are certainly affordable and many numerical analysis papers handle efficiently the problem of minimizing or finding roots of univariate polynomials [48]. Recall that, in this case, the model satisfies the approximation requirements for every value of p. Therefore we may choose the value of p that promises better efficiency, which, according to Theorem 5.8, should be $p = 1$ giving complexity $O(\varepsilon^{-2})$ as gradient-like methods.
4. In most practical situations one is interested in finding global minimizers or, at least, feasible points at which the objective function value is smaller than a given f_{target}. Complexity and convergence analyses in the nonconvex world concern only the approximation to stationary points although every practical algorithm must be devised taking into account the global implicit goal. It turns out that low coordinate global strategies for finding initial points are available in many real-life problems. These strategies fit well with CD algorithms as we will illustrate in Sect. 7.
5. The reader will observe that in our experiments we used $p = 2$, in spite that, according to the complexity results, the optimal p should be 1. The reason is that, as we stated in the convergence section, the employment of $p = 2$ guarantees convergence to points that satisfy second order conditions that are not guaranteed by $p = 1$. Moreover, subproblems with $p = 2$ are computationally affordable in the applications considered. Summing up, we could say that making an informal balance regarding theoretical results, using $p = 2$ should be the default choice for practical applications.

7 Implementation and experiments

This section illustrates with numerical experiments the applicability of Algorithm 4.1. The Multidimensional Scaling (MS) problem [28, 45, 50] adopted for the experiments is described

in Sect. 7.1. Implementation details of Algorithms 3.1 and 4.1 are described in Sect. 7.2. Problem-dependent strategies for generating an initial point and for generating a sequence of improved initial points are described in Sect. 7.3. The computational results are shown in Sect. 7.4.

7.1 Multidimensional scaling problem

Multidimensional Scaling methods emerged as statistical tools in Psychophysics and sensory analysis. The MS problem considered in this section may be described in the following way: Let $x_1, \ldots, x_{n_p} \in \mathbb{R}^d$ be a set of unknown points. Let $D = (d_{ij}) \in \mathbb{R}^{n_p \times n_p}$ be such that $d_{ij} = \|x_i - x_j\|$; and assume that only entries $\{d_{ij} \mid (i, j) \in S\}$ for a given $S \subset \{1, \ldots, n_p\} \times \{1, \ldots, n_p\}$ are known. (Of course, D is symmetric, $d_{ii} = 0$, and $(i, j) \in S$ if and only if $(j, i) \in S$.) Then the MS problem consists of finding $x_1, \ldots, x_{n_p}$ such that $\|x_i - x_j\| = d_{ij}$ for all $(i, j) \in S$. Glunt, Hayden, and Raydan [33] were the first to apply unconstrained continuous optimization tools to the nowadays called Molecular Distance Geometry Problem (MDGP), as defined in [38, 39] in a Multidimensional Scaling context. This problem appears when points $x_1, \ldots, x_{n_p}$ correspond to the positions of atoms in a molecule and distances not larger than 6 Angstroms (i.e. 6×10^{-10} meters) are obtained via nuclear magnetic resonance (NMR) [1]. This problem can be modeled as the following unconstrained nonlinear optimization problem

$$\underset{x_1,\ldots,x_{n_p}\in\mathbb{R}^d}{\text{Minimize}} f(x_1, \ldots, x_{n_p}) := \frac{1}{|S|} \sum_{(i,j)\in S} \left(\|x_i - x_j\|_2^2 - d_{ij}^2\right)^2. \tag{53}$$

7.2 Implementation details

If we wish to apply Algorithm 4.1 to the MDGP problem, it arises quite naturally to associate at iteration k the set I_k with the components of a point $x_{\ell(k)} \in \mathbb{R}^d$ for some $\ell(k)$ between 1 and n_p. Specifically, if we define $x = (x_1^T, \ldots, x_{n_p}^T)^T \in \mathbb{R}^n$ with $n := d\, n_p$, then at iteration k we can define

$$I_k = \{(\ell(k) - 1)d + 1, \ldots, (\ell(k) - 1)d + d\} \text{ with } \ell(k) = \text{mod}(k, n_p) + 1, \tag{54}$$

or any alternative choice of $\ell(k) \in \{1, \ldots, n_p\}$. This is equivalent to say that, at iteration k, the subproblem considered at Step 2 of Algorithm 4.1 is given by

$$\underset{z\in\mathbb{R}^d}{\text{Minimize}} \underline{f}(z), \tag{55}$$

where $\underline{f} : \mathbb{R}^d \to \mathbb{R}$ is defined as

$$\underline{f}(z) := \frac{1}{|S|} \left[\sum_{(i,j)\in S\setminus S(\ell(k))} \left(\|x_i - x_j\|_2^2 - d_{ij}^2\right)^2 + 2 \sum_{(i,\ell(k))\in S} \left(\|x_i - z\|_2^2 - d_{i,\ell(k)}^2\right)^2 \right], \tag{56}$$

$S(\ell(k)) := \{(i, j) \in S \mid i = \ell(k) \text{ or } j = \ell(k)\}$, and $\ell(k)$ is given by (54). Note that the time complexity for evaluating f is $O(d|S|)$; while, since the first summation in (56) does not depend on z, the time complexity for evaluating $\underline{f}$ is, in average $O(d|S|/n_p)$.

For approximately solving (55) in Algorithm 3.1, we consider a second-order Taylor expansion of $\underline{f}$ at $\bar{x} = x^k_{\ell(k)} \in \mathbb{R}^d$, i.e.

$$M_{\bar{x}}(z) := \underline{f}(\bar{x}) + \nabla \underline{f}(\bar{x})^T (z - \bar{x}) + (z - \bar{x})^T \nabla^2 \underline{f}(\bar{x})^T (z - \bar{x}). \tag{57}$$

This means that the underlying model-based subproblem, when Algorithm 3.1 is used at Step 2 of the kth iteration of Algorithm 4.1 is given by

$$\underset{z \in \mathbb{R}^d}{\text{Minimize}} M_{\bar{x}}(z) + \sigma \|z - \bar{x}\|^3. \tag{58}$$

Since problem (53) is unconstrained, i.e. $\Omega = \mathbb{R}^n$, subproblems (55) and model-based subproblems (58) are unconstrained as well. Thus, if in (58) and, in consequence, in (17), for $x \in \mathbb{R}^d$, we consider $\|x\|$ as $\|x\|_3 := (\sum_{i=1}^d |x_i|^3)^{1/3}$, then the *global* minimizer of (58) can be easily obtained at the expense of a single factorization of $\nabla^2 \underline{f}(\bar{x}) \in \mathbb{R}^{d \times d}$, see [8, 18, 43, 44]. (When $\sigma = 0$, (58) may have no solution. This case can be detected with the same cost as well.) Since the exact global minimizer x^{trial} of (58) is being computed at Step 2 of Algorithm 3.1, (15) and (16) always hold, for any $\theta > 0$; thus, in the implementation, their verification can be ignored.

7.3 Initial guess and multistart strategy

As shown in Sect. 4, Algorithm 4.1 has convergence properties towards stationary points which, probably, are local minimizers. Obviously, as we are interested in finding *global* minimizers of MDGP, we need suitable strategies for choosing initial approximations. We employed the combination of two different strategies for this purpose. On the one hand, an initial guess suggested in [32] was adopted. On the other hand, we devised a new coordinate descent procedure based on the structure of MDGP. The Fang-O'Leary strategy [32], based on shortest paths over an underlying graph, is a strategy for computing a single initial solution. Starting from that solution, our new coordinate descent procedure is used iteratively to make successive improvements on the Fang–O'Leary initial point. At each improvement, Algorithm 4.1 is run to find a local solution.

In order to describe the Fang-O'Leary strategy [32], consider the weighted graph $G = (\{1, \ldots, n_p\}, S)$ in which the weight of an edge (i, j) is given by d_{ij}. We assume this graph is connected. Otherwise, the molecule's structure can not be recovered; and problem (53) can be decomposed in as many independent problems as connected components of the graph G in order to recover partial structures. Let $\bar{S} = \{1, \ldots, n_p\} \times \{1, \ldots, n_p\} \setminus S$, i.e. $\bar{S}$ corresponds to the missing arcs in G or, equivalently, the unknown entries of D. For each $(i, j) \in S$, define $\tilde{d}_{ij} = d_{ij}$; and for each $(i, j) \in \bar{S}$, define $\tilde{d}_{ij}$ as the weight of the shortest path between i and j in G. Matrix $\tilde{D} = (\tilde{d}_{ij})$ is a distance matrix that completes D; but with high probability it is *not* an Euclidean distance matrix. Computing $\tilde{D}$ requires $O(n_p^2)$ space and has time complexity $O(n_p^3)$ (using the Floyd–Warshall algorithm as suggested in [32]), which can be an issue for instances with large n_p. Obtaining points $x^0_1, \ldots, x^0_{n_p} \in \mathbb{R}^d$ from $\tilde{D}$ requires to compute the d largest positive eigenvalues of the matrix $\mathcal{T}(\tilde{D})$ given by $\mathcal{T}(\tilde{D}) := -\frac{1}{2} J \tilde{D} J$, where $J := I - \frac{1}{n} e e^T$ and $e = (1, \ldots, 1)^T$. If the truncated spectral decomposition of $\mathcal{T}(\tilde{D})$ is given by $U \Delta_d U^T$ then the initial point $x^0 = ((x^0_1)^T, \ldots, (x^0_{n_p})^T)^T$ is given by $X = (x^0_1, \ldots, x^0_{n_p}) = U \Delta_d^{1/2}$. If the matrix $\mathcal{T}(\tilde{D})$ has only $\underline{d} < d$ positive eigenvalues, then computed points are in $\mathbb{R}^{\underline{d}}$ and their last $d - \underline{d}$ components can be completed with zeros. In

[32], alternative initial guesses are obtained by perturbations of matrix $\tilde{D}$ and/or by stretching the computed points $x_1^0, \ldots, x_{n_p}^0$.

Our coordinate-descent strategy for choosing the initial approximation to the solution of MDGP is inspired on the structure of local solutions. Consider a point $p \in \mathbb{R}^3$ and three other points $q_1, q_2, q_3 \in \mathbb{R}^3$ such that the distances from p to q_i, $i = 1, 2, 3$, are known, i.e., $(p, q_i) \in S$ for $i = 1, 2, 3$. Assume, in addition, that the required distances are satisfied, i.e., that $\|p - q_i\|$ is equal to the corresponding value in matrix D for $i = 1, 2, 3$. Assume that there is an additional point q_4 for which its known distance $d(p, q_4)$ to p is *not* satisfied. Assume, in addition, that $(\|r(p) - q_4\|_2^2 - d(p, q_4)^2)^2 < (\|p - q_4\|_2^2 - d(p, q_4)^2)^2$, where $r(p)$ is the reflection of p on the plane determined by q_i, $i = 1, 2, 3$. If there were no more points in the problem, replacing p by $r(p)$, would produce a reduction in the objective function. Our coordinate descent algorithm with a coordinate-descent strategy for choosing initial points is described in Algorithm 7.1. The coordinate-descent strategy for initial approximations, based on this intuition, is described at Step 4 of Algorithm 7.1.

Algorithm 7.1. Assume $\hat{x}$ is a given arbitrary initial point (that might be obtained using the Fang-O'Leary technique described above).

Step 1. Using $\hat{x}$ as initial guess, run Algorithm 4.1 until the obtention of an iterate $\tilde{x}$ such that $f(\tilde{x}) \leq f_{\text{target}}$ or such that its projected gradient is small enough according to criteria given below.

Step 2. If $f(\tilde{x}) \leq f_{\text{target}}$ then **stop** declaring that $\tilde{x}$ is a global minimizer up to the precision given by f_{target}. Otherwise, update $\hat{x}$ by means of the coordinate-descent strategy in Step 3 below.

Step 3. For $j = 1, \ldots, n_p$ execute Steps 3.1–3.2.

Step 3.1. Let $\hat{f}_j := \sum_{(i,j)\in S} (\|\hat{x}_i - \hat{x}_j\|_2^2 - d_{ij}^2)^2$.

Step 3.2. For every triplet (i_1, i_2, i_3) such that $(i_1, j), (i_2, j), (i_3, j) \in S$, in an arbitrary order, if

$$\sum_{(i,j)\in S} (\|\hat{x}_i - r(\hat{x}_j)\|_2^2 - d_{ij}^2)^2 < \hat{f}_j,$$

where $r(\hat{x}_j)$ is the reflection of $\hat{x}_j$ on the plane determined by $\hat{x}_{i_1}$, $\hat{x}_{i_2}$, and $\hat{x}_{i_3}$, then update $\hat{x}_j \leftarrow r(\hat{x}_j)$. (Note that $\hat{f}_j$ is not updated at this point. This means that a sequence of reflections can be applied to $\hat{x}_j$, with a non-monotone behavior of f, provided it improves the "reference value" $\hat{f}_j$.)

Step 4. If $\hat{x}$ was not updated at Step 3, then stop returning $\tilde{x}$. (Note that f_{target} was not reached in this case.) Otherwise, go to Step 1.

At Step 1 of Algorithm 7.1, we consider that "the projected gradient is small enough" if, during n_p consecutive iterations of Algorithm 4.1, we have that "the final σ" of Algorithm 3.1 is larger than 10^{20} or $f(x^{k+1}) \not\leq f(x^k) - 10^{-8} \min\{1, |f(x^k)|\}$. By (26), (27) and the boundedness of σ, these are practical symptoms of stationarity.

7.4 Computational results

We implemented Algorithms 3.1, 4.1, and 7.1 in Fortran. In the numerical experiments, we considered, $\alpha = 10^{-8}$, $\sigma_{\min} = 10^{-8}$, and $\tau_1 = \tau_2 = 100$, and $f_{\text{target}} = 10^{-10}$. All tests were conducted on a computer with a 3.5 GHz Intel Core i7 processor and 16GB 1600 MHz DDR3 RAM memory, running macOS High Sierra (version 10.13.6). Code was compiled by the GFortran compiler of GCC (version 8.2.0) with the -O3 optimization directive enabled.

Table 1 Description of the instances built with the molecules considered in [1] or [32]

Molecule	n	n_p	$\|S\|$	Time x^0
Points may correspond to protein atoms (ATOM) only or to protein atoms plus atoms in small molecules (HETATM)				
ATOM only				
1ptq	1206	402	14,176 (8.79%)	0.21
1hoe	1674	558	20,356 (6.55%)	0.49
1lfb	1923	641	22,870 (5.57%)	0.70
1pht	2433	811	35,268 (5.37%)	1.41
1poa	2742	914	33,966 (4.07%)	2.03
2igg	2919	973	62,574 (6.62%)	2.54
1ax8	3009	1003	37,590 (3.74%)	2.76
1rml	6192	2064	153,660 (3.61%)	24.14
1ak6	8214	2738	224,568 (3.00%)	52.04
1a24	8856	2952	212,364 (2.44%)	64.90
3msp	11,940	3980	262,876 (1.66%)	157.90
3eza	15,441	5147	356,544 (1.35%)	335.84
ATOM + HETATM				
1ptq	1212	404	14,370 (8.83%)	0.21
1hoe	1743	581	21,422 (6.36%)	0.55
1pht	2964	988	44,542 (4.57%)	2.59
1poa	3201	1067	41,034 (3.61%)	3.23
1ax8	3222	1074	40,866 (3.55%)	3.29
1rml	6273	2091	156,550 (3.58%)	23.90

The Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank [52] is an open access repository that provides access to 3D structure data for large biological molecules (proteins, DNA, and RNA). There are more than 167,000 molecules available. In [32], where Newton and quasi-Newton methods are applied to problem (53), six protein molecules are considered, namely, 2IGG, 1RML, 1AK6, 1A24, 3MSP, and 3EZA (see [32, Table 6.9, p.20]); while in [1], where the Douglas-Rachford method is applied, other six protein molecules are considered, namely, 1PTQ, 1HOE, 1LFB, 1PHT, 1POA, and 1AX8 (see [1, Table 1, p.313]). In the first work, only protein atoms (identified with ATOM in the molecule file) were considered; while in the second work there were considered protein atoms plus atoms in small molecules (identified with HETATM in the protein molecule file). In the current work, both options were considered. Following [32], for each protein molecule, when multiple structures are available, only the first one was considered. Each molecule is given as the set of 3D coordinates of its atoms. An instance of problem (53) is built by computing a complete Euclidean distance matrix and then eliminating distances larger than 6 Angstroms. Since not all molecules have atoms in small molecules, we arrived to eighteen different instances. Table 1 shows, for each instance, the number of variables n of the optimization problem (53), the number of atoms n_p, the number of distances considered to be known $|S|$, and the CPU time in seconds required to construct the initial guess x^0 using the Fang-O'Leary strategy [32].

Note that considered instances are *gedanken* in the sense that points $\bar{x}_1, \ldots, \bar{x}_{n_p} \in \mathbb{R}^3$ such that $f(\bar{x}) = 0$ with $\bar{x}^T = (\bar{x}_1^T, \ldots, \bar{x}_{n_p}^T)^T$ are known. Thus, given x^* such that $f(x^*) \approx 0$, we may wonder whether x^* is close to $\bar{x}$. The answer to this question is "Not necessarily." since any rotation or translation of $\bar{x}$ also annihilates f. So the question would be "How close is x^* to $\bar{x}$ after performing the appropriate rotations and translations?". The answer to this question is obtained by solving an orthogonal Procrustes problem. Let $\bar{X} = (\bar{x}_1, \ldots, \bar{x}_{n_p})$ and $X^* = (x_1^*, \ldots, x_{n_p}^*) \in \mathbb{R}^{3\times n_p}$. It is easy to see that matrices $\bar{X}J$ and X^*J have their centroid at the origin, since $\bar{X}Je = X^*Je = 0$. (Recall that $J = I - \frac{1}{n_p}ee^T$ and $e = (1, \ldots, 1)^T$.) The orthogonal Procrustes problem consists in finding an orthogonal matrix $Q \in \mathbb{R}^{3\times 3}$ which most closely maps X^*J to $\bar{X}J$, i.e.

$$Q = \underset{R\in\mathbb{R}^{3\times 3}}{\operatorname{argmin}} \|RX^*J - \bar{X}J\|_F^2 \text{ subject to } RR^T = I.$$

This problem has a closed form solution given by $Q = VU^T$, where $U\Sigma V^T$ is the singular value decomposition of the matrix $C := X^*J(\bar{X}J)^T$. Thus, the measure we were looking for is given by

$$E(x^*) := \max_{\{j=1,\ldots,n_p\}} \left\{ E(x_j^*) \right\},$$

where

$$E(x_j^*) := \frac{\|[QX^*J - \bar{X}J]_j\|_\infty}{\max\{1, \|[\bar{X}J]_j\|_\infty\}}, \tag{59}$$

and $[A]_j$ denotes the jth column of matrix A.

Table 2 shows the performance of Coordinate Descent, the Spectral Projected Gradient (SPG) method [10–13], and Gencan [6, 9]. In all cases, the initial point given by the Fang-O'Leary technique was used. Since problem (53) is unconstrained, applying SPG corresponds to applying the Spectral Gradient methods as proposed in [33]; while applying Gencan corresponds to applying a line search Newton's method as considered in [32]. All three methods used as stopping criterion $f(x^k) \le f_{\text{target}} := 10^{-10}$. In addition, SPG and Gencan also stopped if $\|\nabla f(x^k)\|_\infty \le \varepsilon_{\text{opt}} := 10^{-8}$. For all three methods the table shows the number of iterations (#iter), the CPU time in seconds (Time), the value of the objective function at the final iterate ($f(x^*)$), and the error with respect to the known solution ($E(x^*)$). In addition, the table shows, for the coordinate descent method the number of evaluations of f; while it shows for the other two methods, the number of evaluations of f and $\|\nabla f(x^*)\|_\infty$. In the table, underlined figures in column $f(x^*)$ are the ones that correspond to local minimizers. Underlined figures in column $E(x^*)$ correspond to final iterates that are far from the known solution. In most cases, this fact is associated with having found a local minimizer. However, in some cases, it corresponds to an alternative global minimizer. We may observe that coordinate descent stands out as the only method to have found a global minimizer in all the eighteen considered instances. Figures 2 and 3 illustrate three molecules in which the coordinate descent method found a global solution while SPG and Gencan found local non-global minimizers. It is worth mentioning that the numerical experiments reported in [1] show that the Douglas-Rachford method, that requires an SVD decomposition of a $n_p \times n_p$ matrix per iteration, with a limit of 5,000 iterations, was able to reconstruct the two smallest molecules (1PTQ and 1HOE) only. As reported in [1], the reconstruction of molecules 1LFB and 1PHT was "satisfactory"; while the reconstruction of molecules 1POA and 1AX8 was "poor".

Table 2 Performance of coordinate descent, SPG, and Gencan applied to the instances of problem (53) built with the molecules considered in [1] or [32]

Molecule	Coordinate descent					Spectral projected gradient					Gencan					
	#iter	#f	Time	$f(x^*)$	$E(x^*)$	#iter	#f	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$	#iter	#f	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$
Points may correspond to protein atoms (ATOM) only or to protein atoms plus atoms in small molecules (HETATM)																	
ATOM only																	
1ptq	57,671	57,686	0.13	9.99e−11	1.66e−06	333	334	0.05	1.12e−11	3.32e−07	2.60e−06	9	13	0.42	5.82e−13	1.45e−07	2.58e−06
1hoe	135,886	135,907	0.30	9.99e−11	2.36e−06	126	128	0.03	8.52e−11	4.39e−07	3.62e−06	7	10	0.62	5.49e−11	1.26e−06	7.25e−06
1lfb	811,486	811,613	1.79	9.99e−11	7.56e−06	738	755	0.19	1.77e−11	5.19e−07	1.11e−06	13	20	1.15	5.96e−11	1.05e−06	4.27e−06
1pht	786,655	786,831	1.99	9.99e−11	1.79e−05	5945	6856	2.50	2.85e−02	5.04e−09	2.08e−01	127	340	28.67	2.85e−02	9.10e−07	2.08e−01
1poa	704,652	704,762	1.59	9.99e−11	9.79e−06	7367	8716	3.00	9.95e−11	3.00e−08	5.84e−04	18	19	2.71	1.79e−11	3.68e−07	2.32e−04
2igg	484,388	484,473	1.56	9.99e−11	9.12e−06	304	305	0.21	8.79e−11	3.18e−07	3.43e−06	11	22	4.58	2.45e−13	1.24e−08	2.58e−07
1ax8	353,820	353,895	0.80	9.99e−11	2.54e−06	325	326	0.14	8.11e−11	1.74e−07	2.02e−05	14	20	3.59	7.98e−13	1.97e−08	2.14e−06
1rml	340,528	340,586	1.24	9.99e−11	4.07e−06	236	238	0.39	1.21e−12	9.05e−08	1.46e−06	9	10	30.48	3.77e−13	6.47e−08	1.23e−06
1ak6	15,138,479	15,138,810	229.85	9.99e−11	1.35e−05	1662	1755	4.06	5.18e−02	9.92e−09	1.97e−01	166	421	953.67	5.18e−02	7.47e−09	1.97e−01
1a24	2,840,577	2,840,834	9.87	9.99e−11	1.39e−05	322	325	0.74	8.10e−11	5.88e−08	1.15e−05	19	48	74.23	8.76e−12	1.76e−07	7.89e−06
3msp	12,873,352	12,874,426	42.40	9.99e−11	1.61e−05	672	688	1.93	1.41e−10	8.47e−09	1.86e−05	31	55	138.70	1.24e−11	1.56e−08	5.46e−06
3eza	17,122,466	17,123,479	58.89	9.99e−11	1.03e−05	580	586	2.26	4.43e−10	9.66e−09	2.11e−05	23	51	224.11	1.24e−10	3.08e−09	1.18e−05
ATOM+HETATM																	
1ptq	57,640	57,659	0.13	9.99e−11	1.61e−06	334	335	0.05	8.45e−11	2.81e−07	3.60e−05	10	15	0.45	3.83e−17	9.27e−10	2.24e−08
1hoe	129,571	129,590	0.31	9.99e−11	2.25e−06	143	144	0.04	3.48e−11	3.47e−07	2.82e−06	8	11	0.76	8.61e−18	4.80e−10	3.14e−09
1pht	946,496	946,610	8.26	9.99e−11	1.60e−05	1541	1608	0.78	1.61e−05	9.85e−09	1.04e−01	21	31	8.48	1.61e−05	1.49e−09	1.04e−01
1poa	409,610	409,655	0.93	9.99e−11	5.20e−05	12,996	15,710	6.43	1.84e−10	9.99e−09	1.57e−02	15	18	4.31	1.93e−11	4.49e−07	1.38e−02
1ax8	308,962	309,026	0.70	9.99e−11	2.18e−06	148	149	0.07	9.43e−11	2.25e−07	1.04e−05	8	11	3.18	1.54e−12	2.35e−07	6.49e−07
1rml	344,977	345,021	1.28	9.99e−11	4.01e−06	305	307	0.52	9.48e−11	1.55e−07	4.36e−05	10	11	36.41	9.82e−17	5.53e−10	4.35e−08

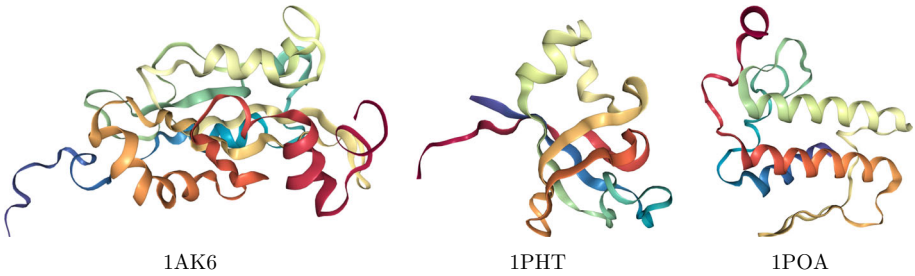

Fig. 2 Representation of molecules 1AK6, 1PHT, and 1POA for which Coordinate Descent found a global minimizer; while SPG and Gencan found a local minimizer

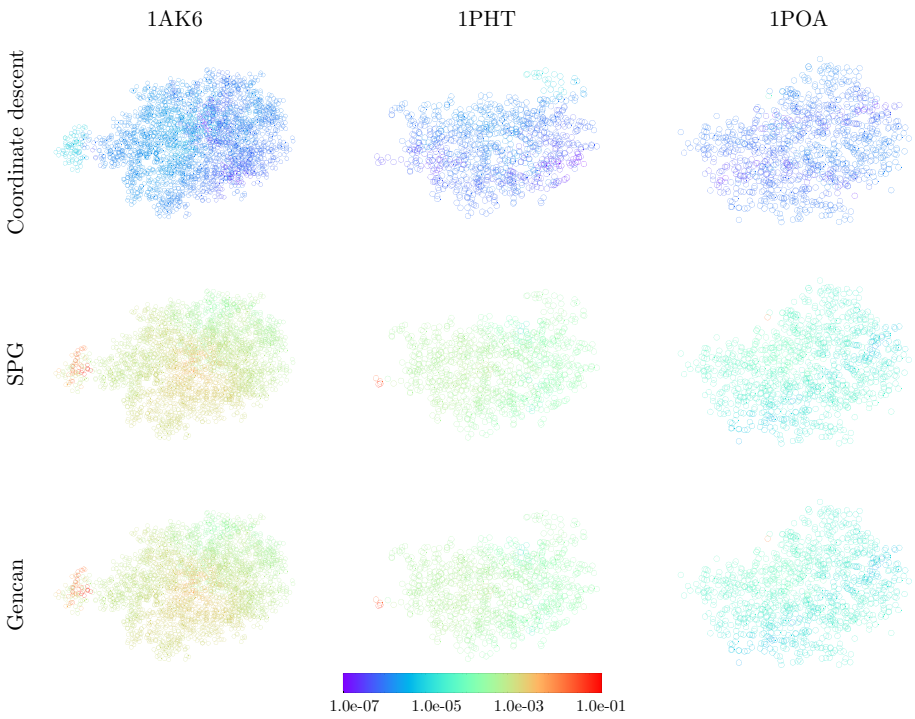

Fig. 3 Molecules 1AK6, 1PHT, and 1POA for which Coordinate Descent found a global minimizer; while SPG and Gencan found a local minimizer. To the naked eye, solutions would appear to be indistinguishable. Therefore, the figures show, for each point $x_1^*, \ldots, x_{n_p}^*$, the value of $E(x_j^*)$ as defined in (59)

At this point the following question arises: how does solving the subproblems with cubically-regularized second-order models affect the performance of the CD method? To answer this question, we solved the same 18 problems tackling the subproblems with quadratically-regularized linear models. This means that, to approximately solve (55) with Algorithm 3.1, we considered $p = 1$. In other words, instead of (57,58), **(a)** we considered the first-order Taylor expansion of $\underline{f}$ at $\bar{x} = x_{\ell(k)}^k \in \mathbb{R}^d$ given by $M_{\bar{x}}(z) := \underline{f}(\bar{x}) + \nabla \underline{f}(\bar{x})^T (z - \bar{x})$, and **(b)** we computed x^{trial} as the global minimizer of

Table 3 Performance of coordinate descent with $p = 1$, i.e. considering quadratically-regularized linear models for solving subproblems, applied to the same instances already shown in Table 2

Molecule	Coordinate descent with $p = 1$				
	#iter	#$\underline{f}$	Time	$f(x^*)$	$E(x^*)$
ATOM only					
1ptq	1,115,103	1,672,658	1.97	9.99e−11	3.98e−05
1hoe	1,862,919	2,794,382	3.10	9.99e−11	2.04e−06
1lfb	7,059,295	10,588,949	9.50	9.99e−11	7.52e−06
1pht	21,056,147	31,584,233	38.52	9.99e−11	2.73e−04
1poa	107,284,920	160,927,383	105.32	9.99e−11	5.85e−04
2igg	3,602,906	5,404,362	30.38	9.99e−11	8.43e−06
1ax8	2,059,932	3,089,901	4.56	9.99e−11	4.05e−06
1rml	9,186,681	13,780,025	98.21	9.99e−11	3.23e−06
1ak6	160,256,027	240,384,044	465.43	9.99e−11	1.62e−05
1a24	79,008,635	118,512,956	238.59	9.99e−11	1.40e−05
3msp	236,434,288	354,651,435	458.60	9.99e−11	1.61e−05
3eza	34,134,889	51,202,336	216.98	9.99e−11	1.07e−05
ATOM+HETATM					
1ptq	1,466,069	2,199,107	2.30	9.97e−11	4.26e−05
1hoe	683,645	1025,474	3.53	9.99e−11	1.98e−06
1pht	16,112,116	24168,177	23.29	9.99e−11	3.38e−05
1poa	32,496,533	48744,802	34.40	9.99e−11	1.46e−02
1ax8	6,829,569	10244,357	9.37	9.99e−11	2.47e−06
1rml	2,302,956	3454,437	87.64	9.99e−11	1.99e−06

$$\underset{z\in\mathbb{R}^d}{\text{Minimize}} M_{\bar{x}}(z) + \sigma\|z - \bar{x}\|^2. \tag{60}$$

Since (60) has no solution when $\nabla \underline{f}(\bar{x}) \neq 0$ and $\sigma = 0$, we skip the case $\sigma = 0$ by substituting $\sigma \leftarrow 0$ with $\sigma \leftarrow \sigma_{\min}$ at Step 1 of Algorithm 3.1. Apart from this, the settings for the case $p = 1$ were identical to those already described for the case $p = 2$. Table 3 shows the results. The numbers in the table show that the method found a global solution in all instances, a feature shared with its counterpart with $p = 2$. (Only in one instance an alternative global minimizer was found.) The numbers in the table also show that, on average, the method does 1.0001 function evaluations per iteration when $p = 2$, while that same amount is 1.5000 when $p = 1$. This means that, on the one hand, in the case $p = 1$, half of the times the solution of the regularized model is discarded for not satisfying the descent condition and the regularization parameter must be increased. On the other hand, this situation is extremely rare (once every ten thousand iterations) when $p = 2$. Moreover, the method with $p = 1$ uses, on average, 26 times more iterations, 39 times more function evaluations and 22 times more time than the case $p = 2$. The conclusion is that using quadratic models with cubic regularization whose global solution can be calculated using the method introduced in [8], greatly improves the performance of the proposed method.

Another natural question that arises is whether the tendency of the coordinate descent method in finding global minimizers could be observed in a larger set of instances. To check this hypothesis, we downloaded 64 additional *random* molecules with no more than 6,000

Table 4 Performance of coordinate descent and SPG methods in the 46 instances that consider protein atoms only

Molecule	n	n_p	$\|S\|$	Time x^0	Coordinate descent					Spectral projected gradient					
					#iter	$\#f$	Time	$f(x^*)$	$E(x^*)$	#iter	$\#f$	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$
6kbq	7554	2518	98,650 1.56	40.49	10,543,341	10,543,995	36.22	9.99e−11	2.65e−05	810	911	0.96	2.65e−02	7.65e−09	1.87e−01
6kc2	7530	2510	98,480 1.56	39.97	7,682,589	7,683,021	20.93	9.99e−11	2.62e−05	954	984	1.11	4.48e−12	3.43e−08	1.29e−05
6khu	3147	1049	39,372 3.58	3.09	316,876	316,959	0.83	9.99e−11	6.12e−06	411	413	0.19	5.66e−11	1.05e−06	7.83e−06
6kir	3861	1287	48,596 2.94	5.58	7,574,444	7,574,767	54.37	1.60e−03	1.50e−01	871	895	0.49	5.27e−11	1.01e−07	3.82e−05
6kk9	17,538	5846	218,662 0.64	479.82	215,549,505	215,561,546	712.59	9.29e−01	1.19e+00	6262	7030	17.33	9.09e−01	9.83e−09	1.15e+00
6kki	8193	2731	109,472 1.47	53.06	2,113,286	2,113,472	5.68	9.99e−11	5.04e−06	432	434	0.56	9.34e−11	1.33e−07	2.99e−05
6kkj	7866	2622	105,642 1.54	47.70	4,068,836	4,070,082	10.88	9.99e−11	5.18e−06	5868	6787	7.70	3.24e−10	9.99e−09	1.58e−03
6kkl	8262	2754	112,646 1.49	54.76	6,064263	6,064,648	16.61	9.99e−11	5.68e−06	592	604	0.78	9.47e−11	5.99e−08	6.48e−06
6kkv	14,607	4869	357,016 1.51	290.74	31,543,917	31,545,196	128.60	9.99e−11	1.86e−05	1095	1140	4.65	2.88e−11	6.93e−08	2.00e−06
6kx0	9885	3295	128,930 1.19	91.69	38,237,232	38,239,417	196.30	1.57e−01	1.02e+00	1428	1546	2.26	1.57e−01	9.87e−09	1.02e+00
6kys	5442	1814	70,296 2.14	16.13	984,382	984,559	2.49	9.99e−11	4.00e−06	359	360	0.29	8.44e−11	1.22e−07	2.95e−05
6l29	5427	1809	70,480 2.15	16.68	965,426	965,620	2.49	9.99e−11	4.51e−06	433	436	0.36	8.43e−11	7.93e−07	8.26e−06
6l2a	2463	821	29,876 4.44	1.55	411,298	411,381	1.04	9.99e−11	5.55e−06	1612	1699	0.59	9.95e−11	7.47e−08	6.46e−05
6laf	8442	2814	105,164 1.33	58.06	31,413,895	31,418,665	104.66	9.99e−11	2.51e−05	7706	9068	10.22	1.53e−02	9.76e−09	2.74e−01
6li7	7515	2505	98,374 1.57	40.21	10,533,446	10,534,072	37.27	9.99e−11	2.64e−05	698	713	0.83	8.73e−11	4.32e−07	1.54e−05
6lik	7515	2505	97,354 1.55	39.67	7,579,646	7,580,087	19.88	9.99e−11	2.63e−05	727	749	0.85	8.89e−11	2.61e−07	6.42e−05
6lty	5964	1988	73,296 1.86	19.95	3,800,264	3,800,792	9.82	9.99e−11	7.86e−06	672	683	0.58	9.76e−11	9.54e−08	1.78e−05
6ltz	3432	1144	41,230 3.15	3.97	975,177	975,323	2.48	9.99e−11	3.13e−06	8025	9404	4.08	1.27e−10	9.94e−09	9.66e−04
6m37	9999	3333	125,394 1.13	91.51	130,035,728	130,040,179	422.49	5.07e−02	4.33e−01	4936	5479	7.63	5.06e−02	9.99e−09	4.30e−01
6m5n	5781	1927	73,890 1.99	18.48	8,183,149	8,183,657	27.54	9.99e−11	6.22e−06	6419	7461	5.81	3.06e−03	9.98e−09	2.74e−01
6m6j	759	253	13,914 21.82	0.07	13,076	13,076	0.04	9.99e−11	1.84e−06	59	61	0.01	3.99e−12	1.99e−07	6.82e−07
6m6k	747	249	13,672 22.14	0.07	11,376	11,376	0.04	9.97e−11	1.29e−06	53	55	0.01	2.83e−11	5.59e−07	1.41e−06
6pq0	6087	2029	84,104 2.04	22.54	2,346,681	2,346,842	31.31	9.99e−11	3.83e−06	440	442	0.43	2.39e−04	8.43e−09	1.83e−01

Table 4 continued

Molecule	n	n_p	$\|S\|$	Time x^0	Coordinate descent					Spectral projected gradient					
					#iter	#f	Time	$f(x^*)$	$E(x^*)$	#iter	#f	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$
6pup	4035	1345	50,372 2.79	6.57	544,519	544,617	1.42	9.99e−11	4.87e−06	409	410	0.24	2.52e−11	7.99e−08	2.38e−05
6pxf	4944	1648	64,944 2.39	11.70	811,879	812,002	2.13	9.99e−11	2.77e−05	4907	5583	3.88	1.81e−10	9.41e−09	2.91e−03
6q08	741	247	13,232 21.78	0.07	22,723	22,744	0.07	9.99e−11	7.19e−06	173	176	0.03	5.75e−11	1.85e−06	3.82e−06
6sx6	2340	780	44,862 7.38	1.28	143,230	143,260	0.49	9.99e−11	2.50e−06	136	137	0.07	5.51e−12	1.80e−07	2.60e−07
6syk	2718	906	54,052 6.59	1.99	156,648	156,707	0.55	9.99e−11	2.50e−06	585	592	0.36	9.41e−12	2.34e−07	1.42e−05
6t1z	8943	2981	119,580 1.35	65.75	14,818,888	14,819,492	40.30	9.99e−11	8.88e−06	3247	3539	4.71	9.94e−11	1.37e−08	2.70e−04
6tad	4362	1454	58,736 2.78	8.07	2,385,243	2,385,423	6.35	9.99e−11	6.84e−06	632	643	0.44	7.87e−11	3.81e−07	5.70e−06
6twe	7902	2634	163,598 2.36	0.18	5,773,930	5,774,426	20.85	9.99e−11	8.20e−06	598	612	1.16	7.04e−11	1.66e−07	6.93e−06
6ubh	9009	3003	113,766 1.26	69.74	8,782,138	8,782,736	22.99	9.99e−11	1.64e−05	3565	4019	4.95	1.23e−10	9.86e−09	1.63e−03
6ucd	8199	2733	97,910 1.31	52.10	86,618,396	86,621,926	278.99	1.35e+00	1.88e+00	9391	11,180	11.51	9.92e−01	9.29e−09	1.10e+00
6veh	7431	2477	182,676 2.98	42.54	4,087,012	4,087,391	16.46	9.99e−11	1.43e−05	658	662	1.37	3.50e−11	1.38e−07	5.83e−06
6vk2	4704	1568	108,520 4.42	11.94	463,141	463,360	1.79	9.99e−11	9.46e−06	3069	3419	3.95	1.40e−10	9.62e−09	2.22e−03
6vnz	1392	464	25,364 11.81	0.32	88,484	88,530	0.29	9.99e−11	3.40e−06	206	208	0.06	6.02e−11	2.16e−07	4.36e−06
6vv6	7464	2488	92,878 1.50	45.42	7,583,602	7,584,292	33.37	9.99e−11	4.04e−06	1846	1943	2.05	6.23e−02	1.00e−08	2.23e−01
6vv7	7452	2484	93,102 1.51	44.46	7,692,189	7,692,886	41.06	9.99e−11	3.80e−06	1981	2233	2.26	1.07e−01	7.39e−09	2.23e−01
6vv9	7452	2484	92,506 1.50	44.29	6,251,096	6,251,759	29.79	9.99e−11	3.11e−06	1022	1040	1.14	7.95e−02	1.25e−09	2.17e−01
6wcr	11,766	3922	151,164 0.98	158.07	118,185,068	118,209,777	421.33	1.67e−01	3.74e−01	7460	8498	13.92	1.99e−01	9.96e−09	2.38e−01
6yuc	8637	2879	107,258 1.29	60.03	17,737,727	17,738,988	117.20	3.77e−01	6.86e−01	1450	1668	1.91	1.09e−04	9.93e−09	1.19e−01
6z4c	5838	1946	72,838 1.92	18.87	1,951,179	1,951,337	5.00	9.99e−11	2.72e−06	369	370	0.31	6.24e−11	2.43e−07	2.91e−06
6zcm	7899	2633	102,030 1.47	46.05	12,338,443	12,339,335	40.78	9.99e−11	2.53e−05	7445	8812	9.41	1.38e−10	9.93e−09	9.87e−04
7ckj	4731	1577	59,608 2.40	10.24	2,681,962	2,682,163	11.61	9.99e−11	3.27e−06	768	784	0.54	6.51e−07	5.85e−09	2.03e−01
7jjl	9690	3230	125,976 1.21	83.34	77,851,519	77,854,837	303.65	4.82e−01	4.52e−01	4830	5451	7.49	7.94e−01	8.12e−09	4.73e−01

Table 5 Performance of coordinate descent and SPG methods in the 37 instances that consider protein atoms plus atoms in small molecules

Molecule	n	n_p	$\|S\|$	Time x^0	Coordinate descent					Spectral Projected Gradient					
					#iter	#f	Time	$f(x^*)$	$E(x^*)$	#iter	#f	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$
6kbq	8106	2702	108,066 (1.48%)	50.64	6,476,123	6,476,435	17.57	9.99D-11	2.35D-05	571	580	0.71	9.97D-11	6.32D-08	1.85D-05
6kc2	8397	2799	111,198 (1.42%)	56.89	15,115,487	15,118,534	50.50	9.99D-11	2.15D-01	1102	1121	1.42	4.03D-10	9.36D-09	2.19D-01
6khu	3465	1155	44,672 (3.35%)	4.24	334,415	334,473	0.87	9.99D-11	6.35D-06	490	500	0.25	6.20D-11	1.63D-06	7.45D-06
6kir	4203	1401	54,634 (2.79%)	7.42	560,278	560,406	1.49	9.99D-11	4.20D-06	450	454	0.28	9.28D-11	4.63D-07	6.28D-05
6kk9	17,895	5965	225,776 (0.63%)	515.33	202,467,161	202,477,953	691.77	4.00D-01	3.09D-01	5084	5637	13.87	3.82D-01	9.95D-09	3.70D-01
6kki	8364	2788	111,596 (1.44%)	56.23	2,049,210	2,049,408	5.51	9.99D-11	3.93D-06	592	594	0.76	9.92D-11	1.13D-07	5.68D-05
6kkj	7992	2664	106,472 (1.50%)	49.62	17,809,921	17,816,613	132.85	9.54D-04	2.81D-01	2921	3188	3.67	9.54D-04	9.12D-09	2.81D-01
6kkl	8421	2807	114,184 (1.45%)	58.35	6,082,607	6,082,924	16.57	9.99D-11	5.67D-06	521	537	0.70	6.88D-11	2.32D-07	6.82D-06
6kkv	14820	4940	364,756 (1.49%)	304.81	27,357,834	27,358,998	113.43	9.99D-11	1.80D-05	1193	1220	5.01	7.35D-10	7.99D-09	4.74D-05
6kx0	10,044	3348	131,624 (1.17%)	94.64	45,983,700	45,985,561	226.68	7.16D-02	2.47D-01	1044	1096	1.61	1.78D-01	9.27D-09	1.01D+00
6kys	5886	1962	77,926 (2.03%)	20.28	816,852	816,930	2.19	9.99D-11	3.60D-06	2389	2688	2.22	9.98D-11	3.11D-08	1.72D-04
6l29	5841	1947	77,602 (2.05%)	19.25	1,807,474	1,807,572	18.75	9.99D-11	1.26D-01	589	592	0.52	5.31D-04	4.39D-09	1.60D-01
6l2a	2643	881	32,644 (4.21%)	1.82	787,753	787,881	4.57	9.99D-11	5.77D-06	1769	1892	0.67	1.79D-10	9.03D-09	1.24D-01
6laf	8535	2845	106,084 (1.31%)	57.40	38,880,745	38,890,853	174.71	1.57D-02	3.40D-01	10,824	12,773	13.95	1.71D-02	9.71D-09	3.41D-01

Table 5 continued

Molecule	n	n_p	$\|S\|$	Time x^0	Coordinate descent					Spectral Projected Gradient					
					#iter	$\#f$	Time	$f(x^*)$	$E(x^*)$	#iter	$\#f$	Time	$f(x^*)$	$\|\nabla f(x^*)\|_\infty$	$E(x^*)$
6li7	8520	2840	114,120 (1.42%)	57.40	6,141,620	6,141,906	16.33	9.99D-11	2.29D-05	443	453	0.58	9.37D-11	5.62D-08	1.50D-05
6lik	8208	2736	108,364 (1.45%)	51.66	12,686,358	12,686,897	52.81	9.99D-11	2.48D-05	7235	8363	9.40	2.99D-03	9.91D-09	1.81D-01
6ltz	3798	1266	47,246 (2.95%)	5.62	767,531	767,612	1.93	9.99D-11	7.56D-06	985	1002	0.54	9.73D-11	5.68D-08	1.28D-04
6m5n	6687	2229	88,996 (1.79%)	29.41	2,380,904	2,381,175	6.33	9.99D-11	1.41D-01	14,921	17,730	15.90	6.98D-10	9.55D-09	1.42D-01
6m6j	840	280	15,602 (19.97%)	0.09	18,319	18,319	0.06	9.99D-11	1.86D-06	76	78	0.01	9.94D-11	3.25D-07	2.06D-06
6m6k	828	276	15,388 (20.27%)	0.09	15,964	15,964	0.05	9.99D-11	1.63D-06	74	76	0.01	1.00D-11	3.36D-07	7.45D-07
6pq0	6360	2120	89,018 (1.98%)	0.12	1,086,898	1,086,994	12.19	9.99D-11	3.98D-06	3540	4285	3.81	9.00D-11	1.21D-07	6.60D-05
6pup	4272	1424	55,442 (2.74%)	7.63	593,071	593,135	1.55	9.99D-11	3.60D-06	363	372	0.23	3.28D-11	6.55D-07	2.12D-06
6pxf	5661	1887	76,154 (2.14%)	17.47	6,753,157	6,775,873	25.50	9.97D-11	1.10D-01	4541	5069	4.07	1.04D-05	9.49D-09	1.16D-01
6t1z	9492	3164	127,488 (1.27%)	79.93	3,427,330	3,427,847	9.17	9.99D-11	1.14D-02	7688	9017	11.70	2.94D-10	9.82D-09	1.23D-02
6tad	5172	1724	71,178 (2.40%)	13.52	1,050,635	1,050,702	2.89	9.99D-11	3.64D-06	273	275	0.22	9.83D-11	3.61D-08	3.95D-06
6twe	7905	2635	163,694 (2.36%)	45.84	5,768,235	5,768,740	20.83	9.99D-11	8.19D-06	637	643	1.17	9.14D-11	1.78D-07	8.01D-06
6ubh	9999	3333	130,348 (1.17%)	91.62	22,598,823	22,602,027	107.35	9.99D-11	3.60D-01	1234	1279	1.90	6.89D-11	3.25D-07	3.63D-01
6veh	7566	2522	186,586 (2.93%)	42.40	4,241,879	4,242,258	17.14	9.99D-11	1.52D-05	381	384	0.80	8.74D-11	2.80D-07	4.54D-05
6vv6	8169	2723	107,072 (1.44%)	52.54	2,824,276	2,824,520	7.62	9.99D-11	9.75D-06	391	395	0.49	7.43D-11	8.50D-08	3.05D-06
6vv7	8247	2749	109,326 (1.45%)	52.54	3,807,178	3,807,395	10.23	9.99D-11	2.33D-06	4434	5002	5.83	5.68D-11	3.59D-07	2.89D-04
6vv9	8250	2750	108,784 (1.44%)	52.41	3,494,562	3,494,812	9.30	9.99D-11	8.41D-06	404	409	0.51	6.69D-11	2.00D-07	7.49D-06
6wcr	12,225	4075	157,032 (0.95%)	167.40	229,852,446	229,885,273	721.26	9.77D-05	8.68D-02	6972	7906	13.17	8.93D-02	9.97D-09	1.97D-01
6yuc	8640	2880	107,366 (1.29%)	59.34	50,987,720	50,988,983	203.00	1.09D-04	1.19D-01	1879	1942	2.37	1.09D-04	7.65D-09	1.19D-01
6z4c	5994	1998	76,300 (1.91%)	20.35	1,697,728	1,697,882	4.45	9.99D-11	2.95D-06	270	271	0.24	9.71D-11	2.20D-07	3.12D-06
6zcm	9696	3232	135,448 (1.30%)	83.59	6,978,627	6,978,943	19.30	9.99D-11	7.42D-06	2131	2288	3.43	9.67D-11	5.81D-08	1.55D-04
7ckj	5199	1733	68,624 (2.29%)	13.55	1,630,610	1,630,694	10.52	9.99D-11	4.11D-06	541	549	0.43	2.14D-05	9.60D-09	1.96D-01
7jjl	9693	3231	126,082 (1.21%)	83.84	102,233,476	102,237,339	369.96	2.46D-01	3.25D-01	5332	6097	8.12	7.94D-01	8.91D-09	4.73D-01

atoms from the ones that were uploaded in 2020; 56 of which have, other than protein atoms, atoms in small molecules. However there were 19 molecules for which, considering protein atoms only or protein atoms plus atoms in small molecules, the graph associated with the incomplete Euclidean matrix obtained by eliminating distances larger than 6 Angstroms is disconnected. Therefore, we were left with 45 and 37 molecules in each set, totalizing 82 new instances. Table 4 shows the performance of Coordinate Descent and SPG when applied to the 45 instances that consider protein atoms only; while Table 5 shows the performance of both methods when applied to the 37 instances that consider protein atoms plus atoms in small molecules. In the 45 instances in Table 4, Coordinate Descent found 37 global minimizers; while SPG found 30 global minimizers. In the 37 instances in Table 5, Coordinate Descent found 30 global minimizers; while SPG found 26 global minimizers.

8 Conclusions

Methods based on high-order models for optimization are difficult to implement due to the necessity of computing and storing high-order derivatives and the complexity of solving the subproblems. These difficulties are not so serious if the subproblems are low-dimensional, which is the most frequent situation in the case of CD methods. In the extreme case, in which one solves only univariate problems, the number of high-order partial derivatives that are necessary is a small multiple of the number of variables. Therefore, the theory that shows that CD algorithms with high-order models enjoy good convergence and complexity properties seems to be useful to support the efficiency of practical implementations. In this context, higher-order techniques allow to escape from attraction points that tend to satisfy lower-order optimality conditions; see [43].

Sometimes the fulfillment of a necessary high-order optimality condition can be expressed as fulfillment of $\Phi(x) = 0$, where Φ is a continuous nonnegative function. In this case, it makes sense to say that $\Phi(x) \leq \varepsilon$ is an approximate high-order optimality condition. Moreover, instead of requiring globality for the solution to the regularized model-based subproblem (18), we may require only that $\Phi(x^{k+1}) \to 0$ when $k \to +\infty$, where Φ corresponds to the high-order optimality condition of (18). Careful choices of Φ and the subproblems' stopping criterion may give rise to complexity results associated with the attainment of these high-order optimality conditions, see [24–26]. This will be the subject of future research.

In this paper the defined algorithms were applied to the identification of proteins under NMR data. Moreover, we extended the CD approach to the computation of a suitable initial approximation that avoids, in many cases, the convergence to local non-global minimizers. Our choice of the most adequate parameter p, that defines the approximating models, and the strategy for choosing the groups of variables were dictated by theoretical considerations discussed in Sect. 6 and by the specific characteristics of the problem. Our computing results are fully reproducible and the codes are available in http://www.ime.usp.br/~egbirgin/.

In future works we will apply the new CD techniques to the case in which data uncertainty is present and outliers are likely to occur. Possible improvements also include the choice of different models at each iteration or at each group of variables with the aim of making a better use of current information.

Data availability: The datasets generated during and/or analyzed during the current study are available in the corresponding author web page, http://www.ime.usp.br/\protect\unhbox\voidb@x\penalty\@M\egbirgin/.

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