A NUMERICAL STUDY OF THE LIMITED MEMORY BFGS METHOD AND THE TRUNCATED-NEWTON METHOD FOR LARGE SCALE OPTIMIZATION*

STEPHEN G. NASH[†] AND JORGE NOCEDAL[‡]

Abstract. This paper examines the numerical performances of two methods for large-scale optimization: a limited memory quasi-Newton method (L-BFGS), and a discrete truncated-Newton method (TN). Various ways of classifying test problems are discussed in order to better understand the types of problems that each algorithm solves well. The L-BFGS and TN methods are also compared with the Polak–Ribière conjugate gradient method.

Key words. large scale nonlinear optimization, limited memory method, truncated-Newton method, conjugate-gradient method

AMS(MOS) subject classifications. 65, 49

1. Introduction. Suppose we had to solve an unconstrained optimization problem,

$$(1.1) \quad \min f(x),$$

where f is a smooth function, the number of variables n is large, and a subroutine to evaluate $f(x)$ and $\nabla f(x)$ is available. What method should we choose?

The answer will depend on how much knowledge we have about the structure of the objective function, and on the size of the problem. Newton's method using sparse matrix estimation techniques [2], and the partitioned quasi-Newton method of Griewank and Toint [8] can be highly efficient if sufficient information is supplied to the algorithms. However, it is sometimes too difficult for the user to provide this information, and efficient and reliable software that supplies it automatically is not yet available. In addition, the storage and arithmetic costs for these methods can be prohibitive if the Hessian matrix is not very sparse, or if the problem is extremely large. In these cases, it is better to use other, less ambitious, algorithms. The limited memory BFGS method (L-BFGS) and the discrete truncated-Newton method (TN) represent two classes of methods in this category. They use a low and predictable amount of storage, and only require the function and gradient values at each iterate—and no other information about the problem. Both methods have been tested on large problems and their performance appears to be satisfactory.

In this paper we study the relative performance of L-BFGS and TN on a set of 45 large test problems with a number of variables ranging from 100 to 10,000. Our goal is to study the two methods in a controlled environment to highlight the differences between them and to indicate to the reader the types of problems that are well suited to each algorithm. Our study is limited by the collection of test problems we have used; however, we have tried to produce a test set of considerable breadth. Some test problems arise from applications, whereas others are artificial. Some of the

* Received by the editors January 10, 1990; accepted for publication (in revised form) January 8, 1991.

[†] Operations Research and Applied Statistics Department, George Mason University, Fairfax, Virginia 22030.

[‡] Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, Illinois 60208. This author was supported by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U.S. Department of Energy, under contract DE-FG02-87ER25047-A001, and by National Science Foundation grant ASC 87-19583.

problems are quadratic or nearly quadratic, while others are highly nonlinear. Some are nonconvex. There are varying degrees of ill-conditioning. Our conclusions can only be based on this sample of results, but we hope that they may be more generally useful—both to readers who solve practical problems, and to readers who develop and test new algorithms.

Many limited memory methods have been proposed; some resemble the conjugate-gradient method, and others, the BFGS method. We chose the L-BFGS method because the studies of Gilbert and Lemaréchal [4] and Liu and Nocedal [10] seem to indicate that it is the best limited memory method available to date. Several implementations of the truncated-Newton method have also been proposed, but few codes are as developed as that of Nash [13], which we have chosen for our tests.

Since the authors of the present paper have been closely involved in the development of the methods tested here, a careful effort was made to run them in their best form. This probably also avoided a conscious or unconscious bias towards one of the methods, while setting the test problems or while interpreting the results. The two codes used for this study are not new; they have both been refined during the last years, and neither was especially modified for these runs. We were aware of the dangers of “tuning” methods to a set of test problems. As a result, the nature of the computational tests was specified in detail in advance: A single, fixed version of each algorithm was provided, with all parameters such as tolerances and stopping conditions chosen beforehand. The set of test problems was also chosen in advance, and a *single* run on each test problem was made. (One exception had to be made. On three runs, the algorithms were unable to satisfy our prespecified convergence tolerance. These three problems were run again with a slightly less stringent convergence tolerance.)

Our results indicate that, for L-BFGS and TN, two properties of the problems can be used to make an informed decision on the choice of method. These are the cost of the function-gradient evaluation and the “degree of nonlinearity” of f (this latter property is defined more precisely in §4).

What follows is a brief outline of the paper. The L-BFGS and TN algorithms are described in §2; the test problems and numerical results are presented in §3. The analysis of the test problems, their classification into types, and the correlation of these types with the two methods, appear in §§4 and 5. In the final part of the paper, we compare the two methods to the Polak–Ribière conjugate-gradient method, to obtain another measure of their efficiency.

2. Description of the TN and L-BFGS methods. The truncated-Newton algorithm and the limited memory BFGS method used in this study have already been published, and hence we will only describe them in outline. The L-BFGS has been incorporated into the Harwell Library under the name VA15, and is described by Liu and Nocedal [10]. The TN method is described by Nash [13] (a more precise description of many parts of the method is in Nash [14]). We now give a brief description of their major components.

2.1. The truncated-Newton algorithm. At each “outer” iteration, an approximate solution is found to the Newton equations

$$(2.1) \quad G_k p_k = -g_k,$$

where $g_k = g(x_k) = \nabla f(x_k)$ is the gradient at the k th iteration, and $G_k = \nabla^2 f(x_k)$ is the Hessian. This is done using an “inner” iteration based on a preconditioned linear

conjugate-gradient method [3]. If indefiniteness in the Hessian is detected, the inner iteration is terminated. The approximate solution p_k (the search direction) is then used in a linesearch to get a new point $x_{k+1} = x_k + \alpha_k p_k$ where $f(x_{k+1}) < f(x_k)$ and $\alpha_k > 0$. More precisely:

- (1) The outer iteration is terminated when

$$(2.2) \quad \|g(x_k)\|_\infty < 10^{-6}(1 + |f(x_k)|).$$

- (2) The linesearch was performed using the iteration described by Gill and Murray [6]. It is based on cubic interpolation, and is terminated when

$$(2.3) \quad |g(x_k + \alpha_k p_k)^T p_k| \leq \eta |g(x_k)^T p_k|$$

and

$$(2.4) \quad f(x_k) - f(x_k + \alpha_k p_k) \geq -\mu \alpha_k p_k^T g(x_k),$$

with $\eta = 0.25$ and $\mu = 10^{-4}$. An initial guess of $\alpha_k = 1$ is used. We refer to (2.3)–(2.4) as the *strong Wolfe conditions*.

- (3) The conjugate-gradient inner iteration is preconditioned by a scaled two-step limited memory BFGS method, with Powell's restarting strategy used to reset the preconditioner periodically. It is based on formula (6.5) in [6]: Let t be the iteration where the last restart occurred. Define $s_1 = x_k - x_t$, $y_1 = g_k - g_t$, $s_2 = x_k - x_{k-1}$, $y_2 = g_k - g_{k-1}$, and let D_k be a scaling matrix. Then the approximation H_k to the Hessian is obtained via

$$(2.5) \quad U = \Gamma_{\text{BFGS}}(D_k, y_1, s_1), \quad H_k = \Gamma_{\text{BFGS}}(U, y_2, s_2),$$

where $\Gamma_{\text{BFGS}}(A, y, s)$ represents the formula for the BFGS update initialized with matrix A , and with vectors y and s corresponding to the change in the gradient and parameter vectors, respectively. The scaling matrix D_k used here is a diagonal approximation to the Hessian obtained by BFGS updating; see equation (10) in Nash [14]. This reference also describes the preconditioner in more detail. We note, in particular, that safeguarding is needed to ensure that the scaling matrix is sufficiently positive definite.

- (4) The matrix-vector products required by the inner conjugate-gradient algorithm are obtained by finite differencing [19]. Given a vector v , the product $G_k v$ is approximated by

$$(2.6) \quad G_k v \approx [g(x_k + \delta v) - g_k] / \delta,$$

where $\delta = (1 + \|x_k\|_2) \sqrt{\epsilon}$, and ϵ is the relative machine precision (the “machine epsilon”).

- (5) The inner algorithm is normally terminated when

$$(2.7) \quad i \left(1 - \frac{Q_k(p_{i-1})}{Q_k(p_i)} \right) \leq 0.5,$$

where i is the counter for the inner iteration, p_i is the i th approximation to the search direction, and $Q_k(p) = \frac{1}{2} p^T G_k p + p^T g_k$ is the value of the quadratic model. This test is explained further in [16]; it guarantees a linear rate of convergence for the optimization algorithm, and detects convergence of the

inner iteration. An upper limit of 50 inner iterations is imposed (this limit was encountered on five of the problems). In addition, the inner algorithm is terminated whenever nonpositive-definiteness is detected in the Hessian. In this case, p_k is the iterate obtained prior to detecting indefiniteness.

The truncated-Newton method requires storage for 16 vectors of length n (the vectors x_k , $g(x_k)$, and 14 work vectors). Each outer iteration consists of three stages: setup, computation of the search direction, and the linesearch. These costs are listed in Table 1. The typical cost was obtained by assuming 1 iteration in the linesearch and 5 inner iterations; these are typical values observed in our test runs.

TABLE 1
Cost of truncated-Newton iteration.

Operation	Flops	f-g	Storage
Setup	$81n$	0	$16n$
Search direction iteration	$48n$	1	
Line search iteration	$4n$	1	
Typical cost	$325n$	6	

Here “Flops” denotes additions, multiplications, or divisions, and “f-g” refers to the number of function-gradient evaluations. The setup is performed once per outer iteration. The search direction and linesearch iterations are repeated until appropriate convergence tests are satisfied, although the linesearch is frequently terminated after only one iteration. Note that each inner iteration requires one gradient evaluation to estimate the matrix-vector product (2.6). The number of inner iterations can vary greatly from problem to problem; thus large deviations from this “typical cost” occur in practice. On the test problems in this paper, where an upper limit of 50 inner iterations was imposed, the number of inner iterations varied between 1 and 50 with both extremes achieved.

2.2. The limited memory BFGS method. We view the L-BFGS method as an adaptation of the BFGS method to large problems, and the implementation of both methods is very similar. In the BFGS method, the approximation H_k to the inverse Hessian matrix of f is updated by

$$(2.8) \quad H_{k+1} = V_k^T H_k V_k + \rho_k s_k s_k^T,$$

where

$$(2.9) \quad V_k = I - \rho_k y_k s_k^T,$$

$s_k = x_{k+1} - x_k$, $y_k = g_{k+1} - g_k$, and $\rho_k = 1/y_k^T s_k$. The search direction is given by

$$(2.10) \quad p_{k+1} = -H_{k+1} g_{k+1}.$$

We say that H_{k+1} is obtained by applying one BFGS correction to H_k . In the L-BFGS method, instead of forming the matrices H_k , we save the vectors s_k and y_k that define them implicitly. We choose a number m of corrections that we wish to store, and at the k th iteration (with $k > m$) proceed as follows:

- (1) Define the diagonal matrix

$$(2.11) \quad H_k^0 = \frac{y_k^T s_k}{\|y_k\|_2^2} I,$$

where I denotes the identity matrix. This scaling is suggested by Oren and Spedicato [20].

- (2) Obtain H_k by applying m BFGS corrections to H_k^0 , using the m previous vectors s_i and y_i . Compute the product $H_k g_k$ using the recursive formula described in §4 of [18]. This formula takes advantage of the symmetry of the BFGS updating to reduce the number of arithmetic operations.
- (3) Perform a linesearch along the direction p_k , enforcing the strong Wolfe conditions (2.3)–(2.4), and trying the steplength $\alpha_k = 1$ first. We use the values $\eta = 0.9$ and $\mu = 10^{-4}$. The linesearch is performed by means of the routine CVSRCH of Moré and Thuente [11], which uses cubic interpolation.
- (4) The iteration is finished when (2.2) is satisfied.

We note that once m is chosen, the only parameters in the L-BFGS method are the constants η and μ . The simple scaling of step 1 contributes significantly to the efficiency of the method. Our experience indicates that values of m in the range $3 \leq m \leq 7$ give the best results, and in this paper we use the value $m = 5$. The L-BFGS method requires $2m(n+1) + 4n$ storage locations. Table 2 gives the storage and computational requirements of the L-BFGS method, assuming $m = 5$. We have observed that L-BFGS requires an average of 1.2 iterations within the linesearch; using this value we obtained the typical cost of the iteration, given in Table 2.

TABLE 2
Cost of the limited memory BFGS iteration.

Operation	Flops	f-g	Storage
Setup	$4n$	0	$14n$
Search direction computation	$33n$	0	
Linesearch iteration	$4n$	1	
Typical cost	$42n$	1.2	

Except for the first $m - 1$ iterations, the cost of computing the search direction in the L-BFGS method is uniform and predictable; it is a function of m and n .

Comparing Tables 1 and 2, we see that the storage requirements of TN and L-BFGS (with $m = 5$) are very similar, and that the arithmetic costs are drastically different. TN uses an elaborate, variable-cost iteration with partial second-derivative information, whereas L-BFGS uses a fixed, low-cost formula requiring no extra derivative information. In fact, TN *contains* a limited memory method, since the preconditioner used for the inner iteration is similar to an L-BFGS matrix with $m = 2$, and several multiplications with this matrix are performed in one iteration. TN and L-BFGS therefore use different principles to compute search direction. It should be noted that the routines used for the linesearch are similar: both use cubic interpolation to obtain the strong Wolfe conditions (only the value of the parameter η in (2.3) is different).

3. Numerical tests. All the problems used in our tests have been described elsewhere; approximately half of them were used by Liu and Nocedal in their study of L-BFGS [10]. Table 3 lists the problems and the number of variables used for the runs, and gives references to detailed descriptions of the test functions and starting points. For test problems 8, 9, and 10, starting point 3 from the reference was used. The problems are not numbered consecutively because they belong to a larger collection of test problems to which we may want to refer in future studies. The number of variables in the test set ranges from 100 to 10,000, and, as will be seen in §4, the problems form a varied grouping. We verified that, in each run, both methods converged to the same solution point.

The results of the tests are given in Tables 4 and 5. There “It” and “f-g” record

TABLE 3
List of test functions

Problem	Name	Reference	n
1	Calculus of variations 1	Gill and Murray [5]	100, 200
2	Calculus of variations 2	Gill and Murray [5]	100, 200
3	Calculus of variations 3	Gill and Murray [5]	100, 200
6	Generalized Rosenbrock	Moré, Garbow, and Hillstom [12]	100, 500
8	Penalty 1	Gill and Murray [6]	100, 1000
9	Penalty 2	Gill and Murray [6]	100
10	Penalty 3	Gill and Murray [6]	100, 1000
28	Extended Powell singular	Moré, Garbow, and Hillstom [12]	100, 1000
29	Variably dimensioned	Moré, Garbow, and Hillstom [12]	100, 500
31	Brown almost linear	Moré, Garbow, and Hillstom [12]	100, 200
38	Tridiagonal 1	Buckley and LeNir [1]	100, 1000
39	Linear minimal surface	Toint [23]	121, 961
40	Boundary-value problem	Toint [23]	100
41	Broyden tridiagonal nonlinear	Toint [23]	100
42	Extended ENGVL1	Toint [23]	1000, 10,000
43	Ext. Freudenstein and Roth	Toint [23]	100, 1000
45	Wrong extended Wood	Toint [23]	100
46(1)	Matrix square root ($ns = 1$)	Liu and Nocedal [9]	100
46(2)	Matrix square root ($ns = 2$)	Liu and Nocedal [9]	100
47	Sparse matrix square root	Liu and Nocedal [9]	100, 1000
48	Extended Rosenbrock	Moré, Garbow, and Hillstom [12]	1000, 10,000
49	Extended Powell	Moré, Garbow, and Hillstom [12]	100, 1000
50	Tridiagonal 2	Toint [23]	100, 1000
51	Trigonometric	Moré, Garbow, and Hillstom [12]	100, 1000
52	Penalty 1 (2nd version)	Moré, Garbow, and Hillstom [12]	1000, 10,000
53	INRIA ults0	Gilbert and Lemaréchal [4]	403

the iteration count and the number of function-gradient evaluations, respectively. For the truncated-Newton method, this includes the number of gradient evaluations of the inner iteration (one gradient computation is considered to be as expensive as a simultaneous function and gradient evaluation). The times are measured in seconds and reflect total execution time, including function-gradient evaluations. The runs were made on one processor of an Encore Multimax computer, using Fortran in double precision (about 16 decimal digits). An upper bound of 9,999 function-gradient evaluations was imposed, but was only encountered by L-BFGS on test function one; this is indicated by a “+” next to the function-gradient count. Most of the test functions were run for two values of n . Table 4 presents the results for the smaller dimensions.

Table 5 gives the results for higher dimensions. On three runs, both routines terminated abnormally in the linesearch (a lower point could not be found). This is indicated by a “*.” In all three cases the algorithms were close to the solution. These problems were rerun with the convergence tolerance in (2.2) set to 10^{-5} , to make it less stringent. With this change, these runs were successful and are included in Table 5. As before, “+” indicates that the function evaluation limit was reached.

The results of Tables 4 and 5 are summarized in Table 6. “Much better” is defined to be a difference of more than 30 percent in results. Differences of less than 10 percent were considered to be insignificant (“even”), as were absolute differences of less than one second and differences of less than five function-gradient evaluations. A failure is recorded as “much better” performance for the algorithm that succeeded.

What can we conclude from these results? First, neither algorithm is clearly superior to the other. Second, the limited-memory BFGS method tends to use fewer

TABLE 4
Smaller test problems. Comparison of the limited memory BFGS method ($m = 5$) with the truncated-Newton method.

P	N	L-BFGS			TN		
		It	f-g	Time	It	f-g	Time
1	100	9707	+9999	2380.0	28	466	105.0
2	100	1605	1669	304.0	27	242	41.4
3	100	3095	3216	640.0	45	325	60.8
6	100	257	291	19.0	78	683	35.3
8	100	30	36	2.1	4	26	0.8
9	100	21	23	2.4	8	48	4.4
10	100	82	90	7.1	20	107	7.3
28	100	57	67	3.6	14	70	3.0
29	100	36	37	2.4	9	42	1.3
31	100	24	27	10.7	14	101	38.5
38	100	120	128	8.5	18	77	4.4
39	121	66	70	8.4	18	187	19.6
40	100	2219	2296	188.0	55	2091	146.0
41	100	28	31	2.1	14	77	4.7
42	1000	15	17	10.2	15	75	41.0
43	100	19	21	1.7	10	38	2.9
45	100	48	56	3.8	14	59	3.3
46(1)	100	362	377	75.9	30	339	61.9
46(2)	100	438	453	92.8	35	556	101.0
47	100	87	95	10.1	17	94	8.8
48	1000	38	49	26.4	16	79	32.0
49	100	57	67	3.8	14	70	3.0
50	100	129	133	9.5	17	78	4.2
51	100	53	60	8.9	28	233	30.2
52	1000	5	6	2.3	3	10	4.3

TABLE 5
Larger test problems. Comparison of the limited memory BFGS method ($m = 5$) with the truncated-Newton method.

P	N	L-BFGS			TN		
		It	f-g	Time	It	f-g	Time
1	200	9695	+9999	5040.0	38	929	428.0
2	200	1734	1785	646.0	37	456	154.0
3	200	7248	7482	2960.0	76	599	220.0
6	500	1054	1177	389.0	356	3446	796.0
8	1000	30	34	21.0	12	58	23.9
10	1000	103	*114	89.4	30	*200	142.0
28	1000	54	61	35.8	15	75	34.6
29	500	48	*49	15.4	12	*54	8.8
31	200	3	4	5.8	4	20	24.9
38	1000	405	423	302.0	33	208	121.0
39	961	165	172	187.0	27	387	364.0
42	10,000	14	17	102.0	24	111	696.0
43	1000	16	20	15.4	15	75	59.1
47	1000	145	157	168.0	22	160	145.0
48	10,000	37	50	261.0	29	118	639.0
49	1000	54	61	35.6	14	68	31.8
50	1000	457	476	328.0	30	210	118.0
51	1000	46	*57	80.1	35	*370	467.0
52	10,000	6	8	32.5	5	19	90.9
53	403	57	63	410.0	14	100	656.0

TABLE 6

Summary of results: number of problems for which a method was better in terms of function-gradient evaluations and time.

Result	f-g	Time
L-BFGS much better	18	21
L-BFGS better	6	1
even	8	4
TN better	2	1
TN much better	11	18

function-gradient evaluations. Third, in terms of time, neither algorithm is a clear winner: the higher iteration cost of TN is compensated by a much lower iteration count, on the average. Fourth, the truncated-Newton method solved all the problems, whereas the limited memory BFGS method failed twice (on both versions of the first test problem). In §5 we analyze these results further, and present more detailed conclusions.

Tests of a simulated Newton method were also made. Algorithm TN was modified by changing the termination rule for the inner algorithm from (2.7) to

$$\frac{\|Gp_i + g_k\|_2}{\|g_k\|_2} \leq 10^{-8},$$

and with an upper limit of $\min(n, 500)$ inner iterations imposed. Even though this does not represent a well-designed Newton method for large scale problems, it can indicate how many outer iterations would be required if the costs of the inner algorithm could be ignored. We refer to this simulated Newton method as SN. On the smaller test problems, SN required 313 iterations and TN required 551; in the worst case TN required five times more iterations. On the larger test problems, SN required 598 iterations and TN required 828; in the worst case TN required seven times more iterations. Hence, over the entire test set, TN required about 50 percent more iterations than SN. The L-BFGS method, whose iteration is much cheaper, typically requires between 3 and 10 times more iterations than TN.

We conclude this section with a few comments on the partitioned quasi-Newton method of Griewank and Toint [8]. It assumes that the objective function is partially separable, i.e., that it can be written as

$$f(x) = \sum_{i=1}^{ne} f_i(x),$$

where the ne element functions f_i depend only on a few variables. The partitioned quasi-Newton method (PQN) takes advantage of this structure of f by updating a quasi-Newton approximation to each of the element functions f_i . Liu and Nocedal [10] compared L-BFGS and PQN, and concluded that when the number of variables entering into the element functions is very small (say, less than four), PQN is vastly superior to L-BFGS, both in terms of function evaluations and time. However, if the element functions f_i depend on four or five variables, L-BFGS and PQN are often comparable. Furthermore, if more than five or six variables enter into the element functions, L-BFGS is likely to be more efficient.

4. Classification of the test problems. We would like to better understand the types of problems that each algorithm solves well. This immediately raises the

question of how to classify the test problems. Among the various function characteristics that are relevant to the convergence theory or computational behavior of algorithms, we have selected the following.

- (1) **Deviation from quadratic.** To assess this, we use the Taylor series approximation of the gradient, and define

$$(4.1) \quad \text{DQ} = \frac{\|g(x_0) - g(x^*) - G(x^*)p\|_\infty}{\|p\|_\infty^2},$$

where x_0 and x^* are the starting point and the solution, and $p = x_0 - x^*$. Since we have scaled the difference by $\|p\|_\infty^2$, DQ gives a measure of the size of the third derivatives.

- (2) **Condition number of the Hessian.** Using the l_2 -norm, we measure the condition numbers of the Hessian at the starting point and solution point; these are denoted by K_0 and K_* , respectively.
- (3) **Convexity.** This was sometimes determined by observation; otherwise we performed several computations to guide us. We computed the eigenvalues of the Hessian at x_0 . If any were negative, the problem was clearly nonconvex. In addition, the inner algorithm of the truncated-Newton method can detect indefiniteness (although it is not guaranteed to find it). If none of these indicators suggested indefiniteness, and if we were not able to ascertain this theoretically, the problem was labeled “presumably convex.”
- (4) **Eigenvalue structure.** We plotted the eigenvalue distribution of the Hessian at the starting point and final point. The graphs are not given here due to space limitations, but can be obtained from the authors. The eigenvalue distribution greatly affects the performance of the inner conjugate-gradient algorithm of the truncated-Newton method, and Gill and Murray [6] suggest that it is also related to the efficiency of limited memory methods.

The characteristics of most of our test problems are displayed in Table 7. We have only considered the case when $n \approx 100$, because the eigenvalue analysis for values of n in the thousands is not tractable. In particular, test problem 42 was analyzed for $n = 100$ rather than $n = 1000$ (TN solved this smaller problem in 1.8 seconds using nine iterations and 35 function-gradient evaluations; L-BFGS used .9 seconds, 14 iterations, and 15 function-gradient evaluations). In Table 7, we also indicate which of the two methods performed best, and give the percentage difference in performance.

The next table has been arranged to show that there is a strong correlation between the degree of nonlinearity of the function and the success of the methods. We have concentrated on those problems of Table 7 in which the performance of the two methods is markedly different. Table 8 lists the problems for which one of the methods was better by at least 30 percent in terms of *both* time and function-gradient evaluations. The entries are ordered by degree of nonlinearity DQ.

We now list, in Table 9, three other properties of the test functions that help measure problem complexity, even though they do not appear to be directly useful for purposes of analysis.

- (1) **Sparsity.** The degree of sparsity and the sparsity pattern determine whether Newton’s method with sparse matrix techniques is attractive. Neither TN nor L-BFGS takes advantage of sparsity.
- (2) **Cost of evaluating f and g .** Here we merely timed the function values for most problems by averaging the time for 1000 function-gradient evaluations. For problem 53, only 20 evaluations were used in the timing because of the expense of computing the function.

TABLE 7
Problem characteristics.

P	N	DQ	$1/K_0$	$1/K_*$	Convexity	Winner	Percent difference f-g	Time
1	100	10^{-2}	10^{-8}	10^{-8}	presumed	TN	2045	2167
2	100	10^0	10^{-5}	10^{-5}	presumed	TN	590	634
3	100	10^0	10^{-6}	10^{-6}	presumed	TN	890	953
6	100	10^2	10^{-3}	10^{-4}	no	L-BFGS	135	86
8	100	10^2	10^{-1}	10^{-2}	no	TN	38	163
9	100	10^5	10^{-3}	10^{-2}	presumed	L-BFGS	109	83
10	100	10^2	10^{-2}	10^{-3}	presumed	L-BFGS	18	3
28	100	10^1	10^{-3}	10^{-8}	presumed	even	4	20
29	100	10^{13}	10^{-9}	10^{-6}	no	even	14	85
31	100	10^2	0	10^{-8}	presumed	L-BFGS	274	260
38	100	10^{-2}	0	0	yes	TN	66	93
39	121	10^1	10^{-9}	0	no	L-BFGS	167	133
40	100	10^{-2}	10^{-7}	10^{-7}	no	TN	10	30
41	100	10^1	0	0	no	L-BFGS	148	124
42	100	10^1	10^{-1}	10^{-1}	presumed	L-BFGS	133	100
43	100	10^0	10^{-3}	10^{-4}	presumed	L-BFGS	81	71
45	100	10^3	10^{-3}	10^{-2}	no	even	5	15
46(1)	100	10^1	10^{-4}	10^{-4}	no	TN	11	23
46(2)	100	10^1	10^{-3}	10^{-4}	no	L-BFGS	23	9
47	100	10^1	10^{-2}	10^{-2}	no	even	1	15
49	100	10^1	10^{-3}	10^{-7}	presumed	even	4	27
50	100	10^{-4}	0	0	yes	TN	58	126
51	100	10^2	10^{-3}	10^{-2}	no	L-BFGS	288	239
53	403	10^0	0	0	no	L-BFGS	59	60

TABLE 8
Selected test problems, ordered by degree of nonlinearity.

P	N	DQ	Winner	Percent difference f-g	Time
9	100	10^5	L-BFGS	109	83
31	100	10^2	L-BFGS	274	260
8	100	10^2	TN	38	163
6	100	10^2	L-BFGS	135	86
51	100	10^2	L-BFGS	288	239
41	100	10^1	L-BFGS	148	124
42	100	10^1	L-BFGS	133	100
39	121	10^1	L-BFGS	167	133
3	100	10^0	TN	890	953
2	100	10^0	TN	590	634
43	100	10^0	L-BFGS	81	71
53	403	10^0	L-BFGS	59	60
1	100	10^{-2}	TN	2045	2167
38	100	10^{-2}	TN	66	93
50	100	10^{-4}	TN	58	126

(3) **Laboriousness.** This is an attempt to measure the difficulty of solving a problem. We considered both algorithms, and recorded the minimum number of function-gradient evaluations and the minimum time to solve the problem.

One final point about the test problems should be made. Of those analyzed here, 13 out of 24 (and all eight of the most laborious problems) are singular, nearly singular, or nonconvex. The fact that all these problems were successfully solved by both methods seems to indicate that their implementations are very robust.

TABLE 9
Other problem characteristics.

P	N	Sparsity	Cost	Laboriousness		Winner	Percent difference	
				f-g	Time		f-g	Time
1	100	7-diagonal	.155	466	105.0	TN	2045	2167
2	100	7-diagonal	.123	242	41.4	TN	590	634
3	100	7-diagonal	.121	325	60.8	TN	890	953
6	100	tridiagonal	.014	291	19.0	L-BFGS	135	86
8	100	dense	.011	26	0.8	TN	38	163
9	100	dense	.054	23	2.4	L-BFGS	109	83
10	100	dense	.026	90	7.1	L-BFGS	18	3
28	100	4 × 4 block diagonal	.007	67	3.0	even	4	20
29	100	dense	.009	37	1.3	even	14	85
31	100	dense	.322	27	10.7	L-BFGS	274	260
38	100	tridiagonal	.014	77	4.4	TN	66	93
39	121	9 non-zero diagonals	.054	70	8.4	L-BFGS	167	133
40	100	5-diagonal	.026	2091	146.0	TN	10	30
41	100	5-diagonal	.018	31	2.1	L-BFGS	148	124
42	100	tridiagonal	.013	15	0.9	L-BFGS	133	100
43	100	tridiagonal	.032	21	1.7	L-BFGS	81	71
45	100	tridiagonal	.015	56	3.3	even	5	15
46(1)	100	dense	.137	339	61.9	TN	11	23
46(2)	100	dense	.131	453	92.8	L-BFGS	23	9
47	100	9-diagonal	.046	94	8.8	even	1	15
49	100	4 × 4 block diagonal	.009	67	3.0	even	4	27
50	100	tridiagonal	.011	78	4.2	TN	58	126
51	100	dense	.094	60	8.9	L-BFGS	288	239
53	403	dense	5.980	63	410.0	L-BFGS	59	60

5. Further analysis of the numerical results. Using the tables of results and of function characteristics of the previous sections, we now try to correlate the types of test problems with the success of TN and L-BFGS. Since we have seen that in terms of time the two methods are similar, we concentrate on the number of function-gradient evaluations.

The first, very visible, trend is that the performance of the two algorithms appears to be correlated with the degree of nonlinearity DN: for quadratic and approximately quadratic problems, TN outperforms L-BFGS. In fact, TN was better almost exclusively for these types of problems. Among the 11 problems for which TN was considered “much better” in Table 6, four are quadratic (both versions of problems 38 and 50) and six are approximately quadratic (both versions of problems 1, 2, and 3). Moreover, one of the two problems for which TN was considered “better” in this table is approximately quadratic (problem 40). For most of the highly nonlinear problems, L-BFGS performed better. It appears that TN’s effort to approximate the Newton step is not paying off on highly nonlinear problems. Continuing work on trying to improve the performance of TN by reducing the number of inner iterations on problems that are detected to be highly nonlinear will be reported in a future paper [17].

A study of the eigenvalue distribution of the Hessian matrices shows no clear correlation between the success of the methods and the eigenvalue structure. For problems with ill-conditioned Hessians, TN is perhaps better, but this is difficult to ascertain from our tests. Clustering of eigenvalues at the solution does not seem to benefit one method more than the other. There is little or no correlation between the other measures of the test problems and the performance of the two methods.

L-BFGS did very poorly on the calculus of variations problems 1, 2, and 3. These

problems are not only ill conditioned; their Hessians have many eigenvalues near zero (for problem 1 for $n = 100$, about half the eigenvalues are near zero). We ran L-BFGS with a more accurate linesearch and using more memory, and even though the performance improved substantially, it was still far from competitive with TN. For example, using $m = 20$ corrections and setting $\eta = 10^{-3}$ in (2.3) resulted in 418 iterations, 861 function-gradient evaluations, and 183 seconds for problem 2 with $n = 100$. The calculus of variations problems also caused difficulties for earlier versions of the TN method that used no preconditioning; the performance was as bad as for L-BFGS. If n is increased to 1000, TN has trouble solving the problem; however, block versions of the TN method (requiring greater storage and work per iteration) are capable of solving it [15]. We should note that Newton's method is very effective on this problem, suggesting that an accurate approximation to the Newton direction is needed.

It appears from this test set that, in terms of function evaluations, L-BFGS is preferable to TN for more highly nonlinear (not approximately quadratic) problems. However, TN almost always requires many fewer iterations than L-BFGS, and therefore, if the number of gradient evaluations in the inner iteration could be significantly reduced, TN would be competitive or more efficient than L-BFGS. How to realize these savings is a question that deserves further investigation. It does not appear that automatic differentiation (see, for example, [7]) will help, because the cost is of the same order as that of the gradient differences used here. Differencing along selective directions determined by the sparsity of the problem could be useful, but in this case both Newton's method with sparse matrix techniques and the partitioned quasi-Newton method may be preferable.

6. The nonlinear conjugate-gradient method. Now that we have studied the relative performances of L-BFGS and TN, we will use another, well-established, algorithm to measure their efficiency. To this end, we will solve our set of test problems with the Polak–Ribière version of the conjugate-gradient method, which is one of the classical methods for solving large problems. We chose the Polak–Ribière method for the following reason.

More recent implementations of the conjugate-gradient method, like the Harwell routine VA14 of Powell [21] or the routine CONMIN of Shanno and Phua [22], which include automatic restarts, and store additional information, require fewer function evaluations than the Polak–Ribière method. However, Liu and Nocedal [10] found that L-BFGS clearly outperforms CONMIN, both in terms of computer time and function evaluations—and it is known that CONMIN is more efficient than VA14. On the other hand, the Polak–Ribière method appeared to be often competitive with L-BFGS in terms of computer time (but not in terms of function evaluations). Therefore, we chose the Polak–Ribière method for this study, since it appears to be the only implementation of the conjugate-gradient method that could be competitive (at least in terms of computer time) with TN and L-BFGS.

The Polak–Ribière iteration is

$$(6.1) \quad x_{k+1} = x_k + \alpha_k p_k,$$

where the steplength α_k satisfies the strong Wolfe conditions (2.3)–(2.4), and where

$$(6.2) \quad p_k = -g_k + \beta_k p_{k-1},$$

TABLE 10
Smaller problems. Results of the Polak–Ribière conjugate-gradient method (CG).

P	N	CG			L-BFGS		TN	
		It	f-g	Time	f-g	Time	f-g	Time
1	100	4915	+9999	1910.0	≈	≈		
2	100	656	1506	201.0	+	*		
3	100	2082	4243	641.0		≈		
6	100	275	1129	24.2				*
8	100	9	28	0.6	+	*		≈
9	100	F						
10	100	119	304	11.3				
28	100	108	277	4.7				
29	100	7	51	1.0				≈
31	100	3	12	4.3	+	*	+	*
38	100	76	154	3.8		*		≈
39	121	63	180	12.6			≈	*
40	100	5001	+9999	363.0				
41	100	27	63	1.8		≈	+	*
42	1000	14	37	8.0		*	+	*
43	100	54	141	7.1				
45	100	36	120	2.8		*		≈
46(1)	100	286	583	89.3				
46(2)	100	313	639	99.4		≈		≈
47	100	73	152	9.6		≈		≈
48	1000	25	108	14.2		*		*
49	100	104	255	4.8				
50	100	79	160	3.6		*		≈
51	100	54	114	12.1			+	*
52	1000	4	10	1.6	≈	≈	≈	*

with

(6.3)
$$\beta_k = \frac{y_{k-1}^T g_k}{\|g_{k-1}\|^2}.$$

The linesearch is performed by means of the routine of Moré and Thuenté [11], previously mentioned in §2, with two small changes: (i) Since the Wolfe conditions do not ensure that descent directions are always generated, we continue the linesearch iteration until the descent condition is guaranteed. (ii) We insist that the linesearch performs at least one quadratic (or cubic) interpolation, and hence the algorithm reduces to the linear conjugate-gradient algorithm if the objective function is quadratic.

We chose $\mu = 10^{-4}$ and $\eta = 0.1$, for the parameters in (2.3)–(2.4), because our earlier experience with the Polak–Ribière method indicated that these values give the best results. The stopping condition was (2.2). The tests were performed, as before, on an Encore Multimax. The algorithm was restarted every n iterations by setting $\beta_k = 0$, which ensures global convergence in exact arithmetic. We note that n is often larger than the number of iterations, so that the algorithm performs no restarts in many of our test runs. The Polak–Ribière method requires $4n$ storage locations, and as shown by (6.2)–(6.3), the computation of d_k is very inexpensive.

Tables 10 and 11 present the results of the Polak–Ribière (CG) method on the whole collection of test problems. Under the column labelled “CG” we give the number of iterations/number of function-gradient evaluations, and the total computing time. As before, a “+” indicates that the function evaluation limit was reached, and a “*” indicates that the weaker convergence test (described in the third paragraph of §3) was used. In the runs marked “F” the search direction was so out of scale that

TABLE 11
Larger problems. Results of the Polak-Ribière conjugate-gradient method (CG).

P	N	CG			L-BFGS		TN	
		It	f-g	Time	f-g	Time	f-g	Time
1	200	4804	+9999	3840.0	≈	≈		
2	200	1106	2491	657.0		≈		
3	200	3336	6847	2060.0	≈	*		
6	500	1098	4889	515.0				*
8	1000	13	36	7.3	≈	*	+	*
10	1000		*F					
28	1000	167	456	72.1				
29	500	8	*98	7.1		*		*
31	200	3	14	20.3			+	*
38	1000	285	573	138.0		*		
39	961	161	519	319.0				*
42	10000	11	33	68.9		*	+	*
43	1000	16	56	23.3			+	*
47	1000	145	302	181.0		≈		
48	10000	18	76	103.0		*	+	*
49	1000	225	615	104.0				
50	1000	294	591	116.0		*		≈
51	1000	41	*91	93.7			+	*
52	10000	5	13	21.0	≈	*	+	*
53	403	62	144	926.0				

overflow occurred. Additional safeguarding could remedy these failures, but was not implemented. We compare the performance of CG with that of L-BFGS and TN by indicating the problems for which CG was more effective. In the column labelled “L-BFGS,” a “+” in the column “f-g” indicates that CG required fewer function calls, and a “*” in the column “Time” indicates that it required less computing time than L-BFGS. The sign “≈” means equal or near-equal performance (measured in the same way as in Table 6: differences of less than 10 percent, less than one second, or less than five gradient evaluations were considered negligible). The same notation is used in the column labelled “TN.” We verified, for each run, that the solution point obtained by CG coincided with that found by L-BFGS and TN.

It is clear that the conjugate-gradient method is not competitive with TN or L-BFGS in terms of function evaluations. However, it is often efficient in terms of computing time, due to its very low iteration cost. From this set of test runs, we conclude that the conjugate-gradient method is not to be recommended when the function evaluation is expensive, but that it may be useful for very large problems whose objective functions are relatively inexpensive.

Acknowledgments. We would like to thank the referees for several valuable comments and suggestions.

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