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PROBABILITY SURFACE MAPPING. AN INTRODUCTION WITH EXAMPLES AND FORTRAN PROGRAMMES

N. Wrigley

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PROBABILITY SURFACE MAPPING

An introduction with examples and Fortran programs

by

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University of Bristol

CONTENTS

Page

I INTRODUCTION

(i) Purpose and pre-requisites 3
(ii) An introductory illustration 4

II THE TREND SURFACE MODEL AND THE SIMPLEST PROBABILITY SURFACE MODELS

(i) The form of the trend surface model, 9
(ii) The simplest kind of probability surface model 11
(iii) Estimating the parameters of the simplest probability surface models 15
(iv) Testing probability surfaces of progressively higher order 17
(v) Goodness-of-fit statistics 19
(vi) An empirical example 20

III EXTENDING THE SIMPLEST PROBABILITY SURFACE MODELS

(i) The generalised probability surface model 31
(ii) Estimating the parameters of the extended probability surface models 33
(iii) Testing probability surfaces and goodness-of-fit statistics 34
(iv) An empirical example 34

IV EXTENSIONS AND PROBLEM AREAS

(i) Introduction 42
(ii) The use of other functional forms 42
(iii) Programs for fitting different surfaces to different responses 42
(iv) Ordered categorizations 43
(v) Inference and estimation considerations 43
(vi) Graphical improvements 43
(vii) Spatial distribution of the data points 43
(viii) The problem of multicollinearity 44
(ix) Conclusion 45

Page

BIBLIOGRAPHY 45

APPENDICES

1 Computer programs for probability surface mapping 48

(a) A Fortran program for the two response category case 48
(b) A Fortran program for the three response category case 56
(c) A Fortran program for the four response category case 63
(d) The common subroutines 63

2 Alterations to the size restrictions of computer programs 63

3 Derivation of the standard errors and variance-covariance matrix of parameter estimates 72

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I INTRODUCTION

(i) Purpose and pre-requisites

Since its introduction into geography in the early 1960's (Chorley and Haggett, 1965) trend surface mapping has become one of the most widely known and widely used methods of spatial analysis in geographical research. Basically the aim of trend surface mapping is to decompose or separate a spatial series into two components, a trend or regional component and an error or local component. This separation is accomplished by specifying and fitting an appropriate trend surface model; appropriate in the sense that it captures the underlying regional structure or trend of the spatial series and leaves a local component showing no discernible systematic spatial variation. A trend surface model is essentially a linear regression model in which the explanatory variables are the geographical co-ordinates of each site or locality in the spatial series.

During the past fifteen years, as geographers have become increasingly aware of the assumptions, limitations and potentialities of regression models, a deeper understanding of trend surface models has developed. However, despite this deeper understanding, the range of applicability of trend surface mapping has remained virtually unaltered. One of the major reasons for this is the fact that until recently the trend surface method has been unable to handle one of the most important types of data collected and analysed by geographers. There appears to have been universal acceptance that variables to be mapped using the trend surface method must be measured at a high level, at least interval scale. Unfortunately for the geographer, a large proportion of the variables measured and utilized in geographical research, particularly in human geography, are measured at lower levels, at the nominal or ordinal scales of measurement. That is to say they are categorizations of an unordered (nominal scale) or ordered (ordinal scale) nature. As a result many of the variables measured and utilized in the course of geographical research have traditionally been viewed as unmappable by the trend surface method, and this has severely limited its range of applicability. Recently an attempt has been made by the author to free the method from this limitation. A technique has been presented (Wrigley, 1977) which allows the extension of surface mapping to the realms of categorized data, and which as a result provides an approach suitable for the imperfect types of data which are faced in geographical research. The technique has been given the name probability surface mapping and the maps produced are termed probability surface maps.

In the original paper outlining the probability surface mapping method, there was only space to introduce and illustrate the method in the briefest of fashions. The aim of this monograph is to consider the topic at greater length, to present examples and computer programs, and give sufficient detail to make the method available to all those who require it for practical research purposes. In the following sections the method will be reviewed and worked examples and the necessary FORTRAN computer programs will be discussed. The monograph assumes the reader is familiar with trend surface mapping as it has traditionally been used in geography (see the earlier CATMOG 5 by Unwin, 1975a) and with multiple linear regression (see CATMOG 15 by Ferguson, 1977). Prior consideration of the original probability surface paper (Wrigley, 1977) and the author's CATMOG 10 (Wrigley, 1976) will prove useful but is not essential.

(ii) An introductory illustration

Before we embark upon discussion of the technical aspects of probability surface mapping the reader may find it helps to sustain his interest if he first has a taste of the potential of the method. Consider the following case. A marketing geographer wishes to investigate the trade area characteristics of a recently opened hypermarket. To assess the extent of the trade area and the level of market, penetration within it, he conducts a household survey of shopping habits. Amongst other questions in the survey he elicits information from each housewife interviewed on whether or not she shops at the hypermarket and if she does, whether she shops there regularly or occasionally. Mapping the responses of the 144 housewives interviewed in the survey he draws the map shown in Figure 1. In this form the map is rather complex in appearance. There is some evidence of systematic spatial variation in the responses but the picture is by no means clear. By using the probability surface method, however, he is able to sift out the underlying systematic spatial variation in responses. He finds that the appropriate probability surfaces to fit are those shown in Figures 2, 3 and 4. These are, respectively, the probability surfaces of, regularly shopping at the hypermarket, occasionally shopping at the hypermarket and never shopping at the hypermarket. (The reader should note that these surface maps were produced automatically by the computer and the hand drawn contours were added to aid interpretation, using the key printed below each map).

Inspection of Figure 2 shows that the underlying regional structure of regularly shopping at the hypermarket is a 'dome' centred on the hypermarket. The probability of regularly shopping at the hypermarket falls away rapidly in all directions as one moves away from the hypermarket. In contrast, Figure 4 shows that the underlying regional structure of never shopping at the hypermarket is a flat-bottomed 'basin' centred on the hypermarket. The probability of never shopping at the hypermarket is low in the area surrounding the hypermarket but becomes high at the edges of the survey area. Finally, Figure 3 shows that the underlying regional structure of occasionally shopping at the hypermarket has a 'ring doughnut' type of structure, with the highest predicted probabilities 0.5 to 0.6 occurring in a broken ring or horseshoe some distance from the hypermarket. Immediately surrounding the hypermarket, the probability of occasionally shopping at the hypermarket falls to between 0.3 and 0.4, a level similar to that found in a ring some way from the hypermarket beyond the ring of higher probabilities.

Countless similar illustrations could have been provided. In the context of human geography for example, probability surfaces of aircraft noise annoyance around Manchester (Ringway) Airport have been described in Wrigley (1977), whilst in the context of physical geography and geology potential illustrations would include the use of probability surfaces of 'barren' or 'producing' oil wells in oil exploration, or probability surfaces of 'presence' or 'absence' of particular components in regional geochemical analyses.

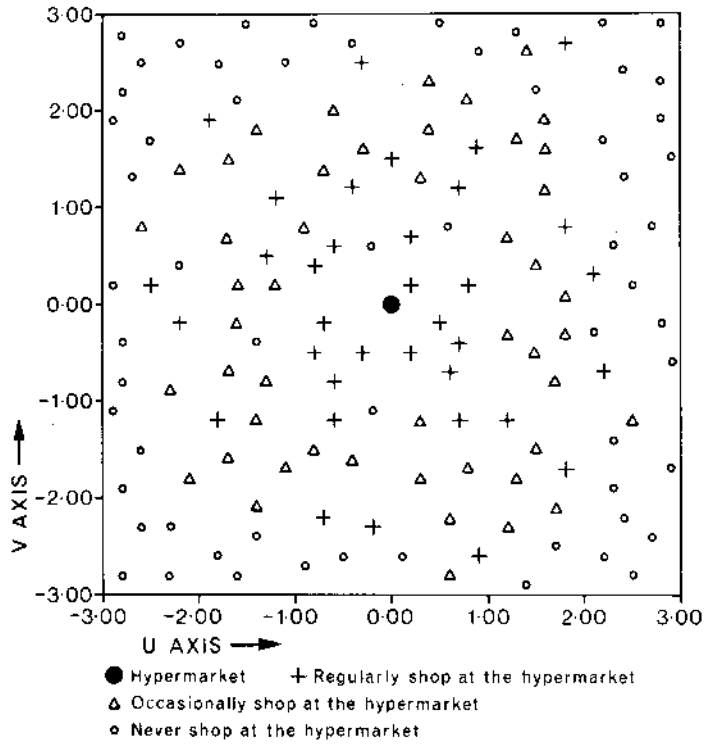

Fig. 1 Distribution of types of shoppers and non-shoppers around a hypermarket

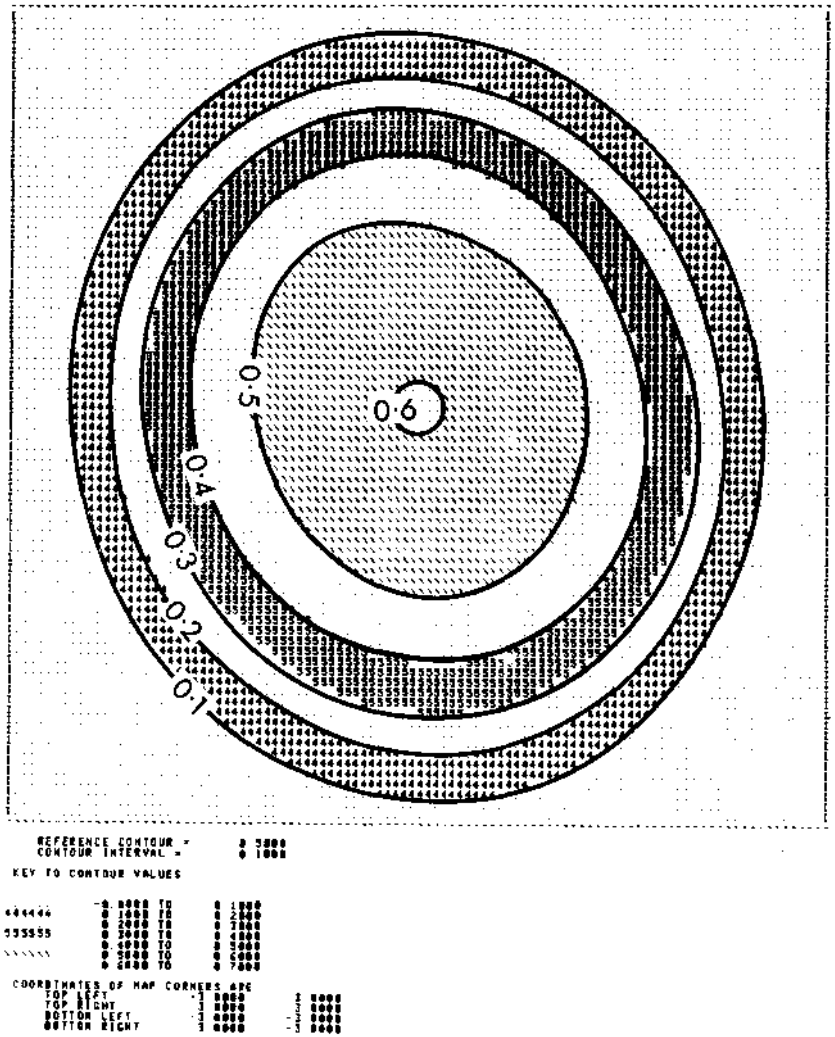

Fig. 2 2nd order probability surface of regularly shopping at the hypermarket

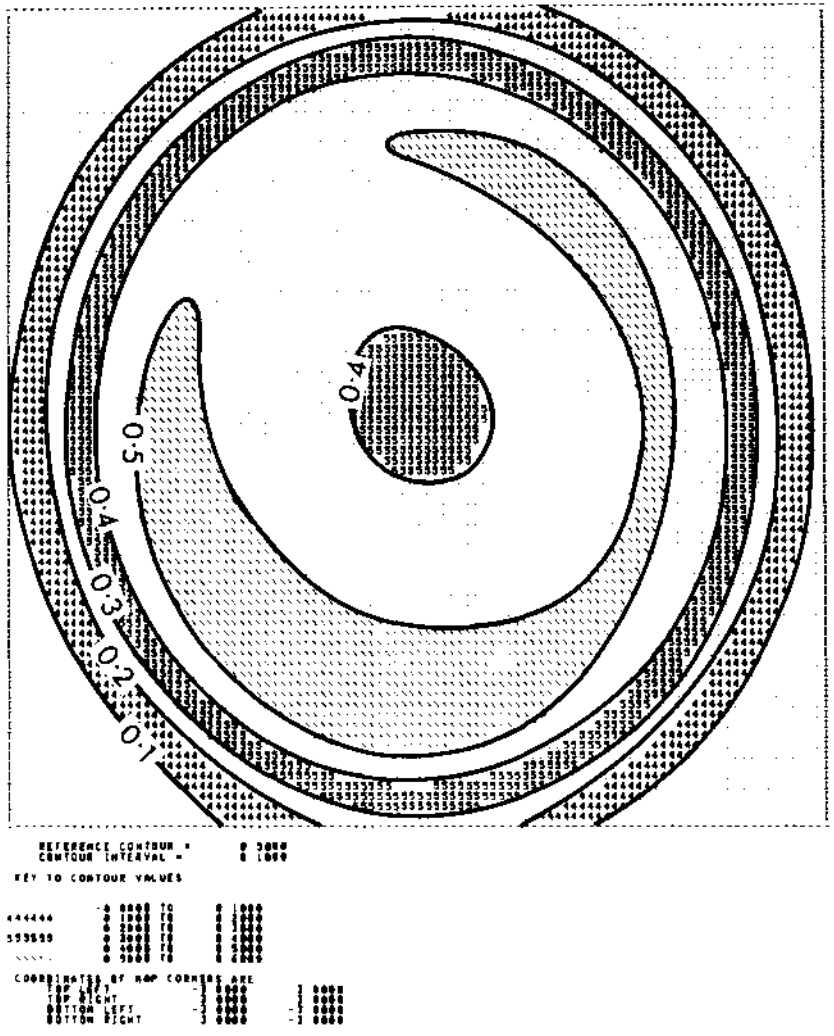

Fig. 3 2nd order probability surface of occasionally shopping at the hypermarket

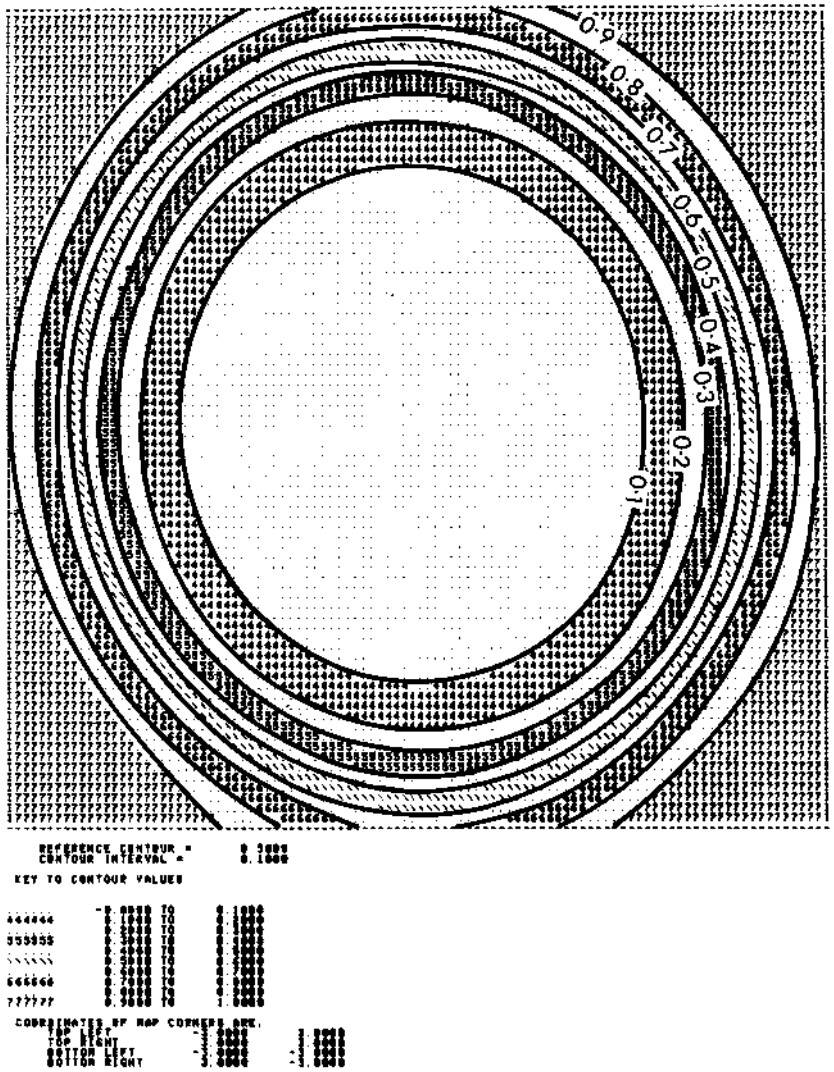

Fig. 4 2nd order probability surface of never shopping at the hypermarket

II THE TREND SURFACE MODEL AND THE SIMPLEST PROBABILITY SURFACE MODELS

(i) The form of the trend surface model

To understand probability surface models it is necessary to understand how they differ from traditional trend surface models. To help clarify these differences we will first briefly summarise the major features of trend surface models.

The traditional trend surface model can be written for each of a series of i localities (i=1,...N) as

$$Z_i = f(U_i,V_i) + \varepsilon_i \quad (1)$$

Z_i is the response variable or variable to be mapped; a metrically (interval or ratio) scaled random variable, and U_i and V_i are the geographical coordinates of locality i. The trend surface model assumes that Z_i is composed of two components, a 'trend' or 'regional' component $f(U_i,V_i)$ and a 'local' component ε_i. In geographical research the most widely used form of the function $f(U_i,V_i)$ is the polynomial power series expansion which has the general form

$$f(U_i,V_i) = \alpha + \beta_1 U_i + \beta_2 V_i + \beta_3 U_i^2 + \beta_4 U_i V_i + \beta_5 V_i^2 + \ldots \quad (2)$$

but other functional forms such as the double Fourier series (Bassett, 1972; Unwin, 1975a; Whitten, 1975) have also been used.

In the polynomial ,case, trend surface models of increasing complexity can be specified by including more and more terms in the power series expansion on the right hand side of. equation (2). The more complex the trend surface model, the higher the so called 'order' of the trend or regional component of Z_i. The simplest polynomial trend surface model is of 1st order and has the form

$$Z_i = \alpha + \beta_1 U_i + \beta_2 V_i + \varepsilon_i \quad (3)$$

The next most complex model is of 2nd order and has the form

$$Z_i = \alpha + \beta_1 U_i + \beta_2 V_i + \beta_3 U_i^2 + \beta_4 U_i V_i + \beta_5 V_i^2 + \varepsilon_i \quad (4)$$

Three additional terms have been added to the 1st order model, and it can be seen that these new terms include squares or second powers of the coordinates. Higher order models follow the same pattern, the highest power included in the expansion at any point denotes the order of the trend surface model. For example a third order trend surface model has the form

$$Z_i = \alpha + \beta_1 U_i + \beta_2 V_i + \beta_3 U_i^2 + \beta_4 U_i V_i + \beta_5 V_i^2 + \beta_6 U_i^3 + \beta_7 U_i^2 V_i + \beta_8 U_i V_i^2 + \beta_9 V_i^3 + \varepsilon_i \quad (5)$$

In most of the following discussion, rather than distinguish a particular order of model, it will be useful to refer to polynomial trend surface models as a class. For this purpose we will use the general form of the expansion given in equation (2).

The trend surface model, equation (1), describes a stochastic dependence relationship between U_i, V_i and Z_i. The error term or stochastic disturbance ε_i is random and therefore for every pair of values U_i, V_i, there exists a whole probability distribution of possible values of Z_i. The trend surface model is therefore essentially a multiple regression model, and furthermore, because the forms of the function $f(U_i,V_i)$ used are normally linear in the unknown parameters (i.e. equation (2) is linear in the unknown parameters α, β_1, β_2...) the trend surface model is normally a multiple linear regression model. As a result, a full specification of the trend surface model must consist of the same assumptions as an equivalent multiple linear regression model (see Ferguson, 1977). In the case of most geographical applications, this means that the specification of the trend surface model must embody the same assumptions as in what is termed the classical normal multiple linear regression model. These assumptions are as follows.

(A1) The linearity assumption. The regression equation should be linear in the unknown parameters. For example, whereas equation (4) is nonlinear in the variables, it is linear in the parameters and thus is an intrinsically linear model.

(A2) The assumption that the values of the explanatory variables in the regression model can be measured without error.

(A3) The assumption that the values of the explanatory variables are fixed or nonstochastic. (This assumption can easily be relaxed.)

(A4) The assumption that no exact linear relationship exists between two or more of the explanatory variables. This is known as the no multicollinearity assumption.

(A5) The assumption that the number of observations exceeds the number of parameters to be estimated.

(A6) The zero error mean assumption. This is written $E(\varepsilon_i) = 0$. ($E(\varepsilon_i)$ is known as the expectation or expected value of ε_i, it is simply the mean of the probability distribution of possible values of ε_i.)

(A7) The constant error variance or homoscedasticity assumption. This is written $E(\varepsilon_i^2) = Var(\varepsilon_i) = \sigma^2$.

(A8) The independent error terms assumption. This is written $E(\varepsilon_i\varepsilon_j) = 0$, for $i \neq j$. In the case where i and j refer to geographical localities this assumption is known as the spatially independent error terms or no spatial autocorrelation assumption.

(A9) The assumption that ε_i is normally distributed.

In the case of the trend surface model, assumptions (A3) and (A6) imply that if we take expectations of both sides of (1), it follows that

$$E(Z_i) = E\left[f(U_i,V_i) + \varepsilon_i\right]$$
$$= f(U_i,V_i) \qquad (6)$$

(By assumption (A3), U_i and V_i are fixed values, thus $E(U_i) = U_i$ and $E(V_i) = V_i$. By assumption (A6) $E(\varepsilon_i) = 0$.) In the case of the widely used polynomial form of the function $f(U_i,V_i)$, equation (6) can be written as

$$E(Z_i) = \alpha + \beta_1U_i + \beta_2V_i + \beta_3U_i^2 + \beta_4U_iV_i + \beta_5V_i^2 \ldots \qquad (7)$$

This relationship gives the mean value of Z_i associated with the pair of geographical co-ordinates U_i and V_i for each of the i possible localities in a particular area. Across the i localities it defines what might be

termed the 'true' or population trend surface. The parameters of this equation α, β_1, β_2 ... are unknown however, and consequently we must estimate their values from the observed Z_i, U_i, V_i values of a sample of the possible localities in the area. When the α and β parameters are estimated in this way we write them as $\hat{\alpha}$ and $\hat{\beta}$, and on the basis of their values (still using the polynomial form of the function) we define the equation

$$\hat{Z}_i = \hat{\alpha} + \hat{\beta}_1U_i + \hat{\beta}_2V_i + \hat{\beta}_3U_i^2 + \hat{\beta}_4U_iV_i + \hat{\beta}_5V_i^2 \ldots \qquad (8)$$

This gives $\hat{Z}_i$, the predicted or fitted value of the trend or regional component at locality i, which serves as a sample estimate of the 'true' or population trend component at locality i. Across the i localities equation (8) defines what might be termed the sample trend surface.

In practice few of the observed values of Z_i will lie exactly on the sample trend surface, most will lie either above or below it, and so the values of Z_i and $\hat{Z}_i$ will differ. This difference is called a residual and is designated e_i

$$Z_i - \hat{Z}_i = Z_i - (\hat{\alpha} + \hat{\beta}_1U_i + \hat{\beta}_2V_i + \hat{\beta}_3U_i^2 + \hat{\beta}_4U_iV_i + \hat{\beta}_5V_i^2 \ldots)$$
$$= e_i \qquad (9)$$

In general, because $\hat{\alpha}$, $\hat{\beta}_1$, $\hat{\beta}_2$ ... are likely to differ from the true values of α, β_1, β_2 ..., the residual e_i is different from the stochastic disturbance or error component term ε_i, for ε_i is given by the relationship

$$Z_i - E(Z_i) = Z_i - (\alpha + \beta_1U_i + \beta_2V_i + \beta_3U_i^2 + \beta_4U_iV_i + \beta_5V_i^2 \ldots)$$
$$= \varepsilon_i \qquad (10)$$

ε_i is a population term and cannot be observed. The value of the residual e_i can thus be regarded as a sample estimate of ε_i.

The method normally used by geographers to estimate the parameters of a trend surface model is the method of least squares. (See for example Unwin, 1975a, p.8-16, 19-21.) Under the assumptions (A1) to (A9) outlined above, the so called ordinary least squares (O.L.S.) estimators $\hat{\alpha}$, $\hat{\beta}_1$, $\hat{\beta}_2$ ... can be shown to be what are termed the best linear unbiased estimators (BLUES). Best linear unbiased estimators have a number of properties which intuitively we would like a 'good' estimator to possess. (See the discussion by Kmenta, 1971, p.154-93; Huang, 1970, p.26-32; Wonnacott and Wonnacott, 1970, p.40-47.) They are unbiased; in other words each estimator has a sampling distribution with a mean equal to the parameter to be estimated. Each estimator also has a variance which is smaller than that of any other unbiased estimator (best linear unbiasedness).

(ii) The simplest kind of probability surface model

Having summarised the major features of trend surface models we are

variable to be mapped, Z_i, is not a metrically (interval or ratio) scaled random variable as it is assumed to be in traditional trend surface models, but is instead a categorized (nominal or ordinal scaled) variable.

The simplest case we can encounter of such a categorized response variable is a random variable with only two possible outcomes. For example, returning to the hypermarket trade area mapping illustration given earlier, the survey conducted might simply ask housewives to indicate whether they shop at the hypermarket or not, that is to say, to give a simple yes/no response. If we then code these two possible responses 1 and 0, 1 representing the response 'yes I shop at the hypermarket' and 0 representing the response no I do not shop at the hypermarket', and try to use such a response variable in the traditional trend surface model we will encounter three problems.

(i) The first problem we will encounter concerns the predicted values which are generated if we use the traditional trend surface model (1). Since Z_i in this case can only assume two different values, 1 and 0, $E(Z_i)$, the expected value of Z_i is a simple weighted average of the two possible values of Z_i with weights given by the respective probabilities of occurrence of the possible values. Purely arbitrarily we will say that the probability that $Z_i=1$ is P_i and that the probability that $Z_i=0$ is $1-P_i$. The expected value of Z_i is then

$$E(Z_i) = \{1xP_i\} + \{0x(1-P_i)\} = P_i \tag{11}$$

Using the result we found in equation (6) we then have

$$P_i = E(Z_i) = f(U_i,V_i) \tag{12}$$

In other words, it is useful and reasonable to interpret the expectation of of Z_i given the co-ordinates of locality i, U_i and V_i, as the probability of giving the specified response 'yes I shop at the hypermarket' at locality i. The problem with this interpretation however, concerns the predicted values $\hat{Z}_i$ generated using the traditional trend surface model (1). Using the polynomial form of the function, $\hat{Z}_i$ equals

$$\hat{Z}_i = \hat{\alpha} + \hat{\beta}_1U_i + \hat{\beta}_2V_i + \hat{\beta}_3U_i^2 + \hat{\beta}_4U_iV_i + \hat{\beta}_5V_i^2 \ldots \tag{13}$$

In view of the probability interpretation of $E(Z_i)$, these predicted values are interpreted as predicted probabilities, i.e. $\hat{Z}_i = \hat{P}_i$. However, whereas probability is defined to lie between 0 and 1, the predictions (13) generated using the traditional trend surface model are unbounded and may take values from $-\infty$ to $+\infty$. Consequently the predictions may lie outside the meaningful range of probability and thus be inconsistent with the probability interpretation advanced.

(ii) The second problem we will encounter concerns the violation of the constant error variance assumption (A7). This follows from the fact that the error term

$$\varepsilon_i = Z_i - f(U_i,V_i) \tag{14}$$

can in this case only have one of two possible values

$$\varepsilon_i = \begin{cases} 1 - f(U_i,V_i) & \text{if } Z_i = 1 \\ - f(U_i,V_i) & \text{if } Z_i = 0 \end{cases} \tag{15}$$

These two possible values of ε_i must occur with probabilities P_i and $1-P_i$ respectively. Thus the assumption (A6) ($E(\varepsilon_i)=0$) implies

$$E(\varepsilon_i) = P_i\{1-f(U_i,V_i)\} + (1-P_i)\{-f(U_i,V_i)\} = 0 \tag{6}$$

Solving for P_i or from (12) directly, we have that

$$P_i = f(U_i,V_i) \tag{7}$$

$$1-P_i = 1 - f(U_i,V_i) \tag{8}$$

The error variance can therefore be written

$$E(\varepsilon_i^2) = P_i\{1-f(U_i,V_i)\}^2 + (1-P_i)\{-f(U_i,V_i)\}^2$$

or using (17)

$$E(\varepsilon_i^2) = P_i(1-P_i)^2 + (1-P_i)(-P_i)^2$$

$$= P_i(1-P_i) \tag{16}$$

Clearly the error variance is not a constant. Localities where P_i is close to 0 or close to 1 will have relatively low variances while localities where P_i is close to 0.5 will have higher variances. When the constant error variance assumption is violated the problem of heteroscedasticity is said to be present. Heteroscedasticity does not result in biased parameter estimates, but it does result in a loss of efficiency. In addition, heteroscedasticity implies that the estimated variances of the estimated parameters will be biased estimators of the true variances of the estimated parameters. If these biased estimators are used, then the statistical tests commonly used in trend surface mapping will be incorrect.

(iii) The third problem we will encounter, and an additional reason for not using the statistical tests employed in trend surface mapping is that in the categorized response variable case the error distribution is not normal. Assumption (A9) therefore does not hold and the commonly used statistical tests can not be applied since the tests depend on the normality of the errors.

As a means of handling a simple categorized response variable the traditional trend surface model is thus seriously deficient. The probability surface models which we will now consider attempt to overcome these deficiences.

We have seen that in the case of a simple categorized response variable with only two possible outcomes, the expected value of Z_i can be interpreted as a probability. That is to say, in our example $E(Z_i) = P_i$, where P_i is the probability of giving the response 'yes I shop at the hypermarket'. In view of this probability interpretation, the predicted values $\hat{Z}_i$ generated when the parameters of the trend surface model are estimated, are interpreted as predicted probabilities. In order to allow the probability interpretation it is necessary therefore that the condition

$$0 \leq \hat{P}_i \leq 1 \tag{20}$$

is satisfied by the predicted values of the trend surface model. Unfortunately, as we have seen, this condition is not necessarily satisfied by the usual trend surface model for it produces predicted values which can range from $-\infty$ to $+\infty$. If we are to improve upon the traditional trend surface model as a means of handling categorized response variables we must therefore seek a model which produces predicted values which satisfy condition (20).

There are a number of potential models which do this, (see Wrigley, 1976, p.9-11; Domencich and McFadden, 1975, p.102-108; Pindyck and Rubinfeld, 1976, p.238-249) but perhaps the most convenient of them is based upon the logistic function.

$$P_i = \frac{e^{f(U_i,V_i)}}{1+e^{f(U_i,V_i)}} \qquad (21)$$

As the value of $f(U_i,V_i)$ ranges from $-\infty$ to $+\infty$, P_i ranges in value from 0 to 1. As an alternative this model can be rewritten as follows to produce a linear model

$$1 + e^{f(U_i,V_i)} = \frac{e^{f(U_i,V_i)}}{P_i}$$

$$P_i = e^{f(U_i,V_i)} - e^{f(U_i,V_i)} P_i$$

$$P_i = (1-P_i)e^{f(U_i,V_i)}$$

$$\frac{P_i}{1-P_i} = e^{f(U_i,V_i)}$$

Then remembering that by the definition of a logarithm if $y=e^x$, $\log_e y=x$, we have

$$\log_e \frac{P_i}{1-P_i} = f(U_i,V_i) \qquad (22)$$

The left hand side of this model is a transformation of P_i known as the logit transformation and we can abbreviate it as L_i. The important point to note about this transformation is that it increases from $-\infty$ to $+\infty$ as P_i increases from 0 to 1. What this means is that the predicted logit values $\hat{L}_i$ derived when the parameters of the model are estimated (using in this case the polynomial form of the function as an example)

$$\hat{L}_i = \log_e \frac{\hat{P}_i}{1-\hat{P}_i} = \hat{\alpha} + \hat{\beta}_1 U_i + \hat{\beta}_2 V_i + \hat{\beta}_3 U_i^2 + \hat{\beta}_4 U_i V_i + \hat{\beta}_5 V_i^2 \ldots \qquad (23)$$

can take any values in the range $-\infty$ to $+\infty$, but the predicted probabilities which can be found by substituting $\hat{\alpha}$, $\hat{\beta}_1$, $\hat{\beta}_2$ ... into equation (21) remain confined within the range 0 to 1.

We call the linear model (22) the linear logit probability surface model or simply the linear probability surface model. The nonlinear model (21) from which it was derived can therefore be termed the nonlinear probability surface model. Both satisfy the predicted probabilities condition (20) and both represent feasible alternatives to the traditional trend surface model for the categorized response variable case.

In the case of our example, P_i represents the probability of giving the response 'yes I shop at the hypermarket' at locality i. $1-P_i$ therefore represents the probability of giving the response no I do not shop at the hypermarket' at locality i, and the equivalent nonlinear model for this case is

$$1-P_i = \frac{1}{1+e^{f(U_i,V_i)}} \qquad (24)$$

It should be clear therefore that for the simplest categorized response variable, a dichotomous variable, one with only two possible outcomes, two probability surfaces can be mapped on the basis of models (21) and (24). In the case of our example, these two surfaces are the probability surface of shopping at the hypermarket, and the probability surface of not shopping at the hypermarket. It should also be clear that the probabilities of giving the two possible responses sum to one at each locality i. This means that in the two response category situation the nonlinear probability surface model is actually a set of two linked models (21) and (24); the models being linked by the fact that response probabilities must sum to one at each locality.

(iii) Estimating the parameters of the simplest probability surface models

Having found models which are more suited to the categorized response variable situation, how do we then estimate the parameters of these models? There are in fact two ways of doing this, a weighted least squares procedure and a direct maximum likelihood procedure.

In the case of the linear probability surface model we can use a least squares estimation method. Least squares is a method of estimation familiar to most geographers and the so called ordinary least squares (O.L.S.) method is the estimation procedure normally adopted for the traditional trend surface model. In the case of the linear probability surface model however, because the assumption (A7) of constant error variance is violated, the least squares method which must be employed is that known as weighted least squares (W.L.S). The method is discussed in the context of linear logit models in Wrigley (1976, p.12-18).

As an alternative to weighted least squares we can use a direct maximum likelihood procedure. This procedure uses the probability expressions (21) and (24) directly and thus it can be thought of as a method of estimating the parameters of the nonlinear probability surface model without first having to convert the model into the linear form (22).

Although both estimation methods give equivalent results in situations where the categorized variable is sampled at a large number of localities, and there are few parameters in the probability surface model to be estimated (i.e. in the polynomial case, when the order of the probability surface to be fitted is low), the maximum likelihood estimation method has significant practical advantages over the weighted least squares method. In the weighted least squares method it is necessary to grbup localities into sets (see Wrigley, 1976, p.12; Pindyck and Rubinfeld, 1976, p.249-250). This is a laborious procedure which does not lend itself to the development of the type of computer programs to be presented in Appendix 1. Moreover, it necessitates partitioning the continuous explanatory variables U_i and V_i (the geographical co-ordinates). In other words it involves reducing continuously distributed explanatory variables to a categorized form, with a consequent waste of information, and the risk of introducing bias into the estimation procedure. The only drawbacks to the maximum likelihood method are that it is less familiar to most geographers, and that it demands a numerical optimization computer routine. In this monograph the appropriate numerical optimization routine will be supplied and moreover it is hoped to show that in the case of probability surface models the maximum likelihood estimation procedure is readily understandable even by geographers totally unfamiliar with the method. As a result, from this point onwards, the method of probability surface mapping will be developed and illustrated assuming direct maximum likelihood estimation, and the use of the nonlinear form of the probability surface model.

In the case of the categorized response variable with only two possible outcomes, the first thing required when using the maximum likelihood estimation method is what is termed the <u>likelihood</u> of the set of observations. Because in this case the observations are drawn from a discrete distribution the likelihood is simply their joint probability of occurrence. This can be written

$$\text{Likelihood} = \Lambda = \prod_{i=1}^{N_1} P_i \prod_{i=N_1+1}^{N} (1-P_i) \qquad (25)$$

(Π simply means multiply the elements together e.g. $\prod_{i=1}^{N} P_i = P_1 \times P_2 \times \ldots P_N$)

P_i is the probability that the housewife at locality i gives the response 'yes I shop at the hypermarket' and $1-P_i$ is the probability that she gives the response 'no I do not shop at the hypermarket'. N is the total sample size; N_1 is the total number of housewives in the sample who claim to shop at the hypermarket, and $N-N_1$ is the number who claim not to shop at the hypermarket. In other words, whenever $Z_i = 1$ (the housewife at locality i claims to shop at the hypermarket) the likelihood contains a term (21). Whenever $Z_i = 0$ (the housewife at locality i claims not to shop at the hypermarket) the likelihood contains a term (24). Substituting from (21) and (24) we thus have

$$\Lambda = \prod_{i=1}^{N_1} \frac{e^{f(U_i,V_i)}}{1+e^{f(U_i,V_i)}} \prod_{i=N_1+1}^{N} \frac{1}{1+e^{f(U_i,V_i)}} \qquad (26)$$

As specified the likelihood depends upon a set of unknown parameters (e.g. in the case of the polynomial $f(U_i,V_i) = \alpha + \beta_1 U_i + \beta_2 V_i + \beta_3 U_i^2 + \beta_4 U_i V_i + \beta_5 V_i^2 \ldots$). These parameters must then be estimated by taking as estimates the values which maximize the overall value of this likelihood equation. In practice, rather than maximize the likelihood itself, it is usual to maximize instead the logarithm of the likelihood. In the case of (26) this implies maximizing

$$\log_e \Lambda = \sum_{i=1}^{N_1} f(U_i,V_i) - \sum_{i=1}^{N} \log_e (1+e^{f(U_i,V_i)}) \qquad (27)$$

The maximum can be found by partially differentiating equation (27) with respect to its parameters and setting the partial derivatives equal to zero. The solution of the resulting set of equations yields the maximum likelihood parameter estimates. Provided no exact linear relationship exists between two or more of the explanatory variables, in other words, provided the data are not perfectly multicollinear, then the existence of a unique maximum is virtually certain in empirical samples of more than ten or twenty observations (Domencich and McFadden, 1975, p.111).

In practical terms the user of probability surface mapping need only know that the maximum likelihood estimation method employed has the logic described above. The computer routine described in Appendix 1(a) performs the estimation automatically.

(iv) <u>Testing probability surfaces of progressively higher order</u>

When discussing the widely used polynomial trend surface model (see II (i)) we noted that trend surface models of increasing complexity were denoted by the so called 'order' of the trend component they specified. A considerable amount of discussion in traditional polynomial trend surface mapping centres on statistical tests to determine what is the appropriate order of trend surface to fit; in other words what order of trend surface captures the underlying regional structure of the original spatial series (see Unwin, 1975a, p.21-24). Now that the form of the simplest probability surface models and methods of parameter estimation have been discussed we must therefore consider the question of what is the appropriate order of probability surface to fit.

In trend surface mapping, for any surface of order N+1, two distinct hypotheses can be tested:
a) A null hypothesis of no trend. That is to say, we test whether all parameters associated with the explanatory variables $U_i, V_i \ldots$ (note that this does not include the α parameter associated with the constant term) in the trend surface of order N+1 equal zero. This is a test of the significance of the surface in isolation from other surfaces.
b) A null hypothesis of no significant reduction in residual sum of squares, or increase in regression sum of squares, between a trend surface of order N and a surface of order N+1. This is a test of the <u>improvement,</u> if any, in the ability of a more complex trend surface of order N+1 to capture the underlying regional structure compared with a less complex surface of order N.

In the case of probability surface mapping, the same type of tests can be conducted, but instead of using residual or regression sums of squares and the F ratio, we now must use inferential tests based upon the maximized log likelihood value for different orders of probability surface. The test statistic we use (see Cox, 1970, p.88) is

$$\log_e\Lambda - \log_e\Lambda^* \qquad (28)$$

$\log_e\Lambda$ is the maximized log likelihood of a set of unrestricted probability surface models, whereas $\log_e\Lambda^*$ is the maximized log likelihood of a set of restricted probability surface models embodying q constraints on the parameters of the set of unrestricted models. This test statistic is distributed asymptotically as one half chi-squared with g degrees of freedom.

Using this statistic, hypotheses equivalent to those in trend surface mapping, (a) and (b) above, can be tested.

a*) A null hypothesis of no trend, that is to say a test of whether all parameters associated with the explanatory variables U_i, V_i ... in the set of linked probability surface models of order N+1, equal zero. In this case $\log_e\Lambda$ is the maximized log likelihood for the set of linked probability surface models of order N+1, and $\log_e\Lambda^*$ is the maximized log likelihood for the set of linked probability surface models of order zero (in other words for the set of probability surface models containing only intercept/constant terms). For convenience we can write this as $\log_e\Lambda^*(C)$.

b*) A null hypothesis of no significant improvement in the ability of a linked set of more complex probability surface models of order N+1 to capture the underlying regional structure compared with a linked set of less complex probability surface models of order N. In this case $\log_e\Lambda$ is the maximized log likelihood for the set of probability surface models of order N+1, and $\log_e\Lambda^*$ is the maximized log likelihood for the set of probability surface models of order N.

In trend surface mapping, when determining the appropriate order of trend surface to fit it is wise to use in addition to the F ratio tests of hypotheses (a) and (b) described above, tests of the amount of systematic spatial variation in the maps of residuals from surfaces of different orders In recent years the ability to test residual maps for systematic spatial variation in this way has been significantly improved by the development of a spatial autocorrelation statistic for use with regression residuals by Cliff and Ord (1972) (see Cliff and Ord, 1973, p.122-127 for a trend surface mapping example).

In probability surface mapping, similar residual map tests would be a useful addition to the tests described in (a*) and (b*) above. To this end we first need therefore a definition of a residual. In the simple two response category case a residual can be defined as

$$Z_i - \hat{P}_i = e_i \qquad (29)$$

Cox (1970, p.96) has suggested standardising such residuals to have a mean of zero and a unit variance as follows

$$\frac{Z_i - \hat{P}_i}{\sqrt{\hat{P}_i(1-\hat{P}_i)}} = e_i \qquad (30)$$

Although this residual has useful properties, because Z_i can only take the value 0 or 1 its distribution like that of (29) will typically be highly non-normal. In particular, residuals close to the value zero will not occur except for extreme values of $\hat{P}_i$. In these locations where there is a high or low probability of the first response category being selected (or in terms of the example discussed above, of shopping at the hypermarket) the residuals have a very skew distribution. Thus in locations where the probability of selecting the first response category is high, the residuals are either small and positive or large and negative. In locations where the probability of selecting the first response category is low, the residuals are either small and negative or large and positive.

In attempts to extend the spatial autocorrelation statistic to the case of residuals (29-30) from probability surface maps, we are hampered not only by the extreme non-normality of the residuals but also by the fact that the Cliff-Ord spatial autocorrelation statistic for regression residuals is not applicable to residuals derived from a nonlinear model. Some form of generalisation of the Cliff-Ord regression residuals statistic is required. In the absence of such a statistic we might perhaps attempt purely visual or ad hoc statistical assessment of the presence of spatial autocorrelation amongst our mapped residuals, or employ in an informal manner Cliff and Ord's (1969) earlier spatial autocorrelation statistic for spatially distributed variables using the version of the test based upon the assumption of randomisation rather than that based upon the assumption of normality. These suggestions are however only tentative and much work remains to be done in this area.

(v) Goodness-of-fit statistics

In traditional trend surface mapping, so called 'goodness-of-fit' statistics are widely used to answer the question, how closely does a trend surface fit the original observations? (see Unwin, 1975a, p.14; Whitten, 1975, p.286-291). These statistics are based upon the R^2 value, the squared multiple correlation coefficient, and they range in value from either 0 to 1, or from 0% to 100%.

In probability surface mapping a goodness-of-fit statistic is available which fulfills the same purpose, but in this case it is based upon the likelihood ratio index (see Tardiff, 1976 and Domencich and McFadden, 1975, p.123). It has the form

$$\rho^2 = 1 - \frac{\log_e\Lambda}{\log_e\Lambda^*(C)} \qquad (31)$$

As noted in II (iv), $\log_e\Lambda^*(C)$ is the maximized log likelihood for a set of linked probability surface models containing only intercept/constant terms (i.e. for the set of probability surface models of order zero). $\log_e\Lambda$ is the maximized log likelihood for the set of linked probability surface models which generate the probability surfaces whose goodness-of-fit is to be assessed. Like goodness-of-fit statistics in traditional trend surface mapping its value ranges from 0 to 1, or from 0% to 100% if multiplied by 100.

The reader should note however, that (31) is not the only goodness-of-fit statistic based upon the likelihood ratio which has been suggested. The economist John Cragg has suggested and used (see for example Baxter and Cragg, 1970, p.230) a 'pseudo' R^2 value which is defined as

$$R^2_p = \frac{1-e^{\{2(\log_e\Lambda^*(C)-\log_e\Lambda)/N\}}}{1-e^{\{2\log_e\Lambda^*(C)/N\}}} \qquad (32)$$

The definition of its components is the same as in (31) with the addition of N which is the total number of observations in the sample. This statistic also ranges in value from 0 to 1 but it gives results which differ from those produced by (31). Clearly therefore the question of what constitutes an appropriate goodness-of-fit statistic is not yet fully resolved.

(vi) An empirical example

Now that we have discussed the form of the simplest probability surface models, methods of parameter estimation, and how to conduct inferential tests, we will work through an actual example of probability surface mapping. As in the discussion above, we will consider the case of a marketing geographer who wishes to investigate the trade area characteristics of a recently opened hypermarket. To assess the extent of the trade area and the level of market penetration within it he conducts a household survey of the shopping habits of 108 housewives in the area surrounding the hypermarket. Amongst other questions in the survey he asks each housewife whether she shops at the hypermarket or not. This information can either be portrayed in map form, as in Figure 5, or in tabular form, as in Table 1. Notice that in Table 1 the home of each housewife has been given a four figure map reference.

Given this survey data, the marketing geographer then wishes to fit probability surfaces of a polynomial type. To achieve this he uses the program supplied in Appendix 1(a). This program allows the user to fit, in a sequential manner, polynomial probability surfaces from order 1 up to order 4. For each surface order the program produces: probability surface maps for both the possible responses, i.e. the probability surface of shopping at the hypermarket and the probability surface of not shopping at the hypermarket; the maximized log likelihood; parameter estimates; standard errors; the variance-covariance matrix of the parameter estimates; predicted probabilities of giving each response for each of the sample respondents; raw residuals (see equation 29) and standardised residuals (see equation 30). Prior to this, the maximized log likelihood for the set of probability surface models containing only an intercept term is printed. This provides the $\log_e\Lambda^*(C)$ value required in the tests described in II (iv) and the goodness-of-fit statistics described in II (v). By using this program to fit probability surfaces up to order 3 he achieves the results shown in Table 2 and Figures 6, 7 and 8.

Table 2 gives the maximized log likelihoods for probability surface models of orders 0 to 3; the differences between these maximized log likelihoods; the differences expected under the null hypothesis (H_0) of no significant improvement between surface models of different orders (see II (iv) hypothesis b*), and the decision on the null hypothesis at conventional

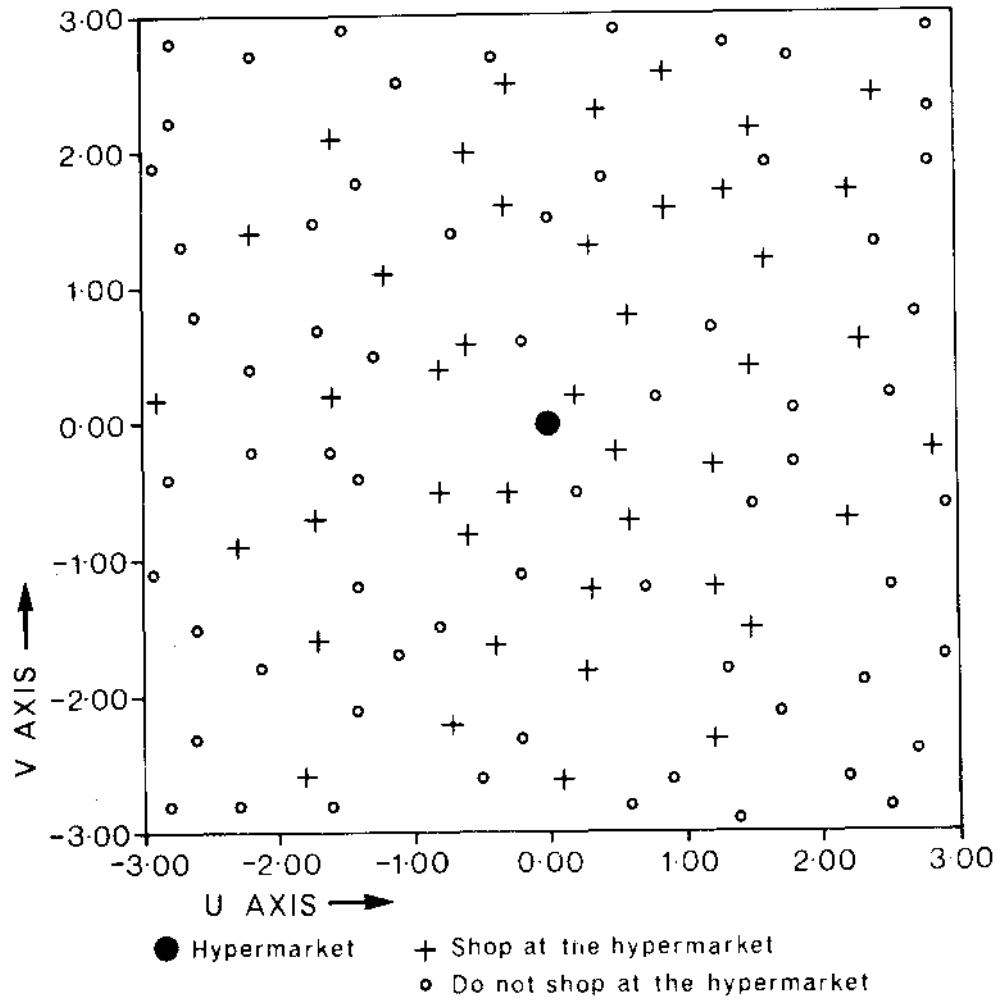

Fig. 5 Map plot of responses to shopping survey

Table 1

Respondent	U	V	Shopping at hypermarket	Respondent	U	V	Shopping at hypermarket
1	-2.8	-2.8	N	55	-2.9	0.2	Y
2	-2.6	-2.3	N	56	-2.6	0.8	N
3	-2.3	-2.8	N	57	-2.2	0.4	N
4	-1.8	-2.6	Y	58	-1.7	0.7	N
5	-1.6	-2.8	N	59	-1.6	0.2	Y
6	-1.4	-2.1	N	60	-1.3	0.5	N
7	-0.7	-2.2	Y	61	-0.8	0.4	Y
8	-0.5	-2.6	N	62	-0.6	0.6	Y
9	-0.2	-2.3	N	63	-0.2	0.6	N
10	0.1	-2.6	Y	64	0.2	0.2	Y
11	0.6	-2.8	N	65	0.6	0.8	Y
12	0.9	-2.6	N	66	0.8	0.2	N
13	1.2	-2.3	Y	67	1.2	0.7	N
14	1.4	-2.9	N	68	1.5	0.4	Y
15	1.7	-2.1	N	69	1.8	0.1	N
16	2.2	-2.6	N	70	2.3	0.6	Y
17	2.5	-2.8	N	71	2.5	0.2	N
18	2.7	-2.4	N	72	2.7	0.8	N
19	-2.9	-1.1	N	73	-2.9	1.9	N
20	-2.6	-1.5	N	74	-2.7	1.3	N
21	-2.1	-1.8	N	75	-2.2	1.4	Y
22	-1.7	-1.6	Y	76	-1.7	1.5	N
23	-1.4	-1.2	N	77	-1.4	1.8	N
24	-1.1	-1.7	N	78	-1.2	1.1	Y
25	-0.8	-1.5	N	79	-0.7	1.4	N
26	-0.4	-1.6	Y	80	-0.3	1.6	Y
27	-0.2	-1.1	N	81	0.0	1.5	N
28	0.3	-1.2	Y	82	0.3	1.3	Y
29	0.3	-1.8	y	83	0.4	1.8	N
30	0.7	-1.2	N	84	0.9	1.6	Y
31	1.2	-1.2	Y	85	1.3	1.7	Y
32	1.3	-1.8	N	86	1.6	1.9	N
33	1.5	-1.5	V	87	1.6	1.2	Y
34	2.3	-1.9	N	88	2.2	1.7	Y
35	2.5	-1.2	N	89	2.4	1.3	N
36	2.9	-1.7	N	90	2.8	1.9	N
37	-2.8	-0.4	N	91	-2.8	2.2	N
38	-2.3	-0.9	Y	92	-2.8	2.8	N
39	-2.2	-0.2	N	93	-2.2	2.7	N
40	-1.7	-0.7	Y	94	-1.6	2.1	Y
41	-1.6	-0.2	N	95	-1.5	2.9	N
42	-1.4	-0.4	N	96	-1.1	2.5	N
43	-0.8	-0.5	V	97	-0.6	2.0	Y
44	-0.6	-0.8	Y	98	-0.4	2.7	N
45	-0.3	-0.5	Y	99	-0.3	2.5	Y
46	0.2	-0.5	N	100	0.4	2.3	Y
47	0.5	-0.2	Y	101	0.5	2.9	N
48	0.6	-0.7	Y	102	0.9	2.6	Y
49	1.2	-0.3	Y	103	1.3	2.8	N
50	1.5	-0.5	N	104	1.5	2.2	Y
51	1.8	-0.3	N	105	1.8	2.7	N
52	2.2	-0.7	Y	106	2.4	2.4	Y
53	2.8	-0.2	Y	107	2.8	2.3	N
54	2.9	-0.6	N	108	2.8	2.9	N

Table 2.

Order of surfaces	Maximized log likelihood	Difference between the maximized log likelihoods of surface orders					Goodness of fit	
			Expected under H_0					
		Observed	1%	5%	D.F.	Decision on H_0	ρ^2	R^2_p
0	−72.603							
		0.458	4.605	2.996	2	Fail to reject		
1	−72.145						0.0063	0.0114
		9.746	5.672	3.907	3	Reject at 1% level		
2	−62.399						0.1405	0.2329
		0.285	6.638	4.744	4	Fail to reject		
3	−62.114						0.1445	0.2388

significance levels. Also given are the values of the two goodness-of-fit statistics discussed in II (v).

Using test statistic (28) and the method explained in II (iv) hypothesis b*, the first time a step from surface order N to surface order N+1 is encountered that does not significantly improve our ability to capture the underlying regional structure, we should stop fitting surfaces of higher order and accept the probability surface models of order N. There is, however, a generally acknowledged exception to this rule in the trend surface context (see Whitten, 1975, p. 289) which also applies in the case of the example under consideration. The exception occurs where the underlying regional structure is a symmetrical 'dome' or 'basin'. In this case, first order surfaces will capture little of this underlying structure and the improvement over zero order surfaces will be insignificant. The second order surfaces, however, will capture a significant amount of this underlying regional structure, and it is clearly worthwhile extending the models to this higher order.

Table 2 shows clearly that it is the second order probability surfaces which are the appropriate surfaces to fit. The increased complexity (i.e. the increased number of parameters to be estimated) associated with moving from second order probability surface models to third order models is associated with only a minor improvement in the maximized log likelihood, and consequently there is no advantage to be gained.

The conclusions drawn using Table 2 are borne out in an examination of the probability surfaces themselves. Figures 6 (a) and (b), 7 (a) and (b), and 8 (a) and (b), show respectively the first, second and third order probability surfaces of shopping at the hypermarket and not shopping at the hypermarket. Clearly the third order surfaces add little to the picture of the underlying regional structure given in Figures 7 (a) and (b) by the second order surfaces. This underlying regional structure is a 'dome' centred on the hypermarket in the case of Figure 7 (a), the probability surface of shopping at the hypermarket, and a 'basin' centred on the

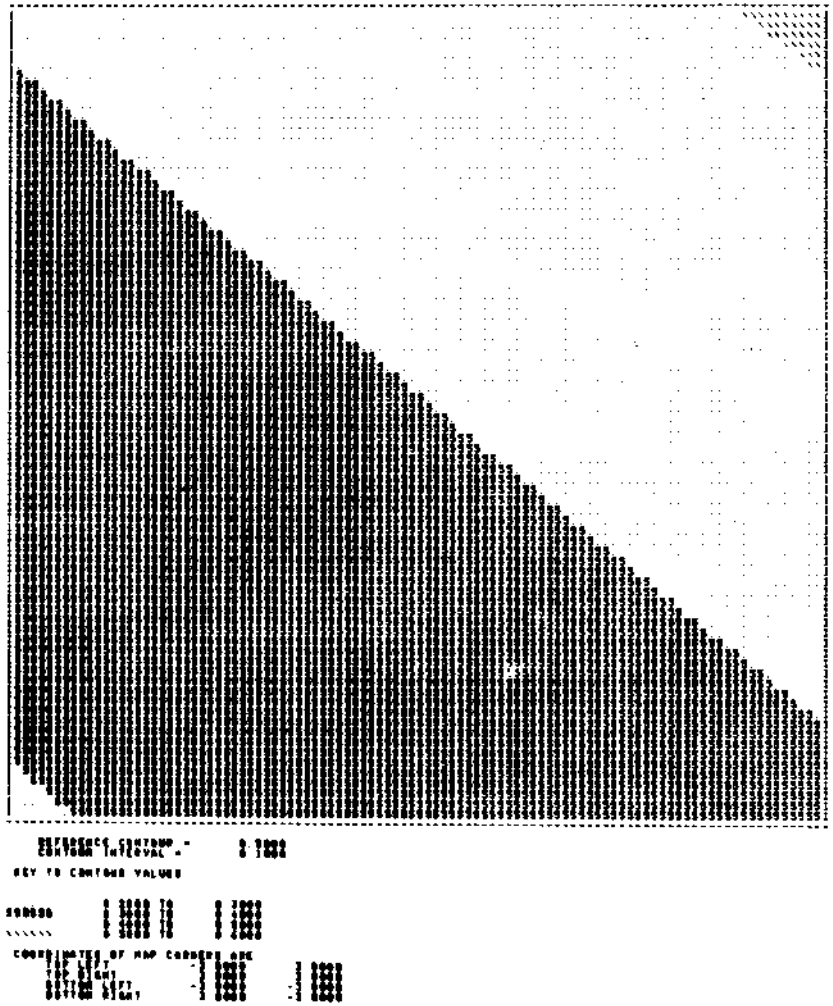

Fig. 6(a) 1st order probability surface of shopping at the hypermarket

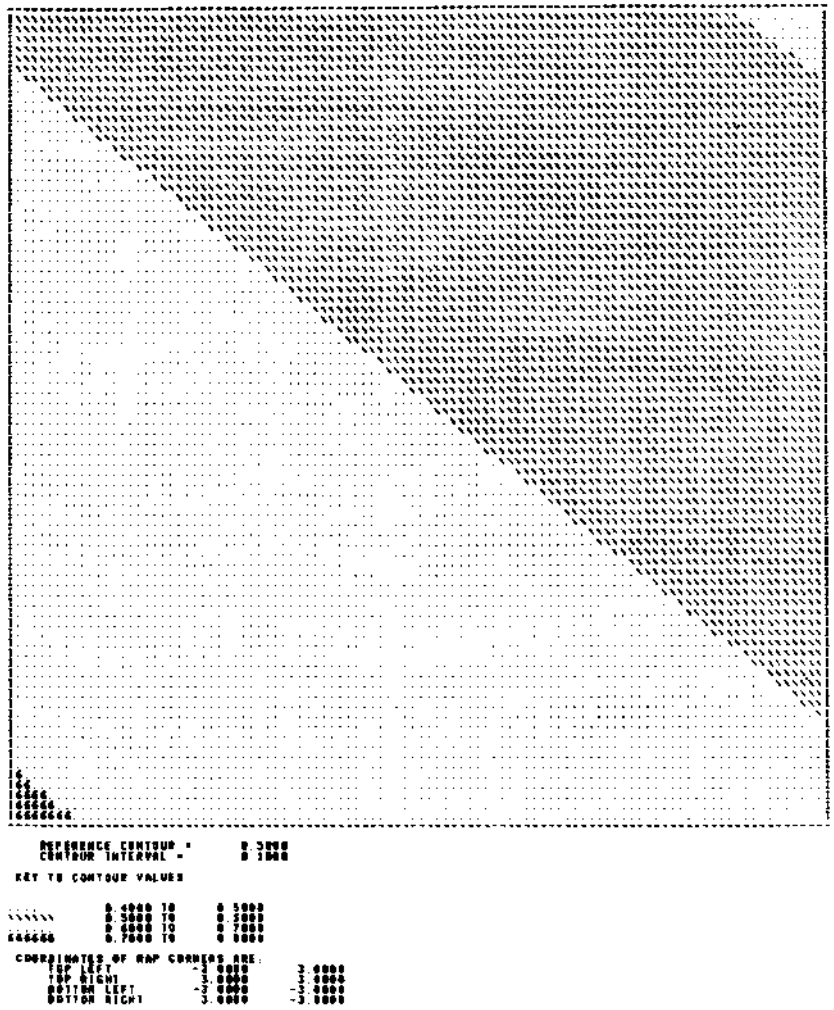

Fig. 6(b) 1st order probability surface of not shopping at the hypermarket

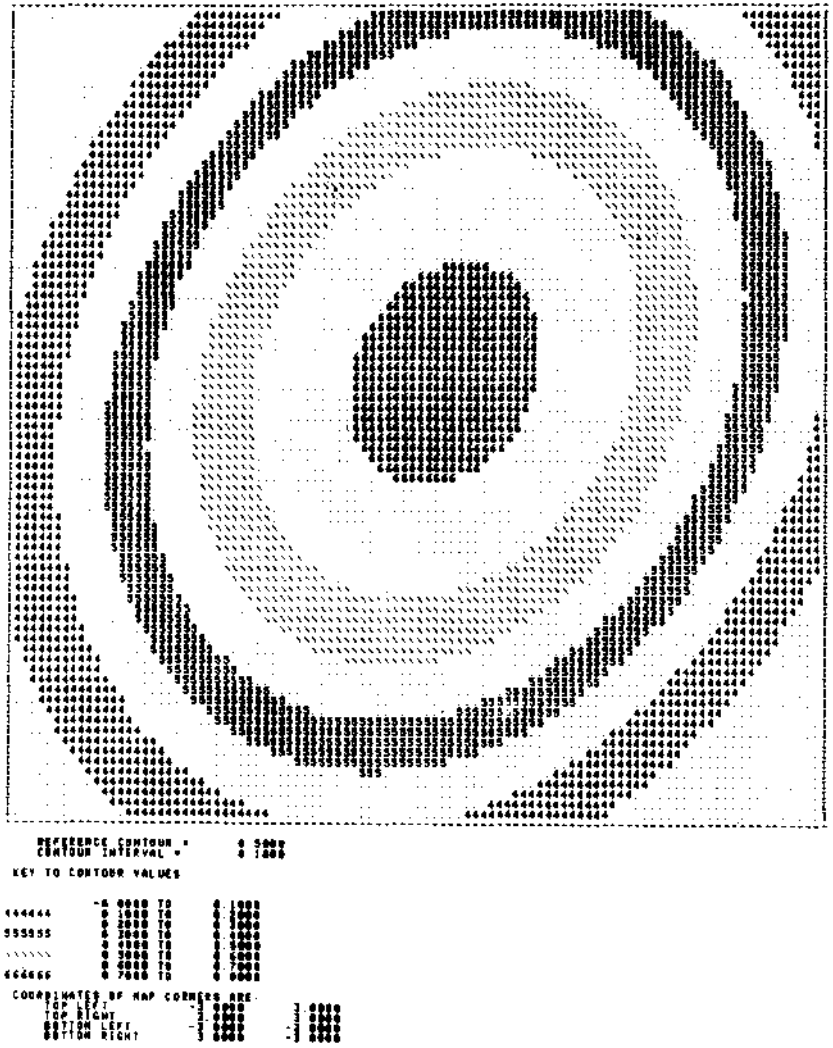

Fig. 7(a) 2nd order probability surface of shopping at the hypermarket

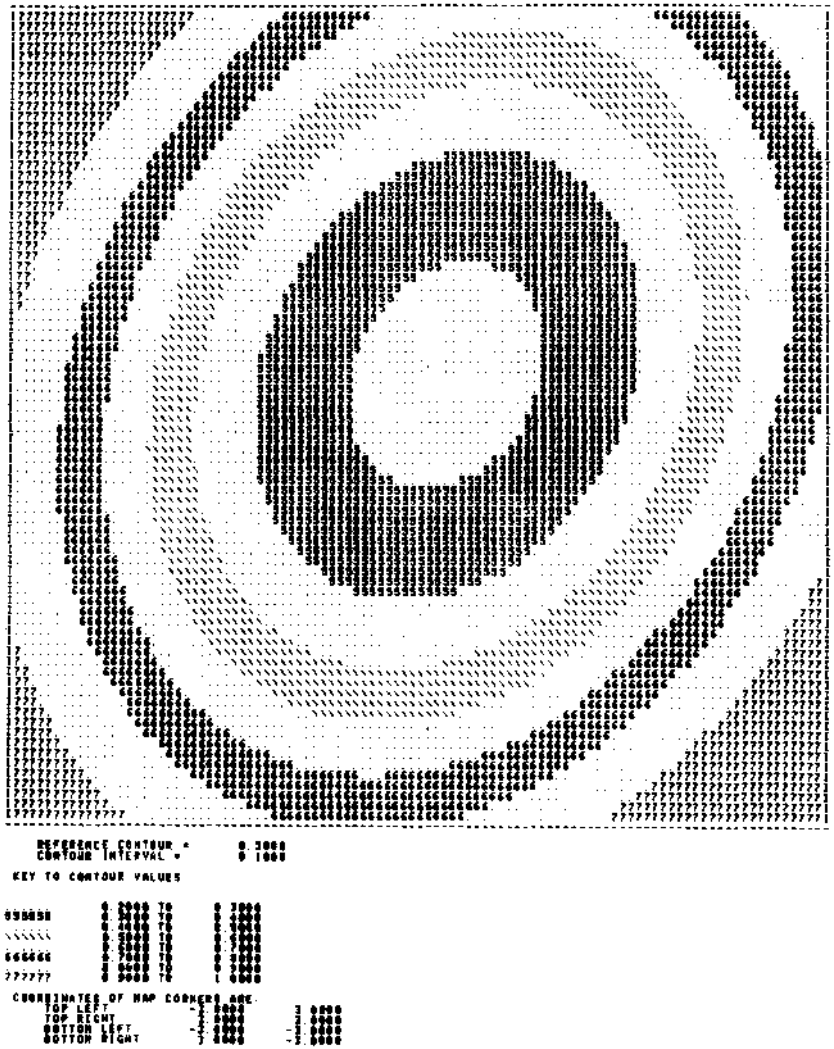

Fig. 7(b) 2nd order probability surface of not shopping at the hypermarket

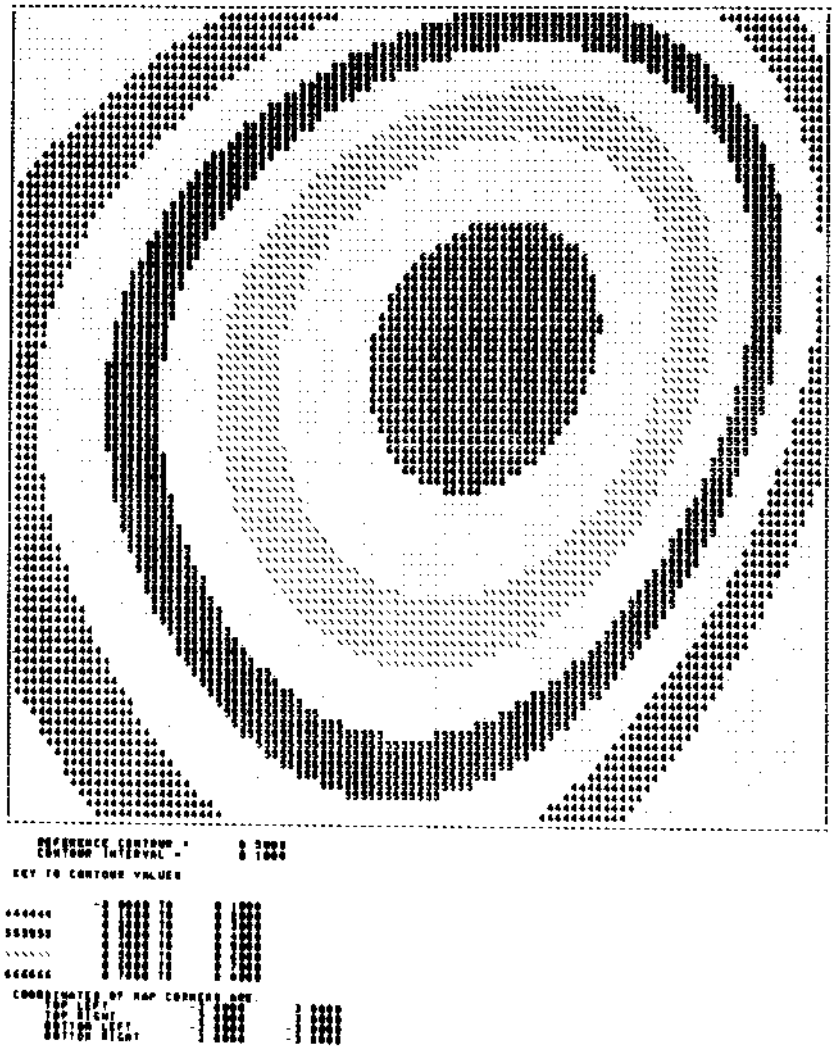

Fig. 8(a) 3rd order probability surface of shopping at the hypermarket

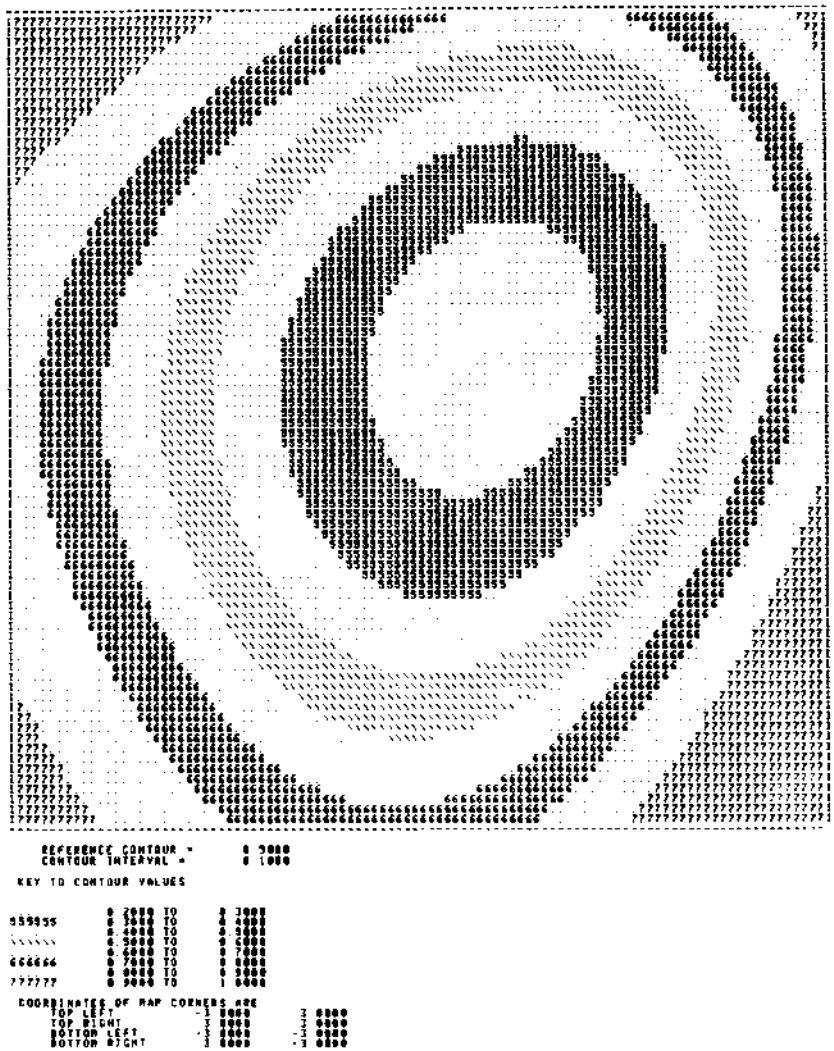

Fig. 8(b) 3rd order probability surface of not shopping at the hypermarket

Table 3 Part of the information printed by the probability surface mapping program for each surface order fitted

MAXIMIZED LOG LIKELIHOOD VALUE • -62.39922

PARAMETER ESTIMATES	STANDARD ERRORS	PARAMETER EST/STANDARD ERROR
0.9685544	8.3718716	2.6045481
8.8925432	0.1335535	0.6929388
8.1837769	8.1289748	8.8046292
-8.2911291	0.0917605	-3.1727865
8.1856475	0.0976147	1.2858208
-0.2151272	0.8840652	-2.5598529

VARIANCE-COVARIANCE MATRIX OF PARAMETER ESTIMATES

COLUMN	1	2	3	4	5	6	
ROY							
ROW 1	0.13829						
ROW 2	8.08732	0.81784					
ROM 3	-0.80434	-8.88178	8.81663				
ROW 4	-8.82452	-8.00885	-0.08822	8.80842			
ROW 5	0.88967	-8.08161	8.88836	-8.80129	0.88768		
ROW 6	-8.01896	-0.88109	-8.89013	8.00129	-0.00223	8.887	

FOR EACH SAMP E LOCALITY

PREDICTED PRO ABILITES		RAW RESIDUALS		STANDARDISED RESIDUALS	
RESP CAT 1	RESP CAT 2	RESP CAT 1	RESP CAT 2	RESP CAT 1	RESP CAT 2
8.28247	.79753	8.79753	-8.79753	1.98469	-1.98478
9.41442	.59558	8.58558	-0.58558	1.18869	-1.18869
0.31584	.68496	0.68496	-0.68496	1.47451	-1.47451
8.26739	.73261	8.73261	-8.73261	1.65526	-1.65526
8.38710	.61290	8.61298	-0.61290	1.25831	-1.25831
0.55868	.44132	0.44132	-0.44132	0.88878	-8.88878
0.62193	.37807	0.37807	-8.37887	0.77967	-0.77967
0.50731	.49269	0.49269	-0.49269	0.98548	-0.98548
8.51847	.48153	8.48153	-0.48153	8.96371	-8.96371
0.39530	.68470	8.68478	-0.68478	1.23681	-1.23682

hypermarket in the case of Figure 7 (b), the probability surface of not shopping at the hypermarket.

The probability surface maps shown in Figures 6, 7 and 8 are the line printer maps produced by the computer. Contours occur at the dividing line between symbols. (As an exercise the reader may wish to draw in these contours following the example of Figures 2, 3 and 4.) A key is automatically printed below each map to aid interpretation. The small page size of this monograph makes this key difficult to read but the reader• should remember that in practice the computer prints these maps and the key at a much larger.size.

In addition to the inferential tests presented in Table 2, residuals from the probability surface maps should be mapped and an attempt made to assess the amount of systematic spatial variation in these maps (see II (iv)). As can be seen in Table 3 (which shows part of the information printed by the program for each surface order fitted) residuals are automatically printed by the program presented in Appendix 1(a) and construction of these residual maps will be left as an exercise for the reader.

III EXTENDING THE SIMPLEST PROBABILITY SURFACE MODELS

(i) The generalised probability surface model

The case we have examined so far, the case in which the categorized response variable has only two possible outcomes, is only the simplest probability surface problem. There are far more cases in which the geographer is faced with categorized response variables with more than two possible outcomes. We call these polychotomous rather than dichotomous variables. Probability surface models can, however, be readily extended to handle such cases. For example, in our hypermarket survey instead of housewives simply indicating whether they shop at the hypermarket or not, let us presume that they indicate whether they regularly shop at the hypermarket, occasionally shop at the hypermarket, or never shop at the hypermarket. In other words, let us return to the introductory illustration in I (ii). For this three response category case, the nonlinear probability surface model generalises to the form

$$P_{r/i} = \frac{e^{f_r(U_i,V_i)}}{\sum_{s=0}^{2} e^{f_s(U_i,V_i)}} \qquad r = 0,1,2 \qquad (33)$$

$P_{r/i}$ represents the probability of the rth response being given by the housewife at locality i, and the 3 responses 'regularly shop at the hypermarket', 'occasionally shop at the hypermarket' and 'never shop at the hypermarket' are arbitrarily coded 0,1 and 2. It should be stressed that there is no assumption of ordering in this coding.

In the polynomial case, equation (33) therefore can be written

$$P_{r/i} = \frac{e^{\alpha_r+\beta_{1r}U_i+\beta_{2r}V_i+\beta_{3r}U_i^2+\beta_{4r}U_iV_i+\beta_{5r}V_i^2 \ldots}}{\sum_{s=0}^{2} e^{\alpha_s+\beta_{1s}U_i+\beta_{2s}V_i+\beta_{3s}U_i^2+\beta_{4s}U_iV_i+\beta_{5s}V_i^2 \ldots}} \quad r=0,1,2 \qquad (34)$$

As was implicit in the simple 2 response category model, one of the response categories is now arbitrarily chosen and the parameters associated with that category are set to zero. The reasons for this are given by Wrigley (1976, p.22-24), and Pindyck and Rubinfeld (1976, p.256-259). If we choose the response category 'never shop at the hypermarket' and set its associated parameters to zero in equation (34), this implies

$$\alpha_2 = \beta_{12} = \beta_{22} = \beta_{32} = \beta_{42} = \beta_{52} \ldots = 0 \qquad (35)$$

Remembering that by definition $e^0 = 1$, the generalised probability surface model (34) thus becomes

$$P_{r/i} = \frac{e^{\alpha_r+\beta_{1r}U_i+\beta_{2r}V_i+\beta_{3r}U_i^2+\beta_{4r}U_iV_i+\beta_{5r}V_i^2 \ldots}}{1+\sum_{s=0}^{1} e^{\alpha_s+\beta_{1s}U_i+\beta_{2s}V_i+\beta_{3s}U_i^2+\beta_{4s}U_iV_i+\beta_{5s}V_i \ldots}} \quad r=0,1,2 \qquad (36)$$

Using for convenience the general function $f(U_i,V_i)$ instead of the polynomial, we can write the generalised probability surface model (36) out as

$$P_{0/i} = \frac{e^{f_0(U_i,V_i)}}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}}$$

$$P_{1/i} = \frac{e^{f_1(U_i,V_i)}}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}} \qquad (37)$$

$$P_{2/i} = \frac{1}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}}$$

This shows that the generalised probability surface model for the three category situation is actually a set of three linked models; just as in the two category situation we saw that there was a set of two linked models given by equations (21) and (24). In (37) the reader should note that the numerator of the right hand side of the equation for $P_{2/i}$ is 1 because

$$e^{f_2(U_i,V_i)} = e^{\alpha_2+\beta_{12}U_i+\beta_{22}V_i+\beta_{32}U_i^2+\beta_{42}U_iV_i+\beta_{52}V_i^2 \ldots}$$
$$= e^0 = 1 \qquad (38)$$

This extension of the nonlinear probability surface model to the three response category case, generalises to any number of categories. For example, with J possible response categories the model (33) simply takes the form

$$P_{r/i} = \frac{e^{f_r(U_i,V_i)}}{\sum_{s=0}^{J-1} e^{f_s(U_i,V_i)}} \qquad r = 0, \ldots J-1 \qquad (39)$$

and this can be expanded out, just as (37) was expanded from (33), to show that it is actually a set of J linked models.

(ii) Estimating the parameters of the extended probability surface models

Maximum likelihood estimation of the parameters of the 3 response category model demands a simple expansion of the likelihood for the two response category case. Instead of (25) we now have

$$\Lambda = \prod_{i=1}^{N_1} P_{0/i} \prod_{i=N_1+1}^{N_2} P_{1/i} \prod_{i=N_2+1}^{N} P_{2/i} \qquad (40)$$

or substituting from equation (37)

$$\Lambda = \prod_{i=1}^{N_1} \frac{e^{f_0(U_i,V_i)}}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}} \prod_{i=N_1+1}^{N_2} \frac{e^{f_1(U_i,V_i)}}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}} \prod_{i=N_2+1}^{N} \frac{1}{1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}} \qquad (41)$$

N is the total sample size; N_1 is the number of housewives in the sample who claim to shop regularly at the hypermarket; N_2-N_1 is the number of housewives who claim to shop occasionally at the hypermarket, and $N-N_2$ is the number of housewives who claim never to shop at the hypermarket.

As in the simple two response category case, instead of maximizing the likelihood itself, it is usual to maximize the logarithm of the likelihood. In the 3 response category case the log likelihood function (27) generalises to

$$\log_e \Lambda = \sum_{i=1}^{N_1} f_0(U_i,V_i) + \sum_{i=N_1+1}^{N_2} f_1(U_i,V_i) - \sum_{i=1}^{N} \log_e\left(1+\sum_{s=0}^{1} e^{f_s(U_i,V_i)}\right) \qquad (42)$$

The maximum can be found by partially differentiating equation (42) with respect to its parameters and setting the partial derivatives equal to zero. The solution of the resulting set of equations yields the maximum likelihood

parameter estimates. The computer routine described in Appendix 1(b) performs the estimation automatically.

Extension of the maximum likelihood estimation procedure to the case of a 4 response category model or ultimately to a J response category model follows exactly the same principles as those outlined above in the extension of the estimation procedure from the 2 response category case to the 3 response category case. The computer routine described in Appendix 1(c) performs the estimation automatically for the 4 response category case.

(iii) Testing probability surfaces and goodness-of-fit statistics

The inferential tests and goodness-of-fit statistics discussed in II (iv) and II (v) apply equally as well in the multiple response category case as in the two response category case. The reader should therefore consult II (iv) and II (v). The only difference is that in the multiple response category case the definitions of a residual (29) and (30) must be generalised to the form

$$Z_{r/i} - \hat{P}_{r/i} = e_{r/i} \tag{43}$$

$$\frac{Z_{r/i} - \hat{P}_{r/i}}{\sqrt{\hat{P}_{r/i}(1-\hat{P}_{r/i})}} = e_{r/i} \tag{44}$$

$\hat{P}_{r/i}$ is the predicted probability that the individual at locality i will choose the rth response category, and $Z_{r/i} = 1$ if category r is chosen and 0 otherwise. In the multiple response category case there are thus as many residual maps as there are response categories.

(iv) An empirical example

To illustrate the use of probability surface mapping in the multiple response category case, we will use once again the example of a marketing geographer who conducts a survey to investigate the trade area characteristics of a recently opened hypermarket. In this case he conducts a survey of the shopping habits of 144 housewives in the area surrounding the hypermarket and amongst other questions in the survey he asks each housewife whether she regularly shops at the hypermarket, occasionally shops at the hypermarket, or never shops at the hypermarket. Once again this information can be portrayed in map form as in Figure 9 (which is Figure 1 repeated for convenience), or in tabular form as in Table 4. Given this survey data, he then fits probability surfaces of a polynomial type using the program supplied in Appendix 1(b) and he achieves the results shown in Table 5.

Table 5 gives the maximized log likelihoods for probability surface models of orders 0 to 3; the differences between these maximized log likelihoods; the differences expected under the null hypothesis of no significant improvement between surface models of different orders; and the decision on the null hypothesis at conventional significance levels. Also given are the values of the two goodness-of-fit statistics discussed in II (v).

As in the example of Section II, the fact that the underlying regional structure of each response is symmetrical, results in the first order surfaces capturing little of this underlying structure, and consequently

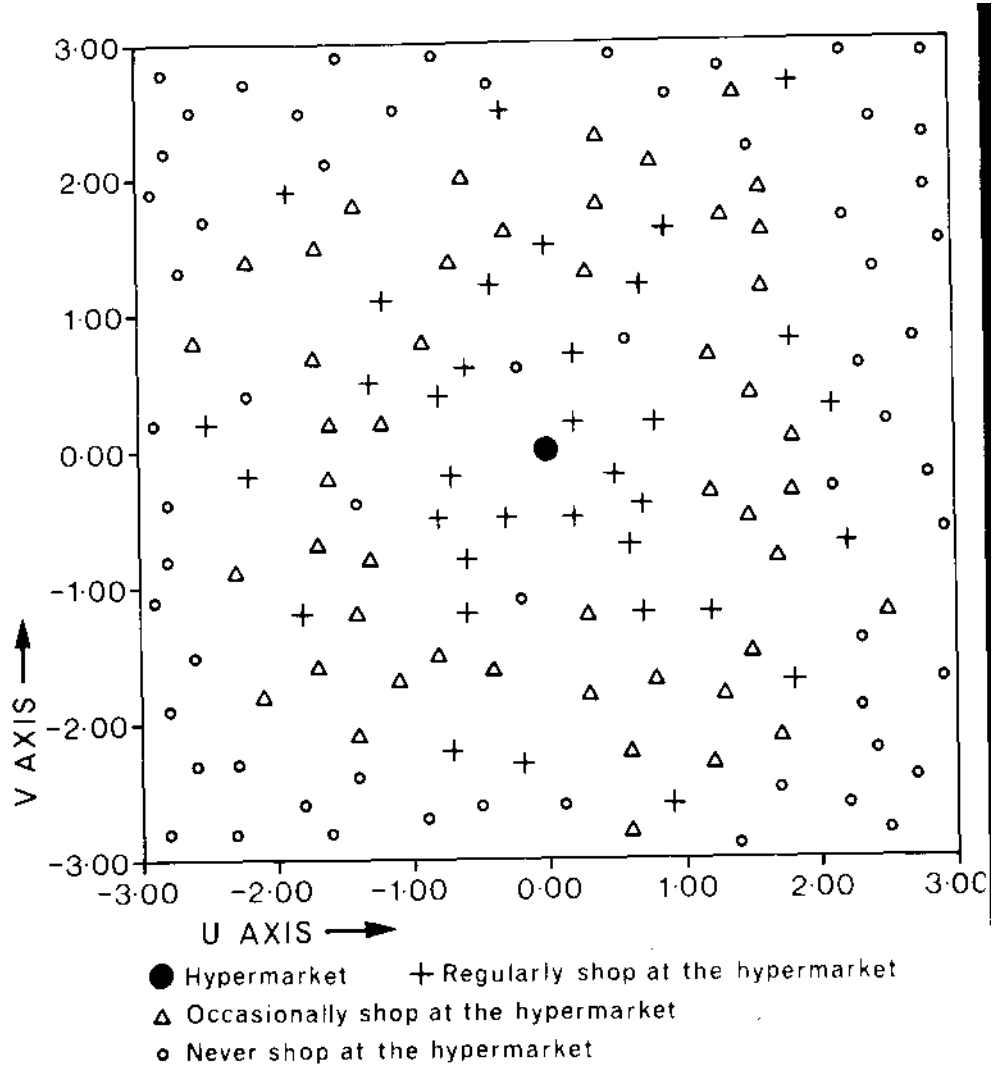

Fig. 9

Table 4

Respondent	U	V	Shopping at hypermarket	Respondent	U	V	Shopping at hypermarket
1	-2.8	-2.8	N	55	-1.4	-0.4	N
2	-2.6	-2.3	N	56	-1.3	-0.8	O
3	-2.3	-2.8	N	57	-0.8	-0.5	R
4	-2.3	-2.3	N	58	-0.7	-0.2	R
5	-1.8	-2.6	N	59	-0.6	-0.8	R
6	-1.6	-2.8	N	60	-0.3	-0.5	R
7	-1.4	-2.1	O	61	0.2	-0.5	R
8	-1.4	-2.4	N	62	0.5	-0.2	R
9	-0.9	-2.7	N	63	0.6	-0.7	R
10	-0.7	-2.2	R	64	0.7	-0.4	R
11	-0.5	-2.6	N	65	1.2	-0.3	O
12	-0.2	-2.3	R	66	1.5	-0.5	O
13	0.1	-2.6	N	67	1.7	-0.8	O
14	0.6	-2.2	O	68	1.8	-0.3	O
15	0.6	-2.8	O	69	2.1	-0.3	N
16	0.9	-2.6	R	70	2.2	-0.7	R
17	1.2	-2.3	O	71	2.8	-0.2	N
18	1.4	-2.9	N	72	2.9	-0.6	N
19	1.7	-2.1	O	73	-2.9	0.2	N
20	1.7	-2.5	N	74	-2.6	0.8	O
21	2.2	-2.6	N	75	-2.5	0.2	R
22	2.4	-2.2	N	76	-2.2	0.4	N
23	2.5	-2.8	N	77	-1.7	0.7	O
24	2.7	-2.4	N	78	-1.6	0.2	O
25	-2.9	-1.1	N	79	-1.3	0.5	R
26	-2.8	-1.9	N	80	-1.2	0.2	O
27	-2.6	-1.5	N	81	-0.9	0.8	O
28	-2.1	-1.8	O	82	-0.8	0.4	R
29	-1.8	-1.2	R	83	-0.6	0.6	R
30	-1.7	-1.6	O	84	-0.2	0.6	N
31	-1.4	-1.2	O	85	0.2	0.2	R
32	-1.1	-1.7	O	86	0.2	0.7	R
33	-0.8	-1.5	O	87	0.6	0.8	N
34	-0.6	-1.2	R	88	0.8	0.2	R
35	-0.4	-1.6	O	89	1.2	0.7	O
36	-0.2	-1.1	N	90	1.5	0.4	O
37	0.3	-1.2	O	91	1.8	0.1	O
38	0.3	-1.8	O	92	1.8	0.8	R
39	0.7	-1.2	R	93	2.1	0.3	R
40	0.8	-1.7	O	94	2.3	0.6	N
41	1.2	-1.2	R	95	2.5	0.2	N
42	1.3	-1.8	O	96	2.7	0.8	N
43	1.5	-1.5	O	97	-2.9	1.9	N
44	1.8	-1.7	R	98	-2.7	1.3	N
45	2.3	-1.4	N	99	-2.5	1.7	N
46	2.3	-1.9	N	100	-2.2	1.4	O
47	2.5	-1.2	O	101	-1.9	1.9	R
48	2.9	-1.7	N	102	-1.7	1.5	O
49	-2.8	-0.8	N	103	-1.4	1.8	O
50	-2.8	-0.4	N	104	-1.2	1.1	R
51	-2.3	-0.9	O	105	-0.7	1.4	O
52	-2.2.	-0.2	R	106	-0.4	1.2	R
53	-1.7	-0.7	O	107	-0.3	1.6	O
54	-1.6	-0.2	O	108	0.0	1.5	R

Table 4 - continued

Respondent	U	V	Shopping at hypermarket	Respondent	U	V	Shopping at hypermarket
109	0.3	1.3	O	127	-1.5	2.9	N
110	0.4	1.8	O	128	-1.1	2.5	N
111	0.7	1.2	R	129	-0.8	2.9	N
112	0.9	1.6	R	130	-0.6	2.0	O
113	1.3	1.7	O	131	-0.4	2.7	N
114	1.6	1.9	O	132	-0.3	2.5	R
115	1.6	1.6	O	133	0.4	2.3	O
116	1.6	1.2	O	134	0.5	2.9	N
117	2.2	1.7	N	135	0.8	2.1	O
118	2.4	1.3	N	136	0.9	2.6	N
119	2.8	1.9	N	137	1.3	2.8	N
120	2.9	1.5	N	138	1.4	2.6	O
121	-2.8	2.2	N	139	1.5	2.2	N
122	-2.8	2.8	N	140	1.8	2.7	R
123	-2.6	2.5	N	141	2.2	2.9	N
124	-2.2	2.7	N	142	2.4	2.4	N
125	-1.8	2.5	N	143	2.8	2.3	N
126	-1.6	2.1	N	144	2.8	2.9	N

Table 5.

Order of surfaces	Maximized log likelihood	Difference between the maximized log likelihoods of surface orders					Goodness of fit	
		Observed	Expected under H_0 1%	Expected under H_0 5%	D.F.	Decision on H_0	ρ^2	R^2_p
0	−154.634							
		0.213	6.638	4.744	4	Fail to reject		
1	−154.421						0.0014	0.0033
		47.370	8.406	6.296	6	Reject at 1% level		
2	−107.051						0.3077	0.5475
		3.019	10.045	7.754	8	Fail to reject		
3	−104.032						0.3272	0.5715

the first order surfaces provide an insignificant improvement over the zero order surfaces. The second order surfaces, however, capture a significant amount of the underlying regional structure and it is clearly worthwhile making an exception to the test procedure explained in II (iv) hypothesis b* and extending the models to this higher order. The increased complexity of the probability surface models associated with moving from second order surfaces to third order surfaces is associated with only a minor improvement in the maximized log likelihood, and thus, once again, there is no significant advantage to be gained in fitting third order surfaces. The second order surfaces are therefore the appropriate surfaces to fit and they represent expressions of the underlying regional structure. Figures 10 (a), (b) and (c) (which are Figures 2, 3 and 4 repeated for convenience but without the hand drawn contours) show respectively the second order probability surfaces of regularly shopping at the hypermarket, occasionally shopping at the hypermarket and never shopping at the hypermarket. The reader should note, once again, how the probability surface of regularly shopping at the hypermarket is a 'dome' centred on the hypermarket, how the probability surface of occasionally shopping at the hypermarket has a 'ring doughnut' type of structure with the highest predicted probabilities occurring in a ring or horseshoe some distance from the hypermarket, and how the probability surface of never shopping at the hypermarket is a flat-bottomed 'basin' centred on the hypermarket.

In addition to the inferential tests presented in Table 5, residuals from the probability surface maps should be mapped and an attempt made to assess the amount of systematic spatial variation in these maps. As in the previous example, the program presented in Appendix 1(b) automatically prints both raw residuals (see equation 43) and standardised residuals (see equation 44) and the construction of these maps will be left as an exercise for the reader.

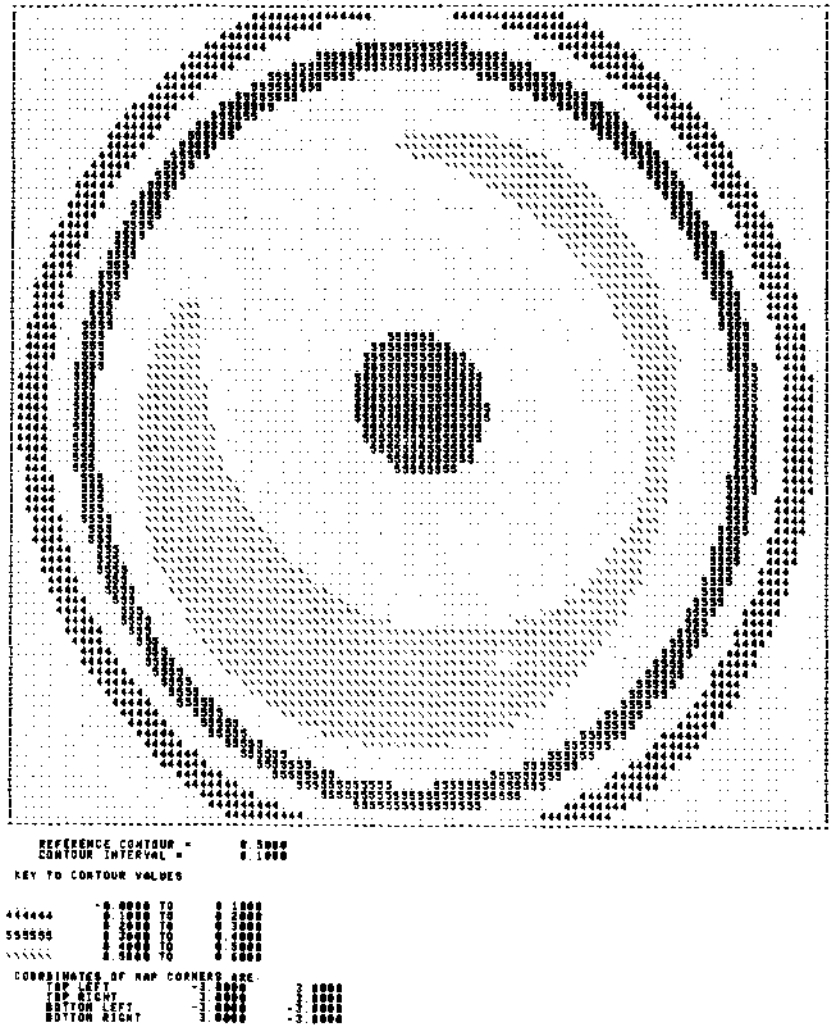

Fig. 10(a) 2nd order probability surface of regularly shopping at the hypermarket

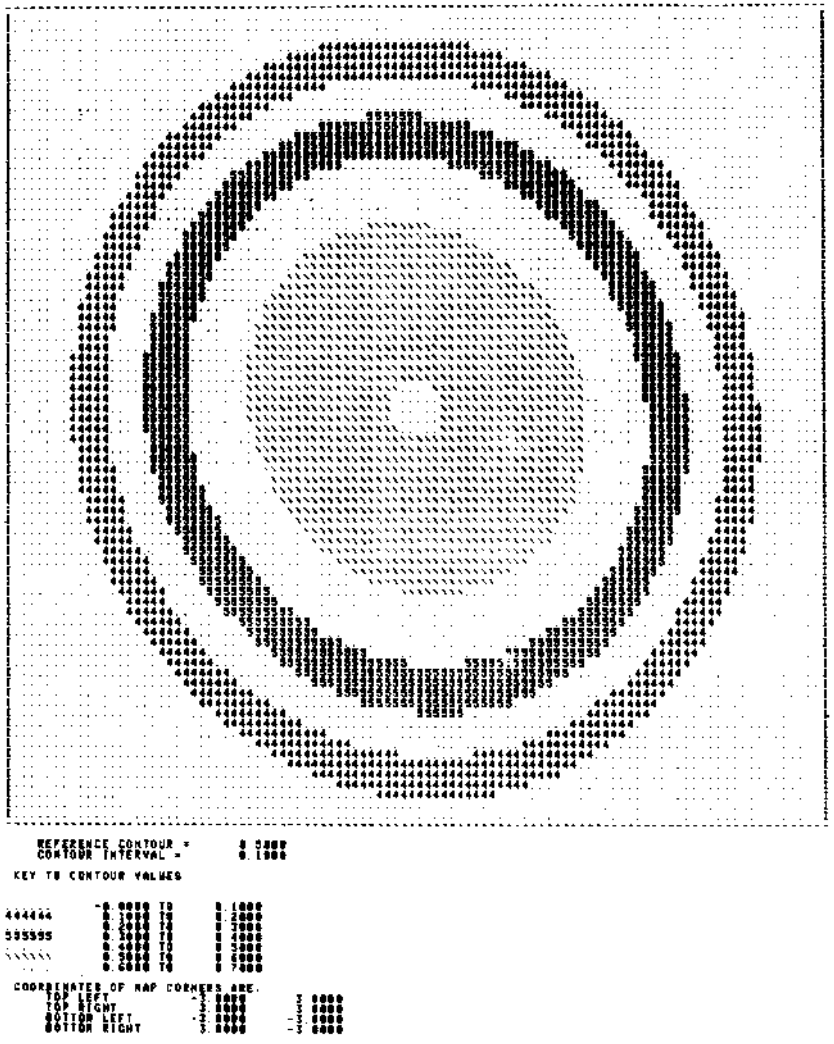

Fig. 10(b) 2nd order probability surface of occasionally shopping at the hypermarket

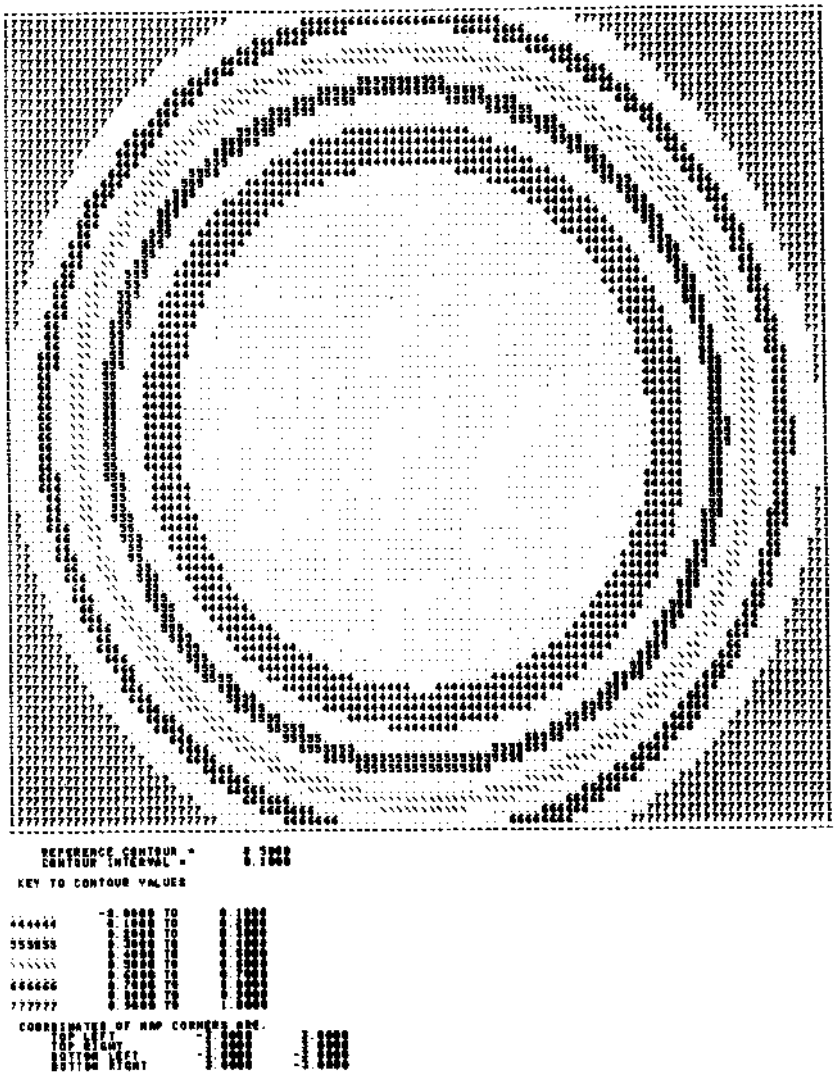

Fig. 10(c) 2nd order probability surface of never shopping at the hypermarket

IV EXTENSIONS AND PROBLEM AREAS

(i) Introduction

Probability surface mapping is an extension of one of the oldest and simplest techniques in spatial analysis. It enables the researcher to use the type of categorized variables which frequently are available but which previously were viewed as unmappable by the trend surface method. It therefore allows the geographer to pose and answer new questions and helps him to come to terms with the imperfect types of data which are often faced in geographical research. It is a method in its infancy and there is much developmental work yet to be done. The user should remember, however, that many of the problems identified in normal trend surface mapping remain problems in probability surface mapping. Consequently these problems must be treated with the same degree of caution. In this concluding section we will therefore briefly consider some of the many possible extensions to probability surface mapping, and some of the problem areas the user must be aware of.

(ii) The use of other functional forms

Although the most widely used form of the function $f(U_i, V_i)$ in traditional trend surface models is the power series polynomial, many other functional forms have also been used. These other functional forms can equally be used in the case of probability surface models, and perhaps the simplest potential extensions of the procedures outlined in this monograph involve the modification of the programs presented to handle these other functional forms.

Three potentially valuable extensions of this type would involve:
a) the use of a double Fourier series functional form. In trend surface mapping this form of function has been found to be of value where the response variable, the variable to be mapped, behaves in a spatially oscillatory or repetitive manner (see Davis, 1973, p.358-374).
b) the use of a functional form with three rather than two constituent coordinates. In this case the function has the general form $f(U_i, V_i, W_i)$. Trend surfaces using this functional form were first developed in petrology by Peikert (1962) and others for use with three-dimensional rock bodies. Using this functional form contour lines on normal trend surfaces become contour envelopes, and the effect is to define hypersurfaces (see Davis, 1973, p.355). The use of such a functional form in probability surfaces would result in the mapping of probability hypersurfaces.
c) the use of an orthogonal polynomial functional form. This form of function has become increasingly important in trend surface mapping in recent years, (see Whitten 1,970, 1972) for it has a number of advantages over the more widely used nonorthogonal polynomial form. These advantages include the added numerical accuracy it is possible to achieve in the computation of the parameter estimates (see Mather, 1976, p.139-142) and the provision of information concerning the importance of each orthogonal parameter.

(iii) Programs for fitting different surfaces to different responses

Probability surface models are essentially sets of linked models; two linked models in the two response category case producing two probability surface maps, three linked models in the three response category case

producing three probability surface maps and so on. The predicted probabilities at any locality i in each set of maps sum to one. To produce the J probability surface maps in a J response category case, the programs presented in Appendix 1(a), 1(b) and 1(c) fit the same order of surface to each response. A logical extension of these programs would be to allow a different order of surface to be fitted to each of the J responses, whilst retaining the property that the predicted probabilities of the J responses at any locality must sum to one. This extension is simply a computer programming problem, it involves no alterations to the structure of the probability surface models outlined above.

(iv) Ordered categorizations

Throughout the monograph no account has been taken of any ordering which might exist amongst the response categories. A potential extension to the probability surface models outlined is to attempt to take account in the specification of the models and in the estimation procedures of any ordering which might exist amongst the response categories. Cox (1970, p.104) presents a nonlinear model which takes account of the ordering of the responses in a particular three category situation.

(v) Inference and estimation considerations

In II (iv) and (v) we discussed the need for a test statistic to evaluate the amount of systematic spatial variation in the maps of residuals from probability surfaces of different orders, and the need to resolve what constitutes an appropriate goodness-of-fit statistic. Although these are perhaps the most urgent inferential matters to be resolved, consideration must also be given to the question of how appropriate is the maximum likelihood estimation method and inferential tests (see equation 28) based upon it, in the case of small samples. Some limited Monte Carlo experiments described by Domencich and McFadden (1975, p.112-117) suggest that the maximum likelihood estimators perform reasonably well when compared with the alternative weighted least squares estimators in small samples, but further small sample Monte Carlo experiments would be useful.

(vi) Graphical improvements

Although the line printer maps produced by the programs given in Appendix 1(a), 1(b) and 1(c) provide a quick and reasonably accurate method of displaying probability surfaces, there is clearly considerable potential for improving the quality of the maps produced, either by using more elaborate line printer techniques, or drum or flat bed plotter methods (see Peuker, 1972; Davis and McCullagh, 1979; Rhind, 1977). The additional use of three-dimensional perspective views of the probability surfaces would also help to improve the graphical output from the programs presented.

(vii) Spatial distribution of the data points

In most text book discussions of traditional trend surface mapping the user is warned that the spatial arrangement of the data points can have profound effects on the shape of the computed trend surfaces (Davis, 1973, p.349-352; Mather, 1976, p.120-130; Unwin, 1975a, p.31-32). Given that there are at least as many, preferably many more, data points than there are parameters to be estimated in the trend surface model, the user is warned

that the data points should have an even spatial distribution, and that the map area should be approximately square.

If thesetwoconditions are not satisfied, the shape of the trend surface fitted can be greatly distorted. For example, if there are few data points at the edges of the map area, the fitted surfaces lack constraints on their form in these areas. Whatever slope exists in the region of the map in which there is data point control, is extrapolated without limits along the map edges. This creates what are termed 'edge effects', and these effects can be very serious in the case of higher order surfaces. To guard against these effects it is wise to form a 'buffer region' (Davis, 1973, p.350) of control points around the map, so that edge effects can be concentrated into this buffer region, leaving the area of interest with adequate data point control. In addition to having sufficient data point control at the edges of the map, the user must also take care that the data point distribution is in no way peculiar, for example, highly clustered or restricted to a narrow strip across the map area (Doveton and Parsley, 1970). He should also ensure that the map area is not markedly rectangular in shape. If it is there will be a pronounced tendency for contours on higher order surfaces to become elongated parallel to the long axis of the map area.

These problems associated with the spatial distribution of the data points are potentially as great a threat to the user of probability surface mapping as they are to the user of trend surface mapping. The user of probability surface mapping should therefore attempt to ensure an even spatial distribution of data points and an approximately square map area. If he is in the position of being able to construct a sample design for the collection of data to be used in probability surface mapping, he should consider using the spatially stratified random sampling method which underlies Figures 5 and 9.

(viii) The problem of multicollinearity

In trend surface mapping, accurate calculation of the parameter estimates of traditional polynomial trend surface models is difficult, for the matrix of sums of squares and cross-products of the explanatory variables (the Ui, Vi terms) is almost certain to be nearly singular for surfaces of order three or more. This results from the fact that the explanatory variables will be approximately linearly related, or in other words because of the presence of a high degree of multicollinearity.

In the presence of such a high degree of multicollinearity, the ordinary least squares estimation methods employed by many of the standard trend surface computer programs produce inaccurate results, particularly when the problem is compounded by a poor data point distribution, a poorly selected origin for the co-ordinate system, and a computer with a short word length (see Unwin, 1975b; Mather, 1977). Such problems can be minimized by using the orthogonal polynomials mentioned in IV (ii) above, by the choice of a sensible origin for the co-ordinate system and/or scaling of the explanatory variables, by choice of a sampling design which produces a better data point distribution and the use of a computer with as long a word as possible.

In the case of probability surface mapping we use a maximum likelihood method of parameter estimation, however, a high degree of multicollinearity still causes problems. Cox (1970, p.90) for example, discussing maximum likelihood estimation of nonlinear logit models, states that 'there is likely to be difficulty in finding (the parameter estimates) if the columns of the (matrix of explanatory variables) are nearly linearily dependent. Therefore it may be good to have a preliminary calculation of the formal 'correlation' matrix of the regressor (i.e. explanatory) variables, followed if necessary by a linear transformation of the regressor variables to ones more nearly orthogonal in the usual least squares sense'. In this monograph no such transformation has been conducted in the examples given, for a sensible origin for the co-ordinate system was chosen, the sampling design employed produced a good data point distribution, and the programs presented have been restricted to fitting surfaces no higher than fourth order. No difficulties were encountered in finding the parameter estimates. In less favourable circumstances, however, or if the user felt that it was absolutely essential to fit probability surfaces of higher order, the use of orthogonal polynomials, and the extension of the computer programs presented here to handle them, appears to be a possible way forward. Even in the absence of such a need, however, it would be interesting to compare the results presented in II (vi) and III (iv) based on the more traditional nonorthogonal polynomials, with those achieved using orthogonal polynomials.

(ix) Conclusion

Probability surface mapping extends one of the oldest, simplest and most widely known techniques in spatial analysis, and it offers the geographer a method capable of handling the type of categorized data which are often faced in geographical research. The aim of this monograph has been to make the method available to all those who require it, and it is hoped that this will stimulate further empirical application, theoretical development, and programming refinement.

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APPENDIX 1 Computer programs for probability surface mapping

Fortran programs for the two, three and four response category cases are provided in this Appendix. All the programs share certain common subroutines which are listed in (d) below, and all allow the user to fit, in a sequential manner, polynomial probability surfaces from order 1 up to order 4. It should be noted in this context that although users of traditional trend surface mapping have fitted polynomial trend surfaces more complex than 4th order, and although the programs provided in the Appendix could be extended to allow similar fitting of surfaces more complex than 4th order, this facility is not provided because there are marked dangers, both theoretical and numerical, associated with the fitting of such higher order surfaces.

The programs provided in this Appendix must be viewed as first generation probability surface programs, capable of considerable future refinement and extension. They are presented simply to allow the method to break through what might otherwise prove to be an initial computational barrier to its wider implementation. Readers so inclined, are encouraged to develop and refine the programs presented here.

Appendix 1(a) A Fortran program for the two response category case

The program presented in Table 6 has the following stages.

a) Input It starts by reading a card which specifies the highest order of sur ace the user wishes to fit (IORD); the number of respondents in the sample (NSAMPL), and the number of respondents who have chosen response category one, in terms of the example in II (vi) the number who have claimed to shop at the hypermarket (N1). It then reads another card which specifies the overall dimensions the user wishes the probability surfaces to be drawn to (10.0 inches by 10.0 inches in the example in II (vi) before reduction to the monograph page size); the Ui and Vi values of the corners of the maps; the contour interval required (0.10 in the example), and the so called reference contour, a contour which should be set to a figure in the middle of the expected range of predicted probabilities (set at 0.50 in the example for convenience). Following this it reads a set of cards. These give the geographical co-ordinates of the sample localities (see Table 1). The input order required of these cards demands that all respondents choosing response category one form the first N1 cards. The next set of cards N1+1 to NSAMPL are the respondents choosing response category two. In the example in II (vi) Table 1, must therefore be reorganized so that the first N1 cards are the housewives claiming to shop at the hypermarket, whilst the next set of cards N1+1 to NSAMPL are the housewives claiming not to shop at the hypermarket. This completes the input.
b) Calculations After receiving the input information the program then fits in a sequential manner, probability surfaces of order 1 to IORD. For each order of probability surface the parameter estimates of the probability surface models are estimated using the maximum likelihood method, and these parameter estimates are then used as the basis of a line printer subroutine which draws the probability surface maps.
c) Output The geographical co-ordinates of the sample households in the order in which they were input, see (a) above, are listed first. Then for each order 1 to IORD, the following is provided: the maximized log likelihood, parameter estimates, standard errors, variance-covariance matrix of the parameter estimates, predicted probabilities of giving each response for each of the sample respondents, raw residuals, standardised residuals, and finally the probability surface maps for both the possible responses. Prior to this the maximized log likelihood for the probability surface models of order 0, that is to say for the probability surface models containing only an intercept term, is printed.

The program given in Table 6 has the following size restrictions. The maximum number of respondents in the sample (NSAMPL) allowed is 250. The maximum number who choose response category one (N1) allowed (i.e. the number who have claimed to shop at the hypermarket) is 125. The maximum number who choose response category two (NSAMPL-N1) allowed (i.e. the number who have claimed not to shop at the hypermarket) is 200. These size restrictions are easily changed however and in Appendix 2(a) the changes required in the program when NSAMPL = AT1, N1 = AT2 and (NSAMPL-N1) = AT3 (where All, AT2, and AT3 represent any arbitrary numbers) are given, thus allowing the user to modify the size restrictions of the program to suit his own needs.

Before using the program for his own research, the reader is advised to check, using the example data set of Table 1, that he has punched and implemented the program correctly. Minor differences in numerical results from those given in the next section can be expected to occur if the computer used by the reader nas a level of precision which differs from that of the University of Bristol machine.

After ensuring that the program has been implemented correctly and reproduces the results reported in II (vi), other possible (but rare) errors which the user may encounter are as follows.
a) Program exits from subroutine VA06AD with message 'Error exit from VA06AD'. The subroutine may finish in this way because the gradients are wrong or because computer rounding errors make it impossible to continue the calculation efficiently. If this message occurs and if the final derivative vector (the G vector printed immediately before the 'Maximized Log Likelihood Value' statement) does not have small components, then it is probably due to incorrect derivatives. The user should note that this error has never been encountered by the author and should check that he has implemented the program correctly.
b) Program exits from subroutine VA06AD with message 'VA06AD has made 2000 calls of CALCFG'. The program has failed to achieve a maximum after 2000 iterations (the arbitrarily set upper limit). The program normally achieves a maximum in less than max(100, 10xn) where n here is the total number of parameters in the set of probability surface models, and therefore this suggests serious problems caused by linear dependence between the explanatory variables. The user should read Section IV (viii). He should also, check that additional comment instruction (b) given in the next paragraph has been obeyed, and try following the instructions given in (c) below to see if this improves the position.
c) Negative square root problem immediately after VA06AD. The user should change the arbitrarily set initial parameter estimates given in lines 33 and 35 of subroutine SURF. It is suggested that line 35 be changed from X(I)=0.01D0 to X(I)=0.02D0, or X(I)=0.03D0.

Additional comments.
a) The probability surface maps are printed on the line printer. The pro-

gram assumes that the line printer prints 8 lines per vertical inch. The user should check what number of lines per vertical inch are printed by his local line printer. In many computer centres 6 lines per vertical inch may be the norm. If this is the case, the user should change line 24 in the main part of the program from NL=INT(VERTx8.0+0.5) to NL=INT(VERTx6.0+0.5).

b) Subroutine VA06AD works most efficiently when the observed values of the explanatory variables differ in scale by a factor of no more than 100. In the polynomial probability surface case the kth order models have a range of values from U_i to U_i^k and V_i to V_i^k. To ensure that this range of values approximates to the range in which subroutine VA06AD works most efficiently, it is essential that the origin (the zero point) of the co-ordinate system coincides with the centre of the study area (see Figure 5). Also the units in which Ui and Vi are expressed should follow the pattern of Figure 5. That is to say, ideally there should be only one number to the left of the decimal point.

c) The DATA statement in subroutine PMAP sets the characters to be used in the line printer maps (see Figures 6, 7 and 8, III (vi)). The user should note that the small dot symbol is used for every other probability division to aid the visual appearance of the maps. He should also note that the eleventh probability division is denoted in the DATA statement and in Figures 6, 7 and 8, by the symbol\ . Users unable to punch this symbol at their local computer centre should replace it in the DATA statement with a $ symbol .


```
      ..... PROBABILITY SURFACE PROGRAMME FOR A 2 CATEGORY SITUATION
      WRITTEN BY NEIL WRIGLEY, DEPT OF GEOGRAPHY, UNIVERSITY OF BRISTOL

      COMMON/ONE/A(250,15),A2(125,15),A1(280.15),NSAMPL.NI.NIA,K,H4B

      .... READ IN IORDsHIGNEST SURFACE ORDER TO BE FITTED, 1,2,3, OR 4
      NSAMPL■IUMBER OF SAMPLE LOCALITIES, NI=NUMBER OF LOCALITIES WHERE
      RESPONSE CATEGORY ONE IS RECORDED
      **** DATA CARD. COL 1■10RD, COL 2-BLANK, COL 3-101SAMPL, COL Gs
C     BLANK, COL 7-9041 .....
      READ(5.1) IORD.NSAMPLAI
    1 FORMAT M,IX.I3.01X.I3)

      ***s READ IN VERTsLENGTH OF PROBABILITY SURFACE MAP REQUIRED IN
      INCHES, WIDsVIDTH IN INCHES, REFCsVALUE OF REFERENCE CONTOUR, CINT
      -CONTOUR INTERVAL, UMAXIUMINsMAXIMUM AND MINIMUM ALONG HORIZONTAL
C     AXIS, VMAX.VNIN■MAXIMUM AND MINIMUM ALONG VERTICAL AXIS *** ***** *
      *** DATA CARD. COLS 1-7sVERT. COLS 13-14■41D. COLS 15-19=REFC,
C     COLS 2B-24-CINT, COLS 25-31sUMAX, COLS 32-38sUMIN, COLS 39-45=VMAX
C     COLS 46-52-VMIN .....
      READC5,18) VERT,WILREFC,CINT,UMAX.UNINIVMAX,VMIN
   18 FORMAT(2F7.4,2F5.3.4F7.4)
      HL-INT(VERT*8.8*81.5)
      NC=INT(VID*141.13+9.5)
      UAXsCUMAX-UMIN)/FLOATCHC-.1)
      VAXARCVNAX.-VNIN)/FLOAT/NL•1)
      UAXsUAX49.8110001*UAX
      VAX*VAX49.9811091*VAX

C     **** READ IN GEOGRAPHICAL CO-ORDINATES OF EACH SAMPLE LOCALITY,
C     U M-HORIZONTAL CO-ORDINATE, V(I)-VERTICAL CO-ORDINATE, IN FORMAT
C     (F8.4.1X.F8.4) (N.B. IN THE PROGRAMME THESE CO-ORDINATES ARE
C     STOPED IN MATRIX A) *** ORDER OF CARDS-ALL SAMPLE LOCALITIES WHERE
C     RESPONSE CATEGORY ONE IS RECORDED, FOLLOWED BY ALL LOCALITIES
C     WHERE REMAINING RESPONSE CATEGORY IS RECORDED *** CREATE CONSTANT
C     TERM s** PRINT SAMPLE LOCALITIES .....
      WRITE(6, 11)
   /1 FORNATCB      U           V')
      DO 3 IsIoNSAMPL
      A(I.1)■1.8
      READ(5.4) ACI.2).ACI.3)
    3 WRITE46,44) (A41,J),Js2.3)
    4 FORMATU8.4.1X.F8.4)
   44 FORMAT4".2F9.4)

C     ***** START OF MAIN LOOP .....
      ID=S
      DO 7 1-1,IORD
      ID-ID41
      CALL  SURFCID.HL.NC.UAX.VAX#UMAX,UNIN,VMAXIVNINoREFC,CINT)
    7 CONT INUE
      STOP
      END



      SUBROUTINE SURFOORD,HL.NC.UAX.VAX,UMAX.UMIN,VMAX,VMIN,REFC,CINT)
      COMMON/ONE/A(259.15) A2(123.15),A1/280.15),NSAMPL,H1,NIA.K.H4B
      DOUBLE PRECISION BZ1.DBLE
      DOUBLE PRECISION X.F.G,STEP.ACC.W.FMINUS,STER,TSTAT
      DIMENSION CIB(258).C13(250)
      DIMENSION PROB1(258),PROB4(250).0ZA(258,1).XZ1(13,1)
      DIMENSION X415) G<IS),TSTAT(15).STER/15),WORK(15),PESTS(15),W(541)

C     *** THIS IS THE MAIN PART OF THE PROGRAMME. IT CALCULATES THE
C     PARAMETER ESTIMATES OF THE PROBABILITY SURFACE MODEL USING MAXIMUM
C     LIKELIHOOD ESTIMATION. IT USES POWELL'S HYBRID STEEPEST DESCENT
      AND GENERALISED NEWTON METHOD

C     1 *** FOLLOWING ARBITRARILY SETS THE ITERATION INSTRUCTIONS *****
      MAXFUN■2888
      IPRINT-28
```

```
      82•FLOAT(IORD)
      821■DOLE(02*8.113)
      STEP•8214.8.83110
      IF(IORD.E8.1) ACC=8.8808
      IF(IORD.E8.2) ACC.8.1600
      IF(IORD.E(4.3) ACC*8.2708
      IF(IORD.E41.4) ACC.8.4000
C
C      • CALCULATE NUMBER OF PARAMETERS ******** ****** ************
      K.((I0RD+1)*(10RD4.2))/2
      NSK
      N1A•N1+1
      N48•NSAMPL—N1
      J92•8

C              GENERATE ARBITRARY INITIAL PARAMETER ESTIMATES ..........
      X(1)•0.0D0
      DO 2 1.2,N
 2    X(I)=0.1D8
C
C     ******* GENERATE POLYNOMIAL TERMS ************** ****** **********
      IF(IORD.E11.1) GO TO 12
      1(11210RD-1
      KDA■((K8+1)*(KI)+2))/2
      KDB*KDA+1
      KE-IORD-2
      KE•((KE+1)*(KE4.2))/2
      KEB-KEA+1
      DO 15 J•KEB,KDA
      DO 14 Ig1,NSAMPL
 14   A(I,KDB)•A(I,J)*A(1.2)
      KDO*KDB+1
 15   CONTINUE
      DO 16 101,NSAMPL
      A(1,KDB).A(1,KDA)*A(I,3)
 16   CONTINUE
C12   CONTINUE

C     ***** CALCULATE PARAMETER ESTIMATES ** ***** **********************
      DO 5 1.1,N1
      DO 5 ,1■1,K
 5    A2(1...1)■A(1,J)
      DO 8 I■NIA,NSAMPL
      J92-J92+1
      DO 8 J■1.1(
 8    A1(J92,J)■11(1,J)
      IF(IORD.NE.1) GO TO 8690
      1118EFLOAT(NSAMPL)
      819■FLOAT(N1)
      828*(1118-819)/818
      1121■818-11119
      W22-W21.ALOC(W28)
      823•119/U18
      825•U19*ALOG(U23)
      826■825+822
      WRITE(6,8691)
8691  FORMAT(////1,1X,'FOLLOWING IS THE MAXIMIZED LOG LIKELIHOOD VALUE F
     IOR INTERCEPT ONLY MODEL')
      URITE(6,369) U26
8698  WRITE(6,6288) IORD
6208  FORMAT(///////10X,'PROSABILITV SURFACE MODEL OF ORDER         NOW
     1FITTED AND SURFACES DRAWN')
      CALL VA86AD(N,X,F,C,STEP,ACC,MAXFUN,IPRINT,W)
      FMINUS.-1.8D8*F
      WRITE(6,369) FMINUS
369   FORMAT(//,1X,'MAXIMIZED LOG LIKELIHOOD VALUE    '.F12.5)
      NW12.8.5*N*(N*1)
      NW13•N1112*1
      NLESS•14-1
      1478•14013
      N280•14013+NLESS'
      DO 6881 K2804.1,N
      N71.NLESS—K2884
      STER(K2884)•DSORT(W(N78))
      H78-N208+1
6881  N208.1478+N71
      WRITE(6,2088)
2888  FORMAT(//,1X,'PARAMETER ESTIMATES STANDARD ERRORS PARAMETER  EST/
     ISTANDARD ERROR')
      DO 280? I.1,N
      TSTAT(I).X(I)/STER(I)
288?  WRITE(6,2889) X(I),STER(I),TSTAT(I)
```

```
2889  FORMAT(1XF15.7,F18.7,F22.7)
      VRITE(6,6889)
6809  FORNAT(//.1X,'YARIANCE—COVARIANCE MATRIX OF PARAMETER ESTIMATES')
8891  FORMAT(  ,  ,'3Xo'COLUMN',16,9111)
8883  FORMAT(//,1x,'ROW')
8892  FORMAT(  ,'ROY   , 13,3)618F11.5)
      IBEGIN•1113-1-.N
      DO 7902 1210618
      ILESS1011-1
      !END■1+9
      IF(IEND.GT.N) IEND•4
      WRITE(6.8801)  (ICOL,ICOL=1,IEND)
      WRITE(6, 8883)
      DO 7802 J•1.14
      MAX■,1
      If(MAX.GT.IEND)  MAX.IEND
      18ASE010EGIN+J
      DO 7991 K17•I.MAX
      INDEX•IBASE+K17*N—(1(17*K17—K17)/2
       •1(17-1LESS1
7801  PROBI(O■SNGL(U(INDEX))
      MAX•MAX—ILESS1
7002  WRITE(6.8982) J.(PROB1(L),L.1,MAX)
      DO 639 I01,K
638   X21(1,11ASNGL(X(1))
C             COMPUTE ESTIMATED PROBABILITIES ...  ***** **************
      CALL MC81AS(A,X21,02A,NSAMPL,K,1,258,15,258)
      DO 633 I01,14SAMPL
      EIZA(1,1)◦EXP(OZA(1,1))
      Z2■1.8+0211(1,1)
      PROB1(1)•0ZA(1,1)/22
633   PROB4(1)■1.8/ZZ
      DO 8918 1111,11SAMPL
      IF(PROB1(1).E0.1.0) PRO81(1)■8.9999999
      IF(14081(1).E0.8.8) PRO81(1).8.0080081
      IF(PROB4(I).EQ.1.8) PRO84(1)=8.9999999
      IF(PRO84(1),E0.0.9) PR084(1)=8.8080881
      C10(1)•4ART(PROB1(1).0(1.8—PRO81(1)))
      C13(1)•SORT(PRO1340)*(1.8—PRO84(1)))
8910  CONTINUE
      WRITE(6, 8981)
8901  FORMAT(///,11WFOR EACH SAMPLE LOCALITY'/'PREDICTED PROBABILITES
     IRAW RESIDUALS              STANDARDISED RESIDUALS')
      WRITE(6.8939)
8930  FORMAT(/.1X.'RESP CAT 1 RESP CAT 2 RESP CAT 1 RESP CAT 2 RESP
     ICAT 1 RESP CAT 2')
      DO 8928 1•1,N1
      RAVRI•(1.9—PRO81(I))
      RAVR4■—PROB4(1)
      RES1■RAVR1/C18(1)
      RES•RAWR4/C13(1)
8929  WRITE(6,8982) PRO81(1),F1084(I),RAVR1,RAWR4,RESI,RES4
      DO 8921 I•NIA,NSAMPL
      RAVR1•—PRO81(1)
      RAWR40(1.0..41084(1))
      RES1■RAWRI/C18(1)
      RES•RAWR4/C13(1)
8921  WRITE(6.8902) PRO81(1),PRO84(1),RAWRI,RAWR4,RES1,RES4
8982  FORMAT(  ,F8.5.4X,F8.5,4X,4(F9.5,3X))
      DO 243 I•1,K
243   PESTS(I)2X21(1,1)
      CALL PMAP(NL,NC.PESTS,WORK,REFC,CINT,UAX,VAX,N,IORD,VMAX,UMIN,UMAX
     1, VNIN)
      RET
      RETUR
      N

      SUBROUTINE CALCFG(N,X,F,G)
      DOUBLE PRECISION X,C,U12,U13,F,D8LE
      COMMON/ONE/A(258,15),A2(125,15).A1(288,15),NSAMPL,N1,NIA,K,N48
      DIMENSION X(15),C(15)
      DIMENSION )041(15,1),01(125.1),U6(258,1),U9(258.1),ROW1(1  258)
      DIMENSION ROV2(1.125),(111(258,15).U12(1,15),U13(1,15)
      DO 66 Iml,K
66    XN1(1,1)•SNGL(X(I))
      U1.11.0
```

```
      2148.8
      CALL MCSIAS(A2,XN1,81,N1,K11,125,15,125)
      DO 169 I-1, N1
  169 U14111401(1,1)
      2=U1
      CALL MC81AS<AAN1,U6,NSAMPL,Kt1,258,15,258)
      DO 87 141,NSAMPL
   87 U60,1)■EXP(U6(1,1))
      DO 98 101,NSAMPL
      U9(1,1)4116(1,1)
   98 U9(I,1)°1.8+U9(I,I)
      DO 91 I=1,NSAMPL
   91 Z1421+ALOG(U9(I,1))
      FA4-1.8*(2-21)
      F■DBLE(FA)
C     ***** -F IS THE LOG LIKELIHOOD VALUE .....
C
C     *** CALCULATE 1ST DERIVATIVES OF LOG LIKELIHOOD FUNCTION ***** 44*
      DO 44 I■1,NSAMPL
   44 ROB1(1,1)41.0
      DO 45 I41/N1
   45 ROV2(1,1)41.8
      DO 94 141,NSAMPL
   94 U6(I,1)=U6(I,1)/U9(I,I)
      DO 92 .141.1(
      DO 92 I41,NSAMPL
   92 U11(1,04A(LJ)*Q6(I,1)
      CALL MATNV(R01111,U11,U12,1,NSAMPLIK,1,258,1)
      CALL MAT WROU2,A2,U13,1,N1,K,1,125,1)
      DO 93 J41,K
   93 U13(1,041/13(1.41)-U12(1,J)
      DO 181 I•tik
  181 G(I)*U13(1,1)
      DO 184 I41,N
  184 G(I)•-G(I)
C     ***** G IS TUE VECTOR OF 1ST DERIVATIVES 444 * .... * ***** 41 0*****
      RET URN
      END
```

```
      SUBROUTINE PM$PCNL,NCoPESTS,WORK,REFC,CINT,UAX,VAX,N,IORD,VMAX,UNI
     IN.UMAX.VMIN)
      DIMENSION PESTS(H),VORK(N),SLINE(128),SYMB(23)
      DATA SYMB/IN1.1H.,1H2,1H.,1H3,1H.,1H4,1H.,11.15,1H.,1}6,1H.,1H6,1m.,
     11117,1H.,1148.1N.,1H9,1H.,1H8,1H1,1H-/
    1 FORMAT('1       PROBABILITY SURFACE OF ORDER ',I8/' PART'I14//)
    2 FORMAT(' '.120A1)
      DO 66 JZ41,2
      KNAX-8
      KMIN*28
      NO24118
      NSTR-NC/118
      LEFT-HC-1184NSTR
      IF(LEFT.GT.8) NSTR4NSTR+1
      DO 96 KOUNT41,NSTR
      IF(KOUNT.EQ.NSTR.AND LEFT.GT.8) NO24LEFT
      URITE(6/1) IORDiKOUNT
      NO22040242
      BRITE(6,2) (SYMB(23),141,NO22)
      V4VMAX+VAX
      BO 12 L01,NL
      Y-Y-VAX
      U■UMIN--UAX4(KOUNT-.1)41184UAX
      DO 6 I.1, NO2
      U4U+UAK
      PR°PROB(PESTS,VORK,N,IORD,U, '0,J2)
      KCC■11+PNT((PR-.REFC)/CINT)
      IF(PRAT.REFC) KCC-KCC-1
      IF(KCC.LT.1) KCC■!
      IF(KCC.GT.29) KCCO20
      IF(KCC.GT.KMAX) KMAX-KCC
      IF(KCCAT.KMIN) KMIN=KCC
    6 SLINE(I)-SYMB(KCC)
   12 URITE(6,2) SYMB(22),(SLINE(1).I41,NO2),SYMB(22)
                (SYMB(23),I41,NO22)
   96 CONTINUE
```

```
      WRITE(6,4) REFC,CINT
    4 FORMAT('8     REFERENCE CONTOUR = ',F11.4/'      CONTOUR INTERVAL =
     1',F12.4)
      WRITE(6,3)
    3 FOORM3AT4KM KEY TO CONTOUR VALUES'//)
      D    IC9 IN,K MAX
      J411-I
      P=REFC-J4CINT
      Q=P4CINT
      IF(I.EQ.1) GO TO 7
      IF(I.EQ.28) GO TO 8
      WRITE(6,9) (SYMB(1),J=1,6),P,(4
      GO TO 5
    7 WRITE(6,11) (SYMB(I),J=1,6),P
   10 FORMAT(",6A1,2X,F18.4.'AND BELOW)
      GO TO 5
    8 WRITE(6,11) (SYMB(I),J■1,67',P
   11 FORMAT(",6A1,2X,F18.4,'AND ABOVE')
    9 FORMAT(     6A1,2X,F18.4,' TO ',F18.4)
    5  ONTINUE
      WRITE(6,13) UMIN.SIMAX,UMAX,IIMAX,UMIN ' MIN ' UMAX ' SIMIN
   13 FORMAT('O COORDINATES OF MAP CORNERS ARE:'/
     15X,' TOP LEFT',5X/2F12.4/
     15X,' TOP RIGHT     ',2F12.4/
     15X,' BOTTOM LEFT   ',2F12.4/
     15X,' BOTTOM RIGHT ',2F12.4)
   66 CONTINUE
      RET N
      RNDUR
```

```
      FUNCTION PROB(PESTS,WORK,N,NORD,U,V JZ)
C     *** COMPUTES VALUE ON PROBABILITY SURFACE AT EACH POINT ■ ■ ■ ■
      DIMENSION PESTS(N),VORK(N)
      OZI4PESTS(1)4(PESTS(2)4U)+(PESTS(3) 4V)
      e22■EXP(:121)
      2241.84822
      IF(J2.E8.2) GO TO 8
      PROD-822/22
      GO TO 9
    8      /22
      CONTINUE
      IF(NORD.LT.2) RETURN
      WORK(2)4U
      WORK(3)06
      DO 1 M■2,NORD
      LI-N-I
      L2014(M+1)/2
      DO 2 I4I'M
      L2=1.241
      NW28841.2.-M
      WORK(L2)=VORK(NQ208) 4U
    2 821411214PESTS(L2)44ORK(L2)
      N11281•L2+1
      NW282•L2-M
      WORK(N14281)=VORK(HU282) °
      82108214PESTS(NU281)411ORK(NW281)
      022•EXP(821)
      22.1.0+822
      IF(JZ.EQ.2) GO TO 4
      PROB4022/22
      GO TO
    4 PROB41.1 8/ZZ
    1 CONTINUE
      RETURN
      END
```

Appendix 1(b) A Fortran program for the three response category case

The program presented in Table 7 basically follows the same structure as that in Table 6 and discussed in (a) above. The reader should therefore ensure that he has understood that discussion and should then take note of the following alterations.

a) Input alterations The first card now specifies the highest order of surface the user wishes to fit (IORD); the number of respondents in the sample (NSAMPL); the number of respondents in the sample who have chosen response category one, in terms of the example in III (iv) the number who have claimed to shop regularly at the hypermarket (N1); and the number who have chosen response category two, in terms of the example in III (iv) the number who have claimed to shop occasionally at the hypermarket (N2B). The input order of the set of cards which follow and which give the geographical co-ordinates now demands that all respondents choosing response category 1 are read in first, followed by all respondents choosing response category 2, followed by all respondents choosing response category 3 (this is the arbitrarily chosen response category whose parameters have been set to zero, see III (i)). In the example in III (iv) Table 4 must therefore be re-organised so that all housewives claiming to shop regularly at the hyper-market are read in first, followed by all housewives claiming to shop occasionally at the hypermarket, followed by all housewives claiming never to shop at the hypermarket.

b) Output alterations The output follows the structure outlined in (a) above and illustrated in Figures 6, 7, 8, 10 and Table 4. The user should be aware however, of the manner in which the parameter estimates, standard errors and parameter estimate/standard error ratios are printed in the multiple response case. Using 1st order probability surface models of the 3 response category kind as an example, the parameter estimates, standard errors and parameter estimate/standard error ratios are printed as follows.

PARAMETER ESTIMATES	STANDARD ERRORS	PARAMETER EST/STANDARD ERROR
-0.5533	0.1960	-2.8225
0.0131		
-0.0454		
-0.2395		
0.0112		
-0.0699		

The first three parameter estimates are α_0, β_{10}, β_{20}; the second three are α_1, β_{11}, β_{21} (see III (i) for clarification). That is to say, the full set of parameter estimates associated with category 1 are printed prior to the full set of parameter estimates associated with response category 2.

c) Size restriction alterations The maximum number of respondents in the sample (NSAMPL) allowed remains the same as in the earlier program, i.e. 250. The maximum number who choose response category one (N1) allowed, is set at 100. The maximum number who choose response category two (N2B) allowed, is set at 100. The maximum number who choose response category three (NSAMPL-N2B-N1) allowed, is set at 150. These size restrictions, like those of the earlier program, are easily changed however, and in Appendix 2(b) the changes required in the program when NSAMPL=AT1, N1=AT2, N2B=AT3 and (NSAMPL-N28-N1)=AT4 are given, thus allowing the user to modify the size restrictions of the program to suit his own needs.

Table 7

```
C
C      ..... PROBABILITY SURFACE PROGRAMME FORA 3 CATEGORY SITUATION.
C      WRITTEN BY NEIL WRIGLEY, DEPT OF GEOGRAPHY, UNIVERSITY OF BRISTOL
C
       COMNON/ONE/A(250,15)/A2(100/15),A3(180.15)/A1(150,15),NSAMPL,NI,N2
      1,NIA/N2A,N2B,N48,K/K1.KA2

C      .... READ IN IORD=HIGNEST SURFACE ORDER TO BE FITTED/ 1,2,3, OR 4
C      NSAMPL=NUMBER OF SAMPLE LOCALITIES, N1=NUMBER OF LOCALITIES WHERE
C      RESPONSE CATEGORY ONE IS RECORDED, N2B=NUMBER OF LOCALITIES WHERE
C      RESPONSE CATEGORY TWO IS'RECORDED ******************************
C      **** DATA CARD: COL 1=IORD, COL 2=BLANK, COL 3-5=NSAMPL, COL 6=
C      BLANK, COL 7-9=N1/ COL 10=BLANK, COL 11-13=N2B ******************
       READ(511) IORDoNSAMPL,H1/N28
  1 FORMAT(I1,1X.I3/1X,13.1X,I3)
C
C      **s* READ IN VERT=LENGTH OF PROBABILITY SURFACE MAP REQUIRED IN
C      INCHES, WID■WIDTH IN INCHES, REFC=VALUE OF REFERENCE CONTOUR, CINT
C      =CONTOUR INTERVAL. UMAX,UMIN=MAXIMUM AND MINIMUM ALONG HORIZONTAL
C      AXIS. VMAX,VNIN=MAXIMUN AND MINIMUM ALONG VERTICAL AXIS *********
C      *** DATA CARD: COLS 1-7=VERT, COLS 8-14=WID, COLS 15-19=REFC,
C      COLS 28-24=CINT, COLS 25-31=UMAX, COLS 32-38=UMIN, COLS 39-45=VMAX
C      COLS 44-52=VNIN .....
       READ(5. 18) VERT,WID,REFC,CINT/UMAX,UMIN,VMAX/VMIN
   18  FORMAT(2F7.4,2F5.3,4F7.4)
      441=INTLVERT*8.0+8.5)
       NC=INT(WID*18.0+0.5)
       UAX=(UMAX—UMIN)/FLOAT(NC-1)
       YAX=(VMAX—VMIN)/FLOAT(NL-1)
       UAX=UAX+8.888801*UAX
       VAX=VAX*0.800801*VAX
C
C      **** READ IN GEOGRAPHICAL CO—ORDINATES OF EACH SAMPLE LOCALITY,
C      U(I)=HORIZONTAL CO—ORDINATE/ V(I)=VERTICAL CO—ORDINATE, IN FORMAT
C      (F8.4,1X,F8.4) (N.B. IN THE PROGRAMME THESE CO—ORDINATES ARE
C      STORED IN MATRIX A) *** ORDER OF CARDS—ALL SAMPLE LOCALITIES WHERE
C      RESPONSE CATEGORY ONE IS RECORDED/ FOLLOWED BY ALL LOCALITIES
C      WHERE RESPONSE CATEGORY TWO IS RECORDED, FOLLOWED BY ALL
C      LOCALITIES WHERE REMAINING RESPONSE CATEGORY IS RECORDED ** CREATE
C      CONSTANT TERM *** PRINT SAMPLE LOCALITITIES **********************
       WRITE(6, 11)
   11  FORMATCO      U           V')
       DO 3 I=1,NSAMPL
       A(1,1)=1.8
       READ(5,4) A(I,2),A(I,3)
    3  WRITE(6,44) (A(I,J),J=2,3)
    4  FORMAT(FS.4,1X,F8.4)
   44  FORMAT("2F9.4)
C
C            START OF MAIN LOOP ****************** ******** ***********,
       ID=O
       CALL SURF(IDINL,NC,UAX,VAX,UMAX,UMIN,VMAX,VMIN,REFC,CINT)
       DO 7 I=1, IORD
       11)=10+1
         LL SURF(IDoNL,NC/UAX,VAX,UMAX/UMIN,VMAX,VMIN,REFC,CINT)
    7  CONTINU
       STOP
       END


       SUBROUTINE SURF(IORDoNL.NC.UAX/VAX/UMAX,UMIN,YMAX,VMIN,REFC,CINT)
       COMMON/ONE/A(250.15).A2(180,15),A3(180,15),A1(150,15),NSAMPL,NI.N2
      1,N1A,N2A,N2B,N4B,K,K1oKA2
        OUBLE PRECISION BZ1.DBLE
        OUBLE PRECISION X,F,G,STEP,ACC,W,FMINUS,STER,TSTAT
        IMENSION C19(258),C11(250),C13(258)
        INENSION PROB1(2541),PROB2.(250),PROB4(258),XZ1(15,1),X22(15,1)
        INENSION OZA(258,1),QZ8(259,1).W(1981)/PESTS2(30)
        IMENSION X(30),G(39),TSTAT(30),STER(38),WORK(30),PESTS1(30)
C
C      *** THIS IS THE MAIN PART OF THE PROGRAMME. IT CALCULATES THE
C      PARAMETER ESTIMATES OF THE PROBABILITY SURFACE MODEL USING MAXIMUM
C      LIKELIHOOD ESTIMATION. IT USES POWELL'S HYBRID STEEPEST DESCENT
C      AND GENERALISED NEWTON METHOD *************** ****** **************
C
C      **** FOLLOWING ARBITRARILY SETS THE ITERATION INSTRUCTIONS ****s
       MAXFUN=2000
```

```
      IPRINT■28
      IF(IORD.EQ.8) GO TO 9658
      82=FLOAT(IORD)
      821=DBLE(82118.84)
      STEP■821+9.83D8
      IF(IORD.EQ.1) ACC=0.16D8
      IFOORD.E0.2) ACC=9.32D8
      IF(IORD.E0.3) ACC=9.5480
      IF(IORD.EQ.4) ACC=0.8888
      GO TO 9651
 9658 STEP=0406D8
      ACC=0.88D0
C
C     ..... CALCULATE NUMBER OF PARAMETERS **********   * ** *** ******
 9651 K=(<IORD+1)*(10RD+2))/2
      14=K*2
      NIA=N/1.1
      N20928+91
      N2A0142+1
      N48=NSAMPL—N2
      K1=K+1
      KA2■K*2
      KI2=K1+1
      J81■8
      J92=0
C
C     ■ ■ ▮ GENERATE ARBITRARY INITIAL PARAMETER ESTIMATES **********
      IF(IORD.E8.8) GO TO 9652
      X(1)=1.080
      DO 2 I=2.1(
    2 X(I)=8.1D8
      X(K1)=1.000
      DO 703 I0KILN
  783 X(I)=8.1D8
      GO TO 9655•
 9652 DO 9653 1.01,N
 9653 X(I)=8.1D8
      GO TO 9654
C
C     ******* GENERATE POLYNOMIAL TERMS ****************************4
 9655 IF(IORD.EQ.1) GO TO 12
      KD0IORD-1
      KDA■(((D+1)*(1(D+2))/2
      KDB0KDA+1
      KE=IORD-2
      KEA0((KE+1)*(KE+2))/2
      KEB■KEA+1
      DO 15 J=KEBoKBA
      DO 14 I=1.NSAMPL
   14 A(I,KDB)=A(I,J)*A(1,2)
      KDB=KDB+1
   15 CONTINUE
      DO 16 I-1,NSAMPL
      A(I,KDB)=A(I,KDA)*A(I,3)
   16 CONTINUE
   12 CONTINUE
C
C     ***** CALCULATE PARAMETER ESTIMATES ****** ***** ****************.
 9654 DO 5 I=1,N1
      DO 3 J=I*K
    5 A2(I,J)=A(IsJ)
      DO 6 I=N1A,N2
      J8014181+1
      DO 6 41=1,K
    6 A3(.181,J)=A(I,J)
      DO 8 I=N2A,NSAMPL
      J92=J92+1
      DO 8 41,01.K
    8 A1(J92,J)-A(I,J)
      1F(IORD,EQ.8) WRITE(6,9668)
 9668 FORMAT(/////.1X,'FOLLOWING IS THE MAXIMIZED LOG LIKELIHOOD VALUE F
     !OR INTERCEPT ONLY MODEL')
      IFOORD.E0.8) GO TO 9661
      WRITE(6,6208),LORD
 6280 FORMAT(/////“//1X,'PROBABILITY SURFACE MODEL OF ORDER '.11 ' NoW
     !FITTED AND SURFACES DRAWN')
 9661 CONTINUE
      CALL VA86AD(NoX/F,G,STEPIACC,MAXFUN,IPRINT,W)
      FMINU8=-1.8D8*,
      WRITE(6,369) FNINUS
  369 FORMAT(//,1X,'MAXIMIZED LOG LIKELIHOOD VALUE    ',F12 5)
      IF(IORD.EQ.0) RETURN
      NV12=8.50*(11+1)
      N813=N1112+1
      NLESS=N-1
      N700813
      N288=N1113+NLESS
      DO 6081 K2884=1,N
      N71=NLESS—K2984
      STER(K2884)=DSORT(W(N78))
      N79=N280+1
 6801 N288=978+971
      WRITE(6,2088)
 2088 FORMAT(//,1X,'PARAMETER ESTIMATES STANDARD ERRORS PARAMETER EST/
     1STANDARD ERROR')
      DO 2087 I=1,N
      TSTAT(I)=X(I)/STER(I)•
 2807 WRITE(6,2889) X(I),STER(I),TSTAT(I)
 2889 FORMAT(IX,F15.7/F18.71F28.7)
      WRITE(6,6099)
 6889 FORMAT(//,1X.'VARIANCE—COVARIANCE MATRIX OF PARAMETER ESTIMATES')
 8881 FORMAT('—'.3X,'COLUMN',I6.9111)
 8883 FORMAT(//.IX.'ROW'/)
 8002 FORMAT(' ','ROW ',13,3X,18F11.5)
      IBEGIN=NW13-1—N
      DO 7882 I=1,No10
      ILESS1=I-1
      IEND=14.9
      IF(IEND.GT.N) IEND0N
      WRITE(6,8881) (ICOL,ICOL.I,IEND)
      WRITE(6.8883)
      DO 7882 J=I,N
      MAX =J
      IF(MAX.GT.IEND) MAX=IEND
      IBASE=IBEGIH+.1
      DO 7001 K17=I,MAX
      INDEX=IBASE+K17*N—(1(17*K17—K17)/2
      L-K17—ILESSI
 7881 PROBI(L)=SNGL(V(INDEX))
      MAX=MAX—ILESS1
 7882 WRITE(6.8882) J.(PROBI(L).L.1,MAX)
      J2208
      DO 68 011/K
  630 X21(I ,1)=SNGL(X(I))
      DO 631 I=K1,KA2
      JZ2=4122+1
  631 X22(J22,1)=SNGL(X(I))
C
C     ***** COMPUTE AND PRINT ESTIMATED PROBABILITIES AND RESIDUALS ***
      CALL MC91AS(A.X21,OZA,NSAMPL,K,1,250,15,258)
      CALL MC0IAS(A.X22,828,NSAMPL.K,1,250,15.250)
      DO 633 I-1,NSANPL
      92A(I,1)=EXP(OZA(1,1))
      QZ8(I,1)=EXP(C28(I,1))
      22=1.8+QZA(I.01)+QZ8(I.1)
      PROB1(1)=Q2A(1,1)/ZZ
      PRO82(1)=028(1,1)/22
  633 PRO84(I)01.8/22
      DO 8918 ImIoNSAMPL
      IF(PROB1(I).EQ.1.0) PROB1(I)=8.9999999
      IF(PRO81(I).E9.8.8) PRO81(1)=8.0880881
      IF(PROB2(I).EQ.1.9) PRO82(1)=8.9999999
      IF(PROB20).E0.8.9) PRO82(I)=8.8880801
      IF(PROB4(I).E8.1.8) PRO84(1)=8.9999999
      IF(PRO84(I).EG.8.0) PRO84(I)=0.0888801
      C10(I)=SQRT(PRO81(1)*(1.9—PROB1(I)))
      CII(I)=SORT(PR0820)*(1.8—PROB2(I)))
      C13(I)=SeRT(PRO84(I)*(1.8—PRQB4(1)))
 8918 CONTINUE
      WRITE(6,8981)
 8981 FORMAT(///.1X.'FOR EACH SAMPLE LOCALITY'/'PREDICTED PROBABILITES
     1          RAW RESIDUALS                    STANDARDISED RES
     1I DUALS')
      WRITE(618938)
 8938 FORMAT(/.1X.'RESP CAT 1 ((ESP CAT 2 RESP CAT 3 RESP CAT 1 RESP
     1CAT 2 RESP CAT 3 RESP CAT 1 RESP CAT 2 RESP CAT 3')
      DO 8928 1=1,N1
      RAWRI=(1.8—PROBI(I))
      RAWR2=-.PRO82(I)
      RAWR4=—•PRO84(I)
      RES1=RAVRI/C18(I)
      RES2=RAWR2/C11(I)
      RES4=RAWR4/C13(I)
```

```
8920 WRITE(6.8982) PRO81(1),PROB2(I),PRO84(1),RAWR1,RA0R2,RAMR4 ' RESI ' RE
     1S2.RES4
      DO 8921 IaN1A,N2
      RABRIa-PROBI(I)
      RAWR2-(1.0-PRO82(I))
      RAIIIR4a•-PRO84(I)
      RESI=RAMR//C10(I)
      RES2aRAWR2/C11(1)
      RES4aRAIOR4/C13(1)
8921 WRITE(6,8902) PROBI(I),PROB2(1),PRO84(I),RAWR1,RAWR2 . RAWR4 . RESI . RE
     152. RES4
      DO 8922 I=N2A,NSAMPL
      RAVR1a-PROBI(I)
      RAVR2m-PROB2(I)
      RAVR40(1.0-PRO84(I))
      RESIaRAWRI/C18/I)
      RES2aRAWR2/C11/D
      RES4-RAWR4/C13(I)
8922 WRITE/6.8982) PROB1(1),PROB2(I),PROB4(1),RAWRI,RAWR2,RAWR4 . RESI . RE
     182, RES4
8962 FORMAT(",F8.5,4X,F8 5,4X,F8.5,3X,6(F9.5,3X))
      DO 243 Ial,K
      PESTSICl/aX21(1,1)
243   PESTS2(I)=X22(I,1)
      CALL PMAP(NL,NC,PESTS1,PESTS2,WORK,REFC,CINT,UAX,VAX,N,IORD . VMAX . U
     IMIN,UMAX,VMIN)
      RET URN
      END
```

```
      SUBROUTINE CALCFG(N,X,F,G)
      DOUBLE PRECISION X,G,U12,U13,U18,F,DBLE
      COMMON/ONE/A(258,15),A2(188,15),A3(180,15),A1(158,15) . NSAMPL . H1 . N2
     1,N1A,N2A,N2B,N4B,K,K1,KA2
      DIMENSION X(38),G(38)
      DIMENSION 101(15,1),XN2(15,1),01(188,1),02(188,1)
      DIMENSION U6(258,1),U7(258,1),U9(258,1)
      DIMENSION ROW1(1,258),ROW2(1,108),ROW3(1,108)
      DIMENSION 011(258,15),U12(1,15),U13(1,15),U18(1,15)
      J2=8
      DO 66 I=1,K
66    X141(I,1)=SNGL(X(I))
      DO 67 I■1(1,1(A2
      J2=J2+1
67    XN2(J2,1)=SNGL(X(I))
      U1=8.8
      U2-8.B
      21■6.0
      CALL MC6IAS(A2, )(NI, Q1 , H1, K, 1 , 188, 15, 188)
      CALL MCOIAS(A3,XN2,82,H2B,K,1,188,15,188)
      DO 169 I.1,141
169   U1=U1+01(I,1)
      DO 70 I-1. 1428
78    U2aU2+02(1.1)
      2aUl+U2
      CALL MC6IAS(A,XN1,U6,NSAMPL,K,1,258,15 . 258)
      DO 87 I=1,NSAMPL
87    U6(I.1)0EXP<U6(1,1))
      CALL MCISIAS(A.XN2.U7,NSAMPL,K,1,258,15,250)
      DO 88 IalaNSAMPL
88    U7(1.1)*EXP<U7(I,1)/
      DO 90 laloNSAMPL
      U9(I,1)-U6(I.1)+U7(1,1)
98    U9(I/1)=1.0+U9(I,1)
      DO 91 IaLNSAMPL
9.1   Z1-Z1+ALOG(U9(I.1))
      FAa-1.0*(2-21)
      F-DBLE(FA)
C     * ..... F IS THE LOG LIKELIHOOD VALUE ****************************
C
C     *** CALCULATE 1ST DERIVATIVES OF LOG LIKELIHOOD FUNCTION ********
      DO 44 Ial/NSAMPL
44    R081/1,1)-1.0
      DO 45 1=1,N1
45    R082(1,1).1.0
      DO 46 1-1,N213
46    ROW3(1,I)-1.0
      DO 94 IaltNSAMPL
94    U6(1,1 )aU6(1,1)/09(1,1)
      DO 92 Ja1:1(
      DO 92 Ial,NSAMPL
92    U11(I,J)=A(I,J)*U6(I,1)
      CALL MATIWROW1,U11,U12,1,NSAMPL,K,1,258,1)
      CALL MATNV(ROW2,A2,1/13, I,N1,K,1,188,1)
      DO 93 Ja1,K
93    U13(1,J)=U13(1,J)-U12(1,J)
      DO 95 Ial,NSAMPL
95    U7(1,1)aU7(1,1)/U9(I,1)
      DO 96 4.101.K
      DO 96 Ial,NSAMPL
96    UI1(I,J)=A(1,J)*U7(I,1)
      CALL MATNV(ROW1,U11,U12,1,NSAMPL,K,1,258,1)
      CALL MATNW(120413,A3,U18,1,N2B,K,I, 188,1)
      DO 97 Jal.K
97    U18(1,J)■U18(1,J)-U12(1,J)
      DO 101 I=1,K
181 GM-1113(1,D
      DO 102 IaliK
      J410I+K
182   G(J4)-U18(1,I)
      DO 184 I=1,N
184   G(I)■-G(I)
C     *IP**  N G IS THE VECTOR OF 1ST DERIVATIVES ....■ ■ ■ ■ ■ ■ ■ ■ ■ ■
      RET
      END UR
```

```
      SUBROUTINE PNAP(NL,NC,PESTSI,PESTS2/WORK,REFC,CINT,UAX,VAX,No1ORD,
     1VMAX,UNIN,UMAX,VMIN)
      DIMENSION PESTSI(M)IPESTS2(N),WORK(N),SLINE(128),SYMB(23)
      DATA SYMB/114/,1H.,1H2,1H.,1143.1H.,1H4,114..1145,114..1H\,IN.,1146.1H.,
     11N7.111.,1118,111.,1149rIN.:1148,INI,IN-/
      FORMAT/ 1 PROBABILITY SURFACE OF ORDER ',I81' PART'oI4//)
2     FORMAT(' ',120A1)
      DO 66 4201,3
      KMAX08
      KNINO20
      NO2■/10
      NSTROIC/110
      LEFTOIC...118*NSTR
      IF(LEFT.GT.0) NSTR=NSTR+1
      DO 96 KOUNT"1,NSTR
      IF(KOUNT.E0.148TR.AND.LEFT.GT . 8) NO2aLEFT
      WRITE(6,1) IORD, KOUNT
      40220NO24.2
      WRITE(6,2) (SYMB(23),I=104022)
      ValiMAX+VAX
      DO 12 La1,11L
      V-V-VAX
      U■UMIN-UAX+(KOUNT-1)4.118*UAX
      DO 6 I=1,NO2
      U-U+UAX
      PRARPROB(PESTS1,PESTS2,WORK,N,IORD,U,Y,J2)
      KCC=11+INT((PR-REFC)/CINT)
      IF(PR.LT . REFC) KCC=KCC-1
      IF(KCC.LT.1) KCC=1
      IF(KCC.GT.28) KCCI.28
      IF(KCC.GT.KMAX) KMAX=KCC
      IF(KCC.LT.KMIN) KMIN=KCC
6     SLINE(I)=SYMB(KCC)
12    WRITE(6,2) SYMB(22),(SLINE(I),I=1,NO2),SVME1(22)
      WRITE(6,2) (SVMB(23),I=1,NO22)
96    CONTINUE
      WRITE(6,4) REFC,CINT
4     FORMAT('8 REFERENCE CONTOUR - ',F11.4/' CONTOUR INTERVAL -
     1',F12.4)
      BRITE(6,3)
3     FORMATC8 KEY TO CONTOUR VALUES'//)
      DO 5 I■KMINoKMAX
      4011-I
      PaREFC-J*CINT
      0=P+CINT
      IF(I.EQ.1) GO TO 7
      IF(I.E0.20) GO TO 8
      MRITE(6,9) (SYMB(I),J=1,6),P,Q
      CO TO 5
7     WRITE(6,10) <SYMB(1),Jal,6),P
```

```
18    FORMAT(".6A1.2%,F18.4,'AND BELOW)
      GO TO 5
8     WRITE(6.11) (SYMB(I).4.1=1■6),P
11    FORMAT(".6A1.2X.F18.4,'AND ABOVE')
9     FORMATC".6A1.224.F18.4.' TO '■F18.4:
5     CONTINUE
      WRITE(6.13) UNIN.YMAX,UMAX.YMAX,UMIN■YMIN,UMAX,YMIN
13    FORMAT('O COORDINATES OF MAP CORNERS ARE,'
     15X.' TOP LEFT . 5}G2F12.4/
     15X.' TOP RIGHT     ',2F12.4/
     15X/' BOTTOM LEFT   ',2F12.4/
     15X.' BOTTOM RIGHT ',2F12.4)
66    CONTINUE
      RET
      RETUR
```

```
      FUNCTION PROB(PESTS1IPESTS2/BORK,N,NORDoUJY,JZ)
C     .04,4 COMPUTES VALUE ON PROBABILITY SURFACE AT EACH POINT ********,
      DIMENSION PESTSI(N),PESTS2(N)IWORK(N)
      0210PESTS/(1)*(PESTS1(2)4U)+(PESTS1(3)*Y)
      0218.PESTS2(1)4(PESTS2(2)4U)+(PESTS2(3)*Y)
      022B=EXP<Q21A)
      0228mEXPCQZ1B)
      22-1.844122A+0228
      IF(JZ.E0.2) GO TO 8
      IF(JZ.EQ.3) GO TO 9
      PROB=OZ2A/ZZ
      GO TO 18
8     PROBwIlZ2B/ZZ
      GO TO 18
9     PROBa1.8/22
18    CONTINUE
      IF(HORD.LT.2) RETURN
      WORK/2)-U
      WORK(3)2Y
      DO 1 M=2,NORD
      L1-11-1
      L2.114.(M4.1)/2
      DO 2 I=101
      L201.2+1
      HB298■1.2-M
      WORK(L2).VORK(Ni1288)4U
      021A01221A+PESTSI<L2)411ORK(L2)
2     Q21801221B+PESTS2(L2)4WORK(L2)
      NO281=1.2+1
      Ni1202-L2-M
      BORK(N11291)0VORK(NB282)*Y
      OZIAIIQZ1A+PESTS1(NB281) 000RK(NO201)
      021801221B+PESTS2(H1n81)01ORK(4U281)
      022ANEXP(0214)
      0228■EXPOZ1B)
      22-1.8+QZ2A+OZ28
      IF(JZ.EQ.2) GO 40 4
      IF(JZ.E0.3) GO TO 5
      PROB■022A/Z2
      GO T I
4     PRO8n 022B/22
      GO TO 1
5     PROB=1.8/ZZ
      CONTINUE
      RET
      RETUR
```

Appendix 1(c) A Fortran program for the four response category case

The program presented in Table 8 follows the same structure as that discussed in (b) above and the minor alterations from the program in Table 7 are explained in the program itself. Appendix 2(c) contains the changes necessary to allow the user to modify the size restrictions of the program to suit his own needs. The program, Table 8, begins on page 65.

Appendix 1(d) The common subroutines

The programs listed in Tables 6, 7 and 8 utilise the common subroutines presented in Table 9. Subroutine VA06AD is taken from the Harwell Algorithm Package and was written by M.J.D. Poweil. The listing given below Incorporates some minor changes by the author but it is essentially in its origina form. It is reproduced here with the kind permission of the Controllers of the Harwell Algorithms Package.

APPENDIX 2 Alterations to size restrictions of computer programs

Appendix 2(a)

The following are the card changes necessary in the program listed in Table 6 when NSAMPL=AT1, N1=AT2 and (NSAMPL-N1)=AT3.

In main part of program:

```
COMMON/ONE/A(AT1,15),A2(AT2,15),A1(AT3,15),NSAMPL,N1,N1A,K,N4B
```

In subroutine SURF:

```
COMMON/ONE/A(AT1,15),A2(AT2,15),A1(AT3,15),NSAMPL,N1,N1A,K,N4B
DIMENSION C10(AT1),C13(AT1)
DIMENSION PROB1(AT1),PROB4(AT1),QZA(AT1,1),XZ1(15,1)
CALL MCOlAS(A,XZ1,QZA,NSAMPL,K,1,AT1,15,AT1)
```

In subroutine CALCFG:

```
COMMON/ONE/A(AT1,15),A2(AT2,15),A1(AT3,15),NSAMPL,N1,N1A,K,N4B
DIMENSION XN1(15,1),Q1(AT2,1),U6(AT1,1),U9(AT1,1),ROW1(1,AT1)
DIMENSION ROW2(1,AT2),U11(AT1,15),U12(1,15),U13(1,15)
CALL MCOlAS(A2,XN1,Q1,N1,K,1,AT2,15,AT2)
CALL MCOIAS(A,XN1,U6,NSAMPL,K,1,AT1,15,AT1)
CALL MATNW(ROW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW2,A2,U13,1,N1,K,1,AT2,1)
```

Appendix 2(b)

The following are the card changes necessary in the program listed in Table 7 when NSAMPL=AT1, N1=AT2, N2B=AT3 and (NSAMPL-N2B-N1)=AT4.

In main part of program:

```
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A1(AT4,15),NSAMPL,N1,N2
```

In subroutine SURF:

```
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A1(AT4,15),NSAMPL,N1,N2
DIMENSION C10(AT1),C11(AT1),C13(AT1)
DIMENSION PROB1(AT1),PROB2(AT1),PROB4(AT1),XZ1(15,1),XZ2(15,1)
```

```
DIMENSION QZA(AT1,1),QZB(AT1,1),W(1981),PESTS2(30)
CALL MCOlAS(A,XZ1,QZA,NSAMPL,K,1,ATI,15,AT1)
CALL MCOlAS(A,XZ2,QZB,NSAMPL,K,1,AT1,15,AT1)

In subroutine CALCFG:
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A1(AT4,15),NSAMPL,N1,N2
DIMENSION XN1(15,1),XN2(15,1),Q1(AT2,1),Q2(AT3,1)
DIMENSION U6(AT1,1),U7(AT1,1),U9(AT1,1)
DIMENSION ROW1(1,AT1),ROW2(1,AT2),ROW3(1,AT3)
DIMENSION Ull(AT1,15),U12(1,15),U13(1,15),U18(1,15)
CALL MCOlAS(A2,XN1,Q1,N1,K,1,AT2,15,AT2)
CALL MCOlAS(A3,XN2,Q2,N2B,K,1,AT3,15,AT3)
CALL MCOlAS(A,XN1,U6,NSAMPL,K,1,AT1,15,AT1)
CALL MCOlAS(A,XN2,U7,NSAMPL,K,1,AT1,15,AT1)
CALL MATNW(ROW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW2,A2,U13,1,N1,K,1,AT2,1)
CALL MATNW(ROW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW3,A3,U18,1,N2B,K,1,AT3,1)
```

Appendix 2(c)

The following are the card changes necessary in the program listed in Table 8 when NSAMPL=AT1, N1=AT2, N2B=AT3, N3B=AT4 and (NSAMPL-N3B-N2B-N1) =AT5.

```
In main part of program:
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A4(AT4,15),A1(AT5,15),N

In subroutine SURF:
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A4(AT4,15),A1(AT5,15),N
DIMENSION C10(AT1),C11(AT1),C12(AT1),C13(AT1)
DIMENSION PROB1(AT1),PROB2(AT1),PROB3(AT1),PROB4(AT1)
DIMENSION QZA(AT1,1),QZB(AT1,1),QZC(AT1,1),TSTAT(45),STER(45)
CALL MCOlAS(A,XZ1,QZA,NSAMPL,K,1,AT1,15,AT1)
CALL MCOlAS(A,XZ2,QZB,NSAMPL,K,1,AT1,15,AT1)
CALL MCOlAS(A,XZ3,QZC,NSAMPL,K,1,AT1,15,AT1)

In subroutine CALCFG:
COMMON/ONE/A(AT1,15),A2(AT2,15),A3(AT3,15),A4(AT4,15),A1(AT5,15),N
DIMENSION X(45),G(45),Q1(AT2,1),Q2(AT3,1),Q3(AT4,1)
DIMENSION U6(AT1,1),U7(AT1,1),U8(AT1,1),U9(AT1,1)
DIMENSION ROW1(1,AT1),ROW2(1,AT2),ROW3(1,AT3),ROW4(1,AT4)
DIMENSION Ull(AT1,15),U12(1,15),U13(1,15),U18(1,15),U23(1,15)
CALL MCOlAS(A2,XN1,Q1,N1,K,1,AT2,15,AT2)
CALL MCOlAS(A3,XN2,Q2,N2B,K,1,AT3,15,AT3)
CALL MCOlAS(A4,XN3,Q3,N3B,K,1,AT4,15,AT4)
CALL MCOlAS(A,XN1,U6,NSAMPL,K,1,AT1,15,AT1)
CALL MCOlAS(A,XN2,U7,NSAMPL,K,1,AT1,15,AT1)
CALL MCOlAS(A,XN3,U8,NSAMPL,K,1,AT1,15,AT1)
CALL MATNW(ROW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW2,A2,U13,1,N1,K,1,AT2,1)
CALL MATNW(RQW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW3,A3,U18,1,N2B,K,1,AT3,1)
CALL MATNW(ROW1,U11,U12,1,NSAMPL,K,1,AT1,1)
CALL MATNW(ROW4,A4,U23,1,N3B,K,1,AT4,1)
```

Table 8

```
C     ***so PROBABILITY SURFACE PROGRAMME FOR A•4 CATEGORY SITUATION
C     WRITTEN BY NEIL WRIGLEY. DEPT. OF GEOGRAPHY, UNIVERSITY OF BRISTOL

      COMMON/ONE/A(2561,15),A2(188,15),A3(188,15),A4(108,13),A1(150,15),N
     1SANPL.NI,N2,N3,N1A,N2A,N3A,N28,N3B,K,K1,KA2,K2

C     ***** READ IN IORDsHIGNEST SURFACE ORDER TO BE FITTED, 1,2,3, OR 4
C     NSAMPL■IUMBER OF SAMPLE LOCALITIES/ HI-HUMBER OF LOCALITIES WHERE
C     RESPONSE CATEGORY ONE IS RECORDED. N2B=NUMSER OF LOCALITIES WHERE
C     RESPONSE CATEGORY TWO IS RECORDED. NU-NUMBER OF LOCALITIES WHERE
C     RESPONSE CATEGORY THREE IS RECORDED
C     ↓*** DATA CARD: COL 1.10RD, COL 2.0LANK, COL 3-5=NSAMPL, COL 6.
C     BLANK, COL 7-9041. COL 18-BLANK, COL 11-130428, COL 14=BLANK, COL
C     15-17■143B
      READ(3.1) IORDoNSAMPL,N1.N2S.N3B
      FORMAT(11.1X.13.1X,13.1X,13.1X,13)

C1    ***4 READ IN VERT■LENGTH OF PROBABILITY SURFACE MAP REQUIRED IN
C     INCHES. YID-WIDTH IN INCHES, REFC=VALUE OF REFERENCE CONTOUR, CINT
C     -CONTOUR INTERVAL, UMAX,UMIN.MAXIMUM AND MINIMUM ALONG HORIZONTAL
C     AXIS. VMAX,VNIN.NAXIMUM AND MINIMUM ALONG VERTICAL AXIS .....
C     *** DATA CARD. COLS 1-7.VERT, COLS 8-14=WID, COLS 15-19=REFC,
C     COLS 20-24■CINT, COLS 25-31=UMAX, COLS 32-38=UMIN, COLS 39-45=VMAX
C     COLS 46-S2sVNIN .....
      READ(5. 18) VERT,WID,REFC,CINT,UMAX,UMIN,VMAX,VMIN
18    FORMAT (2F7. 4, 2F5. 3, 4F7. 4)
      HL.INT(VERT*8.61+8.5)
      NC0INT(VID*19.41+8.5)
      UAX■(UMAX-UMIN)/FLOAT(NC-1)
      VAX.(VMAX-VMIN)/FLOAT(HL-1)
      UAX■UAX+9.080001*UAX
      VAX.VAX+9.6180$01*VAX

C     sae. READ IN GEOGRAPHICAL CO-ORDI HATES OF EACH SAMPLE LOCALITY.
C     U(1)■HORIZONTAL CO-ORDINATE, V(I) -VERTICAL CO-ORDINATE. IN FORMAT
C     (F8.4,1X.F8.4) (N.B. IN THE PROGR ANNE THESE CO-ORDINATES ARE
C     STORED IN MATRIX A) s** ORDER OF CARDS-ALL SAMPLE LOCALITIES WHERE
C     RESPONSE CATEGORY ONE IS RECORDED BY ALL LOCALITIES
C     WHERE RESPONSE CATEGORY TWO IS RE CORDED, FOLLOWED BY ALL
C     LOCALITIES WHERE RESPONSE CATEGOR Y THREE IS RECORDED, FOLLOWED BY
C     ALL LOCALITIES WHERE REMAINING RE SPOHSE CATEGORY IS RECORDED *****
C     CREATE CONSTANT TERM *** PRINT SA NPLE LOCALITIES
      WRITE(6,11)
11    FORMAT('0      U           V')
      DO 3 I.1.NSAMPL
      A(I,1)01.9
      READ(5.4) A(I,2),A(I,3)
3     WRITE(6,44) (A(I,J),J1.2.3)
4     FORMAT(F8.4.1X.F13.4)
44    FORMAT(' '.2F9.4)

C     .... START OF MAIN LOOP .....■ ■ ■ I
      ID-8
      CALL SURF(ID.HL,NC,MAX,VAX,UMAX,UMIN,VMAX,VMIN,REFC,CINT)
      DO 7 In1,10RD
      ID■ID4.1
      CALL SURF(ID,ML.NC,UAX,VAX,UMAX,UMIN,VMAX,VMIN,REFC,CINT)
7     CONTINUE
      STOP
      END



      SUBROUTINE SURF(LORD,HL,MC,UAX,VAX,UMAX,UMIN,YMAX,VMIN,REFC,CINT)
      COMMON/ONE/A(238.15).A2(188,15),A3(180.15),A4(180,15).A1(150. 15),N
     ISAMPL.NI.N2.N3,NIA,N2A,N3A,1429,1431),K,KI,KA2,K2
      DOUBLE PRECISION 021,DBLE
      DOUBLE PRECISION X,F,G,STEP,ACC,W,FMINUS,STER,TSTAT
      DIMENSION C10(238),C11(250),C12(250),C13(258)
      DIMENSION PROB1(258),PROB2(250),PROB3(258),PROB4(258)
      DIMENSION X21(15,1),X22(15,1),X23(15,1),W(4321),WORK(45)
      DIMENSION CIZA(259,1),Q2B(258,1),Q2C(258,1),TSTAT(45),STER(45)
      DIMENSION X(45),G(45),PESTS1(45),PESTS2(45),PESTS3(45)

C     *** THIS IS THE MAIN PART OF THE PROGRAMME. IT CALCULATES THE
C     PARAMETER ESTIMATES OF THE PROBABILITY SURFACE MODEL USING MAXIMUM
C     LIKELIHOOD ESTIMATION. IT USES POWELL'S HYBRID STEEPEST DESCENT
```

```
C      AND GENERALISED NEWTON METHOD ***** ** ****** * ****** **** ***** ******
C
C      **** FOLLOWING ARBITRARILY SETS THE ITERATION INSTRUCTIONS *****
       MAXFUN■2800
       IPRINT■28
       IF(IORD.EQ.8) GO TO 9650
       BZ*FLOATOORD)
       821■DBLEO2*8.85)
       STEP.B21+0.83D8
       IFCIORD.EQ.1) ACC•8.24D8
       IF(IORD.E0.2) ACC-8.48D0
       IFOORD.E0.3) ACC-8.71D8
       IFOORD.E0.4) ACC■1.28D8
       GO TO 9651
 9658 STEP-8.86D0
       ACC-8.88D0
C
C      * ***** * CALCULATE NUMBER OF PARAMETERS * ***** ********************
 9651 K.(<10RD+1)*(10RD+2))/2
       N.K*3
       NIA-N1+1
       N2■N2B+N1
       N2A0112+1
       N3=N3B+N2
       N3A-N3+1
       K1-K+1
       KA2■1(*2
       K2.KA2+1
       KIZ■(1+1
       KIZA.1(2+1
       J81=0
       J91.0
       J9209
C
C      ****** GENERATE ARBITRARY INITIAL PARAMETER ESTIMATES ***********
       IFOORD.EQ.8) GO TO 9652
       X(1).1:8D8
       DO 2 I112,K
  2 X(I)-8.1D8
       X(1(1).1.11D0
       DO 783 IsKIZ,KA2
  783 X(I)•8.1D9
       X(K2)-1.0D8
       DO 704 I.KIZA,N
  784   X(1).8.1D0
       GO TO 9655
 9652 DO 9653 1.1,N
 9653 X(I)•0  1D0
       GO TO 9654
C
C              GENERATE POLYNOMIAL TERMS *******************************
 9655 IFOORD.EQ.1) GO TO 12
       KD=IORD-1
       KDA■((KD+1)*(KD+2))12
       KDB.KDA+1
       KE■IORD-2
       KEA.((KE+1)*(KE+2))12
       KE8■1(EA+1
       DO 15 J.KEB,KDA
       DO 14 I-1,NSAMPL
  14    A(1,1(D8).A(1,J)*A(1,2)
       KDB.KDB+1
  15    CONTINUE
       DO 16 1■1,NSAMPL
       A(1,1(D8).A(1,KDA)*A(1,3)
  16    CONTINUE
c 12    CONTINUE

C              CALCULATE PARAMETER ESTIMATES ****************************
 9654 DO 5 1.1,N1
       DO 5 J,1,K.
  5     A2(1,J).A(I,J)
       DO 6 I.N1A.N2
       J81.J81+1
       DO 6 J.1,1(
  6     A3(J81,J).A(I,J)
       DO 7 I-N2A,H3
       J91■J91+1
       DO 7 J.1,K
  7     A4(.191,J).A(I,J)
       DO 8 I.N3A,NSAMPL
       J92.J92+1
       DO 8 J.1,1(
  8     A1(J92,J)•A(I,J)
       IF(IORD.EQ.8) VRITE(6,9668)
 9660  FORMAT(      1X,'FOLLOING IS THE MAXIMIZED LOG LIKELIHOOD VALUE F
     1OR INTE RCEPT  ONLY MODEL')
       IF(IORD.E(I.8) GO TO 9661
       WRITE(6,6208) IORD
 6288  FORMAT(///////  ,1X,'PROBABILITY SURFACE MODEL OF ORDER ',II,' NOV
     IFITTED AND SURFACES DRAWN')
 9661  CONTINUE
       CALL VA86AD(N,X,F,G,STEP,ACC,MAXFUN,IPRINT,W)
       FNINUS■-1:8D8*F
       URITE(6,369) FNINUS
  369  FORMAT(//,1X,'MAXIMIZED LOG LIKELIHOOD VALUE    ',F12.5)
       IFOORD.EQ.0) RETURN
       N412■0,5*N*(14+1)
       NW13•N412+1
       NLESS•N-1
       N70■413
       N288.N413+NLESS
       DO 6881 K2884.1,14
       N71■11LESS-K2084
       STER(K2004)■DSQRT(W(N78))
       14 70.N280+1
 6891  N208.N70+1171
       WRITE(6,2808)
 2808  FORMAT(//,1X,'PARAMETER ESTIMATES STANDARD ERRORS PARAMETER EST
     1STANDARD ERROR')
       DO 2887 I.11,14
       TSTAT(1).X(1)/STER(1)
 2887  WRITE(6,2089) X(I),STER(I),TSTAT(I)
 2809  FORMAT(1X,F15.7:F18.7,F28.7)
       WRITE(6,6009)
 6889  FORMAT(//,1X,'VARIANCE-COVARIANCE MATRIX OF PARAMETER ESTIMATES')
 8881  FORMAT(  ,3X,'COLUMN',16,9111)
 8083  FORMAT(/,1X,'ROI'/)
 8882  FORMAT(     'ROW   ,I3,3X,18F11.5)
       IBEGIN.N413-1-44
       DO 7002 1•1,11,18
       ILESS1.1-1
       IEND.I+9
       IF(IEND.GT.N) IEND=N
       WRITE(6,8001)  (ICOL,ICOL.LIEND)
       WRITE(6, 8883)
       DO 7082 J.1,14
       MAX.J
       IF(MAX.GT.IEND) MAX-TEND
       IBASE■IBEGIN+J
       DO 7081 K17■1,MAX
       INDEX•I8ASE+K17*N-(K17*K17-K17)/2
       L.K17-ILESS1
 7881  PRO81(0.SNGL(4(INDEX))
       MAX•MAX-ILESS1
 7802  WRITE(6,8082) J,(PROB1(L),L=1,MAX)
       JZ2.0
       J23•8
       DO 630 I.1,K
  630 X21(1,1)=SNGL(X(1))
       DO 631 1.1(1,KA2
       JZ2■J22+1
  631   X22(JZ2,1).SNGL(X(I))
       DO 632 0(2,11
       JZ3.JZ3+1
  632   X23(.123,1) gSNGL(X(1))

C      s**** COMPUTE AND PRINT ESTIMATED PROBABILITIES AND RESIDUALS ***
       CALL MC0IAS(A,X21,4ZA,NSAMPL,K,1,258,15,250)
       CALL MC81AS(A,X22,OZBASAMPL,K,1,258,15,258)
       CALL MC01A8(A,X23,122C,NSAMPL,K,1,258,15,258)
       DO 633 101,NSAMPL
       RZA(111)■EXP(OZA(1,1))
       (1200,1)■EXP(OZO(1,1))
       OZCO,1).EXP(SZC(1,1))
       ZZ=1.0+0ZA(1,1)+82D(I,1)+OZC(I,1)
       PRO81(1)•02A(1,1)/22
       PRO82(1).0Z8(1,1)/ZZ
       PRO830).02C(1,1)/ZZ
  633  PRO84(1)01. 8/ZZ
       DO 8918 1.1.NSANPL
       IF(PRO81(1).EG.1.0) PRO81(1).8.9999999
       IF(PRO81(1).E4.8.8) PRO81(1)•0.8088881
       IF(PROB2(1).EO.1.8) PROB2(1).8.9999999
       IF(PRO82(1).E0.8.0) PRO82(1)■8.8880881
```

```
      IF<PRO83(1).EQ.1.8)  PRO83(I)=8.9999999
      IF(PROB3(1).EQ.8.8)  PRO83(1)=8.0080801
      IF(PRO84(1).EQ.1.0)  PRO84(1)=8.9999999
      IF(PROB4(1).EQ.8.8)  PR084(1)=0.0800801
      C18(I)=SQRT(PROB1(1)*(1.0—PRO81(1)))
      C11(1)=SQRT(PRO82(1)*(1.0—PRO82(I)))
      C12(1)=SQRT(PRO83(I)*(1.8—PRO83(I)))
      C13(1)=SORT(PROB4(I)*(1.0—PROB4(I)))
8918  CONTINUE
      WRITE(6,8981)
8901  FORMAT(///,IXo'FOR EACH SAMPLE LOCALITY'''PREDICTED PROBABILITES
     1                  RAW RESIDUALS                                STANDARD!
     ISED RESIDUALS')
      IIRITE(6,8938)
8938  FORMATO,IX,'RSP CAT1 RSP CAT2 RSP CAT3 RSP CAT4 RSP CATI RSP
     1 CAT2 RSP CAT3 RSP CAT4 RSP CAT1 RSP CAT2 REP CAT3 REP CAT4'
     I)
      DO 8928 I=1,N1
      RAVR1=(1.0—PROB/(I))
      RAWR2■—PROB2<I)
      RAWR3=—PROB3(I)
      RABR4=—PROB4(I)
      RES10RAWR1/C18(I)
      RES2=RAUR2/C11<1)
      RES3=RAWR3/C12(1)
      RES4=RAUR4/C13(I)
8928  BRITE(6.8902)  PRO81(I)/PRO82(I),PRO83(I),PR084(I),RAWRI,RAWR2,RAUR
     13,RAVR4,RES1,RES2,RES3oRES4
      DO 8921 1=N1A/N2
      RABR1■—PROBI(I)
      RAgR2=(1.0—PROB2(I))
      RAUR3=—PROB3(1)
      RAVR4=—PRO84(I)
      RESI=RAIIR1/C100)
      RES2=RAVR2/C11(I)
      RES3=RAWR3/C12(1)
      RES■RAVR4/C13(I)
8921  BRITE(6.8982)  PRO81(I),PRO820),PRO83(I),PRO84(I),RAWRI,RAWR2,RAUR
     13,RAVR4,RES1,RES2,RES3,RES4
      DO 8922 I=N2A,N3
      RAMR1=—PROBI(I)
      RABR2■—PROB2(I)
      RAWR3=0.8—PRO83(1))
      RAM114■—PRO84(I)
      RESI=RAVRI/C180)
      RES2=RAWR2/C11(1)
      RES3■RABR3/C12(1)
      RES■RAVR4/C13(1)
8922  WRITE(6,8902)  PRO81(I)/PRO82(I),PRO83(I),PRO84(I),RAWRI/RAWR2,RAWR
     13,11AVR4,RESI,RES2,RES3IRES4
      DO 8923 I=N3A.NSAMPL
      RA611210—PROBI(I)
      RAVR2=—PROB2(1)
      RAVR3=—PRO83(I)
      RAUR4=(1.8—PROB4(1))
      RESI=RABRI/C18(1)
      RES2■RAVR2/C11<1)
      RES3=RAVR3/C12(I)
      RES4■RAVR4/C13(1)
8923  BRITE(6,8982)  PRO81(1).PRO82(I),PRO83(I),PRO84(I),RAWRI,RAWR2oRAWR
     13,RAWR4,RESI,RES2,RES3,RES4
8982  FORMAT(",12(F8.502X))
      DO 243 1=1,1(
      PESTS1(I)=X21(I,1)
      PESTS2(!)=X22(1,1)
243   PESTS3(1)=X23(1,1)
      CALL PMAP(NL,NC.PESTSI/PESTS2/PESTS3,WORK.REFC,CINT,UAX,YAX/N,IORD
     1,VMAX,UMIN,UMAX,VMIN)
      RET URN
      END
```

```
      SUBROUTINE CALCFG(N,X,F,G)
      DOUBLE PRECISION X,G,U12,1113,1118,U23,F,DBLE
      COMMON/ONE/A(258,15),A2(188,15),A3(188,15),A4(180,15),A1(158,15),N
     1SAMPL,N1A2oN3,NIA,N2AsH3A,N28,N38,K,K1,KA2,K2
      DIMENSION X(45),G(45),Q1(188,1),(12(180,1),(13(188,1)
      DIMENSION KNI(15,1),XN2(15,1),XN3(15,1)
      DIMENSION U6(258,1),U7(250,1),U8(258,1),U9(250,1)
      DIMENSION R001(1,258),ROV2(1o108),ROW3(1,180),ROG4(1,100)
      DIMENSION U11(258.15),U12(1,15),U13(1,15) UI8(1 15) U23(1 15)
      J2=8
      J3=8
      DO 66 I=1,K
66    XN10.1)PSNOL(X(1))
      DO 67 I=K1.102
      J2=42+1
67    012(J2.1)=SNDL(X(I))
      DO 68 I=K2,N
      J3=J3+1
68    XN303,1)=X(I)
      U1=8.8
      U2=8.8
      U3=8. 8
      Z1=8.8
      CALL MCOIAS(A2,XN1,01,N1,K11,188, 15)188)
      CALL MC01AS(A3/XN2,02,N28,K,1,180,15,100)
      CALL MC8IAS(A4.KN3,1113,N3B,K,1, 188,15,180)
      DO 169 I=1,N1
169   U1=U14.01(1,1)
      DO 70 1=1,N28
78    020U2+02(1,1)
      DO 71 I=1,1438
71    U3=113+03(1.1)
      Z=U1+112+U3
      CALL MCOIAS(A)XN1.116.NSAMPL.K,I.258.15.258)
      DO 87 I"I.NSAMPL
87    U60.1)=EXP(U6</o1))
      CALL MC81ASCAAN2,U7,NSAMPL,K,1,258$15,258)
      DO 88 I 21INSAMPL
88    U7(1,1)=EXP(U70,1))
      CALL MCOIAS(A,XN3oU8,NSAMPL,K,1,258/15.258)
      DO 89 I=1,NSAMPL
89    U8(I/1)=EXP(U80,1))
      DO 98 I=1,NSAMPL
      U9M1)0U6<I,1)+U7(1,1)+08(I,1)
98    U9(I,1)=1.0+U9(1,1)
      DO 91 I=1.NSAMPL
91    21=21+ALOG(U9(1,1))
      FA=-1.8*(2-21)
      F=DBLE(FA)
C     ***** —F IS THE LOG LIKELIHOOD VALUE ****************************
CC
C     *** CALCULATE 1ST DERIVATIVES OF LOG LIKELIHOOD FUNCTION *** *****
      DO 44 I=1,NSAMPL
44    ROW1(1,I)=1.0
      DO 45 I=1,N1
45    ROV2(1,I)=1.8
      DO 46 I=1,N28
46    R0113<1,1)=1.8
      DO 47 I=1,1438
47    R0114(1,1)=1.0
      DO 94 I=1,NSAMPL
94    U6(1,1)0U60/1)/U9(1,1)
      DO 92 J01,K
      DO 92 I=1,NSAMPL
92    U11(1,41)=A(1,J)*U6(I,1)
      CALL MATWROVI.U11,U12,1,NSAMPL,K,1,250,1)
      CALL MATNIII(ROW2.A2,013,1,N1,K,1,100,1)
      DO 93 J=1/K
93    U13<1.0=U13(1,J)—U12(1,J)
      DO 95 I=1.NSAMPL
95    U70,1)=U7(1,1)/U9(I,1)
      DO 96 J=1,K
      DO 96 11aNSMPL
96    U11(I,J)=A<I, J)*U7(1,1)
      CALL MATNV(ROW/,011,U12,1,NSAMPL,K,1,258,1)
      CALL NATNU(R0113,A3,018,1,N2BaK,1, 180,1)
      DO 97 J=1*K
97    U18(1,J)=U18(1,J)—U12(1,J)
      DO 98 I1,NSAMPL
98    U8(1,1)=U8(1,/)/U9(1,1)
      DO 99 J=1,K
      DO 99 I=1,NSAMPL
99    U11<I,J)=A(I,J)*U8(1,1)
      CALL MATNUROW1,1111,U12,1,NSAMPL,K,1,258,1)
      CALL MATNB(ROW4,A4,023,1,N38,K,I, 180,1)
      DO 108  J  1,K
188   U23(1,0 =023(1,J)—U12(1,J)
      DO 101 I=1,K
101   G(I)=U13(1,I)
      DO 102 I=1,K
      J4=I4K
```

```
182   G(J4).U18(1,1)
      DO 183 1=1,K
      J5.14KA2
183   G(J5).U23(1,I)
      DO 184 I.1,N
184   C(I)=-G(I)
C     **** G 16 THE VECTOR OF 1ST DERIVATIVES .....................
      RET  N
      END UR
```

```
      SUBROUTINE PMAP(NLAC,PESTS1,PESTS2,PESTS3,WORK REFC CINT UAX VAX
     IN,IORD,VMAX,UMIN,UMAX MIN)
      DIMENSION PESTS1(N),PESTS2(N),PESTS3(N)
      DIMENSION VORK(N),SLINE(128),SYMB(23)
      DATA SYMB/IN1,1H.11H2,1H.,1H311N.,1H411N.  1H5 1H./1 i\ 1H.  1H 6,1 H.
     1110,1N.,11111,111. IN9 11 1H8 1H1 1N /
1     FORMAT('1        PROBABILITY SURFACE OF ORDER ',I8/' PART',I4//)
2     FORMAT(' ',128A1)
      DO 66 J2=1,4
      KMAX.8
      KMIN.28
      NO20118
      1STR■IC/118
      LEFT.NC-118*NSTR
      IF(LEFT.GT.8) NSIR=NSTR41
      DO 96 KOUNT.1,NSIR
      IF(KOUNT.EQ.NSTR.AND.LEFT.GT .8) NO2.LEFT
      WRITE(6,1) IORD,KOUNT
      NO22010242
      WRITE(6,2) (SYMB(23)/1.1,NO22)
      V.VMAX4VAX
      DO 12 1.01,NL
      V=V-VAX
      U.UMIN-UAX4(KOUNT-1).118*UAX
      DO 6 1.1,NO2
      U=U+UAX
      PR.PROB(PESTSI/PESTS2,PESTS3 WORK N IORD U V J2)
      KCC■1141NT((PR-REFC)/CINT)
      IF(PR.LT.REFC) KCC.KCC-1
      IF(KCC.LT.1) KCC=1
      IF(KCC.GT.28) KCC.28
      IF(KCC.GT.KMAX) KMAX=KCC
      IF(KCC.LT.KMIN) KMIN=KCC
6     SLINE(I)=SYMB(KCC)
12    WRITE(6,2) SYMB(22),(SLINE(1)/1=1,NO2),SYMB(22)
      WRITE(6,2) (SYMB(23),I=1,14022)
96    CONTINUE
      WRITE(6,4) REFC,CINT
4     FORMAT('8     REFERENCE CONTOUR = ',F11.4/'      CONTOUR INTERVAL
     1',F12.4)
      WRITE(6, 3)
3     FORMAT('8 KEY TO CONTOUR VALUES''')
      DO 5 1.KMIN.KMAX
      J.11-I
      P■REFC-J4CINT
      Q.P4CINT
      IF(I.EQ.1) GO TO 2
      IF(I.EQ.28) GO TO 8
      WRITE(6,9) (SYMB(I),J=1,6),P,Q
      CO TO 5
2     WRITE(6,19) (SYMB(I),J=1,6)/P
18    FORMAT(",6A1r2X/F18.4,'AND BELOW')
      GO TO 5
8     WRITE(6,11) (SYMB(1),J=1,6),P
11    FORMAT("s6A1,2X,F18.4,'AND ABOVE')
9     FORMAT(",6A1,2X,F18.4,' TO ',F18.4)
5     CONTINUE
      WRITE(6,13) UMIN,VMAX,UMAX,VMAX,UMIN VMIN UMAX/VMIN
13    FORMAT('e COORDINATES OF MAP CORNERS ARE:' '
     15X,' TOP LEFT's5X/2F12.4
     15X,' TOP RIGHT     ',2F12.4'
     15X,' BOTTOM LEFT   ',2F12.4'
     15X,' BOTTOM RIGHT ',2F12.4)
66    CONTINUE
      RET URN
      END
```

```
      FUNCTION PRO8(PESTS1,PESTS2,PESTS3,WORK,N,NORD,U,V,J2)
C     *** COMPUTES VALUE ON PROBABILITY SURFACE AT EACH POINT *********
      DIMENSION PESTS1(N),PESTS2(N),PESTS3(N),WORK(N)
      02/A=PESTS1(1)4(PESTS1(2)*U)4(PESTS1(3)*V)
      021B.PESTS2(1)4(PESTS2(2)*U)4(PESTS2(3)*V)
      021C.PESTS3(1)4(PESTS3(2)*(1)4(PESTS3(3)4 0)
      022M.EXP(02IA)
      QZ28=EXP(QZ1B)
      QZ2C=EXP(021C)
      22.1.841222A+022B+0220
      IF(JZ.EQ.2) GO TO 8
      IF(JZ.EQ.3) GO TO 9
      IF(JZ.EQ.4) GO TO 98
      PRO13.0224/22
      GO TO 18
8     FR08=0228/22
      CO T 1e
9     PROB=0 Q22C/ZZ
      GO TO 18
98    PROB1.8/22
10    CONTINUE
      IF(NORD.LT.2) RETURN
      WORK(2)=U
      WORK(3).V
      DO 1 M.2,NORD
      L1=M-1
      L2=11*(M41)/2
      DO 2 I=1,M
      L2=L2+1
      NW2138.L2-M
      WORK(L2)=WORK(NW280)*U
      021A=021A+PESTS1(L2)*WORK(L2)
      0218=02184PESTS2(L2)*WORK(L2)
2     021C.Q21C+PESTS3(L2)*WORK<L2)
      NW281.1241
      NW282.1-2-M
      WORK(NW281)=WORK(NW282)*V
      021A=Q21A4PESTS1(NW281)*WORK(NW201)
      02113=122184PESTS2(NW281)*WORK(NW201)
      021C.021C+PESTS3(NW281)*WORK(NW201)
      022A=EXP(021A)
      022B.EXP(1121B)
      022C.EXP(021C)
      22.1.84822A+61228+0Z2C
      IF(JZ.EQ.2) GO TO 4
      IF(JZ.EQ.3) GO TO 5
      IF(JZ.EQ.4) GO TO 99
      PRO8...QUA/2Z
      GO TO 1
4     PROB=02213/22
      GO T 1
S     PROBO 022C/22
      GO TO 1
99    PRO8.1.8/22
      CONTINUE
      RETURN
      END
```

APPENDIX 3 Derivation of the standard errors and variance-covariance matrix of parameter estimates

When the method of maximum likelihood is used to compute the parameter estimates, the asymptotic variance-covariance matrix is given by the inverse of the so called 'information matrix', $\underline{I}(\underline{\beta})$, (see Edwards, 1972; Cox, 1970, p.87) where

$$\underline{I}(\underline{\beta}) = -E\left[\frac{\partial^2 \log_e \Lambda}{\partial \underline{\beta} \partial \underline{\beta}'}\right]$$

and is consistently estimated by $\underline{I}(\hat{\underline{\beta}})$. $\underline{\beta}$ in this case is a vector of parameters, e.g. $\underline{\beta}' = [\alpha, \beta_1, \beta_2 \ldots]$. The programs listed in Tables 6, 7 and 8 print both the asymptotic variance-covariance matrix of parameter estimates and the asymptotic standard errors found by taking square roots of the diagonal of $\underline{I}^{-1}(\hat{\underline{\beta}})$.

Table 9

```
      SUBROUTINE VA86AD(N.X.F.C/STEP/ACC/MAXFUNIIPRINT.W)
      DOUBLE PRECISION ACCLACC/DSS.STEP/X.F.G.GSW,GGDIAG,NDIAG/W,DGSDIS
     1GDD.SUM.DSQ.C.GGGG/CD,CAICC.THETA,S.DC.DCA/WOMFA/SDN.CHDISEC/DND
     I.HDIV/CD.CE
      DIMENSION X(1)/G(1)/W(1)
      THE NEXT SEVEN INTEGERS PARTITION THE ARRAY
       DD.N*H+N
       N■IDD/2
       XA.IDD+N*N
       GA=IXA+N
       WA.ISA+N
       W8.19A+N
       WC■IWB+N
C     SET SONE CONSTANTS
      ACCT=ACC*ACC
      1PP■IPRINT*IPRINT
C     GIVE INITIAL VALUES TO SOME VARIABLES
      DSS*STEP*STEP
      MAXC.I
      ITSPEC=1
      IPTEST.1
C     CALCULATE THE INITIAL GRADIENT
      CALL CALCFG (N.X.F.G)
C     GIVE INITIAL VALUES TO THE COMPONENTS OF GC/ H AND DD
      GS0=9,D8
      DO 1 1.1,N
    1 CSQ*CSQ+C(1)**2
      IF (GSW) 5.5,2
    2 GGDIAG.8.81118*DSORT(GSQ) ' STEP
      HDIAG=1.1118/GGDIAG
      K.0
      KDD■IDD
      DO 4 1.1,N
      J.1
  181 IF (J-1) 192,183.183
  182 KDD.KDD+1
      W(KDD).9.88
      J=J+1
      GO TO 181
  183 K
      KDD.KDD+1
      W(K)*GGDIAG
      NW/.IH+K
      W(NW1)=NDIAG
      V(KDD)=1.D8
    3 J*J+I
      IF (J-N) 184,194,4
  184 K=K+1
      KDD=KDD+I
      V(K)=8.D8
      NV2.IH+K
      W(NW2).8.D8
      W(K10)=8.D8
      GO TO 3
    4 CONTINUE
    5 IF OPP) 18,18/6
    6 PRINT 7
    7 FORMAT(///:IX.'THE FOLLOWING OUTPUT IS PROVIDED BY VA86AD')
      GO TO 18
C     BEGIN AN ITERATION BY TESTING FOR CONVERGENCE
    8 GSQ.9.D0
      DO 9 1.1,N
    9 GSW=GSQ+C(1)**2
   18 IF (GSQ-ACCT) 11.11,18
C     PRINT THE FINAL VALUES OF THE FUNCTION AND GRADIENT
   11 IF (IPP) 17.17,12
   12 PRINT 13,MAXC,F
   13 FORMAT(/5WAFTER'.14.' CALLS OF CALCFG, THE FINAL F .'t
     11114.6)
      PRINT 14.(X(I)/1.1,N)
   14 FORMAT(5X.'X ='.(81114 6))
      IF (IPRINT) 17.17/15
   15 PRINT 16/(C(1).1.1tH)
   16 FORMAT(5X.'G ....(8D14 6))
   17 RETURN
C     TEST WHETHER MAXFUN CALLS OF CALCFG HAVE BEEN MADE
   18 IF (MAXC-MAXFUN) 21.19/19
   19 PRINT 28oMAXC
```

```
   20 FORMAT(/ 5X,'VA86AD HAS MADE',I5,' CALLS OF CALCFG')
      GO TO 1 1
C     PRINT THE CURRENT BEST VALUE OF F ETC
   21 IPTEST=IPTEST-IABSCIPRINT)
      IF (IPTEST) 22,22,25
   22 IPTEST=IPP
      PRINT 23,MAXC,F
   23 FORMAT(/5X,'AT THE START OF ITERATION',I4,5X,'F =',014.6)
      PRINT 14,(X(I),I=1,N)
      IF (IPRINT) 25,25,24
   24 PRINT 16.(G(I),I=1,N)
C     TEST WHETHER A SPECIAL ITERATION IS NEEDED, AND CALCULATE
C     THE CHANGE IN GRADIENT ALONG THE DIRECTION OF
C     A SPECIAL ITERATION
   25 ITSPEC=ITSPEC-1
      IF(ITSPEC)26,32,32
   26 DGGD=0.D0
      SGDD=0.D0
      KDD=IDD
      DO 28 I=1,N
      SUM=0.D8
      K=I
      KD=IDD
      J=1
  105 IF (J-I) 186,107,107
  186 KD=KD+1
      SUM=SUM+V(K)*W(KD)
      K=K+N-J
      J=J+1
      GO TO 185
  107 DO 27 J=I,N
      KD=KD+1
      SUM=SUM+W(K)*W(KD)
   27 K=K+1
      KDD=KDD+1
      SGDD=SGDD+G(I)*W(KDD)
   28 DGGD=DGGD+SUM*SUM
C     CALCULATE THE CORRECTION FOR A SPECIAL ITERATION
C     AND REVISE THE ARRAY DD
      DSQ=DMIN1(DSS,GSQ/DGGD)
      C=DSIGH<DSORT(DS12),-SGDD)
      DO 29 I=1,N
      NW3=I+IDD
      NW4=1+IWA
      N1,15=1+1WB
      W(NW4)=C*14(NW3)
   29 W(NW5)=4(NW3)
      KDD=IDD
      DO 30 I=2,N
      DO 38 J=1,N
      KDD=KDD+1
      NW6=KDD+H
   30 W(KDD)=W(NW6)
      DO 31 I=1,N
      KDD=1(00+1
      NW7=I+IWB
   31 W<KDD)=11(14W7)
      ITSPEC=2
      GO TO 51
C     CALCULATE THE GENERALIZED NEWTON CORRECTION TO X
C     AND PREDICT THE CURVATURE OF F ALONG THE GRADIENT
   32 GGGG=8.D0
      DO 34 I=1,N
      NW8=I+IWA
      W(NW8)=0.D0
      SUM=8. D0
      J=1
      K=I
  108 IF <J-I) 189,110,118
  109 NW9=IH+K
      W(NW8)=W(NW8)-W<NW9)*G(J)
      SUM=SUM+W(K)*G(J)
      K=K+N-J
      J=J+1
      CO TO 188
  110 DO 33 J=I,N
      NW11=1H+K
      W(NW8)=W(NW8)-W(NW11)*G(J)
      SUM=SUM+W(K)*G(J)
   33 K=K+1
   34 GGGG=GGGG+SUM*G<I)
```

```
C     TEST WHETHER TO SET THE CORRECTION TO A MULTIPLE OF
C     THE GRADIENT
      IF (GGGG*DABS(GGGG)*DSS-GSQ**3) 35.35,37
C     SET THE CORRECTION VECTOR TO A MULTIPLE OF THE GRADIENT
   35 C=-DSORT(DSS/GSO)
      DO 36 I=1,N
      NW12=I+IWA
   36 W(NW12)=C*G(I)
      GO TO 41
C     SET THE OPTIMAL STEEPEST DESCENT CORRECTION IN WB
C     AND THE DIFFERENCE BETWEEN WA AND W8 IN WC
   37 C=-GSO/GGGG
      CB=0.D8
      DO 38 I=1,N
      NW13=I+IWB
      NW14=I+IWA
      NW15=I+IWC
      W(NW13)=C*G(I)
      W(NW15)=W(NW14)-W<NW13)
   38 CB=CB+W(HU15)**2
      IF (CB) 35,35,85
C     CALCULATE THE SCALAR PRODUCT (-W.GW)
   85 CA=8.D8
      DO 98 I=1,N
      CC=8. D8
      J=1
      K=I
   86 IF (J-I) 87,88,88
   87 NW16=J+IWC
      CC=CC+W(K)*W(NV16)
      K=K+N-J
      J=J+1
      GO TO 86
   88 DO 89 J=I,N
      NW17=J+IWC
      CC=CC+W(K)*W(NW17)
   89 K=K+1
      NW18=I+IWC
   90 CA=CA-CC*V(NW18)
C     INTERPOLATE FOR THE CORRECTION VECTOR ON THE LINE WA - W8
      CA=C*CA
      C=DSS-C*C*GSO
      THETA=DSIGN<C/(DABS(CA)+DSORT(CA*CA+C*C8)),CA)
C     TEST WHETHER TO USE THE GENERALIZED NEWTON CORRECTION
      IF (THETA-1.08) 39,41,41
   39 DO 48 I=1,N
      NW19=1+IWA
      NW28=I+IWB
      NW21=I+IWC
   48 W(NW19)=W(NW28)+THETA*W(NW21)
c     EXPRESS THE CORRECTION VECTOR IN TERMS OF THE ROWS OF DD
   41 D50=8.08
      KDD=IDD
      DO 42 I=1,N
      NW22=I+IWA
      NW23=I+IWB
      NW24=1+IWC
      DSO=DSO+W(NW22)**2
      W(NW23)=0.D0
      U(NW24)=0.D0
      DO 42 J=1,N
      KDD=KDD+1
      NW26=IWA+J
   42 W(NW23)=W(NW23)+W(KDD)*W(NW26)
c     REVISE THE DIRECTIONS IN THE ARRAY DD
      S=0.D0
      KK=N
   43 NW27=KK+1W8
      IF (1,1(H1427)) 45,44,45
   44 KK=KK-1
      GO TO 43
   45 KK=KK-1
      IF (KK) 48,48,46
   46 NW28=1618+KK+1
      S=S+W(NW28)**2
      NW29=IWB+KK
      C=DSORT(S*(S+W(NW29)**2))
      CA=S/C
      CB=W(NW29)/C
      KDD=IDD+N*KK
      DO 47 J=1,N
```

```
      KDD=KDD+1
      NW38=J+IWC
      NW31=IWB+KK+1
      W(NW38)=1,1(NW38)+W(N1431)*W(KDD)
      NW32=KDD-H
 47   W(KDD)=CA*W(HW32)-C8*W(NW30)
      GO TO 45
   48 KDD=IDD
      DO 49 I=2,14
      DO 49 J=1,14
      KDD=KDD+1
      NW33=KDD+N
 49   W(KDD)=W(NW33)
      C=1.D8/DSORT(DSQ)
      DO 58 I1,14
      .KDD=KDD+1
      NW34=1+IWA
 58   W(KDD)=C*W(NW34)
C     APPLY THE CORRECTION VECTOR AND CHECK WHETHER
C     ROUND OFF MAKES THE CORRECTION ZERO
   51 DSQ=0.DO
      DO 52 I=1,N
      NW35=1+IXA
      NW36=I+IWA
      W(NW35)=X(I)+W(NW36)
      W(NW36)=W(NW35)-X(I)
   52 DSQ=DSQ+W(NW36)**2
      IF (DSQ) 80,80,82
   88 PRINT 81
   81 FORMAT ('SX,'ERROR EXIT FROM VA$36AD')
      GO TO 11
C     CALCULATE THE NEXT VALUE OF THE OBJECTIVE FUNCTION
   82 MAXC=MAXC+1
C     NOTE THAT THE NEXT INSTRUCTION IS NOT STANDARD FORTRAN
      NWI08=IXA+1
      NW101=1GA+1
      CALL CALCFG(N,W(NW100),FA,W(NW101))
C     SET THE ERROR OF THE PREDICTED GRADIENT IN WB
C     ALSO CALCULATE SOME NUMBERS FOR REVISING THE STEP-BOUND
      DG=0.DO
      DGA.O.D0
      DGGD=13.D8
      WBSQ=0.DO
      DO 54 I=1,N
      SUM=0.DO
      J=1
      K=1
  111 IF (J-I) 112,113,113
  112 NW37=J+IWA
      SUM=SUM+W(K)*W(NW37)
      K=K+N-J
      J=J+1
      GO TO III
  113 DO 53 J=I,N
      NW38=J+1WA
      SUM=SUM+W(K)*W(NW38)
   53 K=K+1
      NW39=I+IWB
      NW40=I+IGA
      NW41=I+IWA
      W(NW39)=W(NW48)-G(1)-SUM
      DG=DG+G(I)*W(NW41)
      DGA=DGA+W(14440)*W(NW41)
      DGGD=DGGD+SUM*W(NW41)
 54   WBSQ=WBSQ+W(NW39)**2
      IF (ITSPEC-2) 55,68,60
C     CHECK WHETHER ROUND OFF ERRORS ARE SERIOUS
   55 C=DG+.51118*DGGD
      IF (C) 83,80,80
   83 CA=F+C
      CB=CA-F
      IF((C8-,5D0*C)*(CB-1.5D8*C))84,80,80
C     TEST WHETHER TO DECREASE THE STEP BOUND
   84 IF(FA-F-1D8*C)57,57,56
   56 DSS=0.25D0*DSO
      GO TO 60
C     TEST WHETHER TO INCREASE THE STEP-BOUND
   57 DSS=DSQ
      IF (WBSQ-0.25D0*GSQ) 59,59,58
   58 IF (DG-DGA-DGA) 68,59,59
   59 DSS=4.D0*DSO
```

```
C     SET THE DIFFERENCE BETWEEN GRADIENTS
   68 DO 61 I=1,N
      NW42=I+1WC
      NW43=I+IGA
   61 W<N1142)=W(N1143)-G(I)
C     SET X, F AND G TO THE BEST CALCULATED VALUES
      ITHETA=1
      IF (F-FA) 64,64,62
   62 F=FA
      DO 63 I=1,N
      NW44=1+IXA
      NW45=1+IGA
      X(I)=D(NW44)
 63   G(I)=W(NW45)
C     CALCULATE SOME VECTORS AND SCALAR PRODUCTS TO
C     REVISE GG AND H
   64 SDK=8.D8
      GHD=8.D8
      SEG=8.88
      DHD=0.D8
      DO 66 I=1,N
      NW46=1+IXA
      NW47=1+IWA
      NW4B=I+IGA
      W(111146)=-W<HD47)
      W(NW48)=8.D8
      K=IN+I
      J■1
  114 IF (J-I) 115,116,116
  115 NW50=J+IWC
      NW52=J+IWA
      W(NW46)=W(NW46)+W(K)*W<NW58)
      W(H11411)=W(NW413)+W(K)*W<N1452)
      K=K+H-J
      J=J+1
      GO TO 114
  116 DO 65 J=1,N
      NW54=J+IWC
      NW56=J+IWA
      W(NW46)=11(N1146)+W(K)*W<NV54)
      W(NW48)=W(NW413)+W(K)=W<NW56)
   65 K=K+1
      N1'158=1+110
      NW59=I+IWC
      SDM=SDPI+W(NW47)*W<N1158)
      GHD=GH8+W(146159)*W(NW48)
      SEG=SEG+W(NW59)011(H146)
 66   DND=DHD+W(NW47)*W(ND48)
C     TEST WHETHER THE USUAL CORRECTION TO GG GIVES
C     NEAR SINGULARITY
      HDISI=SEG*DND-GHD*GHD
      GO TO (67,70),ITHETA
   67 IF (DABS(HDIV)-8.1DO*DSQ*DSQ) 68,78,78
C     CHANGE THE DIFFERENCE IN GRADIENTS TO AVOID SINGULARITY
   68 CA=1011//(DSQ*DSQ)+0.1D0
      CB=GHD/DSQ-8.1811
      CA=CA/(CA+CB+DSIGN(DSORT(0.9D8*CA+CB*C8) , CA+CB))
      C13=(1.D0-CA)*SDM/DSQ
      DO 69 I=1,N
      NW68■I+IWA
      N1161=1+1118
      NW62=I+IWC
      C=CA*(CB*W(N6168)-D(NW61))
      W(NW61)=111(11W61)+C
 69   W(NW62)=W(NW62)+C
      ITHETA=2
      GO TO 64
C     REVISE THE MATRICES GG AND H
   78 CA=1.80/DSQ
      CB=SDM*CAsCA
      CC=DHD/HDIV
      CD=GHD/HD1 4
      CE=SEG/HD1 1
      K=0
      DO 71 I=1,N
      DO 71 J=I,H
      K=K+1
      NW63=I+IWA
      NW64=J+1110
      N6165=J+IWA
      NW66=1+IWB
      NW67=K+TH
```

```
      Nii68=1.1.1XA
      N1,169=J+IXA
      NW7B=I+IGA
      N1117l=J+IGA
      W(K)=16(K)+CA*(41(N11163)*W(NW64)+W(NU65)*W(NW66))-CB*W(NW63)*W(NW65)
71    W(NW67)=111041167)-CC041(NW68)*W(NW69)-CE*W(NW7B)*W(N6171)+CD*(W<NW68)*
     1W(NU71)+111(NW69)=41(Nil78))
      CO TO 8
      END




      SUBROUTINE MCBIAS<A,B,C,L,M,N,IDA,IDB,IDC)
      DOUBLE PRECISION DA,DB,SUM.DBLE
      DIMENSION A(IDA,IDB),B(IDB,N),C(IDC,N)
      L1=L
      M1=1.1
      N1=N
      DO 1 1=1,1.1
      DO 1 J=1,141
      SUM=8.8DO
      DO 2 K=1,111
      DA=DBLE(A<I,K))
      DB=DBLE(B<K,J))
2     SUM=SUM*DA*DB
1     C(1,J)=SNGLCSUM)
      RETURN
      END




      SUBROUTINE MATN11(/1, 42,V3,1VI,IY2,IV3,IY4,IV5,1V6)
      DOUBLE PRECISION DY1,DY2,Y3,VSUM,DBLE
      DIMENSION Y1(1Y4,1 /5),Y2(1Y5,1V3),V3(1Y6,1V3)
      LY1=IYI
      MY1=IY2
      NY1=IV3
      DO 1 I=1,LVI
      DO 1 J=1,NV1
      VSUM=9.888
      DO 2 10.1,MY1
      DYI=DBLE(V1(I,K))
      DY2=DBLE<Y2(K,J))
2     YSUM=VSUM+DV1*DV2
1     Y3(I, J)=VSUM
      RETURN
      END
```