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Chapter 2

Reflections on Geostatistics and Stochastic Modeling

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ABSTRACT

In recent years, geostatistics and stochastic modeling have made a tremendous impact on scientific investigation. This chapter describes the relationship between these two ideas, provides a historical perspective on their development, and discusses the ways in which they have evolved, both separately and in concert with each other. Important issues impacting future development are also addressed.

INTRODUCTION

In recent years, geostatistics and stochastic modeling have found their way into several scientific endeavors where they have been used in significant ways to address a diverse array of problems that are important to the well-being of mankind. Interest in these particular problem-solving approaches has expanded from rather modest beginnings to the point that individuals across almost all disciplines recognize their value and actively incorporate them into research and applications. This has become increasingly more evident as the importance of space and geography have become recognized in science and industry, and as scientists have come to embrace the ideas of spatial analysis and spatial statistics.

The increased interest in geostatistics and stochastic modeling has also roughly tracked a series of conferences on these topics that have been conducted throughout the last 30 yr. In 1975, for example, there was a North Atlantic Treaty Organization Advanced Study Institute entitled Advanced Geostatistics in the Mining Industry (although it included applications in petroleum and hydrology as well). A 1993 conference entitled Geostatistics for the Next Century provided a look at how geostatistics might impact the succeeding decades. Finally, the quadrennial International Geostatistics Congress was established nearly 30 yr ago, with the most recent installment (2004) being conducted in Banff, Alberta, Canada.

Throughout the years, many have reflected on the future of geostatistics and stochastic modeling, with at least one entire conference being dedicated to the subject (Dimitrakopoulos, 1994). At the 1996 International Geostatistics Congress held in Wollongong, New South Wales, Australia, Srivastava (1997) posed a timely question, asking, "Where are we going?" Although the question might not have been completely answered, it certainly inspired considerable debate; and since that time, there seems to have been a greater effort to give the discipline more overall focus. Clearly, not all the problems have been solved, nor all the issues addressed. The objective of the present discussion is to underscore some of the situations, both technical and philosophical, that, from the author's perspective, represent ongoing distractions

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in the field. Obviously, this will not be the last time someone reflects on the state of geostatistics and stochastic modeling; but perhaps this exchange will help to stimulate still more lively conversation, more open communication, and possibly even resolution of some of the ongoing difficulties.

It is necessary to make a few general comments at the outset of this dialog to set the stage for what is to follow. First, the distinction between stochastic methods (which for now will encompass both geostatistics and other stochastic modeling approaches) and deterministic methods is, today, somewhat blurred. In fact, the distinction is somewhat more of a perception or convenience instead of a reality. In their book entitled An Introduction to Stochastic Modeling, Karlin and Taylor (1998, p. 492) stated the following:

> A quantitative description of a natural phenomenon is called a mathematical model of that phenomenon ... A deterministic model predicts a single outcome for a given set of circumstances. A stochastic model predicts a set of possible outcomes weighted by their likelihoods or probabilities... However, phenomena are not in and of themselves inherently stochastic. Rather, to model the phenomenon as stochastic or deterministic is the choice of the observer.

Although the title of the book is An Introduction to Stochastic Modeling, it is, in fact, really about stochastic processes, which is a different topic with a different focus than is implied in the present context. Stochastic modeling, then, might be understood as somewhat more general than geostatistics, although both emphasize stochastic phenomena. However, in stochastic modeling, more emphasis is placed on modeling, whereas in geostatistics, more emphasis is placed on data analysis.

Second, most developments in geostatistics and stochastic modeling have been, and likely always will be, strongly driven by applications. Note that Holden et al. (2003) interpreted stochastic modeling as simply pertaining to the modeling of a petroleum reservoir. In fact, it is probably fair to say that not many really new ideas in this field have been promulgated through fundamental theoretical research, in the same sense that new ideas in mathematics and traditional statistics are developed from first principles. The applications-driven nature of geostatistics and stochastic modeling is broadly evident by the number and diversity of examples appearing in an ever-widening literature. As a result, some of the issues that have arisen throughout the years really stem from the proliferation of methodologies beyond the conventional boundaries of earth science in which geostatistics and stochastic modeling have evolved. Such issues are both theoretical and practical in nature and sometimes simply reflect the kind of conflict that emerges at the interface of history, language, terminology, and culture. Therefore, to understand some of the difficulties currently plaguing the discipline of geostatistics and stochastic modeling, the best place to start may be in the past.

A BIT OF HISTORY

Geostatistics is a relatively new discipline, and much of its development has occurred throughout the last 30–40 yr. Through its flagship journal, *Mathematical Geology*, the International Association for Mathematical Geology (IAMG) has largely been responsible for disseminating many of the theoretical advances in geostatistics, with other organizations, corporations, and academic institutions making many important contributions in both theory and applications. The IAMG dates from 1968, and almost from its inception, the association recognized the significance of this emerging discipline. However, even well before that time, there were many examples of probability and statistics being applied to earth science investigations. For example, the crucial work of Gandin (1963), Matheron (1965), and Matérn (1986) all predate the establishment of the IAMG. Perhaps because of language differences (Swedish in the case of Matérn and Russian in the case of Gandin) as well as Matheron's affiliation with Ecole des Mines in Paris, his work and those of his students became better known.

In retrospect, Michel David's move from Fontainebleau to the University of Montreal in 1968 (see Dimitrakopoulos and Dagbert, 2001) and Andre Journel's move from Fontainebleau to Stanford University in 1978 were watershed events that greatly increased the interest in geostatistics, particularly in the United States and Canada. Together, David (1977) and Journel and Huijbregts (1978) profoundly influenced the theoretical and methodological development of geostatistics for several decades and fundamentally altered the way scientists view the physical world. The impact of these two scholars on spatial thinking and the practice and mechanics of stochastic modeling is well known, and their names are commonly associated with the expansion of geostatistics from the earth sciences into other disciplines, including medicine, public health, business, and the environment.

Despite the extensive influence of these and other individuals, there was not a large number of people using geostatistical methods in the 1970s and into the 1980s. The knowledge base and number of practitioners have grown tremendously since then, but the community of geostatisticians and stochastic modelers remains comparatively small even today. In fact, formal academic training programs in these disciplines are still not widely available, with only a handful of universities in the United States offering such programs.

One particular problem has to do with an ongoing conflict between the practitioners of geostatistics and traditional statistical methods. Geostatistics is viewed in some circles as a reinvention and repackaging of statistical principles that were already well known; however, the most devoted of geostatisticians contend that traditional statistical methods are totally ineffectual at incorporating spatial variability. One thing seems true: the emergence of geostatistics has forced practitioners of traditional statistical methods to embrace the importance of spatial variation. In fact, interest in spatial statistics has exploded in the statistical community in the last decade. In turn, geostatisticians have come to embrace more of the traditional ideas of statistics. The two camps have certainly not yet become one; but there does seem to be a greater level of cooperation and mutual appreciation than in years gone by. Such a convergence of ideas can only be good for quantitative problem solving in general because it diminishes the distrust and misunderstanding of the techniques harbored by those who are peripheral to the conflict and who are in need of real solutions to their problems.

GEOSTATISTICS VS. STOCHASTIC MODELING

As noted above, stochastic modeling is perhaps more general than geostatistics, but other differences exist. Stochastic differential equations are models, Markov chains are models, there are models for time series, and fractals are commonly used for models. In contrast, kriging in its various forms is not really modeling. Although kriging is closely linked to modeling of the variogram or covariance function, the kriging process itself is not quite the same as modeling in the traditional sense.

Although the term geostatistics has became synonymous with the stochastic approach to spatial estimation, there are those who contend that this view is far too narrow. Given the breadth of work in spatial statistics and spatial estimation in recent years (see Anselin, 1988; Davis, 2002; Haining, 2003), this complaint could certainly be afforded some credence.

Stochastic modeling, to the extent that it is distinct from geostatistics, has, perhaps, had stronger mathematical ties. The link to mathematics is readily apparent in its many applications (e.g., turbulence problems; see Batchelor, 1953; Lumley, 1970; and the work of Kolmogorov as summarized by Hunt et al., 1991; Frisch and Kolmogorov, 1995). The principal upshot of stochastic modeling research has been to replace deterministic differential equations with stochastic differential equations, which are especially important when considering transport problems in the subsurface.

Although the breadth of applications for geostatistics has been steadily increasing, stochastic modeling is probably better known in disciplines such as hydrology and petroleum engineering. The principles of stochastic modeling are also known beyond the realm of earth and environmental science, with applications in fields such as mathematical finance and actuarial science (Actuarial Foundation, 2003). Geostatistics, however, finds most of its applications in the exploration and characterization of natural resources, with a particular historical link to the mining industry.

A natural question that might be asked, then, is whether sufficient cross-fertilization is occurring among disciplines; that is, whether the ideas and results generated in one discipline or area of application are being sufficiently used in other areas. Although it would be hard to give a definitive answer, simply asking the question raises the level of interest and consideration. Unquestionably, more interdisciplinary interaction is needed throughout all the sciences, along with more integration of science and business; and so, acknowledging the need for increased cooperation and communication could only serve to enhance the understanding of geostatistical and stochastic modeling approaches and their applications in scientific investigations.

COMPUTING AND SOFTWARE CONSIDERATIONS

To a considerable extent, it is possible to link and trace the development of geostatistics and stochastic modeling, as well as growth in their applications, to the advent of inexpensive and accessible computing (e.g., interactive multiuser systems such Digital Equipment's virtual address extension (VAX) machines and the personal computer). Ready access to computational resources has given rise to several individualized and customized computer programs, because individuals and groups have tended to develop their own software throughout the years. This is in strong contrast to the way in which software for performing more traditional statistical computation. Many of today's geostatistical algorithms were developed during the same time frame that computing capabilities were expanding, and so the algorithms had to be refined in concert with computational enhancements. Traditional statistical methods and algorithms, however, are somewhat older, and some of them predate the modern computer.

Because many of the procedures and routines used to perform traditional statistical computations were already on the shelf, it was fairly straightforward when the computer came along to operationalize and compile them into integrated packages that could be further developed and commercially distributed. Consequently, as computing organizations began to flourish in businesses and universities, statistical software packages such as the Statistical Analysis System and the Statistical Package for the Social Sciences, although in their infancy, were already available for distribution; and so, as demand increased, it was natural for these packages to be routinely acquired. In most cases, the purchase and acquisition decision, along with the provision of subsequent maintenance and support, was assigned to central computing organizations, and the code was commonly accessible only on mainframe machines. At the same time, because many organizations were obtaining and using the same software, there was a strong move toward standardization (of the algorithms) and widespread testing of the code, thereby increasing their appeal. As a direct consequence, a strong market for statistical software evolved that persists even today, with continued enhancement of the procedures and codes being almost totally commercially driven.

As suggested above, the manner in which software evolved to perform traditional statistical computations is quite different from the evolution of geostatistical programs and software for stochastic modeling. Although there is, indeed, some commercially available geostatistical software, such as the venerable Bluepack and its successor Isatis, as well as geostatistical add-ons for comprehensive statistical packages like S-Plus and geographic information systems such as ArcView developed by the Environmental Systems Research Institute, commercialization has not been the primary driver, and the market for these products is considerably smaller. For petroleum and mining companies, cost has been less of an impediment; but for many practitioners, there is a strong reliance on free software such as the aging GeoEas, GSLIB, and more recently, Gstat and GeoR, both of which have been ported to the freeware platform R. Although there are obvious advantages to this approach, there are also distinct disadvantages. For example, there is little in the systems, or by way of geostatistical practice, to ensure that the same data processed by two different software packages will produce the same results. Further, the options and features of the different implementations are not likely to be the same. In general, the algorithms are moderately well understood, but there may be extensive differences in their implementation. The advent of Fortran-based GSLIB perhaps set some standards; but GSLIB has not been systematically updated as a package. Now, many algorithms are not included, and the use of the Fortran code in batch operations is becoming outdated.

This situation is complicated, of course, by the wide variety of people, groups, and disciplines that use geostatistics and stochastic modeling. Few are exposed to the broad range of journals that now publish papers whose results are based on geostatistical analysis or stochastic modeling. In addition, companies and businesses are reluctant to divulge proprietary codes and systems because they want to maintain their competitive advantages.

Such circumstances suggest the need for increased standardization. One possible solution would be to establish a formal mechanism by which similar codes or packages could be operationally and numerically compared, with the results of such comparisons being widely disseminated. This is a common practice with regard to commercially available statistical (traditional) analysis packages (see the regular reviews that appear in publications such as *The American Statistician*). Without diminishing the uniqueness of individual codes, the objective might be to establish some common performance benchmarks that could be recognized and accepted throughout the geostatistical community.

SIMULATION

Simulation is a term that evokes different meanings for individuals working in different disciplines. It may be deterministic in character (e.g., numerical solution of a differential equation), or it may be probabilistic (e.g., Monte Carlo methods). Simulation is used for a variety of problems and applications, particularly when it is difficult or costly to obtain live data. For example, the U.S. Geological Survey has developed several routines to simulate fluid flow in the subsurface that have been widely adopted. In geostatistics and stochastic modeling, simulation commonly refers to the process of generating multiple realizations of a random function to obtain an acceptable numerical solution to a problem. One or more of these realizations may serve as the input for other computer programs (e.g., MODFLOW, the modular, three-dimensional [3-D], finite-difference ground-water–flow model developed by the U.S. Geological Survey uses simulated cell values for hydraulic conductivity to generate alternative flow patterns).

By its very nature, simulation cannot produce an answer that is absolutely correct. Although the process may yield a very good approximation that is altogether admissible, uncertainty is always associated with the result. This uncertainty arises in several ways. Obviously, assumptions that are improperly imposed, or imperfections in the estimates of one or more process parameters, can lead to questionable results; but there is also uncertainty in knowing which of the many results (or realizations) to choose from among all those that can be produced through simulation. In addition, there can be many different ways to simulate the same process or phenomenon, and so the choice of an approach, or algorithm, can also contribute to uncertainty about the result.

Several different algorithms are associated with the geostatistical or stochastic approach to simulation, including the turning-bands algorithm (which is really a procedure to generate 3-D realizations from multiple one-dimensional [1-D] realizations), covariance matrix decomposition (variously called Cholesky decomposition, LU decomposition, etc.), sequential Gaussian simulation (and multiple variants thereof), and simulated annealing (which is really based on an optimization approach of the same name). Some of these implicitly rely on assumptions pertaining to the multivariate Gaussian distribution, and all of them essentially require use of a known covariance function (i.e., only second-order properties of the random function are reproduced). Each has been developed because of perceived weaknesses or difficulties with competing or alternative approaches; but unfortunately, in many cases, it is not immediately clear how to choose among them. Little effort has been devoted to theoretical comparisons, and empirical examinations are generally complicated by the several restrictions previously suggested.

First, it is commonly the case in practice that only a small number of realizations can be generated (because of cost, time, or other constraints), with each realization encompassing only a finite (although perhaps large) number of locations. In this situation, it would be essentially impossible to conduct any meaningful numerical comparisons among the results of several competing algorithms. Second, little work has been done on the problem of selecting the best realization from among all those that can be produced through simulation. Because process parameters are commonly assumed to be characterized by statistical distributions (e.g., Gaussian), any number of different realizations can be randomly produced, and identification of one or more that appear to be optimum is largely a subjective process. Finally, on an even more fundamental level, the initial choice of the algorithm(s) itself is important if the simulation results (i.e., the realizations) are to be used for further analysis or for decision making because those results are likely to change if a different algorithm is selected. Note that, with the exception of simulated annealing, the various algorithms only reproduce the distributional characteristics of the quantity of interest in an average sense (i.e., averaged across realizations), and so, direct comparisons of individual realizations produced by different algorithms using essentially the same inputs would not be completely valid anyway.

An additional aspect of simulation that has received inadequate attention is random-number generation. All geostatistical-simulation algorithms rely on random-number generators when producing various results, and yet there is a tendency in the literature to ignore the possible effects arising from inappropriate or inadequate procedures (see Van Niel and Laffan, 2001). This situation begs for more theoretical and empirical investigation, but virtually no work has been done on it within the geostatistical community. A solid research effort to examine and substantiate the quality of random-number generation algorithms could yield great dividends and broaden the collective understanding of simulation in the geostatistical context.

THE NOTION OF SUPPORT

One of the crucial distinctions between spatial statistics (which could be interpreted as including both geostatistics and stochastic modeling) and what might be called classical or traditional statistics is the explicit recognition of the importance of the support of the data. Support has to do with the idea that the value of some quantity of interest is related to the physical size (and possibly the dimensions) of the unit on which it is recorded. For example, in the context of ore reservation estimation, it is commonly the case that assay values are associated with the volume and shape of a core, and average grades are associated with the size and shape of mining blocks. A fundamental understanding of this notion has developed over the years in various disciplines. For example, in geography, it is widely known as the "modifiable areal unit" problem; and in a classic paper, Smith (1938) recognizes its implications for agriculture. For a discussion of Smith's results in the context of geostatistics, see Zhang et al. (1990). Although much of the investigation of support predates the more recent expansion of geostatistical methodology, the ideas of block kriging and regularized variograms are, in fact, tools for incorporating the idea of support into geostatistical analyses.

The theory pertaining to these tools is fairly well known, yet practical problems of application still need to be solved. For example, computing point-to-block and block-to-block covariances is commonly accomplished through numerical integration, which is imbedded in software. However, the software options often do not accommodate the irregularly shaped regions that are commonly found in practice, and so, the notion of support is incompletely or inaccurately addressed. Furthermore, whereas a regularized variogram or covariance can be theoretically related to a point support model, it is difficult in practice to obtain such a model from nonpoint support data. Such difficulties arise, for example, in the contexts of upscaling and downscaling geological, petrophysical, or engineering properties. Still other complications may occur in practice when determining the actual support of the data (e.g., when hydraulic conductivity is measured using a pumping test), resulting in restricted application of the currently known theory.

BAYES, ENTROPY, AND MULTIPOINT CORRELATION

As suggested above, an even more diverse array of ideas from traditional statistics have made their way into geostatistical thinking and research in recent years. Three such ideas, in particular, have captured the interest and imagination of practitioners.

The first has to do with multipoint correlation. Both the variogram and the covariance function are two-point functions (i.e., each quantifies the similarity or dissimilarity of the values at a pair of locations in space). Each is a second-moment function. Geostatistics and, to some extent, stochastic modeling are strongly based on the assumption that knowledge of second-order moments is sufficient. The kriging equations depend only on the variogram or covariance (with appropriate assumptions about the mean) and not on other properties or characteristics of the random function. However, it is also known that second-order moments are far from adequate in characterizing even a second-order stationary random function. The variogram is somewhat analogous to a derivative in the sense that both filter out constants because both are based on first-order differences. In contrast, higher order generalized functions are based on higher order differences. First-order differences are essentially dimension-free, whereas higher order differences are not. As seen in Delfiner (1976), to generate sample-generalized covariances, it is necessary to construct higher order differences. To obtain acceptable multiple first-order differences, one may rigidly translate any pair of points. The coefficients in the difference (+1,−1) remain unchanged; but the same is not true for a second-order difference. In 1-D space, one can take the trio of points ($s - h, s, s + h$) with coefficients (1,−2,1), respectively. Moreover, if the pattern of points is rigidly translated, then the coefficients will likely change. Hence, what might seem to be an obvious extension to two-dimensional space does not work.

Although a multiple-point correlation function is not quite the same as a generalized covariance, some analogies are present. Under a second-order stationarity assumption, $\mathrm{Cov}(Z(s + h), Z(s))$ is a function of h alone. Even without this assumption, the geometrical pattern determined by the pair of points is the same (a line segment; although its orientation might change) and is not dependent on the magnitude of h. In contrast, the assumption that $\mathrm{Cov}(Z(s), Z(s + h_1), Z(s + h_1), \ldots, Z(s + h_K))$ is only a function of $(h_1, \ldots, h_K)$ is much stronger. Moreover, the geometrical pattern of the points $(s, s + h_1, \ldots, s + h_K)$ can change greatly as the relative magnitudes and the orientations of the $(h_1, \ldots, h_K)$ change. Clearly, $\mathrm{Cov}(Z(s), Z(s + h_1), Z(s + h_1), \ldots, Z(s + h_K))$ captures more information than $\mathrm{Cov}(Z(s + h), Z(s))$.

Various authors (e.g., Guardano and Srivastava, 1993; Krishman and Journel, 2003) have proposed some form of multipoint correlation function that would characterize the random function to a greater degree. This idea does not seem to have progressed very far, and practical difficulties still exist. In particular, estimating and modeling such functions would likely require large data sets. There is also the question of how to actually apply such functions.

The second issue concerns the evolution of geostatistical methods that have been developed from the Bayesian point of view (see Diggle et al., 2003). In the traditional statistics literature, there are commonly heated disputes about whether the Bayesian or frequentist approach is better. Both the successes of Bayesian statistics and the advent of greater computing power have led to an interest in Bayesian geostatistical methods. The geoR package for R incorporates basic Bayesian geostatistical tools (also, see Diggle and Tawn, 1998). Whether such approaches continue to be developed likely depends on the availability of appropriate software, and currently, such software is not widely available.

The third issue has to do with an evolving understanding about the results obtained with kriging, which, of course, is a widely used spatial estimation procedure. The usual kriging equations are obtained by minimizing the estimation variance (with the unbiasedness constraint); and, yet, it is now well known that the resulting kriging variance is not exactly a variance in the usual sense of the term. The kriging variance does not directly depend on the data and, hence, provides only a relative measure of reliability. This has led to an interest in entropy, best exemplified by the work of G. Christakos (e.g., Journel and Deutsch 1993; Christakos and Li, 1998; Hristopulos and Christakos, 2001). Several definitions of entropy exist, and one must be careful to distinguish between the discrete and the continuous case (see Cover and Thomas, 1991, especially chapters 9 and 11). First, consider the discrete case. Suppose there are outcomes $E_1, \ldots, E_n$ with associated probabilities $p(E_1), \ldots, p(E_n)$. Then, the information-theoretic entropy is given by

$$-\sum p(E_i) \ln p(E_i)$$

This is also known as Shannon's (1948) entropy but is also found in Pauli (1933). It can be interpreted as the average loss of ignorance or gain in knowledge.

For many applications, however, one must consider continuous distributions. If $f(x)$ is the density function of a univariate continuous random variable, then the entropy is defined as

$$H(f) = -\int f(x) \ln f(x) \mathrm{d}x$$

This expression is different from the entropy for a discrete random variable. The values of the density function are not probabilities, and in particular, they are not bounded by the interval [0,1]. Thus, the entropy may not exist (i.e., the [improper] integral may not converge to a finite value). Moreover, it need not be positive.

To make this definition consistent with the previous one, it is necessary to introduce a reference density $g(x)$ and consider the following integral:

$$-\int f(x) \ln[f(x)/g(x)] \mathrm{d}x$$

The justification for maximizing the entropy can be made from various perspectives, but even then, the solution is not unique. It is commonly noted or claimed that the normal distribution has maximum entropy. This is not quite complete; a question about additional constraints must be addressed. If the density function is only nonzero on an interval $[a,b]$, then the uniform distribution has maximum entropy. If the density is only nonzero for $[0, \infty)$ and the expected value is fixed, then the exponential distribution has maximum entropy. If the density function is nonzero on $(-\infty,\infty)$ with fixed expected value and fixed variance, then the normal distribution has maximum entropy. The actual maximal value will depend on the variance. In Bayesian maximum entropy, it is the posterior distribution for which the entropy is maximized.

Unfortunately, this higher level of mathematical complexity and a lack of readily available software have precluded a formal test of whether the entropy results are really better than those obtained with the usual forms of kriging. Additional investigation is clearly needed, but such work may simply have to wait until practice and operational implementation catches up more with theory.

With regard to each of these issues (as well as others), an impediment to further development and expanded application seems to be the absence of software, especially at the commercial or semicommercial level. That such software is not yet readily available likely reflects a lack of easily translatable algorithms and a general immaturity of the scientific principles. Although this situation is expected to change, the extent to which such ideas will permeate geostatistical thinking in practice is yet to be determined.

DESCRIPTIVE OR INFERENTIAL?

Traditional statistics operates at two levels: descriptive and inferential. If the objective is to summarize the measurements represented by a given data set, then the task is a descriptive one (hence, the term "descriptive statistics"). However, if the data are assumed to be a random sample from a larger population and the objective is to use such sample data to draw conclusions or make inferences about the entire population, the task is one of inference (hence, the term "inferential statistics"). Both geostatistics and stochastic modeling are somewhat closer to descriptive statistics than to inferential statistics. That is, drawing conclusions about the specific data set and/or the specific source of the data is more common than drawing conclusions about the entire population in question. In particular, the geostatistical literature is almost void of references to tests of hypotheses, which is a fundamental approach to traditional statistical inference, particularly from the frequentist viewpoint. However, hypothesis testing could be a valuable factor. For example, it might be desirable to test the underlying assumptions of the modeling approach (such as second-order or intrinsic stationarity) or to evaluate the goodness of fit of the variogram and covariance function. The book by Stein (1999) is perhaps one of the few texts that devotes any space to such ideas. Whitten (2003) raises a more general question about the function of hypothesis testing and questions why this has received less attention. Pardo-Igúzquiza and Dowd (2004) provide one example of applying hypothesis testing in the context of geostatistics.

UNCERTAINTY AND RELIABILITY

Statistics, by its very nature, is intended to deal with problems and data in a manner that acknowledges conclusions will be couched in terms of uncertainty (e.g., probabilities of types I and II errors associated with hypothesis testing; confidence level and margin of error associated with confidence interval estimates of population parameters). When kriging was first introduced and promoted as a superior estimation technique (i.e., superior to the nearest neighbor technique commonly in use at the time), one of the claimed advantages was that the estimates have minimum variance (i.e., the kriging variance is minimum). As suggested above, it was subsequently recognized that the kriging variance is more a function of the data location pattern and the variogram model than it is of the data themselves. At best, it is a relative measure of reliability because it can be artificially increased or decreased without changing the estimated values. Moreover, as what has been pointed out by several authors, the kriging variance does not truly incorporate the uncertainty associated with estimating and modeling the variogram. This point is addressed, at least in part, by Stein (1999) but under rather strong assumptions. Consequently, the question might be asked as to whether there are more adequate ways to quantify the uncertainties associated with spatial estimation; and if so, how can they be used in a practical problem?

Although interest in quantifying the uncertainty associated with variogram modeling goes back at least to Davis and Borgman (1979, 1982), there have been a series of more recent papers (e.g., Pardo-Igúzquiza and Dowd, 2001; Ortiz and Deutsch, 2002; Marchant and Lark, 2004). One important point is commonly ignored: the sample variogram estimates the values of the variogram but does not directly estimate the variogram itself (i.e., the function). In practice, then, one must choose a family of variograms (e.g., Matérn, spherical, and power with one or more parameters). Then, the sample variogram or the variogram cloud is used to estimate the parameters. The problem is even more complicated in the case of a nested model variogram. Neither maximum likelihood nor weighted least squares do a good of job of detecting the different components in a nested model (or even the need for one). Although Matheron (1973) gives an integral representation for variograms, it is more difficult to translate this into practical use. Several extant results also make use of a multivariate normality assumption, and hence, they are most applicable in the case of variograms linked to covariance functions. Again, this is an area in which more work is needed.

COLLABORATIVE EFFORTS IN RESEARCH AND SOFTWARE DEVELOPMENT

A great deal has already been made of the importance of software to the proliferation of geostatistical methodology and stochastic modeling approaches. As already suggested, it appears that future developments will be strongly intertwined with the creation of software packages that implement the various ideas, algorithms, and approaches. Such an effort requires substantial financial and intellectual resources. The geostatistical community has greatly benefited in this respect from collaboration between industry and academia. One successful approach, which became popular in the 1980s, has been for the consortia of companies to provide financial backing of academic research programs in the form of a participation fee to obtain proprietary access to research results and computational code. At least four such collaborative efforts are worth noting, each involving one or more academic groups and one or more segments of the petroleum industry.

At the top of this list is the Stanford Center for Reservoir Forecasting (SCRF), which is well known among, and well supported by, oil companies. Over the years of its existence, SCRF has given birth to many new ideas in geostatistics, producing numerous research publications. Most of the actual details of the algorithms, as well as specialized codes, are reserved, of course, for the financial supporters and participants.

The gOcad project at the University of Nancy, which is focused on 3-D Earth modeling, is another such collaboration between industry and academia. The consortium has resulted in the development of the well-known gOcad software package, which provides an alternative to traditional computer-aided drawing of complex geological surfaces based on discrete smooth interpolation. Although the actual software is reserved for supporters and group members, the theory is well documented in the book entitled Geomodeling (Mallet, 2002), and both petroleum and environmental applications have been reported.

A third example is Petbool, which is both a research project and a software package originating out of the collaboration between the Pontifical Catholic University in Rio de Janeiro and Petrobras (see Tavares et al., 2001). The acronym Petbool stands for the combination of Petrobras and Boolean, and the software provides 3-D visualization capabilities, along with object-based geological modeling of oil reservoirs.

Finally, the Statistical Analysis of Natural Resources group at the Norwegian Computing Center has developed multiple software packages largely targeting the petroleum industry, which are summarized and discussed in a recent article by Holden et al. (2003).

The collaborative approach has been both good and bad for the geostatistical community. Although it has resulted in many new discoveries and developments that have greatly expanded the scientific and computational boundaries of the discipline, the proprietary nature of programs has somewhat restricted their application. Individuals and groups without the financial resources to participate are left struggling to devise alternative computational approaches on their own, which has led to unnecessary tension between those who have access to the best algorithms and code and those who do not, as well as incomplete understanding of the solutions to problems that can be obtained. Consequently, both the industry and the scientific community might now be better served by more open communication of geostatistical knowledge and greater accessibility to software than what has been available in the past. Such a suggestion, of course, requires a different kind and level of cooperation and a great deal of leadership and effort to make it work. More immediately, a survey article providing a more detailed summary and comparison of the different analytical and modeling approaches, as well as the software capabilities, would be very useful. The practices common in the broader field of statistics may be relevant here. STATLIB (http://lib.stat

.cmu.edu/) is an archive of algorithms and program codes. As noted previously, *The American Statistician* has a regular section devoted to the review of statistical packages. In addition, a section of the American Statistical Association is devoted to statistical software and graphics.

LANGUAGE DIFFICULTIES

As in the case of all scientific disciplines, there have been many controversies within the geostatistical community over the years. Interestingly, argument about the meaning and intent of some of the fundamental terminology still exists. For example, the term "variogram" was originally used to denote the quantity

$$\mathrm{Var}[Z(s+h) - Z(s)] = 2\gamma(h)$$

under the assumption that it was finite for all values of s and h and did not depend on s (see Matheron, 1971). However, under the second-order stationarity assumption, it is easy to show that

$$0.5\ \mathrm{Var}[Z(s+h) - Z(s)] = \mathrm{Var}[Z(s)] - \mathrm{Cov}[Z(s+h), Z(s)]$$

or

$$\gamma(h) = C(0) - C(h)$$

where $\gamma(h) = 0.5\mathrm{Var}[Z(s+h) - Z(s)]$ and $C(h) = \mathrm{Cov}[Z(s+h), Z(s)]$. Thus, it was natural to focus more on half of the variogram; hence, the term "semivariogram." However, it soon became apparent that there were few, if any, instances in geostatistics where it was really necessary or even useful to consider the (original) variogram instead of the semivariogram (as an example, the kriging equations are easily derived and written in terms of the semivariogram). In the 1980s, many authors began using the term variogram to denote the semivariogram, omitting any reference to the original quantity. There were two principal advantages of this shift: (1) it simplified the language usage in all written and oral communications (e.g., experimental variogram seemed easier to say and communicate than experimental semivariogram); and (2) it avoided the confusion created when the two terms were used interchangeably or incorrectly, even when a distinction might have been technically correct.

Clearly, the shift in terminology was not and is not universal, and there are those who insist on using the original usage, which is certainly their prerogative. It is difficult to say which term is more common today; but, as an example, an examination of the proceedings of the 1988 International Geostatistics Congress in Avignon, France, suggests that most authors (or perhaps the editor) used variogram exclusively, a few used semivariogram exclusively, and a few others used the two terms interchangeably. A similar pattern can be observed in many later texts and compilations. The documentation for some software packages (e.g., GeoEas, http://www.epa.gov/nerlesd1/databases/geo-eas/access.htm) only uses variogram, and several authors (e.g., Chiles and Delfiner, 1999) only acknowledge semivariogram as an older, unused term. The issue is not, and likely never will be, resolved.

Unfortunately, this is not the only inconsistency in geostatistical terminology. At least two other words (or terms) that appear with some frequency in the literature do not always have precise meanings. "Robust" (or robustness) is one example. Kendall and Stuart (1979, p. 492) wrote that "A statistical procedure which is insensitive to departures from the assumptions which underlie it is called robust." This definition is originally attributed to Box (1953). The problem is that the assumptions underlying a particular procedure may not be clearly stated, or their relevance may not be clearly understood; and so, too commonly, the term robust is used as a general catch-all adjective. In the context of geostatistics, it is generally thought that the ordinary kriging estimator is robust with respect to the values of the variogram parameters. However, it may not be so robust with respect to the underlying distribution of the random function or the intrinsic stationarity assumption; and so, as a broadly descriptive term, robustness may not be an appropriate characterization.

Another word that presents some interpretive difficulties is "representativeness." Sometimes, it will be claimed that a sample is representative, and occasionally, other quantities or statistics are called representative. Unfortunately, it is commonly unclear in what sense the characteristic of representativeness applies. Intuitively, representative is a word that sounds desirable, and consequently, it is tempting to claim that some quantity or procedure is representative. It is easy, in fact, to think of ways in which samples might be considered representative. For example, if the empirical distribution of the sample is the same or nearly the same as the distribution of the population, then the sample might be called representative. In this case, the sample mean and variance might be expected to be close to the population mean and variance, respectively. Unfortunately, none of these attributes can be known in advance, and in fact, the population may not have a finite mean or finite variance. Obviously, random samples need not be representative at all. Hence, to remove the ambiguity and to avoid confusion, it would be extremely helpful in all communications of this nature for geostatisticians and their colleagues to explicitly state the sense in which representativeness applies.

Although language differences might not be the primary cause of divisions among practitioners, they still represent a source of irritation and confusion for those outside the immediate geostatistical community, and they do not serve to place the field in the best scientific light. To ensure the future of the discipline, geostatisticians would do well to engage in a conversation aimed at standardizing language and terminology and in making geostatistical communications more effective, more understandable, and more accessible to a wider range of potential users.

FINAL THOUGHTS

It seems obvious that geostatistics and stochastic modeling are alive and well, and that they will continue to be adapted and exploited for the foreseeable future. As suggested earlier, neither discipline has evolved by altogether conventional means through largely theoretical academic endeavors, but instead, through extensive experience, practice, and applied problem solving in the context of a rich and diverse array of applications. It is this focus on applications that makes the tools of these disciplines so attractive in many areas of investigation.

In 50 or even 20 yr, geostatistics and stochastic modeling will no doubt look different. They may continue to converge, or they may diverge along entirely new or different paths. However, if history is a strong indicator of the future, it seems certain they will further evolve within an applications and problem-solving framework. There will be theoretical enhancements, to be sure, and perhaps some truly astonishing breakthroughs; but the need to address both simple and thorny questions from an applied point of view is likely to remain the primary driver.

In a very real sense, the world is becoming smaller with the relentless advances of technology. As a result, science, business, industry, medicine, politics, and the like are becoming increasingly focused on spatial relationships. It is the spatial domain in which stochastic modeling and geostatistics found their beginnings, and it is within this same spatial domain that they will surely continue to flourish.

Obviously, the future is unknown; but stochastic modeling and geostatistics seem destined to exert even greater influence on the way people think about the world around them. Although their past contributions will persist, there will likely be many new applications and developments that will have profound influence on global thinking and well-being. This book catalogs some of the many examples illustrating progress and enhancements throughout the last 10 yr, specifically in the rich areas of earth and petroleum science that have been traditional strongholds for geostatistics and stochastic modeling since their early beginnings. The next decade and beyond promises to be an equally productive and exciting time in which geostatistics and stochastic modeling impact not only the geosciences but important areas of investigation far beyond this traditional base.

REFERENCES CITED

Actuarial Foundation, 2003, Stochastic modeling Symposium, September 4–5, Toronto: http://www.actuaries.ca/meetings/archive_stochasticsymposium_2003_e.html (accessed April 15, 2005).

Anselin, L., 1988, Spatial econometrics: Methods and models: Dordrecht, Kluwer Academic Publishers, 284 p.

Batchelor, G. K., 1953, The theory of homogeneous turbulence: New York, Cambridge University Press, 197 p.

Box, G. E. P., 1953, Non-normality and tests on variances: Biometrika, v. 40, p. 318.

Chiles, J.-P., and P. Delfiner, 1999, Geostatistics: Modeling spatial uncertainty: New York, John Wiley & Sons, 695 p.

Christakos, G., and X. Li, 1998, Bayesian maximum entropy analysis and mapping: A farewell to kriging estimators?: Mathematical Geology, v. 30, p. 435–462.

Cover, T. M., and J. A. Thomas, 1991, Elements of information theory: New York, John Wiley & Sons, 542 p.

David, M., 1977, Geostatistical ore reserve estimation: Amsterdam, Elsevier, 364 p.

Davis, B. M., and L. E. Borgman, 1979, Some exact sampling distributions for variogram estimators: Mathematical Geology, v. 11, p. 643–653.

Davis, B. M., and L. E. Borgman, 1982, A note on the asymptotic distribution of the sample variogram: Mathematical Geology, v. 14, p. 189–193.

Davis, J., 2002, Statistics and data analysis in geology, 3d ed.: New York, John Wiley & Sons, 638 p.

Delfiner, P., 1976, Linear estimation of non-stationary spatial phenomena, *in* M. Guarascio, M. David, and C. J. Huijbregts, eds., Advanced geostatistics in the mining industry: Dordrecht, D. Reidel Publishing Company, p. 49–68.

Diggle, P., P. J. Ribeiro Jr., and O. F. Christensen, 2003, An introduction to model-based geostatistics, *in* J. Møller, ed., Spatial statistics and computational methods: New York, Springer, p. 43–86.

Diggle, P. J., and J. A. Tawn, 1998, Model based geostatistics: Applied Statistics, v. 47, p. 299–350.

Dimitrakopoulos, R., 1994, Geostatistics for the next century: Dordrecht, Kluwer Academic Publishing, 497 p.

Dimitrakopoulos, R., and M. Dagbert, 2001, Farewell to Michel David (1945–2000): Mathematical Geology, v. 33, p. 241–244.

Frisch, U., and A. N. Kolmogorov, 1995, Turbulence: The legacy of A. N. Kolmogorov: New York, Cambridge University Press, 310 p.

Gandin, L. S., 1963, Objective analysis of meteorological fields: Leningrad, Gidrometeorologicheskoe Izsatel'stvo (GIMIZ), 242 p. (reprinted by Israel Program for Scientific Translations, Jerusalem, 1965).

Guardano, F., and M. Srivastava, 1993, Beyond bivariate moments, *in* A. Soares, ed., Geostatistics Troia '92: Dordrecht, Kluwer Academic Publishing, p. 133–144.

Haining, R., 2003, Spatial data analysis: Theory and practice: New York, Cambridge University Press, 432 p.

Holden, L., P. Mostad, B. Nielsen, J. Gjerde, C. Townsend, and S. Ottesen, 2003, Stochastic structural modeling: Mathematical Geology, v. 35, p. 899–914.

Hristopulos, D. T., and C. Christakos, 2001, Practical calculation of non-Gaussian multivariate moments in spatiotemporal Bayesian maximum entropy analysis: Mathematical Geology, v. 33, p. 543–568.

Hunt, J. C. R., O. M. Phillips, and D. Williams, 1991, Turbulence and stochastic processes: Kolmogorov's ideas 50 years on: London, Royal Society, 240 p.

Journel, A. G., and C. V. Deutsch, 1993, Entropy and spatial disorder: Mathematical Geology, v. 25, p. 329–356.

Journel, A. G., and C. J. Huijbregts, 1978, Mining geostatistics: New York, Academic Press, 600 p.

Karlin, S., and H. Taylor, 1998, An introduction to stochastic modeling, 3d ed.: San Diego, Academic Press, 631 p.

Kendall, M., and A. Stuart, 1979, The advanced theory of statistics, 4th ed.: New York, Macmillan Publishing, v. 2, 748 p.

Krishman, S., and A. G. Journel, 2003, Spatial connectivity: From variograms to multiple-point measures: Mathematical Geology, v. 35, p. 915–926.

Lumley, J. L., 1970, Stochastic tools in turbulence: New York, Academic Press, 194 p.

Mallet, J.-L., 2002, Geomodeling: New York, Oxford University Press, 599 p.

Marchant, B. P., and R. M. Lark, 2004, Estimating variogram uncertainty: Mathematical Geology, v. 36, p. 867–898.

Matérn, B., 1986, Spatial variation, 2d ed.: Berlin, Springer-Verlag, 151 p.

Matheron, G., 1965, Les variables regionalisees et leur estimation: Paris, Masson et Cie, 305 p.

Matheron, G., 1971, The theory of regionalized variables and its applications: Fontainebleau, Ecole Nationale Supérieure des Mines de Paris, Les Cahiers du Centre de Morphologie Mathématique, Fascicule 5, 211 p.

Matheron, G., 1973, The intrinsic random functions and their applications: Advances in Applied Probability, v. 5, p. 439–468.

Ortiz, C. J., and C. V. Deutsch, 2002, Calculation of uncertainty in the variogram: Mathematical Geology, v. 34, p. 169–184.

Pardo-Igúzquiza, E., and P. Dowd, 2001, Variance–covariance matrix of the experimental variogram: Assessing variogram uncertainty: Mathematical Geology, v. 33, p. 397–420.

Pardo-Igúzquiza, E., and P. Dowd, 2004, Normality tests for spatially correlated data: Mathematical Geology, v. 36, p. 659–682.

Pauli, W., 1933, Handbuch der physik: Berlin, Springer, v. 24, pt. 1, 151 p.

Shannon, C. E., 1948, A mathematical theory of communication: The Bell System Technical Journal, v. 27, p. 379–423, 623–656.

Smith, H. F., 1938, An empirical law describing heterogeneity in the yields of agricultural crops: Journal of Agricultural Science, v. 28, p. 1–23.

Srivastava, R. M., 1997, Matheronian geostatistics: Where are we going?, *in* E. Y. Baafi and N. A. Schofield, eds., Geostatistics Wollongong '96: Dordrecht, Kluwer Academic Publishing, p. 53–68.

Stein, M., 1999, Interpolation of spatial data: Some theory for kriging: New York, Springer, 247 p.

Tavares, G., H. Lopes, S. Pesco and C. Poletto, 2001, Petbool: A software for stochastic modeling of geometric objects, *in* U. Bayer, H. Burger, and W. Skala, eds., IAMG 2002, Proceedings of the Annual Conference of the International Association for Mathematical Geology: Berlin, Terra Nostra, p. 203–208.

Van Niel, K. P., and S. W. Laffan, 2001, Caveat emptor: Random number generators in geospatial analysis, *in* D. V. Pullar, ed., Proceedings, 6th International Conference on Geocomputation: Queensland, University of Brisbane, 3 p.

Whitten, E. H. T., 2003, Mathematical geology in perspective: Has objective hypothesis testing become overlooked?: Mathematical Geology, v. 35, p. 1–8.

Zhang, R., A. Warrick, and D. E. Myers, 1990, Variance as a function of sample support size: Mathematical Geology, v. 22, p. 107–121.