

Dear Author,

Here are the proofs of your article.

- You can submit your corrections online, via e-mail or by fax.
- For **online** submission please insert your corrections in the online correction form. Always indicate the line number to which the correction refers.
- You can also insert your corrections in the proof PDF and email the annotated PDF.
- For fax submission, please ensure that your corrections are clearly legible. Use a fine black pen and write the correction in the margin, not too close to the edge of the page.
- Remember to note the **journal title**, **article number**, and **your name** when sending your response via e-mail or fax.
- **Check** the metadata sheet to make sure that the header information, especially author names and the corresponding affiliations are correctly shown.
- Check the questions that may have arisen during copy editing and insert your answers/ corrections.
- **Check** that the text is complete and that all figures, tables and their legends are included. Also check the accuracy of special characters, equations, and electronic supplementary material if applicable. If necessary refer to the *Edited manuscript*.
- The publication of inaccurate data such as dosages and units can have serious consequences. Please take particular care that all such details are correct.
- Please **do not** make changes that involve only matters of style. We have generally introduced forms that follow the journal's style. Substantial changes in content, e.g., new results, corrected values, title and authorship are not allowed without the approval of the responsible editor. In such a case, please contact the Editorial Office and return his/her consent together with the proof.
- If we do not receive your corrections within 48 hours, we will send you a reminder.
- Your article will be published **Online First** approximately one week after receipt of your corrected proofs. This is the **official first publication** citable with the DOI. **Further changes are, therefore, not possible.**
- The **printed version** will follow in a forthcoming issue.

Please note

After online publication, subscribers (personal/institutional) to this journal will have access to the complete article via the DOI using the URL: http://dx.doi.org/[DOI].

If you would like to know when your article has been published online, take advantage of our free alert service. For registration and further information go to: <u>http://www.link.springer.com</u>.

Due to the electronic nature of the procedure, the manuscript and the original figures will only be returned to you on special request. When you return your corrections, please inform us if you would like to have these documents returned.

Metadata of the article that will be visualized in OnlineFirst

| Please note: In | mages will appear | in color online but will be printed in black and white. | |
|-----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|--|
| ArticleTitle | An inexact restoration | derivative-free filter method for nonlinear programming | |
| Article Sub-Title | | | |
| Article CopyRight | SBMAC - Sociedade I (This will be the copy | Brasileira de Matemática Aplicada e Computacional right line in the final PDF) | |
| Journal Name | Computational and Ap | oplied Mathematics | |
| Corresponding Author | Family Name | Schuverdt | |
| | Particle | | |
| | Given Name | M. L. | |
| | Suffix | | |
| | Division | CONICET, Department of Mathematics, FCE | |
| | Organization | University of La Plata | |
| | Address | La Plata, Argentina | |
| | Email | schuverd@mate.unlp.edu.ar | |
| Author | Family Name | Echebest | |
| | Particle | | |
| | Given Name | N. | |
| | Suffix | | |
| | Division | Department of Mathematics, FCE | |
| | Organization | University of La Plata | |
| | Address | La Plata, Argentina | |
| | Email | opti@mate.unlp.edu.ar | |
| Author | Family Name | Vignau | |
| | Particle | | |
| | Given Name | R. P. | |
| | Suffix | | |
| | Division | Department of Mathematics, FCE | |
| | Organization | University of La Plata | |
| | Address | La Plata, Argentina | |
| | Email | vignau@mate.unlp.edu.ar | |
| | Received | 20 August 2014 | |
| Schedule | Revised | 19 May 2015 | |
| | Accepted 23 June 2015 | | |
| Abstract | An inexact restoration derivative-free filter method for nonlinear programming is introduced in this paper. Each iteration is composed of a restoration phase, which reduces a measure of infeasibility, and an optimization phase, which reduces the objective function. The restoration phase is solved using a derivative-free method for solving underdetermined nonlinear systems with bound constraints, developed previously by the authors. An alternative for solving the optimization phase is considered. Theoretical convergence results and some preliminary numerical experiments are presented. | | |
| Keywords (separated by '-') | Derivative-free - Nonl | inear programming - Filter methods - Inexact restoration methods | |

Mathematics Subject 65K05 - 90C30 - 90C56 Classification (separated by '-')

Footnote Information

Communicated by Ernesto G. Birgin.



An inexact restoration derivative-free filter method for nonlinear programming

N. Echebest¹ · M. L. Schuverdt² · R. P. Vignau¹

Received: 20 August 2014 / Revised: 19 May 2015 / Accepted: 23 June 2015 © SBMAC - Sociedade Brasileira de Matemática Aplicada e Computacional 2015

- Abstract An inexact restoration derivative-free filter method for nonlinear programming is
- ² introduced in this paper. Each iteration is composed of a restoration phase, which reduces
- ³ a measure of infeasibility, and an optimization phase, which reduces the objective function.
- ⁴ The restoration phase is solved using a derivative-free method for solving underdetermined
- $_{\rm 5}$ nonlinear systems with bound constraints, developed previously by the authors. An alternative
- ⁶ for solving the optimization phase is considered. Theoretical convergence results and some
- 7 preliminary numerical experiments are presented.
- Keywords Derivative-free · Nonlinear programming · Filter methods · Inexact restoration
 methods
- 10 Mathematics Subject Classification 65K05 · 90C30 · 90C56

11 **1 Introduction**

13

¹² In this paper we shall be concerned with the nonlinear programming problem

minimize
$$f(x)$$

subject to $c(x) = 0$ (1)

Communicated by Ernesto G. Birgin.

M. L. Schuverdt schuverd@mate.unlp.edu.ar

> N. Echebest opti@mate.unlp.edu.ar

R. P. Vignau vignau@mate.unlp.edu.ar

- ¹ Department of Mathematics, FCE, University of La Plata, La Plata, Argentina
- ² CONICET, Department of Mathematics, FCE, University of La Plata, La Plata, Argentina

where the functions $f : \mathbb{R}^n \to \mathbb{R}, c : \mathbb{R}^n \to \mathbb{R}^m$ are continuously differentiable but their 14 derivatives are not available. We denote by $J_c(.)$ the Jacobian matrix of c and we consider 15 the function h that measures the constraint infeasibility in each point $x \in \mathbb{R}^n$, h(x) = ||c(x)||16 where ||.|| denotes the Euclidean norm. Such a kind of optimization problems encompasses 17 many real-world problems arising in different fields like, e.g. computational mathematics, 18 physics and engineering, in which it is necessary to minimize functions whose derivatives are 19 not available (see e.g. Alexandrov and Hussaini 1997; Conn et al. 2009; Kolda et al. 2003). 20 Unconstrained techniques based on local explorations, line searches or quadratic models 21 have been suitably adapted to box-constrained and linearly constrained derivative-free opti-22 mization (Arouxét et al. 2011; Conn et al. 1997; Custodio and Vicente 2007; Kolda et al. 23 2006; Lewis and Torczon 1999, 2000; Powell 2006, 2009). Problems with more general con-24 straints are more difficult because they need to obtain optimality and feasibility controlling 25 the number of function evaluations of the objective function and the nonlinear constraints. 26 Derivative-free methods for more general constraints were addressed by means of augmented 27 Lagrangian approaches in Diniz-Ehrhardt et al. (2011), Lewis and Torczon (2002) and Lewis 28 and Torczon (2010). 29 Modern inexact restoration (IR) methods for smooth constrained optimization proceed in 30 two phases (Gonzaga et al. 2004; Martínez 2001; Martínez and Pilotta 2000, 2005). In the 31

restoration phase, feasibility is improved without evaluations of the objective function at all. 32 In the optimization phase, the objective function or a Lagrangian function is minimized. One 33 of the more attractive features of the IR method is that the theory allows us to use any efficient 34 algorithm to perform each phase. Optimality and feasibility can be combined using penalty 35 functions, augmented Lagrangians or can be treated more independently. Inexact restoration 36 algorithms described by Martínez (2001) and by Martínez and Pilotta (2000, 2005), measure 37 the progress by a merit function. Gonzaga et al. (2004) have proposed an inexact restoration 38 algorithm which uses a filter strategy for evaluating candidate points. This idea was proposed 39 by Fletcher and Leyffer (2002) in other contexts. 40

A recent article (Bueno et al. 2013) uses the IR method for solving a nonlinear derivativefree optimization problem where the derivatives of the constraints are available, but the derivatives of the objective function are not. In this case, the second phase must be solved using derivative-free methods. An algorithm introduced by Kolda et al. (2006) for linearly constrained derivative-free optimization is employed for that purpose.

In this paper we propose a derivative-free method, based on the inexact restoration 46 approach introduced in Gonzaga et al. (2004). There the authors define a globally convergent 47 filter method for nonlinear programming considering available the derivatives of the objective 48 function and the constraints. That filter method belongs to the class of methods that treat f49 and h as two independent objectives. Each iteration proceeds in two phases: the restoration or 50 feasibility phase in which feasibility must be improved without using the objective function 51 and the optimization phase in which the objective function on a tangent approximation to the 52 constraints must be minimized. As mentioned in Gonzaga et al. (2004), the filter algorithms 53 define a forbidden region by memorizing the pairs $(f(x^k), h(x^k))$ from well chosen former 54 iterations, avoiding points dominated by those by using the usual Pareto domination rule: 55 "x dominates y if and only if $f(y) \ge f(x)$ and $h(y) \ge h(x)$ ". For bibliography on filter 56 methods see for example (Fletcher et al. 2002; Fletcher and Leyffer 2002; Gonzaga et al. 57 2004) and the references therein. 58

The algorithm developed in this work is based on models built by multivariate interpolation of the objective and the constraint functions (Custodio and Vicente 2007), which is one of the main differences with Gonzaga et al. (2004).



Author Proof

The restoration phase must solve an underdetermined nonlinear system with bound con-62 straints. In our implementation we performed this phase using the derivative-free method 63 developed in Echebest et al. (2012).

On the other hand, the optimization phase must solve a derivative-free optimization prob-65 lem with linear constraints. We shall use a linear constrained trust-region algorithm in which 66 the derivative of the objective function is approximated by a model obtained by linear inter-67 polation. 68

This paper is organized as follows. In Sect. 2 we present the hypotheses, concepts and 69 some results that are fundamental throughout the work. Also we define the Derivative-Free 70 Filter algorithm (DFF) for solving (1). In Sect. 3 we present the internal algorithms used 71 in DFF and we show that they satisfy certain conditions that will be used in the analysis of 72 the convergence. In Sect. 4 we show the global convergence results. In Sect. 5 we describe 73 implementation details and we show some numerical experiments. Finally, Sect. 6 is devoted 74 to conclusions and lines for future research. 75

Notation 76

77

- ||.|| denotes the Euclidean norm.
- Given two non-negative functions $g_1, g_2 : X \to \mathbb{R}, X \subset \mathbb{R}^n$, we denote $g_1(x) =$ 78 $O(g_2(x))$ (or equivalently $g_2(x) = \Omega(g_1(x))$) in $\Gamma \subset X$ if there exists M > 0 such that 79
- $g_1(x) < Mg_2(x)$ for all $x \in \Gamma$. 80

2 Derivative-free filter algorithm 81

We shall develop an algorithm which generates sequences $\{x^k\}, \{z^k\}$ in \mathbb{R}^n and in order to 82 obtain our global convergence we shall assume the following hypotheses. 83

General hypotheses 84

- (H1) The iterates x^k and z^k remain in a convex compact domain $X \subset \mathbb{R}^n$. 85
- (H2) The functions f, c_i for $i = 1, \dots, m$ are continuously differentiable in an open set 86 containing X. 87
- (H3) The functions ∇f , ∇c_i for i = 1, ..., m are Lipschitz continuous in an open set 88 containing X with constants $L_1, L_2 > 0$, respectively: 89
- 90 91

$$\|\nabla f(x) - \nabla f(y)\| \le L_1 \|x - y\|$$

$$\|\nabla c_i(x) - \nabla c_i(y)\| \le L_2 \|x - y\|, \text{ for } i = 1, \dots, m$$

92

for all x, y in the open set containing X.

Before going further into details of the algorithm, we first introduce some concepts and 93 results of multivariate polynomial interpolation models of the objective function and con-94 straints that we make use throughout and that can be found to a more extent in Conn et al. 95 (2009).96

Each interpolation set $Y = \{y^0, y^1, \dots, y^n\} \subset \mathbb{R}^n$, which is contained in the ball 97 $B(y^0, \Delta(Y))$ centered at y^0 and with radius $\Delta(Y) = \max_{1 \le i \le n} ||y^i - y^0||$, is "poised" for linear interpolation, i.e., the matrix of directions $S = [y^1 - y^0 y^2 - y^0 \dots y^n - y^0]^T$ is 98 99 nonsingular. The definition of poisedness is independent of the basis for the space of linear 100 polynomials of degree 1. Hence, if Y is poised for the natural basis then it is poised for any 101 other basis chosen (Conn et al. 2009, Ch. 2). 102

The simplex gradient of f at y⁰ is defined by $\nabla_s f(y^0) = S^{-1} \delta f(Y)$ where $\delta f(Y) =$ 103 $(f(y^1) - f(y^0), f(y^2) - f(y^0), \dots, f(y^n) - f(y^0))^{\mathrm{T}}.$ 104

¹⁰⁵ If we consider $m_f(x) = f(y^0) + g_f^{T}(x - y^0)$ as the linear interpolating model of f(x)¹⁰⁶ on *Y* then we have that $g_f = \nabla_s f(y^0)$ (Conn et al. 2009). Therefore, the simplex gradient ¹⁰⁷ of *f* is closely related to linear multivariate polynomial interpolation.

The geometrical properties of *Y* determine the quality of the corresponding g_f as an approximation to the exact gradient of the objective function. We are interested in the quality of $m_f(x)$ and g_f in the ball $B(y^0, \Delta(Y))$.

The definition of poisedness gives a threshold to the difference between the functions and their interpolation models. Then, for all $x \in B(y^0, \Delta(Y))$, considering the scaled matrix $\bar{S} = \frac{S}{\Delta(Y)}$, we have that

115

121

126

$$|f(x) - m_f(x)| \le \kappa_{ef} \Delta^2(Y), \tag{2}$$

$$\|\nabla f(x) - \nabla m_f(x)\| \le \kappa_{eg} \Delta(Y),\tag{3}$$

where $\kappa_{eg} = L_1(1 + \frac{\sqrt{n}}{2} \|\bar{S}^{-1}\|)$ and $\kappa_{ef} = \kappa_{eg} + \frac{L_1}{2}$, which are given in Theorem 2.11 and Theorem 2.12 in Conn et al. (2009).

Similarly, under the previous hypotheses, if we consider for all $j = 1, ..., m, m_{c_j}(x) = c_j(y^0) + g_{c_j}^{T}(x - y^0)$ as the linear interpolating model of $c_j(x)$ on *Y* then we have that $g_{c_j} = \nabla_s c_j(y^0)$ and the following error bounds

$$|c_j(x) - m_{c_j}(x)| \le \kappa_{ec} \Delta^2(Y), \tag{4}$$

$$\|\nabla c_j(x) - \nabla m_{c_j}(x)\| \le \kappa_{eg_c} \Delta(Y), \tag{5}$$

where $\kappa_{eg_c} = L_2(1 + \frac{\sqrt{n}}{2} \|\bar{S}^{-1}\|)$ and $\kappa_{ec} = \kappa_{eg_c} + \frac{L_2}{2}$.

If we consider as an approximation of $J_c(y)$ the matrix A(y), whose *j*th row is the transpose of $\nabla m_{c_j}(y)$ then we have that

$$\|J_c(y) - A(y)\| \le \kappa_{eJ_c} \Delta(Y), \tag{6}$$

127 where $\kappa_{eJ_c} = \sqrt{m} \kappa_{eg_c}$.

We assume that it is possible to maintain the constants κ_{ef} , κ_{eg} and κ_{eJ_c} uniformly bounded along the iterative process of our algorithm (Conn et al. 2009, Ch. 3 and 6).

Given an iterate z^k we consider the following hypothesis

(H4) The simplex gradient used to approximate the objective function gradient satisfies the error bound: $\|\nabla f(z^k) - \nabla_s f(z^k)\| \le k_{eg} \Delta_f^k$ where Δ_f^k is the radius of the ball that contains the interpolation points.

The simplex derivatives used to approximate the true Jacobian satisfy the error bound: $\|J_c(z^k) - A(z^k)\| \le k_{eJ_c} \Delta_c^k$ where Δ_c^k is the radius of the ball that contains the interpolation points.

The global convergence result of the method in Gonzaga et al. (2004) is obtained without discussing details of the algorithms used in the internal phases. The authors proved that their algorithm produces feasible points \bar{x} satisfying

$$\liminf_{x \to \bar{x}} \|P_{T(x)}(x - \nabla f(x)) - x\| = 0, \tag{7}$$

where $P_{T(z)}(w)$ is the orthogonal projection of $w \in \mathbb{R}^n$ onto the closed set

140

$$T(z) = \{ x \in \mathbb{R}^n : J_c(z)(x - z) = 0 \}$$

that is a linearization of the set $\{x \in \mathbb{R}^n : c(x) = c(z)\}$ at the point z.

Journal: 40314 Article No.: 0253 TYPESET DISK LE CP Disp.:2015/7/3 Pages: 26 Layout: Small

The direction $P_{T(z)}(z - \nabla f(z)) - z$ appears as a sequential optimality condition in the 144 Approximate Gradient Projected condition defined by Martínez and Svaiter (2003). 145

In this paper we address nonlinear problems in which the derivatives of the involved 146 functions are not available. When this is the case we cannot compute in an exact form the set 147 T(z) and the gradient of the objective function. 148

Thus, in this context, we will be able to prove that our derivative-free filter algorithm 149 generates a sequence $\{x^k\}$ which has a feasible limit point $\overline{x} \in \mathbb{R}^n$, $\overline{x} = \lim_{k \in \mathcal{X}} x^k$ for some 150 infinite subset $\mathscr{K} \subset \mathbb{N}$, satisfying

$$\lim_{k \in \mathscr{K}} \|d_c(x^k)\| = 0, \tag{8}$$

where $d_c(z) = P_{L(z)}(z - \nabla_s f(z)) - z$ and $L(z) = \{x \in \mathbb{R}^n : A(z)(x - z) = 0\}.$ 153

This feasible point \overline{x} will be called *quasi-stationary* throughout this work.

Now, following the ideas in Gonzaga et al. (2004), we present the inexact restoration derivative-free filter algorithm with no specification of the internal algorithms.

This algorithm constructs a sequence $F_0 \subset F_1 \subset \cdots \subset F_k \subset \cdots$ of filter sets composed 157 of pairs $(f_i, h_i) \in \mathbb{R}^2$. In the following, we also mention the sets of forbidden points, 158 $\mathscr{F}_k \subset \mathbb{R}^n, \mathscr{F}_k = \{x \in \mathbb{R}^n : f(x) \ge f_i, h(x) \ge h_i, \text{ for some}(f_i, h_i) \in F_k\}, \text{ which are}$ 159 formally defined in each step of algorithm for clarity, but are never actually constructed. 160 Each iteration starts with a filter and the corresponding forbidden region. 161

Given an iterate x^k , the filter slack at x^k is defined by 162

163

$$H_k = \min\{1, \min\{h_j : (f_j, h_j) \in F_k, f_j \le f(x^k)\}\}.$$
(9)

Observe that, as it was made in Gonzaga et al. (2004), at the beginning of each iteration, 164 the pair $(f(x^k) - \alpha h(x^k), h(x^k) - \alpha h(x^k))$ is temporarily introduced in the filter. After 165 the complete successful iteration this entry will become permanent in the filter only if the 166 iteration does not produce a decrease in f. 167

In Martínez (2001), under suitable assumptions, Martínez has shown that a point that 168 satisfies the feasibility phase requirements exists. Considering this, if $h(x^k) \neq 0$, it is plausible 169 to believe that a point z^k satisfying $h(z^k) < (1 - \alpha)h(x^k)$ and $||z^k - x^k|| \le \beta h(x^k)$ could be 170 found, for example, by a Broyden-like method to solve the nonlinear system defined by the 171 constraints. 172

In order to accept z^k , it is necessary to check if $z^k \notin \overline{\mathscr{F}}_k$. Since the pair $(f(z^k), h(z^k))$ is 173 not dominated by (\tilde{f}, \tilde{h}) , it is only necessary to verify that $z^k \notin \mathscr{F}_k$. Since $x^k \notin \mathscr{F}_k$, \mathscr{F}_k is 174 closed and the restored point has bounded distance from x^k , it is reasonable to believe that 175 the algorithm has possibilities to complete the restoration phase. However, we do not have 176 guaranties that such point would be found, and so the stopping criterion in Step 2 is essential. 177 Furthermore, when $h(x^k) = 0$ it is necessary to find x^{k+1} satisfying $f(x^{k+1}) < f(x^k)$, to 178 fulfill the condition that $x^{k+1} \notin \overline{\mathscr{F}}_k$. Since we are not working with the true derivatives, the 179 computed direction $d_c(z^k)$ could not be a descent direction of f in z^k over $L(z^k)$, although it 180 is not null. This can happen because the simplex gradients are not good approximations of the 181 true gradients. Consequently, the procedure used in the optimization phase may not be able 182 to find a point x_T such that $f(x_T) < f(z^k)$. If $z^k \neq x^k$, as $z^k \notin \overline{\mathscr{F}}_k$, it is possible to accept 183 $x_T = z^k$ and $x^{k+1} = z^k$. But when $z^k = x^k$ and the algorithm cannot find a point x_T such 184 that $f(x_T) < f(z^k)$, we propose to restart the optimization phase recomputing the simplex 185 gradient of f and the matrix A_k with the new radiuses $\alpha \Delta_f^k$ and $\alpha \Delta_c^k$ of the interpolation 186 187 points.

The following lemma gives conditions for which $d_c(z^k)$ is a descent direction of f in z^k 188 over $L(z^k)$. 189

D Springer MM

154

155

156

151

Author Proof

190 **Lemma 1** Given $\varepsilon > 0$, $z^k \in \mathbb{R}^n$, if $||d_c(z^k)|| > \varepsilon$ and $||\nabla f(z^k) - \nabla_s f(z^k)|| < \frac{\varepsilon}{4}$ then

191 192

194

1

1

19

202

204

$$\|z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}))\| > \frac{3}{4}\varepsilon, \qquad (10)$$

$$\nabla^{\mathrm{T}} f(z^k) \, d_c(z^k) < -\frac{1}{4} \| d_c(z^k) \|^2. \tag{11}$$

¹⁹³ *Proof* Since the projection $P_{L(z^k)}$ is non-expansive,

$$\|P_{L(z^{k})}(z^{k} - \nabla f(z^{k})) - P_{L(z^{k})}(z^{k} - \nabla_{s} f(z^{k}))\| \le \|\nabla f(z^{k}) - \nabla_{s} f(z^{k})\|,$$

195 then it follows that

$$||z^{k} - P_{L(z^{k})}(z^{k} - \nabla_{s}f(z^{k}))|| \le ||z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}))|| + ||\nabla f(z^{k}) - \nabla_{s}f(z^{k})||.$$
(12)

197 Then we have that

$$\begin{aligned} \|z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}))\| &\geq \|z^{k} - P_{L(z^{k})}(z^{k} - \nabla_{s}f(z^{k}))\| - \|\nabla f(z^{k}) - \nabla_{s}f(z^{k})\| \\ &> \frac{3}{4}\varepsilon > 0, \end{aligned}$$

as we wanted to prove.

Since
$$\nabla^{\mathrm{T}} f(z^k) d_c(z^k) = (\nabla f(z^k) - \nabla_s f(z^k))^{\mathrm{T}} d_c(z^k) + \nabla_s^{\mathrm{T}} f(z^k) d_c(z^k)$$
, then

$$\nabla^{\mathrm{T}} f(z^{k}) \, d_{c}(z^{k}) \leq \|d_{c}(z^{k})\| \, \|\nabla f(z^{k}) - \nabla_{s} f(z^{k})\| + \nabla_{s}^{\mathrm{T}} f(z^{k}) \, d_{c}(z^{k}).$$

203 Therefore, considering

$$\nabla_s^{\mathrm{T}} f(z^k) \, d_c(z^k) \le -\frac{\|d_c(z^k)\|^2}{2},\tag{13}$$

which is obtained by a similar form to one of Martínez and Pilotta (2000, Sec. 2.6, page 140) replacing $\nabla f(z^k)$ by $\nabla_s f(z^k)$, we obtain that

207

$$\nabla^{\mathrm{T}} f(z^{k}) \, d_{c}(z^{k}) \leq \|d_{c}(z^{k})\|^{2} \left(\frac{\|\nabla f(z^{k}) - \nabla_{s} f(z^{k})\|}{\|d_{c}(z^{k})\|} - \frac{1}{2} \right)$$

Hence, we get $\nabla^{\mathrm{T}} f(z^k) d_c(z^k) < \|d_c(z^k)\|^2 (\frac{1}{4} - \frac{1}{2}) = -\frac{1}{4} \|d_c(z^k)\|^2$. Therefore, under the hypotheses given, $d_c(z^k)$ is a descent direction of f in z^k .

Remark 1 Under the hypotheses of the previous lemma, if z^k is not in $\overline{\mathscr{F}}_k$, which is a closed set, then there must exist $\Delta > 0$ and t > 0 such that if $t ||d_c(z^k)|| < \Delta$ then $z^k + td_c(z^k)$ does not fall into the region $\overline{\mathscr{F}}_k$ and $f(z^k + td_c(z^k)) < f(z^k)$. Similarly when $h(x^k) = 0$, by construction $z^k = x^k$ and $z^k \in \overline{\mathscr{F}}_k$. In this case, since $z^k \notin \mathscr{F}_k$, which is a closed set, there exist $\Delta > 0$ and t > 0 such that if $t ||d_c(z^k)|| < \Delta$ then $z^k + td_c(z^k)$ does not fall into the region \mathscr{F}_k . Furthermore, since $f(z^k + td_c(z^k)) < f(z^k)$ it obtains that $z^k + td_c(z^k) \notin \overline{\mathscr{F}}_k$.

216 Lemma 2 Algorithm 1 is well defined.

Proof If the method used in the restoration phase is not able to find a point z^k satisfying the required conditions then the Algorithm 1 stops.

In the optimization phase, when $z^k \neq x^k$ there always exists $x_T \notin \overline{\mathscr{F}}_k$ such that $f(x_T) \leq f(z^k)$ since $z^k \notin \overline{\mathscr{F}}_k$ and then it is possible to accept $x_T = z^k$.

Journal: 40314 Article No.: 0253 TYPESET DISK LE CP Disp.:2015/7/3 Pages: 26 Layout: Small

Algorithm 1. Derivative-Free Filter Algorithm (DFF). Given $x^0 \in \mathbb{R}^n$, $F_0 = \emptyset$, $\mathscr{F}_0 = \emptyset$, $\alpha \in (0,1)$, $\beta > 0$, $\varepsilon_f > 0$, $\varepsilon_l > 0$, $\{\delta_k\}_{k \in \mathbb{N}}$, $\delta_k > 0$, $\delta_k \to 0$. Set $k \leftarrow 0$. Step 1 : Define $(\tilde{f}, \tilde{h}) = (f(x^k) - \alpha h(x^k), (1 - \alpha)h(x^k)).$ Construct the set $\overline{F}_k = F_k \cup \{(\widetilde{f}, \widetilde{h})\}.$ Define the set $\overline{\mathscr{F}}_k = \mathscr{F}_k \cup \{x \in \mathbb{R}^n : f(x) \ge \widetilde{f}, h(x) \ge \widetilde{h}\}.$ Step 2 : Restoration Phase If $h(x^k) = 0$ then set $z^k = x^k$. Otherwise, compute $z^k \notin \overline{\mathscr{F}}_k$ such that $h(z^k) < (1-\alpha)h(x^k)$ and $||z^k - x^k|| \leq \beta h(x^k)$. If it is impossible then stop without success. END. Step 3 : Optimization Phase 3.1 Construct or update $Y_c^k = \{z^k, y_c^1, \dots, y_c^n\}$, a set of interpolation points centered at z^k , such that $\Delta_c^k = \max_{i=1,\dots,n} \{ \|y_c^i - z^k\| \}$ verifies $\Delta_c^k \leq \beta \min\{\max\{h(x^k), H_k\}, \delta_k\}$. Compute $A(z^k) = A_k$ using simplex derivatives, by interpolation on Y_c^k . Define $L(z^k) = \{x \in \mathbb{R}^n : A_k(x - z^k) = 0\}.$ Construct or update $Y_f^k = \{z^k, y_f^1, \dots, y_f^n\}$, a set of interpolation points centered at z^k , such that $\Delta_f^k = \max_{i=1,...,n} \{ \|y_f^i - z^k\| \}$ verifies $\Delta_f^k \leq \delta_k$. Compute $\nabla_s f(z^k)$ by interpolation on Y_f^k and $d_c(z^k) = P_{L(z^k)}(z^k - \nabla_s f(z^k)) - z^k$. 3.2 If $h(x^k) = 0$, max $\{\Delta_f^k, \Delta_c^k\} < \varepsilon_I$ and $\|d_c(z^k)\| < \varepsilon_f$ then stop with finite convergence. 3.3 Compute, by an algorithm without derivatives, $x_T \notin \overline{\mathscr{F}}_k$ such that $x_T \in L(z^k)$ and $f(x_T) \leq f(z^k).$ If $z^k = x^k$ and there is not a x_T such that $f(x_T) < f(z^k)$ then set $\Delta_f^k = \alpha \Delta_f^k$, $\Delta_c^k = \alpha \Delta_f^k$ $\alpha \Delta_c^k$ and go to step 3.1. Otherwise, define $x^{k+1} = x_T$. Step 4 : Filter Update If $f(x^{k+1}) < \overline{f}(x^k)$ then $F_{k+1} = F_k$, $\mathscr{F}_{k+1} = \mathscr{F}_k$ (*f*-iteration). *Else*, $F_{k+1} = \overline{F}_k$, $\mathscr{F}_{k+1} = \overline{\mathscr{F}}_k$ (*h*-iteration). Set $k \leftarrow k+1$, go to Step 1.

221

When x^k is feasible, $z^k = x^k$, if it is possible to find x_T with $f(x_T) < f(z^k)$ then x^{k+1} is 223 defined. If that is not possible then the algorithm restarts the optimization phase with smaller 224 Δ_f^k and Δ_c^k , with the aim of improving the approximation of the gradients of f and c_i , for 225 $i = 1, \ldots, m$. In this case, in a finite number of iterations the radiuses Δ_f^k and Δ_c^k will 226 become sufficiently small and if $||d_c(z^k)||$ is large enough, by Lemma 1 and Remark 1, it is 227 possible to obtain $x_T \notin \overline{\mathscr{F}}_k$ such that $f(x_T) < f(x^k)$ and then x^{k+1} is defined. Otherwise, 228 if $||d_c(z^k)|| < \varepsilon_f$ and $\max\{\Delta_f^k, \Delta_c^k\} < \varepsilon_I$ then the algorithm finishes satisfying the finite 229 termination criterion. 230

Remark 2 When $h(x^k) > 0$, in the previous lemma we have used the possibility to accept $x^{k+1} = z^k$. When this happens an infinite number of iterations a feasible limit point is obtained. Until this moment, the internal algorithms have not been given. In the following section, we will study the characteristics of the limit points using the properties of the internal algorithms.

As it was mentioned in Gonzaga et al. (2004) there are some facts that follow directly from the construction of the algorithm:

Deringer Springer

Fact 1. Given $k \in \mathbb{N}$, $x^{k+p} \notin \mathscr{F}_{k+1}$ for all $p \ge 1$.

Fact 2. Given $k \in \mathbb{N}$, at least one of the following two situations must occur:

240 241 242

243

238

239

1.
$$h(x^{k+1}) < (1 - \alpha)h(x^k)$$
.
2. $f(x^{k+1}) < f(x^k) - \alpha h(x^k)$

Fact 3. Given $k \in \mathbb{N}$, $h_i > 0$ for all $j \in \mathbb{N}$ such that $(f_i, h_i) \in F_k$. Consequently $H_k > 0$ for all $k \in \mathbb{N}$.

Remark 3 By definition of H_k , $H_k < 1$. Therefore, when x^k is in a neighborhood of a feasible 244 point, assuming $h(x^k) < 1$, if $H_k = 1$ then $h(x^k) \le H_k$ holds. If $H_k < 1$ then there exists a 245 $h_i < 1$ such that $(f_i, h_i) \in F_k, f_i \leq f(x^k)$, such that $H_k = h_i$. In this case, since $x^k \notin \mathscr{F}_k$ 246 and $f(x^k) \ge f_i$, it must be $h(x^k) < h_i$. Hence, if x^k is in a neighborhood of a feasible point 247 then $h(x^k) < H_k$ holds. 248

3 Internal algorithms 249

xact restoration methodology gives the possibility of using different methods to solve each phase. In this section, we describe the algorithms that we use in each phase. We will 251 also show that they verify the conditions required to obtain global convergence of DFF. 252

3.1 Restoration phase 253

We use the BCDF-QNB algorithm (Echebest et al. 2012) in the restoration phase of the 254 DFF algorithm. BCDF-QNB (Box-Constrained Derivative-Free Quasi Newton), based on the 255

Broyden update formula, is a derivative-free method for solving underdetermined nonlinear 256 systems with bound constraints. 257

Given an iterate x^k , in Step 2 of DFF we apply BCDF-QNB starting from the initial 258 point $y^0 = x^k$, until it finds a new point $z^k \notin \overline{\mathscr{F}}_k$ satisfying the descent condition $h(z^k) < \infty$ 259 $(1-\alpha)h(x^k)$ and $||z^k - x^k|| \le \beta h(x^k)$ for fixed parameters $0 < \alpha < 1, \beta > 0$. 260

BCDF-QNB generates a sequence $\{y^j\}$, for j = 0, 1, 2, ..., with $y^j \in \Omega_k$, being $\Omega_k =$ 261 $\{y \in \mathbb{R}^n : \|y - x^k\|_{\infty} \le \frac{\beta}{\sqrt{n}}h(x^k)\}$. At each iterate y^j , this algorithm computes a direction 262 d_i , considering two possibilities: in a first attempt, as the solution of the constrained linear 263 system 264

$$B_j d + c(y^j) = 0 \quad \text{and} \quad y^j + d \in \Omega_k,$$
 (14)

if this is possible. Otherwise, the direction is computed as an approximate solution of the 266 problem 267

$$\min_{y^j + d \in \Omega_k} \|B_j d + c(y^j)\| \tag{15}$$

where B_i is the matrix defined as: 269

$$B_j = B_{j-1} + \frac{(w_j - B_{j-1}s^j)(s^j)^1}{\|s^j\|^2}$$
(16)

where $w_j = c(y^j) - c(y^{j-1}), s^j = y^j - y^{j-1}$. 271

Once the current direction d_i is computed, the line search algorithm looks for a step length 272 $\lambda_i \leq 1$ such that 273

$$h(y^{j} + \lambda_{j}d_{j})^{2} \le \max_{0 \le i \le M-1} h(y^{j-i})^{2} + \eta_{j} - \gamma\lambda_{j}^{2} ||d_{j}||^{2}$$
(17)

Journal: 40314 Article No.: 0253 🔲 TYPESET 🔄 DISK 🔄 LE 🔤 CP Disp.: 2015/7/3 Pages: 26 Layout: Small

274

265

268

Algorithm 2. BCDF-ONB

Given $x^k \in \Omega_k$, $0 < \alpha < 1$, $\beta > 0$, W_k an approximation of $J_c(x^k)$, $0 < \gamma < 1$, $M \in \mathbb{N}$, M > 0, $\eta = \sum_{j=0}^{\infty} \eta_j < \infty, \ \eta_j > 0, \ 0 \le \theta_0 < \overline{\theta} < 1, \ ind = 0, \ imax > 0, \ imax \in \mathbb{N}, \ MaxIter > 0.$ Set $i \leftarrow 0, v^0 = x^k, B_0 = W_k$. Step 1: If $h(y^j) < (1-\alpha)h(x^k)$ and $y^j \notin \overline{\mathscr{F}}_k$, define $z^k = y^j$ and return with success. If j > Maxiter then return without success. Step 2: Computing the matrix B_i If j > 0 and ind < imax compute B_j using the Broyden update (16). If ind = imax compute B_i by finite differences as an approximation to the Jacobian matrix in y^j . *Step 3: Computing the direction* d_i 3.1: Find d satisfying (14). If such direction d is found, define $d_i = d$, $\theta_{i+1} = \theta_i$, ind = 0 and go to Step 4. 3.2: Find an approximate solution d of the problem (15). If d satisfies $||B_j d + c(y^j)|| \le \theta_j ||c(y^j)||$, define $d_j = d$, $\theta_{j+1} = \theta_j$, ind = 0 and go to Step 4. 3.3: Set $d_j = 0$, $y^{j+1} = y^j$, $\theta_{j+1} = \frac{\theta_j + \overline{\theta}}{2}$. If ind < imax, set ind \leftarrow ind + 1 and go to Step 5. If ind = imax, define $\overline{\theta} = \frac{\theta+1}{2}$. Set ind $\leftarrow 0$ and go to Step 5. Step 4: Find λ_i and $y^{j+1} = y^j + \lambda_j^2 d_j$, $0 < \lambda_j \le 1$, using the derivative-free nonmonotone line search algorithm (Algorithm 1 in [11]), satisfying (17). Step 5: Set $j \leftarrow j + 1$ and go to Step 1.

276

275

where *M* is a positive integer, $0 < \gamma < 1$ and $\sum_{j=0}^{\infty} \eta_j = \eta < \infty$, $\eta_j > 0$. This procedure is 277 a combination of the well-known nonmonotone line search strategy for unconstrained opti-278 mization introduced by Grippo et al. (1986) with the Li-Fukushima derivative-free line search 279 scheme in Li and Fukushima (2000). The combined strategy produces a robust nonmonotone 280 derivative-free line search that takes into account the advantages of both schemes. Under 281 suitable conditions we have established in Echebest et al. (2012) the global convergence 282 results for the BCDF-ONB method. 283

We describe the application of BCDF-QNB for solving the Restoration Phase. 284

The matrix W_0 is an approximation of $J_c(x^0)$, which is obtained by finite differences. The 285 initial matrix W_k , k > 0, is the updated Broyden matrix of A_{k-1} , where A_{k-1} is the matrix 286 defined at z^{k-1} in the optimization phase. 287

Remark 4 Since $\{y^j\} \subset \Omega_k$, the obtained z^k satisfies the condition $||z^k - x^k|| \leq \beta h(x^k)$, 288 $\beta > 0.$ 289

As a result, more formally, the procedure generates iterates that verify the following 290 condition. 291

(C1) Restoration step condition: At all iterations $k \in \mathbb{N}$, the restoration step satisfies 292

293

$$\|z^{k} - x^{k}\| = O(h(x^{k})).$$
(18)

Using (C1) and that ∇f is bounded in X, it follows that 294

$$|f(z^{k}) - f(x^{k})| = O(||z^{k} - x^{k}||) = O(h(x^{k})).$$
(19)

Deringer

(23)

3.2 Optimization phase

Given $z^k \in X$, generated in the restoration phase, Step 3.3 of DFF must find $x^{k+1} \in L(z^k)$ such that $f(x^{k+1}) \leq f(z^k)$ and $x^{k+1} \notin \overline{\mathscr{F}}_k$ employing a derivative-free method.

We shall describe a linear trust region method and then we show that the resulting step satisfies a special condition needed for obtaining convergence.

 $m_k(x) = f(z^k) + \nabla_{-}^{T} f(z^k)(x - z^k)$

At each iterate z^k , the trust region algorithm associated to z^k uses the linear model

302

304

305

308

312

314

301

³⁰³ where the simplex gradient of the objective function is considered.

The trust region step uses a radius $\Delta > 0$ and solves the problem

subject to
$$x \in L(z^k)$$

 $\|x - z^k\| \le \Delta.$

As the model is linear we know that the solution of this problem is a point $z^k + d(z^k, \Delta)$ such that

$$d(z^k, \Delta) = \Delta \frac{d_c(z^k)}{\|d_c(z^k)\|}$$
(20)

if $d_c(z^k) \neq 0$, where $d_c(z^k)$ is the projected gradient direction defined by $P_{L(z^k)}(z^k - \nabla_s f(z^k)) - z^k$.

We define the *predicted reduction* produced by the step $d(z^k, \Delta)$ as

6

$$\operatorname{pred}(z^k, \Delta) = m_k(z^k) - m_k(z^k + d(z^k, \Delta))$$
(21)

and the *actual reduction* of f as

$$ared(z^{k}, \Delta) = f(z^{k}) - f(z^{k} + d(z^{k}, \Delta)).$$
 (22)

The step $d(z^k, \Delta)$ is only accepted if the sufficient decrease condition is satisfied, i.e.

320

321

322

for a given $\eta \in (0, 1)$.

Since pred $(z^k, \Delta) = -\nabla_s^{\mathrm{T}} f(z^k) d(z^k, \Delta) = -\nabla_s^{\mathrm{T}} f(z^k) \frac{d_c(z^k)}{\|d_c(z^k)\|} \Delta$, considering (13), we get

 $\operatorname{ared}(z^k, \Delta) > \eta \operatorname{pred}(z^k, \Delta),$

$$\operatorname{pred}(z^k, \Delta) \ge \frac{\Delta}{2} \|d_c(z^k)\|.$$
(24)

We briefly describe the linear trust region method for solving the optimization phase.

Algorithm 3. *Minimization on* $L(z^k)$

Given $\eta \in (0,1)$, $\Delta_{min} > 0$, x^k , $z^k \notin \mathscr{F}_k$, $d_c(z^k)$, $\Delta \ge \Delta_{min} > 0$, tol > 0. Set $x^+ = z^k$. While $(||d_c(z^k)||\Delta > tol and f(x^+) \ge f(z^k))$ do Compute $d = d(z^k, \Delta)$, $pred(z^k, \Delta)$ and $ared(z^k, \Delta)$ as in (20), (21) and (22) respectively. If $ared(z^k, \Delta) > \eta$ $pred(z^k, \Delta)$ and $z^k + d \notin \widehat{\mathscr{F}}_k$, define $x^+ = z^k + d$. Else, set $\Delta = \frac{\Delta}{2}$. End While. If $f(x^+) < f(z^k)$ or $z^k \neq x^k$, define $x_T = x^+$, $\Delta_k = \Delta$. Otherwise, return without success.

😧 Journal: 40314 Article No.: 0253 🗍 TYPESET 🗍 DISK 🗌 LE 🗌 CP Disp.:2015/7/3 Pages: 26 Layout: Small

The procedure terminates in a finite number of steps with $f(x^+) < f(z^k)$ or with $x^+ = z^k$. 324 In particular, it finishes in the first iteration when $||d_c(z^k)|| = 0$. If it finishes with $x^+ = z^k$ 325 and $z^k = x^k$, when x^k is feasible, then it is not possible to define $x_T \notin \overline{\mathscr{F}}_k$. Hence it returns 326 without success and so Δ_f^k and Δ_c^k are reduced in Algorithm 1, which means that better 327 models are built. In other cases successfully returns with $x_T = x^+$. 328

Now we study the optimality step near a feasible non-quasi-stationary limit point $\overline{x} \in X$.

Lemma 3 Let $\overline{x} \in X$ be a feasible non-quasi-stationary limit point. Then there exists a 330 neighborhood \widetilde{V} of \overline{x} , $\widetilde{\Delta} > 0$ and a constant $\widetilde{c} > 0$ such that for any $z^k \in \widetilde{V}$ and for any 331 $\Delta \in (0, \Delta),$ 332

341

329

323

$$\operatorname{ared}(z^k, \Delta) > \eta \operatorname{pred}(z^k, \Delta) \ge \eta \widetilde{c} \Delta.$$

Proof As \overline{x} is a non-quasi-stationary limit point, there exists a neighborhood \widetilde{V} such that for 334 $z^k \in \widetilde{V}, ||d_c(z^k)|| \ge \widetilde{\varepsilon} > 0$ for all $k \ge k_0$. 335

Since f is continuously differentiable and ∇f is Lipschitz continuous, we know that 336

ared
$$(z^{k}, \Delta) = f(z^{k}) - f(z^{k} + d(z^{k}, \Delta)) \ge (-\nabla f(z^{k}))^{\mathrm{T}} d(z^{k}, \Delta) - L_{1} \Delta^{2}$$

= $(-\nabla f(z^{k}) + \nabla_{s} f(z^{k}))^{\mathrm{T}} d(z^{k}, \Delta) - (\nabla_{s} f(z^{k}))^{\mathrm{T}} d(z^{k}, \Delta) - L_{1} \Delta^{2}.$

In particular, if $||d_c(z^k)|| \ge \tilde{\varepsilon}$, using (24) we have that $-\nabla_s^{\mathrm{T}} f(z^k) d(z^k, \Delta) = \operatorname{pred}(z^k, \Delta) \ge$ 339 $\frac{\Delta}{2} \| d_c(z^k) \| \ge \frac{\Delta}{2} \tilde{\varepsilon}$. Then, considering 340

$$\operatorname{pred}(z^k, \Delta) = \eta(-\nabla_s^{\mathrm{T}} f(z^k) d(z^k, \Delta)) + (1 - \eta)(-\nabla_s^{\mathrm{T}} f(z^k) d(z^k, \Delta))$$

it obtains $\operatorname{pred}(z^k, \Delta) \ge \eta(-\nabla_s^{\mathrm{T}} f(z^k) d(z^k, \Delta)) + (1-\eta) \frac{\Delta}{2} \tilde{\varepsilon}.$ 342 Hence 343

ared
$$(z^k, \Delta) \ge \eta \operatorname{pred}(z^k, \Delta) + (1 - \eta) \frac{\Delta}{2} \tilde{\varepsilon} + (-\nabla^{\mathrm{T}} f(z^k) + \nabla^{\mathrm{T}}_s f(z^k)) d(z^k, \Delta) - L_1 \Delta^2.$$

By (H4), we have $\| - \nabla^{\mathrm{T}} f(z^k) + \nabla^{\mathrm{T}}_s f(z^k) \| \le k_{eg} \Delta_f^k$. Since $\Delta_f^k \le \delta_k$ and $\delta_k \to 0$, when 345 k goes to infinity, there exists $k_1 \ge k_0$ such that for $k \ge k_1$, $k_{eg}\Delta_f^k < \frac{(1-\eta)}{4}\tilde{\varepsilon}$. Then, 346

ared
$$(z^{k}, \Delta) > \eta \operatorname{pred}(z^{k}, \Delta) - \frac{(1-\eta)}{4} \tilde{\varepsilon} \|d(z^{k}, \Delta)\| + (1-\eta) \frac{\Delta}{2} \tilde{\varepsilon} - L_{1} \Delta^{2}$$

 $\geq \eta \operatorname{pred}(z^{k}, \Delta) - \frac{(1-\eta)}{4} \tilde{\varepsilon} \Delta + (1-\eta) \frac{\Delta}{2} \tilde{\varepsilon} - L_{1} \Delta^{2}.$

Hence, $\operatorname{ared}(z^k, \Delta) > \eta \operatorname{pred}(z^k, \Delta) + (1 - \eta) \frac{\Delta}{4} \tilde{\varepsilon} - L_1 \Delta^2$. Therefore if $\Delta < \widetilde{\Delta} = \frac{(1 - \eta)}{4L_1} \tilde{\varepsilon}$ we obtain that $\operatorname{ared}(z^k, \Delta) > \eta \operatorname{pred}(z^k, \Delta)$ and $\operatorname{pred}(z^k, \Delta) \ge \frac{\Delta}{2} \|d_c(z^k)\| \ge \tilde{c}\Delta$ where 349 350 $\tilde{c} = \frac{\tilde{\varepsilon}}{2}$, as we wanted to prove. 351

Remark 5 In the previous lemma we have seen that if z^k , the point found in restoration 352 phase, is in the neighborhood of a non-quasi-stationary feasible point, then it is possible to 353 find a step $d(z^k, \Delta)$ by (20) such that $f(z^k + d(z^k, \Delta)) < f(z^k)$. Furthermore, when z^k 354 is not in $\overline{\mathscr{F}}_k$, which is a closed set, then there must be a $\Delta < \tilde{\Delta}$ for which $z^k + d(z^k, \Delta)$ 355 does not fall into the forbidden region $\overline{\mathscr{F}}_k$. Similarly when $h(x^k) = 0$, by construction 356 $z^k = x^k$ and $z^k \in \overline{\mathscr{F}}_k$. By Lemma 3 as $f(z^k + d(z^k, \Delta)) < f(z^k)$ for all $\Delta \in (0, \tilde{\Delta})$, 357 $z^k + d(z^k, \Delta) \notin \{x \in \mathbb{R}^n : f(x) \ge f(z^k), h(x) > 0\}$. Then considering that $z^k \notin \mathscr{F}_k$, 358 which is a closed set, we get a similar result to the case when z^k is not in $\overline{\mathscr{F}}_k$. Hence, under 359 the hypothesis of Lemma 3, Algorithm 3 finds a point $x^+ \notin \overline{\mathscr{F}}_k$ and then defines $x_T = x^+$. 360

Deringer Springer

Lemma 4 Suppose that the matrix A_k is computed as an approximation of $J_c(z^k)$ by simplex 361 derivatives using an interpolation radius Δ_c^k . Then if $z^k + d \in L(z^k)$, 362

365

366

367

$$|h(z^{k}+d) - h(z^{k})| \le \kappa_{eJ_{c}} \Delta_{c}^{k} ||d|| + O(||d||^{2}).$$
⁽²⁵⁾

Proof Since $z^k + d \in L(z^k)$, $A_k d = 0$, considering the general hypotheses we have that $\|c(z^k + d) - c(z^k) - J_c(z^k)d\| \le \sqrt{m} L_2 \|d\|^2$. Then $\|c(z^k + d) - c(z^k)\| \le \|(J_c(z^k) - d)\|$ $A_k d \| + \sqrt{m} L_2 \| d \|^2$.

Hence, $|||c(z^k + d)|| - ||c(z^k)||| \le ||c(z^k + d) - c(z^k)|| \le ||(J_c(z^k) - A_k)|| ||d|| +$ $\sqrt{m} L_2 \|d\|^2$. Therefore, considering (6), $|h(z^k + d) - h(z^k)| \le \kappa_{eJ_c} \Delta_c^k \|d\| + \sqrt{m} L_2 \|d\|^2$, 368 as we wanted to prove. 369

The bound in (25) is O(||d||) because we are not using true derivatives. A similar bound 370 appears in Gonzaga et al. (2004), section 4.3, where the authors proposed a simplified tan-371 gential step. 372

Under the hypotheses of Lemmas 3 and 4 and the condition (C1) it can be established that 373 the proposed procedure generates iterates that verify the following condition. 374

(C2) Optimality step condition: Given a feasible non-quasi-stationary point $\overline{x} \in X$, 375 there exists a neighborhood V of \overline{x} such that for any iterate $x^k \in V$, 376

$$f(z^k) - f(x^{k+1}) = \Omega(\sqrt{H_k}).$$
 (26)

Lemma 5 Let $\overline{x} \in X$ be a feasible non-quasi-stationary limit point. Let assume that (C1) 378 and the hypothesis of Lemma 4 hold. Then there exists a neighborhood V of \overline{x} such that if 379 $x^k \in V$ then 380

$$f(z^k) - f(x^{k+1}) = \Omega(\sqrt{H_k}),$$

where $x^{k+1} = x_T$, x_T is computed by Algorithm 3. 382

Proof Let $\{x^k\}_{k \in \mathscr{K}}$ a subsequence such that $\lim_{k \in \mathscr{K}} x^k = \overline{x}$. 383

By (C1) $||x^k - z^k|| = O(h(x^k))$, as $h(x^k)$ tends to zero, it follows that $\lim_{k \in \mathcal{K}} z^k = \overline{x}$. 384 Let $\widetilde{V} \subset X$ and $\widetilde{\Delta} > 0$ be the neighborhood of \overline{x} and the radius given by Lemma 3, such 385 that for any $z^k \in \widetilde{V}$, $k \in \mathscr{K}$ and for any $\Delta \in (0, \widetilde{\Delta})$, $\operatorname{ared}(z^k, \Delta) > \eta \operatorname{pred}(z^k, \Delta) \ge \eta \widetilde{c} \Delta$. 386 Algorithm 3 starts with a radius $\Delta \ge \Delta_{min}$ and computes $d(z^k, \Delta_j), \Delta_j = 2^{-j}\Delta$ for

387 $j = 0, 1, \dots$, until $z^k + d(z^k, \Delta_j) \notin \overline{\mathscr{F}}_k$ and $\operatorname{ared}(z^k, \Delta_j) > \eta \operatorname{pred}(z^k, \Delta_j)$. Then, define 388 $\Delta_k = \Delta_i.$ 389

Let us define $\widehat{\Delta}$ as the first Δ_i such that 390

$$\operatorname{ared}(z^k, \Delta_j) > \eta \operatorname{pred}(z^k, \Delta_j), \text{ and}$$
 (27)

 $z^k + d(z^k, \Delta_i) \notin \overline{\mathscr{F}}_k$ or $f(z^k + d(z^k, \Delta_i)) \ge \widetilde{f}$, (28)where $(\tilde{f}, \tilde{h}) = (f(x^k) - \alpha h(x^k), (1 - \alpha)h(x^k))$ is the temporary entry in the filter.

393 Let us denote $\widehat{d} = d(z^k, \widehat{\Delta})$ and $\widehat{x} = z^k + \widehat{d}$. Note that $\widehat{\Delta} \ge \Delta_k$, and $\widehat{\Delta} > \Delta_k$ happens 394 only when $f(\hat{x}) > f$. 395

Observe that, from Lemma 4, for a fixed Δ we have that there is a constant $\kappa_{eJ_c} \Delta_c^k > 0$ 396 such that 397

398

401

$$|h(z^{k} + d(z^{k}, \Delta)) - h(z^{k})| \le \kappa_{eJ_{c}} \Delta_{c}^{k} ||d(z^{k}, \Delta)|| + \sqrt{m} L_{2} ||d(z^{k}, \Delta)||^{2}$$

By Remark 3 we know that if x^k is in a neighborhood of a feasible point then $h(x^k) \le H_k$. 399 So, considering that $||d(z^k, \Delta)|| \leq \Delta$ and $\Delta_c^k \leq \beta \min\{\max\{h(x^k), \hat{H}_k\}, \delta_k\}$ we have that 400

$$|h(z^{k} + d(z^{k}, \Delta)) - h(z^{k})| \le \kappa_{eJ_{c}}\beta H_{k}\Delta + \sqrt{m} L_{2}\Delta^{2}.$$
(29)

Journal: 40314 Article No.: 0253 🔲 TYPESET 🔄 DISK 🔄 LE 🔤 CP Disp.: 2015/7/3 Pages: 26 Layout: Small

Let us consider
$$\overline{A}$$
 such that $\overline{A} \leq \frac{\alpha}{4\beta\kappa_{e,l_{e}}}$ and $\overline{A} < \frac{\overline{A}}{2}$.
(i) Assume that $\widehat{A} \geq \overline{A}$. Then, by (24),
 $pred(z^{k}, \widehat{A}) \geq \frac{\overline{A}}{2} ||d_{e}(z^{k})|| \geq \frac{\overline{b}}{2} \widehat{A}$.
By considering $\overline{c} = \frac{\overline{b}}{2}$ as in the proof of Lemma 3 we have that
 $pred(z^{k}, \widehat{A}) \geq \overline{c} \widehat{A} \geq \overline{c} \overline{A}$.
By definition of \widehat{A} , (27) holds, then
 $f(z^{k}) - f(\widehat{x}) > \eta pred(z^{k}, \widehat{A}) \geq \eta \overline{c} \widetilde{A} = \Omega(1)$.
Hence, since $H_{k} \leq 1$, it follows
 $f(z^{k}) - f(\widehat{x}) = \Omega(\sqrt{H_{k}})$.
(ii) Assume that $\widehat{A} < \overline{A}$. Then $2\widehat{A} < 2\widehat{A} < \overline{A}$ and $2\widehat{A}$ does not verify (28). By Lemma 3,
 $ared(z^{k}, d(z^{k}, 2\widehat{A})) > \eta pred(z^{k}, d(z^{k}, 2\widehat{A}))$
and, by (28) it follows that $z^{k} + d(z^{k}, 2\widehat{A}) \in \overline{\mathscr{F}}_{k}$ and $f(z^{k} + d(z^{k}, 2\widehat{A})) < \overline{f}$. Conse-
quently by definition of H_{k} , we must have $h(z^{k} + d(z^{k}, 2\widehat{A})) \geq H_{k}$.
By construction, $h(z^{k}) < (1 - \alpha)h(x^{k}) \leq (1 - \alpha)H_{k}$. Therefore,
 $h(z^{k} + d(z^{k}, 2\widehat{A})) - h(z^{k}) \geq \alpha H_{k}$.
 $H_{k} \leq \frac{2\beta}{\alpha}\kappa_{e,l_{k}}H_{k}\widehat{A} + O(\widehat{A}^{2}) \leq \frac{1}{2}H_{k} + O(\widehat{A}^{2})$.
Hence
 $H_{k} \leq \frac{2\beta}{\alpha}\kappa_{e,l_{k}}H_{k}\widehat{A} + O(\widehat{A}^{2}) \leq \frac{1}{2}H_{k} + O(\widehat{A}^{2})$.
Hence
 $\frac{1}{2}H_{k} = O(\widehat{A}^{2})$ or $\widehat{A} = \Omega(\sqrt{H_{k}})$.
Using Lemma 3 with $\widehat{A} < \overline{A}$.
 $f(z^{k}) - f(\widehat{x}) = arcd(z^{k}, \widehat{A}) \geq \eta \overline{c}\widehat{A} = \eta \overline{c}\Omega(\sqrt{H_{k}})$. (30)
Thus, for both cases, we have that $f(z^{k}) - f(\widehat{x}) = \Omega(\sqrt{H_{k}})$. Then the step \widehat{d} satisfies
the conditions in the Lemma.
 $f(z^{k}) - f(\widehat{x}) \geq M\sqrt{H_{k}}$
and
 $f(\widehat{x}) = f(z^{k}) - M\sqrt{H_{k}}$.

432 From (19) there is a positive constant N such that

$$f(z^k) \le f(x^k) + Nh(x^k).$$

⁴³⁴ Then, combining the last two inequalities we have that

$$f(\hat{x}) \le f(x^{k}) + Nh(x^{k}) - M\sqrt{H_{k}} \le f(x^{k}) + Nh(x^{k}) - M\sqrt{h(x^{k})}$$

= $f(x^{k}) - \sqrt{h(x^{k})}(M - N\sqrt{h(x^{k})})$

and, for large $k \in \mathscr{K}$ such that $M - N\sqrt{h(x^k)} > \alpha\sqrt{h(x^k)}$, which means that $\sqrt{h(x^k)} < \frac{M}{N+\alpha}$, we have that $f(\widehat{x}) < f(x^k) - \alpha h(x^k) = \widetilde{f}$, completing the proof.

439 4 Convergence results

In this section, based on conditions (C1), (C2) and considering the general hypotheses we
 will show the global convergence of DFF to a quasi-stationary point.

As it was done in Gonzaga et al. (2004), it can be shown that (C1) and (C2) imply the following condition.

(C3) Given a feasible non-quasi-stationary point $\overline{x} \in X$, there exists a neighborhood V of \overline{x} such that for any iterate $x^k \in V$,

 $f(x^k) - f(x^{k+1}) = \Omega(\sqrt{H_k})$ (31)

where H_k is the filter slack at x^k defined in (9).

The difference between the conditions (C2)–(C3) and the analogous in Gonzaga et al. (2004) is that here they are defined in neighborhood of a non-quasi-stationary point while the others are in a neighborhood of a non-stationary point.

451 **Lemma 6** (C1) and (C2) imply (C3).

Proof Let \overline{x} be a feasible non-quasi-stationary point and let V_1 be the neighborhood defined by (C2). Since $||z^k - x^k|| = O(h(x^k))$ and \overline{x} is a feasible point there exists a neighborhood $V_2 \subset V_1$ of \overline{x} such that for $x^k \in V_2$, $z^k \in V_1$. Consider an iterate $x^k \in V_2$. By (19) there is a positive constant N such that $|f(z^k) - f(x^k)| \le Nh(x^k)$ and $f(x^k) - f(z^k) \ge -Nh(x^k)$. By (C2) there is a positive constant M such that $f(z^k) - f(x^{k+1}) \ge M\sqrt{H_k}$. Then, considering that $h(x^k) \le H_k$, we obtain

461

$$(f(x^{k+1}) = f(x^k) - f(z^k) + f(z^k) - f(x^{k+1}) \ge M\sqrt{H_k} - Nh(x^k)$$

= $M\sqrt{H_k} - N\sqrt{h(x^k)}\sqrt{h(x^k)} \ge M\sqrt{H_k} - N\sqrt{H_k}\sqrt{h(x^k)}.$

460 Thus,

 $f(x^k)$

$$f(x^k) - f(x^{k+1}) \ge (M - N\sqrt{h(x^k)})\sqrt{H_k}$$

By continuity of *h* at the feasible point \overline{x} , there exists a neighborhood $V \subset V_2$ such that, for any $x \in V, \sqrt{h(x)} \le 0.5 \frac{M}{N}$. Therefore, for any iterate $x^k \in V, f(x^k) - f(x^{k+1}) \ge 0.5M\sqrt{H_k}$, completing the proof.

The following lemmas are adaptations of Lemma 2.5 and Lemma 2.6 in Gonzaga et al. (2004) for the definition of quasi-stationary point for the derivative-free case. Such results are obtained considering the validity of the (C3) condition. We state them here for completeness.

Journal: 40314 Article No.: 0253 TYPESET DISK LE CP Disp.:2015/7/3 Pages: 26 Layout: Small

433

Lemma 7 Let $\overline{x} \in X$ be a non-quasi-stationary limit point. Then there exist $\overline{k} \in \mathbb{N}$ and a neighborhood V of \overline{x} such that whenever $k > \overline{k}$ and $x^k \in V$, the iteration k is an f-iteration.

Lemma 8 Suppose that $\{x^k\}_{k \in \mathbb{N}}$ has no quasi-stationary accumulation point. Then for k sufficiently large, all iterations are f-iterations.

Finally, we can obtain the following main theorem. The proof of this theorem follows straightforward from Gonzaga et al. (2004).

Theorem 1 The sequence $\{x^k\}_{k \in \mathbb{N}}$ has a quasi-stationary accumulation point.

476 4.1 Convergence to a Karush–Khun–Tucker point

From the previous section we know that the sequence $\{x^k\}_{k \in \mathbb{N}}$ generated by the DFF algorithm has a quasi-stationary limit point \overline{x} . Then there exists $\mathscr{K} \subset \mathbb{N}$ such that $\lim_{k \in \mathscr{K}} x^k = \overline{x}$. Furthermore, by (C1), we have that $\lim_{k \in \overline{x}} z^k = \overline{x}$ and consequently

480

Author Proof

$$\lim_{k \in \mathscr{K}} \|P_{L(z^k)}(z^k - \nabla_s f(z^k)) - z^k\| = 0.$$
(32)

In this section, we will prove that, using the linear independence constraint qualification (LICQ) (Bertsekas 1999), \overline{x} is a Karush–Kuhn–Tucker (KKT) point of (1).

The following Lemma shows that (32) still holds when we replace $\nabla_s f(z^k)$ by $\nabla f(z^k)$ but maintaining the projection onto $L(z^k)$.

Lemma 9 Let $\{x^k\}_{k \in \mathbb{N}}$ be a sequence generated by the DFF algorithm. Then there exists $\mathscr{K} \subset \mathbb{N}$ such that

$$\lim_{k \in \mathscr{K}} \|P_{L(z^k)}(z^k - \nabla f(z^k)) - z^k\| = 0.$$
(33)

488 *Proof* From condition (H4),

489

487

$$\|\nabla f(z^k) - \nabla_s f(z^k)\| \le k_{eg} \Delta_f^k \le k_{eg} \delta_k, \tag{34}$$

where the sequence $\{\delta_k\}$ tends to zero. Then considering

and using (12) we have that

493

$$\|z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}))\| \le \|z^{k} - P_{L(z^{k})}(z^{k} - \nabla_{s} f(z^{k}))\| + \|\nabla f(z^{k}) - \nabla_{s} f(z^{k})\|.$$

 $\|z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}))\| = \|z^{k} - P_{L(z^{k})}(z^{k} - \nabla f(z^{k}) - \nabla_{s}f(z^{k}) + \nabla_{s}f(z^{k}))\|$ (35)

Therefore, using (32) and (34) and taking limit when k goes to infinite, $k \in \mathcal{K}$, we have (33) as we wanted to prove.

The main difference between the condition (7) and the condition (32) is that in the last one just estimations of the true derivatives are used.

In Gonzaga et al. (2004, Lemma 1.1) the authors prove that condition (7), together with the Mangasarian–Fromovitz constraint qualification (Bertsekas 1999), is equivalent to the KKT conditions.

We are able to prove that if a quasi-stationary point of the sequence generated by the algorithm verifies the Linear Independence constraint qualification then this point is a KKT point of the problem (1).

Theorem 2 Let $\{x^k\}_{k \in \mathbb{N}}$ be a sequence generated by the DFF algorithm and \overline{x} a quasistationary accumulation point of $\{x^k\}$ that satisfies the Linear Independence constraint qualification. Then \overline{x} is a KKT point of (1).

D Springer JDMAC

507

508

510

511

such that $\lim_{k \in \mathscr{K}} x^k = \overline{x}$.

Let $\tilde{z}^k = P_{L(z^k)}(z^k - \nabla f(z^k))$, then by definition \tilde{z}^k is the solution of the problem 509 $\min \|z - (z^k - \nabla f(z^k))\|^2$ subject to $A_k(z - z^k) = 0.$

Since \overline{x} is a quasi-stationary accumulation point and using the previous lemma we have that

Proof Since \overline{x} is a quasi-stationary accumulation point of $\{x^k\}$, then there exists $\mathscr{K} \subset \mathbb{N}$

$$\lim_{k\in\mathscr{K}}(\widetilde{z}^k-z^k)=0$$

Since the feasible set of (36) is defined by linear constraints we know that there exists $\overline{\mu}^k \in \mathbb{R}^m$ 513 such that 514

$$-(\tilde{z}^k - (z^k - \nabla f(z^k))) = A_k^{\mathrm{T}} \overline{\mu}^k$$

$$A_k(\tilde{z}^k - z^k) = 0.$$

$$z^k - \tilde{z}^k = \nabla f(z^k) + \sum_{i=1}^m \overline{\mu}_i^k a_i^k$$

where a_i^k denotes the *i*th column of $A_k^{\rm T}$. By Carathéodory's theorem (see for example Bert-519 sekas 1999, page 689), for each $k \in \mathcal{K}$ there exist $I_k \subset \{1, \ldots, m\}$ and $\{\mu^k\} \subset \mathbb{R}^m$ such 520 that 521

518

$$z^k - \widetilde{z}^k = \nabla f(z^k) + \sum_{i \in I_k} \mu_i^k a_i^k$$

where the set $\{a_i^k\}_{i \in I_k}$ is linearly independent. 523

Since the number of possible sets I_k is finite, then there exists $\mathcal{K}_1 \subset \mathcal{K}$ such that for all 524 $k \in \mathscr{K}_1$, 525

$$I_k = I \subset \{1, \ldots,$$

and

526

 $z^{k} - \tilde{z}^{k} = \nabla f(z^{k}) + \sum_{i \in I} \mu_{i}^{k} a_{i}^{k}$ (37)

where the set $\{a_i^k\}_{i \in I}$ is linearly independent. 529

If $\{\mu^k\}$ is not bounded, let $M_k = \|\mu^k\|_{\infty}$. Then $\lim_{k \in \mathcal{K}_1} M_k = \infty$ and we may take an 530

appropriate subsequence such that $\lim_{k \in \mathscr{K}_2} \frac{\mu^k}{M_k} = \mu \neq 0$, where $\mathscr{K}_2 \subset \mathscr{K}_1$. Then 531

$$\frac{z^k - \tilde{z}^k}{M_k} = \frac{\nabla f(z^k)}{M_k} + \sum_{i \in I} \frac{\mu_i^k}{M_k} a_i^k.$$
(38)

532

534



$$\sum_{i \in I} \mu_i \nabla c_i(\overline{x}) = 0$$

Journal: 40314 Art icle No.: 0253 TYPESET DISK LE CP Disp.: 2015/7/3 Pages: 26 Layout: Small (36)

$$I_k = I \subset \{1, \ldots, n\}$$

which contradicts the Linear Independence constraint qualification. So $\{\mu^k\}$ is bounded and there exists $\mathscr{K}_3 \subset \mathscr{K}_1$ such that $\lim_{k \in \mathscr{K}_3} \mu^k = \mu$. Then using (H4) and taking limit in (37) when k goes to infinite, $k \in \mathscr{K}_3$, we obtain that

538

$$\nabla f(\overline{x}) + \sum_{i \in I} \mu_i \nabla c_i(\overline{x}) = 0.$$

⁵³⁹ Hence, \overline{x} is a KKT point of (1).

540 **5 Numerical experiments**

In this section, we present some preliminary computational results obtained with a Fortran 77 implementation of the DFF algorithm. These experiments were run on a personal computer with INTEL(R) Core (TM) 2 Duo CPU E8400 at 3.00 GHz and 3.23 GB of RAM.

As it is usual in derivative-free optimization articles we are interested in the number of function evaluations needed for satisfying the stopping criteria.

546 5.1 Details on the implementation of the DFF algorithm

We have considered two versions of DFF: DFF1 and DFF2. The only difference between them is the form to compute the matrix A_k . In DFF1 it is computed by simplex derivatives as was described in Algorithm 1 and used in the theoretical results. In DFF2, once z^k is computed in the restoration phase, we consider a new Broyden matrix by updating the last one computed in that process, which is used as the matrix A_k .

In our experiments the parameters used in DFF1 and DFF2 are $\alpha = 0.1$, $\beta = 100$, $\varepsilon_f = 10^{-6}$ and $\varepsilon_I = 10^{-6}$.

In this implementation we declare convergence, if breakdown does not occur at the restoration phase, when $h(x^k) \le \varepsilon_f$, max $\{\Delta_f^k, \Delta_c^k\} \le \varepsilon_I$ and $\|d_c(z^k)\| \le \varepsilon_f$.

In the implementation of the optimization phase we use the subroutine DLSVRR of the IMSL Fortran Numerical Libraries, which is based on the LINPACK routine SSVDC (Dongarra et al. 1979), for computing the singular value decomposition (USV) of the matrix A_k to obtain the projection of $z^k - \nabla_s f(z^k)$ onto $L(z^k)$.

Step 3 of DFF requires the calculation of the simplex gradients of c_j , for j = 1, ..., m, which requires to select a set of interpolation points. In the first iteration we construct the set $Y_c^0 = \{z^0, y_c^1, ..., y_c^n\}$ for obtaining the models $m_{c_j}(x) = c_j(z^0) + \nabla_s c_j(z^0)^T(x - z^0), j = 1, ..., m$, generating the matrix A_0 , as an approximation of $J_c(z^0)$. We consider $y_c^i - z^0 = \rho_0 e_i$ and the corresponding values $c_j(y_c^i)$, for i = 1, ..., n and j = 1, ..., m, $\rho_0 < \beta \max\{\delta_0, h(x^0)\}$.

Also, it requires to compute the model $m_f(x) = f(z^k) + \nabla_s f(z^k)^T (x - z^k)$. In the first iteration, we used the vectors of the matrix V of the decomposition USV of A_0 to obtain the model $m_f(x) = f(z^0) + \nabla_s f(z^0)^T (x - z^0)$, considering the set $Y_f^0 = \{z^0, y_f^1, \dots, y_f^n\}$, where $y_f^i = z^0 + \rho_0 v_i$ and $f(y_f^i)$, for $i = 1, \dots, n$.

In the following iterations Y_c^k and Y_f^k are updated, adding the new z^k as the center of them and eliminating a point y_t , the farthest from the center, trying to maintain the independence of directions. In this preliminary implementation, in some iterations the interpolation sets are newly constructed, while in others they are updated from the previous ones. The construction takes place in the first iteration and whenever it is not possible to preserve the independence of

Deringer Springer

the directions easily. To check the independence of the directions we use a similar algorithm 575 to the one proposed in Gratton et al. (2011). 576

The parameters used in BCDF-QNB are the same used in Echebest et al. (2012).

Finally, the parameters used in Algorithm 3 are the following: $\eta = 0.1$, $\Delta_{min} = 0.5$ and $tol = 10^{-16}$.

5.2 Test problems 580

We have used a set of nonlinear programming problems defined in Hock and Schittkowski 581 (1981). Also, we have considered one problem which was used firstly in Gonzaga et al. 582 (2004) and in our previous paper (Echebest et al. 2012) where we introduced the basic 583 ideas of the actual algorithm. The selected problems from Hock and Schittkowski (1981) 584 are those that have equality constraints. Also, we have considered some problems from 585 Hock and Schittkowski (1981) with inequality constraints. In these problems the inequality 586 constraints have been replaced by equality constraints since they are active at the solu-587 tion. 588

In Table 1 we show the data of the problems. The number of variables ranges from 2 to 589 10 and the number of equality constraints from 1 to 4. Initial points were the same as in the 590 cited references. 591

5.3 Numerical results 592

In Table 2 we show the results obtained taking into account the number of iterations (Iter), the 593 number of objective function evaluations (ObjEval), the number of constraints evaluations 594 (ConstEval), the final value $f(x^{\text{end}})$ and the final value of the infeasibility $h(x^{\text{end}})$. 595

We can notice that the DFF1 version has done fewer iterations than the DFF2 version 596 in 70% of the problems. We believe that this behavior is due to the fact that DFF1 uses a 597 better approximation of $J_c(z^k)$ in many iterations, and as consequence the initial updated 598 matrix in the restoration phase is better. When we consider $h(x^{end})$ as a measure of the 599 performance of the algorithms we can see that DFF1 outperforms DFF2 in 70% of the 600 problems. 601

From the results of test problems we can conclude that the restoration algorithm was 602 successful in almost all iterations of all the problems. The only exception was the problem 603 HS 56 for DFF2. 604

For algorithmic comparison we use *performance profile* described in Dolan and Moré 605 (2002) and *data profile* for derivative-free optimization presented in Moré and Wild (2009). 606 The performance profile of a solver s is defined as the fraction of problems where the 607 performance ratio is at most α , that is, $\rho_s(\alpha) = \frac{1}{|\mathcal{P}|} \text{size} \{ p \in \mathcal{P} : r_{p,s} \leq \alpha \}$, where $r_{p,s} =$ 608 $\frac{t_{p,s}}{\{\min t_{p,s}:s \in \mathscr{S}\}}, t_{p,s}$ is the number of function evaluations required to satisfy the convergence 609 test, \mathscr{P} is the set of problems and $|\mathscr{P}|$ denotes the cardinality of \mathscr{P} .

We are also interested in the percentage of problems that can be solved, according to the 611 convergence test mentioned in Sect. 5.1, by a solver s with a particular number of function 612 evaluations. The percentage of problems that can be solved with α function evaluations is 613 computed by $d_s(\alpha) = \frac{1}{|\mathcal{P}|} \operatorname{size} \{ p \in \mathcal{P} : t_{p,s} \leq \alpha \}.$ 614

As it was mentioned in Moré and Wild (2009), the definition of d_s is independent of the 615 number of variables of the problem $p \in \mathcal{P}$. However, we know that the number of function 616 evaluations grows when the number of variables grows. We thus consider the data profile 617 of a solver s by $d_s(\alpha) = \frac{1}{|\mathscr{P}|} \operatorname{size} \{ p \in \mathscr{P} : \frac{t_{p,s}}{n+1} \leq \alpha \}$, where n is the number of variables 618



577

578

579

| Problem | п | т | Problem | n | т | Problem | п | т |
|------------------------------------------------|---|---|------------------------------------------------|---|---|-------------------------------------------------|----|---|
| HS 6 of Hock and Schittkowski (1981) | 2 | 1 | HS 39 of Hock and Schittkowski (1981) | 4 | 2 | HS 60 of Hock and Schittkowski (1981) | 3 | 1 |
| HS 7 of Hock and Schittkowski (1981) | 2 | 1 | HS 40 of Hock and Schittkowski (1981) | 4 | 3 | HS 61 of Hock and Schittkowski (1981) | 3 | 2 |
| HS 8 of Hock and Schittkowski (1981) | 2 | 2 | HS 42 of Hock and Schittkowski (1981) | 4 | 2 | HS 63 of Hock and Schittkowski (1981) | 3 | 2 |
| HS 9 of Hock and Schittkowski (1981) | 2 | 1 | HS 43 of Hock and Schittkowski (1981) | 4 | 3 | HS 77 of Hock and Schittkowski (1981) | 5 | 2 |
| HS 14 of Hock and Schittkowski (1981) | 2 | 2 | HS 46 of Hock and Schittkowski (1981) | 5 | 2 | HS 78 of Hock and Schittkowski (1981) | 5 | 3 |
| HS 22 of Hock and Schittkowski (1981) | 2 | 2 | HS 47 of Hock and Schittkowski (1981) | 5 | 3 | HS 79 of Hock and Schittkowski (1981) | 5 | 3 |
| HS 26 of Hock and Schittkowski (1981) | 3 | 1 | HS 48 of Hock and Schittkowski (1981) | 5 | 2 | HS 80 of Hock and Schittkowski (1981) | 5 | 3 |
| HS 27 of Hock and Schittkowski (1981) | 3 | 1 | HS 52 of Hock and Schittkowski (1981) | 5 | 3 | HS 81 of Hock and Schittkowski (1981) | 5 | 3 |
| HS 29 of Hock and Schittkowski (1981) | 3 | 1 | HS 53 of Hock and Schittkowski (1981) | 5 | 3 | HS 111 of Hock and Schittkowski (1981) | 10 | 3 |
| HS 35 of Hock and Schittkowski (1981) | 3 | 1 | HS 56 of Hock and Schittkowski (1981) | 7 | 4 | Example of Gonzaga et al. (2004) | 2 | 1 |

| Table 1 Data of the probl | ems |
|---------------------------|-----|
|---------------------------|-----|

⁶¹⁹ in $p \in \mathscr{P}$. The value of $d_s(\alpha)$ can be interpreted as the percentage of problems that can ⁶²⁰ be solved with the equivalent of α simplex gradient estimates, considering that n + 1 is ⁶²¹ the number of evaluations needed to compute a one-sided finite-difference estimate of the ⁶²² gradient (Moré and Wild 2009).

We analyze separately the number of objective function evaluations (ObjEval) and the number of constraints evaluations (ConstEval).

In the following figures we compare DFF1 and DFF2 using the number of objective function evaluations as a measure of the performance.

Deringer JDMAC

Author Proof

| Prob | Iter | | ObjEval | | ConstEval | | $f(x^{end})$ | | $h(x^{end})$ | |
|-------|------|------|------------|------|-----------|------|--------------|--------------|--------------|--------------|
| | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 |
| HS 6 | 24 | 49 | 76 | 151 | 103 | 103 | 3.050E - 05 | 3.023E-05 | 8.644E-10 | 2.383E-11 |
| HS 7 | 10 | 10 | 33 | 33 | 46 | 24 | -1.732E00 | -1.732E00 | 2.620E-13 | 9.645E-11 |
| HS 8 | 3 | L | 5 | 6 | 18 | 12 | -1.000E00 | -1.000E00 | 2.764E-12 | 3.157E-07 |
| 6 SH | 27 | 49 | 58 | 101 | 36 | 53 | -5.000E - 01 | -5.000E - 01 | 5.329E-15 | 3.695 E - 09 |
| HS 14 | 3 | 5 | 5 | L | 16 | 6 | 1.393E00 | 1.393E00 | 2.428E-10 | 6.547E-09 |
| HS 22 | 3 | 4 | 5 | 9 | 15 | 8 | 1.000E00 | 1.000E00 | 2.085E - 09 | 5.116E-07 |
| HS 26 | 15 | 18 | 74 | 107 | 93 | 72 | 8.787E-07 | 5.367E-08 | 1.858E-12 | 4.981E-11 |
| HS 27 | 9 | 45 | 81 | 355 | 270 | 267 | 4.001E - 02 | 4.005E-02 | 2.254E-11 | 1.113E-11 |
| HS 29 | 19 | 24 | 80 | 148 | 106 | 104 | -2.263E01 | -2.262E01 | 1.040E - 11 | 9.216E-08 |
| HS 35 | 41 | 45 | 210 | -186 | 255 | 26 | 1.111E - 01 | 1.111E - 01 | 9.159E - 09 | 5.271E-10 |
| HS 39 | 31 | 36 | 127 | 156 | 193 | 202 | -1.000E00 | -9.999E - 01 | 1.036E - 07 | 1.644E - 08 |
| HS 40 | 21 | 14 | 68 | 87 | 138 | 76 | -2.500E-01 | -2.500E - 01 | 9.352E-11 | 1.522E-08 |
| HS 42 | 18 | 45 | 123 | 269 | 165 | 181 | 1.386E01 | 1.386E01 | 9.108E-13 | 3.686E-14 |
| HS 43 | 24 | 32 | <i>L</i> 6 | 156 | 181 | 187 | -4.400E01 | -4.400E01 | 1.882E - 08 | 1.740E - 07 |
| HS 46 | 31 | 37 | 182 | 214 | 249 | 105 | 5.774E-05 | 5.265E-05 | 1.323E - 08 | 4.828E-09 |
| HS 47 | 30 | 40 | 129 | 182 | 222 | 105 | 1.461E - 05 | 2.582E-05 | 1.852E-09 | 1.824E-07 |
| HS 48 | 57 | 62 | 249 | 317 | 165 | 133 | 7.521E-09 | 1.150E-09 | 9.108E - 09 | 7.326E-09 |
| HS 52 | 41 | 41 | 289 | 286 | 230 | 207 | 5.327E00 | 5.327E00 | 1.959E-08 | 9.141E-09 |
| HS 53 | 19 | 19 | 87 | 81 | 87 | 46 | 4.093E00 | 4.093E00 | 8.408E-09 | 8.067E-09 |
| HS 56 | 58 | 79 | 364 | 437 | 685 | 207 | -3.456E00 | -3.346E00 | 8.545E-07 | 1.217E-05 |
| | Ţ | | ļ | | | | | | | |

Author Proof

Table 2 continued

| Prob | Iter | | ObjEval | | ConstEva | | $f(x^{end})$ | | $h(x^{end})$ | |
|-----------------------------------------------|--------------|---------------|----------------|---------------|----------|------|--------------|-------------|---------------|-------------|
| | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 | DFF1 | DFF2 |
| HS 61 | 16 | 18 | 67 | 94 | 115 | 82 | -1.436E02 | -1.436E02 | 4.715E-09 | 2.985E-10 |
| HS 63 | 12 | 30 | 43 | 93 | 78 | 67 | 9.617E02 | 9.617E02 | $3.141E{-10}$ | 1.806E - 10 |
| LL SH | 25 | 26 | 133 | 270 | 190 | 198 | 2.415E-01 | 2.415E-01 | 1.021E-11 | 4.608E-07 |
| HS 78 | 5 | 30 | 27 | 167 | 50 | 110 | -2.919E00 | -2.919E00 | 5.694E - 09 | 1.824E - 08 |
| 62 SH | 8 | 10 | 41 | 51 | 73 | 34 | 7.878E-02 | 7.878E-02 | 6.064E-12 | 1.570E - 07 |
| HS 80 | 11 | 10 | 48 | 44 | 89 | 27 | 5.395E - 02 | 5.396E - 02 | 7.441E-09 | 1.282E - 07 |
| HS 81 | 11 | И | 48 | 48 | 89 | 29 | 5.395E - 02 | 5.395E - 02 | 1.215E - 08 | 1.835E-07 |
| HS 111 SH | 99 | 101 | 595 | 1084 | 805 | 397 | -4.776E01 | -4.764E01 | 3.849 E - 07 | 8.760E-07 |
| Ex. of Gonzaga et al. (2004) | 11 | 20 | 46 | 64 | 70 | 45 | -2.210E00 | -2.211E00 | 1.278E - 09 | 1.783E-09 |
| ^a The final solution does not read | ch the enoug | th decrease o | f the infeasit | oility measur | o | | | | | |





Fig. 2 Data profiles for the comparison between DFF1 and DFF2: objective function evaluations

In the performance profile of Fig. 1, we can notice that DFF1 expended less objective function evaluations in more than 80% of the problems, while DFF2 expended less objective function evaluations in approximately 20% of the problems. The performance difference between DFF1 and DFF2 is approximately 20% when the performance ratio is 2.

The data profile of Fig. 2a shows that DFF1 solves the largest percentage of problems for all sizes of the number of objective function evaluations. We can observe that DFF1 solves 80 % of problems with 200 evaluations while DFF2 solves approximately 70 %. The biggest difference is 30 % and it happens when the number of function evaluations is approximately 180. We believe that this behavior is due to the fact that DFF1 uses a better approximation of $J_c(z^k)$ in many iterations as well as it makes fewer iterations.

Figure 2b shows that DFF1 solves the largest percentage of problems for all sizes of the number of simplex gradient estimates (ObjEval/(n + 1)). With 60 evaluations DFF1 solves





Fig. 4 Data profiles for the comparison between DFF1 and DFF2: constraints evaluations

approximately 30% of them.
 approximately 50% of them.

In the following figures we compare DFF1 and DFF2 using the number of constraints evaluations as a measure of the performance.

In the performance profile of Fig. 3 we can notice that DFF2 expended less constraints function evaluations in approximately 80% of the problems while DFF1 expended less constraints function evaluations in more than 20%.

In Fig. 4a the data profile shows that DFF2 solves the largest percentage of problems for all sizes of the number of constraints evaluations. We believe that this result is associated to the fact that DFF2 does not require new constraints evaluations to define the matrix A_k because it updates the last matrix used in the restoration phase. With 400 eval-

Deringer Springer

uations DFF2 solves all the problems, while DFF1 needs 800 evaluations to solve all of them.

Figure 4b shows that DFF2 solves the largest percentage of problems for all sizes of the number of simplex gradient estimates (ConstEval/(n + 1)). With 70 evaluations DFF2 solves almost 100 % of the problems, while DFF1 solves approximately 90 % of the problems. The biggest difference between DFF1 and DFF2 happens when the number of constraints evaluations is 20 % and in this case DFF2 solves 60 % of the problems while DFF1 solves approximately 40 % of them.

Taking into account the performance and data profiles, we believe that better results can be obtained developing another alternative that combines DFF1 and DFF2 implementations. That could be made considering the DFF2 implementation, computing A_k by simplex gradients after a fix number of iterations. In addition, in the application of BCDF-QNB in the restoration phase, we could replace the use of finite differences to compute B_k by the use of simplex gradients. That will be a subject of future study.

668 6 Conclusions

We have presented an inexact restoration filter algorithm for equality constrained nonlinear programming without using derivatives. The main contribution of the paper is to extend the theory of a filter-based optimization method to the derivative-free context, but future research about numerical behavior of the algorithm is still necessary to understand if there exists a class of problems that would be better solved with the DFF algorithm than with other benchmark DF algorithm.

From the theoretical point of view, under suitable conditions, we were able to prove global convergence to quasi-stationary points. Furthermore, we have shown that if a quasi-stationary accumulation point satisfies the Linear Independence constraint qualification then this point is a KKT point of (1).

From the practical point of view, two versions of the proposed algorithm were implemented and tested considering a set of small-scale problems. The main difference between the two versions is the way in which an approximation of the true Jacobian $J_c(z^k)$ is computed. Two main aspects can be taken into account from the numerical experiments:

 They suggest plausible the use of Quasi Newton for computing the Jacobian approximations and this will be one of the subject of forthcoming research.

The implemented algorithms behave as expected; however, it will be desirable to test the
 execution of the algorithm with a more challenging set of problems. Also, we would like
 to compare the performance of the tested algorithms with other derivative-free algorithms
 defined for solving the same problem.

pgAs the method proposed is the type of inexact restoration, different alternatives can be studied in order to solve the two phases. In particular, to solve the optimality phase, we would like to define a derivative-free algorithm based on a quadratic model, instead of a linear one. In this case the use of quadratics models must be consistent with the theory, especially with the condition (C2), in order to preserve the convergence.

Acknowledgments The authors are indebted to the two anonymous referees whose comments helped a lot to improve the quality of the paper.

Journal: 40314 Article No.: 0253 TYPESET DISK LE CP Disp.:2015/7/3 Pages: 26 Layout: Small

696 **References**

- Alexandrov N, Hussaini MY (1997) Multidisciplinary design optimization: state of the art. In: SIAM proceed ings series. SIAM, Philadelphia
 - Arouxét MB, Echebest N, Pilotta EA (2011) Active-set strategy in Powell's method for optimization without derivatives. Comput Appl Math 30(1):171–196
 - Bertsekas DP (1999) Nonlinear programming, 2nd edn. Athena Scientific, Belmont
 - Bueno LF, Friedlander A, Martínez JM, Sobral FNC (2013) Inexact restoration method for derivative-free optimization with smooth constraints. SIAM J Optim 23(2):1189–1213
 - Conn AR, Scheinberg K, Toint PhL (1997) Recent progress in unconstrained nonlinear optimization without derivatives. Math Program 79(3):397–414
 - Conn A, Scheinberg K, Vicente LN (2009) Introduction to derivative-free optimization. In: SIAM book series on optimization, Philadelphia
 - Custodio AL, Vicente LN (2007) Using sampling and simplex derivatives in pattern search methods. SIAM J Optim 18(2):537–555
- Diniz-Ehrhardt MA, Martínez JM, Pedroso LG (2011) Derivative-free methods for nonlinear programming
 with general lower-level constraints. Comput Appl Math 30(1):19–52
- Dolan E, Moré J (2002) Benchmarking optimization software with performance profiles. Math Program
 91:201–213
- 714 Dongarra JJ, Bunch JR, Moler CB, Stewart GW (1979) LINPACK users' guide. SIAM, Philadelphia
- Echebest N, Schuverdt ML, Vignau RP (2012) A derivative-free method for solving box-constrained under determined nonlinear systems of equations. Appl Math Comput 219(6):3198–3208
- Fletcher R, Gould NIM, Leyffer S, Toint PhL, Wächter A (2002) Global convergence of a trust-region SQP filter algorithm for general nonlinear programming. SIAM J Optim 13:635–659
- Fletcher R, Leyffer S (2002) Nonlinear programming without a penalty function. Math Program 91(2):239–269
 Gomes-Ruggiero MA, Martínez JM, Santos SA (2009) Spectral projected gradient method with inexact restora-
- tion for minimization with nonconvex constraints. SIAM J Sci Comput 31:1628–1652
- Gonzaga CC, Karas EW, Vanti M (2004) A globally convergent filter method for nonlinear programming.
 SIAM J Optim 14(3):646–669
- Gratton S, Toint PhL, Tröltzsch A (2011) An active-set trust region method for bound-constrained nonlinear
 optimization without derivatives. Optim Methods Softw 26(4–5):875–896
- Grippo L, Lampariello F, Lucidi S (1986) A nonmonotone line search technique for Newton's method. SIAM
 J Numer Anal 23:707–716
- Hock W, Schittkowski K (1981) Test examples for nonlinear programming codes. In: Springer series lectures
 notes in economics mathematical systems
- Kolda TG, Lewis RM, Torczon V (2003) Optimization by direct search: new perspectives on some classical
 and modern methods. SIAM Rev 45:85–482
- Kolda TG, Lewis RM, Torczon V (2006) Stationarity results for generating set search for linearly constrained
 optimization. SIAM J Optim 17(4):943–968
- Lewis RM, Torczon V (1999) Pattern search algorithms for bound constrained minimization. SIAM J Optim
 9(4):1082–1099
- Lewis RM, Torczon V (2000) Pattern search algorithms for linearly constrained minimization. SIAM J Optim 10(3):917–941
- Lewis RM, Torczon V (2002) A globally convergent augmented Lagrangian pattern search algorithm for
 optimization with general constraints and simple bounds. SIAM J Optim 12(4):1075–1089
- Lewis RM, Torczon V (2010) A direct search approach to nonlinear programming problems using an augmented
 Lagrangian method with explicit treatment of linear constraints. In: Technical report WMCS- 2010–01,
 College of William & Mary, Department of Computer Sciences, Department of Computer Sciences
- 743 Li DH, Fukushima M (2000) A derivative-free line search and global convergence of Broyden-like method 744 for nonlinear equations. Optim Methods Softw 13:181–201
- Martínez JM (2001) Inexact-restoration method with Lagrangian tangent decrease and a new merit function
 for nonlinear programming. J Optim Theory Appl 111(1):39–58
- Martínez JM, Pilotta EA (2000) Inexact restoration algorithm for constrained optimization. J Optim Theory
 Appl 104(1):135–163
- Martínez JM, Pilotta EA (2005) Inexact restoration methods for nonlinear programming: advances and per spectives. In: Qi L, Teo K, Yang X (eds) Optimization and control with applications. Springer, Berlin,
 271–292
- Martínez JM, Svaiter BF (2003) A practical optimality condition without constraint qualifications for nonlinear
 programming. J Optim Theory Appl 118(1):117–133

699

700

701

702 703

704

705

706

707

708

Moré JJ, Wild SM (2009) Benchmarking derivative-free optimization algorithms. SIAM J Optim 20(1):172–
 191

Powell MJD (2006) The NEWUOA software for unconstrained optimization without derivatives. In: Di Pillo
 G, Roma M (eds) Large-scale nonlinear optimization. Springer, New York, pp 255–297
 Powell MJD (2009) The BOBYOA algorithm for bound constrained optimization without derivatives. In:

Powell MJD (2009) The BOBYQA algorithm for bound constrained optimization without derivatives. In:
 Cambridge NA report NA2009/06. University of Cambridge, Cambridge

≦ Springer 𝔅𝔅𝔅𝔅



Author Query Form

Please ensure you fill out your response to the queries raised below and return this form along with your corrections

Dear Author

During the process of typesetting your article, the following queries have arisen. Please check your typeset proof carefully against the queries listed below and mark the necessary changes either directly on the proof/online grid or in the 'Author's response' area provided below

| Query | Details required | Author's response |
|-------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------|
| 1. | Kindly check and confirm if the edit made in the following sentence is correct: "This idea was proposed by Fletcher and Leyffer in [13] in other contexts." | 0 |
| 2. | Reference (Gomes-Ruggiero et al. 2009) is given in list but not cited in text. Please cite in text or delete from list. | |