Optimization Methods and Software
Vol. 20, Nos. 4–5, August–October 2005, 493–508

Taylor & Francis
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Optimizing partially separable functions without derivatives

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(Received 5 November 2003; revised 31 March 2004; in final form 7 April 2004)

We present an algorithm for solving nonlinear programming problems involving a partially separable objective function whose derivatives are assumed to be unavailable. At each iteration, we construct a quadratic interpolation model of the objective function around the current iterate and minimize this model to obtain a trial step. The whole process is embedded within a trust-region framework. We further propose to use ideas of Curtis, Powell and Reid to minimize the number of calls to the objective function in the part of the derivative-free algorithm that improves the geometry of the interpolation set. Numerical experiments tend to confirm the promising behaviour of the algorithm.

Keywords: Partially separable functions; Derivative-free optimization; Multivariate interpolation; Trust-region algorithms

1. Introduction

Derivative-free optimization (DFO) is concerned with the design and analysis of algorithms for solving mathematical programmes involving functions whose derivatives are not available. This may be due to the fact that the evaluation of these derivatives is very difficult, unreliable or time consuming or because their computation requires the solution of another problem or even because the objective and/or constraint functions themselves are complex. The last situation may occur when the computation of the accurate value of such a function at a given point requires calls to extremely expensive codes and solvers or because the related source codes may be unavailable or unmodifiable, in which case they must be considered as black boxes. Also, such complex functions may be the output of a simulation or some physical, chemical or econometrical measurements or experiments, for instance.

DFO algorithms are designed in such a way that the number of function evaluations they require is minimized, which makes this number the usual criterion for the assessment and comparison of algorithms. Existing methods may be grouped in four broad categories. Direct search and pattern search methods (see refs. [1,18,30] may be viewed as sampling methods in the sense that they are based on an exploration of the space region under consideration; they perform a search by means of exploratory moves, considering the behaviour of the objective

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Optimization Methods and Software
ISSN 1055-6788 print/ISSN 1029-4937 online
http://www.tandf.co.uk/journals
DOI: 10.1080/10556780500140227

function at a 'pattern' of points that is independent of this function. A second class of methods was introduced by Powell [20] who described a line search method which proceeds in stages, each of them consisting of a sequence of $n + 1$ one-dimensional searches; the searches are governed by the minimization of a quadratic interpolant computed for each direction. Lucidi and Sciandrone [19] reported some numerical experiments obtained with the algorithm of Grippo *et al.* [17], who introduced a line search procedure where the usual conditions involving the gradient of the objective function are replaced by requirements on the values of f at points of the form $x \pm \alpha d$, which in turn allowed the design of another algorithm for minimizing f using the set of orthonormal coordinate vectors as directions at each step. Powell [21,22] also introduced another approach where finite-difference techniques are coupled with quasi-Newton algorithms, which constitute the third class of algorithms for DFO problems. The fourth and last class contains trust-region methods (see, e.g. refs. [8,25]), in which all available function values are used to build a polynomial model interpolating the objective function at all those points at which its value is known. The model is then minimized within a trust region and a new point is obtained. The latter point is evaluated, and while this enlarges the interpolation set, this also allows to check whether the objective function is improved. The whole process is then repeated until convergence occurs.

Several recent contributions considered unconstrained DFO problems where the objective function is known to have some structure, despite the fact that its derivatives are not available (see, e.g. refs. [3,4,24]). The reason for studying algorithms adapted to these particular problems is that a suitable exploitation of the problem structure is expected to result in important savings in terms of computational effort. The research work we describe in this paper is in line with refs. [3,4] in which we considered algorithms for solving unconstrained problems exploiting the banded and sparse structure of the objective function, respectively. In this article, we introduce another trust-region algorithm for solving unconstrained problems where this time the objective function is partially separable, i.e. it may be expressed as

$$\min f(x) = \sum_{i=1}^{M} f_i(x), \tag{1}$$

where $f: \mathbb{R}^n \to \mathbb{R}$ and each individual function $f_i(x)$ is a function depending on some of the components x_j, $j \in I_i$ for some index sets $I_i \subseteq \{1, \ldots, n\}$ $(i = 1, \ldots, M)$. We assume that the cardinality of these M subsets is given by $|I_i| = n_i$ and that the n_i-dimensional subspace of $\mathbb{R}^n$ is denoted by R_i $(i = 1, \ldots, M)$.

The concept of partial separability was introduced by Griewank and Toint [14,16], and it was also studied by Conn *et al.* [6] in the framework of the development of the LANCELOT package. Many optimization problems involve partially separable functions (see, e.g. the test problems collected by Toint [29]) and Griewank and Toint [15] show that every twice continuously differentiable function with a sparse Hessian is partially separable. It is remarkable that although this is only an existence result and does not specify the particular decomposition (1), we are not aware of any practical problem of having a sparse Hessian and whose partially separable decomposition is not explicitly known. In the context of problems where derivatives are unavailable, the partially separable structure often arises from the observation that the objective has a block structure involving different subsets of variables, even if each block is a black box in itself.

Section 2 provides some background material consisting of multivariate interpolation tools, before describing the aforementioned algorithm of Conn *et al.* [8]. The reason for presenting it is that it served as a basis for the development of our algorithm for partially separable functions, which is described in section 3. Section 4 details the numerical experience gained

so far, and it is followed by a short conclusion and several ideas for improving our algorithm further.

2. Trust regions and multivariate interpolation models

The new algorithm discussed in the present paper is a variation of that proposed by Conn *et al.* [8,9] and is of trust-region type. At iteration k, this algorithm first constructs a quadratic model

$$m_k(x_k + s) = f(x_k) + \langle g_k, s\rangle + \frac{1}{2}\langle s, H_k s\rangle, \tag{2}$$

for some $g_k \in \mathbb{R}^n$ and some symmetric n-by-n matrix H_k, which is intended to be valid in a neighbourhood of the current iterate $x_k \in \mathbb{R}^n$ (the trust region) defined by

$$\mathcal{B}_k = \{x_k + s : s \in \mathbb{R}^n \text{ and } \|s\| \leq \Delta_k\}, \tag{3}$$

for some trust-region radius Δ_k.

In our approach, the model (2) is chosen to interpolate the value of a function f at a set $Y_k = \{y_i\}$ of points containing x_k, yielding

$$f(y_i) = m_k(y_i) \quad \text{for all } y_i \in Y. \tag{4}$$

We refer the interested reader to de Boor and Ron [12], Sauer [27], Sauer and Xu [28] and Conn *et al.* [7,10] for details of how the

$$p = n + \frac{1}{2}n(n+1) = \frac{1}{2}(n+1)(n+2) - 1 \tag{5}$$

entries of g_k and H_k can be computed given the set Y (of fixed cardinality p) and the collection of associated function values $F = \{f(y_i)\}_{y_i \in Y}$. It is, however, important to point out that the knowledge of Y and F is not sufficient to guarantee the existence and uniqueness of suitable g_k and H_k but that a further geometric condition (known as poisedness) is also required. This condition ensures that the points of Y do not collapse in a lower dimensional space or do not lie on a quadratic curve (which would then span an infinite set of interpolating quadratic polynomials). If one chooses to build the interpolating quadratic using quadratic Newton fundamental polynomials as a basis (which is the approach taken by Conn *et al.* [7,9]), poisedness is ensured if and only if the pivots, i.e. the values of the nonnormalized Newton fundamental polynomials at their associated[†] interpolation point $|N_i^u(y_i)|$, are all different from zero (we denote the nonnormalized Newton fundamental polynomials by N_i^u and their normalized version by N_i). Although from a theoretical point of view this may be sufficient to ensure poisedness, in practice we must verify that,

$$|N_i^u(y_i)| \geq \theta \quad \text{for all } y_i \in Y \tag{6}$$

for some pivoting threshold $\theta > 0$. If condition (6) is satisfied, then the interpolation problem (4) is said to be well poised, and the entries of g_k and H_k can be computed safely. If this condition fails, we may have to improve the geometry of our interpolation set to ensure it. Following Conn *et al.* [7,9], a reasonable strategy for improving the geometry of this set might be to replace a point $y_- = y_i \neq x_k$ by another point y_+ such that $|N_i(y_+)|$ is larger, for instance by choosing

$$y_+ = \text{argmax}_{y \in \mathcal{B}_k} |N_i(y)| \tag{7}$$

[†]We again refer the reader to de Boor and Ron [12], Sauer [27], Sauer and Xu [28] and Conn *et al.* [7,10] for details on how fundamental Newton polynomials are associated with interpolation points and normalized.

provided $|N_i(y_+)| \geq 1 + \theta$ because otherwise the geometry was already fine. Note that solving (7) reduces to solving two instances of the classical trust-region subproblem for which good algorithms exist (see, e.g. ref. [7, chapter 7]).

Once we have computed the model $m_k(x_k + s)$ in the neighbourhood of the current iterate x_k, we follow the classical procedure of trust-region methods and compute the step $s_k \in \mathbb{R}^n$ by minimizing the polynomial model m_k over the trust region defined by (3). Again, this can be done using any of the well-known algorithms described in ref. [7, chapter 7]. If

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)} \tag{8}$$

is sufficiently positive, we say that iteration k is successful, define our next iterate x_{k+1} to be $x_k + s_k$ and possibly enlarge our trust-region radius Δ_k. If ρ_k is not sufficiently positive, our iteration is deemed unsuccessful, the current iterate is not altered and the trust-region radius is potentially reduced.

We now consider three particular issues arising in the particular framework of DFO. The first point regards the convergence test at the end of each iteration. Although in classical trust-region methods it may be sufficient to check that the gradient of f is small enough at the current point, our derivative-free framework makes things more difficult because we cannot compute the gradient $\nabla f(x)$. It is nevertheless the case that if the model (2) is a sufficiently accurate representation of the objective function, we may assume that

$$\|g_k\| \approx \|\nabla f(x_k)\|.$$

Hence, as soon as the quadratic model m_k has been updated, we compute $\|g_k\|$ and check whether it is small enough (in practice: $\|g_k\| < \epsilon_c$ for some constant $\epsilon_c > 0$). If this is the case, we ensure that the model is sufficiently accurate by making it valid in some ball centred at x_k, which is the case when

$$|f(x) - m_k(x)| \leq \kappa \Delta^2$$

for all x such that $\|x - x_k\| \leq \Delta$, where κ is a positive constant independent of x [7, p. 308]. It is important that we are able to verify this condition in a finite number of steps (see ref. [7, section 9.1, Assumption AM.7]) by checking that the points of the interpolation set are sufficiently close to x_k and that the associated Newton fundamental polynomials are bounded (see ref. [7, Theorem 9.4.4]). If $\|g_k\|$ remains small after this verification, convergence is declared and the algorithm terminates (see ref. [7, Lemma 9.1.2] for a proof that this process is well defined and finite whenever $\epsilon_c > 0$). Otherwise, the optimization process is continued.

The second issue is the way to use new available function values in a suitable way. To see this, let us now assume that at some iteration k, we get a point $x_k^+ = x_k + s_k$ of associated function value $f(x_k^+)$; one may consider the problem of finding the best way to make x_k^+ play a role in the next iterations when building the interpolating quadratic. Indeed, because in our DFO framework the function evaluations are expensive, it is natural to take advantage of the fact that $f(x_k^+)$ is known to check whether x_k^+ may be added to the set of interpolation points or not. If $|Y| < p$, which generally occurs in the first few iterations of the process, and if the inclusion of x_k^+ within Y does not destroy poisedness, we may simply add x_k^+ to Y, which allows to progressively complete the set of interpolation points. Otherwise, if $|Y| = p$, we try to find a point in Y, say y_-, which can advantageously be replaced by x_k^+. This replacement is performed in a way that makes the pivots as large as possible in order to obtain a well-poised interpolation problem. More precisely, we proceed as follows:

Let p_i $(i = 1, \ldots, M)$ denote the size of a complete interpolation set for function f_i. We first initialize the radius Δ_{geom} as follows:

$$\Delta_{\text{geom}} = \begin{cases} \min(\|s_k\|, \Delta_k) & \text{if the iteration is successful,} \\ \min(\|s_k\|, \Delta_k)/\gamma_{\text{div}} & \text{if the iteration is unsuccessful} \\ & \text{and the model is valid,} \\ \min(\|s_k\|, \Delta_{\text{ref}}/\gamma_{\text{lim}}) & \text{otherwise,} \end{cases} \tag{9}$$

where $\gamma_{\text{div}} = 1.75$, Δ_{ref} is the trust-region radius of the most recent successful iteration and

$$\gamma_{\text{lim}} = \max(10, p_i)\gamma_{\text{div}}.$$

We then look for the point y_- whose distance to the base is the largest.

- If $\|y_- - x_{k+1}\|$ is not too small (e.g. larger than $1.5\Delta_k$) and the value of the fundamental polynomial associated to y_- evaluated at x_k^+ is larger than

$$2\left(\frac{\Delta_{\text{geom}}}{\|y_- - x_{k+1}\|}\right)^2,$$

  then we replace y_- by x_k^+;
- Otherwise, we choose y_- to be the point associated to the fundamental polynomial whose absolute value is maximal at x_k^+, and we replace y_- by x_k^+ provided this absolute value is sufficiently large (e.g. larger than 1).

Note that this procedure also provides a finite algorithm for obtaining an interpolation set such that the model is valid in the trust region (see ref. [7, section 9.1, Assumption AM.8]).

Finally, a third issue is the management of the trust-region radius. In classical trust-region methods, the radius Δ_k is always decreased at unsuccessful iterations. In our framework, however, we must first verify that the interpolation set is poised before reducing Δ_k because a bad geometry might be the main reason for the iteration to be unsuccessful. If Y is not well poised, we thus have to improve its geometry (using, again, the procedure described previously) possibly reducing Δ_k. It is particularly important not to modify Δ_k too early in the process as this would often impose too small steps and cause the algorithm to be excessively slow.

3. Trust-region algorithm for minimizing partially separable functions

We now turn back to the case of unconstrained problems involving a partially separable function (1). Intuitively, we may compute a solution to problem (1) by applying the interpolation ideas outlined previously to each individual function $f_i(x)$ $(i = 1, \ldots, M)$. We thus consider M interpolation sets Y_i whose points are used to construct M quadratic models approximating f_i around the current iterate x_k:

$$m_{i,k}(x_k + s) = f_i(x_k) + g_{i,k}^T s + \frac{1}{2} s^T H_{i,k} s, \quad i = 1, \ldots, M, \tag{10}$$

where each $g_{i,k}$ is a vector of $\mathbb{R}^{n_i}$ and $H_{i,k}$ is an n_i-by-n_i matrix with real coefficients for $i = 1, \ldots, M$. Note that each model $m_{i,k}$ actually depends on the n_i-dimensional vectors of the subspace R_i $(i = 1, \ldots, M)$ and approximate the f_i's around the projection of x_k onto R_i, even if, for the sake of simplicity, our notations in model (10) keep this projection implicit.

Once the model (10) interpolating the individual functions is computed, a quadratic model of the global objective function f at x_k is trivially obtained as

$$\begin{aligned} m_k(x_k + s) &= \sum_{i=1}^{M} m_{i,k}(x_k + s), \\ &= f(x_k) + g_k^T s + \frac{1}{2} s^T H_k s, \end{aligned} \tag{11}$$

where the vector $g_k \in \mathbb{R}^n$ and the matrix $H_k \in \mathbb{R}^{n \times n}$ are built from 'incomplete' – or 'partial' – vectors $g_{i,k}$ and matrices $H_{i,k}$ $(i = 1, \ldots, M)$. As usual, in trust-region methods, the model (11) can then be minimized within the current trust region $\mathcal{B}_k$, which yields a new point $x_k + s_k$ at which the objective function f may be evaluated.

However, we now have to manage M interpolation sets Y_i $(i = 1, \ldots, M)$ instead of a single one. We then have to consider two possible cases: either it is possible for the user to evaluate a single element function $f_i(x)$ independently of the others or the objective function must always be evaluated as a whole (i.e. only the collection of values $\{f_i(x)\}_{i=1}^M$ can be computed for a given x). In the second case, a straightforward implementation of our algorithm could be very expensive in terms of function evaluations if we blindly apply procedures similar to those of section 2 to each Y_i for geometry improvement or for replacing an existing interpolation point with a new one. Indeed, computing a vector that improves the geometry of the jth interpolation set yields a vector having only n_j 'useful' components, and it is not clear which values should be assigned to the remaining $n - n_j$ components. Our strategy in this case is to group the necessary individual function evaluations by applying the CPR procedure of Curtis *et al.* [11] for estimating sparse Jacobian matrices to the $n \times M$ occurence matrix of variables x_j into elements f_i defined by

$$d_{ji} = \begin{cases} 1 & \text{if function } f_i \text{ depends on } x_j \\ 0 & \text{otherwise,} \end{cases}$$

with $i \in \{1, \ldots, M\}$ and $j \in \{1, \ldots, n\}$.

Now, at some iteration k, we denote by L_k the set of indices corresponding to the interpolation sets for which a geometry improvement is requested. If $L_k = \{i_1, i_2, \ldots, i_l\} \neq \emptyset$ (i.e. $|L_k| > 0$), we partition the set of columns of D in a number of groups, each of them containing columns corresponding to individual functions whose associated index sets have an empty intersection. Hence, the individual functions whose associated columns belong to the same subset depend on strictly different components of a vector $x \in \mathbb{R}^n$. There are various ways to obtain such a grouping. For the experiments reported subsequently, we have chosen the greedy approach originally proposed by Curtis *et al.*, which is summarized as follows for $L_k = \{i_1, i_2, \ldots, i_L\}$:

- a new group $L_{k,1}$ is first created that contains column i_1;
- the function i_2 is then considered and one checks whether f_{i_1} and f_{i_2} have common variables (i.e. whether $d_{j1} + d_{j2} > 1$ for all $j = 1, \ldots, n$): if this is not the case, then $L_{k,1}$ is replaced by $L_{k,1} \cup \{i_2\}$; otherwise, a new group $L_{k,2}$ is created containing column i_2;
- the process is repeated, considering the remaining elements of L_k in increasing order and adding the corresponding columns to one of the existing subsets when possible or creating a new group when this proves impossible.

The authors are aware that it might be more efficient to use more sophisticated techniques, such as the graph colouring method of Coleman and Moré [2], to further improve the efficiency of this approach.

We now summarize the main steps of our algorithm. Note that at this point we must consider the two aforementioned possible frameworks: the first one corresponds to the situation where the functions f_i $(i = 1, \ldots, M)$ are accessible individually, whereas in the second one, the value of an individual function f_i can only be obtained by calling the routine for evaluating the whole function f. We denote the corresponding versions of the algorithm by I and G, respectively.

3.1 *Partially separable functions and DFO*

Step 0 Initialization. An initial point x_0 is given, as well as a trust-region radius $\Delta_0 > 0$, a user defined tolerance $\epsilon_c > 0$ and constants $\alpha \in (0, 1)$, $\mu > 0$, γ_1, γ_2, η_1 and η_2 satisfying $0 < \gamma_1 \leq \gamma_2 < 1$ and $0 < \eta_1 \leq \eta_2 < 1$. We also initialize the parameters for geometry improvements γ_{div}, γ_{lim} and we choose $\Delta_{\text{ref}} = \Delta_0$. It is assumed that for each $i = 1, \ldots, M$, there exists a (possibly incomplete) set Y_i of interpolation points. The iteration counter k is set to 0.

Step 1 Computing the models. Compute quadratic interpolation polynomials $m_{i,k}$ (for $i = 1, \ldots, M$) approximating each f_i around the projection of x_k onto each R_i as defined by model (10). Form the complete model m_k defined by model (11).

Step 2 Convergence test. If $\|g_k\| \leq \epsilon_c$ and Y is well poised in a ball of radius $0 < \delta \leq \mu\|g_k\|$ centred at x_k stop. Otherwise, improve the geometry until Y is well poised in a ball of radius $0 < \delta \leq \alpha\mu\|g_k\|$ centred at x_k and return to the beginning of Step 2.

Step 3 Minimizing the models. Solve

$$\begin{aligned} &\min_{s \in \mathbb{R}^n} && m_k(x_k + s) \\ &\text{s.t.} && \|s\| \leq \Delta_k, \end{aligned}$$

and obtain s_k.

Step 4 Step acceptance. Compute ρ_k from (8). If $\rho_k > \eta_1$, then $x_{k+1} := x_k + s_k$ and $x^+ := x_k$, otherwise set $x_{k+1} := x_k$ and $x^+ := x_k + s_k$.
Update Δ_k as follows:

$$\Delta_{k+1} \in \begin{cases} [\Delta_k, \infty) & \text{if } \rho_k \geq \eta_2, \\ \left[\gamma_2\Delta_k, \Delta_k\right] & \text{if } \rho_k \in [\eta_1, \eta_2), \\ \left[\gamma_1\Delta_k, \gamma_2\Delta_k\right] & \text{if } \rho_k < \eta_1. \end{cases}$$

Step 5 Improve the geometry. Update Δ_{geom} as in model (9).

Version I: for $i = 1, \ldots, M$, compute the projection of x^+ on R_i and see whether it can be advantageously added to Y_i (i.e. making its geometry better, as described in section 2), possibly replacing an existing point. If this is the case, modify Y_i and update the fundamental polynomials related to it. Otherwise, try and compute an additional point that could improve the geometry Y_i (yielding larger pivots); if this is possible, compute this point as described in section 2, update Y_i and the corresponding fundamental polynomials.

Version G: first set $L_k := \emptyset$ and then loop over the individual functions f_i and their interpolation sets Y_i $(i = 1, \ldots, M)$ as mentioned previously. If the insertion or replacement of a point in the interpolation set Y_i is possible, then proceed as before. Otherwise, add the index i to L_k. If $L_k \neq \emptyset$, apply the previously described CPR procedure to group the indices in L_k. The number of resulting groups gives the number of new points to compute for improving the geometry of the interpolation sets Y_j such that $j \in L_k$.

If incidentally one of the new points computed within this step has a better objective function value than x_{k+1}, then replace x_{k+1} and update all fundamental polynomials.

Go to Step 1.

Note that the trust-region radius Δ_k remains 'global', i.e. it is related to f and not to the (possible) individual improvements in terms of the f_i's.

4. Numerical experience

The Fortran code resulting from the implementation of this algorithm is named `PSDFO` and the purpose of this section is to discuss preliminary numerical results obtained with it to solve unconstrained problems involving a partially separable objective function. The two previously described versions of our algorithm were implemented and are denoted by `PSDFO(I)` and `PSDFO(G)` in the sequel. Table 1 provides the list of tested test problems, whereas figure 1 shows the sparsity patterns of the sparse problems considered. All problems in table 1 are part of the `CUTEr` (see ref. [13]) collection, most of them being already described in Toint [29]. Note that because the primary goal of the `CUTEr` collection is to regroup test problems for general nonlinear programming software packages, most `CUTEr` problems are not derivative-free problems. Besides their availability in the public domain, the main advantage of using the `CUTEr` problems is that their solution is known, a very useful feature for testing.

Before describing the test results, we emphasize that the framework of partially separable functions makes it necessary to distinguish two different types of function evaluations: those related to the global objective function f and those related to the element functions f_i ($i = 1, \ldots, M$). The `PSDFO` package is implemented in such a way that a subroutine (named `UFN_I`) allows to evaluate one particular individual function at a time. As a result, when the value of the global objective function is required (e.g. after computation of an improvement step s_k), `PSDFO` calls the subroutine `UFN_I` M times (once for every element function). As we wish to compare the number of function evaluations required by our algorithm with that required by other approaches, we report subsequently the equivalent number of objective function evaluations, which is obtained by dividing the total number of element functions evaluations by M. As we did not observe major variations in the number of calls to `UFN_I` for

Table 1. Problem specifications.

Problem name	Dimension (n)	Structure	M
ARWHEAD	10, 15, 20, 25, 50, 100, 200	Sparse	$n-1$
BDQRTIC	10, 15, 20, 25, 50, 100, 200	Banded	$n-4$
BDVALUE	10, 20, 50, 100, 200	Banded	n
BRYDN3D	10, 20, 50, 100, 200	Banded	n
CHROSEN	10, 15, 20, 25, 50, 100, 200	Banded	$n-1$
CRAGGLVY	10, 20, 50, 100, 200	Banded	$(n-2)/2$
DQDRTIC	10, 20, 50, 100, 200	Banded	$n-2$
EXTPOWELLSG	10, 22, 49, 100, 202	Sparse	$(n-1)/3$
EXTROSNB	10, 20, 50, 100, 200	Sparse	$n-1$
GENHUMPS	10, 20, 50, 100, 200	Banded	$n-1$
LIARWHD	10, 20, 50, 100, 200	Sparse	$n-1$
MOREBV	10, 20, 50, 100, 200	Banded	n
ROSENBR	10, 20, 50, 100, 200	Banded	$n-1$
SCHMVETT	10, 20, 50, 100, 200	Banded	$n-2$
WOODS	12, 20, 48, 100, 200	Sparse	$n/4$

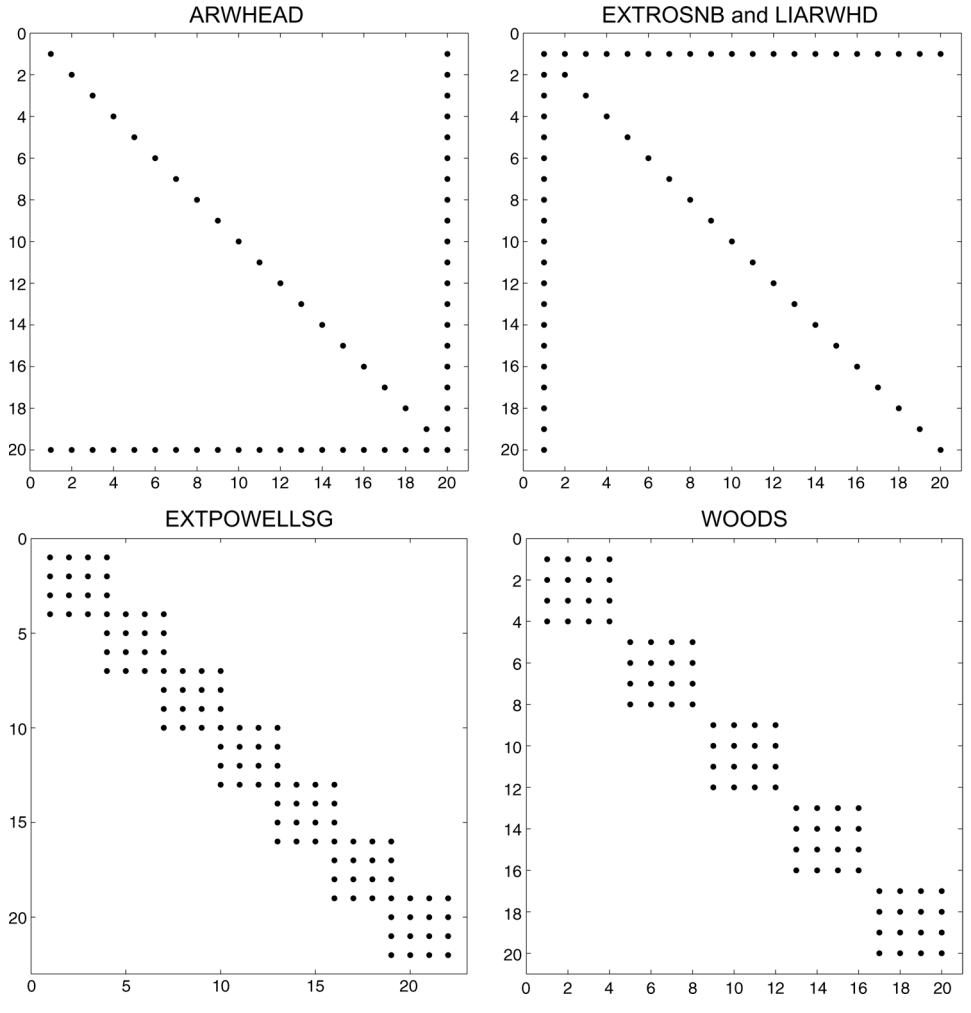

Figure 1. Sparsity patterns of the sparse problems considered for numerical experiments with PSDFO.

evaluating the different element functions, we consider that this equivalent number of objective function evaluations is an appropriate measure for the assessment of the performance of PSDFO.

4.1 *Comparison of the approaches*

We first provide some numbers to compare PSDFO with two other packages: UDFO is the basic implementation of the algorithm of Conn *et al.* [8] and UDFO(S) is one of its two extensions considered in refs. [3,4] (for banded and sparse Hessian matrices); UOBYQA is Powell's package described in ref. [25], whereas UOBSQA and UOBDQA are its extensions taking sparsity into account and constructing approximations having a diagonal Hessian, respectively (see ref. [24]).

Table 2 summarizes the performance of these five packages for the three problems of the CUTE collection considered by Powell (see ref. [24, table 1]). We also consider the same problem dimensions, i.e. $n = 10$, 15, 20 and 25 and as in ref. [24], we focus on the number

Table 2. Comparison of the number of function evaluations required by DFO solvers for solving medium-size instances of problems.

Problem	Dimension (n)	UDFO	UDFO(S)	UOBSQA	UOBDQA	PSDFO(I)	PSDFO(G)
ARWHEAD	10	311	150	118	105	30	54
	15	790	339	170	164	30	56
	20	1,268	333	225	260	35	161
	25	1,478	448	296	277	37	198
BDQRTIC	10	519	327	350	288	348	358
	15	1,014	639	594	385	345	382
	20	1,610	893	855	534	509	596
	25	2,615	940	1,016	705	360	542
CHROSEN	10	2,032	775	247	3,652	85	123
	15	4,901	1,660	431	4,590	91	154
	20	>10,000	3,268	553	5,871	95	168
	25	>10,000	5,015	736	5,943	98	173

of function evaluations required for solving the problems. Figure 2 shows the evolution of the number of function evaluations required by the five solvers. As shown by this figure and the results in table 2, both versions of PSDFO generally require much fewer function evaluations than the other packages. The reason for these savings in function evaluations may be explained by the fact that PSDFO obtains complete interpolation sets more rapidly because the dimensions n_i $(i = 1, \ldots, M)$ are (sometimes considerably) smaller than the dimension n of the problem. More precisely, the number of p function evaluations that is required by UDFO to obtain a full interpolation set is given by (see (5))

$$\begin{cases} \frac{1}{2}(n+1)(n+2) - 1 & \text{for UDFO} \\ n + n_H & \text{for UDFO(S)} \\ \frac{1}{2}(\bar{n}+1)(\bar{n}+2) - 1 & \text{for PSDFO} \end{cases}$$

where n_H is the number of nonzero entries in the lower triangular part of the Hessian and where

$$\bar{n} = \max_{1 \le i \le M} n_i \ll n$$

which is typically independent of the actual size of the problem. (Owing to the involved quasi-Newton mechanism, this comparison is not really relevant for UOBSQA and UOBDQA, except that in both cases p is bounded subsequently by n.)

4.2 *Performance of* PSDFO

We now concentrate on PSDFO and analyze the complete results we obtained with this package. These results are reported in table 3 and they were obtained with a PC Pentium 4, 2.00 GHz (900 MB Ram) running Linux. The three measures we collected with both PSDFO(I) and PSDFO(G) are the number of function evaluations, the number of iterations and the CPU time required for solving the problems of table 1.

We first examine the performance of PSDFO(I), i.e. the version for which it is assumed that the functions f_i $(i = 1, \ldots, M)$ are accessible individually. As expected, the number of function evaluations does not increase much when higher dimensions are considered, except for some difficult problems like ROSENBR. This is illustrated in figure 3, where the evolution of the number of function evaluations required by PSDFO(I) for the various sizes of the

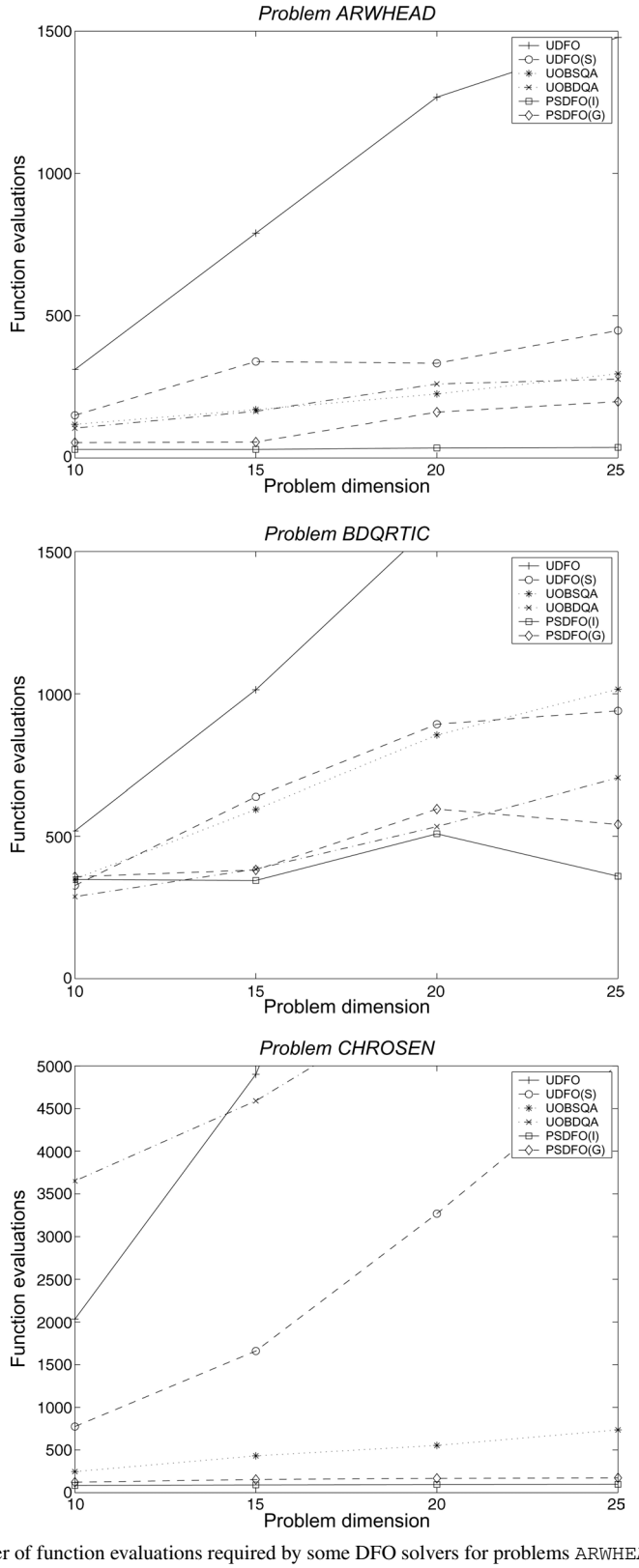

Figure 2. Number of function evaluations required by some DFO solvers for problems ARWHEAD, BDQRTIC and CHROSEN.

Table 3. Further results for PSDFO.

		$n = 10$		$n = 20$		$n = 50$		$n = 100$		$n = 200$	
Problem	Measure	I	G	I	G	I	G	I	G	I	G
ARWHEAD	Evaluations	30	54	35	161	34	226	43	925	40	1,624
	Iterations	18	18	19	19	22	22	26	26	24	24
	CPU time	0.02	0.02	0.04	0.04	0.11	0.12	0.49	0.49	2.96	3.47
	Groups	–	1.5	–	7.0	–	9.0	–	34.2	–	66.3
BDQRTIC	Evaluations	348	358	509	596	627	1,275	343	2,263	336	5,786
	Iterations	214	214	408	408	567	561	295	295	279	279
	CPU time	1.68	1.75	8.33	4.68	33.58	33.60	37.74	39.23	118.80	117.50
	Groups	–	0.05	–	0.2	–	1.2	–	6.5	–	19.6
BDVALUE	Evaluations	46	57	45	73	44	72	42	79	27	42
	Iterations	28	28	24	24	23	23	20	20	9	9
	CPU time	0.05	0.04	0.03	0.09	0.27	0.26	0.71	0.72	1.54	1.60
	Groups	–	0.5	–	1.4	–	1.4	–	2.1	–	2.0
BROYDN3D	Evaluations	53	70	56	84	68	144	153	342	123	278
	Iterations	38	38	40	40	42	42	116	116	84	84
	CPU time	0.05	0.06	0.13	0.14	0.48	0.49	2.83	3.98	16.82	17.01
	Groups	–	0.5	–	0.8	–	2.1	–	1.8	–	2.2
CHROSEN	Evaluations	85	123	95	168	143	262	177	313	226	396
	Iterations	63	63	67	67	99	99	111	111	141	141
	CPU time	0.03	0.05	0.11	0.11	0.57	0.58	2.50	2.54	22.67	21.58
	Groups	–	0.8	–	1.4	–	1.6	–	1.7	–	1.7
CRAGGLVY	Evaluations	392	455	390	530	525	878	713	1,228	1,040	1,841
	Iterations	327	327	334	334	424	424	562	562	799	799
	CPU time	0.55	0.70	1.73	1.73	6.13	6.14	23.58	23.10	160.43	159.58
	Groups	–	0.3	–	0.5	–	1.0	–	1.1	–	1.3
DQDRTIC	Evaluations	191	289	337	726	342	747	274	834	484	775
	Iterations	151	162	233	275	212	212	170	226	283	204
	CPU time	0.21	0.26	0.93	1.18	2.20	2.59	6.59	6.78	49.27	43.98
	Groups	–	0.6	–	2.4	–	2.4	–	2.6	–	2.7
EXTPOWELLSG	Evaluations	270	276	256	308	401	525	504	772	844	1319
	Iterations	225	225	213	213	354	354	441	441	746	746
	CPU time	0.37	0.41	0.85	0.75	3.70	3.71	14.42	14.38	132.52	132.30
	Groups	–	0.05	–	0.3	–	0.4	–	0.6	–	0.7
EXTROSNB	Evaluations	60	108	103	571	113	1,553	205	6,575	168	10,864
	Iterations	46	46	70	70	78	78	135	135	112	112
	CPU time	0.04	0.04	0.11	0.11	0.42	0.43	3.08	3.46	17.98	20.47
	Groups	–	1.2	–	7.0	–	18.9	–	47.7	–	96.0
GENHUMPS	Evaluations	114	168	200	345	202	357	249	433	253	436
	Iterations	86	86	142	142	131	131	152	154	154	154
	CPU time	0.08	0.08	0.26	0.27	0.79	0.81	3.05	3.21	15.39	19.18
	Groups	–	0.8	–	1.4	–	1.65	–	1.75	–	1.80
LIARWHD	Evaluations	45	95	58	173	63	589	67	1,345	93	4,460
	Iterations	31	31	45	45	46	46	46	46	66	66
	CPU time	0.03	0.03	0.05	0.09	0.23	0.26	0.94	1.01	10.20	10.62
	Groups	–	1.8	–	2.7	–	11.7	–	28.1	–	66.5
MOREBV	Evaluations	32	40	32	41	34	49	37	65	23	34
	Iterations	15	15	16	16	15	15	17	17	6	6
	CPU time	0.03	0.04	0.07	0.08	0.18	0.18	0.60	0.61	1.11	1.11
	Groups	–	0.6	–	0.6	–	1.1	–	1.8	–	1.8
ROSENBR	Evaluations	187	321	418	759	1158	2,057	2,502	4,420	6,728	11,811
	Iterations	136	136	276	276	738	738	1,553	1,553	4,005	4,070
	CPU time	0.13	0.13	0.53	0.56	4.78	4.94	40.32	33.3	707.91	731.69
	Groups	–	1.3	–	1.7	–	1.8	–	1.8	–	1.9

(*continued*)

Table 3. Continued.

Problem	Measure	$n = 10$		$n = 20$		$n = 50$		$n = 100$		$n = 200$	
		I	G	I	G	I	G	I	G	I	G
SCHMVETT	Evaluations	61	75	51	82	65	144	89	191	150	285
	Iterations	44	44	33	33	41	41	62	62	97	97
	CPU time	0.09	0.10	0.12	0.13	0.46	0.47	0.78	0.87	21.37	21.49
	Groups	–	0.4	–	1.1	–	2.2	–	1.9	–	1.8
WOODS	Evaluations	963	1,080	1,046	1,183	477	518	671	758	1,366	1,714
	Iterations	840	840	933	933	416	416	585	585	1,044	1,044
	CPU time	1.53	1.56	2.54	2.91	3.46	3.49	18.05	18.24	192.22	192.72
	Groups	–	0.2	–	0.2	–	0.2	–	0.3	–	0.6

problems is displayed (note that these numbers are normalized in the sense that, for a given line of table 3, the various values it contains are divided by the average of these values). For some problems (e.g. EXTROSNB and GENHUMPS), intermediate dimension instances require more computational effort than for the larger instances we considered.

Let us now consider the results obtained with PSDFO(G). As could be expected, this version of the algorithm requires more function evaluations than PSDFO(I), which is a clear illustration of the advantages of the previous framework. However, it seems that the grouping strategy described in section 3 allows to limit the increase in the computational cost. To show this, we reported a further measure regarding the results obtained with PSDFO(G), namely, the average number of groups (per iteration) constructed by the algorithm when geometry improvements occur (for PSDFO(I), the corresponding cells are filled with a dash). For some problems, this number varies much from $n = 10$ to $n = 200$, whereas for others it remains between 0.5 and 2.0. This is due to the fact that some problems (like ARWHEAD or EXTROSNB) have individual functions that can never be grouped because they all depend on (at least) one

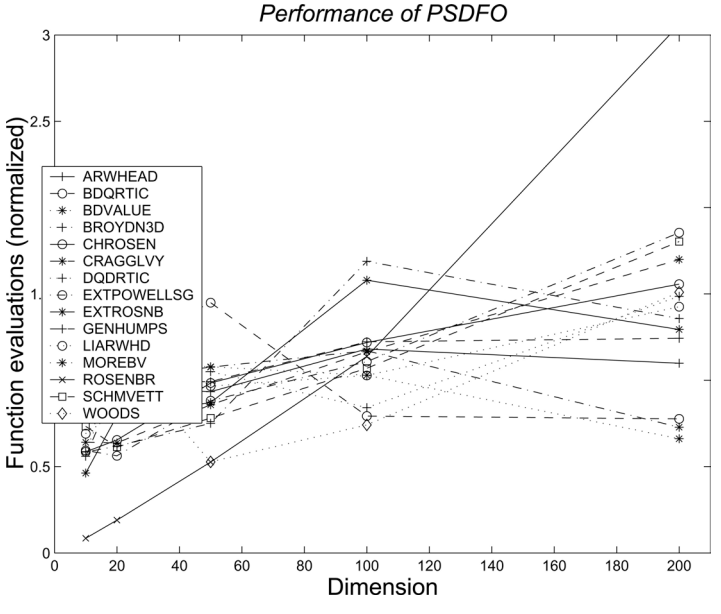

Figure 3. Performance of PSDFO(I) in terms of function evaluations when the size of problems increases.

common variable (for ARWHEAD, function f_i depends on x_i and x_{10}, while for EXTROSNB it depends on x_1 and x_i) whereas other problems (like BDVALUE or WOODS) involve individual functions that can be grouped easily (see figure 1). As a consequence, solving the former problems with PSDFO(G) requires much more function evaluations (with the same number of iterations as that observed with PSDFO(I)), whereas the latter can be solved at a cost which is only slightly higher than with PSDFO(I).

Finally, we should mention that although PSDFO is clearly better than UDFO in terms of computational effort, the latter remains advantageous from the point of view of storage issues, should this become an issue. Indeed, because PSDFO constructs models for the M individual functions forming the objective, it must manage M interpolation sets, M bases of Newton fundamental polynomials and M models $m_{i,k}$. Despite the fact that each of these components is smaller than that corresponding to the single model m_k generated by UDFO (because $n_i < n$ for each $i \in \{1, \ldots, M\}$), the need to consider M such spaces in PSDFO makes it more demanding in terms of storage.

5. Discussion

We have presented a new algorithm for solving unconstrained DFO problems whose objective function is partially separable. This algorithm proves to be very efficient in terms of function evaluations, the latter being the most important criterion for the assessment of derivative-free methods.

We believe that our algorithm can be extended further and we would like to mention here some possible refinements. The first one is related to Powell's methods and consists in using only the dominant parts of the Hessian matrix. Indeed, it seems that introducing artificial sparsity and ignoring some of the entries of the Hessian that may be considered as being negligible are likely to yield the same improvements as those reported by Powell [24]. A more promising approach would be to combine the least Frobenius norm update of Powell within our partially separable scheme and to apply Powell's technique at the level of individual functions and their models. Furthermore, we could use a criterion like that of Conn *et al.* [5] for selecting negligible individual functions whose model might be left unchanged in a larger region. Their criterion suggests to define the index set of negligible functions as follows:

$$\{i \in \{1, \ldots, M\}: |m_{i,k}(x^{(k)}) - m_{i,k}(x^{(k)} + s^{(k)})| \leq \frac{\mu}{M} |m_k(x^{(k)}) - m_k(x^{(k)} + s^{(k)})|\},$$

where $m_{i,k}$ and m_k denote the model of the individual function f_i and that of the global objective f, respectively, whereas μ is a parameter such that $0 < \mu < 1$.

Also note that the current version of the algorithm assumes that we can only evaluate the f_i's at any point x but we might have a more complete knowledge concerning the gradient and/or the Hessian of some individual functions $f_i(\cdot)$. The use of all available derivatives is straightforward in model (10). Combination with quasi-Newton methods is also possible for the element functions whose gradient but not the Hessian is available.

Acknowledgements

The authors are indebted to two anonymous referees for their valuable comments and suggestions for improving this paper.

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