

## APPROXIMATE NORM DESCENT METHODS FOR CONSTRAINED NONLINEAR SYSTEMS

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ABSTRACT. We address the solution of convex-constrained nonlinear systems of equations where the Jacobian matrix is unavailable or its computation/storage is burdensome. In order to efficiently solve such problems, we propose a new class of algorithms which are “derivative-free” both in the computation of the search direction and in the selection of the steplength. Search directions comprise the residuals and quasi-Newton directions while the steplength is determined by using a new linesearch strategy based on a nonmonotone approximate norm descent property of the merit function. We provide a theoretical analysis of the proposed algorithm and we discuss several conditions ensuring convergence to a solution of the constrained nonlinear system. Finally, we illustrate its numerical behaviour also in comparison with existing approaches.

### 1. INTRODUCTION

Solving nonlinear systems of equations is a ubiquitous task in applied mathematics, and has generated considerable interest for a long time. In this paper, we focus on an important variant of this task: that of solving a nonlinear system subject to convex constraints (such as bounds). More precisely, let  $F : X \rightarrow \mathbb{R}^n$  be a continuous mapping and  $X \subseteq \mathbb{R}^n$  be an open set. We address the problem of finding a vector  $x \in \mathbb{R}^n$  satisfying the nonlinear system with convex-constraints

$$(1) \quad F(x) = 0, \quad x \in \Omega,$$

where  $\Omega \subset X$  is a convex set whose relative interior is nonempty.

The solution of problem (1) has been intensively investigated in the last years. Most of the proposed methods require the calculation of the derivatives of  $F$  and are Newton-based methods belonging to the class of affine-scaling procedures; see e.g., [3, 4, 19, 26, 29, 31]. However, such methods may become computationally expensive for medium and large scale problems, due to the evaluation cost of the Jacobian  $J$  of  $F$ , unless this matrix has structure which can be exploited. Whenever this is not the case, spectral residual methods [21, 22] and quasi-Newton methods [6, 27] may become competitive, and implementations which do not involve derivatives at

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all (derivative-free algorithms) are of special interest, as exemplified by the algorithms proposed in [1, 17, 21, 23] for unconstrained problems and in [12, 20, 30] for constrained problems.

Our interest in this paper is in a class of derivative-free methods covering both spectral residual and quasi-Newton algorithms. As it turns out (and as we demonstrate in the paper), these methods can be used for relatively large problems and can be surprisingly efficient in terms of computing a solution of (1), as opposed to the easier task of computing a local minimizer of the residual

$$(2) \quad f(x) = \|F(x)\|_2^2.$$

However, it is also known that they may fail. Our objective is thus to propose an efficient algorithm which avoids some of the convergence pitfalls present in similar approaches and also to investigate conditions under which convergence to a solution of (1) can be ensured.

The algorithm developed in this paper generates feasible iterates  $x_k$ , where  $k$  is the iteration index. If  $F$  is continuous, then the residuals  $\pm F(x_k)$  are used as search directions. Alternatively, if  $F$  is differentiable, search directions can be computed by using approximations  $B_k$  to the Jacobian matrices  $J$  of  $F$  at the iterates. In both cases, large savings can be obtained in the computation of the search directions compared with Newton's method. A derivative-free linesearch strategy is proposed so that, for any initial iterate, either  $\|F(x_k)\|$  converges to zero or the iteration fails to do so in a small and characterized number of ways. Since the solutions of problem (1) are global minimizers of the function  $f$  and the search directions generated may be uphill directions for  $f$ , we introduce a nonmonotone *approximate norm descent condition* inspired by both the linesearch proposed by Li and Fukushima [23], and the globalization schemes for inexact Newton methods due to Eisenstat and Walker [13].

The paper is organized as follows. Section 2 introduces the context and the PSANE method [20]. Our proposal is then developed in Section 3. We next investigate (in Section 4) some simple convergence properties of the sequences of residuals and iterates. The theoretical core of the paper is Section 5 where we discuss several conditions ensuring convergence to a solution of (1). Section 6 then illustrates the numerical properties of the proposed method and its variants, and compares it with PSANE. Some conclusions and perspectives are finally presented in Section 7.

**1.1. Notation.** Throughout this paper,  $(x)_i$  represents the  $i$ th component of the vector  $x$ , and  $\mathcal{B}(y, \delta)$  represents the closed ball with center  $y$  and radius  $\delta$ . The symbol  $\|\cdot\|$  denotes the Euclidean norm. The (orthogonal) projection map onto  $\Omega$  is denoted with  $P(\cdot)$ . When discussing iterative methods for (1), the term *breakdown* refers to the case in which an iterate cannot be determined. Finally, given a sequence of vectors  $\{x_k\}$ , for any function  $f$ , we let  $f_k = f(x_k)$ .

## 2. PRELIMINARIES

In this section we review both linesearch strategies which do not require directional derivatives of  $f$  and the projected derivative-free algorithm PSANE for nonlinear equations with convex constraints given in [20].

A useful contribution in global convergence of Broyden-like methods for unconstrained nonlinear systems is due to Li and Fukushima [23]. Starting from an earlier contribution by Griewank [15], they proposed a new derivative-free linesearch which

is well-defined and easy to implement. At the  $k$ th iteration, given the iterate  $x_k$  and a search direction  $p_k$ , the successive iterate takes the form  $x_{k+1} = x_k + \lambda p_k$ ,  $\lambda > 0$ , and satisfies

$$(3) \quad \|F(x_k + \lambda p_k)\| \leq (1 + \eta_k)\|F(x_k)\| - \alpha\lambda^2\|p_k\|^2,$$

for some constant  $\alpha \in (0, 1)$  and some positive  $\eta_k$ . The sequence  $\{\eta_k\}$  is supposed to meet the following requirement.

**Assumption 2.1.** *The positive sequence  $\{\eta_k\}$  satisfies*

$$(4) \quad \sum_{k=0}^{\infty} \eta_k \leq \eta < \infty.$$

Due to the continuity of  $F$ , condition (3) holds for all  $\lambda$  sufficiently small, and it is called an approximate norm descent linesearch since

$$(5) \quad \|F(x_k + \lambda p_k)\| \leq (1 + \eta_k)\|F(x_k)\|.$$

La Cruz, Martínez and Raydan [21] then developed the derivative-free nonmonotone iterative method for unconstrained nonlinear systems named Derivative Free Spectral Algorithm for Nonlinear Equations (DF-SANE). The linesearch strategy proposed has the form

$$(6) \quad \phi(x_k + \lambda p_k) \leq \max_{0 \leq j \leq \min\{k, M\}} \phi(x_{k-j}) + \eta_k - \alpha\lambda^2\phi(x_k),$$

where  $\phi(x) = \|F(x)\|^\tau$ ,  $\tau \in \{1, 2\}$ ,  $M$  is a nonnegative integer. The first term on the right-hand side of (6) is responsible for the nonmonotone behaviour of  $\phi$ , while the second term  $\eta_k > 0$  guarantees that the linesearch strategy is well-defined, and the third term provides the arguments for proving global convergence. The sequence  $\{\eta_k\}$  is supposed to satisfy Assumption 2.1. In [17] condition (6) is combined with a nonmonotone watchdog rule and is used with  $\eta_k = 0$  for all  $k$ .

A further proposal was made by Birgin, Krejić and Martínez [5] in the context of inexact quasi-Newton methods for unconstrained systems. Restricting to the “exact” solution of the linear systems, the linesearch is given by

$$(7) \quad \|F(x_k + \lambda p_k)\| \leq (1 - \alpha\lambda)\|F(x_k)\| + \eta_k,$$

and, again,  $\alpha \in (0, 1)$  and the sequence  $\{\eta_k\}$  is supposed to satisfy Assumption 2.1. We refer to previously mentioned papers for the analysis of the resulting procedures.

In addition, La Cruz recently proposed a projected derivative-free method for the constrained nonlinear system (1), named PSANE [20]. Since the PSANE algorithm motivated the definition of our method, we restate its details in Algorithm 2.1.

One distinguishing feature of PSANE is that the computation of the search directions  $d_-$  and  $d_+$  does not involve the solution of linear systems. The spectral coefficient  $1/b_k$  formed in Step 6 is closely related to the Barzilai-Borwein’s steplength [2]; it may be positive or negative, and the absolute value  $|1/b_k|$  is constrained to belong to the given interval  $[\beta_{\min}, \beta_{\max}]$  [21]. The iterate  $x_{k+1}$  is determined through a backtracking strategy and each repetition of Step 4 requires a number of evaluations of  $F$  between 1 and 2. It is easy to observe that each iterate  $x_{k+1}$  is feasible as it is the convex combination of the feasible points  $x_k$  and  $P(x_k \pm \beta_k F(x_k))$ .

**Algorithm 2.1: The PSANE algorithm**

Given  $x_0 \in \Omega$ ,  $\alpha, \sigma \in (0, 1)$ ,  $\lambda_{\max} \in (0, 1]$ ,  $0 < \beta_{\min} < \beta_{\max} < \infty$ ,  $\beta_0 \in [\beta_{\min}, \beta_{\max}]$ , a positive sequence  $\{\eta_k\}$  that satisfies (4).

For  $k = 0, 1, 2, \dots$  do

1. If  $\|F(x_k)\| = 0$  stop.
2. Set  $d_- = P(x_k - \beta_k F(x_k)) - x_k$  and  $d_+ = P(x_k + \beta_k F(x_k)) - x_k$ .
3. Choose  $\lambda \in (0, \lambda_{\max}]$ .
4. Repeat

4.1 If

$$(8) \quad \|F(x_k + \lambda d_-)\|^2 \leq \|F(x_k)\|^2 + \eta_k - \alpha \lambda^2 \beta_k^2 \|F(x_k)\|^2,$$

set  $\lambda_k = \lambda, d_k = d_-$  and go to Step 5.

4.2 If

$$(9) \quad \|F(x_k + \lambda d_+)\|^2 \leq \|F(x_k)\|^2 + \eta_k - \alpha \lambda^2 \beta_k^2 \|F(x_k)\|^2$$

set  $\lambda_k = \lambda, d_k = d_+$  and go to Step 5.

4.3 Set  $\lambda = \sigma \lambda$ .

5. Set  $x_{k+1} = x_k + \lambda_k d_k$ ,  $s_k = x_{k+1} - x_k$ ,  $y_k = F(x_{k+1}) - F(x_k)$ .
6. Update  $\beta_k$ :

$$\text{Set } b_k = \frac{s_k^T y_k}{s_k^T s_k}.$$

$$(10) \quad \text{If } \left| \frac{1}{b_k} \right| \in [\beta_{\min}, \beta_{\max}], \text{ set } \beta_{k+1} = \frac{1}{b_k},$$

$$\text{else } \beta_{k+1} = \min \left[ \beta_{\max}, \max \left[ \beta_{\min}, \left| \frac{1}{b_k} \right| \right] \right].$$

Convergence properties of both  $\{\|F(x_k)\|\}$  and  $\{x_k\}$  have been established under Assumption 2.1. In particular, it is shown that the sequence  $\{\|F(x_k)\|\}$  converges [20, Proposition 2.4] and that, if an isolated solution of (1) is a limit point of  $\{x_k\}$ , then the whole sequence converges to such a solution [20, Theorem 2.7].

As such, the PSANE algorithm is not without drawbacks. We first note that the acceptance conditions (8) and (9) depend on the spectral coefficient  $\beta_k$  such that  $|\beta_k| \in [\beta_{\min}, \beta_{\max}]$  (Step 6). Since in practice  $1/\beta_{\min}$  and  $\beta_{\max}$  are large values, the term  $\alpha \lambda^2 \beta_k^2 \|F(x_k)\|^2$  may become either negligible for small values of  $|\beta_k|$ , or excessively large for big values of  $|\beta_k|$ . In the latter case, a large number of backtracks may be necessary to generate the new iterate  $x_{k+1}$ .

Moreover, PSANE may breakdown prematurely if an iterate  $x_k$  lies on the boundary of  $\Omega$ , the step  $d_-$  has zero norm and  $d_-$  is accepted in Step 4.1. In this case,  $x_{k+1} = x_k$  and therefore  $b_k$  in Step 6 is not well-defined. This can be observed when solving the nonlinear system [20, eqn. (28)]

$$(11) \quad F(x) = \begin{pmatrix} 54 - 18x_1 + 3x_3 \\ 78 - 26x_2 + 2x_3 \\ x_3(18 - 3x_1 - 2x_2) \end{pmatrix} = 0, \quad x \in \Omega,$$

where  $\Omega$  is the box  $\{x \in \mathbb{R}^n \text{ s.t. } l \leq x \leq u\}$ ,  $l = (0, 0, 0)^T$ ,  $u = (4, 6, \infty)$ . This system admits the unique solution  $x^* = (3, 3, 0)^T$ . Breakdown occurs at the starting point when running a MATLAB implementation of PSANE with the parameters declared in [20], and initial guesses  $x_0^{(1)} = (0, 0, 0)^T$  and  $x_0^{(2)} = (4, 6, 0)^T$ .

### 3. THE NEW ALGORITHM

Building on the concepts developed above, we now introduce our new Projected Approximate Norm Descent algorithm (PAND), which builds a sequence of feasible iterates  $\{x_k\}$  satisfying the approximate norm descent property (5) for all  $k$  by using the projection operator onto  $\Omega$  and a linesearch strategy,

At the  $k$ th iteration, let  $x_k$  be the current feasible iterate and let  $B_k$  be a suitable invertible matrix. First, the linear system

$$(12) \quad B_k p_k^{\text{QN}} = -F(x_k)$$

is solved and two steps

$$(13) \quad p_+(p_k^{\text{QN}}, \lambda) \stackrel{\text{def}}{=} P(x_k + \lambda p_k^{\text{QN}}) - x_k, \quad p_-(p_k^{\text{QN}}, \lambda) \stackrel{\text{def}}{=} P(x_k - \lambda p_k^{\text{QN}}) - x_k$$

are formed, where  $\lambda \in (0, 1]$ ; see e.g. [7]. A feasible point of the form

$$x_{k+1} = x_k + p_k = x_k + p_k(\lambda)$$

is then selected such that, for some  $\alpha \in (0, 1)$ ,  $\eta_k > 0$ , and  $\{\eta_k\}$  satisfying (4),

$$(14) \quad \|F(x_k + p_k(\lambda))\| \leq (1 - \alpha(1 + \lambda))\|F(x_k)\|$$

or

$$(15) \quad \|F(x_k + p_k(\lambda))\| \leq (1 + \eta_k - \alpha\lambda)\|F(x_k)\|,$$

where  $p_k(\lambda) = p_{\pm}(p_k^{\text{QN}}, \lambda)$ .

In this procedure,  $p_k^{\text{QN}}$  is a quasi-Newton step (which explains its superscript). The matrix  $B_k$  can be chosen as a two-point approximation to the secant equation by letting

$$(16) \quad B_k = \beta_k^{-1}I, \quad |\beta_k| \in [\beta_{\min}, \beta_{\max}],$$

with  $\beta_k$  given in (10) [2, 21]. Alternatively,  $B_k$  can be built by using Broyden's update or any other secant formula; see e.g., [9, 24, 27]. The use of such matrices  $B_k$  is intended to make the computation of  $p_k^{\text{QN}}$  cheap.

The formal description of the PAND method is given in Algorithm 3.1.

Trivially,  $x_k + p_{\pm}(p_k^{\text{QN}}, \lambda)$  is feasible. If  $F$  is continuously differentiable, either  $p_+$  or  $p_-$  is a descent direction for  $f$  in (2), unless  $\nabla f(x_k)^T p_+ = \nabla f(x_k)^T p_- = 0$ . Thus, the use of both  $p_+$  and  $p_-$  promotes a decrease of  $\|F\|$ ; cf. [21, 22].

We also observe that the vector

$$(17) \quad v_k^{\text{QN}} = P(x_k + p_k^{\text{QN}}) - x_k$$

is the first step tested in the PAND algorithm. From the properties of the projection map  $P$ , we may deduce that

$$(18) \quad \|v_k^{\text{QN}}\| \leq \|p_k^{\text{QN}}\|,$$

$$(19) \quad \|p_{\pm}\| \leq \lambda \|p_k^{\text{QN}}\|,$$

and, by Steps 3 and 4 of the PAND algorithm, we have that

$$(20) \quad \|p_k\| \leq \lambda_k \|p_k^{\text{QN}}\|.$$

**Algorithm 3.1: The PAND algorithm**

Given  $x_0 \in \Omega$ ,  $B_0 \in \mathbb{R}^{n \times n}$  nonsingular,  $\alpha, \sigma \in (0, 1)$ ,  $\{\eta_k\}$  satisfying (4).

For  $k = 0, 1, 2, \dots$  do

1. Solve the linear system (12).
2. Set  $\lambda = 1$ .
3. Repeat
  - 3.1 Set  $p_+ = p_+(p_k^{\text{QN}}, \lambda)$  and  $p_- = p_-(p_k^{\text{QN}}, \lambda)$  as in (13).
  - 3.2 If  $p_k(\lambda) = p_+$  satisfies (14), go to Step 4.
  - 3.3 If  $p_k(\lambda) = p_-$  satisfies (14), go to Step 4.
  - 3.4 If  $\|p_+\| \neq 0$  and  $p_k(\lambda) = p_+$  satisfies (15), go to Step 4.
  - 3.5 If  $\|p_-\| \neq 0$ , and  $p_k(\lambda) = p_-$  satisfies (15), go to Step 4.
  - 3.6 Otherwise set  $\lambda = \sigma \lambda$ .
4. Set  $p_k = p_k(\lambda)$ ,  $\lambda_k = \lambda$ ,  $x_{k+1} = x_k + p_k$ .
5. If  $\|F(x_{k+1})\| = 0$  stop.  
Else form an invertible matrix  $B_{k+1}$ .

Acceptance of the trial steps is tested in Step 3, which terminates in a finite number of steps. Indeed, from the continuity of  $F$  and the positivity of  $\eta_k$ , there exists a scalar  $\bar{\lambda}$  such that

$$(F(x_k + p_k(\lambda)))_i^2 \leq (1 + \eta_k - \alpha \bar{\lambda})^2 (F(x_k))_i^2,$$

with  $\lambda \in (0, \bar{\lambda}]$  and for  $i = 1, \dots, n$ . Trivially the above inequalities imply that (15) holds for  $\lambda$  small enough. The number of  $F$ -evaluations performed at each loop within Step 3 is either 1 or 2.

The linesearch conditions (14) and (15) are derivative-free. The first is related to globally convergent inexact Newton methods [13] where a sufficient decrease in  $\|F\|$  is imposed at each iteration. It is tested on both  $p_+$  and  $p_-$  in order to promote a decrease in  $\|F\|$ . The second allows for an increase in  $\|F\|$ , possibly for  $\lambda$  small enough. We exclude the use of zero-norm steps as in this case the inequality (15) is trivially satisfied as long as  $(\eta_k - \alpha \lambda) \geq 0$ .

It is important to observe that inequality (14) implies (15), and the latter implies (5). Thus, the approximate norm descent condition (5) holds for all  $k$ .

As in (3), (7) and (8), the scalar  $\eta_k$  in (15) allows a nonmonotone behaviour of  $\|F\|$ . Conditions (14) and (15), however, differ from (3) and (8) in two respects. First, they are independent from the norm of the step used, which may be convenient whenever this norm is very large; see §2. Second,  $\eta_k$  appears as a multiplicative term for  $\|F(x_k)\|$  in (15), while the impact of  $\eta_k$  on the value  $\|F(x_k)\|^2 + \eta_k$  in (6) is unpredictable as  $\eta_k$  is not adjusted to reflect the size of  $\|F(x_k)\|$ .

Finally, the sufficient decrease condition (14) with  $p_+$  and  $p_-$  is important for establishing theoretical results on the convergence of  $\{\|F(x_k)\|\}$  to zero (see next section). Such results are valuable as convergence to stationary points of (2) cannot be obtained in our framework; cf. [17, 20, 21, 23]. We are aware that (14) may slow the convergence of the method but the numerical experience presented in §6 shows that it does not either prevent the nonmonotone behaviour of  $\|F\|$  or slow convergence down compared with PSANE.

Detailed numerical experience with PAND will be presented in §6. We only observe at this stage that the implementation of PAND (with  $B_k$  given by (16), and the PSANE parameters as used in [20]) is successful on problem (11) starting from the initial guesses  $x_0^{(1)}, x_0^{(2)}$  given in §2: the algorithm converges to a solution in 8 and 10  $F$ -evaluations, respectively.

4. CONVERGENCE ANALYSIS

This section is devoted to the theoretical study of the PAND algorithm. Summarizing our main results:

- We show that the sequence  $\{\|F_k\|\}$  is convergent.
- We show that sequence  $\{x_k\}$  is convergent and give an upper bound on the distance between  $x_0$  and the limit point  $x^*$ .
- We investigate some conditions under which  $\lim_{k \rightarrow \infty} \|F_k\| = 0$ , i.e.  $F(x^*) = 0$ .

The following technical result shown in [23, Lemma 2.1] will be useful.

**Lemma 4.1.** *Let  $\{\eta_k\}$  satisfy Assumption 2.1. Then  $\prod_{i=0}^k (1 + \eta_i) \leq e^\eta$  with  $k \geq 0$ .*

**4.1. Analysis of the sequences  $\{\|F_k\|\}$  and  $\{\lambda_k\}$ .** We start by analyzing the asymptotic behaviour of the sequences  $\{\|F_k\|\}$  and  $\{\lambda_k\}$  and make a first attempt to detect both occurrences where  $\lim_{k \rightarrow \infty} \|F_k\| = 0$  and where the PAND method fails to solve (1). The following theorem characterizes the behaviour of  $\{\|F_k\|\}$  and is valid for any continuous function  $F$ . The proof relies on inequality (5).

**Theorem 4.2.** *Let Assumption 2.1 hold and  $\{x_k\}$  be generated by the PAND algorithm. Then:*

- (i) *The sequence  $\{\|F_k\|\}$  is bounded and*

$$(21) \quad \|F_{k+1}\| \leq e^\eta \|F_0\|,$$

for all  $k \geq 0$ .

- (ii) *The sequence  $\{\|F_k\|\}$  is convergent.*

- (iii)

$$(22) \quad \lim_{k \rightarrow \infty} \lambda_k \|F_k\| = 0.$$

- (iv)

$$(23) \quad \liminf_{k \rightarrow \infty} \lambda_k > 0 \quad \text{implies that} \quad \lim_{k \rightarrow \infty} \|F_k\| = 0.$$

- (v) *If (14) is satisfied for infinitely many  $k$ , then  $\lim_{k \rightarrow \infty} \|F_k\| = 0$ .*

- (vi) *If  $\|F_k\| \leq \|F_{k+1}\|$  for infinitely many iterations, then  $\liminf_{k \rightarrow \infty} \lambda_k = 0$ .*

- (vii) *If  $\|F_k\| \leq \|F_{k+1}\|$  for all  $k$  sufficiently large, then  $\{\|F_k\|\}$  does not converge to 0.*

*Proof.* (i) Applying (5) recursively, we obtain that

$$\|F_{k+1}\| \leq \prod_{i=0}^k (1 + \eta_i) \|F_0\|,$$

for all  $k \geq 0$ . The proof is then completed by using Lemma 4.1.

- (ii) We know that any positive sequence  $\{a_k\}$  satisfying

$$a_{k+1} \leq (1 + r_k)a_k + r_k,$$

with  $r_k > 0$  and  $\sum_{k=0}^\infty r_k < \infty$ , is convergent by [10, Lemma 3.3]. Hence, since  $\{\|F_k\|\}$  satisfies (5) for all  $k$ , it converges.

(iii) By (15), we have that

$$(24) \quad \alpha\lambda_k\|F_k\| \leq (1 + \eta_k)\|F_k\| - \|F_{k+1}\|.$$

Using  $\lim_{k \rightarrow \infty} \eta_k = 0$  and the convergence of  $\{\|F_k\|\}$  we obtain (22).

(iv) The implication (23) directly follows from (22).

(v) If the norm decrease (14) holds for infinitely many  $k$ , there exists a subsequence  $\{\|F_{k_j}\|\}$ ,  $1 \leq k_0 < k_1 < \dots$ , such that

$$\|F_{k_j}\| \leq (1 - \alpha - \alpha\lambda_{k_j})\|F_{k_{j-1}}\| \leq (1 - \alpha)\|F_{k_{j-1}}\|,$$

whereas by (5)

$$\|F_{k_{j-1}}\| \leq (1 + \eta_{k_{j-2}})\|F_{k_{j-2}}\| \leq \prod_{i=k_{j-1}}^{k_j-2} (1 + \eta_i)\|F_{k_{j-1}}\|.$$

Thus,

$$\begin{aligned} \|F_{k_j}\| &\leq (1 - \alpha)\|F_{k_{j-1}}\| \\ &\leq (1 - \alpha) \prod_{i=k_{j-1}}^{k_j-2} (1 + \eta_i)\|F_{k_{j-1}}\| \\ &\leq (1 - \alpha)^2 \prod_{i=k_{j-1}}^{k_j-2} (1 + \eta_i)\|F_{k_{j-1}-1}\| \\ &\leq \dots \\ &\leq (1 - \alpha)^{j+1} \prod_{i=k_0}^{k_j-2} (1 + \eta_i)\|F_{k_0-1}\| \\ &\leq (1 - \alpha)^{j+1} \prod_{i=0}^{k_j-2} (1 + \eta_i)\|F_0\| \\ &\leq (1 - \alpha)^{j+1} e^\eta \|F_0\|, \end{aligned}$$

where the last inequality follows from Lemma 4.1. Hence,  $\lim_{k_j \rightarrow \infty} \|F_{k_j}\| = 0$  and the convergence of  $\{\|F_k\|\}$  implies  $\lim_{k \rightarrow \infty} \|F_k\| = 0$ .

(vi) If  $\|F_k\| \leq \|F_{k+1}\|$  for infinitely many steps, then there exists a subsequence of indices  $\{k_j\}$  such that

$$\|F_{k_j}\| \leq \|F_{k_j+1}\| \leq (1 + \eta_{k_j} - \alpha\lambda_{k_j})\|F_{k_j}\|,$$

and this gives

$$\alpha\lambda_{k_j} \leq \eta_{k_j}.$$

Since  $\lim_{k \rightarrow \infty} \eta_k = 0$ , we get  $\liminf_{k \rightarrow \infty} \lambda_k = 0$ .

(vii) In case we have that

$$\|F_k\| \leq \|F_{k+1}\| \leq (1 + \eta_k - \alpha\lambda_k)\|F_k\|,$$

for all  $k$  sufficiently large, we trivially conclude that  $\{\|F_k\|\}$  does not converge to 0. □



4.2. **Analysis of the sequence**  $\{x_k\}$ . Now we analyze the sequence of iterates generated by the PAND algorithm and make the following assumption.

**Assumption 4.1.** *Matrices  $B_k^{-1}$  are uniformly bounded for  $k \geq 0$ , i.e.  $\|B_k^{-1}\| \leq c_B$  for some positive scalar  $c_B$ .*

Assumption 4.1 immediately yields that the step  $p_k^{QN}$  in (12) satisfies

$$(25) \quad \|p_k^{QN}\| \leq c_B \|F_k\|.$$

We observe that  $B_k$  of the form (16) is guaranteed to fulfill Assumption 4.1 as  $\|B_k^{-1}\| = |\beta_k| \leq \beta_{\max}$ . We start showing that  $\{x_k\}$  is convergent.

**Theorem 4.3.** *Let Assumptions 2.1 and 4.1 hold and let  $\{x_k\}$  be the sequence generated by the PAND algorithm. Then the sequence  $\{x_k\}$  is convergent and, if  $x^*$  is the limit point, then*

$$\|x_0 - x^*\| \leq c_B \left( \frac{1}{\alpha} + \frac{\eta}{\alpha} e^\eta \right) \|F_0\|.$$

*Proof.* First note that (20) and (25) yield

$$(26) \quad \|p_k\| \leq c_B \lambda_k \|F_k\|.$$

Consider  $\sum_{k=0}^\infty \lambda_k \|F_k\|$ . Using (24) and (21), we obtain that

$$\begin{aligned} \sum_{k=0}^\infty \lambda_k \|F_k\| &\leq \sum_{k=0}^\infty \left( \frac{1 + \eta_k}{\alpha} \|F_k\| - \frac{1}{\alpha} \|F_{k+1}\| \right) \\ &= \sum_{k=0}^\infty \frac{1}{\alpha} (\|F_k\| - \|F_{k+1}\|) + \sum_{k=0}^\infty \frac{\eta_k}{\alpha} \|F_k\| \\ &\leq \frac{1}{\alpha} \|F_0\| + \sum_{k=0}^\infty \frac{\eta_k}{\alpha} e^\eta \|F_0\| \\ (27) \quad &\leq \left( \frac{1}{\alpha} + \frac{\eta}{\alpha} e^\eta \right) \|F_0\|. \end{aligned}$$

Then  $\sum_{k=0}^\infty \lambda_k \|F_k\|$  is convergent since the terms  $\lambda_k \|F_k\|$  are nonnegative. Moreover, by (26), we have that

$$(28) \quad \sum_{k=0}^\infty \|p_k\| < \infty.$$

In order to show that  $\{x_k\}$  is convergent, let  $m \geq \ell$  and consider

$$\|x_m - x_\ell\| \leq \sum_{k=\ell}^{m-1} \|p_k\| \leq \sum_{k=\ell}^\infty \|p_k\|.$$

Now,

$$\sum_{k=\ell}^\infty \|p_k\| = \sum_{k=0}^\infty \|p_k\| - \sum_{k=0}^{\ell-1} \|p_k\|$$

tends to zero as  $\ell$  tends to infinity. Consequently, for any  $\epsilon > 0$ , there exists  $\ell$  sufficiently large such that  $\|x_m - x_\ell\| \leq \epsilon$  for  $m \geq \ell$ . This means that  $\{x_k\}$  is a

Cauchy sequence and hence it converges. Finally,

$$\|x_0 - x_\ell\| \leq \sum_{k=0}^{\ell-1} \|p_k\|,$$

and letting  $\ell$  tend to infinity, we obtain that

$$\|x_0 - x^*\| \leq \sum_{k=0}^{\infty} \|p_k\| \leq c_B \sum_{k=0}^{\infty} \lambda_k \|F_k\|.$$

The desired conclusion then follows from (27). □

Assumption 4.1 has an important consequence. The bound on  $\|x_0 - x^*\|$  given above implies that if a solution  $\bar{x}$  of (1) satisfies

$$\|x_0 - \bar{x}\| > c_B \left( \frac{1}{\alpha} + \frac{\eta}{\alpha} e^\eta \right) \|F_0\|,$$

then  $\{x_k\}$  cannot converge to  $\bar{x}$ . Fortunately,  $\alpha$  is typically chosen quite small in practice [9], but this remains a drawback of PAND. An analogous result to the bound (28) was established by Li and Fukushima on the steps taken in their derivative-free Broyden-like method; see [23, Theorem 2,2]. This class of methods is therefore best suited to cases where a solution is known to exist in a reasonable neighbourhood of the initial point.

We conclude our analysis of the convergence of  $\{x_k\}$  by considering the case where the limit point of  $\{x_k\}$  solves (1) and lies in the interior of  $\Omega$ . Part of our results is obtained under the well-known Dennis-Moré condition [9] and the following assumption.

**Assumption 4.2.** *F is continuously differentiable on  $\Omega$  and the Jacobian J is Lipschitz continuous on  $\Omega$  and satisfies*

$$\|J(x) - J(y)\| \leq 2L\|x - y\|, \quad \forall x, y \in \Omega.$$

**Lemma 4.4.** *Let Assumptions 2.1, 4.1 hold, and let  $\{x_k\}$  be the sequence generated by the PAND algorithm. Suppose that the limit point  $x^*$  of  $\{x_k\}$  is such that  $x^* \in \text{int}(\Omega)$  and  $F(x^*) = 0$ . Then the following conclusions hold.*

(i) *For k sufficiently large it holds  $p_+(p_k^{\text{QN}}, 1) = p_k^{\text{QN}}$  and  $x_k + p_\pm(p_k^{\text{QN}}, \lambda) \in \text{int}(\Omega)$  for all  $\lambda \in (0, 1]$ .*

(ii) *If Assumption 4.2 holds,  $J(x^*)$  is nonsingular, and*

$$(29) \quad \lim_{k \rightarrow \infty} \frac{\|E_k p_k^{\text{QN}}\|}{\|p_k^{\text{QN}}\|} = 0,$$

*with  $E_k = B_k - J(x^*)$ , then  $\{x_k\}$  converges to  $x^*$  superlinearly.*

*Proof.* (i) Since  $x^* \in \text{int}(\Omega)$ , there exist  $\rho^* > 0$  such that  $\mathcal{B}(x^*, \rho) \subset \text{int}(\Omega)$  for  $\rho \in (0, \rho^*)$ . Since  $\{x_k\}$  converges to  $x^*$ , we know that  $x_k \in \mathcal{B}(x^*, \rho)$  for all  $k$  sufficiently large. From (25),  $\|p_k^{\text{QN}}\|$  tends to 0, and for  $k$  large enough

$$\|x^* - (x_k + p_k^{\text{QN}})\| \leq \|x^* - x_k\| + \|p_k^{\text{QN}}\| \leq \rho + \|p_k^{\text{QN}}\| < \rho^*.$$

Thus, we have that  $x_k + p_k^{\text{QN}} \in \text{int}(\Omega)$  and  $p_+(p_k^{\text{QN}}, 1) = p_k^{\text{QN}}$  by (13). Further, (19) yields that  $x_k + p_\pm \in \text{int}(\Omega)$  for all  $\lambda \in (0, 1]$ .

(ii) See [9, Chapter 8]. □

5. ENSURING THE CONVERGENCE OF  $\{\|F_k\|\}$  TO ZERO

In Theorem 4.2 we pointed out one case where the PAND algorithm solves problem (1), i.e.,  $\{\|F_k\|\}$  converges to zero. In this section we complete our theoretical analysis of the PAND algorithm by detecting further occurrences where  $\{\|F_k\|\}$  converges to zero. We address this issue considering the use of both spectral residual steps and more general quasi-Newton steps. In order to interpret the results given, it is again useful to remember that  $\alpha$  is typically quite small [9].

We start by recalling a simple observation.

**Lemma 5.1.** *Let  $f$ , defined in (2), be continuously differentiable. For  $p_k = \pm\lambda_k\beta_k F_k$ , it holds that*

$$(30) \quad f(x_{k+1}) = f(x_k) \pm 2\lambda_k\beta_k \int_0^1 F_k^T J(x_k + tp_k) F_k dt \\ \pm 2\lambda_k\beta_k \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt.$$

*Proof.* Using [9, Lemma 4.1.2], we have that

$$f(x_{k+1}) = f(x_k) + \int_0^1 \nabla f(x_k + tp_k)^T p_k dt \\ = f(x_k) \pm 2\lambda_k\beta_k \int_0^1 F(x_k + tp_k)^T J(x_k + tp_k) F_k dt,$$

from which (30) follows. □

Under specific assumptions on the Jacobian  $J$  at the limit point  $x^*$  of  $\{x_k\}$ , the next two theorems analyze the acceptance of the spectral residual steps  $p_k = \pm\lambda_k\beta_k F_k$ ,  $|\beta_k| \in (\beta_{\min}, \beta_{\max})$  for  $k$  large enough. Our first result concerns the case when  $J_S(x^*)$ , the symmetric part<sup>1</sup> of  $J(x^*)$ , is positive (negative) definite and ensures that  $\lim_{k \rightarrow \infty} \|F_k\| = 0$  when the 2-norm condition number of  $J_S(x^*)$  is of order  $O(\alpha^{-1})$ . The notation  $G_k$  is used for the ‘‘average Jacobian’’ matrix along the step  $p_k$ , defined by

$$(31) \quad G_k \stackrel{\text{def}}{=} \int_0^1 J(x_k + tp_k) dt,$$

while  $(G_S)_k$  denotes the average matrix associated to  $J_S$  along the step  $p_k$ , defined by

$$(32) \quad (G_S)_k \stackrel{\text{def}}{=} \int_0^1 J_S(x_k + tp_k) dt.$$

**Theorem 5.2.** *Let Assumptions 2.1, 4.1, 4.2 hold and let  $\{x_k\}$  be the sequence generated by the PAND algorithm with  $B_k$  given by (16). Suppose that for  $k$  sufficiently large, the steps taken have the form  $p_k = \pm\lambda_k\beta_k F_k$ ,  $|\beta_k| \in (\beta_{\min}, \beta_{\max})$ . Moreover assume that the symmetric part  $J_S$  of  $J$  is positive (negative) definite at the limit point  $x^*$  of  $\{x_k\}$ , and that the 2-norm condition number  $\kappa(J_S(x^*))$  satisfies*

$$(33) \quad \kappa(J_S(x^*)) < \frac{\gamma}{\alpha},$$

for some  $\gamma \in (0, 1)$ , and  $\alpha \in (0, 1)$  as in (14)–(15). Then  $F(x^*) = 0$ .

---

<sup>1</sup>We recall here that the symmetric part  $A_S$  of any matrix  $A$  is defined as  $A_S = (A + A^T)/2$ . It holds that  $v^T A v = v^T A_S v$  for any vector  $v$ .

*Proof.* Without loss of generality, let us assume that  $J_S(x^*)$  is positive definite. Then  $J(x^*)$  is nonsingular and by (10) and (31) we get

$$\begin{aligned} \beta_k &= \frac{\|p_{k-1}\|^2}{p_{k-1}^T(F_k - F_{k-1})} = \frac{\|p_{k-1}\|^2}{p_{k-1}^T \int_0^1 J(x_{k-1} + tp_{k-1})p_{k-1} dt} \\ &= \frac{\|p_{k-1}\|^2}{p_{k-1}^T \int_0^1 J_S(x_{k-1} + tp_{k-1})p_{k-1} dt}, \end{aligned}$$

i.e., by (32)

$$\beta_k = \frac{\|p_{k-1}\|^2}{p_{k-1}^T (G_S)_{k-1} p_{k-1}}.$$

Moreover, since  $F_k^T G_k F_k = F_k^T (G_S)_k F_k$ , using Lemma 5.1, we have that

$$\begin{aligned} (34) \quad f(x_{k+1}) &= f(x_k) \pm 2\lambda_k \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} f(x_k) \\ &\quad \pm 2\lambda_k \beta_k \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt. \end{aligned}$$

Now, continuity implies that there exists a scalar  $\rho > 0$  sufficiently small such that, for all  $y \in \mathcal{B}(x^*, \rho)$ ,

$$(35) \quad \sigma_{\min}(J_S(y)) \geq (1 - \epsilon)\sigma_{\min}(J_S(x^*)) \text{ and } \sigma_{\max}(J_S(y)) \leq (1 + \epsilon)\sigma_{\max}(J_S(x^*))$$

and

$$(36) \quad \sigma_{\max}(J(y)) \leq (1 + \epsilon)\sigma_{\max}(J(x^*)),$$

with  $\epsilon \in (0, 1)$  given by

$$(37) \quad \epsilon \stackrel{\text{def}}{=} \frac{1 - \gamma}{1 + \gamma}.$$

Moreover, the convergence of the sequence  $\{x_k\}$  implies that  $x_{k-1} + tp_{k-1}$  and  $x_k + tp_k$  both belong to  $\mathcal{B}(x^*, \rho)$  for large enough  $k$  and all  $t \in [0, 1]$ . As a consequence, we deduce that, for  $k$  sufficiently large,

$$(38) \quad \min[\sigma_{\min}((G_S)_k), \sigma_{\min}((G_S)_{k-1})] \geq (1 - \epsilon)\sigma_{\min}(J_S(x^*))$$

and

$$(39) \quad \max[\sigma_{\max}((G_S)_k), \sigma_{\max}((G_S)_{k-1})] \leq (1 + \epsilon)\sigma_{\max}(J_S(x^*)).$$

This in turn implies that, for  $k$  sufficiently large,  $\beta_k > 0$  lies in the interval

$$(40) \quad \beta_k \in \left[ \frac{1}{\sigma_{\max}((G_S)_{k-1})}, \frac{1}{\sigma_{\min}((G_S)_{k-1})} \right],$$

and that

$$\begin{aligned} \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} &\in \left[ \frac{\sigma_{\min}((G_S)_k)}{\sigma_{\max}((G_S)_{k-1})}, \frac{\sigma_{\max}((G_S)_k)}{\sigma_{\min}((G_S)_{k-1})} \right] \\ &\subseteq \left[ \frac{1 - \epsilon}{1 + \epsilon} \left( \frac{\sigma_{\min}(J_S(x^*))}{\sigma_{\max}(J_S(x^*))} \right), \frac{1 + \epsilon}{1 - \epsilon} \left( \frac{\sigma_{\max}(J_S(x^*))}{\sigma_{\min}(J_S(x^*))} \right) \right], \end{aligned}$$

which yields

$$(41) \quad \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} \geq \frac{\gamma}{\kappa(J_S(x^*))}.$$

Consider  $p_k = -\lambda_k \beta_k F_k$ . The inequality (34) implies that

$$(42) \quad f(x_{k+1}) \leq f(x_k) - 2\lambda_k \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} f(x_k) + 2\lambda_k \beta_k \left| \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt \right|,$$

in which the last absolute value can be written as

$$\left| \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt \right| = \left| \int_0^1 \left( \int_0^1 J(x_k + \zeta tp_k) tp_k d\zeta \right) J(x_k + tp_k) F_k dt \right|,$$

$\zeta \in [0, 1]$ . Again  $x_k + \zeta tp_k \in \mathcal{B}(x^*, \rho)$  for  $t, \zeta \in [0, 1]$ . Thus, proceeding as above and using the form  $p_k = -\lambda_k \beta_k F_k$ , we deduce that

$$(43) \quad \left| \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt \right| \leq \int_0^1 t \lambda_k |\beta_k| \max_{z \in \mathcal{B}(x^*, \rho)} \|J(z)\|^2 \|F_k\|^2 dt = \frac{1}{2} \lambda_k |\beta_k| \max_{z \in \mathcal{B}(x^*, \rho)} \sigma_{\max}(J(z))^2 \|F_k\|^2.$$

Combining this expression with (41), (42), (40), (35), (36) and (37) we obtain that, for  $k$  sufficiently large,

$$f(x_{k+1}) \leq \left( 1 - 2\lambda_k \beta_k \frac{F_k^T (G_S)_k F_k}{\|F_k\|^2} + \lambda_k^2 \beta_k^2 \max_{z \in \mathcal{B}(x^*, \rho)} \sigma_{\max}(J(z))^2 \right) f(x_k) \leq \left( 1 - 2 \frac{\gamma}{\kappa(J_S(x^*))} \lambda_k + \frac{1}{\gamma^2} \left[ \frac{\sigma_{\max}(J(x^*))}{\sigma_{\min}(J_S(x^*))} \right]^2 \lambda_k^2 \right) f(x_k).$$

Thus, for  $k$  sufficiently large, the linesearch condition (15) holds for any  $\lambda$  such that

$$1 - \frac{2\gamma}{\kappa(J(x^*))} \lambda + \frac{1}{\gamma^2} \left[ \frac{\sigma_{\max}(J(x^*))}{\sigma_{\min}(J_S(x^*))} \right]^2 \lambda^2 \leq (1 - \alpha \lambda)^2,$$

i.e., such that

$$(44) \quad \kappa_2 \lambda^2 + 2\kappa_1 \lambda \stackrel{\text{def}}{=} \left( \frac{1}{\gamma^2} \left[ \frac{\sigma_{\max}(J(x^*))}{\sigma_{\min}(J_S(x^*))} \right]^2 - \alpha^2 \right) \lambda^2 + 2 \left( \alpha - \frac{\gamma}{\kappa(J(x^*))} \right) \lambda \leq 0.$$

By definition of  $J_S$ ,  $\|J_S(x^*)\| \leq \|J(x^*)\|$ . Then,

$$\frac{\sigma_{\max}(J(x^*))}{\sigma_{\min}(J_S(x^*))} \geq \kappa(J_S(x^*)),$$

and  $\kappa_2 > 0$  since  $\alpha$  and  $\gamma$  belong to  $(0, 1)$ . This implies that (44) is satisfied for a sufficiently small and positive  $\lambda$ , since (33) gives  $\kappa_1 < 0$  and (15) is satisfied (for  $k$  large enough) if  $\lambda \leq \lambda_* \stackrel{\text{def}}{=} -2\kappa_1/\kappa_2$ . The mechanism of Step 3.6 of the PAND algorithm then guarantees that, for  $k$  sufficiently large, the loop in Step 3 terminates with  $\lambda_k \geq \min\{1, \sigma \lambda_*\}$ , and  $\lambda_*$  independent of  $k$ . As a consequence,  $\liminf_{k \rightarrow \infty} \lambda_k > 0$  and (23) allows us to conclude the proof.  $\square$

Convergence of  $\{\|F_k\|\}$  to zero was also obtained in [22] by assuming the positive (negative) definiteness of  $J_S$  for all  $x$  in the lower level set  $\{x : 0 \leq f(x) \leq f(x_0)\}$ .

In the next theorem, we analyze the acceptance of the spectral residual step under the assumption that  $J$  is strongly diagonally dominant and the diagonal entries have constant sign. We use the following notation:

$$(45) \quad \zeta_i(x) \stackrel{\text{def}}{=} \frac{1}{|(J(x))_{ii}|} \sum_{\substack{j=1 \\ j \neq i}}^n |(J(x))_{ij}|, \quad i = 1, \dots, n,$$

$$(46) \quad m(x) \stackrel{\text{def}}{=} \min_{1 \leq i \leq n} (J(x))_{ii}, \quad M(x) \stackrel{\text{def}}{=} \max_{1 \leq i \leq n} (J(x))_{ii},$$

$$(47) \quad \tilde{m}(x) \stackrel{\text{def}}{=} \min_{1 \leq i \leq n} |(J(x))_{ii}|, \quad \widetilde{M}(x) \stackrel{\text{def}}{=} \max_{1 \leq i \leq n} |(J(x))_{ii}|.$$

Observe that all of these quantities only depend on the Jacobian matrix at  $x$ . The value of  $\zeta_i(x)$  measures the degree of diagonal dominance of the  $i$ th row of  $J(x)$ ,  $m(x)$  and  $M(x)$  measure the signed range of its diagonal elements while  $\tilde{m}(x)$  and  $\widetilde{M}(x)$  measure the diagonals' absolute values' range. If  $J(x)$  has positive diagonal entries, then  $\tilde{m}(x) = m(x) = |m(x)|$  and  $\widetilde{M}(x) = M(x) = |M(x)|$ . If the diagonal elements are negative, then  $\tilde{m}(x) = -M(x) = |M(x)|$  and  $\widetilde{M}(x) = -m(x) = |m(x)|$ . The conditions used are

$$(48) \quad \max \left[ \frac{\widetilde{M}(x^*)}{|m(x^*)|}, \frac{\widetilde{M}(x^*)}{|M(x^*)|} \right] \sum_{i=1}^n \zeta_i(x^*) \leq \frac{1 - \nu}{1 + \nu}$$

and

$$(49) \quad \frac{\widetilde{M}(x^*)}{\tilde{m}(x^*)} < \left( \frac{\nu}{2 - \nu} \right) \left( \frac{1 - \nu}{1 + \nu} \right) \frac{1}{\alpha},$$

where  $\nu \in (0, 1)$  and  $\alpha \in (0, 1)$  is the constant in (14)–(15). Such conditions are satisfied by matrices which are close to being diagonal and have a condition number of order  $\alpha^{-1}$ . In fact, for decreasing values of  $\max_{1 \leq i \leq n} \zeta_i$ , the ratio  $\widetilde{M}/\tilde{m}$  approaches  $\kappa(J(x^*))$  and (49) implies a bound on such a condition number in terms of  $\alpha^{-1}$ . For example, if  $\nu = 1/2$ , the right-hand side of (48) is  $1/3$  and that of (49) is  $1/(9\alpha)$ .

**Theorem 5.3.** *Let Assumptions 2.1, 4.1, 4.2 hold and let  $\{x_k\}$  be the sequence generated by the PAND algorithm with  $B_k$  given by (16). Suppose that for  $k$  sufficiently large, the steps taken have the form  $p_k = \pm \lambda_k \beta_k F_k$ ,  $|\beta_k| \in (\beta_{\min}, \beta_{\max})$ , and that  $J(x^*)$  is nonsingular, where  $x^*$  is the limit point of  $\{x_k\}$ . Suppose in addition that  $J(x^*)$  has diagonal entries of constant sign and satisfies (48) and (49), for some  $\nu \in (0, 1)$  and  $\alpha \in (0, 1)$  being the constant in (14)–(15). Then  $F(x^*) = 0$ .*

*Proof.* Because  $J(x)$  is continuous, there exists a  $\rho > 0$  such that

$$(50) \quad \max \left[ \frac{\widetilde{M}(x)}{|m(x)|}, \frac{\widetilde{M}(x)}{|M(x)|} \right] \sum_{i=1}^n \zeta_i(x) < 1 - \nu$$

and

$$\widetilde{M}(x) \leq (1 + \nu)\widetilde{M}(x^*) \quad \text{and} \quad \tilde{m}(x) \geq (1 - \nu)\tilde{m}(x^*),$$

for all  $x \in \mathcal{B}(x^*, \rho)$ . Moreover, for  $k$  sufficiently large  $x_{k-1}$  and  $x_k$  belong to  $\mathcal{B}(x^*, \rho)$  and the same holds for  $x_k + tp_k$ ,  $x_{k-1} + tp_{k-1}$ ,  $t \in [0, 1]$ . Hence (50)

holds for  $J(x_k)$  and  $J(x_k + tp_k)$  for all  $k$  sufficiently large and all  $t \in [0, 1]$ . As a consequence, we obtain that, for sufficiently large  $k$ ,

$$(51) \quad \max \left[ \frac{\widetilde{M}_k}{|m_k|}, \frac{\widetilde{M}_k}{|M_k|} \right] \sum_{i=1}^n \zeta_{i,k} \leq 1 - \nu$$

and

$$\widetilde{M}_k \leq (1 + \nu)\widetilde{M}(x^*) \text{ and } \widetilde{m}_k \geq (1 - \nu)\widetilde{m}(x^*),$$

where  $\zeta_{i,k}$ ,  $M_k$ ,  $m_k$ ,  $\widetilde{m}_k$  and  $\widetilde{M}_k$  are defined as in (45)–(47) using the average Jacobian  $G_k$  instead of  $J(x)$ .

As in the previous theorem, the steps used have the form  $p_k = \pm \lambda_k \beta_k F_k$  and we analyze (30). As for  $F_k^T G_k F_k$ ,  $t \in [0, 1]$ , with  $G_k$  as in (31), we have that

$$F_k^T G_k F_k = \sum_{i=1}^n (F_k)_i \left[ (G_k)_{ii}(F_k)_i + \sum_{\substack{j=1 \\ j \neq i}}^n (G_k)_{ij}(F_k)_j \right].$$

Then, for  $i$  fixed,

$$\begin{aligned} (G_k)_{ii}(F_k)_i^2 + \sum_{\substack{j=1 \\ j \neq i}}^n (G_k)_{ij}(F_k)_i(F_k)_j &\geq (G_k)_{ii}(F_k)_i^2 - \sum_{\substack{j=1 \\ j \neq i}}^n |(G_k)_{ij}| |(F_k)_i| |(F_k)_j| \\ &\geq (G_k)_{ii}(F_k)_i^2 - \sum_{\substack{j=1 \\ j \neq i}}^n |(G_k)_{ij}| \|F_k\|_\infty^2 \\ &\geq (G_k)_{ii}(F_k)_i^2 - \zeta_{i,k} |(G_k)_{ii}| \|F_k\|^2. \end{aligned}$$

The entries of  $(G_k)_{ii}$  are of constant sign. If they are positive, by using (51) we obtain that, for  $k$  large enough,

$$F_k^T G_k F_k \geq m_k \left( 1 - \sum_{i=1}^n \zeta_{i,k} \frac{\widetilde{M}_k}{|m_k|} \right) \|F_k\|^2 \geq m_k \nu \|F_k\|^2.$$

Similarly, for  $k$  large enough, we have

$$\begin{aligned} (G_k)_{ii}(F_k)_i^2 + \sum_{\substack{j=1 \\ j \neq i}}^n (G_k)_{ij}(F_k)_i(F_k)_j &\leq (G_k)_{ii}(F_k)_i^2 + \sum_{\substack{j=1 \\ j \neq i}}^n |(G_k)_{ij}| |(F_k)_i| |(F_k)_j| \\ &\leq (G_k)_{ii}(F_k)_i^2 + \zeta_{i,k} |(G_k)_{ii}| \|F_k\|^2 \end{aligned}$$

and

$$F_k^T G_k F_k \leq M_k \left( 1 + \sum_{i=1}^n \zeta_{i,k} \frac{\widetilde{M}_k}{|M_k|} \right) \leq M_k (2 - \nu) \|F_k\|^2,$$

where the last inequality again follows from (51). Proceeding analogously when the entries of  $(G_k)_{ii}$  are negative, we have

$$m_k (2 - \nu) \|F_k\|^2 \leq F_k^T G_k F_k \leq M_k \nu \|F_k\|^2.$$

Hence, for sufficiently large  $k$  the scalars  $F_k^T G_k F_k$  have constant sign and

$$(52) \quad |F_k^T G_k F_k| \geq \nu \widetilde{m}_k \|F_k\|^2 \geq (1 - \nu) \nu \widetilde{m}(x^*) \|F_k\|^2.$$

Moreover,

$$\beta_k = \frac{\|p_{k-1}\|^2}{p_{k-1}^T(F_k - F_{k-1})} = \frac{\|p_{k-1}\|^2}{p_{k-1}^T \int_0^1 J(x_{k-1} + tp_{k-1})p_{k-1} dt} = \frac{\|p_{k-1}\|^2}{p_{k-1}^T G_{k-1} p_{k-1}}.$$

Thus, using similar arguments, for  $k$  large enough the scalars  $\beta_k$  have the same sign as  $F_k^T G_k F_k$ , and

$$(53) \quad |\beta_k| \in \left[ \frac{1}{(2-\nu)\widetilde{M}_{k-1}}, \frac{1}{\nu\widetilde{m}_{k-1}} \right] \subseteq \left[ \frac{1}{(1+\nu)(2-\nu)\widetilde{M}(x^*)}, \frac{1}{(1-\nu)\nu\widetilde{m}(x^*)} \right].$$

Consequently,

$$(54) \quad \beta_k F_k^T G_k F_k = |\beta_k F_k^T G_k F_k| \geq \left( \frac{\nu}{2-\nu} \right) \frac{(1-\nu)\widetilde{m}(x^*)}{(1+\nu)\widetilde{M}(x^*)} \|F_k\|^2,$$

for  $k$  large enough. Now, without loss of generality, consider  $p_k = -\lambda_k \beta_k F_k$ . Lemma 5.1 then gives that

$$(55) \quad f(x_{k+1}) \leq f_k - 2\lambda_k \beta_k F_k^T G_k F_k + 2\lambda_k |\beta_k| \left| \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt \right|,$$

and the last absolute value above satisfies (43). Denoting the diagonal and off diagonal part of a matrix as  $\text{diag}(\cdot)$  and  $\text{off}(\cdot)$ , respectively, and using  $\|J(z)\| \leq \|\text{diag}(J(z))\| + \|\text{off}(J(z))\|$  we obtain that

$$\|J(z)\| \leq \widetilde{M}(z) + \sqrt{n}\|\text{off}(J(z))\|_\infty \leq \widetilde{M}(z) \left( 1 + \sqrt{n} \max_{1 \leq i \leq n} \zeta_i(z) \right).$$

Using this bound, (43), (53) and the fact that (50) implies that  $\zeta_i(z) \leq 1$  in  $\mathcal{B}(x^*, \rho)$ , we deduce that, for  $k$  large enough,

$$\begin{aligned} & \left| \int_0^1 (F(x_k + tp_k) - F_k)^T J(x_k + tp_k) F_k dt \right| \\ & \leq \frac{1}{2} \lambda_k |\beta_k| \max_{z \in \mathcal{B}(x^*, \rho)} \|J(z)\|^2 \|F_k\|^2 \\ & \leq \frac{1}{2} \lambda_k |\beta_k| \|F_k\|^2 \max_{z \in \mathcal{B}(x^*, \rho)} \left[ \widetilde{M}(z) \left( 1 + \sqrt{n} \max_{1 \leq i \leq n} \zeta_i(z) \right) \right]^2 \\ & \leq \frac{(1 + \sqrt{n})^2}{2\nu} \frac{((1 + \nu)\widetilde{M}(x^*))^2}{(1 - \nu)\widetilde{m}(x^*)} \lambda_k \|F_k\|^2. \end{aligned}$$

This bound, (55) and (53) then imply that

$$\begin{aligned} f(x_{k+1}) \leq & \left[ 1 - \left( \frac{2\nu}{2-\nu} \right) \frac{(1-\nu)\widetilde{m}(x^*)}{(1+\nu)\widetilde{M}(x^*)} \lambda_k \right. \\ & \left. + \frac{(1 + \sqrt{n})^2}{\nu^2} \frac{((1 + \nu)\widetilde{M}(x^*))^2}{(1 - \nu)^2 \widetilde{m}(x^*)^2} \lambda_k^2 \right] f(x_k). \end{aligned}$$

The linesearch condition (15) thus holds for  $k$  large enough and for any  $\lambda$  such that

$$1 - \left( \frac{2\nu}{2-\nu} \right) \frac{(1-\nu)\widetilde{m}(x^*)}{(1+\nu)\widetilde{M}(x^*)} \lambda + \frac{(1 + \sqrt{n})^2}{\nu^2} \frac{(1 + \nu)^2 \widetilde{M}(x^*)^2}{(1 - \nu)^2 \widetilde{m}(x^*)^2} \lambda^2 \leq (1 - \alpha\lambda)^2,$$



that is, such that

$$(56) \quad \left( \frac{(1+\sqrt{n})^2}{\nu^2} \frac{(1+\nu)^2 \widetilde{M}(x^*)^2}{(1-\nu)^2 \widetilde{m}(x^*)^2} - \alpha^2 \right) \lambda^2 + 2 \left( \alpha - \left( \frac{\nu}{2-\nu} \right) \frac{(1-\nu) \widetilde{m}(x^*)}{(1+\nu) \widetilde{M}(x^*)} \right) \lambda \leq 0.$$

Again,

$$\kappa_2 \stackrel{\text{def}}{=} \frac{(1+\sqrt{n})^2}{\nu^2} \frac{(1+\nu)^2 \widetilde{M}(x^*)^2}{(1-\nu)^2 \widetilde{m}(x^*)^2} - \alpha^2 > 0,$$

by (47) and the fact that  $\alpha$  and  $\nu$  belong to  $(0, 1)$ , and

$$\kappa_1 \stackrel{\text{def}}{=} \alpha - \left( \frac{\nu}{2-\nu} \right) \frac{(1-\nu) \widetilde{m}(x^*)}{(1+\nu) \widetilde{M}(x^*)} < 0$$

by (49). Thus (15) holds for  $\lambda \leq \lambda_* \stackrel{\text{def}}{=} -2\kappa_1/\kappa_2$  and all  $k$  sufficiently large,  $\liminf_{k \rightarrow \infty} \lambda_k \geq \min[1, \sigma \lambda_*] > 0$  and (23) finally allows us to deduce that  $F(x^*) = 0$ . □

We conclude our investigation of some cases where the PAND algorithm can be proved to converge to a solution by showing that  $\{\|F_k\|\}$  converges to zero if the limit point  $x^*$  lies in the interior of  $\Omega$  and the step  $p_k^{\text{QN}}$  in (12) is, eventually, an inexact Newton step.

**Theorem 5.4.** *Let Assumptions 2.1, 4.1 and 4.2 hold and  $\{x_k\}$  be generated by the PAND algorithm. If the limit point  $x^*$  of  $\{x_k\}$  is such that  $x^* \in \text{int}(\Omega)$  and the step  $p_k^{\text{QN}}$  in (12) satisfies*

$$(57) \quad \|J_k p_k^{\text{QN}} + F_k\| = \tau_k \|F_k\|, \quad \tau_k \leq \tau_{\max} < 1 - \alpha,$$

for all  $k$  sufficiently large, then  $\lim_{k \rightarrow \infty} \|F_k\| = 0$ .

*Proof.* Let  $\rho^* > 0$  and  $\rho \in (0, \rho^*)$  such that  $\mathcal{B}(x^*, \rho) \subset \text{int}(\Omega)$ . Since  $\{x_k\}$  converges to  $x^*$ , we have  $x_k \in \mathcal{B}(x^*, \frac{\rho}{2})$  for all  $k$  sufficiently large. Suppose  $k$  is large enough so that  $x_k \in \mathcal{B}(x^*, \frac{\rho}{2})$ . Then, possibly for  $\lambda$  small enough,  $P(x_k + \lambda p_k^{\text{QN}}) - x_k = \lambda p_k^{\text{QN}}$ , i.e.,  $x_k + \lambda p_k^{\text{QN}}$  belongs to the interior of  $\Omega$ . In particular, if  $\|\lambda p_k^{\text{QN}}\| = \frac{\rho}{2}$ , then  $x_k + \lambda p_k^{\text{QN}} \in \mathcal{B}(x^*, \rho)$ . By using (21) and (25), and setting  $\underline{\lambda} = \frac{\rho}{2c_B e^{\eta} \|F_0\|}$ , independent of  $k$ , we get that equation  $\|\lambda p_k^{\text{QN}}\| = \frac{\rho}{2}$  is satisfied for some  $\lambda \geq \underline{\lambda}$ ; namely,  $x_k + \lambda p_k^{\text{QN}}$  belongs to the interior of  $\Omega$  for some  $\lambda$  uniformly bounded away from zero.

Now we show that  $\lambda p_k^{\text{QN}}$  satisfies (15) for some  $\lambda$  uniformly bounded away from zero, which implies our claim. Since Assumption 4.2 holds, we know that

$$\begin{aligned} F(x_k + \lambda p_k^{\text{QN}}) &= F(x_k) + \int_0^1 J(x_k + t \lambda p_k^{\text{QN}}) \lambda p_k^{\text{QN}} dt \\ &= (1 - \lambda) F(x_k) + \lambda (J(x_k) p_k^{\text{QN}} + F(x_k)) \\ &\quad + \int_0^1 (J(x_k + t \lambda p_k^{\text{QN}}) - J(x_k)) \lambda p_k^{\text{QN}} dt; \end{aligned}$$

see [9, Lemma 4.1.9]. Hence, using (57) and the bounds (25) and (21) we obtain

$$\begin{aligned} \|F(x_k + \lambda p_k^{\text{QN}})\| &\leq (1 - \lambda)\|F_k\| + \lambda\tau_k\|F_k\| + L\lambda^2\|p_k^{\text{QN}}\|^2 \\ &\leq (1 - \lambda + \lambda\tau_{\max})\|F_k\| + L\lambda^2 c_B^2 \|F_k\|^2 \\ &\leq (1 - \lambda + \lambda\tau_{\max} + L\lambda^2 c_B^2 e^\eta \|F_0\|)\|F_k\|. \end{aligned}$$

Now observe that if

$$1 - \lambda + \lambda\tau_{\max} + L\lambda^2 c_B^2 e^\eta \|F_0\| \leq 1 - \alpha\lambda,$$

then (15) is satisfied and the step is accepted. In particular, if

$$\lambda \leq \lambda_* \stackrel{\text{def}}{=} \frac{1 - \alpha - \tau_{\max}}{L c_B^2 e^\eta \|F_0\|},$$

then (15) is fulfilled for all  $k$  sufficiently large. Now, considering Step 3.6 of PAND algorithm, we conclude that the repeat-loop at Step 3 terminates with  $\lambda \geq \min\{1, \sigma\lambda_*\}$ ,  $\lambda_*$  independent of  $k$ . Combining this bound with  $\lambda \geq \underline{\lambda}$ , we get  $\liminf_{k \rightarrow \infty} \lambda_k > 0$  and (23) implies  $\lim_{k \rightarrow \infty} \|F_k\| = 0$ .  $\square$

## 6. NUMERICAL EXPERIMENTS

In this section we present the results of some numerical experiments conducted with different implementations of the PAND algorithm. Our goal is to test its behaviour in terms of robustness and computational cost and to compare it with PSANE [20].

**6.1. The problem sets.** We considered two sets of problems: the first comprises small and medium-size smooth nonlinear systems with box constraints from a variety of applications; the second is made of semismooth systems with nonnegative constraints which reformulate well-known nonlinear complementarity problems from the literature.

**6.1.1. Bound-constrained nonlinear systems.** We selected 14 constrained nonlinear systems listed in Table 1 along with their description and dimension. The convex set  $\Omega$  in (1) is the  $n$ -dimensional box  $\{x \in \mathbb{R}^n \text{ s.t. } l \leq x \leq u\}$ , where  $l \in (\mathbb{R} \cup -\infty)^n$ ,  $u \in (\mathbb{R} \cup \infty)^n$ , and the inequalities are meant componentwise. Therefore, the projection map is given by  $P(x) = \max[l, \min[x, u]]$ .

The first 8 problems have been frequently used as a test set and are fully described in [14]; their dimension is small. The remaining problems have variable dimension and their Jacobian matrices cannot be formed at a low computational cost by finite difference procedures for sparse matrices such as [8]. Hence, computing  $B_k = J(x_k)$  by finite differences is expensive and solving (12) with such  $B_k$ 's cannot take advantage of sparse/structured linear algebra solvers. As for the definition of  $\Omega$ , it is the positive orthant for problem 9;  $l = (0, \dots, 0)^T$ ,  $u = (10, \dots, 10)^T$  in problems 10, 11 and 14;  $l = (5, \dots, 5)^T$ ,  $u = (15, \dots, 15)^T$  in problem 12,  $l = (-10, \dots, -10)^T$ ,  $u = (0, \dots, 0)^T$  in problem 13.

All problems were run starting from three different initial guesses  $x_0$  given by

$$(x_0)_i = \begin{cases} l_i + \gamma(u_i - l_i)/2 & \text{if } l_i > -\infty \text{ and } u_i < \infty, & \gamma = 1, 2, 3, \\ l_i + \gamma 10^\gamma & \text{if } l_i > -\infty \text{ and } u_i = \infty, & \gamma = 0, 1, 2. \end{cases}$$

TABLE 1. Bound-constrained nonlinear system.

Pb#	Name and Source	$n$
1	Himmelblau function [14, 14.1.1]	2
2	Equilibrium Combustion [14, 14.1.2]	5
3	Bullard-Biegler system [14, 14.1.3]	2
4	Ferraris-Tronconi system [14, 14.1.4]	2
5	Brown’s almost linear system [14, 14.1.5]	5
6	Robot kinematics problem [14, 14.1.6]	8
7	Series of CSTRs, $R = .945$ [14, 14.1.8]	2
8	Series of CSTRs, $R = .990$ [14, 14.1.8]	2
9	Chandrasekar’s H-equation, $c = 0.9999$ [23, Problem 6]	1000
10	Problem 74 [25]	1000
11	Problem 77 [25]	2000
12	Trigonometric function [22, Test 8]	2000
13	Function 15 [22, Problem 15]	2000
14	Zero Jacobian function [22, Problem 19]	2000

TABLE 2. Nonlinear complementarity problems.

Pb#	Name and Source	$n$
15	Kojima-Shindo’s problem [11]	3
16	Josephy’s problem [11]	4
17	Mathiensen’s problem[11]	4
18	Harker’s Nash-Cournot-5 problem [18]	5
19	Harker’s Nash-Cournot-10 problem [18]	10
20	Pang and Murphy’s Nash-Cournot-5 problem [28]	5
21	Pang and Murphy’s Nash-Cournot-10 problem [28]	10

6.1.2. *Nonlinear complementarity problems.* We consider the nonlinear complementarity problems listed in Table 4 and defined as

$$G(x)^T x = 0, \quad x \geq 0, \quad G(x) \geq 0,$$

where  $G : \mathbb{R}^n \rightarrow \mathbb{R}^n$  is continuous differentiable. Following [20], we solved the following nonlinear systems with nonnegative constraints

$$F(x) = \min[x, G(x)] = 0, \quad x \in \Omega,$$

where  $\Omega$  is the positive orthant and the function  $F$  is continuous but not everywhere differentiable. All runs were started using  $x_0 = 10^\gamma$  with  $\gamma = 0, 1, 2$ .

**6.2. Implementation issues and numerical results.** All the tested algorithms have been implemented in MATLAB and run using MATLAB R2015A version on an Intel(R) Core(TM) i5-6600K CPU @3.50 GHz x 4, 16.0 GB RAM.

The main implementation issues are as follows. Two rules for choosing matrices  $B_k$  were implemented. The former corresponds to the choice made in PSANE, i.e.  $B_k = \beta_k^{-1}I$  with  $\beta_k$  given in (10), and the resulting implementation is named PAND-SR (PAND algorithm with Spectral Residual step). The latter consists in starting from a given  $B_0$  and generating matrices  $B_k$  by using the Broyden’s formula

$$(58) \quad B_{k+1} = B_k + \frac{(y_k - B_k p_k) p_k^T}{p_k^T p_k},$$

where  $y_k = F(x_{k+1}) - F(x_k)$ ; see [6]. The resulting implementation is named PAND-BR (PAND algorithm with Broyden step).

In order to perform a fully derivative-free implementation of PAND-BR, our default choice for  $B_0$  was the identity matrix. The current matrix  $B_k$  was refreshed and set equal to the identity matrix every 30 iterations and whenever  $\|v_k^{QN}\| = 0$ , with  $v_k^{QN}$  defined in (17).

The linear systems (12) arising in PAND-BR were solved via QR factorizations. Specifically, given the QR factorization of  $B_k$ , the QR factorization of  $B_{k+1}$  was formed by the rank one update (58) using the MATLAB function `qrupdate`.

The parameters used in PAND-SR and PAND-BR were set equal to those declared in PSANE, i.e.  $\beta_{\min} = 10^{-30}$ ,  $\beta_{\max} = 10^{30}$ ,  $\beta_0 = 1$ ,  $\alpha = 10^{-4}$ ,  $\sigma = 0.5$ ,  $\eta_k = 0.99^k(100 + \|F(x_0)\|^2)$ ,  $k \geq 0$ . This allows comparing PAND-SR, PAND-BR and PSANE in terms of their distinctive features, i.e. definition of the search directions and linesearch strategy. Following [20], PSANE was tested using  $\lambda_{\max} = 1$ , and  $\lambda = \lambda_{\max}$  in Step 3 of Algorithm 2.1.

Tables 3 and 4 collect the results obtained with PSANE, PAND-SR and PAND-BR. The problem number refers to Tables 1 and 2 and the scalar  $\gamma$  is associated to the starting point. We report the number of iterations (**It**) and  $F$ -evaluations (**Fe**) performed on successful runs, i.e., runs where the criterion

$$(59) \quad \|F_k\| \leq 10^{-6},$$

was met within a maximum number of iterations (**maxIt**) and function evaluation (**maxFe**) both equal to  $10^5$  as in [20]. For the remaining runs, we eventually stopped the iterations on the base of the behaviour of  $\lambda_k$  and  $\|F_k\|$ : the symbol  $F_\lambda$  indicates that  $\lambda$  has been reduced 40 times by a factor  $\sigma$  in the linesearch strategy; the symbol  $F_i$  indicates that

$$\|F_{k+1}\| > (1 - \alpha)\|F_k\|,$$

occurred for 50 iterations consecutively, i.e., repeatedly  $\|F_k\|$  either increased or slightly decreased. We remark that the occurrences  $F_\lambda$  and  $F_i$  are suggested by the convergence properties of the PAND algorithm presented in Theorem 4.2. For large values of  $k$ , the first occurrence may indicate that  $\{\lambda_k\}$  is converging to zero while the second occurrence may indicate that  $\{\|F_k\|\}$  does not converge to zero. Breakdowns in PSANE, described in §2, are denoted as  $F_b$ .

The reported results show that on a total of 63 tests, PSANE and PAND-SR fail 22 and 9 times, respectively, while PAND-BR solves all the tests. Most of the failures in PSANE are due to a breakdown ( $F_b$ ); on successful runs the performance of PSANE is quite similar to that of PAND-SR algorithm. In several runs where PAND-SR is successful, its computational cost is comparable to that of PAND-BR procedure in terms of  $F$ -evaluations, but the former is more efficient as it does not require forming and solving linear systems. This fact is shown in Table 5 where we report the CPU times of the methods under analysis on problems with dimension larger than or equal to 1000. On the other hand, the version of PAND based on Broyden matrices is more robust as it allows us to avoid failures of the spectral residual procedures on problems 2, 6 and 17.

Finally, Figure 1 shows the nonmonotone behaviour of  $\|F_k\|$  observed in two runs performed and is representative of the tests presented.

TABLE 3. Computational results obtained with PSANE, PAND-SR and PAND-BR algorithms on bound-constrained nonlinear systems

Pb#	$\gamma$	PSANE		PAND-SR		PAND-BR	
		It	Fe	It	Fe	It	Fe
1	1	11	14	12	15	14	18
	2	11	18	12	16	11	14
	3	14	25	17	23	14	20
2	1	$F_\lambda$		$F_\lambda$		284	433
	2	$F_\lambda$		$F_\lambda$		54	80
	3	$F_\lambda$		$F_\lambda$		119	180
3	1	$F_b$		26	41	14	19
	2	$F_b$		192	319	58	88
	3	$F_b$		1090	1817	1581	2568
4	1	25	26	27	46	10	12
	2	31	32	24	42	106	164
	3	$F_b$		23	39	28	39
5	1	26	27	26	34	13	15
	2	26	27	26	35	12	15
	2.5	19	22	26	35	11	13
6	1	$F_i$		$F_i$		144	234
	2	$F_\lambda$		$F_i$		46	69
	3	$F_b$		$F_i$		44	62
7	1	$F_b$		642	2427	51	79
	2	$F_\lambda$		430	849	546	1316
	3	$F_b$		825	1426	659	1098
8	1	13	14	9	13	6	9
	2	12	14	12	16	7	10
	3	11	13	11	14	8	11
9	0	30	31	30	41	13	14
	1	60	61	122	192	15	16
	2	37	38	37	50	15	16
10	1	14	15	14	16	13	14
	2	20	25	18	24	43	50
	3	29	31	15	19	16	19
11	1	$F_b$		8	11	34	61
	2	$F_b$		7	10	15	19
	3	$F_b$		6	9	16	20
12	1	92	99	21	24	2937	6911
	2	56	59	24	27	2736	6506
	3	372	645	29	35	1728	4858
13	1	115	116	243	375	418	596
	2	511	521	447	745	497	711
	3	71	72	221	356	412	586
14	1	$F_b$		19	22	2	4
	2	$F_b$		20	23	2	4
	3	$F_b$		20	23	2	4

TABLE 4. Computational results obtained with PSANE, PAND-SR and PAND-BR algorithms on nonlinear complementarity problems.

		PSANE		PAND-SR		PAND-BR	
Pb#	$\gamma$	It	Fe	It	Fe	It	Fe
15	0	181	371	75	108	15	20
	1	110	111	110	167	22	32
	2	29	30	29	39	30	40
16	0	24	25	24	33	14	18
	1	22	23	22	28	19	24
	2	21	22	21	26	15	18
17	0	$F_\lambda$		$F_\lambda$		9	15
	1	$F_i$		$F_\lambda$		45	63
	2	$F_i$		$F_\lambda$		41	60
18	0	6	11	1	3	1	3
	1	20	30	24	39	26	35
	2	1	2	1	2	1	2
19	0	3	4	3	4	6	8
	1	63	72	97	132	260	375
	2	2	5	4	6	4	6
20	0	21	22	21	23	22	23
	1	16	17	16	17	15	16
	2	17	18	17	19	15	16
21	0	24	25	24	27	46	52
	1	27	28	27	34	40	43
	2	22	23	22	26	49	57

TABLE 5. CPU time (in seconds) obtained with PSANE, PAND-SR and PAND-BR algorithms on bound-constrained nonlinear systems.

		Execution time		
Pb#	$\gamma$	PSANE	PAND-SR	PAND-BR
9	0	0.20	0.26	0.27
	1	0.38	1.23	0.36
	2	0.24	0.32	0.32
10	1	0.09	0.09	0.31
	2	0.15	0.14	1.00
	3	0.18	0.11	0.42
11	1	$F_b$	0.01	2.24
	2	$F_b$	0.01	1.04
	3	$F_b$	0.01	0.96
12	1	0.08	0.02	182.80
	2	0.04	0.02	170.73
	3	0.50	0.02	108.98
13	1	0.06	0.20	25.73
	2	0.28	0.40	30.26
	3	0.04	0.16	25.23
14	1	$F_b$	0.01	0.08
	2	$F_b$	0.01	0.08
	3	$F_b$	0.01	0.08

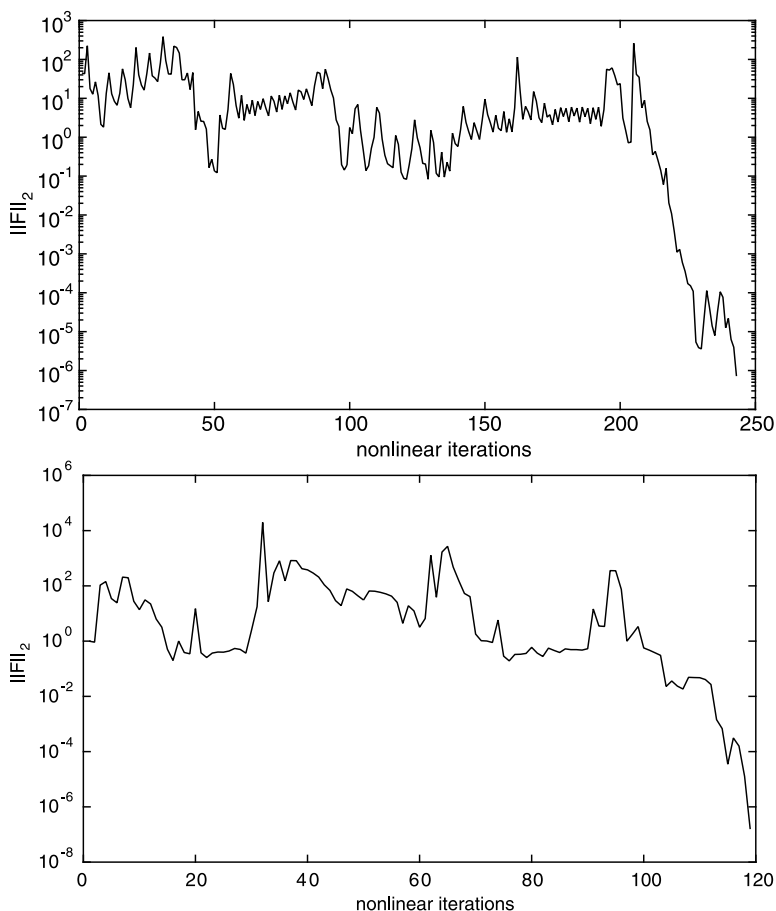


FIGURE 1. Norm of  $F$  on a log scale against the number of iterations. Top: problem 13 solved by PAND-SR,  $\gamma = 1$ . Bottom: problem 2 solved by PAND-BR,  $\gamma = 3$

## 7. CONCLUSION

We have proposed a new class of derivative-free methods for the solution of constrained nonlinear systems which combines the use of simple search directions with a new suitable approximate norm linesearch. The methods are suitable for both continuous and/or differentiable nonlinear systems and their convergence properties have been studied in both cases. In particular, we have focused on methods based on spectral residual steps (PAND-SR) and quasi-Newton directions (PAND-BR). These methods exhibit good numerical performance on relatively large problems. PAND-SR has turned out to be very efficient and competitive with PAND-BR; on the other hand PAND-BR has solved a larger set of problems than PAND-SR.

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