Benchmarking the BFGS Algorithm on the BBOB-2009 Function Testbed

Raymond Ros
Univ. Paris-Sud, LRI
UMR 8623 / INRIA Saclay, projet TAO
F-91405 Orsay, France
raymond.ros@lri.fr

ABSTRACT

The BFGS quasi-Newton method is benchmarked on the noiseless BBOB-2009 testbed. A multistart strategy is applied with a maximum number of function evaluations of 10^5 times the search space dimension, resulting in the algorithm solving six functions.

Categories and Subject Descriptors

G.1.6 [Numerical Analysis]: Optimization—*global optimization, unconstrained optimization*; F.2.1 [Analysis of Algorithms and Problem Complexity]: Numerical Algorithms and Problems

General Terms

Algorithms

Keywords

Benchmarking, Black-box optimization, BFGS, Quasi-newton

1. INTRODUCTION

The Broyden-Fletcher-Goldfarb-Shanno (BFGS) method [1, 3, 4, 7] is a real-parameter unconstrained non-linear optimization method. The BFGS method belongs to the class of quasi-Newton methods which, by supposing that the objective function can be locally approximated by a quadratic function near its optimum, tries to approximate the Hessian matrix of this quadratic function. The BFGS method is tested here on a testbed of noiseless functions.

2. ALGORITHM PRESENTATION

Quasi-Newton methods address the problem of unconstrained black-box optimization by the determination of the stationary point of a function using a second-order approximation. The Hessian matrix is iteratively approximated by finding a search direction using the gradient of the current point and operating a line search to find the step size. For

each iteration $D + 1$ function evaluations (where D denotes the problem dimension) or double if the step size changes, are done to evaluate the gradient and the function value at the current point. A simple stochastic independent restart procedure (as advised in [5]) was added.

3. EXPERIMENTAL PROCEDURE

The Matlab implementation of the BFGS method was used. It is accessible using the generic function `fminunc` (revision 1.1.6.3) that proposes, among others, the BFGS method for the update of the Hessian Matrix. The starting point is chosen uniformly in $[-5, 5]^D$. The stopping criteria were chosen such that a restart occurs due to numerical errors. The multistart strategy was used with at most 100 restarts to reduce the duration of an experiment. For the same reason, a run is limited to at most $10^5 \times D$ function evaluations. The algorithm used is presented in Figure 1. No parameter tuning was done, the CrE [5] is computed to zero.

4. RESULTS AND DISCUSSION

Results from experiments according to [5] on the benchmark functions given in [2, 6] are presented in Figures 2 and 3 and in Table 1. As expected, poor results were obtained on multimodal functions $f_3, f_4, f_{15-19}, f_{24}$. The algorithm could not solve the rugged functions f_7, f_{13}, f_{23} neither. It only solves f_6 , in dimensions lesser than 5. Though the functions f_{21} and f_{22} are multimodal and have weak global structure, the algorithm still solves them even for dimensions larger than 10. The algorithm solves f_1 and f_5 with a scaling of its performances close to linear. The scaling is close to quadratic for f_2, f_8 and f_9 . The algorithm is coordinate-dependent as a result of the computation of the gradient using finite differences which can yield numerical errors on ill-conditioned functions as can be seen in the results on f_{10} compared to f_9 . The effects of ill-conditioning on the performances of the algorithm can also be seen in the results on f_{11} and f_{14} .

5. CPU TIMING EXPERIMENT

For the timing experiment, the proposed algorithm was run on f_8 and restarted until at least 30 seconds have passed (according to Figure 2 in [5]). The experiments were conducted with an Intel Core 2 6700 processor (2.66GHz) with Matlab R2008a on Linux 2.6.24.7. The results were 6.0, 4.7, 3.7, 3.0, 2.9, 2.9 and 2.8×10^{-4} seconds per function evaluations in dimension 2, 3, 5, 10, 20, 40 and 80 respectively.

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f1 in 5-D, N=15, mFE=18						f1 in 20-D, N=15, mFE=63					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
1	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
1e-1	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
1e-3	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
1e-5	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
1e-8	15	1.3e1	1.3e1	1.3e1	1.3e1	15	4.3e1	4.3e1	4.3e1	4.3e1	
f3 in 5-D, N=15, mFE=18540						f3 in 20-D, N=15, mFE=129192					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	3	7.6e4	4.6e4	2.2e5	1.8e4	0	28e+1	18e+1	32e+1	5.6e4	
1	0	21e+0	70e-1	24e+0	7.1e3						
1e-1	.	.	.	.	.						
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f5 in 5-D, N=15, mFE=48						f5 in 20-D, N=15, mFE=189					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.9e1	1.8e1	2.0e1	1.9e1	15	9.6e1	9.1e1	1.0e2	9.6e1	
1	15	3.0e1	2.7e1	3.2e1	3.0e1	15	1.1e2	1.1e2	1.2e2	1.1e2	
1e-1	15	3.1e1	2.9e1	3.3e1	3.1e1	15	1.1e2	1.1e2	1.2e2	1.1e2	
1e-3	15	3.1e1	2.9e1	3.3e1	3.1e1	15	1.1e2	1.1e2	1.2e2	1.1e2	
1e-5	15	3.1e1	2.9e1	3.3e1	3.1e1	15	1.1e2	1.1e2	1.2e2	1.1e2	
1e-8	15	3.1e1	2.9e1	3.3e1	3.1e1	15	1.1e2	1.1e2	1.2e2	1.1e2	
f7 in 5-D, N=15, mFE=600						f7 in 20-D, N=15, mFE=2100					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	0	32e+0	13e+0	58e+0	3.2e2	0	67e+1	56e+1	10e+2	1.3e3	
1	.	.	.	.	.						
1e-1	.	.	.	.	.						
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f9 in 5-D, N=15, mFE=936						f9 in 20-D, N=15, mFE=14028					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.3e2	1.0e2	1.5e2	1.3e2	15	3.8e3	3.6e3	3.9e3	3.8e3	
1	15	3.8e2	3.1e2	4.5e2	3.8e2	15	6.7e3	5.7e3	7.7e3	6.7e3	
1e-1	15	4.4e2	3.7e2	5.1e2	4.4e2	15	6.9e3	5.9e3	7.9e3	6.9e3	
1e-3	15	4.8e2	4.2e2	5.5e2	4.8e2	15	7.1e3	6.1e3	8.1e3	7.1e3	
1e-5	15	5.0e2	4.3e2	5.7e2	5.0e2	15	7.1e3	6.1e3	8.2e3	7.1e3	
1e-8	15	5.1e2	4.4e2	5.8e2	5.1e2	15	7.2e3	6.2e3	8.2e3	7.2e3	
f11 in 5-D, N=15, mFE=49422						f11 in 20-D, N=15, mFE=211239					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.4e2	1.3e2	1.5e2	1.4e2	15	1.0e3	8.5e2	1.2e3	1.0e3	
1	15	2.0e2	1.8e2	2.3e2	2.0e2	15	2.2e3	1.8e3	2.7e3	2.2e3	
1e-1	15	8.4e2	6.4e2	1.1e3	8.4e2	15	8.3e3	4.7e3	1.2e4	8.3e3	
1e-3	14	9.6e3	6.2e3	1.3e4	9.6e3	2	1.4e6	7.3e5	>3e6	2.0e5	
1e-5	2	2.9e5	1.5e5	>6e5	4.5e4	0	31e-4	83e-5	47e-4	7.9e4	
1e-8	0	32e-6	80e-7	33e-5	2.8e4						
f13 in 5-D, N=15, mFE=55584						f13 in 20-D, N=15, mFE=580545					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.3e2	1.2e2	1.4e2	1.3e2	15	1.1e3	1.0e3	1.1e3	1.1e3	
1	15	1.9e2	1.9e2	2.0e2	1.9e2	15	2.0e3	2.0e3	2.0e3	2.0e3	
1e-1	15	2.5e2	2.5e2	2.5e2	2.5e2	15	2.8e3	2.7e3	2.8e3	2.8e3	
1e-3	14	6.2e3	1.7e3	1.1e4	6.2e3	9	4.2e5	2.8e5	6.5e5	2.4e5	
1e-5	3	2.4e5	1.4e5	7.2e5	4.4e4	0	96e-5	20e-6	19e-4	1.8e5	
1e-8	0	37e-6	46e-7	79e-5	2.8e4						
f15 in 5-D, N=15, mFE=18486						f15 in 20-D, N=15, mFE=128646					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	5	4.4e4	2.9e4	7.9e4	1.4e4	0	25e+1	18e+1	32e+1	7.1e4	
1	0	13e+0	70e-1	22e+0	1.1e4						
1e-1	.	.	.	.	.						
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f17 in 5-D, N=15, mFE=22386						f17 in 20-D, N=15, mFE=410025					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	6.2e2	3.7e2	8.9e2	6.2e2	15	2.3e4	1.3e4	3.3e4	2.3e4	
1	2	1.4e5	7.0e4	>3e5	1.8e4	0	56e-1	46e-1	68e-1	2.5e5	
1e-1	0	19e-1	87e-2	28e-1	1.3e4						
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f19 in 5-D, N=15, mFE=37734						f19 in 20-D, N=15, mFE=255570					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.7e3	1.2e3	2.2e3	1.7e3	3	1.2e6	7.0e5	3.5e6	2.5e5	
1	12	2.2e4	1.7e4	2.8e4	1.7e4	0	12e+0	71e-1	15e+0	1.6e5	
1e-1	1	4.3e5	2.1e5	>4e5	2.8e4						
1e-3	0	62e-2	22e-2	12e-1	1.8e4						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f21 in 5-D, N=15, mFE=12012						f21 in 20-D, N=15, mFE=140112					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.6e2	9.4e1	2.3e2	1.6e2	15	1.1e3	6.4e2	1.6e3	1.1e3	
1	15	1.6e3	1.1e3	2.1e3	1.6e3	15	3.6e4	2.4e4	4.7e4	3.6e4	
1e-1	15	3.2e3	2.1e3	4.3e3	3.2e3	13	6.5e4	4.8e4	8.6e4	5.3e4	
1e-3	15	3.3e3	2.2e3	4.3e3	3.3e3	13	6.6e4	4.9e4	8.7e4	5.4e4	
1e-5	15	3.4e3	2.3e3	4.4e3	3.4e3	13	6.7e4	5.0e4	8.7e4	5.5e4	
1e-8	15	3.7e3	2.5e3	4.9e3	3.7e3	2	8.6e5	4.3e5	>2e6	9.1e4	
f23 in 5-D, N=15, mFE=26718						f23 in 20-D, N=15, mFE=115269					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	3.2e1	1.9e1	4.6e1	3.2e1	15	1.5e2	7.9e1	2.2e2	1.5e2	
1	12	1.6e4	1.3e4	2.0e4	1.4e4	3	4.9e5	3.0e5	1.5e6	1.1e5	
1e-1	0	69e-2	31e-2	13e-1	1.4e4	0	13e-1	85e-2	23e-1	5.6e4	
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f2 in 5-D, N=15, mFE=948						f2 in 20-D, N=15, mFE=12516					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	3.2e2	2.8e2	3.7e2	3.2e2	15	7.5e3	7.2e3	7.9e3	7.5e3	
1	15	4.9e2	4.5e2	5.4e2	4.9e2	15	9.2e3	8.7e3	9.7e3	9.2e3	
1e-1	15	5.5e2	5.1e2	5.9e2	5.5e2	15	1.0e4	9.5e3	1.0e4	1.0e4	
1e-3	15	5.9e2	5.6e2	6.3e2	5.9e2	15	1.1e4	1.0e4	1.1e4	1.1e4	
1e-5	15	6.4e2	6.0e2	6.8e2	6.4e2	15	1.1e4	1.0e4	1.1e4	1.1e4	
1e-8	15	6.9e2	6.4e2	7.3e2	6.9e2	15	1.1e4	1.1e4	1.1e4	1.1e4	
f4 in 5-D, N=15, mFE=20964						f4 in 20-D, N=15, mFE=169596					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	2	1.4e5	7.2e4	>3e5	2.0e4	0	40e+1	29e+1	45e+1	6.3e4	
1	0	24e+0	99e-1	34e+0	1.0e4						
1e-1	.	.	.	.	.						
1e-3	.	.	.	.	.						
1e-5	.	.	.	.	.						
1e-8	.	.	.	.	.						
f6 in 5-D, N=15, mFE=155790						f6 in 20-D, N=15, mFE=2.00e6					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	3.5e2	2.8e2	4.1e2	3.5e2	15	4.6e3	4.1e3	5.1e3	4.6e3	
1	15	7.1e2	6.3e2	7.9e2	7.1e2	15	8.1e3	7.4e3	8.9e3	8.1e3	
1e-1	15	9.5e2	8.6e2	1.0e3	9.5e2	15	1.2e4	1.1e4	1.3e4	1.2e4	
1e-3	15	1.4e3	1.3e3	1.6e3	1.4e3	15	1.8e4	1.7e4	2.0e4	1.8e4	
1e-5	15	2.1e3	1.9e3	2.3e3	2.1e3	15	2.4e4	2.3e4	2.6e4	2.4e4	
1e-8	15	7.1e4	5.5e4	8.7e4	7.1e4	0	44e-9	31e-9	77e-9	8.9e5	
f8 in 5-D, N=15, mFE=1968						f8 in 20-D, N=15, mFE=6531					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	1.5e2	1.3e2	1.8e2	1.5e2	15	3.7e3	3.5e3	3.8e3	3.7e3	
1	15	4.9e2	3.7e2	6.3e2	4.9e2	15	4.7e3	4.6e3	4.9e3	4.7e3	
1e-1	15	5.5e2	4.3e2	6.8e2	5.5e2	15	5.0e3	4.8e3	5.1e3	5.0e3	
1e-3	15	5.9e2	4.7e2	7.3e2	5.9e2	15	5.1e3	5.0e3	5.3e3	5.1e3	
1e-5	15	6.0e2	4.9e2	7.4e2	6.0e2	15	5.2e3	5.0e3	5.3e3	5.2e3	
1e-8	15	6.2e2	4.9e2	7.5e2	6.2e2	15	5.2e3	5.1e3	5.4e3	5.2e3	
f10 in 5-D, N=15, mFE=78708						f10 in 20-D, N=15, mFE=1.11e6					
Δf	#	ERT	10%	90%	RTsucc	#	ERT	10%	90%	RTsucc	
10	15	3.5e2	3.1e2	3.9e2	3.5e2	15	7.5e3	7.1e3	7.8e3	7.5e3	
1	15	5.0e2	4.6e2	5.4e2	5.0e2	15	8.7e3	8.3e3	9.0e3	8.7e3	
1e-1	15	5.7e2	5.3e2	6.2e2	5.7e2	15	1.1e4	9.6e3	1.2e4	1.1e4	
1e-3	15	6.3e2	5.8e2	6.7e2	6.3e2	15	1.6e4	1.4e4	1.8e4	1.6e4	
1e-5	15	9.0e2	6.9e2	1.1e3	9.0e2	15	5.2e4	2.5e4	8.2e4	5.2e4	
1e-8	5	2.0e5	1.3e5	3.6e5	6.1e4	0	77e-8	19e-8			

Figure 1: Matlab code: Multistart BFGS

```
function [x, ilaunch] = MY_OPTIMIZER(FUN, D, ftarget, maxfunevals)
% minimizes FUN in D dimensions by independent restarts of fminunc (BFGS).
% ftarget and maxfunevals are additional external termination conditions.
% Search space is [-5, 5]^D

% set options, make sure we always terminate
options = optimset('fminunc');
options = optimset(options, 'LargeScale', 'off'); % BFGS algorithm
options = optimset(options, 'MaxIter', inf, 'Tolfun', 1e-11, 'TolX', 0, ...
    'OutputFcn', @callback, 'Display', 'off');

maxfunevals = min(1e4*DIM, maxfunevals);

% multistart such that ftarget is reached with reasonable prob.
for ilaunch = 1:100; % relaunch optimizer up to 100 times
    options = optimset(options, 'MaxFunEvals', ...
        maxfunevals - feval(FUN, 'evaluations'));
    x = fminunc(FUN, 10*rand(DIM,1)-5, options);
    if (feval(FUN, 'fbest') < ftarget || ...
        feval(FUN, 'evaluations') >= maxfunevals)
        break;
    end
end

function stop = callback(x, optimValues, state)
    stop = false;
    if optimValues.fval < ftarget
        stop = true;
    end
end
end % function
```

6. CONCLUSION

The results of a quasi-Newton method algorithm with restarts were presented. The algorithm performs well on smooth functions, but its performances decrease on rugged and multimodal functions. Furthermore due to numerical error in the computation of the gradient in ill-conditioned problems, the algorithm is affected by coordinate systems transformations.

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Figure 2: Expected Running Time (ERT, $\bullet$) to reach $f_{\text{opt}} + \Delta f$ and median number of function evaluations of successful trials (+), shown for $\Delta f = 10, 1, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-5}, 10^{-8}$ (the exponent is given in the legend of f_1 and f_{24}) versus dimension in log-log presentation. The $\text{ERT}(\Delta f)$ equals to $\#FEs(\Delta f)$ divided by the number of successful trials, where a trial is successful if $f_{\text{opt}} + \Delta f$ was surpassed during the trial. The $\#FEs(\Delta f)$ are the total number of function evaluations while $f_{\text{opt}} + \Delta f$ was not surpassed during the trial from all respective trials (successful and unsuccessful), and f_{opt} denotes the optimal function value. Crosses (x) indicate the total number of function evaluations $\#FEs(-\infty)$. Numbers above ERT-symbols indicate the number of successful trials. Annotated numbers on the ordinate are decimal logarithms. Additional grid lines show linear and quadratic scaling.

Figure 3: Empirical cumulative distribution functions (ECDFs), plotting the fraction of trials versus running time (left subplots) or versus Δf (right subplots). The thick red line represents the best achieved results. Left subplots: ECDF of the running time (number of function evaluations), divided by search space dimension D , to fall below $f_{\text{opt}} + \Delta f$ with $\Delta f = 10^k$, where k is the first value in the legend. Right subplots: ECDF of the best achieved Δf divided by 10^k (upper left lines in continuation of the left subplot), and best achieved Δf divided by 10^{-8} for running times of $D, 10D, 100D \dots$ function evaluations (from right to left cycling black-cyan-magenta). Top row: all results from all functions; second row: separable functions; third row: misc. moderate functions; fourth row: ill-conditioned functions; fifth row: multi-modal functions with adequate structure; last row: multi-modal functions with weak structure. The legends indicate the number of functions that were solved in at least one trial. FEvals denotes number of function evaluations, D and DIM denote search space dimension, and Δf and Df denote the difference to the optimal function value.