A Derivative-free Algorithm for Sparse Unconstrained Optimization Problems

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Abstract: We consider the problem of minimizing a function whose derivatives are not available. This paper first presents an algorithm for solving problems of this class using interplation polynomials and trust-region techniques. We then show how both the data structure and the procedure allowing to build the interpolating polynomials may be adapted in a suitable way to consider problems for which the Hessian matrix is known to be sparse. The favourable behaviour of the resulting algorithm is confirmed with numerical experiments illustrating the advantages of the method in terms of storage, speed and function evaluations, the latter criterion being particularly important in the framework of derivative-free optimization.
Keywords: derivative-free optimization, interpolation models, trust-region methods, sparsity.

1 Introduction

Many optimization problems arising from the industrial world involve complex objective functions whose derivatives are not always available. This may be due to the fact that the evaluation of these derivatives is very difficult or time-consuming, or their computation requires the resolution of another problem, or because the objective function itself is the output of some physical, chemical or econometrical measurements, for instance. Such functions are frequently encountered in engineering and design optimization problems and the result of this is a high demand from practitioners for efficient algorithmic tools and softwares. In this paper, we focus on unconstrained optimization problems that may be formulated as follows:

$$\min_{x \in \mathbb{R}^n} f(x),$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a nonlinear, smooth, real-valued function whose derivatives are not available.

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Algorithms for derivative-free optimization problems have been extensively studied in the literature since the late fifties and various approaches have been proposed. In the class of "pattern search" techniques, where a predefined class of geometrical patterns is used to explore the variable space, early contributions include those of Box [3], Campey and Nickols [7], Hooke and Jeeves [19], Spendley, Hext and Himsworth [33], Nelder and Mead [22], and Dixon [17]. This approach was revisited more recently by Dennis and Torczon [15, 16] [PDS], Buckley [5], Wright [38], Torczon [35], Alexandrov et al. [1], and Audet et al. [2]. Linesearch methods have also been investigated for the problem, including proposals by Powell [24] [VA04,VA24], Brent [4] [PRAXIS], Callier and Toint [6], Lucidi and Sciandrone [20], while finite-difference techniques have been coupled with quasi-Newton algorithms in a very natural way, and are discussed in particular by Powell [25, 27, 26], Stewart [34], Gill, Murray and Wright [18] Dennis and Schnabel [14], Nocedal and Wright [23] or Conn, Gould and Toint [9]. In this paper we consider an algorithm based on a fourth possible approach, namely the use of interpolation methods to model the objective function and their combination with trust-region techniques. This class of methods has been pioneered by Winfield [36, 37], who used full quadratic models but did not study convergence. This technique was later reinvestigated by Powell [28, 29, 30, 31], Marazzi and Nocedal [21], Conn and Toint [13], and Conn, Scheinberg and Toint [10, 11, 12]. The main ideas of these latter contributions may be summarized as follows. Assuming that $f(x)$ is computable for all $x \in \mathbb{R}^n$, the spirit of these methods is to use all the available function values to build a polynomial model interpolating the objective function f at the points at which its value is known. The model is then minimized within a trust region, yielding a new – potentially good – point. To check this possible improvement, the objective f is evaluated at the new point – thus possibly enlarging the interpolation set – and the whole process may then be repeated until convergence is achieved.

The aim of this paper is to specify these methods for the particular case where we know that the Hessian of $f(x)$ is sparse and to do this in a way that takes advantage of this particular structure so as to minimize the computational costs and in particular the number of function evaluations. Such a situation arises when it is known that the objective function can be viewed as the sum of "blocks" that do not individually involve all the variables, for instance. This paper extends the results presented in Colson and Toint [8] – where we focussed the numerical experiments on banded Hessian matrices – to the case of general sparse matrices.

The structure of this paper is as follows. In Section 2 we present the main ingredients of the abovementioned algorithm, including some preliminary considerations as regards the geometry of the interpolation set. The latter topics are extended in Section 3, where we consider the use of Newton fundamental polynomials as a basis for building the function model at each iteration and show how this technique may be specified for the case where the Hessian matrix $\nabla^2_{xx} f(x)$ is known to be sparse. The resulting savings in terms of computational effort are assessed through a series of numerical results reported in Section 4.

2 Description of the algorithm

At iteration k of the process, starting from iterate $x^k \in \mathbb{R}^n$, the algorithm computes the step $s \in \mathbb{R}^n$ minimizing the quadratic model

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

for some $g_k \in \mathbb{R}^n$ and some symmetric $n \times n$ matrix H_k, where $\langle \cdot, \cdot \rangle$ denotes the dot product. It must be emphasized here that g_k and H_k do not necessarily correspond to the first and second derivatives of $f(\cdot)$ respectively since we assume they are not available. Rather, the latter vector and matrix are built by requiring that the model (1) satisfy

$$m_k(y) = f(y) \quad \forall y \in Y, \tag{2}$$

where Y denotes the set of points at which the value of f is known, including the current iterate x^k. Building (1) requires to determine $f(x_k)$, the components of g_k and the entries of H_k, that is

$$p = 1 + n + \frac{1}{2}n(n+1) = \frac{1}{2}(n+1)(n+2) \tag{3}$$

parameters. Since the model (1) is entirely determined by the conditions (2), this is equivalent to say that we need to know at least p function values, that is

$$|Y| = p. \tag{4}$$

However this is not sufficient to guarantee the good quality of the model, and we need further geometric conditions – known as *poisedness* – on the points in Y to ensure both the existence and uniqueness of an interpolant. If we denote by $\{\phi_i(\cdot)\}_{i=1}^p$ a basis of the linear space of n-dimensional quadratics, then the model we are looking for may be written as

$$m_k(x) = \sum_{i=1}^{p} \alpha_i \phi_i(x)$$

for some scalars α_i $(i = 1, \ldots, p)$ to be computed. Particularizing conditions (2) to this expression for m_k yields

$$\sum_{i=1}^{p} \alpha_i \phi_i(y) = f(y) \quad \text{for all } y \text{ in } Y,$$

which is a system of $|Y| = p$ linear equations whose unknowns are the α_i's. It follows that $Y = \{y_1, \ldots, y_p\}$ is poised if the determinant

$$\delta(Y) = \det \begin{pmatrix} \phi_1(y_1) & \cdots & \phi_p(y_1) \\ \vdots & & \vdots \\ \phi_1(y_p) & \cdots & \phi_p(y_p) \end{pmatrix} \tag{5}$$

is nonzero. In practice, we consider Y to be poised whenever $|\delta(Y)| \geq \epsilon$ provided the y_j's span the neighbourhood of the current iterate x_k in a "good way". But this measure of poisedness is not the only possible one, and we will use another technique in what follows, that is more consistent with our use of the Newton fundamental polynomials as a basis for constructing the interpolating quadratics.

Before giving the complete formulation of the algorithm, we must mention some more of its ingredients related to the management of the interpolation set and to the fact that the computation of the interpolant is embedded in a trust-region framework.
The first issue deals with the acceptance of a new iterate. Assuming that after a successful iteration we get a point x_k^+ of associated function value $f(x_k^+)$ lower than $f(x_k)$, one may now 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, including x_k^+ in Y means that we need to remove another point y from Y (except maybe in the course of the first few iterations, where Y might be incomplete) in which case we must proceed with care so as not to deteriorate the geometry of Y, making the latter set "as poised as possible". Moreover, since x_k^+ is obtained through a minimization process which does not take the geometry of Y into account, there is no guarantee that the quality of the geometry of the interpolation set remains acceptable once x_k^+ is included in Y. This means that the quality of the geometry of Y as well as its poisedness might be deteriorated as and when new iterates are computed and accepted by the algorithm.
A second feature of trust-region algorithms is the management of the trust-region radius. At iteration k, the trust region is defined by $\mathcal{B}_k = \{x_k + s \mid \|s\| \leq \Delta_k\}$. In classical setups, the radius Δ_k is decreased when no significant progress can be made as regards the reduction of the objective function. In our framework, however, we must first verify that the interpolation set is poised before reducing Δ_k since a bad geometry might be the major reason for the algorithm to stall. If Y is not poised, we have to improve its geometry before possibly reducing Δ_k. It is particularly important not to modify Δ_k too early in the process since the geometry improvement is precisely achieved by introducing a new point y^+ in Y such that $\|y^+ - x_k\| \leq \Delta_k$ and using a suitable improvement measure to evaluate the advantage of replacing some past point $y^- \in Y \backslash \{x_k\}$ by y^+.
We will see in Section 3 how the use of the Newton fundamental polynomials provides a way to assess the abovementioned geometry improvements.

This concludes the description of the main ingredients of the algorithm, whose complete formulation may be stated as follows:

Algorithm UDFO

Step 0: Initialization. An initial point x_0 is given, as well as a trust-region radius $\Delta_0 > 0$, an initial model based on a vector g_0 and a matrix H_0, as

well as constants $\gamma_1 \leq 1 \leq \gamma_2$ and $0 < \eta_0 \leq \eta_1 < 1$.

Step 1: Criticality test. If g_k is small, then improve the geometry until Y is poised in a ball of radius $\delta \leq \mu \|g_k\|$ centered at x_k.

Step 2: Subproblem. Compute s_k from

$$\min_{s \in \mathcal{B}_k} m_k(x_k + s).$$

Step 3: Evaluation. Compute $f(x_k + s_k)$ and

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

If $\rho_k \geq \eta_1$, define $\mathcal{X}_k = \{x_k + s_k\}$.
Otherwise $\mathcal{X}_k = \{x_k\}$.

Step 4: Model management.
If $\rho_k \geq \eta_1$, include $x_k + s_k$ in Y.
Otherwise, if Y is not poised, improve the geometry (possibly enlarging $\mathcal{X}_k$).

Step 5: Next iterate. Compute

$$\hat{x}_k = \arg\min_{x \in \mathcal{X}_k} f(x)$$

and

$$\hat{\rho}_k = \frac{f(x_k) - f(\hat{x}_k)}{m_k(x_k) - m_k(x_k + s_k)}.$$

If $\hat{\rho}_k \geq \eta_0$, accept $\hat{x_k}$, and set $x_{k+1} = \hat{x}_k$.
Otherwise let the iterate unchanged, *i.e.* set $x_{k+1} = x_k$.

Step 6: Radius update.
If $\hat{\rho}_k \geq \eta_0$ or Y was poised, set $\hat{\Delta} = \Delta_k$.
If $\rho_k \geq \eta_1$, choose $\Delta_{k+1} \geq \hat{\Delta}$.
Otherwise choose $\Delta_{k+1} \in [\gamma_1 \hat{\Delta}, \gamma_2 \hat{\Delta}]$.
Go to Step 1.

3 Newton fundamental polynomials, geometry and sparsity

As indicated earlier, the interpolating quadratics (1) are built using Newton fundamental polynomials. The scope of this section is to present the basic concepts used when constructing these polynomials as well as to derive from this technique procedures for improving the geometry of Y and for including a new iterate x_k^+ in the interpolation set. Further, we show how to adapt the whole

method so as to consider the case where the Hessian $\nabla^2_{xx} f(x)$ is sparse. For more details on Newton fundamental polynomials – and more generally on multivariate interpolation – we refer the reader to Sauer and Yuan [32].

Newton fundamental polynomials are built with an increasing degree up to the degree d of the desired interpolation polynomial and are arranged by blocks. This is why the set Y is first partitioned into $d+1$ blocks $Y^{[\ell]}$ ($\ell = 0, \ldots, d$). The ℓ-th block contains $|Y^{[\ell]}| = \begin{pmatrix} \ell+n-1 \\ \ell \end{pmatrix}$ points and to each point $y_i^{[\ell]} \in Y^{[\ell]}$ corresponds a single Newton fundamental polynomial of degree ℓ satisfying the conditions

$$N_i^{[l]}(y_j^{[m]}) = \delta_{ij}\delta_{lm} \text{ for all } y_j^{[m]} \in Y^{[m]} \text{ with } m \leq l. \tag{6}$$

The details of the procedure for constructing the Newton fundamental polynomials for a given set Y have been omitted in this presentation (the interested reader is refered to *e.g.* Conn, Scheinberg and Toint [10]) since we prefer to focus on other algorithmic issues. It may be sufficient for now to mention that this procedure may be considered as a particular case in which the well-known Gram-Schmidt orthogonalization procedure is applied to an initial polynomial basis with respect to the inner product

$$\langle P, Q \rangle = \sum_{y \in Y} P(y)Q(y).$$

As an example, in the framework of quadratic interpolation (*i.e.* for the case $d = 2$), one might start with the following polynomials:

$$1, \ \{x_i\}_{1 \leq i \leq n}, \ \{x_i^2\}_{1 \leq i \leq n}, \{x_i x_j\}_{1 \leq i < j \leq n}. \tag{7}$$

Once the Newton fundamental polynomials are built, the interpolating polynomial $m_k(x)$ is given by

$$m_k(x) = \sum_{\ell=0}^{d} \sum_{i=1}^{|Y^{[\ell]}|} \lambda_\ell(y_i^{[\ell]}) N_i^{[\ell]}(x), \tag{8}$$

where the coefficients $\lambda_\ell(y_i^{[\ell]})$ are generalized finite differences defined by the following formulae (see Sauer and Yuan [32])

$$\lambda_0(x) = f(x) \text{ and } \lambda_{\ell+1}(x) = \lambda_\ell(x) - \sum_{i=1}^{|Y^{[\ell]}|} \lambda_\ell(y_i^{[\ell]}) N_i^{[\ell]}(x) \quad (\ell = 0, \ldots, d-1).$$

We now particularize the method to the case where the Hessian matrix $\nabla^2_{xx} f(x)$ is known to be sparse independently of x. This implies that there exists a symmetric index set

$$\mathcal{S} = \{ \ (i,j) \mid 1 \leq i, j \leq n \text{ and } \langle e_i, \nabla^2_{xx} f(x) e_j \rangle = 0 \ \forall x \in \mathbb{R}^n \}. \tag{9}$$

Intuitively, the sparse nature of the Hessian should be reflected in the model (1) approximating $f(x)$ within the trust-region. However, as we said before, working in the framework of derivativre-free optimization implies that the matrix H_k appearing in (1) may be different from the Hessian of $f(\cdot)$ and thus the particular structure of the Hessian is expected to reverberate in a less direct way in the algorithm.
A simple idea for the process for building the interpolating quadratics to take advantage of the simplified structure of the Hessian is to reduce the approximation space to the set of quadratic polynomials satisfying (9). Implementing this strategy in the framework of multivariate interpolation amounts to compute the Newton fundamental polynomials $N_i^{[\ell]}$ by orthogonalizing a *partial* basis of polynomials. For instance, if we consider an initial basis of the type described by (7), we will exclude the polynomials taking the form $x_i x_j$ for $(i,j) \in \mathcal{S}$.
As a result, the number of polynomials to generate is decreased and the algorithm needs fewer interpolation points. In other words, the interpolation set Y may become significantly smaller than for the case for which the Hessian matrix is dense.
This way to proceed and to deal with sparsity has a triple impact on the method and the computations performed at each iteration of the algorithm: first, less data points are needed for complete interpolation since $|Y|$ is now smaller than p, therefore allowing the algorithm to revise its Hessian approximation more quickly; second, less polynomials need being built and stored and, third, each polynomial is smaller. As one could expect, these are advantageously reflected in the numerical tests reported in Section 4.

We now return to the question of measuring poisedness of the interpolation set in conjunction with Newton fundamental polynomials. When constructing these polynomials, the procedure has to normalize them and to this end performs a division by $|N_i^{[\ell]}(y_i^{[\ell]})|$. While from a theoretical point of view it may be sufficient to require this term to be nonzero, in practice we must verify that

$$|N_i^{[\ell]}(y_i^{[\ell]})| \geq \theta \tag{10}$$

for some parameter $\theta > 0$. The values $|N_i^{[\ell]}(y_i^{[\ell]})|$ are known as *pivots* and θ is called the *pivoting threshold*. If condition (10) is satisfied, then the Newton fundamental polynomials are said to be *well poised*.
This connection between geometry, poisedness and Newton fundamental polynomials allows us to derive suitable mechanisms to control and improve the quality of the geometry of Y. When having to *remove a point* y^- from Y, we choose y^- to be the point associated to the smallest orthogonalization pivot, that is the point $y_i^{[\ell]}$ for which $|N_i^{[\ell]}(y_i^{[\ell]})|$ is minimal, thus making the Newton fundamental polynomials well poised for the subsequent computations. On the other side, a reasonable strategy for *improving the geometry* of the interplation set Y might be to replace a point $y^- = y_i^{[\ell]} \neq x_k$ by another point y^+ such that

$|N_i^{[\ell]}(y^+)|$ is larger, for instance

$$y^+ = \arg\max_{y \in \mathcal{B}_k} |N_i^{[\ell]}(y)|$$

provided $|N_i^{[\ell]}(y^+)| \geq 1 + \theta$ since otherwise the geometry was already fine.
Of course these are not the only possible strategies for the management of Y and the interested reader may find a more complete treatment of these issues in Conn, Scheinberg and Toint [11] and Conn, Gould and Toint [9].

For the sake of completeness, we would like to conclude this section by mentioning the two main convergence results allowing us to justify algorithm UDFO. The first result is a bound on the interpolation error; it says that, under appropriate assumptions (see Sauer and Yuan [32] or Theorem 9.4.4 in Conn, Gould and Toint [9] for the details), one has

$$|f(x) - m_k(x)| \leq \kappa \Delta_k^3 \max_{Y,x} |N_i^{[\ell]}(y_j^{[\ell+1]})|$$

for all $x \in \mathcal{B}_k$ and some constant κ independent of k. This result is of crucial importance since it guarantees that the model $m_k(x)$ is sufficiently close to $f(x)$ within the trust region. When particularizing this to the case of quadratic models ($d = 2$), we may deduce that algorithm UDFO converges towards critical points and, more precisely,

- if the model $m_k(x)$ is at least *fully linear* (*i.e.* $|Y| \geq n + 1$) and the interpolation set Y is well poised, the algorithm produces a sequence of iterates converging towards a *first-order* critical point,
- if the model is at least *fully quadratic* (*i.e.* $|Y| \geq p$) and Y is well poised, then convergence to *second-order* critical points is ensured;

(see Conn, Scheinberg and Toint [10] for details).

4 Numerical experience

The software we designed for implementing the algorithm presented above is called UDFO. It is coded in Fortran.
We tested UDFO by selecting a number of problems having a sparse Hessian from the CUTE collection: `TRIDIA`, `SCHMVETT` and `BDQRTIC` have a banded Hessian (with a semi-bandwidth value of 2, 3 and 5 respectively) while the other problems have more general sparsity patterns. We run UDFO for three different problem dimensions, namely $n = 10$, 15 and 20 (except for the `DIXMAAN` problems since the latter require n to be a multiple of 3 – for this reason, we used $n = 9$, 15 and 21 respectively) and compared the results achieved with both possible configurations of UDFO, that is ignoring structure and using suitable data structure and mechanisms so as to take sparsity into account. The results

are summarized in Tables 1, 2 and 3. They show the percentage of nonzero entries (which we denote by s further in this text) in H_k, the size p of the interpolation set Y, the number of function evaluations, the number of iterations and the CPU time required for solving the abovementioned problems using both configurations of UDFO. We found interesting to complete this information by

Problem name	Nonzero	Size of Y		Fct. eval.		Iter.		CPU time	
($n = 10$)	entries	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
TRIDIA	28.0%	65	29	99	63	13	13	1.35	0.32
ARWHEAD	28.0%	65	29	311	150	70	75	26.54	2.69
DIXMAANA	33.3%	54	27	301	108	108	66	25.40	1.92
DIXMAANE	33.3%	54	27	298	152	119	56	28.40	1.63
SCHMVETT	44.0%	65	37	243	138	71	37	27.41	2.55
DIXMAANB	53.0%	54	35	259	188	120	98	28.66	6.51
DIXMAANC	53.0%	54	35	288	255	91	131	20.85	8.90
DIXMAAND	53.0%	54	35	319	211	124	120	29.87	8.11
DIXMAANF	53.0%	54	35	284	232	113	111	26.89	7.48
BDQRTIC	70.0%	65	50	519	327	219	199	95.08	41.32
SPARSINE	84.0%	65	57	356	349	184	197	78.68	61.55

Table 1: Results for $n = 10$. (a) Ignoring the Hessian structure. (b) Exploiting sparsity.

Problem name	Nonzero	Size of Y		Fct. eval.		Iter.		CPU time	
($n = 15$)	entries	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
TRIDIA	19.1%	135	44	182	91	20	20	12.63	1.47
ARWHEAD	19.1%	135	44	790	339	149	175	524.13	21.00
DIXMAANA	20.0%	135	45	534	180	309	110	1181.01	13.43
DIXMAANE	20.0%	135	45	698	238	204	122	735.27	14.99
SCHMVETT	30.7%	135	57	371	185	48	48	97.28	11.10
DIXMAANB	32.4%	135	59	674	285	184	172	650.83	51.64
DIXMAANC	32.4%	135	59	732	330	237	176	881.65	53.31
DIXMAAND	32.4%	135	59	724	467	237	252	882.33	77.96
DIXMAANF	32.4%	135	59	901	371	273	246	1031.14	75.89
BDQRTIC	51.1%	135	80	1014	639	273	267	1044.24	223.89
SPARSINE	71.5%	135	103	1163	690	402	210	1590.30	378.50

Table 2: Results for $n = 15$. (a) Ignoring the Hessian structure. (b) Exploiting sparsity.

adding the three barcharts of Figure 1, showing the evolution of the impact of using structure when the dimension of the problem increases, which is based on

Problem name ($n = 20$)	Nonzero entries	Size of Y (a)	Size of Y (b)	Fct. eval. (a)	Fct. eval. (b)	Iter. (a)	Iter. (b)	CPU time (a)	CPU time (b)
TRIDIA	14.5%	230	59	293	122	23	23	52.13	3.60
ARWHEAD	14.5%	230	59	1268	333	196	183	3264.06	50.22
DIXMAANA	14.3%	252	63	1350	314	208	150	4440.74	48.24
DIXMAANE	14.3%	252	63	1537	354	381	208	9431.37	68.89
SCHMVETT	23.5%	230	77	950	298	128	95	1856.33	56.88
DIXMAANB	23.3%	252	83	1418	486	519	270	13279.99	224.13
DIXMAANC	23.3%	252	83	1740	460	340	328	8217.48	275.12
DIXMAAND	23.3%	252	83	1831	453	311	237	7393.43	194.73
DIXMAANF	23.3%	252	83	1495	565	349	344	8487.44	289.10
BDQRTIC	40.0%	230	110	1610	893	551	375	10822.45	813.37
SPARSINE	61.0%	230	152	1410	1406	566	547	11072.81	3408.54

Table 3: Results for $n = 20$. (a) Ignoring the Hessian structure. (b) Exploiting sparsity.

the following three ratios:

$$\rho_Y = \frac{\text{Size of } Y \text{exploiting sparsity}}{\text{Size of } Y \text{ignoring structure}} \quad ,$$

$$\rho_{\text{eval}} = \frac{\text{Function evaluations exploiting sparsity}}{\text{Function evaluations ignoring structure}} \quad ,$$

$$\rho_{\text{iter}} = \frac{\text{Number of iterations exploiting structure}}{\text{Number of iterations ignoring structure}} \quad ,$$

$$\rho_{\text{CPU}} = \frac{\text{CPU time exploiting structure}}{\text{CPU time ignoring structure}}.$$

Tables 1, 2 and 3 and Figure 1 clearly show that the savings in terms of computational effort are considerable, especially when n is high. Only the number of iterations is not always lower when using structure, but this criterion is less important in terms of numerical performance in the framework of derivative-free optimization.

We next assess the advantages of exploiting the sparse structure of the Hessian matrix as regards storage issues. When ignoring the structure, we store the lower triangular part of H_k in a `DOUBLE PRECISION` array of length $n(n+1)/2$, which involves $d(n) = 4n^2 + 4n$ bytes. By contrast, when allowing UDFO to take sparsity into account, we use a first array of `DOUBLE PRECISION` variables to store the diagonal of H_k as well as its other nonzero entries – note that the whole diagonal must be nonzero, or otherwise the function is unbounded below. Using the percentage s of nonzero elements among the n^2 entries of H_k as a parameter, this first array contains

$$n + \frac{sn^2 - n}{2} = \frac{sn^2 + n}{2}$$

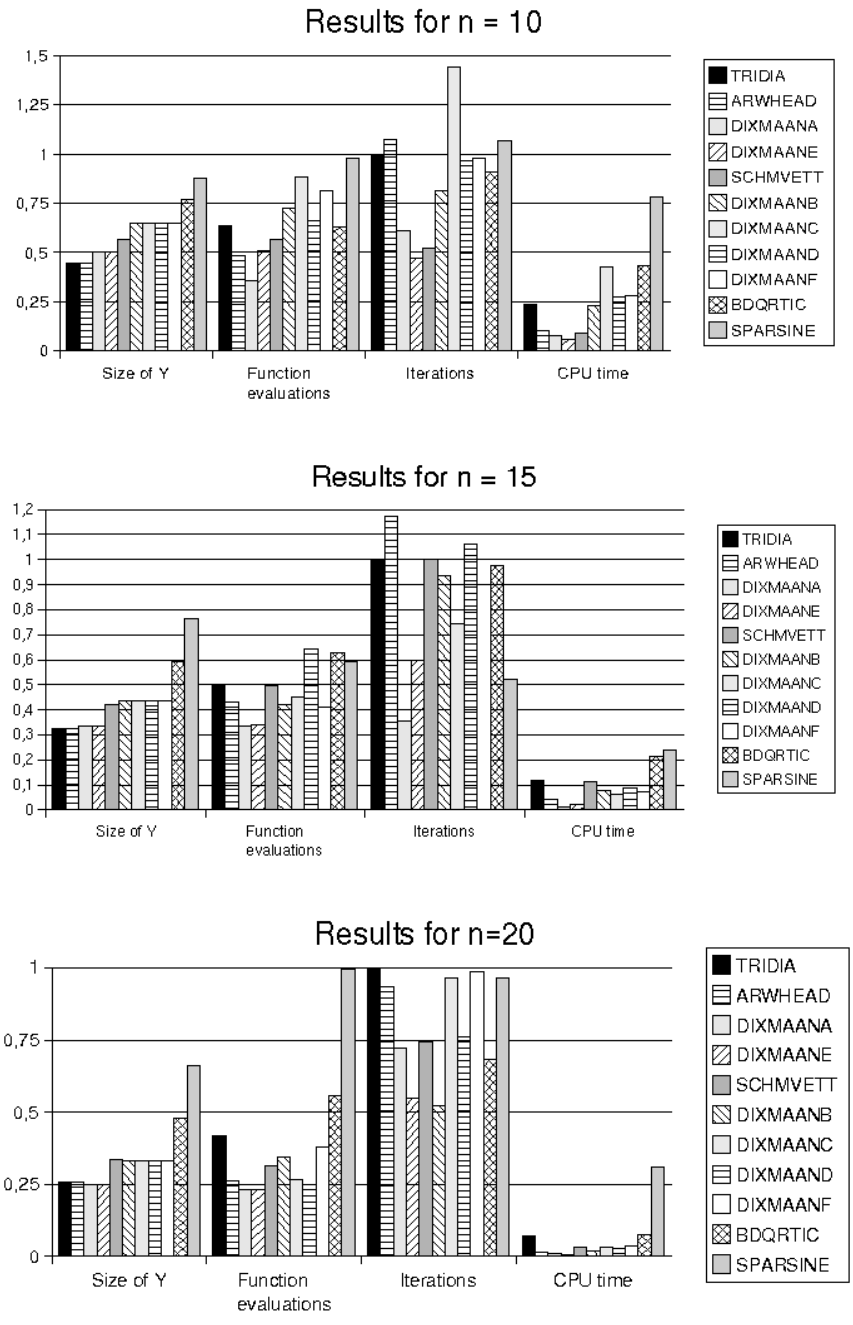

Figure 1: Impact of exploiting structure when the dimension for $n = 10, 15$ and 20.

`DOUBLE PRECISION` elements. But we also need information about the location of the nonzero entries and this is why we also use an array of `INTEGER` variables containing the successive pairs of indices between 1 and n corresponding to the positions of nonzero entries in the strictly lower triangular part of H_k. This second array is thus of length $sn^2 - n$. As a consequence, the overall space required for exploiting structure is

$$u(n, s) = 8 \ \frac{sn^2 + n}{2} + 4 \ (sn^2 - n) = 8 \ sn^2$$

bytes. Figure 2 displays the functions $d(n)$ and $u(n, s)$ for three different values of s – 25%, 33% and 50% – corresponding to the average of nonzero entries in all considered problems for $n = 10$, 15 and 20 respectively. Only the curve for $s = 50\%$ is close to $d(n)$, which leads to the somewhat expected conclusion that matrices with as many nonzero entries as 50% are not much advantageously handled by a code designed for sparse matrices.

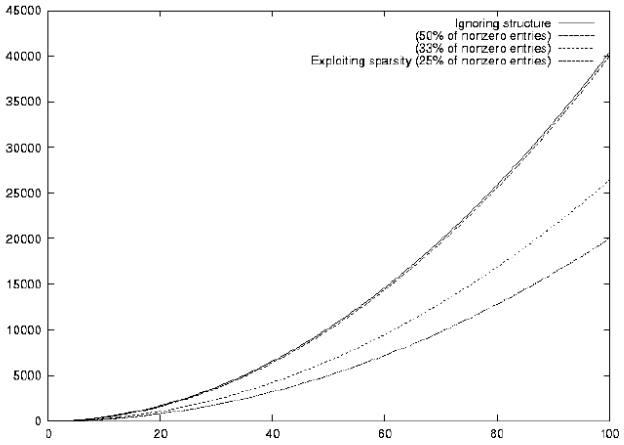

Figure 2: Storage required for the matrix H_k (in bytes).

5 Conclusion and perspectives

The method discussed in this paper proves to be a very useful technique when sparsity is known. Its main advantages are the much smaller dimension of the working space and the increased speed, as was confirmed by a series of numerical experiments.

We believe that the method can be extended so as to use dominant parts of

the Hessian matrix only, *i.e.* introducing "artificial sparsity" and ignoring some of its entries that may be considered as being neglectible. Finding appropriate criteria for selecting such entries and implementing them within the framework described in this paper should yield a further progress from the point of view of storage and speed. Explicit consideration of the partially separable structure of the objective function should also result in important practical savings. Both these extensions are subject of ongoing research.

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