Nelder-Mead User's Manual – The Fminsearch Function –

Michaël BAUDIN

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Contents

Chapter 1

The *fminsearch* function

In this chapter, we analyze the implementation of the *fminsearch* which is provided in Scilab. In the first part, we describe the specific choices of this implementation with respect to the Nelder-Mead algorithm. In the second part, we present some numerical experiments which allows to check that the feature is behaving as expected, by comparison to Matlab's *fminsearch*.

1.1 *fminsearch*'s algorithm

1.1.1 The algorithm

The algorithm used is the Nelder-Mead algorithm. This corresponds to the "variable" value of the "-method" option of the *neldermead*. The "non greedy" version is used, that is, the expansion point is accepted only if it improves over the reflection point.

1.1.2 The initial simplex

The fminsearch algorithm uses a special initial simplex, which is an heuristic depending on the initial guess. The strategy chosen by fminsearch corresponds to the -simplex0method flag of the neldermead component, with the "pfeffer" method. It is associated with the - simplex0deltausual = 0.05 and -simplex0deltazero = 0.0075 parameters. Pfeffer's method is an heuristic which is presented in "Global Optimization Of Lennard-Jones Atomic Clusters" by Ellen Fan [2]. It is due to L. Pfeffer at Stanford. See in the help of optimsimplex for more details.

1.1.3 The number of iterations

In this section, we present the default values for the number of iterations in fminsearch.

The options input argument is an optionnal data structure which can contain the options.MaxIter field. It stores the maximum number of iterations. The default value is 200n, where n is the number of variables. The factor 200 has not been chosen by chance, but is the result of experiments performed against quadratic functions with increasing space dimension.

This result is presented in "Effect of dimensionality on the nelder-mead simplex method" by Lixing Han and Michael Neumann [5]. This paper is based on Lixing Han's PhD, "Algorithms in Unconstrained Optimization" [4]. The study is based on numerical experiment with a quadratic function where the number of terms depends on the dimension of the space (i.e. the number of variables). Their study shows that the number of iterations required to reach the tolerance criteria is roughly 100n. Most iterations are based on inside contractions. Since each step of the Nelder-Mead algorithm only require one or two function evaluations, the number of required function evaluations in this experiment is also roughly 100n.

1.1.4 The termination criteria

The algorithm used by *fminsearch* uses a particular termination criteria, based both on the absolute size of the simplex and the difference of the function values in the simplex. This termination criteria corresponds to the "-tolssizedeltafvmethod" termination criteria of the *neldermead* component.

The size of the simplex is computed with the $\sigma - +$ method, which corresponds to the "sigmaplus" method of the *optimsimplex* component. The tolerance associated with this criteria is given by the "TolX" parameter of the *options* data structure. Its default value is 1.e-4.

The function value difference is the difference between the highest and the lowest function value in the simplex. The tolerance associated with this criteria is given by the "TolFun" parameter of the *options* data structure. Its default value is 1.e-4.

1.2 Numerical experiments

In this section, we analyse the behaviour of Scilab's *fminsearch* function, by comparison of Matlab's *fminsearch*. We especially analyse the results of the optimization, so that we can check that the algorithm is indeed behaving the same way, even if the implementation is completely different.

1.2.1 Algorithm and numerical precision

We consider the unconstrained optimization problem [6]

$$\min f(\mathbf{x}) \tag{1.1}$$

where $\mathbf{x} \in \mathbb{R}^2$ and the objective function f is defined by

$$f(\mathbf{x}) = 100 * (x_2 - x_1^2)^2 + (1 - x_1)^2. \tag{1.2}$$

The initial guess is

$$\mathbf{x}^0 = (-1.2, 1.)^T, \tag{1.3}$$

where the function value is

$$f(\mathbf{x}^0) = 24.2. \tag{1.4}$$

The global solution of this problem is

$$\mathbf{x}^\star = (1, 1.)^T \tag{1.5}$$

where the function value is

$$f(\mathbf{x}^\star) = 0. \tag{1.6}$$

The following Matlab script allows to see the behaviour of Matlab's *fminsearch* function on Rosenbrock's test case.

```
% Matlab
format long
banana = @(x)100*(x(2)-x(1)^2)^2+(1-x(1))^2;
[x,fval,exitflag,output] = fminsearch(banana,[-1.2, 1])
output.message
```

When this script is launched in Matlab, the following output is produced.

```
>> % Matlab
>> format long
>> banana = @(x)100*(x(2)-x(1)^2)^2+(1-x(1))^2;
>> [x,fval] = fminsearch(banana,[-1.2, 1])
>> [x,fval,exitflag,output] = fminsearch(banana,[-1.2, 1])
x =
   1.000022021783570   1.000042219751772
fval =
     8.177661197416674e-10
exitflag =
     1
output =
    iterations: 85
     funcCount: 159
     algorithm: 'Nelder-Mead simplex direct search'
       message: [1x194 char]
>> output.message
ans =
Optimization terminated:
the current x satisfies the termination criteria using
OPTIONS.TolX of 1.000000e-04
and F(X) satisfies the convergence criteria using
OPTIONS.TolFun of 1.000000e-04
```

The following Scilab script allows to solve the problem with Scilab's *fminsearch*.

```
// Scilab
format(25)
function y = banana (x)
  y = 100*(x(2)-x(1)^2)^2 + (1-x(1))^2;
endfunction
[x , fval , exitflag , output] = fminsearch ( banana , [-1.2 1] )
output.message
```

The output associated with this Scilab script is the following.

```
-->// Scilab
-->format(25)
-->function y = banana (x)
-->  y = 100*(x(2)-x(1)^2)^2 + (1-x(1))^2;
-->endfunction
-->[x , fval , exitflag , output] = fminsearch ( banana , [-1.2 1] )
 output  =
   algorithm: "Nelder-Mead simplex direct search"
   funcCount: 159
   iterations: 85
   message: [3x1 string]
 exitflag  =
     1.
 fval  =
     0.0000000008177661099387
 x  =
     1.0000220217835567027009     1.0000422197517710998227
-->output.message
 ans  =

!Optimization terminated:                                                     !
!                                                                             !
!the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-004  !
!                                                                             !
!and F(X) satisfies the convergence criteria using OPTIONS.TolFun of 1.000000e-004     !
```

Because the two softwares do not use the same formatting rules to produce their outputs, we must perform additionnal checking in order to check our results.

The following Scilab script displays the results with 16 significant digits.

```
// Scilab
// Print the result with 15 significant digits
mprintf ( "%.15e" , fval );
mprintf ( "%.15e %.15e" , x(1) , x(2) );
```

The previous script produces the following output.

```
-->// Scilab
-->mprintf ( "%.15e" , fval );
8.177661099387146e-010
-->mprintf ( "%.15e %.15e" , x(1) , x(2) );
1.000022021783557e+000 1.000042219751771e+000
```

Matlab Iterations Scilab Iterations	85 85	
Matlab Function Evaluations Scilab Function Evaluations	159 159	
Matlab $\mathbf{x}^\star$ Scilab $\mathbf{x}^\star$	1.000022021783570 1.000022021783557e+000	1.000042219751772 1.000042219751771e+000
Matlab $f(\mathbf{x}^\star)$ Scilab $f(\mathbf{x}^\star)$	8.177661197416674e-10 8.177661099387146e-010	

Fig. 1.1 : Numerical experiment with Rosenbrock's function – Comparison of results produced by Matlab and Scilab.

These results are reproduced verbatim in the table 1.1.

We must compute the common number of significant digits in order to check the consistency of the results. The following Scilab script computes the relative error between Scilab and Matlab results.

```
// Scilab
// Compare the result
xmb = [1.000022021783570    1.000042219751772 ];
err = norm(x - xmb) / norm(xmb);
mprintf ( "Relative Error on x : %e\n", err );
fmb = 8.177661197416674e-10;
err = abs(fval - fmb) / abs(fmb);
mprintf ( "Relative Error on f : %e\n", err );
```

The previous script produces the following output.

```
// Scilab
Relative Error on x : 9.441163e-015
Relative Error on f : 1.198748e-008
```

We must take into account for the floating point implementations of both Matlab and Scilab. In both these numerical softwares, double precision floating point numbers are used, i.e. the relative precision is both these softwares is $\epsilon \approx 10^{-16}$. That implies that there are approximately 16 significant digits. Therefore, the relative error on x, which is equivalent to 15 significant digits, is acceptable. If we now consider the relative error on f, which is equivalent to only 8 significant digits, that may sound as a problem. This corresponds to the square root of the relative precision, because $\sqrt{\epsilon} =\approx 10^{-8}$. In fact, this is the best that we can expect from an optimization algorithm ([1, 3]).

Therefore, the result is as close as possible to the result produced by Matlab. More specifically :

- the optimum x is the same up to 15 significant digits,
- the function value at optimum is the same up to 8 significant digits,
- the number of iterations is the same,
- the number of function evaluations is the same,
- the exit flag is the same,
- the content of the output is the same (but the string is not display the same way).

The output of the two functions is the same. We must now check that the algorithms performs the same way, that is, produces the same intermediate steps.

The following Matlab script allows to get deeper information by printing a message at each iteration with the "Display" option.

```
% Matlab
opt = optimset('Display','iter');
[x,fval,exitflag,output] = fminsearch(banana,[-1.2, 1] , opt );
```

The previous script produces the following output.

```
% Matlab
 Iteration   Func-count     min f(x)         Procedure
     0            1             24.2
     1            3            20.05         initial simplex
     2            5           5.1618         expand
     3            7           4.4978         reflect
     4            9           4.4978         contract outside
     5           11          4.38136         contract inside
     6           13          4.24527         contract inside
     7           15          4.21762         reflect
     8           17          4.21129         contract inside
     9           19          4.13556         expand
    10           21          4.13556         contract inside
    11           23          4.01273         expand
    12           25          3.93738         expand
    13           27          3.60261         expand
    14           28          3.60261         reflect
    15           30          3.46622         reflect
    16           32          3.21605         expand
    17           34          3.16491         reflect
    18           36          2.70687         expand
    19           37          2.70687         reflect
    20           39          2.00218         expand
    21           41          2.00218         contract inside
    22           43          2.00218         contract inside
    23           45          1.81543         expand
    24           47          1.73481         contract outside
    25           49          1.31697         expand
    26           50          1.31697         reflect
    27           51          1.31697         reflect
    28           53           1.1595         reflect
    29           55          1.07674         contract inside
    30           57         0.883492         reflect
    31           59         0.883492         contract inside
    32           61         0.669165         expand
    33           63         0.669165         contract inside
    34           64         0.669165         reflect
    35           66         0.536729         reflect
    36           68         0.536729         contract inside
    37           70         0.423294         expand
    38           72         0.423294         contract outside
    39           74         0.398527         reflect
    40           76          0.31447         expand
    41           77          0.31447         reflect
    42           79         0.190317         expand
    43           81         0.190317         contract inside
    44           82         0.190317         reflect
    45           84          0.13696         reflect
    46           86          0.13696         contract outside
    47           88         0.113128         contract outside
    48           90          0.11053         contract inside
    49           92          0.10234         reflect
    50           94         0.101184         contract inside
    51           96        0.0794969         expand
    52           97        0.0794969         reflect
    53           98        0.0794969         reflect
    54          100        0.0569294         expand
    55          102        0.0569294         contract inside
    56          104        0.0344855         expand
    57          106        0.0179534         expand
    58          108        0.0169469         contract outside
    59          110       0.00401463         reflect
    60          112       0.00401463         contract inside
    61          113       0.00401463         reflect
    62          115      0.000369954         reflect
    63          117      0.000369954         contract inside
    64          118      0.000369954         reflect
    65          120      0.000369954         contract inside
    66          122      5.90111e-005        contract outside
    67          124      3.36682e-005        contract inside
    68          126      3.36682e-005        contract outside
    69          128      1.89159e-005        contract outside
    70          130      8.46083e-006        contract inside
    71          132      2.88255e-006        contract inside
    72          133      2.88255e-006        reflect
    73          135      7.48997e-007        contract inside
    74          137      7.48997e-007        contract inside
    75          139      6.20365e-007        contract inside
    76          141      2.16919e-007        contract outside
    77          143      1.00244e-007        contract inside
```

```
       78            145      5.23487e-008         contract inside
       79            147      5.03503e-008         contract inside
       80            149       2.0043e-008         contract inside
       81            151      1.12293e-009         contract inside
       82            153      1.12293e-009         contract outside
       83            155      1.12293e-009         contract inside
       84            157      1.10755e-009         contract outside
       85            159      8.17766e-010         contract inside

Optimization terminated:
 the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-004
 and F(X) satisfies the convergence criteria using OPTIONS.TolFun of 1.000000e-004
```

The following Scilab script set the "Display" option to "iter" and run the *fminsearch* function.

```
// Scilab
opt = optimset ( "Display" , "iter" );
[x , fval , exitflag , output] = fminsearch ( banana , [-1.2 1] , opt );
```

```
// Scilab
 Iteration    Func-count     min f(x)          Procedure
     0            3              24.2
     1            3             20.05          initial simplex
     2            5          5.161796          expand
     3            7          4.497796          reflect
     4            9          4.497796          contract outside
     5           11         4.3813601          contract inside
     6           13         4.2452728          contract inside
     7           15         4.2176247          reflect
     8           17         4.2112906          contract inside
     9           19         4.1355598          expand
    10           21         4.1355598          contract inside
    11           23         4.0127268          expand
    12           25         3.9373812          expand
    13           27          3.602606          expand
    14           28          3.602606          reflect
    15           30         3.4662211          reflect
    16           32         3.2160547          expand
    17           34         3.1649126          reflect
    18           36         2.7068692          expand
    19           37         2.7068692          reflect
    20           39         2.0021824          expand
    21           41         2.0021824          contract inside
    22           43         2.0021824          contract inside
    23           45         1.8154337          expand
    24           47         1.7348144          contract outside
    25           49         1.3169723          expand
    26           50         1.3169723          reflect
    27           51         1.3169723          reflect
    28           53         1.1595038          reflect
    29           55         1.0767387          contract inside
    30           57         0.8834921          reflect
    31           59         0.8834921          contract inside
    32           61         0.6691654          expand
    33           63         0.6691654          contract inside
    34           64         0.6691654          reflect
    35           66         0.5367289          reflect
    36           68         0.5367289          contract inside
    37           70         0.4232940          expand
    38           72         0.4232940          contract outside
    39           74         0.3985272          reflect
    40           76         0.3144704          expand
    41           77         0.3144704          reflect
    42           79         0.1903167          expand
    43           81         0.1903167          contract inside
    44           82         0.1903167          reflect
    45           84         0.1369602          reflect
    46           86         0.1369602          contract outside
    47           88         0.1131281          contract outside
    48           90         0.1105304          contract inside
    49           92         0.1023402          reflect
    50           94         0.1011837          contract inside
    51           96         0.0794969          expand
    52           97         0.0794969          reflect
    53           98         0.0794969          reflect
    54          100         0.0569294          expand
    55          102         0.0569294          contract inside
    56          104         0.0344855          expand
    57          106         0.0179534          expand
    58          108         0.0169469          contract outside
    59          110         0.0040146          reflect
    60          112         0.0040146          contract inside
    61          113         0.0040146          reflect
    62          115         0.0003700          reflect
    63          117         0.0003700          contract inside
    64          118         0.0003700          reflect
    65          120         0.0003700          contract inside
    66          122         0.0000590          contract outside
    67          124         0.0000337          contract inside
    68          126         0.0000337          contract outside
    69          128         0.0000189          contract outside
    70          130         0.0000085          contract inside
    71          132         0.0000029          contract inside
    72          133         0.0000029          reflect
```

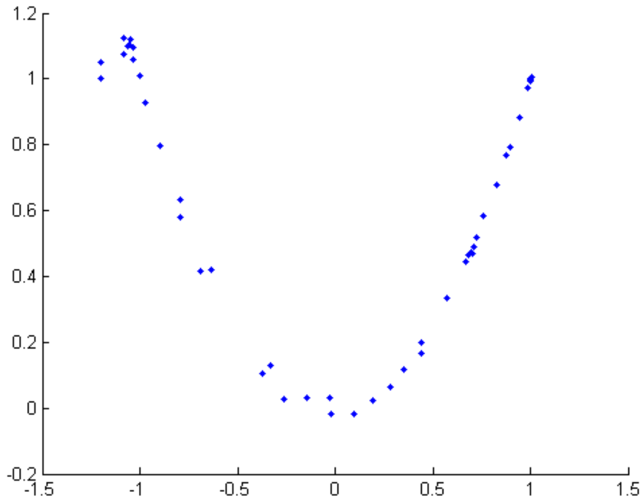

Fig. 1.2 : Plot produced by Matlab's fminsearch, with customized output function.

```
73     135    0.0000007     contract inside
74     137    0.0000007     contract inside
75     139    0.0000006     contract inside
76     141    0.0000002     contract outside
77     143    0.0000001     contract inside
78     145    5.235D-08     contract inside
79     147    5.035D-08     contract inside
80     149    2.004D-08     contract inside
81     151    1.123D-09     contract inside
82     153    1.123D-09     contract outside
83     155    1.123D-09     contract inside
84     157    1.108D-09     contract outside
85     159    8.178D-10     contract inside

Optimization terminated:
 the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-004
 and F(X) satisfies the convergence criteria using OPTIONS.TolFun of 1.000000e-004
```

A close inspection at the data reveals that the two softwares produces indeed the same intermediate results.

1.2.2 Plot features

In this section, we check that the plotting features of the *fminsearch* function are the same.

The following output function plots in the current graphic window the value of the current parameter **x**. To let Matlab load that script, save the content in a .m file, in a directory known by Matlab.

```
% Matlab
function stop = outfun(x, optimValues, state)
stop = false;
hold on;
plot(x(1),x(2),'.');
drawnow
```

The following Matlab script allows to perform the optimization so that the output function is called back at each iteration.

```
% Matlab
options = optimset('OutputFcn', @outfun);
[x fval] = fminsearch(banana, [-1.2, 1], options)
```

This produces the plot which is presented in figure 1.2.

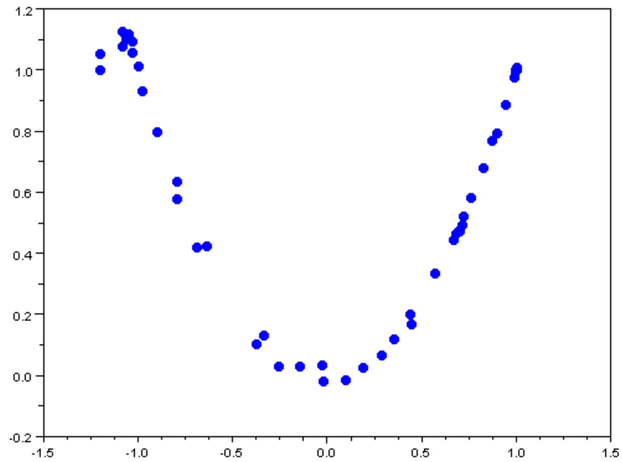

Fig. 1.3 : Plot produced by Scilab's fminsearch, with customized output function.

The following Scilab script sets the "OutputFcn" option and then calls the *fminsearch* in order to perform the optimization.

```
// Scilab
function outfun ( x , optimValues , state )
  plot( x(1),x(2),'.');
endfunction
opt = optimset ( "OutputFcn" , outfun);
[x fval] = fminsearch ( banana , [-1.2 1] , opt );
```

The previous script produces the plot which is presented in figure 1.3.

Except for the size of the dots (which can be configured in both softwares), the graphics are exactly the same.

Bibliography

[1] Richard P. Brent. Algorithms for minimization without derivatives, 1973.

[2] Ellen Fan. Global optimization of lennard-jones atomic clusters. Technical report, McMaster University, February 2002.

[3] P. E. Gill, W. Murray, and M. H. Wright. *Practical optimization*. Academic Press, London, 1981.

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[6] H. H. Rosenbrock. An automatic method for finding the greatest or least value of a function. *The Computer Journal*, 3(3):175–184, March 1960.