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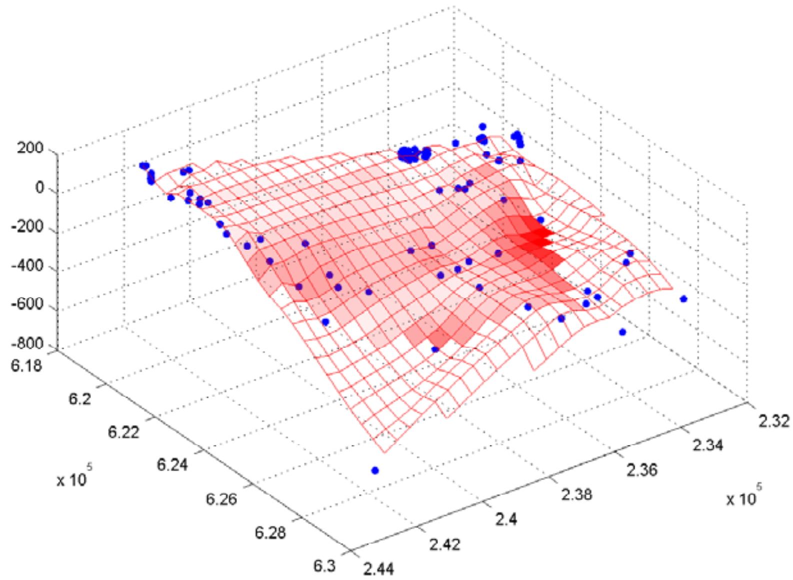
Approaches to the Measurement of Uncertainty in Geoscience Data Modelling

Digital Geoscience Spatial Model

Internal Report IR/02/068



BRITISH GEOLOGICAL SURVEY

INTERNAL REPORT IR/02/068

Approaches to the Measurement of Uncertainty in Geoscience Data Modelling

M R Cave, B Wood

Key words

Uncertainty; geoscience; modelling.

Front cover

Predicted uncertainty expressed as red transparency value and mapped to interpolated surface obtained by gridding of Ayr Hard Coal Seam borehole data.

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Summary

Broadly speaking, geoscientific investigations involve observations or measurements of the natural environment and, through modelling and interpretation, produce an understanding of the objects within the geosphere and the natural processes governing it. The absolute value of the measurements arising from the modelling and interpretation are critically important but equal importance must be given to the confidence that can be placed upon the measurement in terms of how closely it mimicks reality. The aims of this study are to review current methodologies for measurement of uncertainty, to make recommendations for a practical approach to uncertainty measurement within the BGS and to give some practical examples of how this might be achieved.

The major sources of uncertainty in geoscience were found to be:

- Variability - the inherent natural variability that exists in geological objects and processes that exists independently of geoscientist's investigations;
- Measurement uncertainty - the uncertainty arising from imperfections in the measurement procedure;
- Sampling uncertainty - arising from the process of making a measurement at a specific spatial location and takes account of whether the measurement is truly representative of the area/volume being sampled;
- Modelling Uncertainty - the uncertainty at this interpretive stage is a combination of the uncertainties of all of the input parameters and the uncertainty introduced through the data interpretation itself.

The methods used for estimating uncertainty were found to fall into three broad categories:

- The analytical approach - this uses rigorous statistical theory to propagate combined uncertainties through the mathematical functions that use the measured inputs to produce the modelled output.
- Computationally intensive approaches - this procedure requires that the model is calculated a number of times, each time a small change is made to the input parameters (representative of the natural uncertainty of that parameter). The result of each run of the model is stored and, with the use of suitable strategies for the choice input parameter changes, the distribution of results for the repetitions will be representative of the uncertainty in the model.
- Measurement of uncertainty on subjective and semi-quantitative data. - in geoscience applications there are many examples where semi-quantitative data is an important input parameter for modelling. Geological interpretation is a good example of subjective information. Borehole logs and geological maps produced by different geologists will be different according to their experience and background, data from these sources is then digitised and can end up as an input to a solid geology model.

Examples of applying selected measurement uncertainty strategies to three different geoscience data models have been presented. These are:

i) Bootstrap resampling of synthetic borehole data

ii) Bootstrap resampling of coal-field borehole data

iii) Bootstrap resampling on a geostatistical interpretation of G-base arsenic data

From the literature review and the modelling examples a philosophy and strategy for the measurement of uncertainty in BGS geoscience data modelling has been proposed:

- Equal importance should be given to the measurement of uncertainty as is given to the final model.
- It is critical to have a multidisciplinary team with expert representatives from each stage of the modelling project providing information on the uncertainty of each step of the process and to ensure that that emphasis is placed on obtaining good uncertainty estimates for those inputs that critically affect the model outcome.
- There should be a defined mechanism for all geoscience modelling projects that allows all sources of uncertainty within the project to be recorded in a formalised manner. A suitable tool for this is the use of cause and effect diagrams.
- Geoscience data models include both quantitative and subjective/semi-quantitative inputs and outputs. The authors suggest that bootstrap-resampling and fuzzy logic approaches respectively are suitable methods for producing robust estimates of uncertainty on these two types of data.
- The final estimate of uncertainty on any model must include contributions from all of the significant sources of uncertainty identified by the cause and effect diagram of the project.

1 Introduction

In geoscience, the practice of generating models from data is becoming increasingly common. By model we refer generally to any value-added output representing a possible reality that can be produced from raw data which gives us a picture of the general nature of a feature or property; for example a key geological surface, or the distribution of geochemical measurements across an area. Broadly speaking, geoscientific investigations involve the making of observations or measurements of the natural environment and, through modelling and interpretation, produce an understanding of the objects within the geosphere and the natural processes governing it. The absolute value of the measurements arising from the modelling and interpretation are critically important but equal importance must be given to the confidence that can be placed upon the measurement as being representative of natural reality. This confidence is usually expressed as an uncertainty that is defined as (ISO, 1993) "A parameter associated with the result of a measurement, that characterises the dispersion of the values that could reasonably be attributed to the measurand". This is not to be confused with the term 'error' that is defined as the difference between an individual result and the true value of the measurand. As such, error is a single value and, because the true value is usually unknown in geoscience applications, the error cannot be calculated. Uncertainty, however, takes the form of a range, and if estimated for a particular measurement procedure may be applied to all future measurements using the same procedure.

The aims of this study are to review current methodologies for measurement of uncertainty, to make recommendations for a practical approach to uncertainty measurement within the BGS and to give some practical examples of how this might be achieved.

2 Sources of Uncertainty in Geoscience

A review of uncertainty in geology (Mann, 1993) suggested that there are four main categories.

2.1 VARIABILITY

The inherent natural variability that exists in geological objects and processes that exists independently of geoscientist's investigations. The degree of variability varies from low, for homogenous objects, to high in heterogeneous objects. The variability can also be divided into structured (e.g. regular transitions of features in time or space or cyclic structures or events) and unstructured features. Some authors treat variability as a specific component of uncertainty (Carrington and Bolger, 1998) and others (Paustenbach et al., 1992) advise that variability and uncertainty should be distinguished as separate entities. As already stated uncertainty represents a lack of knowledge about factors affecting a specific measurement, whereas variability arises from true heterogeneity in geological objects and processes. Random or systematic error can lead to inaccurate or biased estimates, whereas variability can affect the precision of the estimates and the degree to which they can be generalised.

2.2 MEASUREMENT UNCERTAINTY

The measurement uncertainty arises from imperfections in the measurement procedure. Depending on the type of measurement being made a wide variety factors can contribute to the overall uncertainty and have been discussed in detail for analytical chemistry in a number of texts (e.g. Day and Underwood, 1991; Eurachem, 1995) and in geochemistry, mineralogy and in environmental science (Ferson et al., 1999).

2.3 SAMPLING UNCERTAINTY

The sampling uncertainty that arises from the process of making a measurement at a specific spatial location and takes account of whether the measurement is truly representative of the area/volume being sampled. This source of uncertainty encompasses the natural variability uncertainty discussed in point 1 and will be the limiting factor. Recent literature (Abt et al., 1999; Alden et al., 1997; Benedetti and Palma, 1995; Hyland et al., 1998; Lee and Ramsey, 2001; Longpre et al., 1997; Okx and Stein, 2000; Ramsey, 1997; Ramsey, 1998; Ramsey and Argyraki, 1997; Ramsey et al., 1995; Ramsey et al., 2001; Ramsey et al., 1999; Rathbun, 1998; Smith et al., 1996; Squire et al., 1999; Squire et al., 2000; Strobel et al., 2000; van Groenigen, 2000; van Groenigen et al., 2000a; van Groenigen et al., 2000b; van Groenigen et al., 1999; van Groenigen and Stein, 1998; Winkels and Stein, 1997) discusses many ways of measuring sampling uncertainty and optimising the sampling procedure to minimise uncertainty

The sampling strategies can be based on a number of different sampling point selection algorithms that include:

1. Standard grid based sampling schemes.
2. Probabilistic sampling design.
3. Use of decision trees.
4. Use of geostatistical type spatial methods; optimal sampling distances based on spatial variability, variograms, semi-variograms, kriging, best linear unbiased estimator.
5. Optimisation using simulated annealing taking sample constraints and preliminary information into account.

2.4 UNCERTAINTY DERIVED FROM MODELLING

The modelling and interpretation of the data is usually the final stage of an investigation, using inputs from a number of sources (e.g. borehole records, geophysical data, hydrological data, geochemical data, engineering geology data) all of which have their own associated uncertainties. These data are the inputs to the final interpretation, which may be carried out by expert evaluation or by the use a geoscience computer modelling package (e.g. EarthVision, Vulcan, FracMan) or a combination of both. The uncertainty in this final interpretation is a combination of the uncertainties of all of the input parameters and the uncertainty introduced through the data interpretation.

The petroleum industry uses a variety of models for describing oil/gas field reservoirs where the uncertainty in the model can have a huge financial implication. Recent publications in this area (Ballin et al., 1992; Floris et al., 2001; Hegstad and Omre, 2001; Lecour et al., 2001; Massonnat, 2000; Mishra et al., 2002; Ouenes, 2000; Panigrahi and Mujumdar, 2000; Salas and Shin, 1999; Wakefield et al., 2001; Zhang et al., 2000; Zheng et al., 2000) illustrate the importance of quantifying uncertainty in geoscience modelling. Other workers (Carroll and Warwick, 2001; Christiaens and Feyen, 2001; Davis and Keller, 1997; Goovaerts, 2001; Goovaerts, 2002; Heuvelink and Webster, 2001; Journel, 1996; Lee and Ramsey, 2001; Meinrath and Nitzsche, 2000; Pfingsten et al., 2001; Phillips and Marks, 1996; Robins et al., 2000; Rossel et al., 2001; Tattari and Barlund, 2001; Wiehn et al., 1996) in a diversity of applications, have used a wide variety of techniques including Monte Carlo simulations, Fuzzy logic, stochastic, empirical and Bayesian statistics to measure geoscience modelling uncertainty.

3 Measurement of Uncertainty

An idealised flow chart for the determination of uncertainty in a modelling scenario is shown in Figure 1.

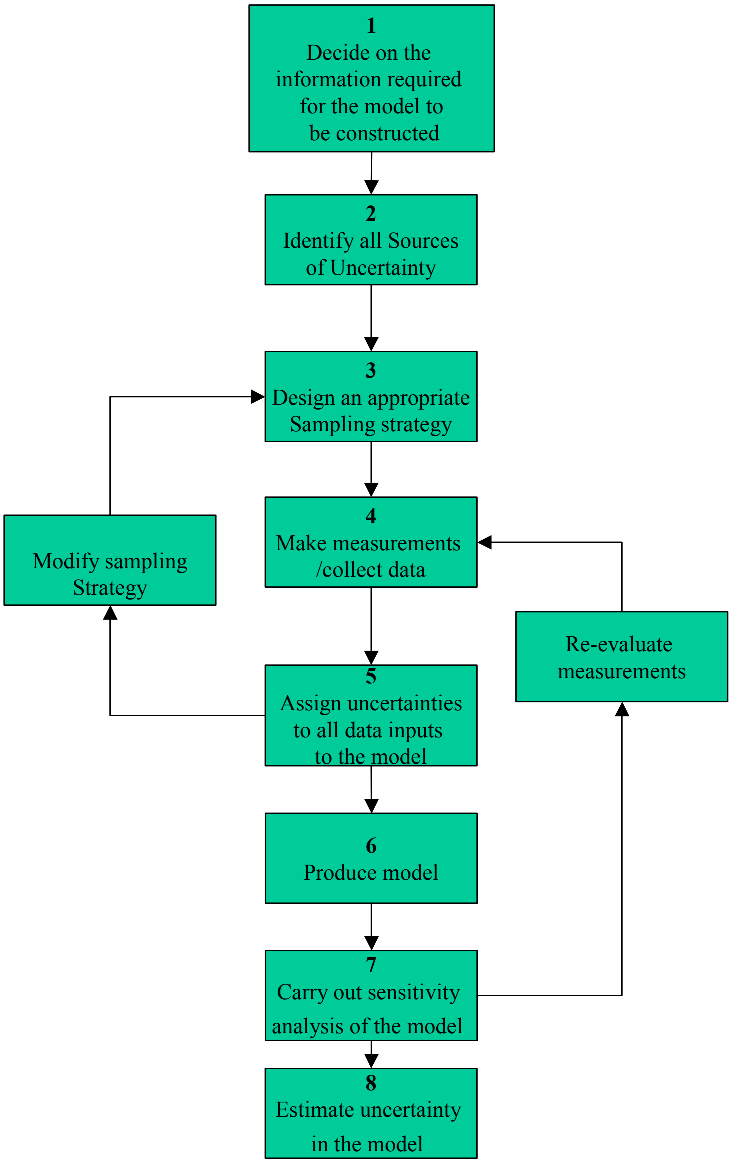

Figure 1 Flow chart for measurement of uncertainty

The first task is to decide what information is required to formulate the final model (Stage 1 Figure 1). Stage 2 of the process (Figure 1), is possibly the most important step in ensuring that the final measured uncertainty is representative of the whole information gathering and modelling process. The final modelling of the data is usually carried out by those familiar with the modelling process but not necessarily fully conversant with the preceding stages in which all of the inputs to the model are obtained. The final model can, therefore, be completed without a full appreciation of all the possible sources of error in the data being used. It is therefore critical to have a multidisciplinary team with expert representatives from each stage of the investigation. The team can provide information on the uncertainty on each step of the process and ensure that emphasis is placed on obtaining good uncertainty estimates for those inputs that critically affect the model outcome. A formalised method for cataloguing all the sources of uncertainty is discussed in Section 4.1.

Under ideal conditions, the design of the sampling procedure (stage 3 Figure 1) also provides a key role in allowing the correct density and replication of measurements to be made allowing sampling uncertainty to be minimised (Section 2.3) and measurement errors to be quantified (Section 2.2). In many situations, however, physical difficulties and monetary constraints can severely curtail the sampling that can be carried out or, in some cases, no sampling strategy can be designed, as the modelling has to be based on existing data.

Once measurements have been made and data has been collected (stages 3 and 4 in Figure1) the uncertainties identified in stage 2 can be assigned to all of data inputs to the model. Methods for assigning the uncertainty are discussed in Sections 3.1, 3.2 and 4. At this stage it may become evident that there is not enough information to measure the uncertainty or that the uncertainty is too high and, given enough resources, additional sampling should be carried out and supplementary measurements made to rectify any problems.

When the data gathering has been completed, the quality of the data has been deemed 'fit for purpose' and all the associated errors have been calculated, preliminary modelling can take place (stage 5). The sensitivity of the model to the input parameters should be assessed. In most cases this information will already be known and it should be the responsibility of the modeller to relay this information to the stage 2 consultation (Figure 1). However, if stage 7 is reached and particular critical inputs are found to have unacceptably high or poorly characterised uncertainties, then additional measurements may need to be made.

The last stage (stage 8 Figure 1) is to produce the final model and combine all the uncertainty analysis of the inputs with additional uncertainties introduced by the modelling to obtain an overall uncertainty for the final interpretation. Methods for producing a combined overall uncertainty on the model outcome are discussed in more detail in Sections 3.1 to 3.3 and methods found in the literature are referred to in section 2.4.

3.1 ANALYTICAL APPROACHES

The analytical approach to measurement of uncertainty uses rigorous statistical theory to propagate combined uncertainties through the mathematical functions that use the measured inputs to produce the modelled output. To give a very simplistic example, assume that there are two measured inputs to a model, **a** and **b,** that have uncertainties of $\mathbf{u_a}$ and $\mathbf{u_b}$ respectively. If **a** and **b** are added together to produce an output **c** then the uncertainty ($\mathbf{u_c}$) on c is given by:

$$u_c = \sqrt{{u_a}^2 + {u_b}^2}$$

Equation 1

and if **a** and **b** are multiplied together to give **c** then the combined uncertainty is given by:

$$u_c = c\sqrt{\frac{u_a}{a} + \frac{u_b}{b}}$$

Equation 2

This is relatively straightforward for mathematical expressions where additions and multiplications are involved, however, most of the mathematics behind geoscience data modelling has a higher degree of complexity and, in these cases, more general expressions for combined uncertainty must be used. The general relationship between the combined standard uncertainty $u_c(y)$ of a value y and the uncertainty of the independent parameters $x_1, x_2, x_3, \ldots x_n$ on which it depends is:

$$u_c(y(x_1, x_2, \ldots)) = \sqrt{\sum_{i=1,n} c_i^2 u(x_i)^2} = \sqrt{\sum_{i=1,n} u(y, x_i)^2}$$

Equation 3

Where $y(x_1,x_2,\ldots)$ is a function of several parameters x_1, x_2, x_3 .., c_i is a sensitivity coefficient evaluated as $c_i = \partial y / \partial x_i$, the partial differential of y with respect to x_i and $u(y,x_i)$ denotes the uncertainty in y arising from the uncertainty in x_i.

Where variables are not independent, then the relationship is more complex:

$$u_c(y(x_{i,j}, \ldots)) = \sqrt{\sum_{i=1,n} c_i^2 u(x_i)^2 + \sum_{\substack{i,k=1,n \\ i \neq k}} c_i c_k \cdot u(x_i, x_k)}$$

Equation 4

Where $u(x_i,x_k)$ is the covariance between x_i and x_k and c_i and c_k are the sensitivity coefficients as described.

Clearly this type of calculation can be very complicated where a large number of complex expressions need to be evaluated. Methods for implementation of equation 4 in a spreadsheet have been described (Kragten, 1994). Equation 4, however, is only applicable under certain conditions. Non-normality, non-linearity correlation and other nuisance factors (Meinrath, 2000) can render the analytical approach impracticable.

3.1.1 Stochastic Response Surface Methods

Stochastic Response Surface Modelling (SRSM) is a generalised form of the analytical approach. Conceptually, the propagation of input uncertainty through a model using SRSM is accomplished as follows:

i) input uncertainties are expressed in terms of a set of random variables;

ii) a functional form is assumed for selected outputs or output metrics;

iii) the parameters of the functional approximation are determined.

SRSMs are founded on the principle that random variables with well-behaved (square-integrable) PDFs can be represented as functions of a set of independent random variables. The above integribility requirement is sometimes but not always satisfied in geoscience, so these methods can be applied in certain situations (Cooper et al., 1996; GomezHernandez and Wen, 1998; Goovaerts, 2001; Lecour et al., 2001; Rood et al., 2001; Zhang et al., 2000). Random variables with standard distributions (e.g. normal and gamma) are often chosen to represent input uncertainties due to the mathematical tractability of functions of these random variables often referred to as Standard Random Variables (srvs). Once the inputs are expressed as functions of the chosen srvs, the output metrics can also be represented as functions of the same set of srvs. The disadvantage to this approach is the need to assume that the input variables either follow or are a close approximation to standard distribution functions, which is not always the case.

3.1.2 Geostatistics

Geostatistics is a special case of stochastic modelling, used widely in geoscience as way of describing the spatial continuity that is an essential feature of many natural phenomena (Isaaks and Srivastava, 1989). The most widely used tools of geostatistics have been presented in a variety of good introductions (e.g. (Isaaks and Srivastava, 1989)) and only a brief outline of the methodology is presented here.

The principal tool of most geostatistical analyses is the variogram, a function that relates half the average squared difference between paired data values to the distance (and direction, where anisotropy is considered) by which they are separated. A mathematical model may be fitted to the variogram and the coefficients of the model may be used to assign optimal weights for interpolation using the technique of kriging. Kriging is a form of weighted average estimator. The weights are assigned on the basis of the form of a model fitted to a function, such as the variogram, which represents spatial variability in the property of interest. Ordinary Kriging (OK) is probably the most widely used variant of kriging. A by-product of OK is the OK variance (or standard error), a measure of confidence in estimates. It is a function of the form of spatial variability of the data (modelled, for example, by the variogram) and the spatial configuration of the observations. The OK variance serves as a measure of confidence in estimates although, since it is independent of the data values, its practical value is frequently severely limited unless the data are segmented into sub-sets within which the spatial variability is similar. For a given sampling configuration, the OK variance will be the same irrespective of the data values locally. If data are measured on a regular grid, the maximum OK variance will be identical for a given location; however, much of the data values vary locally (Goovaerts, 1997). The utility of conventional variograms and ordinary kriging for geostatistical analysis is limited by particular assumptions. The principal problems concern (i) normality and (ii) the independence of the estimation variance on data values. The Indicator Kriging (IK) approach is one means of overcoming both of these limitations. The indicator approach involves the designation of several thresholds, for example the deciles of the sample cumulative distribution (Goovaerts, 1997) that are used to transform the data to a set of binary variables. With IK, a least-squares estimate of the cumulative distribution function (cdf) is made at each cut-off. The cdf is constructed by putting together the IK estimates for each cut-off.

There is considerable work describing developments in the geostatistical approach to measurement of uncertainty which cannot be comprehensively covered within the scope of this report. Some recent examples of applications include (Barabas et al., 2001; Carlon et al., 2001; Goovaerts, 1998; Goovaerts, 2001; Goovaerts, 2002; Lloyd and Atkinson, 2001; Nicholson and Mather, 1996; Phillips and Marks, 1996; Rossel et al., 2001; Van Meirvenne and Goovaerts, 2001).

3.2 COMPUTER INTENSIVE METHODS

The analytical methods described above usually require a detailed mathematical knowledge of the modelling processes to allow the propagation of error through each stage. One method of overcoming problems of finding exact mathematical solutions for estimating uncertainty in complex geoscience models, where statistical theory is not available, is by computationally intensive approaches. This procedure requires that the model is calculated a number of times, each time a small change is made to the input parameters (representative of the natural uncertainty of that parameter). The result of each run of the model is stored and, with the use of suitable strategies for the choice input parameter changes, the distribution of results for the repetitions will be representative of the uncertainty in the model. The advantage of this approach is that the model can be considered a ‘black-box’ since the result is not dependant on any assumptions of the mathematics of the model and there are no constraints on the uncertainty data being normally distributed. There are a number of ways of implementing this type of approach.

3.2.1 Monte Carlo methods and Latin Hypercube Sampling

In this methodology each input parameter is assigned a probability density function (PDF) that describes the natural variability of each parameter. Each parameter PDF is sampled randomly and the model output is calculated. This process is repeated a large number of times (e.g.1000-10000) each with a new random sampling of the input parameter PDF's. The range of results from the model then forms the PDF for the modelled data. If there are a large number of input parameters for a complex model this may require very expensive computing resources to complete the task in a satisfactory manner. One way of significantly reducing the number of iterations without losing information is to use Latin Hypercube Sampling (LHS)(Iman and Helton, 1988; Iman and Helton, 1991; McKay et al., 1979; Meinrath et al., 2000). In the LHS method, the range of probable values for each uncertain input parameter (PDF) is divided into M segments of equal probability. Thus, the whole parameter space, consisting of N parameters, is partitioned into M^N cells, each having equal probability. For example, for the case of 3 parameters and 4 segments, the parameter space is divided into 4x4x4 cells. The next step is to choose M cells from the M^N cells. First, a random sample is generated, and its cell number is calculated. The cell number indicates the segment number the sample belongs to, with respect to each of the parameters. For example, a cell number (2,1,2) indicates that the sample lies in the segment 2 with respect to first parameter, segment 1 with respect to second parameter, and segment 2 with respect to third parameter. At each successive step, a random sample is generated, and is accepted only if it does not agree with any previous sample on any of the segment numbers. The advantage of this approach is that the random samples are generated from all the ranges of possible values, thus giving insight into the tails of the probability distributions. Further, for every M samples, each parameter is sampled from each of its M subranges.

The disadvantage to this approach is that the PDF for the input parameters must be known. In many cases there is likely to be a lack of knowledge of these PDFs in which case standard PDFs (e.g. normal, lognormal), which approximate to the natural variation are used. Other potential problems have also recently been highlighted with regard to Monte Carlo modelling in risk assessment (Ferson, 1996).

3.2.2 Jackknife and Crossvalidation

In contrast to Monte Carlo methods, where additional data in the form of estimated variation in the original data is used to recalculate the model, the jackknife procedure (Iman and Helton, 1988; Iman and Helton, 1991; McKay et al., 1979; Meinrath et al., 2000) generates resampled data by omission. The resampling is carried out by using the *n* original measured data sets as an adequate representation of the true but unknown distribution function. The properties of this distribution function are explored by creating sub-samples from the *n* data sets. In the jackknife approach, eliminating each object in turn from the data sets produces *n* sub samples. Then in an analogous way to the Monte Carlo approach the modelling is carried out for each of the sub-sets of data and the variation in the model output for each modelling scenario and the variation in results is used to construct the PDF for the model. Since the jackknife does not require the uncertainty in the input parameters to follow a certain distribution function, the jackknife is a representative of non-parametric statistics.

If there are many experimental data points the jackknife may be abbreviated by randomly choosing j ($j<n$) data sets that are successively omitted. This procedure can also be referred to as Cross Validation although this terminology is usually used when the prediction properties of a model are being assessed. The jackknife often works well, provided that the output under study does not change drastically with small changes in the data.

There is one great advantage of the full jackknife approach; for each data point omitted a modelled prediction can be calculated and comparisons between the modelled data at the omitted point can be compared to the actual data. This allows actual and estimated uncertainties to be compared and therefore the ability of the procedure to measure uncertainty can be monitored.

3.2.3 Bootstrap sampling

The bootstrap (Davison and Hinkley, 1997; Efron, 1979; Efron and Tibshirani, 1993; Wehrens et al., 2000; Young, 1994) is a Monte Carlo style resampling method. Unlike the jackknife procedure, which creates sub-samples of the data in a predictable way, the bootstrap uses a random sampling method. In this approach the process of sampling is mimicked by picking another sample at random from a hypothetical population of interest, usually based on data from your sample. For example, when resampling 10 points from a data set of 10 values, all 10 values are kept available when selecting each of the re-sampled points. It is as if all 10 values have been written on individual slips of paper and put into a hat. To resample 10 points, one slip at random is selected from the hat and recorded. The slip is then replaced in the hat and the process is repeated until there are 10 values recorded. This means that some of the original data values might appear more than once on the tally sheet; others might not appear at all. This process is repeated a number of times (typically 500 to 1000) and statistics are calculated using a combination of the different outcomes.

An important advantage of the bootstrap, as with the jackknife, is that it is a non-parametric method and it does not matter if the original sample is well behaved or not because it forms its own PDF in the process of resampling. Examples of the use of bootstrap resampling in geoscience modelling are not as widespread as Monte Carlo methods but its use has been reported (Meinrath and Nitzsche, 2000).

3.3 SUBJECTIVE AND SEMI-QUANTITATIVE MEASUREMENTS

The discussion so far has been confined to defining an uncertainty associated with a measured quantitative parameter that is either used as an input to a model or is the final output of the model. In geoscience applications, however, there are many examples where semi-quantitative data is an important input parameter for modelling. Geological interpretation is a good example of subjective information. Borehole logs and geological maps produced by different geologists will be different according to their experience and background, data from these sources is then digitised and can end up as an input to a solid geology model. In some instances these differences may be small but in others they can be significant and have a profound effect on the final model. The question then arises as to which interpretation of the data was correct and how can the uncertainty on the interpretations be calculated so that it encompasses the subjective interpretation process. One approach is to minimise differences in interpretation between geologists by good training and the use of quality assurance and quality control procedures. Nevertheless, formal methodologies for describing the uncertainties in this type of parameter are required.

3.3.1 Fuzzy Logic

Zadeh (1965) introduced fuzzy logic as a methodology for the description of imprecise or vague information. In this methodology, vague linguistic descriptions of parameters (e.g. the use of the terms ‘high’ ‘low’ ‘very long’ or ‘quite short’ describing length) can be incorporated into a mathematical model to give a numerical result and an associated uncertainty. This is achieved by defining fuzzy sets that do not have crisp clear boundaries and can contain elements with only a partial degree of membership. Consider a simple example, illustrated in Figure 2, in which the set of tall people is considered. The membership function illustrated at the top of Figure 2 is a sharp edged membership function such that people are either tall (tall people have a membership value (μ) of 1 and short people have a value of 0) whereas the bottom membership function in Figure 2 is more representative of the real world such that there is a continuous membership function that takes into account the all the subjective interpretations of how tall a person is from μ= 0 to 1. Using this approach and its associated mathematics, fuzzy logic has been used extensively to estimate uncertainty in geoscience data modelling in a wide range of applications of which recent examples include (Bubnicki, 2001a; Bubnicki, 2001b; Cooper et al., 1996; Ouenes, 2000; Ozelkan and Duckstein, 2001; Panigrahi and Mujumdar, 2000; Scherm, 2000; Schulz and Huwe, 1997; Schulz et al., 1999; Torri et al., 1997; Wadia-Fascetti and Gunes, 2000; Wakefield et al., 2001; Wiehn et al., 1996; Zhang and Stuart, 2001; Zhang and Tumay, 1999; Zhu, 1997). Fuzzy logic has also been used in geostatistics, where kriging of imprecise data from fuzzy variograms has been described (Bardossy et al., 1990a; Bardossy et al., 1990b).

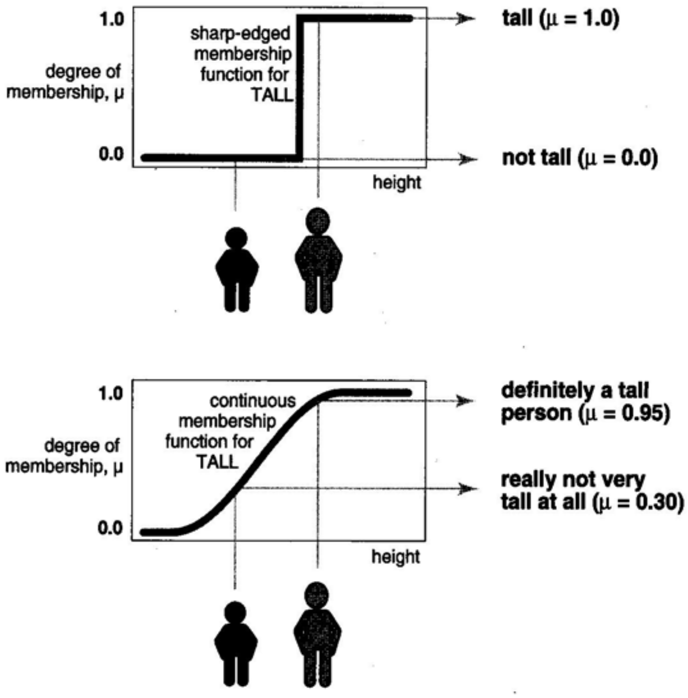

Figure 2 Illustration of a the difference between a crisp (two value) membership function (top) and a fuzzy membership function (bottom)

3.3.2 Bayesian Statistics

Bayesian statistics is used widely in modelling applications to deal with 'soft data' (e.g. probability characteristics, physical laws and experience).

Bayes' theorem can be summarised as follows:

Suppose A is an event and $\{B_1, B_2, \quad B_i, \quad B_n\}$ is a partition of a sample space . If probability $P(A)>0$, then the conditional probability of B_j given that A has occurred ($P(B_j|A)$), is given by:

$$P(B_j \mid A) = \frac{P(B_j)P(A \mid B_j)}{\sum_{i=1}^{n} P(B_i)P(A \mid B)}$$

Equation 5

To give a simple example, suppose four bags are equally likely to be sampled. Number 1 contains one white and two red balls; number 2 has three white and 1 red; number 3 has one white and four red; and number 4 has one white and five red. The probability $P(B_i)$ of a bag being sampled is ¼ ; and if A is the draw of the white ball, $P(A|B_i)$ equals $^1/_3$, ¾, $^1/_5$, and $^1/_6$, respectively for each bag. According to Bayes Theorem the probability $P(B_3|A)$ that a white ball will come from bag number 3 is

$$P(B_3) = \frac{\frac{1}{4}\cdot\frac{1}{5}}{\frac{1}{4}\cdot\frac{1}{3}+\frac{1}{4}\cdot\frac{3}{4}+\frac{1}{4}\cdot\frac{1}{5}+\frac{1}{4}\cdot\frac{1}{6}} = \frac{12}{87}$$

Equation 6

Bayes' theorem can also be formulated in terms of PDFs of unknown parameters of a distribution. According to the Bayesian view, all quantities are of two kinds; those known to the person making the inference and those unknown to such a person. The former situation is described by their known values, the uncertainty surrounding the latter being described by a joint PDF. The statistical model admits a distribution of the random variable x for a parameter θ. When x has a PDF or likelihood function f(x|θ), and g(θ) is the prior PDF of θ, the posterior PDF of θ, g(x|θ), is

$$g(\theta \mid x) = \frac{f(x \mid \theta) g(\theta)}{\int_\theta f(x \mid \theta) g(\theta) d\theta}$$

Equation 7

Both θ and x may be vectors.

The ability of the Bayesian model to incorporate prior PDF's into the stochastic model allows 'soft ' data (e.g. the experience of a geologist) to be incorporated into the final uncertainty calculation. There are a number of ways in which Bayesian statistics has been applied to modelling uncertainty.

3.3.2.1 Bayesian Model Averaging (BMA)

This technique is designed to help account for the uncertainty inherent in the model selection process. By averaging over many different competing models, BMA incorporates model uncertainty into conclusions about parameters and prediction. BMA has been applied successfully to many statistical model classes including linear regression, generalized linear models, Cox regression models, and discrete graphical models, in all cases improving predictive performance. The technique has obvious application to geoscience modelling although there are relatively few examples (Lamon and Clyde, 2000).

3.3.2.2 The Bayesian Maximum Entropy (BME)

This method of spatial analysis and mapping provides definite rules for incorporating prior information as well as hard and soft data into the mapping process. It has certain unique features that allow it to include plausible reasoning under conditions of uncertainty. BME is a general approach that does not make any assumptions regarding the linearity of the estimator, the normality of the underlying probability laws, or the homogeneity of the spatial distribution. The method is used in place of kriging in geostatistical applications and it has been suggested (Christakos and Li, 1998) that it is far superior to the more traditional kriging approach. Recent examples of its use include (Christakos and Li, 1998; Christakos and Serre, 2000a; Christakos and Serre, 2000b; D'Or et al., 2001; Hristopulos and Christakos, 2001; Serre and Christakos, 1999).

3.3.2.3 Bayesian Statistics used in combination with other methods

Bayesian statistics has also been used successfully in combination with some of the other methodologies used in Section 3 of this report (Chatterjee et al., 1994; Copty and Findikakis, 2000; Ellison et al., 1998; Gouveia and Scales, 1998; Hegstad and Omre, 2001; Sohn et al., 2000).

4 A Practical Approach to Uncertainty Measurement

This review of methods for measurement of uncertainty, whilst not pretending to be fully comprehensive, has shown that there are a wide variety of techniques available and there is a large body of active research currently being carried out. Within the BGS the estimation of uncertainty as a part of the modelling process has not been fully formalised. At this initial stage it is necessary to ensure that an uncertainty estimation procedure should try to ensure that all sources of uncertainty are considered and, where they make significant contribution, be taken into account in the final uncertainty estimate. The methodology adopted for carrying this out should be simple (i.e. capable of being carried out without having to have an in depth knowledge of the mathematics and statistics) and robust (i.e. be able to handle non-normally distributed data). A suggested methodology that satisfies these criteria is discussed in Section 4.1 and in the case studies (Section 4.2).

This consists of two stages:

i) a formal methodology to identify all sources of uncertainty.

ii) the use of resampling methods (e.g. bootstrap resampling) to propagate the uncertainty estimation through the modelling process.

Whether this approach is fully practicable to BGS requirement requires further discussion with end users. It is inevitable that a single procedure will not be practicable in all cases but the method suggested here provides a starting place for the development of a BGS protocol that can be built on and modified in the future.

4.1 SOURCES OF UNCERTAINTY – CAUSE AND EFFECT DIAGRAM

Logically, the first step in being able to quantify uncertainty is to identify the causes of uncertainty themselves and consider their relationships. Certain simple techniques for assessing the sources of error or uncertainty in a system have long been used in sectors such as the manufacturing industry by managers trying to understand quality issues. These methods are not necessarily quantitative, nor do they have a statistical basis; rather they are useful tools for understanding and visualising the causality between different steps in some process. This process might traditionally be the manufacture of a product (Kindlarski, 1984), but it is possible to think of the geological modelling process in a similar way.

One method that can be applied is the construction of a cause and effect diagram, otherwise known as the Ishikawa diagram (after the inventor Kaoru Ishikawa) and as the fishbone diagram (Kindlarski, 1984). The concept is simple and begins with the identification of a specific problem resulting from a complex process. In our case this might be 'lack of certainty in sub-surface 3D models' resulting from the modelling process. From this end effect the major categories to which causes might belong are identified. Within each category a series of sub-causes that contribute may be identified and thus built upon in a hierarchical manner. In this way the problem can be explored to greater and greater depth as required. During this process, the cause and effect diagram is developed which documents and visualises the problem; essentially a horizontal 'backbone' arrow represents the effect and branches off this backbone arrow represent the causes of error or uncertainty, which contribute to the effect. These branches in turn have branches of their own and so on, covering smaller and smaller sub-causes.

Generally the construction of such a diagram may be the result of a brainstorming session or a collaborative effort between project workers who each have their own idea of what the uncertainties in their work are and their relative magnitude. In assessing smaller problems the task may be carried out by one or two team members working on a specific area. The usefulness of this approach is not that is places a value on the uncertainty of a geoscientific model but that:

- It forces the project members to think laterally about the uncertainties that may be inherent in their area of work;
- It brings to the attention of all team members the sources of inaccuracy that are inherited from areas of the modelling process other than their own;
- It demonstrates how various factors can interact or influence one-another. The approach allows the individual to understand the complexity of a particular process and the causality that exists between different factors in the modelling.

This is useful because it combats the treatment of a particular stage of the process as being wholly ‘black-box’ and hence readily accepted as being accurate. By providing qualitative uncertainty metadata at each stage of the modelling in a way that is easy to understand, the recipient of some processed material becomes aware that it may be flawed in certain ways, and thus have a 'knock-on' effect. The relative value of the overall uncertainty is thus propagated throughout the entire modelling process and is not ignored at each new stage. Also, the processor of any data or models has a duty to consider what uncertainties they themselves are introducing into the system and should document them in a similar way.

As a relevant case study, an example of constructing a basic cause and effect diagram for assessing the uncertainties in modelling a 3-D surface from limited point depth data is outlined here:

- Firstly, the effect that is being investigated is identified; this effect is essentially the end problem we are trying to resolve or quantify. This is written on the far right of the diagram, and a backbone arrow is drawn pointing towards it;
- Next we consider what are the large-scale causes of uncertainty in the modelling process. These causes are broad classifications identifying the main areas of a process whose uncertainties may contribute to a particular problem. The causes can then be built up hierarchically by investigating the sub-causes. Once they have been identified they are included in the diagram using more arrows which converge upon the backbone arrow thus representing contributing factors (Figure 3);
- Having identified the large scale classifications of causes the process is then iterated for each one to explore the problem to greater levels of detail. Figure 4 demonstrates how this is achieved by adding more arrows that represent sub-causes feeding into the larger ones;

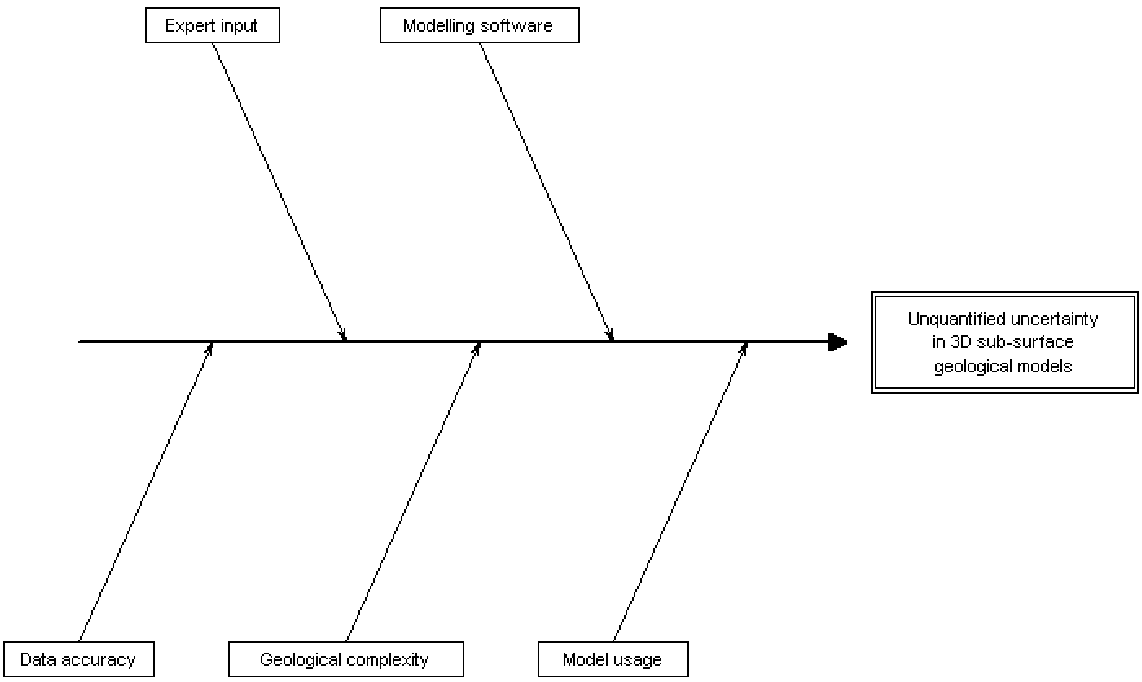

Figure 3 Identification of large-scale causes of a lack of knowledge about the uncertainty present in current 3-D sub-surface geologic models

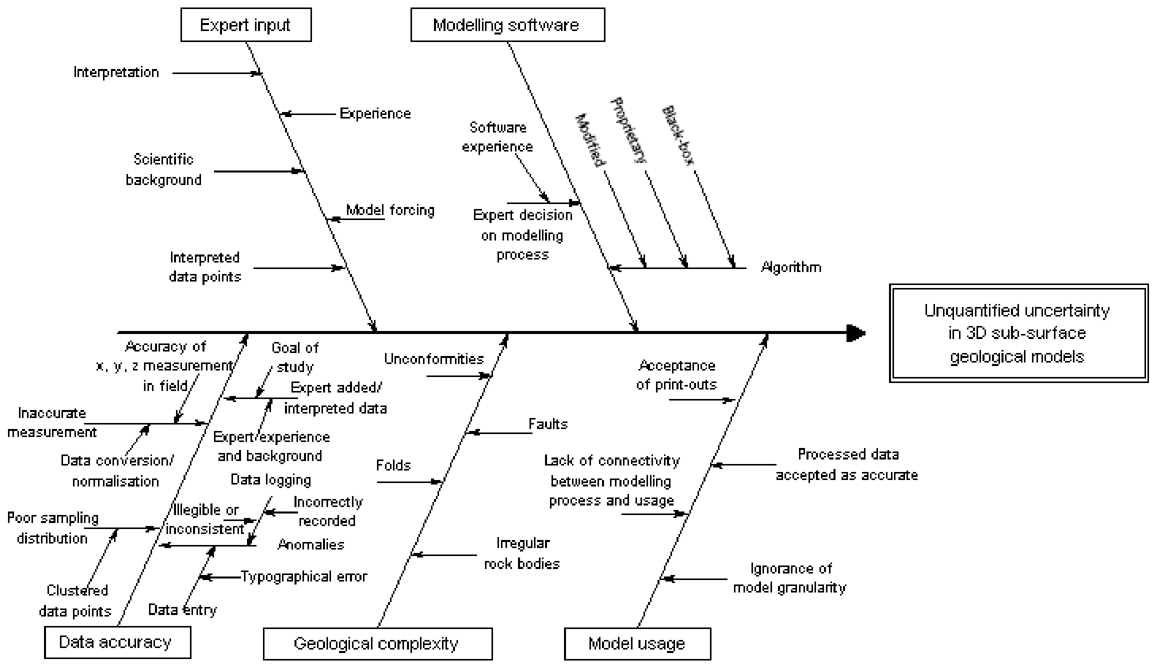

Figure 4 Investigation of some basic causes leading to uncertainty in the modelling process

4.1.1 Towards a system for constructing cause and effect diagrams

Systems are available for developing cause and effect diagrams e.g. http://www.mindtools.com/pages/article/newTMC_03.htm http://www.skymark.com/resources/tools/cause.asp, so would it not be useful for BGS project staff to have access to such software for documenting sources of uncertainty in their work?

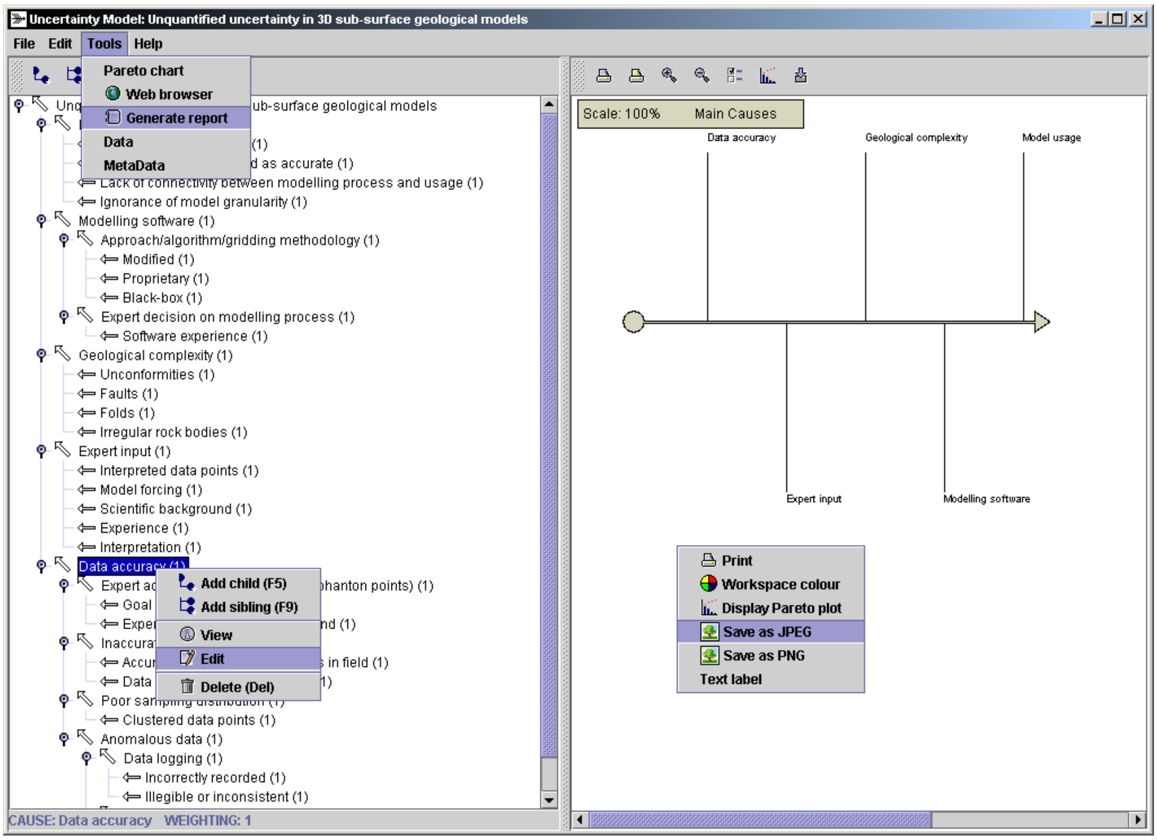

Figure 5 Screenshot of the development application showing various menus

Theoretically it would. However, the following drawbacks are identified:

- Cause and Effect diagrams are often provided as a module for large quality control software packages, and not as stand-alone applications;
- Many people would need access to the software to make it an effective tool; this may be expensive, especially taking into account the above point;
- Much of the software available for carrying out cause and effect analysis are purely graphical tools, requiring manual construction of the diagram, and have no underlying data structure. This is not ideal, as it relies on the software the analysis was carried out on for future edits; there is no database associated with the study;
- The software has been optimised for management applications not for the specific use of identifying uncertainty in geological modelling applications.

Because of these issues, it is thought that a dedicated software system would be a good approach and a start has been made on developing software for constructing cause and effect diagrams that BGS staff will be able to use specifically for modelling applications. The system is being developed with an underlying data structure, and the graphics are generated dynamically from this data (Figure 5). A major advantage of this approach is that the data will be available for compiling reports and for storage in meta data tables. Graphical tools for creating these sorts of diagrams are however currently available within MS Visio, but there is no underlying metadata.

4.2 CASE STUDIES

The principal method of measurement of uncertainty in these examples will be bootstrap resampling (see Section 3.2.3) implemented principally in the MATLAB® (MathWorks, Inc , Natick, MA, USA) programming language and with some data analysis using Microsoft Excel.

4.2.1 Software and Programming languages

4.2.1.1 MATLAB

MATLAB® (MathWorks, Inc , Natick, MA, USA) is a high-performance language for technical computing. It integrates computation, visualization, and programming in an easy-to-use environment where problems and solutions are expressed in familiar mathematical notation. Typical uses include:

- i) Math and computation;
- ii) Algorithm development;
- iii) Data acquisition modelling, simulation, and prototyping;
- iv) Data analysis, exploration, and visualization;
- v) Scientific and engineering graphics;and
- vi) Application development, including graphical user interface building;

MATLAB is an interactive system whose basic data element is an array that does not require dimensioning. This allows you to solve many technical computing problems, especially those with matrix and vector formulations, in a fraction of the time it would take to write a program in a scalar non-interactive language such as C or Fortran. In the mid-1970s, Cleve Moler and several colleagues developed the FORTRAN subroutine libraries called LINPACK and EISPACK under a grant from the National Science Foundation. LINPACK is a collection of FORTRAN subroutines for solving linear equations, while EISPACK contains subroutines for solving eigenvalue problems. Together, LINPACK and EISPACK represented the state of the art software for matrix computation. In the late 1970s, Cleve, who was then chairman of the computer science department at the University of New Mexico, wanted to be able to teach students in his linear algebra courses using the LINPACK and EISPACK software. However, he didn't want them to have to program in FORTRAN, because this wasn't the purpose of the course. So, as a "hobby" on his own time, he started to write a program that would provide simple interactive access to LINPACK and EISPACK. He named his program MATLAB, for MATrix LABoratory. Over the next several years, when Cleve would visit another university to give a talk, or as a visiting professor, he would end up by leaving a copy of his MATLAB on the university machines. Within a year or two, MATLAB started to catch on by word of mouth within the applied math community as a "cult" phenomena. In early 1983, John Little was exposed to MATLAB because of a visit Cleve made to Stanford University. Little, an engineer, recognized the potential application of MATLAB to engineering applications. So in 1983, Little teamed up with Moler and Steve Bangert to develop a second generation, professional version of MATLAB written in C and integrated with graphics. The MathWorks, Inc. was founded in 1984 to market and continue development of MATLAB. projects. Today, MATLAB engines incorporate the LAPACK and BLAS libraries, embedding the state of the art in software for matrix computation. MATLAB has evolved over a period of years with input from many users. In university environments, it is the standard instructional tool for introductory and advanced courses in mathematics, engineering, and science.

MATLAB features a family of add-on application-specific solutions called toolboxes. Very important to most users of MATLAB, toolboxes allow you to learn and apply specialized technology. Toolboxes are comprehensive collections of MATLAB functions (M-files) that extend the MATLAB environment to solve particular classes of problems. Areas in which toolboxes are available include signal processing, control systems, neural networks, fuzzy logic, wavelets, simulation, and many others. User written toolboxes are also available as freeware at the Mathworks website (www.mathworks.com) and at many other url's.

The ease of programming of MATLAB makes it a very powerful tool for carrying out these prototype studies on the measurement of uncertainty on large data sets. In addition to this, once a MATLAB programme has been written and tested it can be compiled into a standalone programme or converted to a Microsoft Excel add-in tool.

4.2.1.2 Resampling software

The resampling software used in the following examples have been developed for MATLAB using the resampling programs described by Kaplan (1999) and for applications implemented in Microsoft Excel, the Resampling Stats add-in was used (Blank et al., 2001). Both sets of software were purchased from Resampling Stats, Inc, Arlington, Virginia, USA through their web site www.resample.com. The software comes with very good manuals that gives a wide range of examples.

4.2.2 Bootstrap resampling of gridded synthetic borehole data

In this example an estimation of the uncertainty introduced in modelling the surface of a geological feature is investigated. This is a simplified example, which assumes that the uncertainty in the spatial co-ordinates is negligible and that all the uncertainty arises from the modelling process itself.

Consider a topographical surface, in this case represented by a mathematical function (Figure 6). Assume that this represents a subsurface geological feature and that the extent of this feature is only known from borehole logs of a 100 non-uniformly spaced boreholes drilled in the area of the feature.

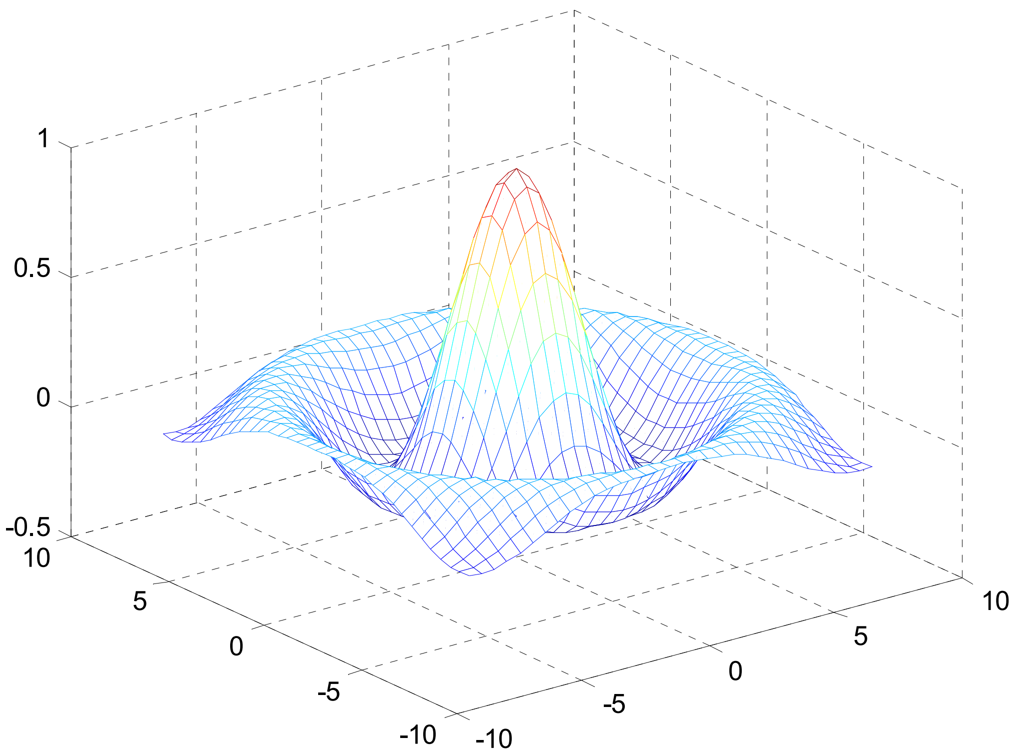

Figure 6 Simulated subsurface geological feature

The XYZ co-ordinates of the feature are then taken from the borehole logs and entered into a geological package that allows the shape of the feature to be modelled by interpolating the data to a regular grid and fitting a surface across it. Generally, in these examples, the standard

MATLAB gridding function was applied and a nearest neighbour algorithm employed. Figure 7 shows a gridded interpolation of the true surface given in Figure 6, produced with the MATLAB programming language gridding function. This surface is an approximation of the true surface because the algorithm has to 'guess' the shape in areas where there is no data. The question then arises as to what is the uncertainty in this approximation. In this case, because we know the true shape it is a simple matter to compare the true surface to the estimated surface point by point. In the real world, however, the shape of the true surface is not known and a different approach to measurement of uncertainty is required.

It may be possible to drill more boreholes to fill in the gaps but this can be a very expensive and time-consuming business. One practical methodology is to use bootstrap resampling (Section 3.3.3).

This would produce a series of gridded surfaces for each resampling of the original data. Measuring the standard deviation at each gridded point then gives an estimate of the uncertainty produced by the gridding procedure.

In this example resampling of the 100 data points was carried out 1000 times and the 95% uncertainty was calculated as twice the standard deviation for each gridded point. This was then compared to the actual measured error between the average of the resampled data and the actual surface. The results are plotted in Figures 8, 9 and 10. Although not a perfect match it is clear that there is good agreement between the predicted uncertainty (which was produced without any knowledge of the true surface) and the true error. Figure 8 (with the uncertainty plotted as contours) shows the position of the simulated boreholes and clearly shows the regions of greatest uncertainty are related to areas where there are fewer data points and also to areas where the shape of the surface is changing rapidly. The MATLAB gridding algorithm has some difficulties in producing interpolated data at the edges of the feature, which explains why the contours in Figure 8 do not extend to the boundaries of the plots. Figures 9 and 10 have the uncertainty and errors plotted as wire mesh surfaces and show the good correspondence of both shape and magnitude between the two confirming that the resampling method has the potential for accurately estimating uncertainty.

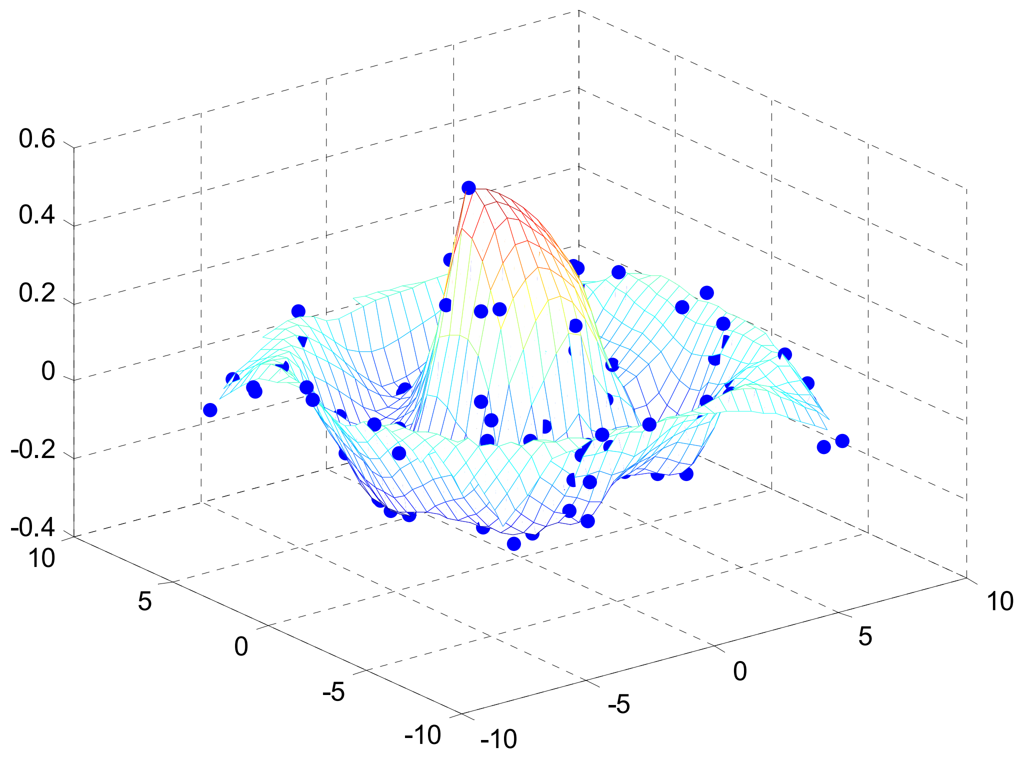

Figure 7 Interpolated surface obtained by gridding of the borehole data

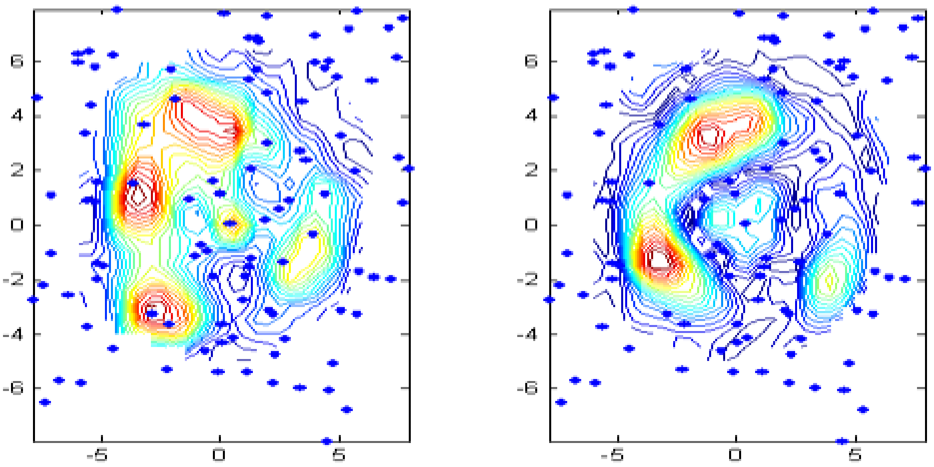

Figure 8 Comparison of predicted uncertainty using resampling (left hand plot) with actual measured error (right hand plot)

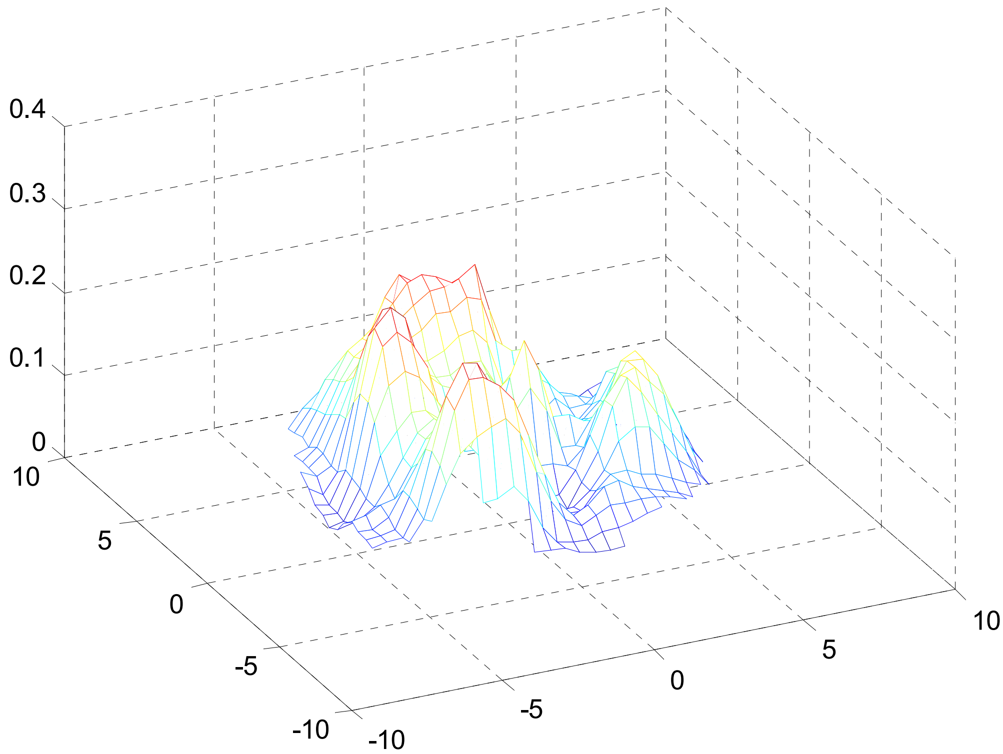

Figure 9 Predicted uncertainty using resampling

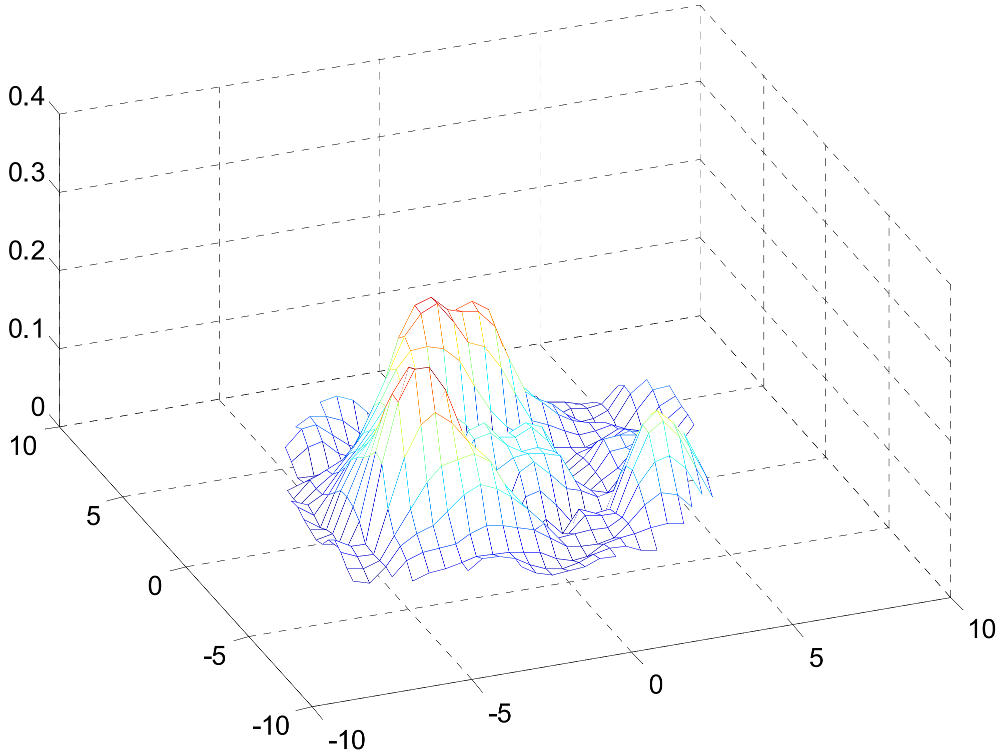

Figure 10 Actual measured error

In this example errors in the X and Y co-ordinates have been neglected and it is assumed that there are no errors in the depths of the surface shown from the borehole log. Examples of estimates of uncertainty for these parameters is given in subsequent sections.

4.2.3 Bootstrap resampling of gridded coal field borehole data

The MATLAB resampling code (Section 4.2.1) has been applied to some borehole data, from the Ayr Hard Coal Seam in the Midland Valley of Scotland, that has a non-uniform spatial distribution. This code (Appendix 1) calculates the uncertainty in the same way as before using the resampling functions provided as part of the resampling toolbox (Kaplan, 1999). In addition to the calculation of uncertainty, the data visualisation capabilities of MATLAB were used to show the uncertainty on the interpolated topographical surface as a colour transparency value. This approach allows both the modelled data and the uncertainty to be visualised simultaneously.

As a control, the approach has been applied to the topographical surface generated by a mathematical function seen in Section 4.2.1. Figures 11 and 12 respectively, show that the uncertainty and the real error can be mapped onto the real data interpolation surface, with darker toned areas representing higher values of uncertainty and error respectively. Again, in this instance, 100 data points taken from the mathematical function have been resampled 1000 times.

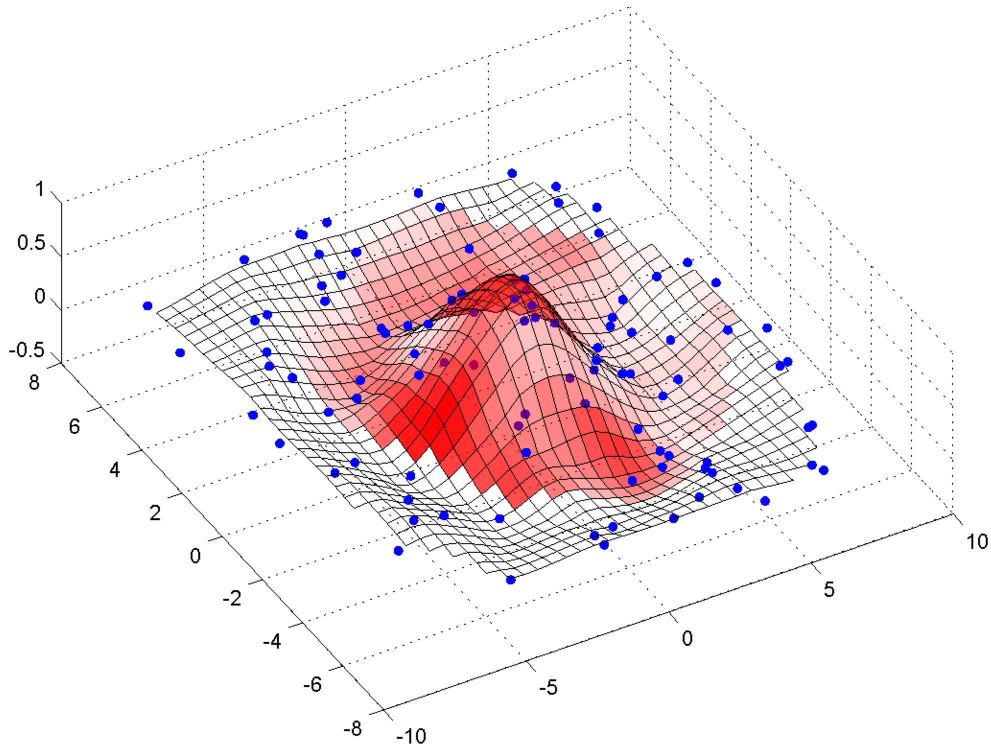

Figure 11 Predicted uncertainty expressed as red transparency value and mapped to interpolated surface obtained by gridding of borehole data

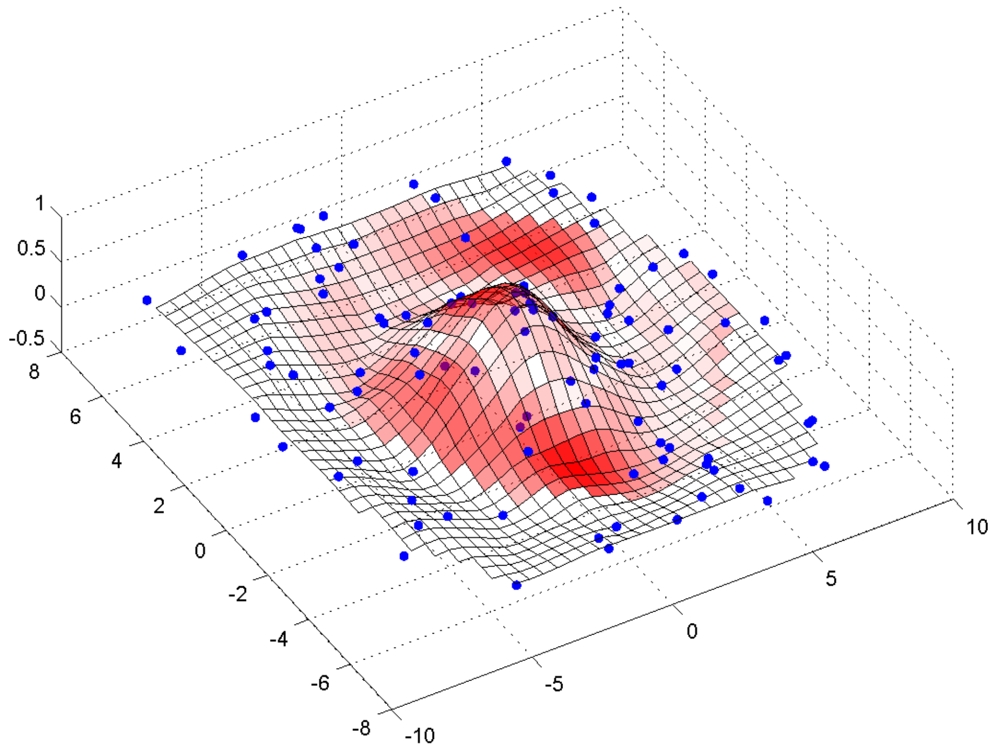

Figure 12 Actual measured error expressed as red transparency value and mapped to interpolated surface obtained by gridding of the borehole data

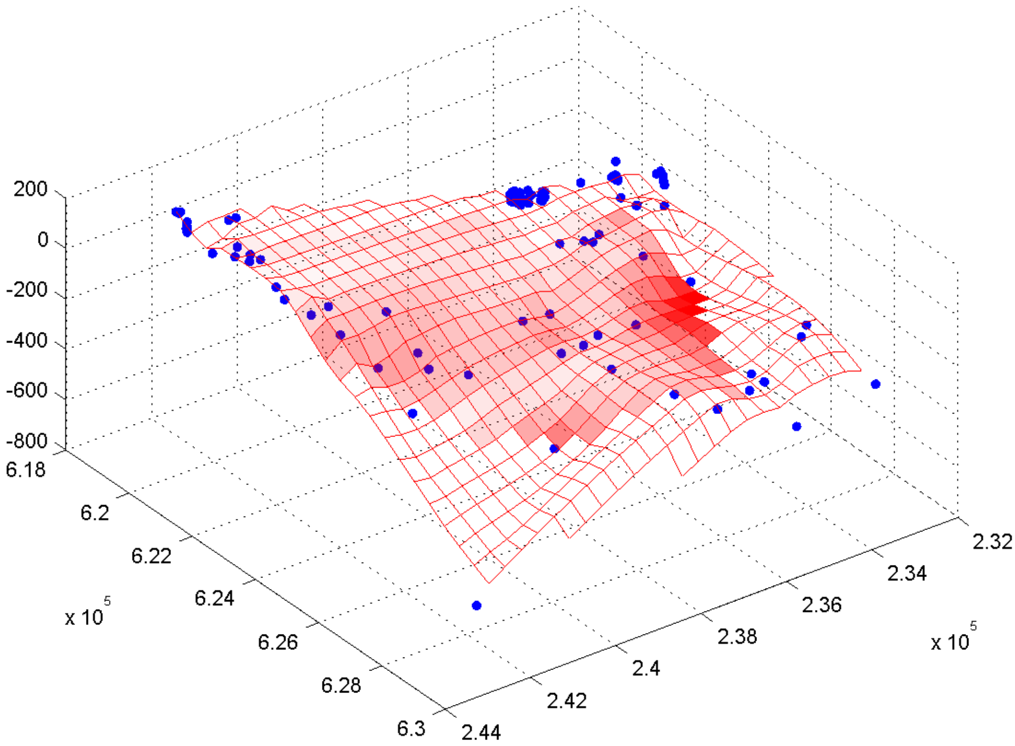

Figure 13 Predicted uncertainty expressed as red transparency value and mapped to interpolated surface obtained by gridding of Ayr Hard Coal Seam borehole data

Figure 13 shows the result of the same methods when applied to the real borehole data describing the Ayr Hard Coal. All 108 borehole data points available for the area were used and resampled 1000 times and the area was separated into a 25 x 25 cell grid for interpolation of the surface. Although this method is still at a preliminary stage, the surface shown in Figure 13 clearly shows how this approach can be applied to real data sets and shows how the results can be displayed in a way which allows users to obtain an instant evaluation of the confidence in the data displayed.

4.2.4 Bootstrap resampling on a geostatistical interpretation of G-base arsenic data

In this example geostatistical methods are used to model the soil arsenic concentrations sampled as part of the BGS Geochemical Baseline Programme (G-base).

The data set consists of 657 data points (a subset of the original 6561 points) made up of sampling site locations (easting and northings) and arsenic concentrations in mg/kg obtained by XRF analysis. In addition to this, there are data for 65 sample locations where duplicate soil samples have been taken and, for each of the duplicate samples, duplicate arsenic concentration measurements have been made.

In this example the uncertainties arising from a number of input parameters are combined to give an overall model uncertainty. Figure 14 shows a simplified cause and effect diagram of the parameter uncertainties being considered.

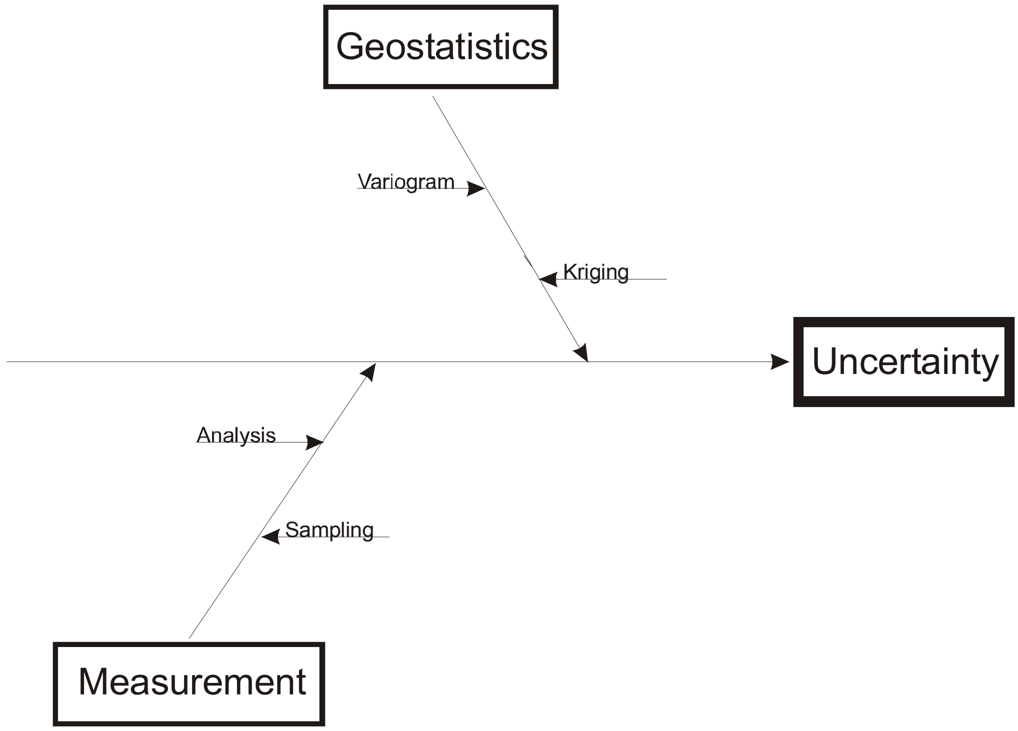

Figure 14 Cause and effect diagram for Arsenic Modelling

The geostatistical modelling of this data presented here does not necessarily represent an optimised data modelling strategy but serves to illustrate how uncertainties from a number of sources can be combined to produce an estimate of the final modelling uncertainty.

4.2.4.1 MEASUREMENT UNCERTAINTY

The combined uncertainty arising from the sampling of the soils and XRF analysis for arsenic was calculated from the duplicate data using the analysis of variance (ANOVA) method described by Ramsey (1998).

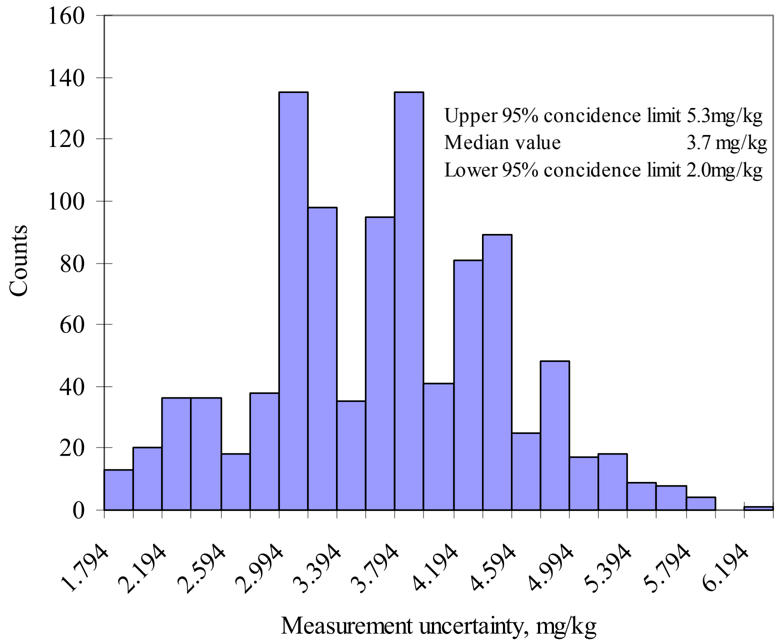

Figure 15 Histogram of the arsenic measurement uncertainty distribution

This combined uncertainty, which measures sampling uncertainty by considering the variance between sampling duplicates and the analysis uncertainty by considering the analysis duplicates, was subjected to bootstrap resampling to allow the confidence limit for the total measurement uncertainty to be calculated.

Figure 15 shows the distribution of uncertainty values for 1000 bootstrap samples and the median value with 95% confidence limits (based on the 97.5 percentile and the 2.5 percentile of the data). This gives a combined measurement error of between 2 and 5 mg/kg for each sample.

4.2.4.2 VARIOGRAM UNCERTAINTY

A variogram of the arsenic test data set was calculated using the robust variogram function (Cressie, 1993) as implemented in MATLAB programming code (Planque, 1996). The functions used to fit the variogram model came from the MATLAB Kriging Toolbox (Gratton, 1996). The variogram was fitted with an exponential model.

Arsenic variograms were calculated for two different scenarios; one with and one without the uncertainty from arsenic measurement as described in Section 4.2.4.1. For each scenario median fit parameters and 95% confidence limits on the fitted variograms were calculated using 1000 iterations of bootstrap resampling. The arsenic measurement uncertainty was included by generating a random noise vector centred on the median arsenic uncertainty of 3.7mg/kg and adding this to each resampled data set. Figure 16 summarises the results showing the original robust variogram trend and the fitted exponential model and its associated uncertainty and the exponential model and associated uncertainty from the scenario where the uncertainty from the measurement was included. This clearly illustrates that the measurement uncertainty has a significant effect on the variogram and reinforces the points made earlier in Sections 3 and 4.1 that all sources of uncertainty must be considered if the true uncertainty in the final model is to be found.

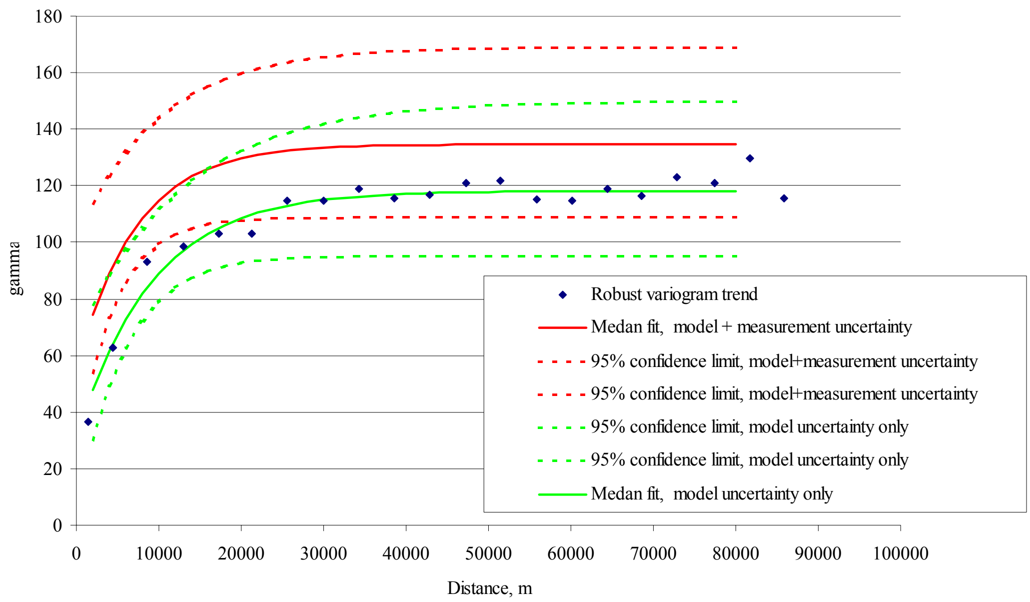

Figure 16 Arsenic Variograms and associated uncertainties

4.2.4.3 KRIGING

Using the variogram coefficients calculated in section 4.2.4.2, an interpolated grid of arsenic values can be calculated using the original arsenic data points and a kriging model (see Section 3.1.2). In a similar manner to the variogram modelling (Section 4.2.4.2), two modelling scenarios were used.

In the first scenario, the kriging was carried out in a conventional manner using the robust fit variogram.

In the second scenario, the kriged values were calculated using a bootstrap resampling protocol. A series of 1000 resampled models for the interpolated grid were calculated. The median arsenic value for each point from each of the 1000 resampled models was obtained along with the variance in the arsenic value at each data point.

To obtain each resampled data set, a three-stage process was carried out:

i) Variogram coefficients were obtained by resampling the variogram coefficient data found in Section 4.2.4.2 for the variogram that included the total measurement error (Figure 16);

ii) The original arsenic data were resampled. To simulate measurement error a random noise vector centred on the median arsenic uncertainty of 3.7 mg/kg (see Section 4.2.4.1) was generated and added to the resampled data. In addition, a random noise vector centred on 5% was added to the sampling locations to simulate spatial uncertainty;

iii) An interpolated grid of data was obtained by kriging the data obtained in point ii) using the variogram coefficients used in point i).

The kriging was carried out using the 'cokrig' program from the MATLAB Kriging Toolbox (Gratton, 1996) and the MATLAB resampling toolbox (Kaplan, 1999). The results of the resampled and kriged data and the normally kriged data are summarised in Figures 17-22.

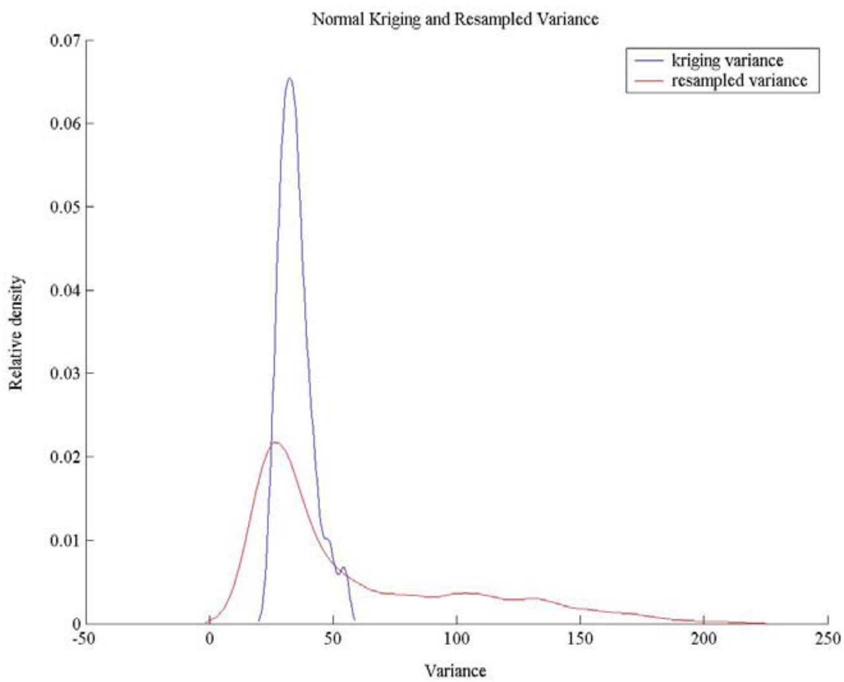

Figure 17 PDF plot of the kriged variance and the resampled variance for the arsenic data

Figures 17 and 18 illustrate the differences in the results obtained for the two kriging scenarios for the arsenic data. Figure 18 compares the kriged variances with the resampled variances. The kriging variance shows an almost symmetric profile over the range of ca. 30-60 whereas the resampled variance shows an extended tail and covers a range of ca. 0-200. This clearly illustrates how the inclusion of measurement uncertainty and modelling uncertainty drastically affects the final uncertainty in the model.

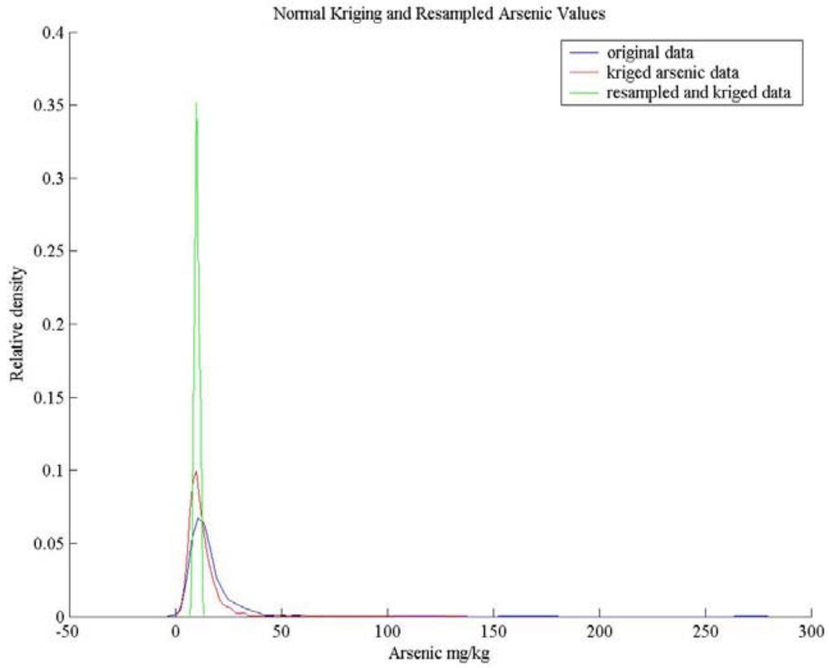

Figure 18 PDF plots of the conventionally kriged data, the resampled and kriged data and the original data set values for arsenic

Figure 18 shows that the resampled and kriged arsenic data have a much tighter distribution than either the conventionally kriged values and the original data. This effect derives from the resampled model taking the median value from 1000 separate models and therefore acting as a filter for outlying data points and provides a more robust estimate in the final model. The spatial plots in Figures 19-21 illustrate this effect.

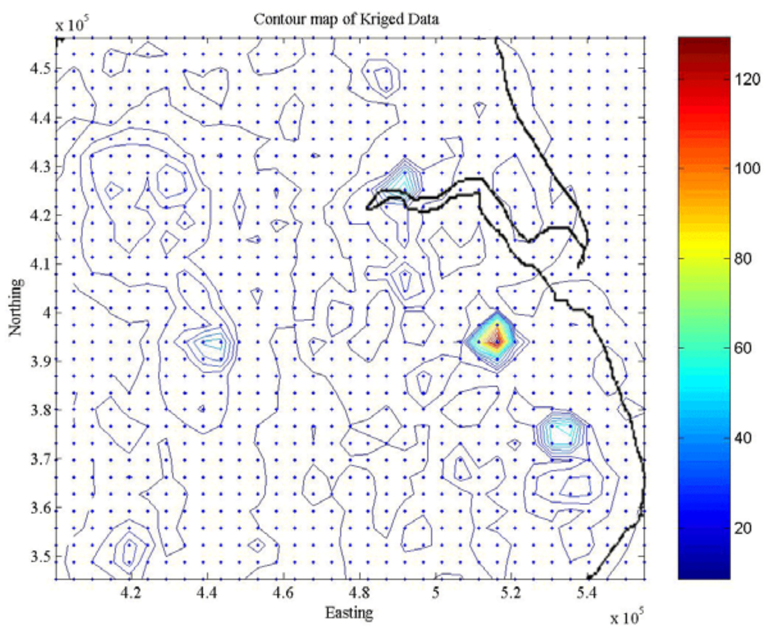

Figure 19 Spatial plot of the conventionally kriged arsenic data in mg/kg (solid black line shows the coastline; blue dots show the position of the interpolated kriging positions).

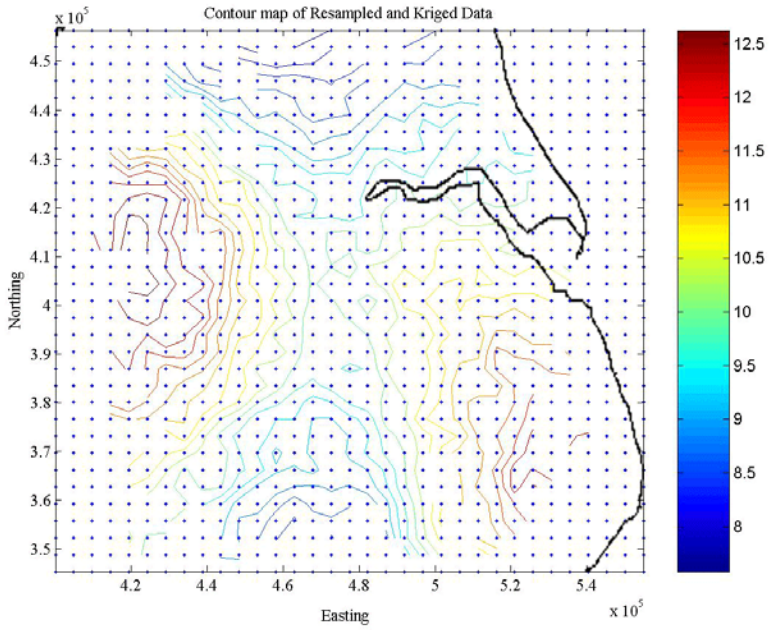

Figure 20 Spatial plot of the resampled and kriged arsenic data in mg/kg (solid black line shows the coastline; blue dots show the position of the interpolated kriging positions).

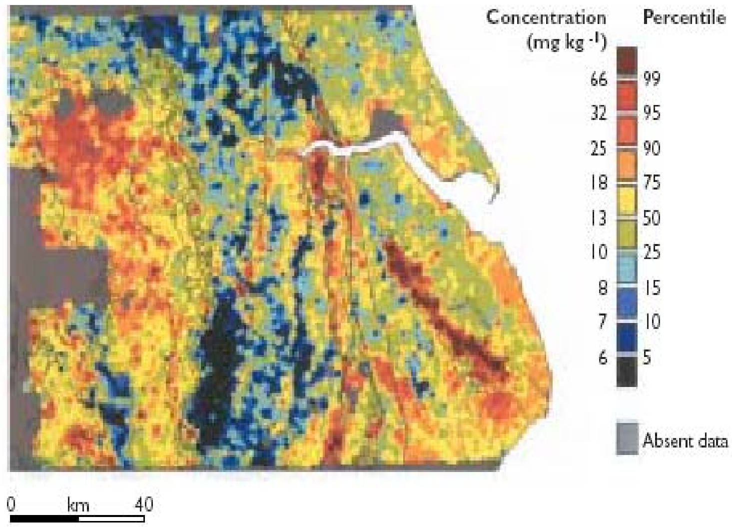

Figure 21 Original high-resolution spatial plot of the arsenic G-Base data

In figures 19 and 20 the conventionally kriged arsenic values and the resampled and kriged values have been plotted as contours, using a nearest neighbour algorithm. In figure 19, the conventionally kriged data produces a few high values causing the formation of 'bulls-eye' hot spots whereas the more robust model produced by the resampled and kriged data (Figure 20) shows clearer trends in the data. Comparing Figure 20 to the high resolution plot (Figure 21) it can be seen that although the resampled and kriged data used in this study (Figure 20) does not show up the individual features of the original data set (this is not surprising since the original data set is based on 6000 data points whereas this study is base on a random sample of 600 of these data points) the high areas of arsenic in the west and south east of the study area are clearly visible. Figure 22 shows a spatial plot of the uncertainty in the arsenic values based on the standard deviation of the arsenic values at each spatial location calculated over the 1000 resampled models.

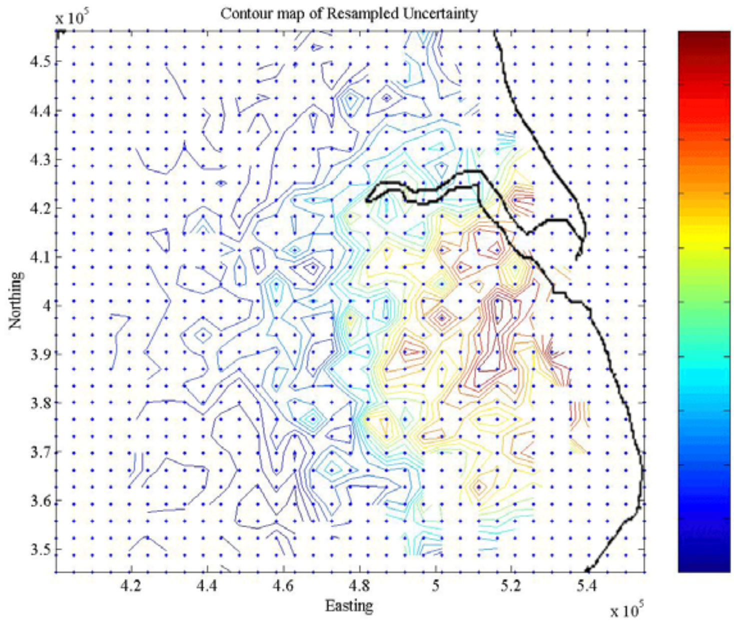

Figure 22 Spatial plot of the resampled uncertainty in the arsenic data in mg/kg (solid black line shows the coastline; blue dots show the position of the interpolated kriging positions)

The highest uncertainties occur in the south east corner of the study area and represent a combination of both measurement uncertainty and modelling uncertainty. Examination of Figure 21 shows this area has the highest contrast in arsenic concentrations going from very low to high in a relatively small topographical distance. This suggests that the uncertainty is mostly derived from the modelling interpolation and not the measurement uncertainty.

Although the geostatistics used in this example may not be fully optimised for the best interpretation of this data set, the exercise serves to illustrate how bootstrap-resampling methods can be used to produce a structured approach to measurement of uncertainty that can be applied to each of the steps in the production of the final model.

5 Conclusions and Recommendations

The literature review element of this study has clearly illustrated that measurement of uncertainty in geoscience applications is a very active area of research, which highlights the importance being given to this topic in the geoscientific community. Although there are many ways of approaching uncertainty measurement, the authors of this report have suggested a structured approach that could be applied to the data modelling projects within BGS. The general philosophy and structure to this approach is as follows:

- Equal importance should be given to the measurement of uncertainty as is given to the final data model.
- It is critical to have a multidisciplinary team with expert representatives from each stage of the modelling project providing information on the uncertainty of each step of the process and to ensure that that emphasis is placed on obtaining good uncertainty estimates for those inputs that critically affect the model outcome.
- There should be a formalised mechanism for all geoscience modelling projects that allows all sources of uncertainty within the project to be recorded in a formalised manner. A suitable tool for this is the use of cause and effect diagrams (See section 4.1)

- Geoscience data models include both quantitative and subjective/semi-quantitative inputs and outputs. The authors suggest that bootstrap-resampling (see Section 3.2.3) and fuzzy logic (see Section 3.3.1) approaches respectively are suitable methods for producing robust estimates of uncertainty on these two types of data.
- The final estimate of uncertainty on any model must include contributions from all of the significant sources of uncertainty identified by the cause and effect diagram of the project.

Appendix 1 Matlab Computer Codes

MATLAB CODE FOR SIMULTANEOUS PLOTTING OF UNCERTAINTY

```
function[uncert]= uncertplot(n,p)

% MATLAB function to simulate the measurement of uncertainty when
% plotting a surface using resampling methods. Relies on the resampling
% toolbox. Plots uncertainty value using proportional colour transparency
% over interpolated data surface.

test=1 % Default (data distribution is bad)

% Allow user to load a text file containing data and check how the data
% is distributed before proceeding
while test<2
     % Read in some data from a text file
      [x y z] = textread('Borehole.txt','%f %f %f','headerlines', 1);

      % Plot data distribution so user can check OK
      plot(x,y,'.','MarkerSize',15)
      title('Data point distribution')

      % If OK, user enters 2
      test=input('Data OK? (y=2/n=1)?');
end



% user selects interpolation method
method = 1;     % default
interptype = 'cubic';
method = input('Interpolation: (1=cubic,2=linear,3=nearest neighbour,4=Matlab v4 ? ');

% test which interpolation method is required and set accordingly
if(method == 1)
    interptype = 'cubic';
elseif(method == 2)
    interptype = 'linear';
elseif(method == 3)
    interptype = 'nearest';
elseif(method == 4)
    interptype = 'v4';
```

```
% default to cubic
elseif(method > 4)
    method = 1;
    interptype = 'cubic';
end

% Set up grid
xlin=linspace(min(x),max(x),p);
max(x)
ylin=linspace(min(y),max(y),p);
max(y)
[X,Y]=meshgrid(xlin,ylin);
surface=[x,y,z];

% Interpolate data across grid
Z1=griddata(surface(:,1),surface(:,2),surface(:,3),X,Y,interptype);


Z1long=reshape(Z1,1,(p*p));
Final=Z1long;

% Loop through n times, re-gridding to get an average
for i=1:n
    % resample original XYZ data
    surface2=resamp(surface);
    % grid resampled data
    Z=griddata(surface2(:,1),surface2(:,2),surface2(:,3),X,Y,interptype);


    Zlong=reshape(Z,1,(p*p));

    Final=[Final;Zlong];
end


% Loop through and calculate mean from Final for each column
average = [];
for j=1:(p*p)
    % get rid of NaN's in each column and store values in tmp
    tmp = weed(Final(:,j), ismissing(Final(:,j)));
    % if all the values were NaN in this column then the length of tmp will be zero
(causing divide by zero error in mean())
    % - catch this possibility and set tmp to 0
    if(length(tmp) == 0)
        tmp = [0];
    % tmp contains real values, so average them
```

```
    else
        tmp = mean(tmp);
    end

    % concatenate mean value for column (tmp) onto average array
    average = [average; tmp];

end



stdev=abs(std(Final));
uncert=reshape(stdev,p,p);
uncert=uncert.*2;
average=reshape(average,p,p);

% Plot uncertainty value across grid as a contour
figure(2)
contour(X,Y,uncert,20)
hold on
plot(x,y,'.','MarkerSize',15)
title('Uncertainty contour')

% Plot uncertainty value across grid as a surface mesh
figure(3)
mesh(X,Y,uncert)
title('Uncertainty mesh');




% Plot surface 1 - use uncertainty value as transparency (darker = greater UC value)

figure(4)
surf(X,Y,Z1,'FaceAlpha','flat','AlphaDataMapping','scaled','AlphaData',uncert,'FaceCol
or','red','LineStyle','-','EdgeColor','red');
hold on
plot3(x,y,z,'.b','MarkerSize', 15)
title(['Interpolated surface - transparency --> uncertainty      ',interptype, '
interpolation'])
```

Glossary

Bayesian statistics Concerned with a theory (as of decision making or statistical inference) involving the application of Bayes' theorem and the use of probabilities based on prior knowledge and accumulated experience. Techniques include Bayesian Model Averaging and Bayesian Maximum Entropy.

Bootstrap sampling A form of randomisation test that involves generating subsets of the data on the basis of random sampling with replacements as the data are sampled.

cdf Cumulative Distribution Function.

Covariance The arithmetic mean of the products of the deviations of corresponding values of two quantitative variables from their respective means.

Cross validation Equivalent to Jackknife sampling

Fuzzy Logic A multi-valued (as opposed to binary) logic developed to deal with imprecise or vague data.

Jackknife procedure A form of randomisation test that involves generating subsets of the data on the basis of sampling by omission of data.

Kriging A stochastic interpolation technique based on a generalised least-squares algorithm, using variograms as weighting functions. A number of variants of kriging are in general use, these are: simple kriging; ordinary kriging; universal kriging; block kriging; co-kriging; and disjunctive kriging.

Latin Hypercube Sampling Sampling so that the range of probable values for each uncertain input parameter (PDF) is divided into segments of equal probability.

Measurand Particular quantity subject to measurement.

Monte Carlo simulation A problem-solving technique that uses random samples and other statistical methods for finding solutions to mathematical or physical problems.

Simulated annealing A technique to find a good solution to an optimization problem by trying random variations of the current solution. This technique stems from the thermal annealing which aims to obtain perfect crystallizations by a slow enough temperature reduction to give atoms the time to attain the lowest energy state.

Semi-variogram See variogram.

SRSM Stochastic Response Surface Modelling.

Stochastic Statistics being or having a random variable.

Variogram A measure of the continuity of spatial phenomena expressed as an average squared difference between measured quantities at different locations.

References

ABT, M., WELCH, W. J. & SACKS, J. 1999. Design and analysis for modeling and predicting spatial contamination. *Mathematical Geology*, **31**(1), 1-22.

ALDEN, R. W., WEISBERG, S. B., RANASINGHE, J. A. & DAUER, D. M. 1997. Optimizing temporal sampling strategies for benthic environmental monitoring programs. *Marine Pollution Bulletin*, **34**(11), 913-922.

BALLIN, P. R., JOURNEL, A. G. & AZIZ, K. 1992. Prediction of Uncertainty in Reservoir Performance Forecast. *Journal of Canadian Petroleum Technology*, **31**(4), 52-62.

BARABAS, N., GOOVAERTS, P. & ADRIAENS, P. 2001. Geostatistical assessment and validation of uncertainty for three-dimensional dioxin data from sediments in an estuarine river. *Environmental Science & Technology*, **35**(16), 3294-3301.

BARDOSSY, A., BOGARDI, I. & KELLY, W. E. 1990a. Kriging with Imprecise (Fuzzy) Variograms .1. Theory. *Mathematical Geology*, **22**(1), 63-79.

BARDOSSY, A., BOGARDI, I. & KELLY, W. E. 1990b. Kriging with Imprecise (Fuzzy) Variograms .2. Application. *Mathematical Geology*, **22**(1), 81-94.

BENEDETTI, R. & PALMA, D. 1995. Optimal Sampling Designs for Dependent Spatial Units. *Environmetrics*, **6**(2), 101-114.

BLANK, S., SEITER, C. & BRUCE, P. (2001) *Resampling Stats in Excel*. Resampling Stats Inc., Arlington, Virginia.

BUBNICKI, Z. 2001a. Uncertain variables and their application to decision making problems. *Ieee Transactions on Systems Man and Cybernetics Part a-Systems and Humans*, **31**(6), 587-596.

BUBNICKI, Z. 2001b. Uncertain variables and their applications for a class of uncertain systems. *International Journal of Systems Science*, **32**(5), 651-659.

CARLON, C., CRITTO, A., MARCOMINI, A. & NATHANAIL, P. 2001. Risk based characterisation of contaminated industrial site using multivariate and geostatistical tools. *Environmental Pollution*, **111**(3), 417-427.

CARRINGTON, C. D. & BOLGER, P. M. 1998. Uncertainty and risk assessment. *Human and Ecological Risk Assessment*, **4**(2), 253-257.

CARROLL, R. W. H. & WARWICK, J. J. 2001. Uncertainty analysis of the Carson River mercury transport model. *Ecological Modelling*, **137**(2-3), 211-224.

CHATTERJEE, N. D., MILLER, K. & OLBRICHT, W. 1994. Bayes Estimation - a Novel-Approach to Derivation of Internally Consistent Thermodynamic Data for Minerals, Their Uncertainties, and Correlations .2. Application. *Physics and Chemistry of Minerals*, **21**(1-2), 50-62.

CHRISTAKOS, G. & LI, X. Y. 1998. Bayesian maximum entropy analysis and mapping: A farewell to kriging estimators? *Mathematical Geology*, **30**(4), 435-462.

CHRISTAKOS, G. & SERRE, M. L. 2000a. BME analysis of spatiotemporal particulate matter distributions in North Carolina. *Atmospheric Environment*, **34**(20), 3393-3406.

CHRISTAKOS, G. & SERRE, M. L. 2000b. Spatiotemporal analysis of environmental exposure-health effect associations. *Journal of Exposure Analysis and Environmental Epidemiology*, **10**(2), 168-187.

CHRISTIAENS, K. & FEYEN, J. 2001. Analysis of uncertainties associated with different methods to determine soil hydraulic properties and their propagation in the distributed hydrological MIKE SHE model. *Journal of Hydrology*, **246**(1-4), 63-81.

COOPER, J. A., FERSON, S. & GINZBURG, L. 1996. Hybrid processing of stochastic and subjective uncertainty data. *Risk Analysis*, **16**(6), 785-791.

COPTY, N. K. & FINDIKAKIS, A. N. 2000. Quantitative estimates of the uncertainty in the evaluation of ground water remediation schemes. *Ground Water*, **38**(1), 29-37.

CRESSIE. (1993) *Statistics for spatial data*. Wiley and Sons, inc.

DAVIS, T. J. & KELLER, C. P. 1997. Modelling uncertainty in natural resource analysis using fuzzy sets and Monte Carlo simulation: Slope stability prediction. *International Journal of Geographical Information Science*, **11**(5), 409-434.

DAVISON, A. C. & HINKLEY, D. V. (1997) *Bootstrap Methods and their Applications*. Cambridge Univesity Press, Cambridge.

DAY, R. A. & UNDERWOOD, A. L. (1991) *Quantitative analysis*. Prentice Hall, New Jersey.

D'OR, D., BOGAERT, P. & CHRISTAKOS, G. 2001. Application of the BME approach to soil texture mapping. *Stochastic Environmental Research and Risk Assessment*, **15**(1), 87-100.

EFRON, B. 1979. Bootstrap methods: another look at the jackknife. *Annals of Statistics*, **7**, 1-26.

EFRON, B. & TIBSHIRANI, R. J. (1993) *An Introduction to the Bootstrap*. Chapman and Hall, New York.

ELLISON, S. L. R., GREGORY, S. & HARDCASTLE, W. A. 1998. Quantifying uncertainty in qualitative analysis. *Analyst*, **123**(5), 1155-1161.

EURACHEM. (1995) *Quantifying uncertainty in Analytical measurement*. Eurachem.

FERSON, S. 1996. What Monte Carlo methods cannot do. *Human and Ecological Risk Assessment*, **2**(4), 990-1007.

FERSON, S., ROOT, W. & KUHN, R. (1999) *RAMAS Risk Calc: Risk assessment with uncertain numbers - Applied Biomathemetics*, New York.

FLORIS, F. J. T., BUSH, M. D., CUYPERS, M., ROGGERO, F. & SYVERSVEEN, A. R. 2001. Methods for quantifying the uncertainty of production forecasts: a comparative study. *Petroleum Geoscience*, **7**, S87-S96.

GOMEZHERNANDEZ, J. J. & WEN, X. H. 1998. To be or not to be multi-Gaussian? A reflection on stochastic hydrogeology. *Advances in Water Resources*, **21**(1), 47-61.

GOOVAERTS, P. (1997) *Geostatistics for Natural Resources Evaluation*. Oxford University Press, New York.

GOOVAERTS, P. 1998. Geostatistical tools for characterizing the spatial variability of microbiological and physico-chemical soil properties. *Biology and Fertility of Soils*, **27**(4), 315-334.

GOOVAERTS, P. 2001. Geostatistical modelling of uncertainty in soil science. *Geoderma*, **103**(1-2), 3-26.

GOOVAERTS, P. 2002. Geostatistical modelling of spatial uncertainty using p-field simulation with conditional probability fields. *International Journal of Geographical Information Science*, **16**(2), 167-178.

GOUVEIA, W. P. & SCALES, J. A. 1998. Bayesian seismic waveform inversion: Parameter estimation and uncertainty analysis. *Journal of Geophysical Research-Solid Earth*, **103**(B2), 2759-2779.

GRATTON, Y. (1996) MATLAB Kriging Toolbox 4.0.

HEGSTAD, B. K. & OMRE, H. 2001. Uncertainty in production forecasts based on well observations, seismic data, and production history. *Spe Journal*, **6**(4), 409-424.

HEUVELINK, G. B. M. & WEBSTER, R. 2001. Modelling soil variation: past, present, and future. *Geoderma*, **100**(3-4), 269-301.

HRISTOPULOS, D. T. & CHRISTAKOS, G. 2001. Practical calculation of non-Gaussian multivariate moments in spatiotemporal Bayesian maximum entropy analysis. *Mathematical Geology*, **33**(5), 543-568.

HYLAND, J. L., SNOOTS, T. R. & BALTHIS, W. L. 1998. Sediment quality of estuaries in the southeastern US. *Environmental Monitoring and Assessment*, **51**(1-2), 331-343.

IMAN, R. L. & HELTON, J. C. 1988. An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer-Models. *Risk Analysis*, **8**(1), 71-90.

IMAN, R. L. & HELTON, J. C. 1991. The Repeatability of Uncertainty and Sensitivity Analyses for Complex Probabilistic Risk Assessments. *Risk Analysis*, **11**(4), 591-606.

ISAAKS, E. H. & SRIVASTAVA, R. M. (1989) *An Introduction to Applied Geostatistics*. Oxford University Press.

ISO. (1993) *International Vocabulary of basic and general standard terms in Metrology*. ISO, Geneva.

JOURNEL, A. G. 1996. Modelling uncertainty and spatial dependence: Stochastic imaging. *International Journal of Geographical Information Systems*, **10**(5), 517-522.

KAPLAN, D. T. (1999) *Resampling Stats in MATLAB*. Resampling Stats Inc, Arlington, Virginia.

KINDLARSKI, E. 1984. Ishikawa Diagrams for Problem-Solving. *Quality Progress*, **17**(12), 26-30.

KRAGTEN, J. 1994. Calculating Standard Deviations and Confidence-Intervals with a Universally Applicable Spreadsheet Technique. *Analyst*, **119**(10), 2161-2165.

LAMON, E. C. & CLYDE, M. A. 2000. Accounting for model uncertainty in prediction of chlorophyll a in Lake Okeechobee. *Journal of Agricultural Biological and Environmental Statistics*, **5**(3), 297-322.

LECOUR, M., COGNOT, R., DUVINAGE, I., THORE, P. & DULAC, J. C. 2001. Modelling of stochastic faults and fault networks in a structural uncertainty study. *Petroleum Geoscience*, **7**, S31-S42.

LEE, J. C. & RAMSEY, M. H. 2001. Modelling measurement uncertainty as a function of concentration: an example from a contaminated land investigation. *Analyst*, **126**(10), 1784-1791.

LLOYD, C. D. & ATKINSON, P. M. 2001. Assessing uncertainty in estimates with ordinary and indicator kriging. *Computers & Geosciences*, **27**(8), 929-937.

LONGPRE, D., JARRY, V. & FORTIN, M. J. 1997. Environmental impact sampling designs used to evaluate accidental spills. *Spill Science & Technology Bulletin*, **4**(3), 133-139.

MANN, C. J. (1993) Uncertainty in Geology. In: *Computers in Geology - 25 Years of Progress* (Ed. by J. C. Davis and U. C. Herzfeld), pp. 241-254.

MASSONNAT, G. J. 2000. Can we sample the complete geological uncertainty space in reservoir-modeling uncertainty estimates? *Spe Journal*, **5**(1), 46-59.

MCKAY, M. D., CONOVER, W. J. & BECKMAN, R. J. 1979. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, **221**, 239-245.

MEINRATH, G. 2000. Computer-intensive methods for uncertainty estimation in complex situations. *Chemometrics and Intelligent Laboratory Systems*, **51**(2), 175-187.

MEINRATH, G., EKBERG, C., LANDGREN, A. & LILJENZIN, J. O. 2000. Assessment of uncertainty in parameter evaluation and prediction. *Talanta*, **51**(2), 231-246.

MEINRATH, G. & NITZSCHE, O. 2000. Impact of measurement uncertainty in chemical quantities on environmental prognosis by geochemical transport modelling. *Isotopes in Environmental and Health Studies*, **36**(3), 195-210.

MISHRA, S., CHOUDHARY, M. K. & DATTA-GUPTA, A. 2002. A novel approach for reservoir forecasting under uncertainty. *Spe Reservoir Evaluation & Engineering*, **5**(1), 42-48.

NICHOLSON, M. C. & MATHER, T. N. 1996. Methods for evaluating lyme disease risks using geographic information systems and geospatial analysis. *Journal of Medical Entomology*, **33**(5), 711-720.

OKX, J. P. & STEIN, A. 2000. Use of decision trees to value investigation strategies for soil pollution problems. *Environmetrics*, **11**(3), 315-325.

OUENES, A. 2000. Practical application of fuzzy logic and neural networks to fractured reservoir characterization. *Computers & Geosciences*, **26**(8), 953-962.

OZELKAN, E. C. & DUCKSTEIN, L. 2001. Fuzzy conceptual rainfall-runoff models. *Journal of Hydrology*, **253**(1-4), 41-68.

PANIGRAHI, D. P. & MUJUMDAR, P. P. 2000. Reservoir operation modelling with fuzzy logic. *Water Resources Management*, **14**(2), 89-109.

PAUSTENBACH, D. J., WENNING, R. J., LAU, V., HARRINGTON, N. W., RENNIX, D. K. & PARSONS, A. H. 1992. Recent Developments on the Hazards Posed by 2,3,7,8-Tetrachlorodibenzo-Para-Dioxin in Soil - Implications for Setting Risk-Based Cleanup Levels at Residential and Industrial Sites. *Journal of Toxicology and Environmental Health*, **36**(2), 103-149.

PFINGSTEN, W., HADERMANN, J. & PERROCHET, P. 2001. Radionuclide release and transport from nuclear underground tests performed at Mururoa and Fangataufa - predictions under uncertainty. *Journal of Contaminant Hydrology*, **47**(2-4), 349-363.

PHILLIPS, D. L. & MARKS, D. G. 1996. Spatial uncertainty analysis: Propagation of interpolation errors in spatially distributed models. *Ecological Modelling*, **91**(1-3), 213-229.

PLANQUE, B. (1996) NUMERICAL ECOLOGY AND DATA ANALYSIS TOOLBOX.

RAMSEY, M. H. 1997. Measurement uncertainty arising from sampling: Implications for the objectives of geoanalysis. *Analyst*, **122**(11), 1255-1260.

RAMSEY, M. H. 1998. Sampling as a source of measurement uncertainty: techniques for quantification and comparison with analytical sources. *Journal of Analytical Atomic Spectrometry*, **13**(2), 97-104.

RAMSEY, M. H. & ARGYRAKI, A. 1997. Estimation of measurement uncertainty from field sampling: Implications for the classification of contaminated land. *Science of the Total Environment*, **198**(3), 243-257.

RAMSEY, M. H., ARGYRAKI, A. & THOMPSON, M. 1995. On the Collaborative Trial in Sampling. *Analyst*, **120**(9), 2309-2312.

RAMSEY, M. H., LYN, J. & WOOD, R. 2001. Optimised uncertainty at minimum overall cost to achieve fitness-for-purpose in food analysis. *Analyst*, **126**(10), 1777-1783.

RAMSEY, M. H., SQUIRE, S. & GARDNER, M. J. 1999. Synthetic reference sampling target for the estimation of measurement uncertainty. *Analyst*, **124**(11), 1701-1706.

RATHBUN, S. L. 1998. Spatial modelling in irregularly shaped regions: Kriging estuaries. *Environmetrics*, **9**(2), 109-129.

ROBINS, A. G., HALL, R., COWAN, I. R., BARTZIS, J. G. & ALBERGEL, A. 2000. Evaluating modelling uncertainty in CFD predictions of building affected dispersion. *International Journal of Environment and Pollution*, **14**(1-6), 52-64.

ROOD, A. S., MCGAVRAN, P. D., AAVENSON, J. W. & TILL, J. E. 2001. Stochastic estimates of exposure and cancer risk from carbon tetrachloride released to the air from the Rocky Flats Plant. *Risk Analysis*, **21**(4), 675-695.

ROSSEL, R. A. V., GOOVAERTS, P. & MCBRATNEY, A. B. 2001. Assessment of the production and economic risks of site- specific liming using geostatistical uncertainty modelling. *Environmetrics*, **12**(8), 699-+.

SALAS, J. D. & SHIN, H. S. 1999. Uncertainty analysis of reservoir sedimentation. *Journal of Hydraulic Engineering-Asce*, **125**(4), 339-350.

SCHERM, H. 2000. Simulating uncertainty in climate-pest models with fuzzy numbers. *Environmental Pollution*, **108**(3), 373-379.

SCHULZ, K. & HUWE, B. 1997. Water flow modeling in the unsaturated zone with imprecise parameters using a fuzzy approach. *Journal of Hydrology*, **201**(1-4), 211-229.

SCHULZ, K., HUWE, B. & PEIFFER, S. 1999. Parameter uncertainty in chemical equilibrium calculations using fuzzy set theory. *Journal of Hydrology*, **217**(1-2), 119-134.

SERRE, M. L. & CHRISTAKOS, G. 1999. Modern geostatistics: computational BME analysis in the light of uncertain physical knowledge - the Equus Beds study. *Stochastic Environmental Research and Risk Assessment*, **13**(1-2), 1-26.

SMITH, V. E., RATHBUN, J. E., ROOD, S. G. & HUELLMANTEL, L. L. 1996. Technical considerations in sediment quality surveys. *Journal of Great Lakes Research*, **22**(3), 512-522.

SOHN, M. D., SMALL, M. J. & PANTAZIDOU, M. 2000. Reducing uncertainty in site characterization using Bayes Monte Carlo methods. *Journal of Environmental Engineering-Asce*, **126**(10), 893-902.

SQUIRE, S., RAMSEY, M. H. & GARDNER, M. J. 1999. Collaborative trial in sampling for the spatial delineation of contamination and the estimation of uncertainty. *Analyst*, **125**(1), 139-145.

SQUIRE, S., RAMSEY, M. H., GARDNER, M. J. & LISTER, D. 2000. Sampling proficiency test for the estimation of uncertainty in the spatial delineation of contamination. *Analyst*, **125**(11), 2026-2031.

STROBEL, C. J., PAUL, J. F., HUGHES, M. M., BUFFUM, H. W., BROWN, B. S. & SUMMERS, J. K. 2000. Using information on spatial variability of small estuaries in designing large-scale estuarine monitoring programs. *Environmental Monitoring and Assessment*, **63**(1), 223-236.

TATTARI, S. & BARLUND, I. 2001. The concept of sensitivity in sediment yield modelling. *Physics and Chemistry of the Earth Part B-Hydrology Oceans and Atmosphere*, **26**(1), 27-31.

TORRI, D., POESEN, J. & BORSELLI, L. 1997. Predictability and uncertainty of the soil erodibility factor using a global dataset. *Catena*, **31**(1-2), 1-22.

VAN GROENIGEN, J. W. 2000. The influence of variogram parameters on optimal sampling schemes for mapping by kriging. *Geoderma*, **97**(3-4), 223-236.

VAN GROENIGEN, J. W., GANDAH, M. & BOUMA, J. 2000a. Soil sampling strategies for precision agriculture research under sahelian conditions. *Soil Science Society of America Journal*, **64**(5), 1674-1680.

VAN GROENIGEN, J. W., PIETERS, G. & STEIN, A. 2000b. Optimizing spatial sampling for multivariate contamination in urban areas. *Environmetrics*, **11**(2), 227-244.

VAN GROENIGEN, J. W., SIDERIUS, W. & STEIN, A. 1999. Constrained optimisation of soil sampling for minimisation of the kriging variance. *Geoderma*, **87**(3-4), 239-259.

VAN GROENIGEN, J. W. & STEIN, A. 1998. Constrained optimization of spatial sampling using continuous simulated annealing. *Journal of Environmental Quality*, **27**(5), 1078-1086.

VAN MEIRVENNE, M. & GOOVAERTS, P. 2001. Evaluating the probability of exceeding a site-specific soil cadmium contamination threshold. *Geoderma*, **102**(1-2), 75-100.

WADIA-FASCETTI, S. & GUNES, B. 2000. Earthquake response spectra models incorporating fuzzy logic with statistics. *Computer-Aided Civil and Infrastructure Engineering*, **15**(2), 134-146.

WAKEFIELD, M. I., COOK, R. J., JACKSON, H. & THOMPSON, P. 2001. Interpreting biostratigraphical data using fuzzy logic: The identification of regional mudstones within the Fleming field, UK North Sea. *Journal of Petroleum Geology*, **24**(4), 417-440.

WEHRENS, R., PUTTER, H. & BUYDENS, L. M. C. 2000. The bootstrap: a tutorial. *Chemometrics and Intelligent Laboratory Systems*, **54**(1), 35-52.

WIEHN, G., GORAK, A. & PEDRYCZ, W. 1996. Cost modelling of waste in incineration plants: An application of fuzzy sets toward decision making under uncertainty. *Ecological Modelling*, **85**(1), 83-91.

WINKELS, H. J. & STEIN, A. 1997. Optimal cost-effective sampling for monitoring and dredging of contaminated sediments. *Journal of Environmental Quality*, **26**(4), 933-946.

YOUNG, G. A. 1994. Bootstrap: More than a stab in the dark? *Statistical Science*, **9**, 382-415.

ZADEH, L. A. 1965. Fuzzy Sets. *Information and Control*, **8**, 338-353.

ZHANG, D. X., LI, L. Y. & TCHELEPI, H. A. 2000. Stochastic formulation for uncertainty analysis of two-phase flow in heterogeneous reservoirs. *Spe Journal*, **5**(1), 60-70.

ZHANG, J. X. & STUART, N. 2001. Fuzzy methods for categorical mapping with image-based land cover data. *International Journal of Geographical Information Science*, **15**(2), 175-195.

ZHANG, Z. J. & TUMAY, M. T. 1999. Statistical to fuzzy approach toward CPT soil classification. *Journal of Geotechnical and Geoenvironmental Engineering*, **125**(3), 179-186.

ZHENG, S. Y., CORBETT, P. W. M., RYSETH, A. & STEWART, G. 2000. Uncertainty in well test and core permeability analysis: a case study in fluvial channel reservoirs, northern North Sea, Norway. *Aapg Bulletin*, **84**(12), 1929-1954.

ZHU, A. X. 1997. Measuring uncertainty in class assignment for natural resource maps under fuzzy logic. *Photogrammetric Engineering and Remote Sensing*, **63**(10), 1195-1202.