USING A SIMPLE GENETIC ALGORITHM TO CALIBRATE SPATIAL INTERACTION MODELS

G. Diplock and S. Openshaw

WORKING PAPER 95/2

SCHOOL OF GEOGRAPHY • UNIVERSITY OF LEEDS

WORKING PAPER 95/2

Using a Simple Genetic Algorithm to Calibrate Interaction Models

Gary Diplock and Stan Openshaw

School of Geography
University of Leeds
Leeds
LS2 9JT

Abstract

The paper investigates the use of a genetic algorithm to obtain globally optimal parameter estimates for a mix of simple and complex spatial interaction models. The genetic algorithm works well and is strongly advocated for use with the more complex multi-parameter models where the differences in both performance and parameter values are judged to be significant.

1 Introduction

In recent years genetic algorithms have attracted considerable attention as an assumption free and robust approach to finding the global optimum of hard to optimise functions with multiple local optima; see for example De Jong (1975), Goldberg (1989) and Fogel (1994). This paper seeks to evaluate the utility of this technology as a means of estimating the unknown parameters in three variants of spatial interaction models that might be potentially considered hard to handle by more conventional methods.

The unknown parameters in a spatial interaction model are usually estimated by seeking the minimum of an unconstrained sum of squares function or the maximum of a likelihood function (Fotheringham and O'Kelly, 1989 and Openshaw, 1976). A number of non-linear optimisation methods exist which are suitable for this type of problem (Scales, 1985) and, apart from being compute intensive, the spatial interaction model is not normally considered to present a hard non-linear optimisation task and can seemingly be readily handled using widely available software libraries, such as NAG. However, this situation is only applicable to the family of spatial interaction models with standard parameterisations; for example those of Wilson (1971). Once more esoteric specifications are investigated then the optimisation problem can rapidly become harder; for example, Wilson and Clarke (1979) showed that the standard shopping model displays chaotic behaviour for attraction parameters less than unity and concern can be expressed that chaotic behaviour might also be observed during model calibration especially with the more complex model specifications. However, even with the standard model, globally optimal parameter values require a well behaved convex function over the range of relevant parameter values. This assumption is usually taken for granted but it need not always hold and may be data specific. Its validity becomes more doubtful when different types of spatial interaction model are investigated. In particular, the intervening opportunity model has always been difficult to calibrate because of the numeric instability of its exponential form. Similar difficulties may well affect a more recent hybrid formulation due to Gonçalves and Ulysséa-Neto (1993). Likewise, Fotheringham's (1983, 1985) competing destinations production-constrained model may also present calibration problems, because of the use of an embedded non-linear destination accessibility function. The paper evaluates the use of a genetic algorithm to estimate the parameters of these models and compares the results with a more conventional approach. This might be considered a useful test of the global optimality of the conventional parameter estimates as well as a demonstration of what even simple genetic algorithms can achieve.

2 Two potentially hard to calibrate spatial interaction models

Gonçalves and Ulysséa-Neto (1993) describe what is considered to be an interesting hybrid spatial interaction model . The production-constrained version can be written as

$$T_{ij} = A_i . O_i . W_j . \exp(-\lambda . Z_{ij} - \beta . C_{ij}) \tag{1}$$

where

$$A_i = \left[\sum_{j=1}^{n_j} W_j . \exp(-\lambda . Z_{ij} - \beta . C_{ij}) \right]^{-1} \tag{2}$$

where Z_{ij} is the number of opportunities intervening between origin zone i and destination zone j when destinations are ranked by distance from zone i, O_i is the number of trips originating from origin i, W_j is the attractiveness of destination j and C_{ij} is the 'cost' of travelling from origin zone i to destination zone j. In this model the gravity and intervening opportunities factors are combined to yield a hybrid deterrence function that has been considered a most useful development (Roy, 1993). The "hardness" of calibrating this model results from the complex exponential form of the deterrence function. The exponential function presents considerable potential for numeric instability once the functions arguments fall outside a fairly narrowly defined range of values. These numeric problems may, if they occur, rapidly propagate through the model via the accounting constraints and, whereas IEEE arithmetic may well handle the computation side, the concern here is that they may adversely affect the performance of the nonlinear optimiser.

The Fotheringham (1983, 1986) competing destinations model is another very interesting form of spatial interaction model. The calibration complexity here concerns whether or not the various parameters are treated as independent and estimated simultaneously or else fixed at constant non-independent values. The model takes the form

$$T_{ij} = A_i . O_i . W_j . Q_{ij}^{\delta} . \exp(\beta . C_{ij}) \tag{3}$$

where

$$A_i = \left[\sum_{j=1}^{n_j} W_j . Q_{ij}^{\delta} . \exp(\beta . C_{ij}) \right]^{-1} \tag{4}$$

Q_{ij} represents the accessibility of destination j to all other destinations available to origin i as perceived by the residents of that origin (Fotheringham, 1983). It can take numerous forms and in this case the term is represented by a common function of attractiveness and distance (see equation 5). It is defined in Fotheringham (1983, 1984, 1985) as

$$Q_{ij} = \sum_{\substack{k=1 \\ k \neq i \\ k \neq j}}^{n_j} W_k . \exp(\sigma . C_{jk}) \tag{5}$$

This model can also be extended from this three parameter (β, δ and σ) version to a five parameter production-constrained model, which is represented as follows;

$$T_{ij} = A_i . O_i . W_j^{\alpha} . Q_{ij}^{\delta} . \exp(\beta . C_{ij}) \tag{6}$$

where

$$A_i = \left[\sum_{j=1}^{n_j} W_j^{\alpha} . Q_{ij}^{\delta} . \exp(\beta . C_{ij}) \right]^{-1} \tag{7}$$

and

$$Q_{ij} = \sum_{\substack{k=1 \\ k \neq i \\ k \neq j}}^{n_j} W_k^{\gamma} . \exp(\sigma . C_{jk}) \tag{8}$$

The optimisation "hardness" here results from the use of the destinations accessibility term Q_{ij} where δ should be simultaneously estimated together with the other parameters in the model on which Q_{ij} depends (γ and σ). It should be noted that the parameters have not been disaggregated to origin-specific specifications as this is not normally done.

Finally, for comparison purposes, a conventional Wilson (1971) origin-constrained entropy-maximising model is included.

$$T_{ij} = A_i . O_i . W_j . \exp(-\beta . C_{ij}) \tag{9}$$

where

$$A_i = \left[\sum_{j=1}^{n_j} W_j . \exp(-\beta . C_{ij}) \right]^{-1} \tag{10}$$

This model is generally regarded as being well behaved although the exponential deterrence function has some potential for numerical instability if the product of $\beta . C_{ij}$ becomes either too large or too small.

3 A simple genetic algorithm

The genetic algorithm (GA) is extremely simple to apply and numerous variations can be readily devised (Holland, 1975, Davis, 1991). Here, attention is restricted to the simplest reproductive plan described in Goldberg (1989). The parameters in the spatial interaction model are coded as binary bit strings (you could use the standard 32 bit floating point representation for each parameter, if desired). The bit strings representing the parameters are concatenated together and subject to genetic operators. The GA functions by mimicking the process of natural evolution, whereby the genes of a life-form adapt to its local environment. The fittest forms survive, breed and adapt to be re-exposed to their environment; others die out. Here, the 'life' is the bit string representing the spatial interaction model's unknown parameters. Its ability to adapt to the local environment is measured by how well the model fits the spatial interaction data on which it is to be calibrated.

A simple GA for estimating the unknown parameters in a spatial interaction model involves the following steps:

<u>Step 1</u> set reproductive plan design parameters; size of population (P), crossover probability (C), mutation probability (M), and number of generations (G).

<u>Step 2</u> generate an initial set of P different, random bit strings representing plausible parameter values.

<u>Step 3</u> evaluate all P sets of bit strings (i.e. decode each bit string as numbers representing the model parameters and then measure the goodness of fit of the resulting model); report the best value.

Step 4 create a new population of P bit strings by

either

Apply a crossover operator (with probability C) on pairs of bit strings selected at random but weighted so that the best performers have the greatest chance of selection; a crossover involves randomly selecting a bit sub-string from one point and inserting it in the second point at the same location. Crossover is the principle search mechanism in a GA

or

Select a single bit string.

Step 5 apply a mutation (flipping a bit) operator to each bit (with probability M), which is designed to provide a finely tuned local search capability and may also prevent premature convergence.

Step 6 repeat steps 4 and 5, P times, to create a new generation of bit strings.

Step 7 repeat steps 3 to 6, G times.

GAs are usually extremely robust but performance can vary according to the reproductive plan used. For this implementation, P=50, C=0.75, M=0.01 and G=50. The problem representation is perhaps the most critical part, as redundancy in the bit string may well reduce performance. Here, the parameters are coded as fixed decimal binary numbers with 15 binary bits per number and an implicit decimal point after the sixth digit.

The attractions of the GA are primarily twofold. Firstly, Holland's (1975) schemata theorem demonstrates that each bit string evaluated also represents many others that now do not need to be considered, due to the explicitly parallel nature of the search process (it looks at many different sub-optimal locations simultaneously). Secondly, its suitability for parallel hardware architectures is increasingly attractive, since the P strings in step 3 can be evaluated in parallel. Indeed the code used here is run on four processors of a Silicon Graphics Challenger XL Server.

4 Empirical evaluation

Two very different data sets are used. The first (data #1) is that of Openshaw (1976) and is a 73 zone journey to work dataset from the 1966 census and the second consists of 1992 car sales data for 86 origins and 35 dealers (data #2); both use car travel times as the distance 'cost' function. For comparison purposes, results for the conventional NAG one parameter optimisation routine "e04abf" and the multi-parameter optimisation routine "e04jaf" are given. The former utilises a quadratic interpolation method whilst the latter is a standard quasi-Newton method that generates derivatives numerically and accepts simple range limits on the parameters (NAG, 1991).

Model performance is measured by computing the mean sum of squares error, given by

$$f(error) = \frac{\sum \left(S_{ij} - T_{ij} \right)^2}{m} \qquad \forall\, i, j \tag{11}$$

where S_{ij} is the observed flow matrix, T_{ij} the model predicted matrix and m the total number of trip pairs. In the GA, these values are adjusted to represent fitness by subtracting the error of each chromosome from the population's maximum and then dividing each value by the average of these adjusted errors, since the GA is more easily implemented when higher function values represent 'fitter' individuals (Davis, 1991).

The results are summarised in Table 1. In the case of the conventional model, it can be seen that the genetic algorithm finds the same solutions as the NAG routine but take much longer to execute, primarily because their run-times are determined by the parameters P and G in the genetic plan outlined previously. GAs have no simple means of knowing when to stop. In

Table 1 Run-times and optimal error values for model calibrations

	DATA #1		DATA #2	
	NAG	Genetic	NAG	Genetic
Conventional production-constrained gravity model				
time*	2.20	197.90	1.10	157.60
error†	260.78	260.78	7.67	7.67
Hybrid gravity and intervening opportunity model				
time*	4.20	177.80	2.70	139.10
error†	260.48	260.68	7.67	7.08
Three parameter competing destination model				
time*	516.40	2,104.70	225.20	1,098.20
error†	253.81‡	253.79	7.37‡	7.19
Five parameter competing destination model				
time*	875.20	2,312.30	401.30	1,321.40
error†	253.16‡	251.42	7.55‡	7.14

Notes

* - actual processing time (seconds), run on a Silicon Graphics multi-processor Challenge XL

† - minimum error function value

‡ - signifies a NAG soft failure, indicating a final solution was not found

the case of data #1 for example, the run times were 2 seconds for the NAG routine and 198 for the genetic algorithm; for data #2, the execution times were approximately 1 and 157 seconds respectively (Table 1).

The similarity of the results is not surprising as plots of β against model performance illustrate clearly identifiable single optimal solutions (Figures 1 and 2) and nice smooth functions, but will similar trends emerge for the more complicated models? The intervening opportunity model behaves in a somewhat similar manner and levels of performance are again almost identical, but with a slightly worse solution for data #1 and a much better solution for data #2 (Table 1). However, the competing destination models do not reflect these trends; the genetic algorithm provides an improved performance for both datasets. This is surprising and perhaps an indication that calibrating spatial interaction models need not always be straightforward. A plot of a three parameter competing destination model treating only β as independent (other parameters specified as outlined by Fotheringham, 1983) can be seen in figures 3 and 4. These graphs are much more complex, with evidence of various local minima far away from the global optimum. The GA is much better equipped to handle this problem than the conventional optimiser, the results of which are dependant on starting values. It is also noticeable that the problem areas occur in parameter value domains different from what would be considered as sensible values. However, how is the conventional optimiser supposed to know this, especially as it is almost certainly going to explore a wide range of non-sensical values, especially when optimising functions with multiple parameters.

Another interesting discovery is that the performance of the conventional model and the hybrid gravity and intervening opportunity model were similar whilst the competing destination models generally yielded slightly lower error values. This may reflect the characteristics of the data with an absence of intervening opportunities, reducing this particular model to a form similar to the conventional model, with the intervening opportunity term contributing very little.

Figure 1: Error function behaviour of a production-constrained spatial interaction model; data #1

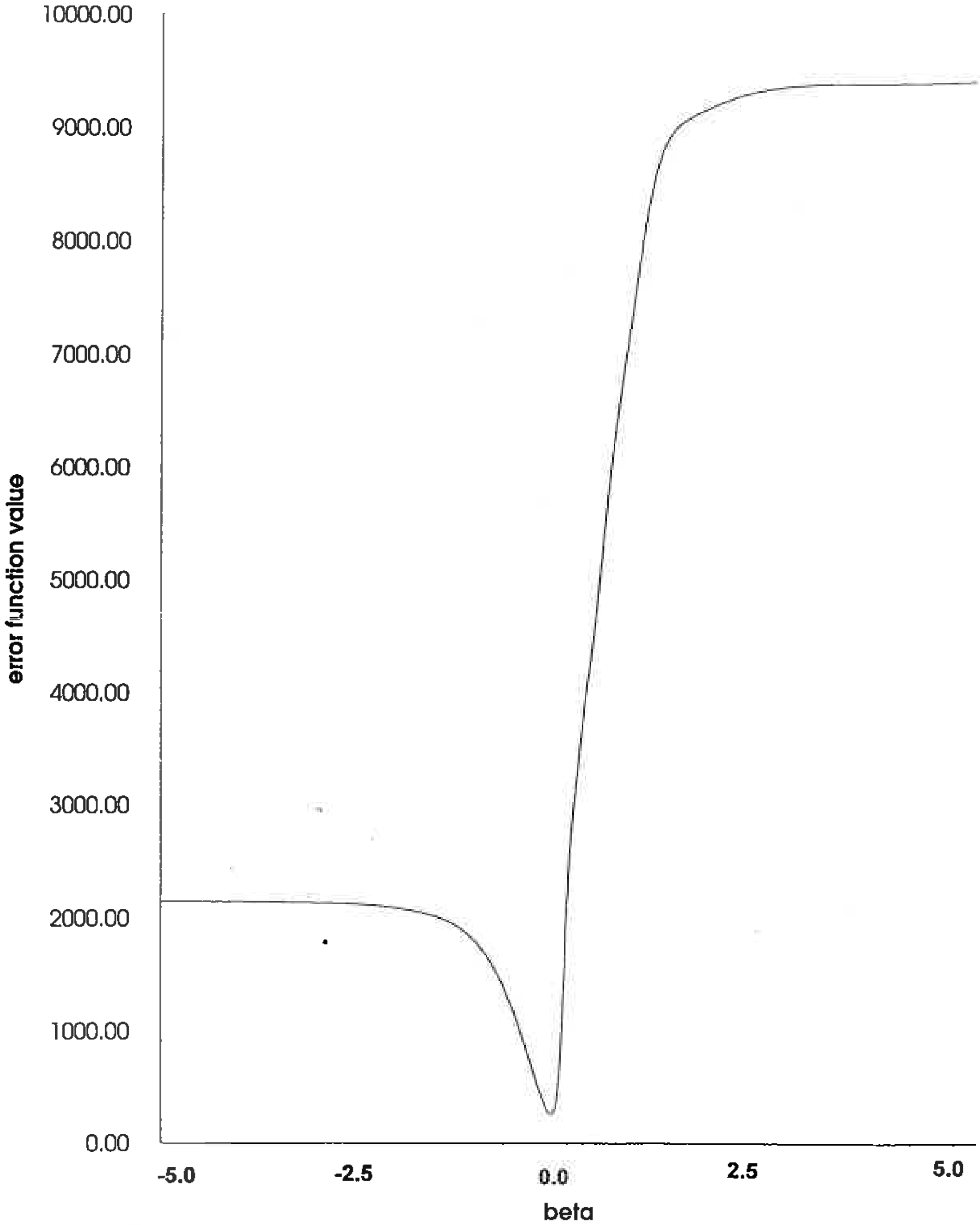


Figure 2: Error function behaviour of a production-constrained spatial interaction model; data #2

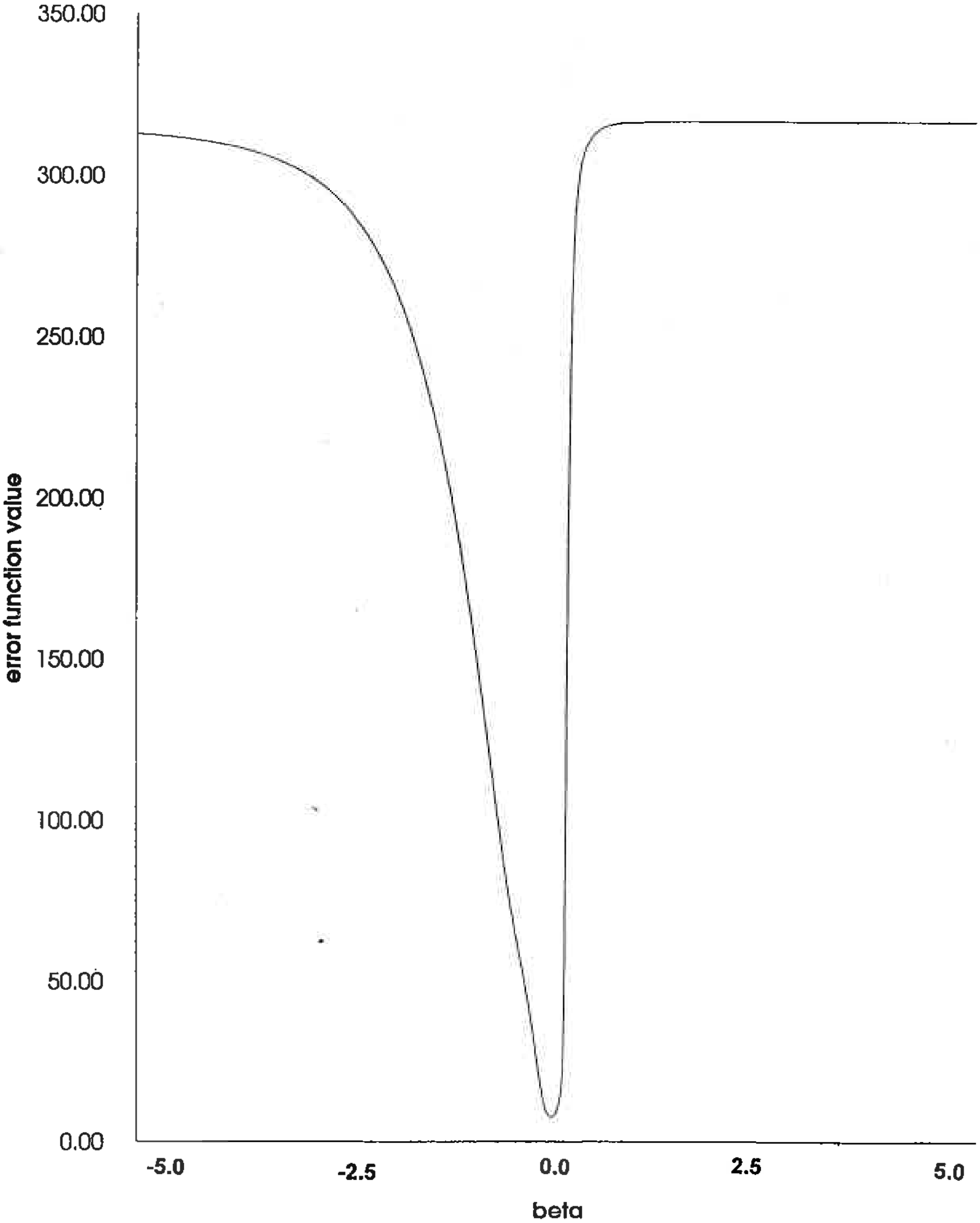


Figure 3: Error function behaviour of a competing destination spatial interaction model; data #1

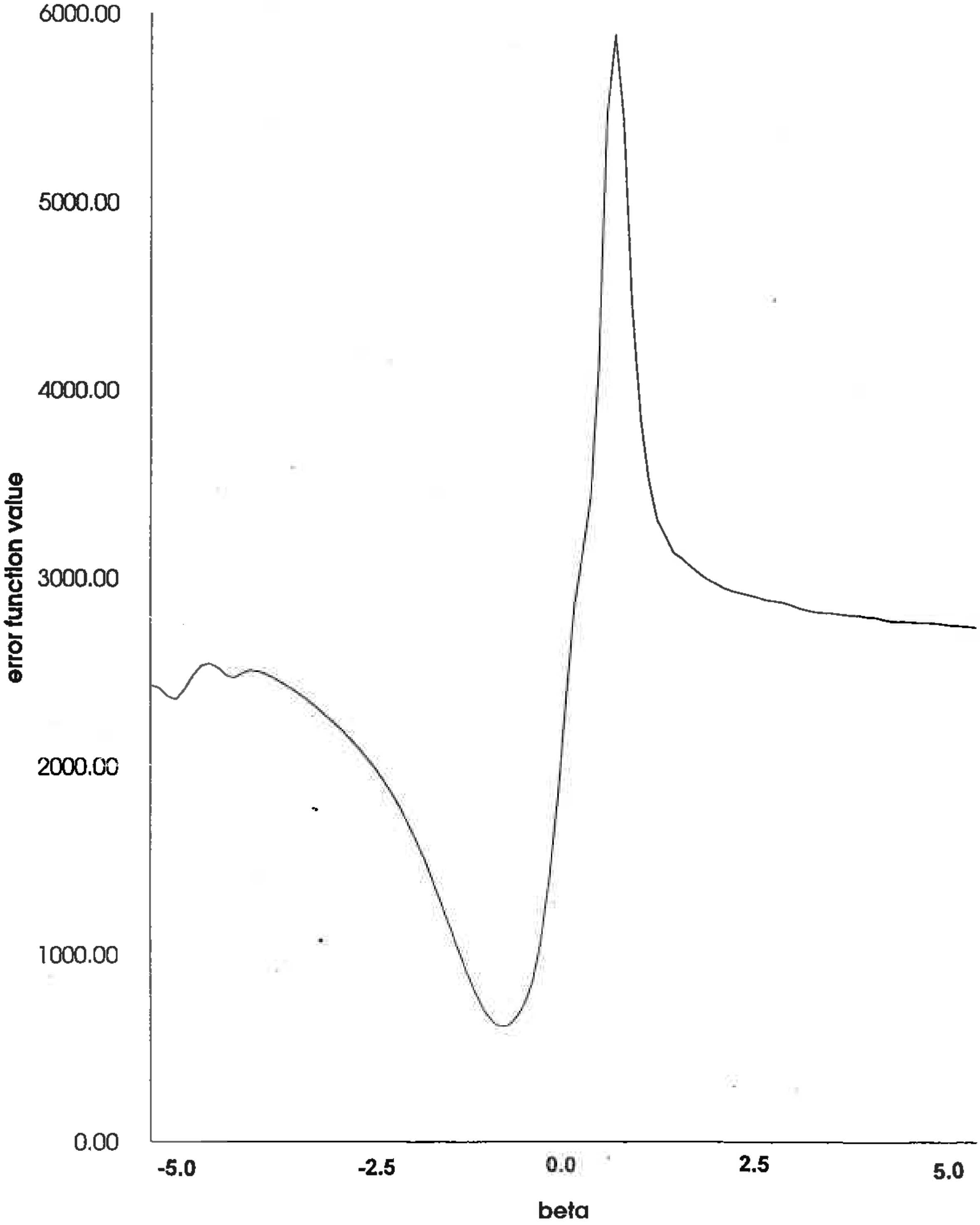
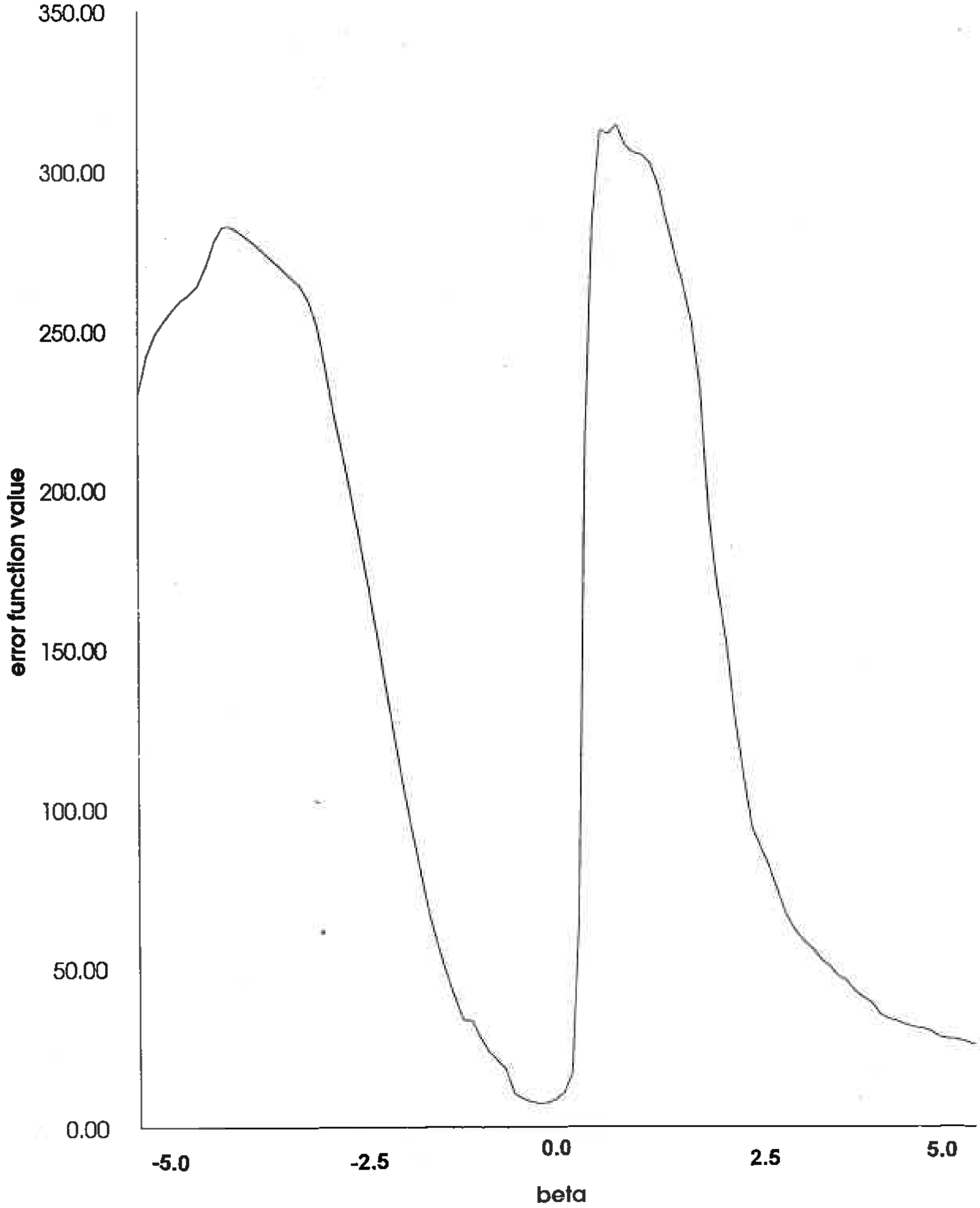


Figure 4: Error function behaviour of a competing destination spatial interaction model; data #2



The parameter values produced by the optimisation methods are also of interest. Table 2 (in conjunction with the values of Table 1) shows that with the exception of the conventional model, there are differences in parameter values even when overall levels of performance are the same, or very similar. For the intervening opportunity model markedly different λ values with similar β values were found to yield similar error function values in the case of data #1, even though the signs of the critical parameters accord with expectations. This feature is also characteristic of the three parameter competing destination model, with the β values being similar whilst the other parameters are very dissimilar. The five parameter version exhibited large differences in all the optimal parameter values, perhaps due to the model's complexity. The conventional method's estimates for β are distinctly odd, having the wrong sign. This looks very much as if the optimiser has either become stuck in the wrong part of the response surface, or inappropriate starting estimates were used. The latter is dismissed because neutral values were used (randomly generated α, β, γ, δ, σ within reasonable limits). The former is investigated by plotting different views of the response surface; see Figures 5 and 6. The plots vary β and δ, but assume σ is equal to β (Fotheringham, 1983). They show complex response surfaces with a mixture of sharp peaks and ravenous discontinuities separated by flat areas. This complex landscape provides possible reasons for similar performance with different parameter values; the optimiser makes it into the valley at a certain point, but not necessarily the same one, or in the case of the five parameter model results, the optimiser gets stuck in the valley associated with large positive β values and cannot subsequently escape.

The results illustrate the varied and unpredictable nature of the systems that are being modelled here, and give rise to a further question concerning whether the differences in parameter values obtained between the GA and NAG solutions matter. Whilst the differences appear large from a numerical point of view they need not be significant. They could be due to the flatness of the objective function in the region of the optimum making it insensitive to parameter values in this critical region. Indeed the optimal β values remained more or less constant for each dataset across the suite of models; indeed, when the NAG

Table 2 Optimal parameter values for model calibrations

	DATA #1		DATA #2	
	NAG	Genetic	NAG	Genetic
Conventional production-constrained gravity model				
β	-0.2211	-0.2211	-0.0756	-0.0756
Hybrid gravity and intervening opportunity model				
β	-0.2206	-0.2208	-0.0757	-0.0804
λ	-0.0008	-0.2262	-0.0002	-0.0015
Three parameter competing destination model				
β	-0.2250	-0.2139	-0.0756	-0.1035
δ	-3.4802	-1.9906	-4.0143	1.0965
σ	1.2669	0.2027	0.4857	0.2092
Five parameter competing destination model				
α	1.1121	0.7985	0.9057	0.7987
β	4.3319	-0.2238	2.1014	-0.0883
γ	1.3411	0.6657	1.6101	-0.7482
δ	0.5963	-0.3635	0.0683	1.7596
σ	-0.4996	0.4296	-1.3412	0.4072

Figure 5: Error function behaviour of a competing destination production constrained spatial interaction model; data #1

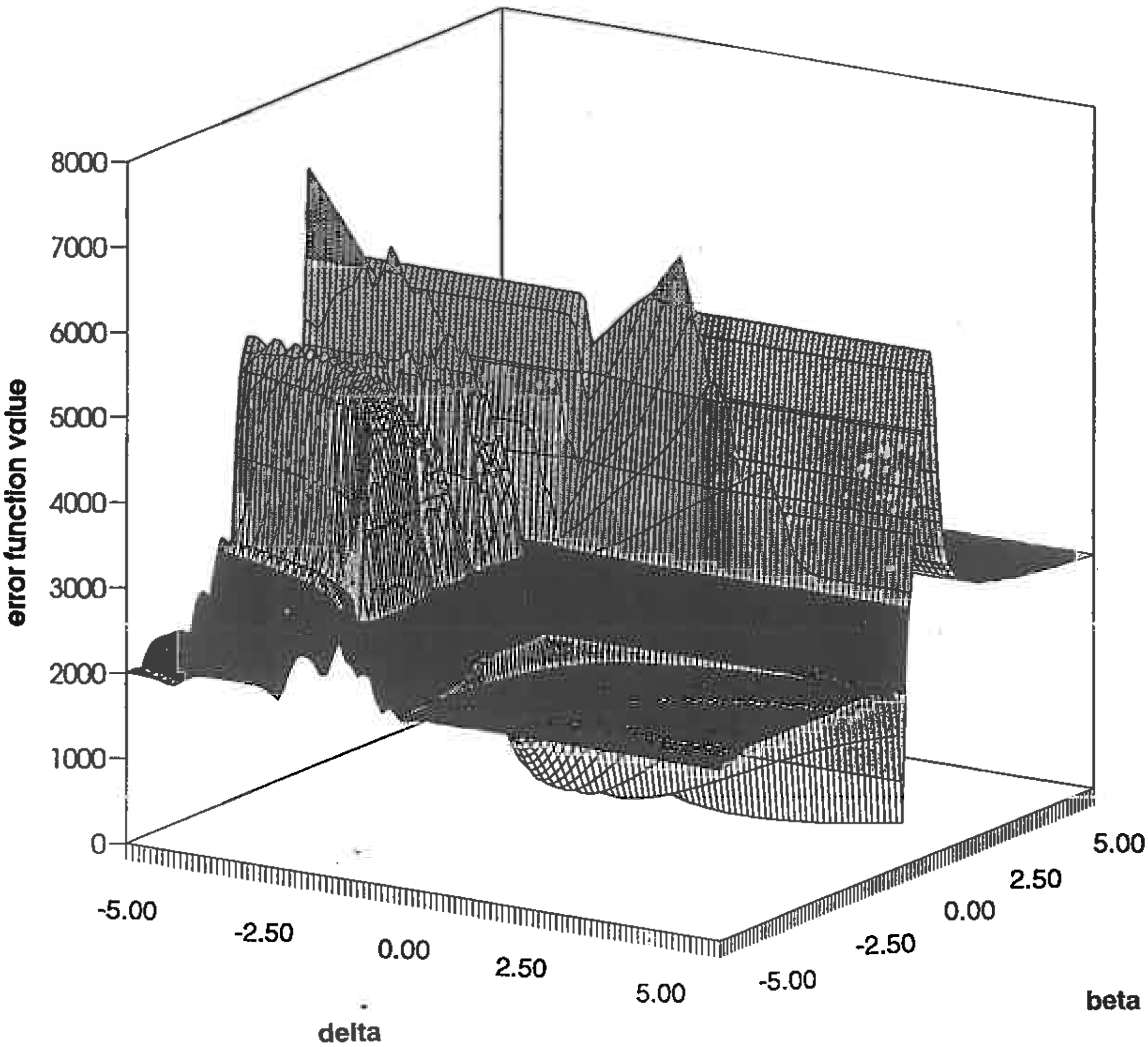
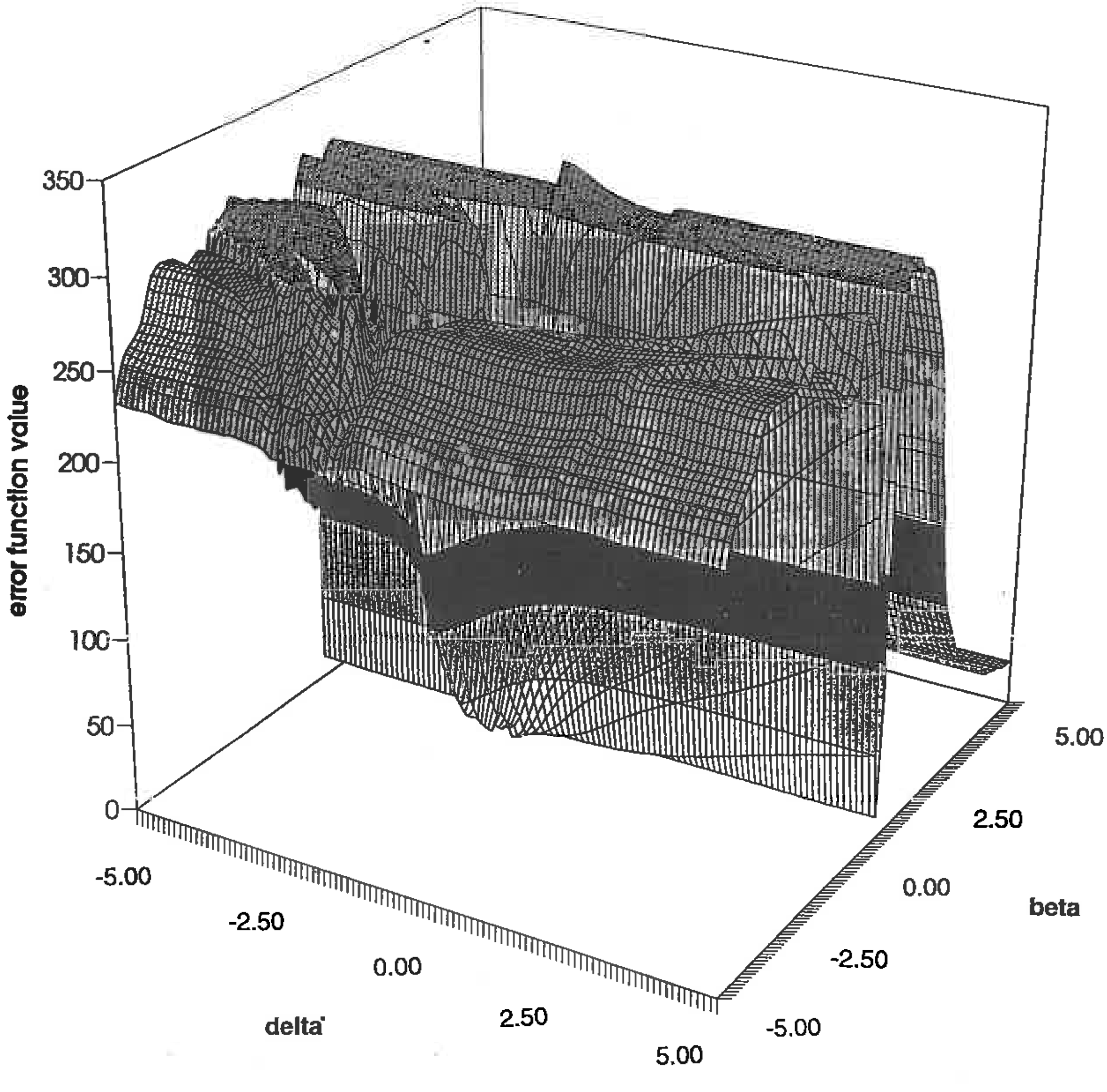


Figure 6: Error function behaviour of a competing destination production constrained spatial interaction model; data #2



routine reports a value differing from that identified in the one parameter model, the genetic algorithm's optimal solution outperforms that given by the library routine, suggesting that the NAG routine had in fact failed.

One way of estimating the "significance" of these differences is to compute standard errors for the NAG results (since they are more quickly found than the GA results) using a bootstrap procedure (Efron and Tibshirani, 1993). This may be contrasted with the asymptotic variance estimates that Fotheringham and O'Kelly (1989) use. The bootstrap provides an easy plug-in method for assessing statistical accuracy that becomes very attractive if the computational costs are acceptable. Here, 400 independent bootstrap samples are created from the trip data by sampling with replacement trip pairs drawn from the observed data. For instance, in data #1 there 5,229 trip pairs. A sample of 5,229 is selected with replacement and new sets of origin and destination totals computed. The model's parameters are then re-estimated using the NAG library conventional non-linear optimiser and saved. This process is repeated 400 times so that the mean and standard deviation of the bootstrap distribution can be computed. these statistics can be used to assign significance to the differences in parameter values; see Table 3. Differences greater than three standard deviations may be well be of interest.

Table 3 highlights the significantly different parameters. In all model specifications, β is the parameter which emerges with the lowest standard deviation, illustrating that if an optimal (or near optimal) β value is identified, the other parameters are perhaps less critical. This may well explain why the genetic algorithm outperforms the NAG routine for the more complex model, since it finds a better value for β. With this in mind it is perhaps not surprising that the majority of the genetic algorithm derived optimal parameter values lie outside the bounds of the bootstrap sample results for the competing destinations models, but not the conventional or hybrid models.

Table 3 Bootstrap estimates of parameter values and standard errors

	DATA #1			DATA #2		
	NAG		GA	NAG		GA
	bootstrap mean	bootstrap se	parameter	bootstrap mean	bootstrap se	parameter
Conventional production-constrained gravity model						
β	-0.2342	-0.0076	-0.2210	-0.0796	0.0094	-0.0756
Hybrid gravity and intervening opportunity model						
β	-0.2341	0.0079	-0.2208	-0.0798	0.0100	-0.0804
λ	-0.0009*	0.0009	-0.2262	-0.0001	0.0018	-0.0015
Three parameter competing destination model						
β	-0.2184	0.0140	-0.2139	-0.0715	0.0211	-0.1035
δ	-3.5684*	0.2634	-1.9906	-4.1503*	0.0145	1.0965
σ	1.3448*	0.0805	0.2027	0.5105*	0.0926	0.2092
Five parameter competing destination model						
α	1.2019*	0.0621	0.7985	0.9465*	0.0470	0.7987
β	4.2719*	0.0013	-0.2238	2.1013*	0.0013	-0.0883
γ	1.1574	0.9981	0.6657	1.3820	0.9974	-0.7482
δ	0.6721*	0.0183	-0.3635	0.0722*	0.0069	1.7596
σ	-0.4776*	0.0072	0.4296	-1.3419*	0.0352	0.4072

Notes

* - difference between GA and bootstrap result greater than three standard deviations

5 Conclusions

The results demonstrate that a simple, very basic GA can provide very good solutions for spatial interaction model recalibration, albeit at the expense of considerable extra compute time for simple models. The benefits are most relevant for relatively more complicated multi-parameter model specifications. The results are both re-assuring (the conventional optimiser works well) and worrying (similar levels of performance can be produced by different parameter values and there are unexplained differences in optimal parameter values). It would be very interesting to investigate further the reasons for these differences and also to determine whether the use of stochastic non-linear global optimisation methods might produce results closer to those obtained here; see Byrd et al (1992). As computer hardware becoming faster so the attractions of simple, relatively assumption free and highly robust approaches to global parameter estimation can only but grow and allow the geographical model builder to focus more on the task of model design, and worry less about the problems of parameter estimation.

References

Byrd, R.H., Eskow, E., Schnabel, R.B., Smith, S.L. (1992): '', in Fincham, A.E. and Ford, B. (eds): *Parallel Computation, New Series, vol. 46, pp.187-207*

Davis, L. (1991), ed: *Handbook of genetic algorithms*, Van Nostrand Reinhold, New York

De Jong, K.A. (1975): '*An analysis of the behaviour of a class of genetic adaptive systems*', Doctoral dissertation, University of Michigan

Efron, B.; Tibshirani, R.J. (1993): *An introduction to the bootstrap*, Chapman & Hall, London

Fogel, D.B. (1994): 'An introduction to simulated evolutionary optimisation', *IEEE Transactions on Neural Networks, vol.1, no.1, pp.3-14*

Fotheringham, A.S. (1983): 'A new set of spatial interaction models; the theory of competing destinations', *Environment & Planning A, vol.15, pp.15-36*

Fotheringham, A.S. (1984): '*Spatial flows and spatial patterns*', Environment & Planning A, vol.16, pp.529-543

Fotheringham, A.S. (1985): '*Spatial competition and agglomeration in urban modelling*', Environment & Planning A, vol.17, pp.213-230

Fotheringham, A.S. (1986): '*Modelling hierarchical destination choice*', Environment & Planning A, vol.18, pp.401-418

Fotheringham A.S.; O'Kelly, M.E. (1989): *Spatial Interaction models; formulations and applications*, Kluwer Academic Press, London

Goldberg, D.E. (1989): *Genetic algorithms in search, optimisation and machine learning*, Addison-Wesley, Reading

Gonçalves, M.B.; Ulysséa-Neto, I. (1993): 'The development of a new gravity-opportunity model for trip distribution', *Environment & Planning A, 1993, vol.25, pp.817-826*

Holland, J.H. (1975): *Adaptation in natural and artificial systems*, MIT Press, Cambridge

NAG (1991): *The NAG Fortran library manual; Mark 15*, The Numerical Algorithms Group Limited, Oxford

Openshaw, S. (1976): 'An empirical study of some spatial interaction models', *Environment & Planning A, vol.8, pp.23-41*

Roy, J.R. (1993): 'Comment of "The development of a new gravity-opportunity model for trip distribution"', *Environment & Planning A, vol.25, pp.1681-1691*

Scales, L.E. (1985): *Introduction to non-linear optimisation*, MacMillan, London

Wilson, A.G. (1971): 'A family of spatial interaction models and associated developments', *Environment & Planning A, vol.3, pp.1-32*

Wilson, A.G.; Clarke, M. (1979): 'Some illustrations of catastrophe theory applied to urban retailing structures', in Breheny, M.J. (ed): *Developments in urban and regional analysis; London papers in Regional Science 10*, Pion, London

Produced By
School of Geography
University of Leeds
Leeds LS2 9JT
From Whom Copies **May Be** Ordered

January 1995