The Nelder-Mead Simplex Procedure for Function Minimization

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The Nelder-Mead simplex method for function minimization is a "direct" method requiring no derivatives. The objective function is evaluated at the vertices of a simplex, and movement is away from the poorest value. The process is adaptive, causing the simplexes to be continually revised to best conform to the nature of the response surface. The generality of the method is illustrated by using it to solve six problems appearing in the May 1973 issue of *Technometrics*.

KEY WORDS

Constraints
Curve Fitting
Estimation
Least Squares
Minimization
Non-Linear
Optimization
Response Surface
Simplex

1. INTRODUCTION

The subject of function minimization is both important and ubiquitous in the physical sciences. This is easily demonstrated by noting that it is involved in a very wide variety of areas ranging from finding roots of polynomials and solving simultaneous equations to estimating the parameters of non-linear functions.

Although no exhaustive investigation was carried out, we were struck by the fact that, for the last eight years, every issue of *Technometrics* contains at least one paper in which a general minimization program was either needed or could have been used to avoid a time-consuming algebraic solution. The May 1973 issue stands out in that seven of its articles make use of function minimization. In some of these, one or more special modifications had to be made in a "standard" procedure to solve the given problem.

In consequence of our two-year experience with the Nelder–Mead simplex procedure [17], and our continuing investigation into its benefits, limitations and potential for improvement, we applied this procedure to six of the problems in the May 1973 issue (no data were given in one of the articles). The simplicity of application, lack of special requirements, and accuracy with which this procedure was able to reproduce (or improve) the answers to these six problems prompted us to prepare this report.

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The article by Nelder and Mead [17] is almost ten years old, yet their procedure has only fairly recently been called to the attention of physical scientists in *Analytical Chemistry* [5], *Industrial and Engineering Chemistry, Process Design and Development* [12], the *Review of Scientific Instruments* [6], and *Applied Statistics* [20].

Garfield [7] published a list of the 78 books and papers most heavily cited in pure mathematics from 1961 to 1972. Of the 22 papers listed, the Nelder and Mead paper stands 15th; a fact made somewhat curious by the totally applied nature of the work. Even more curious is its absence from a similar list of citations in applied mathematics [8].

The main objective of this paper is to call attention to and lend support for the growing enthusiasm for the Nelder–Mead procedure by (1) demonstrating with worked examples its wide applicability for general function minimization, and (2) indicating the existence of both a coding of the procedure in FORTRAN IV [19], and a BASIC program on the General Electric time-share system [9]. To increase the universality of appeal, three of the examples are worked using the FORTRAN IV version; the other three were solved using the BASIC program.

After describing the rationale of the method (Section 2), the six problems are solved and discussed (Section 3). This is followed by a summary and discussion of limitations (Section 4). No criticism of the material in any of the six *Technometrics* articles furnishing the examples is intended. Our sole consideration is the demonstration of an alternative method of solution.

2. TECHNICAL PRELIMINARIES

Detailed accounts of how the simplex procedure operates have been given in a number of papers,

e.g. [17, 18, 19]. Only a very brief review will be given here to provide enough information for the reader unfamiliar with the procedure to appreciate its main ideas and observe its simplicity.

Although Spendley, et al. [23] presented the idea of optimizing either physical processes or mathematical functions by the application of simplexes, Nelder and Mead [17] supplied the idea essential to making the procedure broadly applicable, namely, the *adaptive* feature. This enables the simplex (see Figure 1 for an example in two dimensions) to reflect, extend, contract, or shrink so as to conform to the characteristics of the response surface. These actions are based on the conditions set forth in Table 1 and are applied repeatedly until a termination criterion is reached. For the particular case illustrated in Figure 1, reflection of point A (corresponding to the highest result) through the centroid of the opposite side locates point E. In this instance, an extension would then follow making the next simplex BCF.

The simplex procedure derives its name from the geometric figure which is moved along the response surface in search of the minimum. It is a so-called "direct" procedure in that no derivatives of the objective function are required. For this reason it is readily applicable to situations which are analytically difficult, such as minimization of the maximum absolute deviation.

In contrast to other minimization procedures, the simplex procedure approaches the minimum by moving away from high values of the objective function rather than by trying to move in a line toward the minimum. A casual investigation of modifying the procedure to permit more than one extension, based on a gambler's rule: "don't quit while you're winning", gave no indication that this would be generally beneficial. Disappointment in the behavior of a number of such modifications was expressed by Nelder [16]. The robustness of the procedure and its excellence relative to other general minimization techniques has been reported in some detail [16, 18].

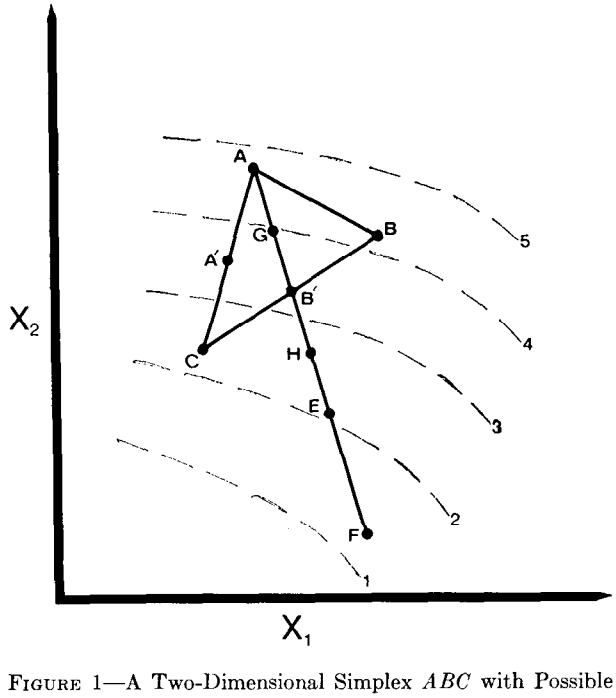

FIGURE 1—A Two-Dimensional Simplex ABC with Possible Subsequent Points (see Table 1).

TABLE 1—*Conditions Governing the Formation of Subsequent Simplexes [$f(A)$ means the value of the objective function at point A]*

Condition	Action	New Simplex*
$f(C) \leq f(E) \leq f(B)$	Reflect	BCE
$f(E) < f(C)$	Extend	BCF
$f(A) < f(E)$	Contract	BCG
$f(B) < f(E) \leq f(A)$	Contract	BCH
$f(A) \leq f(G)$ or $f(E) \leq f(H)$	Shrink	$A'B'C$

* Refer to Figure 1.

3. Worked Examples and Discussion

Example 3.1. *Direct Maximization of a Likelihood Function*

Boardman [12] addresses the problem of obtaining maximum likelihood estimates of the parameters of a compound exponential distribution when the data are grouped. The application of the Nelder–Mead simplex procedure directly to the natural logarithm of the likelihood function obviated the necessity of considering an approximation to its solution. Boardman's iterative approximate solution appears to be an excellent one, usually requiring fewer than half a dozen trials (in contrast to the 48 trials used in the simplex method). However, its development required, in part, skill in applying an expansion of a hyperbolic cotangent function. This first example is especially appropriate because maximization of likelihood functions was the principal motivation for Nelder and Mead's development of the simplex procedure.

The objective function (equation (5) in [2]) to be maximized was

$$\ln L = C + \sum_{i=1}^{k} [r_{1i} + r_{2i}] \ln [\exp(-t_{i-1}/\lambda) - \exp(-t_i/\lambda)] - (n - r)T/\lambda + r_1 \ln(\lambda/\lambda_1) + r_2 \ln(\lambda/\lambda_2)$$

Maximization was accomplished by minimizing the negative of the function $F = \ln(L) - C$. Data consisted of 325 observations grouped into 13

classes. See Table 2 for a coding of an appropriate subroutine in FORTRAN IV, which was used with the program given in [19]. This subroutine contains the data, assigns values to the constants in the function, and expresses the objective function to be minimized. Decisions on the mechanics of the method are never needed; the required subroutine is purely descriptive of the problem. Operational

TABLE 2—*Computer Subroutines Used in the Examples*

EXAMPLE 3.1

```
      DOUBLE PRECISION FUNCTION FN(XLAM)
      DOUBLE PRECISION XLAM(2),XLAMDA,R1,R2,R,T,
     1XN,SUM,TERM1,TERM2,TERM3,FAIL(13),TGRP(14),
     2EX1,EX2,XLOG1,XLOG2
      DATA FAIL/4.1D1,4.4D1,5.0D1,4.8D1,2.8D1,2.9D1,
     11.8D1,1.6D1,1.5D1,1.1D1,7.D0,1.1D1,7.D0/
      DATA TGRP/0.D0,5.D1,1.D2,1.5D2,2.D2,2.5D2,3.D2,
     13.5D2,4.D2,4.5D2,5.D2,5.5D2,6.D2,6.3D2/
      XLAMDA=XLAM(1)*XLAM(2)/(XLAM(1)+XLAM(2))
      R1=2.18D2
      R2=1.07D2
      R=3.25D2
      T=6.3D2
      XN=3.69D2
      SUM=0.D0
      DO 100 J=2,14
      EX1=DEXP(-TGRP(J-1)/XLAMDA)
      EX2=DEXP(-TGRP(J)/XLAMDA)
      TERM1=EX1-EX2
      SUM=SUM+FAIL(J-1)*DLOG(TERM1)
100   CONTINUE
      TERM2=-(XN-R)*T/XLAMDA
      XLOG1=DLOG(XLAMDA/XLAM(1))
      XLOG2=DLOG(XLAMDA/XLAM(2))
      TERM3=R1*XLOG1+R2*XLOG2
      FN=-(SUM+TERM2+TERM3)
      RETURN
      END
```

EXAMPLE 3.2

```
500 DATA 92.13,107.87,129.47,138.50,106.71
510 FØR I=1 TØ 5
520 READ X(I)
530 NEXT I
1000 F1=F2=0
1010 M=0.053
1020 FØR I=1 TØ 5
1030 V=5*I+5
1040 C=(1/V)-M
1050 D=EXP(B(1)-B(2)*C)
1060 E=9*D/X(I)
1070 F1=F1+9-E
1080 F2=F2+C*E
1090 NEXT I
1100 S=ABS(F1)+ABS(F2)
```

EXAMPLE 3.3

```
      DOUBLE PRECISION FUNCTION FN(X)
      DOUBLE PRECISION X(3),YS1,YS2,YS3,YP1,YP2,YP3,
     1YS,YP,BOUND
      BOUND=DSQRT(X(1)*X(1)+X(2)*X(2))
      IF(BOUND .GT. 1.D0) GO TO 100
      YS1=8.217D1-1.01D0*X(1)-8.61D0*X(2)
      YS2=1.4D0*X(1)*X(1)-8.76D0*X(2)*X(2)
      YS3=-7.2D0*X(1)*X(2)
      YS=YS1+YS2+YS3
      YP1=5.369D1+7.26D0*X(1)-1.033D1*X(2)
      YP2=7.22D0*X(1)*X(1)+6.43D0*X(2)*X(2)
      YP3=1.136D1*X(1)*X(2)
      YP=YP1+YP2+YP3
      FN=-YP+DABS(YS-87.8D0)
      RETURN
100   FN=1.D38
      RETURN
      END
```

EXAMPLE 3.4

```
      DOUBLE PRECISION FUNCTION FN(B)
      DOUBLE PRECISION B(2),X(10),Y(10),YHAT,RES,
     1SUMSQ,WGT
      DATA X/8.D0,8.9D0,1.8D0,2.6D0,3.3D0,4.4D0,
     15.2D0,6.1D0,6.5D0,7.4D0/
      DATA Y/5.9D0,5.4D0,4.4D0,4.6D0,3.5D0,3.7D0,
     12.8D0,2.8D0,2.4D0,1.5D0/
      WGT=B(2)*B(2)+1.D0
      SUMSQ=0.D0
      DO 100 I=1,10
      YHAT=B(1)+B(2)*X(I)
      RES=Y(I)-YHAT
      SUMSQ=SUMSQ+RES*RES/WGT
100   CONTINUE
      FN=SUMSQ
      RETURN
      END
```

EXAMPLE 3.5

```
0 DØUBLE PRECISIØN
500 DATA 0.25,0.50,1.00,1.70,2.00,4.00
501 DATA 0.25,0.40,0.60,0.58,0.54,0.27
510 FØR I=1 TØ 6
520 READ X(I)
530 NEXT I
540 FØR I=1 TØ 6
550 READ Y(I)
560 NEXT I
1000 S=0
1010 FØR I=1 TØ 6
1020 H=B(1)*EXP(B(3)*X(I))+B(2)*EXP(B(4)*X(I))
1030 R=Y(I)-H
1040 S=S+R*R
1050 NEXT I
```

EXAMPLE 3.6

```
500 DIM X(18)
501 DIM Y(18)
502 DATA 1,7.7086,2,6.9443,3,6.5914,4,6.3883
503 DATA 5,6.2560,6,6.1631,7,6.0942,8,6.0410
504 DATA 9,5.9986,10,5.9644,12,5.9117,15,5.8578
505 DATA 20,5.8035,24,5.7744,30,5.7459,40,5.7170
506 DATA 60,5.6878,120,5.6581
510 FØR I=1 TØ 18
520 READ X(I),Y(I)
530 NEXT I
1000 S=0
1010 T=0
1020 FØR I=1 TØ 18
1030 R=ABS(Y(I)-(X(I)+B(1))/(B(2)*X(I)+B(3)))
1040 IF R<T THEN 1060
1050 T=R
1060 NEXT I
1070 S=T
```

details are not given here since they appear in [19], and [9] has self-contained instructions.

In the following comparison, starting values and initial step sizes $(\cdot, \cdot)$ for the Nelder–Mead simplex procedure were $\lambda_1 = (500,10)$ and $\lambda_2 = (1000,10)$. The starting values were obtained from a plot of the data. Forty-eight trials were used.

Method	λ_1	λ_2	$-F$
Boardman	451.90	920.82	1120.5245
Nelder-Mead	451.84	920.94	1120.5245

To show the insensitivity (in *this* problem) to different starting values and initial step sizes, the combinations $\lambda_1 = (300,25)$, $\lambda_2 = (500,25)$ and $\lambda_1 = (250,50)$, $\lambda_2 = (630,50)$ were tried. In 57 and 51 trials, respectively both combinations gave $-F = 1120.524$. The estimates obtained were $\hat{\lambda}_1 = 451.85$, $\hat{\lambda}_2 = 920.79$ and $\hat{\lambda}_1 = 451.73$, $\hat{\lambda}_2 = 920.68$, respectively.

Example 3.2. *Non-Linear Simultaneous Equations*

Singpurwalla [22] derives expressions for the maximum likelihood estimators for the parameters of a "slightly amended" Arrhenius reaction rate model. The resulting equations, given as equations (3.1) and (3.2) in [21], are

$$\sum_i^k r_i - \sum_i^k (r_i/\lambda_i) \exp (A - B(V_i^{-1} - \bar{V})) = 0$$

$$\sum_i^k (r_i/\lambda_i)(V_i^{-1} - \bar{V}) \exp (A - B(V_i^{-1} - \bar{V})) = 0$$

These were solved numerically using the Newton–Raphson method, which gave the required estimates in "a few iterations".

For the simplex method of solution, the objective function was taken to be the sum of the absolute values of the two equations. This was to be driven toward zero. After 248 trials, with quite arbitrary starting values of 10 and initial step sizes of 2, the objective function was less than 0.000002 and the estimates shown below were changing in no less than the eighth significant figure.

Method	$\hat{A}$	$\hat{B}$
Newton-Raphson	4.728	4.168
Nelder-Mead	4.7283	4.1680

Two important points need to be made at this time. (1) When the Newton–Raphson procedure is applicable (and considerable experience may be required in making this judgment), it always requires far fewer trials than any "direct" procedure; however (2) for this problem, the central processing cost of running the Nelder–Mead simplex procedure on the General Electric time-share system was approximately one dollar. Even in Example 3.6, the most expensive, the central processing time cost less than two dollars. The advantage of a general, and hence *sometimes* inefficient, program derives from the relatively low cost of modern computing.

Example 3.3. *Maximization Subject to Constraints*

Myers and Carter [15] give an algorithm for maximizing a primary quadratic response subject to a constraint based on a secondary quadratic response in the same variables. We consider the problem given in Section 5 of their article. The two responses were

$$\hat{y}_p = 53.69 + 7.26x_1 - 10.33x_2 + 7.22x_1^2 + 6.43x_2^2 + 11.36x_1x_2$$

$$\hat{y}_s = 82.17 - 1.01x_1 - 8.61x_2 + 1.40x_1^2 - 8.76x_2^2 - 7.20x_1x_2$$

The authors pose the problem: find conditions which maximize $\hat{y}_p$, subject to $\hat{y}_s = 87.8$ and $x_1^2 + x_2^2 \leq 1$. One way to accomodate the specific-value constraint on $\hat{y}_s$ is to incorporate it into the objective function as follows.

$$\text{Obj. func.} = -\hat{y}_p + ABS(\hat{y}_s - 87.8)$$

The inequality constraint on the x's was handled by setting the objective function equal to 10^{38} whenever the inequality was violated. This so-called "penalty function" approach keeps the search in the required region.

These were the approaches taken (cf. Table 2). Starting values of zero and initial step sizes of 0.50 were used for both variables. After 122 trials, the objective function was changing only beyond the sixth decimal place. The comparison is shown below.

Method	x_1	x_2	$\hat{y}_s$	$\hat{y}_p$
Myers and Carter	0.85	−0.6	87.8	67
Nelder-Mead	0.811	−0.585	87.8	67.1

Myers and Carter's approach requires the construction of three graphs from which the estimates, subject to the required constraints, can be read. In view of the graphical precision obtainable, the agreement is satisfactory.

A simple and effective way of handling bounded variables is given by Atwood and Foster [1]. They suggest transformation of the bounded space into an unbounded one by the following equations. Let the X-space have a lower bound L and an upper bound U. An unbounded Z-space is obtained from

$$Z_i = \ln [(X_i - L)/(U - X_i)]$$

the inverse of which is

$$X_i = [L + U \exp (Z_i)]/[1 + \exp (Z_i)].$$

For unbounded lower and upper cases, one can use

$$Z_i = -\ln (U - X_i)$$

$$X_i = U - \exp (-Z_i)$$

and

$$Z_i = \ln (X_i - L)$$

$$X_i = L + \exp (Z_i).$$

Further, it is possible to let L and U be functions rather than constants, thereby allowing the treatment of nonlinear constraints.

Example 3.4. *Linear Least-Squares with Errors in Both Variables*

Britt and Luecke [3] give an algorithm, using Lagrange multipliers, for finding maximum likelihood estimators of the parameters of nonlinear algebraic models. They state, "our algorithm is similar in structure to the Gauss–Newton method for the standard parameter estimation problem, and may be subject to similar convergence problems". Their first example involved finding the least-squares estimate of the slope of a straight line when equal variances were assumed for both variates. This amounts to finding the slope of the line which minimizes the perpendicular distances from the observed points to the line (with equal scaling for the two axes). The simplex procedure produced the correct answer in 65 trials using starting values of 6.0 and −0.625 for the intercept and slope, respectively, and initial step sizes of 0.2 and 0.1. The comparison of slopes shows exact agreement.

Method	Intercept est.	Slope est.
Britt and Luecke	not given	−0.54556
Nelder-Mead	5.7840	−0.54556

The same remarks given at the end of *Example* 3.2 apply with equal force here.

Example 3.5. *Non-Linear Least-Squares*

Guttman, Pereyra, and Scolnik [10] report on a new method for determining least-squares estimators for certain classes of non-linear models. They employed "a relaxed form of the Gauss–Newton procedure". In the first problem, the model $\eta = a_1 e^{\alpha_1 t} + a_2 e^{\alpha_2 t}$ was fitted to six data points.

In applying the Nelder–Mead simplex method, we used the same initial guesses as in [10] for α_1 and α_2, namely, −0.5 and −2.5, respectively. Our other starting values were $a_1 = a_2 = 1$. Initial step sizes were 0.1 for all variables. After 460 trials, the program terminated because the objective function (the residual sum of squares) was changing in no less than the eighth significant figure. The comparison is shown below.

Method	a_1	a_2	α_1	α_2	Residual SS
Guttman et al.	1.645	−1.685	−0.443	−1.258	0.001
Nelder-Mead	1.801	−1.842	−0.463	−1.205	0.0009

There are a number of combinations of parameter values that yield a residual sum of squares of about 0.001. The response surface associated with a model containing a single exponential term is pictured by Lawton and Sylvestre (Figure 1 of [13]) to be a steep-sided valley. The present model, being the sum of two exponential terms, undoubtedly has an analogous terrain in four-space. Such response surfaces are usually associated with both sensitivity to starting values and slow convergence. Even so, when the final values found by Guttman et al. [10] were used as starting values in the Nelder–Mead simplex procedure, together with initial step sizes of 0.00001 for each, the estimates moved to those shown above for the Nelder–Mead method.

Of course, the estimation effort can generally be reduced, as Guttman et al. [10] point out, by iterating on the estimates of the exponent coefficients α_1 and α_2, and treating the estimation of a_1 and a_2 as a problem in linear regression. This same point was made earlier by Lawton and Sylvestre [13], who also specifically discuss the present model. Since the Nelder–Mead method was successful in this problem without such a partial linearization, it should prove useful in similar problems to those who either do not know of this device or do not wish to take the time to use it. However, it is not difficult to incorporate such a partial linearization into a subroutine for the Nelder–Mead method, thereby using the simplex procedure only for the non-linear portion. In complex models, some such device might prove necessary.

Example 3.6. *Fitting Tabular Data*

Johnson [11] fits a number of hyperbolic equations to obtain approximations to tabulated values of the F-distribution. His criterion was least-squares, and his procedure was the "iterative linearization technique". Although the author does not describe, or state the source of, the tabular values he used, we have presumed that the most accurate available [14] were used.

When fitting approximations to tabled functions, the quantity to be minimized is generally taken to be the maximum absolute deviation. In the following list, we compare Johnson's results (line 1) for his Group IV model: $F_{0.95,f_1,4} = (f_1 + A)/(Bf_1 + C)$, with the Nelder–Mead simplex method applied to

both the least-squares and minimax criteria. The maximum absolute deviations for the first two solutions were 20.7×10^{-4} and 11.4×10^{-4}, somewhat larger than the 8.2×10^{-4} given by the minimax procedure, shown in Table 2. Starting values were the least-squares estimates rounded to four decimal places. Initial step sizes were all 0.001.

Method	Criterion	$\hat{A}$	$\hat{B}$	$\hat{C}$	Obj. Func.
Iter. Lin.	Least Sq.	1.349	0.1776	0.1271	23.1[a]
Nelder-Mead	Least Sq.	1.36295	0.177641	0.128913	5.5[a]
Nelder-Mead	Minimax	1.36252	0.177645	0.128867	8.2[b]

[a] Residual sum of squares; multiply by 10^{-6}

[b] Maximum absolute deviation; multiply by 10^{-4}

Johnson's ultimate evaluation of his approximation was based on the maximum absolute percent deviation from the tabular significance level. In principle, this would have been the appropriate criterion for him to use in the minimization procedure. However, the results he obtained are undoubtedly adequate for most practical purposes.

4. Summary

We have shown the straightforward application of the Nelder–Mead simplex minimization method to six problems taken from the May 1973 issue of *Technometrics*. These included direct maximization of the logarithm of a likelihood function, solution of simultaneous equations, maximization of a quadratic function subject to a quadratic constraint, fitting a line by minimizing the sum of squares of perpendicular distances, non-linear least-squares, and fitting approximations to tabular data.

The main points of this demonstration are the generality of the Nelder–Mead simplex method, its accuracy, and the simplicity of the information required for the computer input statements. Additional applications of this method, given to show other kinds of problems it can solve and to compare it with alternative methods are contained in [17, 18].

Our experience with this procedure, extending over two years, has given convincing evidence of its capability to handle a wide variety of optimization problems, without requiring any modifications specialized to the problem at hand. However, in spite of this, it would be unreasonable to imply that the Nelder–Mead method cannot be defeated. Given an extremely sharp ridge, produced by high interdependency among the variables, the method can become inefficient to the point of failure. Similarly, when violation of a bound is treated by assigning a very large value to the objective function, constraints can lead to unwarranted shrinkage followed by stopping when further movement along a bound is needed.

Therefore, we are led to recommend this method for solving the kinds of problems illustrated here. The more the problem tends to be large, with many constraints, the less desirable is the Nelder–Mead simplex procedure. However, for the usual problems encountered in applied statistics, involving no more than (say) half a dozen parameters, this method can be expected to perform very well.

To quote Luecke and Britt [3] again, "No parameter estimation scheme is complete if it does not furnish some information on the distribution of the estimation error". Although such a statement is usually made as an introduction to a section in which standard errors are derived, we certainly agree with the thought. In its presently available forms [9, 19], the Nelder–Mead simplex procedure does not give information on the errors associated with statistical estimates. The subject is, however, discussed in [17] where it is pointed out that such errors can be evaluated by adding a few selected points and generating the Hessian matrix. An alternative approach which might prove fruitful is described in detail by Sillén [21] and by Christian [4]. The addition of a feature which would supply estimates of standard errors, where these are required, would be a welcome addition to the present program.

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