

Function minimisation using the Nelder and Mead simplex Method with limited arithmetic precision: the self regenerative simplex

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The behaviour of a curve fitting program is described which uses the Nelder-Mead simplex method to optimise the fit and which works with limited arithmetic precision. Apparent false minima are shown to be due to the creation of various simplex arrays which are regenerated unchanged by the logic of the process. A simple procedure is suggested for detecting the formation of such arrays and initiating restarting the search for the true minimum.

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I have recently completed a curve analysis (or spectral analysis) program for a Nicolet BNC12 minicomputer, which uses the Nelder and Mead simplex method to minimise the RMS difference between a real and a synthetic spectrum by varying the parameters of the latter (Akitt, 1975) (Nelder and Mead, 1965; O'Neil, 1971; Parkinson and Hutchinson, 1972; Box, Davies and Swan, 1969). To obtain a fast operating program it was necessary to carry out the calculation using almost entirely integer arithmetic with the parameters in the simplex limited to 12 binary bits, single precision (the BNC12 word length is 20 bits). The search for a minimum is thus made over a quite coarsely spaced lattice of function values rather than over the near continuum generally regarded as essential for the successful operation of minimisation procedures. This appears to confer no disadvantage in the early stages of a search and the function value (RMS difference) falls rapidly and by large steps. Progress is slow near the minimum and is hampered by rounding errors made in calculating new simplex parameters though generally at this stage the curve fit is sufficiently close to enable the search to be terminated prior to attainment of the precise true minimum. Using ideal, noise free data the procedure is capable of going quite quickly to the point with function value zero.

However, long before the minimum is reached with either real or ideal data the procedure commonly encounters apparent false minima. This was to be expected (O'Neil, 1971) though its occurrence with ideal data representing a single spectral line—a three or four parameter fit—was surprising since the existence of a real false minimum seemed unlikely. Examination of the behaviour of the simplex at such false minima showed that in fact a stationary self regenerative state had been reached where due to the rounding errors of the calculation the simplex cannot be altered by any of the logical pathways provided. Further progress can only be made if a new simplex is formed around the best set of parameters, i.e. by restarting.

An example of a self regenerating simplex

An example is given involving a four parameter fit to an ideal, noise free Lorenzian line.

The four parameters defining a single line are baseline slope, linewidth at half height, line intensity and line position, giving a 4×5 simplex array. An exact fit is obtained with the set 0, 1,440, 6,200, 6,200 (all octal numbers) and the search was started with a manually entered guess consisting of the set, 0, 1,510, 6,200, 6,320 for which $RMS = 40,151$. The contents of the simplex for a typical stationary state is shown below within the box. The 'RMS store' which contains the RMS error for the curve calculated for each parameter set is to the right and the logical regenerative cycle is shown below the box. This consists of the following steps

(a) form parameter set \bar{P} by taking the average of all sets but that with the highest RMS (marked H) i.e.

$$\bar{P}_i = (\sum^n S_i - H_i)/n .$$

Stationary state with $RMS = 650$

Parameter Set	Simplex				RMS Store
1	0	1,432	6,206	6,177	724
2 (H)	0	1,431	6,206	6,177	1,077
3	0	1,431	6,206	6,200	1,033
4	0	1,432	6,206	6,200	650
5	0	1,431	6,206	6,200	1,033
\bar{P}	0	1,431	6,206	6,177	—
P^*	0	1,431	6,206	6,177	1,077

(b) reflect the values of set H through those of \bar{P} to give a set $P^*(P^* = 2\bar{P}_i - H_i)$ and find its RMS (y^*)

(c) compare this with the values in the simplex RMS store (y_i). Where a self regenerative simplex is about to be formed the RMS of P^* will not be smaller than all numbers in the store. The number, x , of RMS store values \geq the RMS of P^* is counted. In the example chosen only one value in the RMS store $\geq 1,077$ so we form set P^{**} from

$$P^{**} = (\bar{P} + P^*)/2, \text{ giving}$$

$$P^{**} \quad 0 \quad 1,431 \quad 6,206 \quad 6,177$$

which replaces set H without altering the simplex. This obviously could continue indefinitely.

Calculations made with different degrees of precision indicated that increased precision would allow exit to be made from a given self regenerative cycle, but in practice it was found that this approach markedly slowed down the search, suggesting that for optimum results the lattice spacing need not be very much smaller than the expected variance of the real data to be fitted. Limiting the choices which may be made by the simplex may also assist in speeding matters along.

Testing for and exit from the self regenerative state

The occurrence of a self regenerative state is easily detected and within one iterative cycle of the procedure. Two slightly different tests are needed depending upon the pathway chosen by the iteration. In all cases but one it is sufficient simply to check whether the RMS value of the parameter set about to replace set H is the same as that of set H . If it is, the simplex has almost certainly become self regenerative, and a restart should be made immediately. If the pathway chosen however is to shrink the simplex it is necessary to compare all values in the RMS store before shrinkage with the values obtained after shrinkage. If there has been no change then a restart must be made. Modifications to the Nelder-Mead algorithm are shown which make these tests.

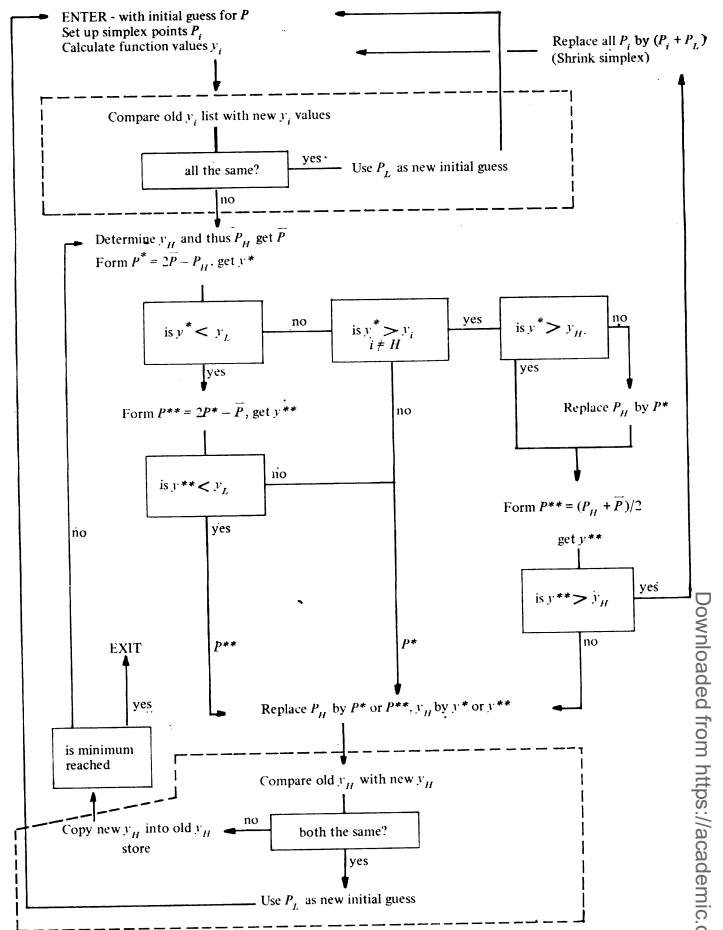
It should be noted that after a series of restarts has been made a new restart may lead to the same self regenerative simplex.

This condition may be avoided by altering the step size used in forming the new simplex at each restart, remembering that when integer arithmetic is used the minimum step size allowed is equal to the number of parameters.

Appendix

Modified Nelder-Mead algorithm including tests for the formation of a self regenerative simplex. P represents a set of parameters from which function y is calculated. Subscript H denotes the highest, L the lowest, i any other, values of y . Note that if the simplex is shrunk then all y_i have to be tested for a change in value. The dashed boxes bracket the additions made.

The algorithm is otherwise set out in the same way as in Nelder and Meads original paper.



References

- AKITT, J. W. (1975). Visual and automatic spectral analysis using a small digital computer, *Applied Spectroscopy*, Vol. 29, pp. 493-496.
- BOX, M. J., DAVIES, D., and SWANN, W. H. (1969). Non linear Optimisation Techniques *ICI Monograph No. 5*, Oliver and Boyd, pp. 16-28.
- O'NEILL, R. (1971). Function Minimisation using a simplex procedure, *Applied Statistics*, Vol. 20, pp. 338-345.
- NELDER, J. A. and MEAD, R. (1965). A simplex method for function minimisation, *The Computer Journal*, Vol. 7, pp. 308-313.
- PARKINSON, J. M. and HUTCHINSON, D. (1972). An investigation into the efficiency of Variants on the Simplex Method, No. 8 in *Numerical Methods for non linear Optimisation*, Ed. F. O. Lortsma, Academic Press, pp. 115-135.

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