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SOME RESULTS OF COMPARATIVE TESTING OF A VARIABLE METRIC CODE



INTRODUCTION

As has been demonstrated in a few papers $^{/1,2/}$, the quasi-Newton Davidon-Fletcher-Powell (DFP) $^{/3/}$ and Broyden-Fletcher-Shanno (BFS) $^{/4/}$ algorithms possess both maximum efficiency 'and reliability when solving the problems of unconstrained and constrained optimization of differentiable multivariate objective functions. On the other hand, practical experience dramatically shows both efficiency and reliability to be critically dependent not so much on the version of the quasi-Newton method as on its real implementation in the form of a specific Fortran code.

The present paper describes some results of testing the DFP-code MIGRAD from the LIBCERN package MINUIT ^{/5/}, which is widely used in physical research.

2. MIGRAD CODE

This code is one of the efficient realizations of the variable metric method in the form of the DEP algorithm. Starting from 1967 and until now the code has been continuously modified to improve its efficiency and reliability.

One of the most distinguishing features of this code is some "global" logic built into it and allowing to search for not only local extrema but the global one, too. This feature can be contrasted by the "common" strategy of searching for the global extremum using numerous program runs with different initial (seed) parameter values and a subsequent sorting of the identified local extrema.

However, until now this code has not been tested, thus leaving intact the problems of its comparative performance.

3. THE TESTING TECHNIQUE

Ref. ^{/1/} contains the results of a comparative testing of two BFS-codes, MINIO2 and MINIO1, as well as two DFP-codes, MINFA and VMMO1. As a convergence criterion the number of

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function calls has been assumed to satisfy the following condition

 $|g_1| = \langle 1.0E - 5,$ (1)

where g_1 is the gradient calculated for the i-th independent variable, using seven two-, three- and four-dimensional unimodal and multimodal continuous test functions and an IBM-370/165 computer running in the double precision mode. The two-dimensional test functions are presented in Table 1. The testing results obtained in ref. ^{/1/} with two-dimensional test functions of Rosenbrock, Beale and Box are presented in Table 2. The overall total ranks registered for the codes MINI02, MINI01, MINFA and VMM01 (the basis code of MIGRAD) are 7, 23, 16 and 13, respectively, thus resulting in the MINI02 code to the best one.

4. THE RESULTS OF TESTING MIGRAD

The results of testing the MIGRAD code on the EC-1055M (IBM compatible) computer in the double precision mode are given for the three above continuous test functions in Table 3.

The overall total rank of the tested MIGRAD version is clearly seen to be much higher than that of any other codes.

The results of testing the MIGRAD code with a discontinuous Joker's test function are presented in Table 4. It is evident that this function is symmetric relative to the origin within an interval of [-1.0, +1.0]. One can assume the zero seed parameter values to end in the final parameter values equal to -1.0 or +1.0 depending on the specific implementation (machine precision) of zero, thus allowing one to investigate a "zero" behaviour of the code under study, i.e. its numerical sensitivity concerning some minute fluctuations in the seed parameter values. One can see, however, that the shift from the final parameter values of +1.0 needs a change in the seed parameter values within an interval of -0.01 to -0.1, i.e. of about 1.0-10.0% of these latter. The explicit reason for this assymmetry shift is as yet unexplained.

5. CONCLUSION

The final results obtained for the DFP-code MIGRAD with the standard continuous two-dimensional test functions demon-

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Table 1. Continuous two-dimensional test functions (TF)

N	Name	Analytical expression and initial (seed) vector	Minimum
1	Rosenbrock's TF	$\frac{100.0(x2 - x1^2)^2 + (1.0 - x1)^2}{F(-1.2, 1.0) = 24.2}$	F(1.0, 1.0) = 0.0
2	Beale's TF	$(1.500 - x1(1.0 - x2))^{2} + (2.250 - x1(1.0 - x2^{2}))^{2} + (2.625 - x1(1.0 - x2^{3}))^{2} + (1.0, -1.2) = 18.95$	F(3.0, 0.5) = 0.0
3	Box's TF	$\sum_{i=1}^{10} [(\exp(-x1*t_i) - \exp(-x2*t_i) - (\exp(-t_i) - \exp(-10.0*t_i))]]$ - (exp(-t_i) - exp(-10.0*t_i))] where t_i ranges from 0.1 to 1.0	F(1.0,10.0) = 0.0

Table 2. Testing results from ref.^{/1/} with continuous two-dimensional test functions (TF) (1 - Rosenbrock's TF, 2 - Beale's TF, 3 - Box's TF) (N - number of function and gradient calls, R - rank of each algorithm)

N	Seed vector	MINI02		MINI01		MINFA		VMM01	
		N	R	N	R	N	R	N	R
1 1	(1.0, -1.2) (2.0, -2.0)	26 18	1 1	42 34	4 3	37 39	3	28 20	2 2
2 2	(1.0, -1.2) (2.0, -2.0)	13 18	1 1	23 26	4 4	15 25	2 3	16 24	3 2
3	(5.0, 0.0) (0.0, 0.0)	24 19	2 1	40 28	4	20 27	1 3	24 21	2 2
Ove	erall Total Rank	(OTR)*	7		23		16		13

* The original Table 1 from ref. $^{/1/}$ contains some minor errors in the OTR line for the MINFA and VMMO1 codes

Table 3. Comparative testing results for MIGRAD code with continuous two-dimensional test functions (TF) (1 - Rosenbrock's TF, 2 - Beale's TF, 3 - Box's TF) (N - number of function and gradient calls, R - rank of each algorithm)

N Seed	vector	MI	NIO2	MINI01		MI	MINFA		MIGRAD	
		N	R	N .	R	N	R	N	R	
1 (1.0, - 1 (2.0, -	-1.2 -2,0)	26 18	1 1	42 34	3 2	37 39	2 3	196 176	4 4	
2 (1.0, - 2 (2.0, -	-1.2) -2.0)	13 18	1 1	23 26	3 3	15 25	2 2	199 184	4 4	
3 (5.0, 0 3 (0.0, 0).0)).0)	24 19	2 1	40 28	3 - 3	20 27	1 2	101 84	4 4	
Overall To	otal Rank	(OTR)	7		17	· · ·	12		24*	

* The typical final value of $|g_i|$ is (0.5E-2 - 0.5E-4) and that of TF = (1-0E-7 - 1.0E-19).

Table 4. The final results of numerical experiments with Joker's function (Joker's TF = $(1.0/(x1^2 - 1.0))$ + + $(1.0/x2^2 - 1.0)$) with breaks at F(+1.0, + 1.0) = ∞ and F(-1.0, -1.0) = ∞ and a maximum at F(0.0,0.0)=-2.0)

N Seed vector	g _i	TF value	x1	x2	Notes
1 (+0.0, +0.0)	0.3E+11	-0.2E+16	+1.0	+1.0	
2 (-0.0, -0.0)	0.3E+11	-0.2E+16	+1.0	+1.0	
3 (-0.01, -0.01)	0.8E+4	-0.1E+16	+1.0	+1.0	
4 (-0.10, -0.10)	0.0	-0.3E+16	-1.0	-1.0	

strate the real rating of this code as compared to four other DFP- and BSF-based ones. These data clearling indicate the real level of a specific realization of an optimization algorithm in the form of an efficient Fortran code.

Discontinuous test functions are shown to be a useful means to detect some unusual features of the codes under test.

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