

This slim volume is the culmination of more years' effort than its modest thickness might suggest. The usual difficulties of inspiration, coordination, and communication common to all committee activities were compounded by traumatic changes in the parent organizations themselves. The directorship of COGEODATA passed from the dynamic hands of W. W. Hutchison (Canada) to those of Richard Sinding-Larsen (Norway), and with the transition came a shift in emphasis from scientific review and synthesis to third-world technology transfer. The subject-area Working Groups of COGEODATA have been phased out; this publication is the final activity of the Working Group on Data Capture and Display.

CODATA itself was not without its vicissitudes. The ambitious project on time- and space-dependent data was to review the state of the art in each of ten scientific disciplines ranging from astronomy to biomedicine to soil science. Synoptic reviews of techniques used in each discipline to gather, store, and analyze time- and space-dependent data were to be published as a single, large volume, extensively cross-indexed to aid interdisciplinary investigations. The central Task Group, chaired by Roger Tomlinson (Canada) and funded by CODATA and UNESCO, established Working Groups in each field. Unfortunately, the fiscal resources necessary to continue the coordination and exhortation of the Working Groups did not appear, and deprived of strong leadership, activity in most areas slowly ground to a halt.

Perhaps geologists are more dogged than other scientists, or perhaps the synergism from the melding of two groups, both in their last hours, was sufficient to propel the geology committee to completion of its task. Perhaps is was just a nagging editor. In any case, here is the result—a unique compendium, complete with glossary, of the methods and techiques used to study time—and space—dependent phenomena in geology. It is the Working Group's hope that this review will be interesting and useful, not only to Earth scientists, but to others who may be able to adopt our approaches.

As Chairman, I would like to extend my sincere thanks to the members of the Working Group who gave so freely of their knowledge and effort in what at times must have seemed a futile cause. I would also like to thank the Kansas Geological Survey for providing the mechanism for final publication of the Working Group's efforts.

John C. Davis, Chairman
CODATA/COGEODATA Working Group on
Time- and Space-Dependent Data in Geology

The picture of Mt. St. Helens, spectacularly engaged in an instantaneous event, was provided by the Photographic Library of the U.S. Geological Survey.

SURVEY ON TIME-AND SPACE-DEPENDENT DATA IN THE EARTH SCIENCES

CODATA/COGEODATA Working Group on Geology

Jo Anne DeGraffenreid, Editor

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ABOUT THIS PUBLICATION

Many scientific disciplines treat phenomena that vary in time or space. To describe and analyze the properties of these phenomena, scientists may use methods that are quite general, such as time series statistics, or they may apply techniques that are unique to a specific field. These methods and special techniques sometimes prove to be useful outside the discipline in which they have been developed, if they are brought to the attention of practitioners in other specialties. Too often such communication is lacking. The scientific literature records an unfortunate incidence of "the reinvention of the wheel"—the same methodologies are developed independently in different fields. This duplication results in confusion and an unnecessary investment of time and effort.



Recognizing the need for cooperation and interdisciplinary exchange of scientific information, a committee was set up for this purpose by the International Council of Scientific Unions (ICSU). CODATA, the Committee on Data for Science and Technology, was established by ICSU in 1966. CODATA was originally concerned only with basic physical properties; however, within a decade the widespread use of computers, the development of scanners, digitizers, and remote-sensing satellites, and the proliferation of special instruments and devices produced enormous quantities of time- and space-dependent data. This vast amount of information created severe data-handling problems and led to a tremendous increase in research on spatial and temporal properties. To draw together representatives of those fields in which time- and space-varying phenomena were of special concern, a CODATA Task Group was established under the chairmanship of Dr. Roger Tomlinson (Canada).



The CODATA Task Group on Space and Time Dependent Data determined to publish a compendium of methods and techniques used to treat spatial and temporal data in ten scientific disciplines, including the field of geology, represented by Task Group member Dr. John Davis (USA). Within each of the ten disciplines, a Working Group was to be chosen to produce a written survey of that particular specialty. At that time Davis served also as Chairman of the Working Group on Data Capture and Data Display of COGEODATA. [The geological sciences had not been included within the purview of CODATA at its inception, so a parallel organization, COGEODATA (Committee on Storage, Automatic Processing and Retrieval of Geological Data), was established the following year by the International Union of Geological Sciences.]



Much of geologic data is spatial in nature, thus the COGEODATA group, already at work in the area of data capture and display, received a dual charge to serve also as members of the Working Group on Geology within the CODATA Task Group. This publication is the result of their survey, and represents a cooperative effort involving the two international bodies and the Kansas Geological Survey, which has provided operational support for the study. It is simultaneously the final contribution of the COGEODATA Working Group on Data Capture and Data Display, the chapter prepared by the Working Group on Geology for the volume to be issued by the CODATA Task Group on Space and Time Dependent Data, and No. 6 in the Kansas Geological Survey's Series on Spatial Analysis.

The names of the CODATA/COGEODATA Working Group members are listed below. Individual sections of this report were submitted by committee members in their areas of speciality, but all were free to comment upon and make contributions to other sections, many of which have been extensively edited and modified. For this reason, specific parts are not identified by author; rather, the publication should be regarded as a contribution by the Working Group as a whole. It is dedicated to the common goals of the sponsoring organizations: improved communication, international cooperation, and interdisciplinary transfer of scientific knowledge and technology.

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SURVEY ON TIME- AND SPACE-DEPENDENT DATA IN THE EARTH SCIENCES CODATA/COGEODATA Working Group on Geology

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INTRODUCTION

The discipline of geology embodies two distinct but intertwined objectives. On one hand it is committed to resolving and understanding the evolution and history of the Earth. On the other, it is equally committed to finding and extracting those natural resources of the Earth that are essential for the maintenance of human civilization. Both of these objectives are closely related; the search for natural resources provides much of the data and financial backing for more basic studies, and "academic" investigations (as into plate tectonics) provide the framework for major exploration efforts.

Both types of investigation are intensely involved with the analysis of temporal and spatial data. All geologic data are characterized by both spatial and temporal aspects, although in specific instances these may not be emphasized. Geologists are concerned with the evolution of a three-dimensional Earth through time, in which changes in the temporal domain are intimately linked to changes in the geographic dimensions. For the sake of comparison with other scientific fields, and to simplify the exceedingly complex interrelations which exist, spatial and temporal methodologies will be separated in this report. This distinction is artificial, for the two aspects are not independent. Indeed, it is this interdependency between changes which have occurred through geologic time with variation in space within the Earth that gives the study of geology its unique character.

The literature of geology contains extensive references to classical methods of univariate and multivariate analysis. Elementary statistical procedures are discussed in the book by Till (1974). Griffiths (1967) has explored the applications of analysis of variance to sedimentary petrology, and Koch and Link (1970, 1971) provide discussions of the use of analysis of variance, regression, and other statistical tests in mine evaluation. Numerous authors, mostly paleontologists, have utilized classification techniques such as cluster analysis to categorize fossil organisms, sedimentary environments, and other geologic entities which possess multiple attributes. Extensive applications of eigenvector techniques, including principal components analysis, canonical correlation, and factor analysis, have been made in the Earth sciences; these are discussed at length in Jöreskog, Klovan, and Reyment (1976). However, these methods and applications do not explicitly make use of the spatial and temporal character of geologic data, and so are indistinguishable in their basic nature from similar studies in chemistry, biology, and other sciences. Such methods and their applications will not be considered further here; an overview of these is given by Davis (1973).

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- Griffiths, J. C., 1967, Scientific Method in Analysis of Sediments: McGraw-Hill Book Co., New York, 508 p.
- Jöreskog, K. G., J. E. Klovan, and R. A. Reyment, 1976, Geological Factor Analysis: Elsevier, Amsterdam, 178 p.
- Koch, G. S., and R. F. Link, 1970, Statistical Analysis of Geological Data, Volume 1: John Wiley & Sons, New York, 375 p.
- Koch, G. S., and R. F. Link, 1971, Statistical Analysis of Geological Data, Volume 2: John Wiley & Sons, New York, 438 p. [Both volumes are now available as a single paperbound edition from Dover Publications, New York.]
- Till, R., 1974, Statistical Methods for the Earth Scientist: John Wiley & Sons, New York, 154 p.

GEOLOGIC DATA BANKS

The geological sciences are concerned with the accumulation and interpretation of spatially distributed data for many purposes. Geologic data represent an enormous range of scale, from the microscopic (for example, the shapes and positions of mineral grains in a rock), to global (the arrangement of continents and their structural features). Data banks of geological information cover the spectrum of the science itself (Hubaux, 1972), and the entries almost always have some spatial attri-In many instances this attribute is a coordinate location representing a sample or observation taken at a point on the Earth's surface. The structure and organization of geologic data banks inevitably reflect both the nature of the data and the requirements of the geological interpretation. The following examples illustrate the variation in type of data, processing requirements, and uses of the data.

FIELD MAPPING DATA

Geological field mapping (Hutchison, 1975) classically is performed by a geologist traversing an area making observations (often personal notes) about type, color, texture, and other properties of rock at various points along the traverse. Physical samples may be collected and sent to laboratories for analyses of various types; the results also relate to the individual points. The data thus include both quantitative and qualitative attributes associated with spatial coordinates. Such data are processed to define map units of consistent rock type in the area, their relationships to each other, and to units in other areas. The ultimate product is a geological map, which consists of entities that may be characterized as areas, lines, and points. The areas are the map units having attributes of rock type or Linear features are most commonly the boundaries between map units, and have attributes of type and confidence of location, but also can occur within the map units. Point features relate to a measurement, observation, or feature at a particular location, such as a measurement of the orientation of a structural feature within a rock unit, the occurrence of a specific mineral of interest, or a well site.

The processing required to produce a usable data assemblage from the raw observations, measurements, and analyses often cannot be predefined. It may involve summaries of notes and measurements, production of graphic displays of various parameters, statistical analysis, comparison with other data in the area, and comparison with data in related areas. It involves pattern recognition and a

high degree of inference, and therefore is rarely performed by automated means.

GEOPHYSICAL REMOTE SENSING DATA

Data are collected by measurement of one or more physical properties at intervals along a shipor airborne traverse or along the track of an orbiting satellite. Typical properties are the value of the Earth's magnetic or gravity field, reflectiontime measurements of seismic waves, the magnitude of naturally occurring gamma-ray radiation, and reflectance of rocks and vegetation in bands of the electromagnetic spectrum. Such data are purely quantitative and the collection process is automated so the raw measurements and corresponding spatial coordinates are collected directly in machine-processible form. A data item consists of a measurement taken at a point on the Earth's surface, although often it is collected and to some extent processed in "lines," that is, as series of measurements along a flight path, a ship's track, or a scanner's orbit. The first steps in processing such data are editing, calibration, and adjustment for instrument effects. Commonly, enormous volumes of data are recorded, as much as several million observations in a map area, and data reduction and compression may be required. Processing also may involve corrections for the nature of the physical measurement, to ensure consistency with control values and between intersecting tracks, and to convert raw navigational information to absolute coordinates. The cleaned and corrected data may be gridded and contoured to detect anomalies, or regions of particularly high or particularly low Magnetic anomalies, for example, may relate to buried rock bodies rich in iron-bearing minerals; anomalies in gamma radiation may indicate surface concentrations of potassium, thorium, or uranium; seismic reflection-time anomalies often represent structures in sedimentary rocks which are potential petroleum reservoirs.

WELL AND DRILL-HOLE DATA

Well data are spatially referenced to a point on the Earth's surface where the exploratory hole is located. The data, however, usually involve a third dimension representing the depth of the hole. For instance, geologic attributes may be depths to the tops or bottoms of different stratigraphic units penetrated, pressure or temperature measurements at various depth, or analyses of samples taken during drilling. Other attributes such as identifiers for a well or drill hole and production data are also related to the point location. Data may be both

quantitative and non-quantitative, originating in some instances from a specific drilling program and in others from a more random collection of data available from pre-existing holes and wells. Subsequent processing is done to construct a three-dimensional model of subsurface geology, perhaps to be used in exploration for natural resources such as oil, gas, or minerals. Production of graphic displays such as contour maps, cross-sections, and fence diagrams is common.

PROBLEMS OF DATA STORAGE

The first attempts to automate storage and retrieval of geologic field data were restricted by the format imposed by the 80-column punched card. Immense effort went into the design of forms to ease the task of the field geologist in recording data in a suitable format. Success was limited, due to the inevitable inadequacies of the coding forms and the physical restrictions of field work. It is now recognized that highly compressed coding is not essential, but it is also recognized that coding helps insure consistency of data, a major problem with non-quantitative attribute values. Terms used in a data bank for field map data often defy strict definitions except in highly controlled situations.

Because of the computation which must be performed on geophysical data, such files are almost always in machine-processible form. This does not necessarily imply efficient storage in data banks. The logical structure of such data can easily be accommodated by the theoretical models (Bie and others, 1977) underlying many of the data base management systems commercially available. However, these may not be adequate to handle the large amounts of numerical data that can be involved in a geophysical program.

Well data commonly are treated as having a hierarchical logical structure, with the geographic location of the drill hole associated with the highest level of hierarchy. This structure echoes the way in which the data are collected but does not easily reflect the three-dimensional nature of the geology penetrated by the drills. For instance, the spatial relationship of one formation above or below another is usually not intrinsic in the data structure, though it can be deduced from attribute values. The association of a formation encountered in one hole with the occurrence of the same formation in another hole is also made only from attribute values.

DERIVED DATA

The preceding examples, including field observations, remote sensing data, and well data, all form banks of raw data at the start. Another type of data bank is composed of derived data. include computed values obtained by processing raw remote sensing data. Other examples are data banks on mineral deposits and petroleum reservoirs (Laznicka, 1975; University of Oklahoma, 1977) in which field observations, well data, and economic information are integrated, and data banks containing chemical or mineralogical data (Chayes and others, 1977) which include all analyses pertaining to a particular rock type. The problem of consistency in meaning and derivation (How and under what conditions were the analyses performed? Which reservoir evaluation procedure was used?) is significant, as is the problem of data entry to assemble the bank in digital form.

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Bie, S. W., R. W. Bowen, K. G. Jeffery, M. Lenci, and G. M. Martin, 1977, Relevant Data Structures: COGEODATA Report from Working Group on Data Structures and Data Management: Netherlands Soil Survey Institute, Wageningen, 53 p.

An explanation, aimed at geologists, of the information science terms used in data base management systems. Five geological examples are used as illustrations.

Chayes, F., C. McCammon, J. Trachimczyka, and D. Velde, 1977, A new edition (RKOC76) of the data base of the Rock Information System RKNFSYS: Annual Report of the Director, Geophysical Laboratory, Carnegie Institution, Washington, D.C., p. 635-637.

Describes a data bank containing over 16,000 analyses of Cenozoic volcanic rocks.

Hubaux, A., 1972, Geological data files, survey of international activity: COGEODATA Report, CODATA Bulletin 8, International Council of Scientific Unions, Paris, 29 p.

Summarizes 186 answers to a survey of geological data files.

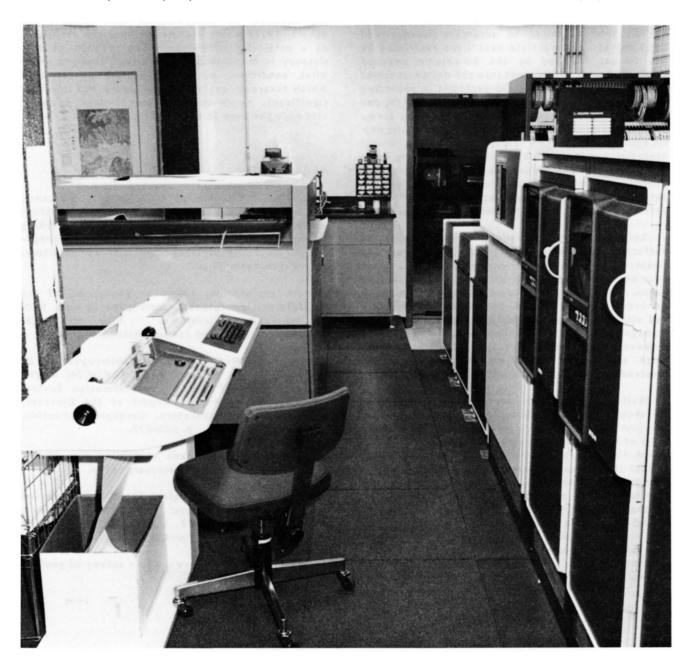
Hutchison, W. W., 1975, Computer-based systems for geological field data: Geological Survey of Canada Paper 74-63, 100 p.

Report of 5-day seminar on the use of computer-based techniques in geological field work and management of geological data.

Laznicka, P., 1975, Manifile: The University of Manitoba computer-based file of world's nonferrous metallic deposits: Geological Survey of Canada Paper 75-20, 11 p. Describes the content, structure, compilation process, and uses of a data file relating to a particular type of mineral deposits.

University of Oklahoma, 1977, Petroleum Data System: Information Systems Programs Documentation Series, The University of Oklahoma, Norman, Okla., 118 p.

Documents the variety of data entered into PDS, how the file is structured, and the available methods of retrieval and display.



ORIENTATION STATISTICS

The first really significant applications of orientation statistics in the geosciences came with the need to analyze directions of residual magnetism in igneous rocks (Irving, 1964). Watson (1969) gives an overview of directional analysis in geology in which some aspects of the work on paleomagnetism have been updated. Directional analysis of a simple kind has long been used as a tool for the study of the motion of continental ice sheets, as expressed by the orientations of glacial striae and other features. In this field, however, mapping of directions has usually been considered sufficient for explaining the features observed and refined statistical analysis has not been thought necessary.

In sedimentology, rudimentary methods of statistical analysis have been employed to analyze paleocurrent directions (Potter and Pettijohn, 1963). Directional data also arise naturally in the form of strike and dip measurements in the mapping of geological formations. Despite the fact that thousands of such orientations are measured annually, little statistical analysis has been used to extract the information contained in the measurements. Directional data also arise in paleoecology, but require relatively advanced methods for their analysis (Reyment, 1971). Examples of directional quantities include: (1) Lines with a sense, technically termed unit vectors (i.e., a vector of length one). Unit vectors occur in the form of directions of remanent magnetism, glacial striations, and current-oriented fossils. (2) Lines without a sense, such as fold axes, the normal to a slate cleavage plane, or the direction of the c-axis in a calcite crystal.

In measuring a directed line such as a glacial striation, a trend angle is determined. This is the angle between two vertical planes through the sampling point, one containing the vector, the other containing the magnetic north pole. The angle is given in degrees east of, or clockwise from, the north; it is also referred to as the azimuth or declination. The "dip" angle (not to be confused with the dip of a formation — see below), also referred to as the inclination or plunge, is the angle between the vector and the horizontal plane. This angle is taken as positive if the vector is above the horizontal plane. The orientation of a plane may be defined by its strike and dip. Choose the smaller of two possible angles made by a horizontal line in the plane with the north; this is the strike of the plane. Thus, strikes run from -90°(W) to +90°(E). The **dip** of the plane is the dihedral angle with the horizontal plane. If a plane has strike s and the up-face dips downward to the west by an amount d, the direction cosines of the normal of the up-face relative to downwards, northwards, eastwards axes are:

 $(-\cos s \sin d, -\cos d, \sin s \sin d)$

Directed lines often are in planes. If the horizontal line in the plane and its strike are found, the angle between the directed line and the strike line, given its northern sense, is the **pitch** of the directed line. Strike, dip, and pitch specify the direction uniquely. Trend-plunge, declination-inclination, azimuth-"dip" angle, also provide unique designations of direction. Expediency and the nature of the problem decide which of these combinations are selected for expressing a directional measurement. Unit vectors may be identified with a point on the surface of a sphere of unit radius. Sample data usually are plotted in this way for visual inspection (Koch and Link, 1971).

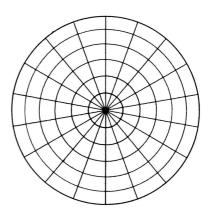


Figure 1. Lambert equal-area projection.

Various projections are available for plotting points on hemispheres and spheres and displaying the results on a page. The Lambert equal-area projection of a hemisphere is used often (Fig. 1). In the geosciences, this projection is known as the "Schmidt net," after W. Schmidt, who first used it in structural geology in 1925. The Wulff or stereographic net is employed in crystallography; it is an equal-angle rather than an equal-area map.

The analysis of two-dimensional observations tends to be simpler. Interpretations based on properties of a circle usually are made by grouping the observations according to their angle into a "rose diagram," a circular histogram having sectors equal to the angular class interval and radial lengths proportional to the class frequency (Fig. 2).

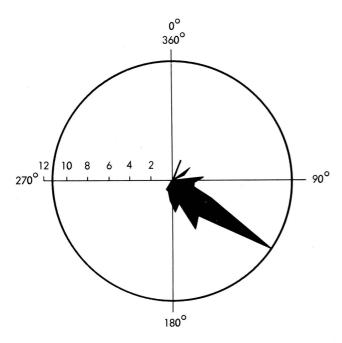


Figure 2. Rose diagram.

For tensor quantities of order greater than one, the usual procedure is to record the orientation of the specimen in the field and then to perform a laboratory measurement, as is done in paleomagnetic determinations. For many second-order tensors such as magnetic susceptibility, the laboratory measurement may result in a 3 x 3 symmetric matrix μ . If B (3 x 1) is the magnetic induction and H (3 x 1) is the magnetic field strength, then B = μ H. The theory and results are similar to those for statistical response surfaces.

The geologist often will want to know if there is a preferred orientation in data, or whether observations could be a random sample from a uniform distribution. Many of the usual statistical testing situations arise; for example, whether two or more samples come from the same distribution. This type of problem may best be treated by non-parametric methods, although in some instances parametric distributions must be sought as an alternative (Mardia, 1972).

If the n observations of a sample are denoted by unit vectors, r_1 , ..., r_n , their sum is designated $R = \sum_{i=1}^{n} r_i$, and |R| is the length of R, then the direction R/|R| is a natural measure of the **mean direction.** If the dispersion of the sample about R/|R| is small, |R| will be almost as large as nothus, n - |R| provides a useful measure of dispersion of the sample about its mean vector. This, and

many other basic results, derive from the work of Watson (1966).

The deposition of sediments is an anisotropic process and orientation problems are common in stratigraphy and sedimentology. Difficulties in direct measurement of many intuitively appealing quantities has led to use of tensor characteristics such as fluid permeability and magnetic susceptibility. In the case of the former, the directions of greatest, intermediate, and least flow through a porous rock are the principal axes of eigenvectors of the tensor corresponding to its greatest, intermediate, and least eigenvalues.

Deformation of rocks is usually referred to as strain. The simplest situation of homogeneous strain may be defined in terms of a point initially at x which is at Bx after deformation; B is a constant matrix. The strain matrix or tensor e is defined by

$$e = \frac{1}{2} (BB^{\dagger} - I)$$

where I is the unit matrix. The strain matrix e is usually of more interest than B. If the rock contained a sphere of radius c, mechanically indistinguishable from the body of the rock, then after deformation the sphere would be an ellipsoid,

$$y'(BB')^{-1}y = c^2$$

where y is specific for the particular geological situation. The estimation of the strain tensor is based on observations of the extent of deformation of objects of known original form in the rock (Fig. 3).

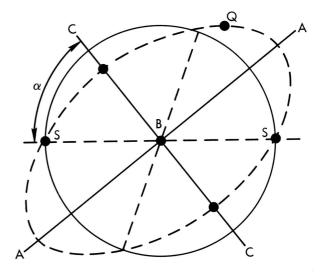


Figure 3. Estimation of the strain tensor.

A special variant of this structural problem is encountered in petrofabric analysis, where small features, such as orientations of the optical axes of crystals in the rock, are of interest. Petrofabric analysis is an aspect of the general statistical problem of mapping orientations (Watson, 1969). Loudon (1964) applied some methods of orientation analysis to problems of structural geology with an emphasis on computer applications.

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Irving, E., 1964, Paleomagnetism: John Wiley &
 Sons, New York, 399 p.

Applications of directional statistics to paleomagnetic problems.

Koch, G. S., and R. F. Link, 1971, Statistical Analysis of Geological Data, Vol. 2: John Wiley & Sons, New York, 438 p.

Contains a useful section on directional analysis, including worked examples for a problem involving a second-order tensor.

Loudon, T. V., 1964, Computer analysis of orientation data in structural geology: Tech. Report No. 13, Office of Naval Research, ONR Task No. 389-135, Northwestern University, Evanston, III., 129 p.

Computer-oriented study of some methods of the analysis of directional data in tectonics.

Mardia, K. V., 1972, Statistics of Directional Data: Academic Press, London, 357 p.

Textbook on directional statistics in which mathematical aspects of the subject are given full coverage. Examples are taken from many spheres, including some from the geosciences.

Potter, P. F., and F. J. Pettijohn, 1963, Paleocurrents and Basin Analysis: Academic Press, New York, 296 p.

Application of simple directional statistical methods to the analysis of sedimentological problems.

Reyment, R. A., 1971, Introduction to Quantitative Paleoecology: Elsevier, Amsterdam, 226 p.

Contains case histories of analyses of directional data for fossils in paleoecological studies.

Watson, G. S., 1966, The statistics of orientation data: Journal of Geology, v. 74, p. 786-797.

Presents basic statistical concepts with reference to geological problems.

Watson, G. S., 1969, Orientation statistics in the earth sciences: Bull. Geol. Inst., NS2, Univ. Uppsala, Sweden, p. 73-89.

Review article of fundamental importance in the application of directional statistics to geological data.

TIME SERIES ANALYSIS

Time series are sequences of observations which are arranged by their order of occurrence, either in time or along a spatial dimension. Many types of time series occur in geology, ranging from the classic form of time series encountered often in hydrogeology (stream flow records, water table measurements), to geophysical measurements which may vary either in time and/or in space (seismic return times measured along traverses, airborne aeromagnetic records), to the less organized and hence less tractable forms of sequences such as measured stratigraphic sections and drill hole descriptions. All of the standard methodologies for analyzing time series have been applied in geology, although many problems remain to be solved. Particularly vexing are problems related to stratigraphic analysis, because a sequence of sedimentary rocks obviously represents a succession of physical changes through time, but as there is only a tenuous relation between the spatial scale (thicknesses of sedimentary units) and the temporal scale, most analyses have been disappointing.

An excellent introduction to time series analysis applied to stratigraphic successions is given by Schwarzacher (1975). Several books treat time series analysis in hydrogeology, including one by Yevjevich (1972). Geophysical treatments abound, but their consideration is beyond the scope of this publication.

Time series may be classified by the informational content of the scales along which they are measured. For example, measured stratigraphic sections are a form of time series in which the "time" dimension consists of a monotonic succession and the measured variable consists of nominal data. Markov chain analysis has been used to study such sequences. Another type of simple time series consists solely of the durations between sudden events such as earthquakes or volcanic eruptions; these are called point processes or series of events. Important sources of time series data in which both scales are of interval or ratio rank are the logs recorded in holes drilled for petroleum exploration; a following section is devoted to the special problems of well log analysis. More conventional types of time series arise in many areas of geology. These are treated by techniques which also are widely used in other disciplines.

MARKOV CHAINS

There are many situations in which a sequence of events in either time or space is observed as a succession of mutually exclusive states. Geological examples include traverses across a thin-section in

which each "event" corresponds to the mineral state recorded at each point; and stratigraphic successions, where observations spaced at constant intervals record the occurrence of a rock type at those points. The relationship between adjacent events may be summarized by a **transition tally matrix** in which each cell sums the number of times that one state (identified by the row) is succeeded by another (identified by the column). A stratigraphic succession consisting of alternating beds of lithologies A, B, C, and D may be summarized as a transition tally matrix by taking observations at successive equally spaced intervals and accumulating transition totals in the appropriate cells. The transition tally matrix might appear as:

Here, for example, lithology C succeeds lithology A three times. The i-th row total is equal to the i-th column total, a property of all transition matrices of this type, since every lithology that is entered is also left (with the exception of the initial and terminal states). These row/column totals may be written as the vector

which represents the number of times a sampling point fell in beds of each of the four lithologies.

Division of each row of the tally matrix by the corresponding row total leads to a transition probability matrix, P:

Similarly, division of the totals vector by the grand total results in an estimate of the **fixed probability** vector

which expresses the proportions of each lithology in the total sequence. Since A, B, C, and D are mutually exclusive events, the probability that one state is followed by another is either a conditional or unconditional probability. P(B|A) is the notation that A will be followed by B, given that A has occurred as the previous event. In the unconditional case,

$$P(B|A) = \frac{P(A \text{ and } B)}{P(A)} = \frac{P(A) P(B)}{P(A)} = P(B)$$

as opposed to the conditional alternative where

$$P(B|A) \neq P(B)$$

If all the transitions are unconditional,

$$P(B|A) = P(B|B) = P(B|C) = P(B|D)$$

and the model is one of independent events. The expected transition probability matrix, A, for independent events consists of rows of the fixed probability vector. In the numerical example,

$$A = \begin{bmatrix} 0.31 & 0.24 & 0.24 & 0.20 \\ 0.31 & 0.24 & 0.24 & 0.20 \\ 0.31 & 0.24 & 0.24 & 0.20 \\ 0.31 & 0.24 & 0.24 & 0.20 \end{bmatrix}$$

A matrix of **expected tallies** is computed by multiplying A by the row totals of the observed tally matrix. The null hypothesis of independent events may be tested using a chi-square procedure with (m-1)² degrees of freedom, where m is the number of states. If the null hypothesis is rejected, the alternative model of a partial dependency between successive events is accepted. Such a model is known as a Markov chain of the first order (Kemeny and Snell, 1960).

Named after its discoverer, A.A. Markov, whose inspiration was the alternation of vowels and consonants in Pushkin's poem, "Onegin," Markov chains are an example of a stochastic process model (Kemeny and Snell, 1960). Markov chain models occur in the range between the extremes of determinism, where every event is exactly specified by its predecessor, and independent events, where there is no relationship between successive events.

If the matrix P is squared so that

$$P^2 = PP$$

the resulting matrix is the expectation of the probability of event (i + 2), given the probability of the i-th event. If this matrix differs significantly from

that observed in the sequence, the succession has **second-order** Markov properties. As the matrix **P** is successively powered, the product approaches a matrix of equilibrium proportions of the states, which corresponds to **A**.

There are several problems that must be resolved before analyzing typical geological sequences for Markov properties:

- (1) The length of the interval between successive observations must be selected. If too small an interval is chosen in analyzing a lithological succession, the number of transitions of a state to itself becomes extremely large and the Markov property reflects the trivial fact that successive observations tend to be within the same bed. If too large an interval is used, many thin beds are missed altogether. The problem may be resolved by structuring the model in terms of an embedded Markov chain, where transitions are recorded between successive lithologic states, rather than at equally spaced sampling points. The transition matrices of the embedded model have zero entries on their leading diagonal.
- (2) A long sequence of events must be recorded to provide an adequate sample, since the number of transition types to be estimated increases as the square of the number of lithologies.
- (3) Each computed transition probability is a sample estimate of its population parameter. Consequently, the transition probabilities must not change systematically over the sequence; that is, the sequence must be stationary.

SPECTRAL ANALYSIS

Spectral analysis is the partitioning of the variation in a time series into components according to the duration of the intervals over which they occur. The methodology is widely used in most fields of science; applications in the various branches of the geologic sciences are described by Yevjevich (1972), Rayner (1971), and Schwarzacher (1975). Spectral analysis constitutes the cornerstone of many types of geophysical interpretation, particularly of exploration seismic data and remote sensing data. In a geologic context, the time series being investigated by spectral methods must consist of measurements of a continuously distributed geologic variable measured either continuously or at discrete points spaced through time or along a line in space. Examples include geophysical measurements taken along a traverse or down a drill hole, pressure changes over time recorded at a point within a petroleum reservoir, and variation in groundwater level in an observation well. The measurements can be regarded as a function of the time (or distance) dimension:

$$Y = f(x)$$

f(x) may also be expressed as the sum of a number of sine and cosine terms. Such a series is called a Fourier series and the determination of the coefficients of this function is called spectral analysis, harmonic analysis, Fourier analysis, or frequency analysis.

Basic Trigonometric Relationships

Figure 1 shows a sinusoidal curve. Assume the wave makes one complete fluctuation in a time (or distance) T. The total duration (or length) of the interval can be expressed in radians by the conversion:

$$\theta = \frac{2\pi}{T}$$
 radians

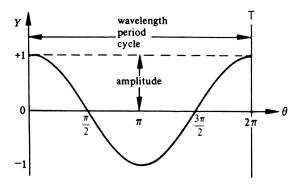


Figure 1. Sinusoidal curve.

Then, the equation of the regular sinusoidal curve may be written

$$Y_k = A_k \cos (k\theta - \phi_k)$$

Because of the trigonometric relationship $\cos (R - S) = \cos S \cos R + \sin S \sin R$, this equation may be rewritten

$$Y = A_k \cos \phi_k \cos (k\theta) + A_k \sin \phi_k \sin (k\theta)$$

If we define

$$\alpha_{\mathbf{k}} = A_{\mathbf{k}} \cos \phi_{\mathbf{k}}$$
 and $\beta_{\mathbf{k}} = A_{\mathbf{k}} \sin \phi_{\mathbf{k}}$

the equation becomes

$$Y_k = \alpha_k \cos(k\theta) + \beta_k \sin(k\theta)$$

In general, any complex time series can be defined as the sum of these sinusoids

$$Y = \sum_{k=0}^{\infty} \alpha_k \cos(k\theta) + \beta_k \sin(k\theta)$$

which is an expression of Fourier's relationship.

Calculation of the Fourier Coefficients

If the time series is sampled at n equally spaced points, one of which is j, the computational equations used to find the $\,\alpha\,$ and $\,\beta\,$ coefficients are

$$\beta_k = \frac{2}{k} \sum_{j=0}^{n-1} Y_j \sin \left(\frac{2\pi j k}{n}\right)$$

$$\alpha_k = \frac{2}{k} \sum_{j=0}^{n-1} Y_j \cos \left(\frac{2\pi j k}{n}\right)$$

Because of trigonometric relationships, β_0 vanishes and α_0 simplifies to

$$\alpha_0 = \frac{1}{n} \sum_{j=0}^{n-1} Y_j$$

which is simply the mean of the time series.

The Fourier coefficients can be combined to obtain the amplitudes

$$A_{k} = \sqrt{\alpha_{k}^{2} + \beta_{k}^{2}}$$

and phase angles of the constituent sinusoids

$$\phi_{\mathbf{k}} = \tan^{-1} \left(\frac{\alpha_{\mathbf{k}}}{\beta_{\mathbf{k}}} \right)$$

The Variance Spectrum

The variance of a sinusoidal wave form sampled at regular intervals is simply half the square of the amplitude of the wave. That is,

$$s_{k}^{2} = A_{k}^{2}/2$$

Therefore, the contribution of any frequency k of the total variance of a time series is

contribution in percent =
$$\frac{s_k^2}{s_k^2}$$
 • 100% = $\frac{A_k^2}{2s_k^2}$ • 100%

The variances of the individual frequencies may be plotted as a variance spectrum or power spectrum (the latter term is favored in engineering applications). The variance spectrum which is calculated for an observed time series is sometimes called the raw spectrum, and is an estimate of the true or population spectrum. If the original time

series is continuous, but sampled only at regular intervals, the computed spectrum is not complete, as wavelengths shorter than twice the sample spacing (the Nyquist frequency) cannot be estimated. Instead these short wavelengths are confounded in the longer wavelengths; this is called aliasing. In addition, the observed time series is usually only a sample from a much longer (or infinite) series and so the variances calculated are statistics estimating the true population parameters. The standard error of these raw spectral estimates commonly is very high, on the same order of magnitude as the raw estimates themselves. Better estimates can be created by first calculating the autocovariance or autocorrelation of the time series, taking the Fourier transform of this function, and then smoothing the spectrum by averaging adjacent values. Alternative equations have been proposed for the smoothing operation. A commonly used procedure calculates the raw spectrum as

$$s_k^2 = 2(1 + 2 \sum_{\tau=1}^m cov_{\tau} cos 2\pi k\tau)$$

where τ is the lag up to a maximum lag of τ = m (usually n/4 or less). The raw spectrum is smoothed by a **filter** such as the Hanning filter:

$$s_k^2 = 1/4 s_{k-1}^2 + 1/2 s_k^2 + 1/4 s_{k+1}^2$$

A third approach is to express the Fourier transform in an exponential form involving the imaginary number i. Then, the **Fast Fourier Transform** (FFT) algorithm can be used to find the complex coefficients for all wavelengths up to the Nyquist frequency, provided the number of points in the time series is some power of 2.

Components of Time Series

Time series may be deterministic or stochastic, or mixtures of the two. **Deterministic** components are those whose behavior can be predicted exactly. These include periodic changes which repeat at regular intervals, and **transients**, most commonly long-term trends and sudden jumps or changes in average value. **Stochastic** components, in contrast, are characterized by their statistical properties. The development of a stochastic time series is governed by probability functions, and its exact state at any instant cannot be predicted with certainty.

Most geologic time series are either completely stochastic or stochastic with a periodic component. For example, hydrologic series such as stream levels may be stochastic with annual periodic components related to spring runoff. Other geologic phenomena may exhibit trends or nonstationarity.

The presence of a suspected periodic component may be tested by calculating the probability that a spectral value s_k^2 will exceed the value σ_k^2 of an independent stochastic process. The test, devised by Fisher, involves calculation of the ratio

$$\hat{g} = \frac{s_{max}^2}{2s^2}$$

where s_{max}^2 is the largest value in the variance spectrum and s^2 is the variance of the time series. The critical value of g for a specified probability P is given by

$$g \approx 1 - e^{\frac{\ln P - \ln m}{m-1}}$$

where $m=\frac{n}{2}$ if the series contains an even number of observations and $m=\frac{n-1}{2}$ if n is odd. If the test value of \hat{g} exceeds the critical value g, the periodic component may be presumed to exist, and may be removed from the time series to isolate the stochastic component. If the test value does not exceed the critical value, the observed variance s_k^2 could have arisen by chance from a purely stochastic process.

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INSTANTANEOUS EVENTS

In some geologic problems, concern lies in estimating the rate at which events take place and whether these events can be related to an underlying process having definable statistical properties (Reyment, 1976). In the context of geologic time, the events are considered to occur instantaneously. Examples include earthquakes, volcanic eruptions, and geomagnetic reversals. Although the duration of such events may extend over days, months, years, or even millennia, considering the long periods of time involved, their occurrences can be treated as **point processes** (Cox and Lewis, 1966).

The primary objective of a study may be to obtain an estimate of the mean rate of occurrence of events; for example, the mean rate of occurrence of earthquakes above a given magnitude within a specified area. The detailed pattern of occurrences is of interest solely for determining the precision of the final estimate of the mean rate, and the appropriateness of various sampling schemes. In general, if n is the number of events observed in a period of length t starting from some arbitrary time origin, the mean rate of occurrence of events is n/t.

Interest may lie, not in the mean rate of occurrence, but rather in the gross pattern of occurrence. This may be viewed as exploratory analysis in which no particular model is put forward but instead the data are examined either to suggest a model or to give direction to a further search for the physical mechanisms which generated the data. An example is the examination of geomagnetic reversal data for the purpose of identifying possibly significant trends in the lengths of time between magnetic field reversals which occurred in the geologic past. Graphical analysis is particularly useful, and a common practice is to plot the cumulative number of events against elapsed time. Changes in the mean rate of occurrence are reflected by changes in the mean slope of a curve statistically fitted to the data. It is important to identify trends which exist in the data, as it is meaningless otherwise to compute a mean rate of occurrence. If no trends are found, the assumption can be made that the series of events is stationary; that is, the mean rate of occurrence is constant regardless of the length of interval considered.

Once the absence of trend has been established or the trend has been removed (detrending), the next step is to search for dependence in the sequence of events, using second-order properties. This usually involves testing for serial correlation between successive events. This might be done to determine if there are relationships between, for

example, successive intervals separating eruptions of a particular volcano over an extended period of time. If there is no indication that a serial correlation exists, it is assumed that the events are independently and identically distributed with some unknown distribution.

In the analysis of series of events, interest may lie in specific models which are to be tested against the data and whose parameters are to be estimated. The models generally are suggested by exploratory analysis or from prior knowledge. In the example of volcanic eruptions, for instance, once the absence of serial correlation is established, a renewal process may be invoked, a special case of which is the Poisson model:

Prob
$$(X \le x) = 1 - e^{-\lambda x}$$

where X is a random variable defined as the interval between successive events and λ is the mean rate of occurrence. Tests for the Poisson model have been made for particular data sets and yield, for example, a close agreement with the sequence of eruptions of Mauna Loa in Hawaii. For the most part, however, the patterns of volcanic activity deviate strongly from a simple Poisson model and must involve more complicated types of point processes. It is unfortunate that the historic record of eruptions is insufficient for more detailed analysis of most active volcanoes. Recent developments in non-homogeneous Poisson processes, however, are promising (Lewis, 1972).

Analysis of series of events or point processes is a useful tool in geological model building and has obvious potential for the future. The number of published applications has been limited, although increasing in recent years. Areas of possible future applications include investigation of the rates of seafloor spreading, magnetic anomalies, glaciologic events, and geotectonic problems related to the rapid accumulation or sudden removal of large volumes of sediments.

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PETROPHYSICAL LOG INTERPRETATION

Petrophysical logs (also known as electrical, mechanical, or geophysical logs) are records of physical variables such as resistivity, spontaneous potential, temperature, acoustic transmission character, and levels of spontaneous and induced radioactivity in subsurface lithologic sections which have been penetrated by drill holes. The petrophysical variables are measured by specialized tools developed by oil industry service companies and conventionally are recorded as analog traces which are a continuous function of depth. The data express variations of physical properties with an ordinal time domain, since stratigraphic depth generally can be equated with some complex (but monotonic) transformation of geologic time.

Conventional log interpretation methods are directed primarily to the evaluation of reservoir rock properties, such as porosity, hydrocarbon saturation, and mineralogical composition. Treatments of well-log data as time series have been more restricted, as such applications are generally secondary to the main objectives of logging.

Because of its construction, each logging tool has a limited "vertical resolution," which may vary from inches to feet. As a result, the recorded analog traces are smoothed transformations of the "real" petrophysical variation. Methods that use discrete sampling and digital logic have been more widely applied to the analysis of these traces than have analog or hybrid procedures. For this purpose, the log responses are either directly recorded as digital information at the drilling site, or are digitally sampled from the log traces at regular depth increments. There has been extensive debate (Lindseth, 1966) on the optimum sampling density that will avoid problems of aliasing. Typically, records are sampled at a frequency of one reading per 6 inches or 1 foot, which is in part a compromise between average tool response and the economics of digitizing and storage of large volumes of data.

The widest time series application of such data has been in attempts to correlate (in the stratigraphic sense) from well to well using the log traces. The simplest procedures have applied a cross-correlation function of the form:

$$C(x) = \sum_{i=1}^{n} f_{1}(x + \lambda) f_{2}(x)$$

where f_1 and f_2 are equivalent logs in two adjacent wells as a function of depth x, and λ is a vertical displacement between the two traces. Usually, a restricted test window length is specified in one

well to minimize effects introduced by non-overlap of correlated sequences. This window is progressively migrated by increments of depth and cross-correlated with the corresponding section of the second well log trace to produce a cross-correlation function. This operation represents a convolution of the second log trace by the window of the first as the convolution operator. A maximum value of the cross-correlation function indicates a position of "best match" for stratigraphic correlation.

This technique works successfully in the correlation of micro-resistivity profiles across a single borehole and is routinely used for this purpose in order to determine the dip of beds in continuous dipmeter analysis (Matuszak, 1972). However, when extended to correlation between wells, numerous problems result from considering depth as a linear function of time, when generally it is non-linear and often discontinuous. Rock units characteristically thicken, thin, or even disappear when traced laterally in the subsurface between wells. At the same time, rock properties such as mineralogy and porosity vary with corresponding changes in petro-physical variables.

Various modifications of the basic cross-correlation procedure have been suggested to accommodate these disturbing factors. A variety of "stretch" coefficients may be applied as simple expansions of the correlated window to generate cross-correlation functions related to both lag and stretch. Rudman and Lankston (1973) outline an iterative method to select an appropriate stretch coefficient, by matching different stretch cross-correlation functions with the autocorrelation of the second well trace.

The selection of a "best match" position for stratigraphic correlation from cross-correlation functions is further complicated by the fact that rock sequences typically are highly repetitive in character. This produces a cyclic character in any cross-correlation function, with numerous local maxima. Changes in the length of the window alter both the cross-correlation periodicity and position of the greatest match. Furthermore, the lateral changes which are known to occur in the character of rock units means that there is no guarantee that the maximum cross-correlation position coincides with a common stratigraphic horizon.

Simple transforms of log traces are helpful in geologic correlation, such as power, derivative, and frequency functions of logs used as a precursor to visual or mechanical correlation. In another

approach, both Gill (1970) and Hawkins and Merriam (1974) have used modified analysis of variance techniques which partition log traces into a series of segments, so that variation within segments is minimized. Their work represents attempts at "optimal zonation" of the stratigraphic sections from which the logs are drawn. Sequences of zones from different wells may be stratigraphically correlative, and also may be suggestive of the subdivision of stratigraphic sections into major and minor rock facies.

More general applications of signal theory to analysis of log traces have been restricted to work done by geophysicists on acoustic logs as an adjunct to interpretation of exploration seismic data. Research has also been directed to the design of inverse filters to sharpen the vertical resolution of logs through deconvolution (Lindseth, 1966). Filter design is most commonly based on the Wiener least-squares criterion, although some recent work has examined the potential of the Kalman filter.

Time series applications to petrophysical logs will continue to develop at a low key, although recent developments in seismic stratigraphy and emphasis on detailed reservoir modelling may encourage additional studies by geophysicists and petroleum engineers.

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INTERPRETATION OF MAP DATA

Maps and other forms of two-dimensional displays, including aerial photographs and remotely sensed images, form the core language of geology. The classic form of geologic research consists of defining the present areal extent of rock bodies and interpreting their origins and subsequent history. The primary product of such research is the geologic map, a cartographic portrayal of the lithic units forming the surface of the Earth, with other information about the three-dimensional configuration of the units and their interrelationships shown by special symbols. A geologic map is a concise expression of very complex spatial relationships and is an extremely efficient storage mechanism (a typical geologic map may contain 10 million bits of information).

In addition to maps of areal geology, geologists make extensive use of other types of maps, which display the form of actual or perceptual surfaces within a geographic area. Examples include contour maps of topography, of subsurface structural configuration, and of geophysical properties such as the intensity of the Earth's gravitational and magnetic fields. Any variable which can be regarded as differing continuously from place to place may be shown as a contour or isoline map.

If geologic map data are captured in computer readable form, they are available for extensive analysis and can be displayed in a variety of alternative ways. The geologist is freed of the constraints of cartographic tradition, and can experiment with map projections, scales, and symbolism to select those which best convey the information and impressions that he wishes to impart. More importantly, once in the computer, geologic data can be manipulated mathematically to yield forms of maps and displays which could not be obtained in any other way. Some of these, for example trend surface and residual maps, are extensively used by geologists. Others, such as factor maps, logit maps, and spatially filtered maps, are the subject of current research.

All types of geologic maps, whether constructed by hand using traditional interpretative procedures, or by computer using a mathematical algorithm, are displays of data having common characteristics. They all derive from observations consisting of one or more variables measured at locations defined in two (or three) spatial dimensions. In a sense, map data are two-dimensional "time" series, although of a very general type. The procedures discussed in previous sections can be expanded and used to analyze maps, and there are additional methodologies unique to the treatment of map information.

MAPPING AND DISPLAY OF CATEGORY DATA (AREAL GEOLOGIC, SOILS, AND OTHER QUALITATIVE MAPS)

Much of the spatial information in geology and other Earth sciences is most clearly represented by categories defined by qualitative or nominal criteria. Maps displaying qualitative information are called chorochromatic maps by Monkhouse and Wilkinson (1974) to differentiate them from choropleth maps, which depict categories based upon quantitative differences. The former group includes conventional geologic, pedologic, and geomorphologic maps, as well as many other maps used in the Earth sciences. Mapping units usually are based upon categories within recognized taxonomic systems, defined and accepted by the scientific discipline. Mapping units need not correspond directly to these taxonomic categories, as map scale and the complexity of a given distribution may require that several categories be combined as a single mapping unit.

The distribution of each mapping unit is represented by an areal symbol, usually a color or shaded pattern. The use of such symbols implies a model of

geographic variation where each mapping unit is a homogeneous body with abrupt boundaries. This model is probably reasonable for many lithologic mapping units, but is only a rough approximation of the true distributions of unconsolidated sediments and soils, which frequently have gradational boundaries and may exhibit considerable variation within mapping units.

Even the most homogeneous mapping units display some degree of internal variation, the result of accidental or deliberate inclusion of two or more taxa within the same mapping unit, and of the inevitable place-to-place variability exhibited by any natural phenomenon. Because an objective of a map is to enable the reader to make accurate statements about a particular place, variability within mapping units is a key element in determining map accuracy. Beckett and Webster (1971) suggest that each definition of a mapping unit should include measures of variability as guides to the precision of the map. They also propose

(Webster and Beckett, 1968) the use of the intraclass correlation as an index of within-class variance in relation to variation within the total area.

A second source of error is the sampling pattern used to collect information for the map (Switzer, 1975). Although regular sampling patterns may be used to take data from an existing map, a field geologist must rely on irregularly spaced observations when he compiles an original map. Under such circumstances the reliability of the map varies from place to place; unless the sampling density is indicated in some manner, this cannot be discerned by the user.

In part because of the potential effects of these kinds of errors, category maps, more than other mapping techniques, require extensive documentation to clearly define characteristics of each mapping unit. Such documentation may be printed (in part) on the map itself, but often is presented in a report accompanying the map.

Several operations can be performed upon category information to generate new versions of the original map (Varnes, 1974). Generalization is the simplification of a map, perhaps so it can be published at smaller scale. Boundary generalization is the smoothing of intricate segments of boundaries, and deletion of small outliers and other inappropriate detail. Taxonomic generalization is the combination of related categories to create a smaller number of mapping units. A generalized map presents a more easily understood pattern, at the cost of decreased detail, accuracy, and precision.

Selection is the isolation of specific mapping units to emphasize their distributions in a revised map, or as a preliminary step to performing other operations. Addition is the process of superimposing two or more category maps to generate new distributions from the combined maps. For example, a map of soil permeability can be combined with a map of topographic slope categories to generate a new map of estimated erosion hazard.

Mapping units can also be interpreted or transformed to create new mapping units. For example, mapping units representing limestone can be assessed in terms of depth of burial, quality, and thickness to generate a new map of the suitability of limestone as a source for construction material.

Other efforts to improve capabilities for handling map information have attempted to store and manipulate category map data in the form of images. A system designed for topographic maps stores map information in the form of microfilm images, and has computer-assisted retrieval and

display capabilities (Gunther, 1974). It greatly reduces storage space for large numbers of maps and permits convenient retrieval, but provides little capability for manipulation or analysis other than changes in scale on a display screen. Analysis of category maps in image form can be accomplished through the use of combined analog-digital computer systems (Anderson and others, 1972), designed primarily for the study of aerial photographs, but also applicable to category maps in image form. Such a system can combine two or more images, redefine categories, and perform other operations, then display results on a television screen. The products are suitable for research, but are unlikely to meet graphic standards for production maps.

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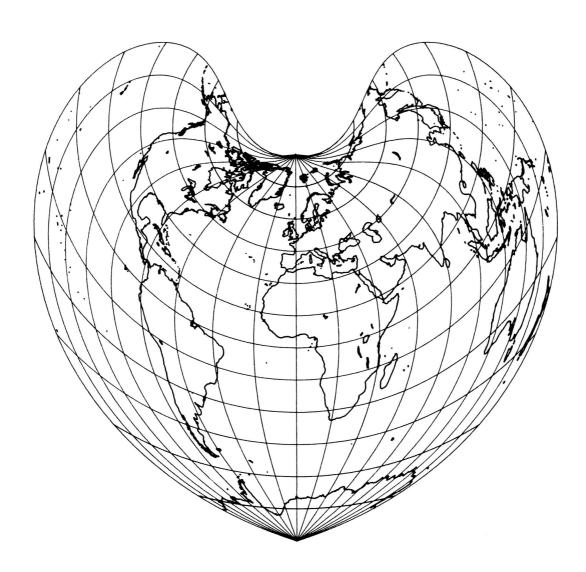
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Bonne projection of the world with the standard parallel at 45° latitude. Drawn by the MAPRO program using World Data Base I.

CARTOGRAPHIC PROJECTIONS

A globe is the only form of representation which can simultaneously possess a constant scale, correct shape, and the true direction of features on the Earth's surface. Any other form of representation requires projection of the spherical form of the Earth onto a flat surface. Although implying a geometric projection, most cartographic projections are best defined in terms of mathematical expressions relating locations on the sphere to their equivalent positions on a map. (Mathematical definitions of most common projections are available in standard references on projections, usually as tables for graphic construction of maps.) In comparison to a globe, a flat map is more convenient but must sacrifice at least some of the qualities required for accurate representation of the Earth's surface.

This fact becomes evident whenever it is necessary to compare two maps compiled using different projections. Even if the scales are the same, the two maps may not register because of differences in projections. Optical devices can be used to manually transform data from some projection to another, although this process is tedious and inaccurate. The most practical methods for transforming map data from one projection to another require use of the computer (CIA, 1974; Colman, 1975).

Usually, information from each map is translated into a standard system of latitude and longitude coordinates which then can be compared directly. In addition, other maps showing a combination of, or differences between, two or more maps can be created at any desired size and projection. By merging information from different source materials, maps showing new features can be generated (Campbell and others, 1979).

The initial step in entering cartographic information into a common data base involves making the data readable by computer. If the source is an existing map, this is accomplished by digitizing.

An operator traces over the selected map features, using an electronic cursor. The digitizing equipment can detect and record the location of the cursor at any time. It also is possible to enter annotations—for example, the drilling date, company, final well status, and depth of wells whose locations are being digitized.

Most digitizing equipment records locations as sets of Cartesian coordinates. For these raw data to be included in a cartographic file, it usually is necessary to transform the coordinates of each point into latitude and longitude. In some instances, the transformation can be obtained by mathematically inverting the equations of the projection used

in the source map (see, for example, Maling, 1973; Richardus and Adler, 1972). This is a fast, highly accurate means of transforming the raw data into the required format. Unfortunately, because of the complexity of some projection equations, a set of inverse equations may not exist. Then, a slower method involving iterative approximation must be used. The computer initially selects a point, generally the center of the map area, to be used as an initial approximation. By using certain mathematical properties of the projection equations, an improvement in the accuracy of this approximation can then be made. This process is continued until a solution of any desired accuracy is obtained.

Once all necessary information has been entered into the data base, the requested map can be produced. This final step involves a computer program to create and plot the map at the desired scale and projection. A typical projection program first requests the user to specify parameters such as size, area to be included, and center point of the area to be mapped. The user can then select any of the several map projection options. Maps may be plotted so rapidly and inexpensively that the programs can be used to generate "one-only" copies for editing or for field use, or highly accurate scribed cartographic masters to be used in the printing process.

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DATA STRUCTURES FOR GEOLOGIC MAPPING

A geologic map stores two types of information: the geometric characteristics of the spatial unit—point, line, or area; and the content, which is the meaning or attribute of the spatial unit. The potential benefits of a cartographic system for geologic mapping are realizable only if the data are organized in a way to provide easy access, updating, and retrieval.

COMPUTER SCIENCE ASPECTS

Due to frequent insertions and deletions of records involved in many cartographic applications, most of the existing cartographic data structures make use of tree and hierarchical arrangements which are combinations of random and list organizations. Descriptions of various forms of data organization are given by Dodd (1969) and a survey of data structures used in computer graphics systems is found in Williams (1971). Graph theory techniques for describing the nature and efficiency of data structures are developed by Pfaltz (1977).

One of the important problems that arise in computer cartography, especially in interactive editing or updating, is partitioning of large data sets into smaller units. Storing a map or portions of a map may require many times the available computer memory, so data must be segmented into pages. Designing an efficient paging mechanism which minimizes swapping between core and secondary memory is a difficult problem and an optimal solution depends greatly upon the data structure adopted.

TOPOLOGICAL STRUCTURES

A neighborhood function is essential for much cartographic analysis to indicate the position of a geographic or geologic entity with respect to its neighbors. Data structures which do not store explicit neighborhood relationships have only limited flexibility and a narrow scope of applications.

One of the first attempts to include topological information in a data structure is the Dual Independent Map Encoding (DIME) system of the U.S. Bureau of the Census. The dual encoding procedure (Fig. 1) is characterized by two (dual) adjacency relations. For every segment, encoding is performed both at its bounds (endpoints) and its cobounds (left region and right region). The DIME system has been used in many urban and regional information data banks and recently was implemented in the U.S. Geological Survey's Digital Cartographic Data Base, DCDB (Edson, 1975).

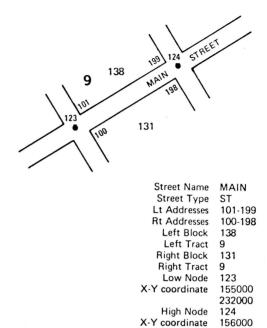


Figure 1. DIME dual encoding procedure.

The DIME concept has been refined in the POLYVRT system developed by Chrisman at Harvard University's Laboratory for Computer Graphics and Spatial Analysis (Peucker and Chrisman, 1975). The new structure uses a "chain file" based on the same topological principles as the DIME system. However, instead of a unique segment, a chain or arc may consist of many line segments which connect two endpoints and separate two polygons. A header attached to each chain contains identifiers for the two ends and the polygons on both sides of the chain. Headers and chains allow construction of a set of directories to link polygons to their constituent chains.

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The relevance of the chain-based concept is demonstrated by the development of topological systems in a broad range of fields. GIRAS (Mitchell and others, 1977) has been created by the U.S. Geological Survey to describe and manipulate landuse data. In a similar approach, Cao (1978) has designed a topological system to handle geologic maps. This system incorporates an inclusion relation which allows specification of the relative locations of simple or compound "islands" with respect to the surrounding zones (Fig. 2). Also, a complete program-generated description of the graph structure of the map is produced, allowing easy retrieval and interactive editing.

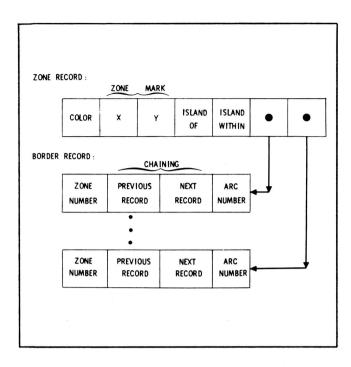


Figure 2. Topological system allowing specification of islands.

Current research includes the GEOGRAF and GDS (Geographic Data Structure) projects of Peucker and Chrisman, both attempts to handle a very large range of two— or three—dimensional geographic data. Such research involves developing new data handling techniques and requires a large computer memory, a limiting factor in many instances. Therefore, as it depends largely upon machine characteristics, a data structure is a compromise between what is desirable and what can be achieved with the available computer resources.

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TREND SURFACE ANALYSIS

A trend surface is the name applied by geologists to a multiple regression technique in which the dependent variable is some property to be mapped, and the independent variables are functions (usually a polynomial expansion) of the geographic coordinates (Krumbein and Greybill, 1965). A typical trend surface can be expressed by an equation of the form

$$Y = \alpha_0 + \beta_1 X_1 + \beta_2 X_2 +$$

$$+ \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 + \epsilon$$

which is for a second-degree surface. The variable X_1 represents one geographic coordinate and X_2 is the orthogonal coordinate. A first-degree trend surface is defined by the first three terms only

$$(\alpha_0, \beta_1, \text{ and } \beta_2),$$

while higher order trend surfaces include additional, higher powers of the geographic coordinates and their cross-products. A first-degree trend surface has the form of a dipping plane; a second-degree surface may exhibit curvature in one or two directions, producing a surface having the form of a ridge, trough, dome, or basin with a single maximum or minimum value. Higher order trend surfaces are more complicated and may have multiple maxima and minima.

The surface defined by a trend equation can be fitted to observational data by ordinary least squares techniques. If Y_i is the value of the mapped variable at point i and \hat{Y}_i is the value of the trend surface at that point, the coefficients of the trend surface equation are found so that the quantity $\Sigma \left(Y_i - \hat{Y}_i\right)^2$ is a minimum. The coefficients can be determined by expanding the trend surface equation into a series of normal equations which can be solved by standard matrix techniques:

$$\begin{bmatrix} n & \Sigma X_{1} & \Sigma X_{2} & \cdots & \Sigma X_{2}^{m} \\ \Sigma X_{1} & \Sigma X_{1}^{2} & \Sigma X_{1} X_{2} & \cdots & \Sigma X_{1} X_{2}^{m} \\ \Sigma X_{2} & \Sigma X_{1} X_{2} & \Sigma X_{2}^{2} & \cdots & \Sigma X_{2}^{m+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \Sigma X_{1}^{m} & \Sigma X_{1} X_{2}^{m} & \Sigma X_{2}^{m+2} & \cdots & \Sigma X_{2}^{2m} \end{bmatrix} \begin{bmatrix} \alpha_{0} \\ \beta_{1} \\ \beta_{2} \\ \vdots \\ \beta_{m} \end{bmatrix} = \begin{bmatrix} \Sigma Y \\ \Sigma X_{1} Y \\ \Sigma X_{2} Y \\ \vdots \\ \Sigma X_{m}^{m} Y \end{bmatrix}$$

Trend surface analysis provides a way to partition the variation in a mapped property into two parts; the gently changing trend surface defined by the fitted equation, and the deviations or residuals from the trend surface. The total variation in the mapped property may be defined as the sum of the squared deviations of the observations from their mean value. Then,

$$\Sigma(Y_i - \overline{Y})^2 = \Sigma(\hat{Y}_i - \overline{Y})^2 + \Sigma(Y_i - \hat{Y}_i)^2$$
or,
$$SS_T = SS_R + SS_D$$
(total variation) (regression) (deviation)

The ratio SS_R/SS_T can be expressed as a percent goodness-of-fit of the trend surface to the data; the square root of the ratio is the multiple correlation coefficient, R_{\bullet}

Trend surfaces may be regarded in two alternative ways (Davis, 1973). One approach considers trend surfaces as special cases of the statistical procedure of multiple regression, in which the Y_{i} values are a random variate. Then, a trend surface is an estimate of the variation in the expected values of Y_i with geographic location, and the deviation is a random error. Standard statistical tests of the trend are available, and can be used to assess the significance of a particular model (Koch and Link, 1971). This approach is appropriate, for example, when using trend surfaces to describe the large-scale variation of a geochemical variable across a pluton, or changes in grain size within a sedimentary body. Here, the trend is the component of interest and the residuals are regarded as noise superimposed upon the trend.

In contrast, trend surface analysis is extensively used as a high-pass filter technique to isolate small anomalies (in the form of deviations) from a general background (the trend). In this application, statistical tests are not appropriate because deviations are not regarded as random, but rather as systematic although small-scale features. For example, trend surface analysis is routinely used in petroleum exploration to isolate residuals corresponding to small features that are structurally higher than surrounding areas. These may be approximately equated to anticlines, and may be favorable targets for petroleum exploration (Harbaugh and Merriam, 1968).

Trend surface analysis may be extended to three dimensions if a three-axis coordinate system is used to define the location of sample points in space

(Davis, 1973). Typically, observations might consist of measurements of grade (the dependent variable) collected from within an ore body at specific locations whose coordinates are the independent variables. The trend representation has the form of a three-dimensional solid in which contour lines are generalized to surfaces which enclose volumes of estimated equal grades.

It is also possible to use functions other than polynomial expansions for trend surfaces. Miesch and Connor (1968), for example, describe a number of approximating equations of linear form which can be used. However, trend surfaces are basically empirical tools for displaying a component of geologic variation through space, and polynomial equations have proved sufficient for this purpose.

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CONTOURING

Procedures for drawing contour or isoline maps from irregularly spaced data points fall into three categories, although the programs which implement these basic procedures contain endless embellishments (Davis and McCullagh, 1975). Triangulation procedures simulate the process of manual contouring. Lines are projected from each data point to the nearest three control points, dividing the map area into triangles. The points where contour lines cross the triangles are established by linear interpolation down the sides of the triangles. The final step is to connect all points of intersection which have equal value to form the contours. Essentially this process represents the surface as a "geodesic dome" composed of flat triangular plates. Modifications include fitting curved rather than flat plates to the triangular areas, subdividing the basic triangles into finer subtriangles of similar form, and restricting the manner in which control points are connected so the resulting triangles are as nearly equilateral as possible.

The principal advantages of this procedure are the directness of the methodology and the fact that all control points must lie on the contoured surface. Unfortunately, some triangulation programs produce a non-unique triangular mesh, which can result in different patterns of contour lines for the same data, and may be extremely slow as compared to gridding routines. Recent developments, however, have led to a rapid algorithm which creates an optimal triangular net (McCullagh and Ross, 1980).

Global fit procedures find the coefficients of a mathematical function relating the geographic coordinates of the control points to the values being mapped. Polynomial trend surfaces and double Fourier surfaces are examples; their computation is discussed in another section. Modifications include two-stage procedures for fitting small "trend surfaces" to local areas of residuals from the global trend surface.

The advantage of global fitting as a contouring procedure is its extreme computational speed. Its disadvantage is that it provides a very poor map of the data, as it is impossible to represent the detail in most mapped variables with any single, tractable equation.

Local fit methods estimate values at the nodes of a regular grid across the map as weighted averages of the control points nearest each grid node. Linear interpolation is used between the nodes to find the points of intersection of specified contour levels with the grid lines. These points of common

elevation are then connected to form the contour lines (Walters, 1969).

Estimating the regular grid of values is called gridding and consists of two steps. First the nearest neighboring control points to each grid intersection must be found. The simplest way in which this can be done is to take the n points nearest to the grid node being estimated without regard to their angular arrangement around the node. With certain distributions of control points, this may result in unconstrained estimates of the surface, if all the nearest points lie on one side of the node to be estimated. This is especially apt to happen if the data are collected at closely spaced locations along widely spaced traverses. Geophysical data, such as reflection seismic measurements and airborne magnetic and radiometric measurements, typically are taken in such patterns. Constraints may be introduced to insure some equitable radial distribution of the control points used in the estimating process. These include a quadrant search, where n control points must be found in each of four quadrants around the estimated grid node, and the octant search which carries the concept one step further, so n control points must be found in each of the eight radial segments around the grid node.

The second step in the estimation procedure is the calculation of grid values from control points that have been located in the first step. The estimates may be simply weighted averages, with the control points weighted by a function of their distance from the location where the surface is being estimated. The most commonly used weighting functions decline with distance at least as rapidly as $1/d^2$ and some decline at rates of up to $1/d^6$.

A more elaborate procedure divides the estimating process into two phases. During the first phase, the dip of the surface at each control point is found by fitting a weighted least-squares plane to the surrounding control points. In the second phase, dips are projected from all the control points in a neighborhood to the location of a grid node being evaluated. An estimate of the surface at that node is then made as a weighted average of these projected dips.

Contouring programs combine different weighting functions, search procedures, and other modifications in great variety. The superiority of specific combinations is loudly proclaimed by their proponents, but the relative merits of the more elaborate procedures are debatable. Commercial contouring packages usually have the ability to construct block diagrams, isopach maps, and maps of other transformations of the surface.

The primary advantages of the local fit method derive from the intermediate gridding step; this allows storage of the mathematical representation of the surface as an array in the computer. Storage requirements are minimized because the explicit locations of points on the surface do not need to be retained, as they are implied by their position within the array. In addition, the process of drawing contour lines is speeded because the geometric relations between all pairs of points are the same. Two or more variables can be compared (by isopaching or other methods) even if they are measured at different geographic locations, because the grids, rather than the control points, are compared. However, the gridding step also is the cause of most of the drawbacks of the method, especially the distressing tendency for contour lines to sometimes pass on the wrong side of control points in areas of low dip (Wren, 1975).

Current research is centered on the use of non-uniform rectangular grids in which every control point lies at the intersection of a pair of perpendicular grid lines, and the fitting of bicubic splines to the grid in order to define the surface on which the contour lines are drawn. Either of these approaches may alleviate some of the problems which exist in many of the present programs.

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GEOSTATISTICS AND REGIONALIZED VARIABLES

Space- and time-dependent data may exhibit behavior which is too complex to be analyzed by standard deterministic methods. Variations are erratic and often unpredictable from one point to another, but there is usually an underlying trend in the fluctuations which precludes regarding the data as resulting from a completely random process. To characterize variables which are partly stochastic and partly deterministic in their behavior, Matheron (1971) introduced the term regionalized variable. The term "geostatistics" has come to mean the specialized body of statistical techniques developed Examples of to treat regionalized variables. regionalized variables are: the porosity of sedimentary rocks; the amount of precipitation per square mile; the depth to subsurface formation tops.

All three of these are regionalized variables, but each has a different geometric support, or characteristics which specify the geometric n-dimensional volume, shape, and orientation of the sample elements. Measurements of porosity, for instance, have a meaning only as averages related to a volume of rock. The "porosity" at a point is a meaningless concept. The geometric support may extend over a three-dimensional volume, a twodimensional area, along a segment of a line, even to a point. The same variable defined over two different geometric supports constitutes two different regionalized variables. Although time is not precluded as support, almost all applications of geostatistics are to space-varying rather than timevarying data.

The three main problems addressed by geostatistics are: (1) Understanding, through mathematical analysis, of the genesis and natural laws ruling phenomena that can be regarded as regionalized variables. (2) Estimation of the regionalized variable itself or some of its spatial characteristics using the information and relationships available in a discrete set of samples. (3) Assessing estimation errors in order to state the degree of reliability in forecasts, and to design optimum sampling patterns which assure that a specified maximum estimation error will not be exceeded.

In order to obtain practical results by the use of geostatistics, the probability density function ruling the occurrence of the regionalized variable must be known, at least partially. As in conventional statistical inference, this knowledge must be based on either a good theoretical model or on an empirical analysis of a large number of samples. The complexity of regionalized variables precludes formulating a theoretical model of their behavior, leaving an empirical or relative frequency determination of the probabilities as the only solution.

Unfortunately, a regionalized variable is a unique outcome of a random function, and it is impossible to base statistical inference on a single sample. To resolve this apparent impasse, geostatistics uses a stationarity constraint similar in concept to ergodicity in time dependent series. The constraint is called the intrinsic hypothesis, and allows the common use of outcomes of a regionalized variable for moment estimation. Let Y(x) and Y(x+h) be two components of the regionalized variable at x and x+h, which are a distance h units apart. The notation h indicates that the distance is a vectorial property having specified direction and orientation. The difference between the two is another random variable [Y(x) - Y(x+h)]. The intrinsic hypothesis states that [Y(x) - Y(x+h)] is second-order stationary. in other words, a regionalized variable satisfies the intrinsic hypothesis if, for any displacement h, the first two moments of the difference [Y(x) - Y(x+h)] are independent of location \dot{x} and are a function only of h:

$$E[\Upsilon(\vec{x}) - \Upsilon(\overset{\rightarrow}{x+h})] = m(\vec{h})$$

$$E[\{\Upsilon(\vec{x}) - \Upsilon(\overset{\rightarrow}{x+h}) - m(\vec{h})\}^{2}] = 2\Upsilon(\vec{h})$$

In the specialized language used in geostatistics, $m(\tilde{h})$ and $\gamma(\tilde{h})$ are referred to as the **drift** and as the **semivariance** or **intrinsic function**. Provided the intrinsic hypothesis is met, both can be estimated.

There are three important cases where geostatistics are applicable even if the intrinsic hypothesis does not hold: (1) The regionalized variable is stationary only for small displacements of h. Geostatistical techniques can be used provided estimation is restricted to small neighborhoods within which the process is stationary. (2) The intrinsic hypothesis holds only within certain areas but not over the region as a whole. Estimation can still be performed by dividing the area of study into more homogeneous portions where the hypothesis holds. (3) The regionalized variable is not firstorder stationary because the drift has a slowly varying trend. The trend may be removed from the regionalized variable yielding a difference called Regionalized variable theory is the residual. applicable if the intrinsic hypothesis holds for the residuals. Alternatively, the theory of intrinsic random functions (Matheron, 1973) can be invoked, which is a weaker generalization of the intrinsic hypothesis. This specifies that generalized increments of the regionalized variable must be stationary in the wide sense (Henley, 1981).

If each observation is regarded as the outcome of the same random variable and if this random

variable is second-order stationary, then the following relationship is true:

$$\sigma^2 = \gamma(h) + cov(h)$$

Here, σ^2 is the variance of the samples, $\Upsilon(\vec{h})$ is the semivariance for a specified displacement of \vec{h} , and $cov(\vec{h})$ is the autocovariance (as used in classical time series statistics) for displacement \vec{h} .

STRUCTURAL ANALYSIS

The semivariance $\Upsilon(\tilde{h})$ can be plotted against values of \tilde{h} to yield a function called the **semivariogram**, which is analogous to the correlogram as used in time series analysis. **Structural analysis** is the term applied to the study of semivariograms for the purpose of characterizing the degree of fluctuation in regionalized variables. The objective of a structural analysis may be to draw inferences about the causes of the behavior of a regionalized variable, or simply to provide parameters for use in further analyses.

To obtain a semivariogram, it is necessary to have a set of samples taken at regular intervals within the same geometric support. Let

$$y(x_1), y(x_2), ..., y(x_i), ..., y(x_n)$$

be n outcomes of a regionalized variable (either regionalized variables or residuals) having a common intrinsic function and satisfying the intrinsic hypothesis. Then, the following is an unbiased estimator of the semivariance (Olea, 1975):

$$\gamma(\vec{h}) = \frac{1}{2(k-p)} \sum_{j=k'}^{k'+k-p-1} [y(\vec{x}_j + \vec{h}) - y(\vec{x}_j)]^2$$

Here, \vec{h} is p times the sampling distance \vec{a} ; $k + k' \le n$; and p = 0, 1, ..., k-1. The study is done in one direction along a traverse or series of parallel traverses. The estimation of a semivariogram for observations of a regionalized variable is fairly straightforward, but this is not true for a semivariogram of residuals. Before the residuals can be obtained, it is necessary to know the semivariogram. The problem may be solved recursively by assuming a semivariogram, computing the drift and the residuals, and comparing the resulting semivariogram to that assumed.

Figure 1 is a typical semivariogram, of depth to the top of the Cretaceous Springhill Formation measured by a marine seismic survey in the Straits of Magellan, Chile. The major characteristics of regionalized variables that can be deduced from the semivariogram include:

(1) Continuity. The shape of the semivariogram, and in particular its behavior near the origin,

reflects the regularity and smoothness of the regionalized variable. A parabolic semivariogram which is horizontally tangent at the origin means the variable is extraordinarily regular relative to the sampling distance. In contrast, highly erratic sequences produce a semivariogram which is almost vertical at the origin.

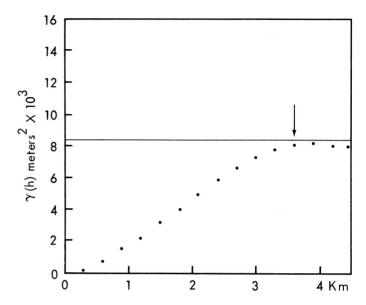


Figure 1. Semivariogram of elevations of top of Springhill Formation measured along marine seismic traverse in Straits of Magellan. Semi-variance is in square meters. Line represents sill, or variance of elevations, and equals 8380 square meters. The range is equal to 3.5 km.

- (2) Zone of influence. Figure 1 is a transitive type of semivariogram. The arrow in Figure 1 indicates the range, which divides the samples into two categories. Samples taken a distance apart which is smaller than the range are statistically dependent and may be used in estimation; samples which are farther apart are statistically independent. In this sense, the range defines a zone of spatial influence around any location. The horizontal portion of the semivariogram to the right of the range is the sill, which asymptotically approaches the variance of the observations (Clark, 1979). The semivariogram shown in Figure 1 is said to exhibit transitive behavior, expressing moderate continuity of the regionalized variables within a local neighborhood, and random behavior over larger distances.
- (3) Repetition. Regionalized variables may tend to repeat if examined over sufficiently large intervals. The semivariogram of a repetitive regionalized variable is also repetitive in appearance.
- (4) Anisotropy. Non-uniform variation of the regionalized variable through the geometric field is

shown as changes in the semivariogram from area to area, or with direction of the sampling traverses. Anisotropy may be related to structural faulting, depositional patterns in sediments, and magmatic and other genetic processes which operated along preferred directions or specific locations.

Interesting results can be obtained by mapping the residuals from a regionalized variable after completion of structural analysis. The objectives of such studies are similar to those of trend surface analysis.

ESTIMATION

Estimation procedures that incorporate regionalized variable theory were originally known as kriging, a term named for D. G. Krige, a South African mining engineer whose pioneer work in ore grade estimation gave Matheron the inspiration to develop geostatistics. Kriging is used only with regionalized variables which are first-order stationary. For variables whose drift is not stationary, but for whose residuals the intrinsic hypothesis holds, universal kriging is used; kriging is a particular case of this more general procedure.

Universal kriging is used for three purposes: (1) To predict the value of a regionalized variable at a location in the geometric field. Universal kriging is an exact interpolation procedure which honors all observations. The procedure can be used to estimate values of a regionalized variable at regularly spaced points across an area, as the first step in automatic contour mapping. (2) To compute the average value of a regionalized variable inside a volume larger than the geometric support. For instance, it is used to estimate the average ore content of mining blocks using grade information from drill cores which have a considerably smaller volume. (3) To estimate the drift in a manner similar to the analysis of trend surfaces.

Certain minimum requirements must be satisfied before universal kriging can be performed. First, the drift M(x) is assumed to have analytical representation inside a neighborhood.

$$M(x) = \sum_{i=0}^{n} a_i f^i(x)$$

where a_i are unknown coefficients and $f(\vec{x})$ are functions of \vec{x} , commonly powers of the spatial coordinates. Second, the residuals $R(\vec{x})$, defined as the difference between the regionalized variable $Y(\vec{x})$ and the drift $M(\vec{x})$, must satisfy the intrinsic hypothesis. The semivariance must be known, either from a structural analysis of the same data or as a result of previous studies.

Universal kriging uses linear estimators for the regionalized variable itself, the drift or any coefficient in the analytical representation of the drift, and for average values. The estimators are of the form

$$Z*(\vec{x}_0) = \overset{k}{\underset{j=1}{\sum}} \lambda_j y(\vec{x}_j)$$

where:

 $Z^*(\overset{\rightarrow}{x_0})$ is the unknown parameter at location $\overset{\rightarrow}{x_0}$ λ_j are (real number) weights $y(\overset{\rightarrow}{x_j})$ are observations at locations $\overset{\rightarrow}{x_j}$ inside the zone of influence.

The k unknown λ_j 's are found by solution of a system of linear equations which result from forcing the estimator to be unbiased and to have minimum estimation variance. The form of the equations differs slightly among estimators. For point estimation of the regionalized variable (Olea, 1975), for instance, the equation is

$$A X = B$$

where A, B, and X are the matrices shown on the following page.

The Lagrangian multipliers μ_i are additional unknowns arising from the constraints on the estimator. $\Upsilon(\vec{x}_j, \vec{x}_k)$ is the semivariance between pairs of samples located at points \vec{x}_j and \vec{x}_k . If the samples are not measurements made at points, the computations become considerably more complex as the semivariances are no longer those in the semivariograms, but are moving averages of pairs of points inside the pair of supports.

Even though point estimations made by kriging are optimal, they yield a predicted surface which is smoother than the unknown actual surface, because spatial variation at a scale smaller than the sampling interval cannot be assessed. If the rate of spatial variability in the geometric field is more important than a best guess of the regionalized variable at a particular location, geostatistics provides a method for **conditional simulation** of the regionalized variable. This is a simulation technique which differs from Monte Carlo methods by its intensive use of the spatial correlation between sample points (Journel and Huijbregts, 1978). The conditional simulation honors the observations, but between the sample points it consists of realizations

 $\mathbf{x} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \dots \\ \lambda_j \\ \dots \\ \lambda_k \\ \mu_0 \\ \mu_1 \\ \mu_2 \\ \dots \\ \mu_i \\ \dots \\ \mu_n \end{bmatrix}$ $\mathbf{B} = \begin{bmatrix} \gamma(\overrightarrow{x}_1, \overrightarrow{x}_0) \\ \gamma(\overrightarrow{x}_2, \overrightarrow{x}_0) \\ \dots \\ \gamma(\overrightarrow{x}_k, \overrightarrow{x}$

which have structural characteristics and dispersion equal to the measured dispersion.

Cokriging is another geostatistical tool which allows estimation considering not only the spatial autocorrelation between samples of the same regionalized variable, but also the cross-correlation between different regionalized variables defined on the same geometric support (Matheron, 1971).

ESTIMATION RELIABILITY

The minimum estimation variances of universal kriging estimators can be used as measures of confidence, as the estimation variance is an expression of the degree of dispersion of the true value of the regionalized variable around its estimated value (Olea, 1982). The estimation variance comes directly from the solution of the system of equations for universal kriging. For point estimation of a regionalized variable, the estimation variance

$$\sigma_{\mathsf{E}}^{2}(\mathbf{x}_{0})$$

is

$$\sigma_{E}^{2}(x_{0}) = x^{T} B$$

where \boldsymbol{X} and \boldsymbol{B} are the matrices defined above, and \boldsymbol{X}^T is the transpose of matrix \boldsymbol{X}_\bullet

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MODELLING METHODS FOR SPATIAL DATA

Modelling spatially distributed data is important in many branches of geology. The types of models vary greatly with the data on which they are based, and with the purpose for which they are made. At the present time there is no coherent discipline of geological modelling.

Each model attempts to describe in some mathematical manner the geometry of a surface, given constraints of one form or another (Tipper, 1979). The surfaces may be real physical entities such as the boundaries of a subsurface sandstone unit, or they may be abstract concepts such as the phase-boundary surfaces in a silicate-melt system. Most can be considered as sharp contacts between two phases; where phases grade imperceptibly into each other the concept of a bounding surface becomes arbitrary. The constraints imposed on the models are twofold: (1) the mathematical form of the model is specified by equations, and (2) boundary conditions are set which enable the equations to be solved.

The most widely used model has been the trend surface, which is reviewed elsewhere in this publication. Its mathematical form is

$$Z = f(X, Y)$$

where the function, f, is chosen arbitrarily. Whitten (1975) has tabulated most of the functions which have been used, of which the most common is a polynomial, usually of less than seventh degree in either of the independent variables. Double Fourier series have also been used to model surfaces which are suspected to contain periodic components. The boundary conditions usually are coordinates of points known to lie on the surface. If there are n of these points and the function f contains m unknown coefficients, a unique solution can be obtained only when n is equal to m. Under such conditions the model passes through all the data points but, if m is large, may vary erratically between the points. In consequence, this exact model can rarely be used except for small data sets. If n > m, a leastsquares fit may be used to give a model that approximates the data points. For the least-squares model to be valid in a statistical sense, certain assumptions must be met which involve testing the model for spatial autocorrelation.

Another modelling method uses bicubic splines (de Boor, 1962), and has been used to represent subsurface horizons. A **bicubic spline** is a set of individual bicubic surfaces, each defined over a rectangular cell in the X-Y plane. The cells are formed into a regular two-dimensional grid, and surfaces in adjacent cells are constrained to have

continuity of position, slope, and curvature across their mutual boundaries. The boundary conditions for this model are again the coordinates of points known to lie on the surface, together with the values of slope of the surface at its edges. The data points must be located at every node of the grid, and the slope values specified at each external node. The major drawbacks to this modelling method are its dependence on gridded data and its poor performance in representing highly inclined surfaces. Trend surfaces also suffer from the latter drawback.

To circumvent the necessity for gridded data and to enable general surfaces to be modelled, Tipper (1977, 1979) introduced the use of **computeraided design** (CAD) methods in geology. These represent a surface as a network of quadrilateral cells, as do bicubic splines, but define cells on the surface itself rather than on the X-Y plane. Each cell is defined in terms of parameters u and v, and the location of any point within the cell in terms of rectangular Cartesian coordinates is determined by the functions f_{1-3} in

$$f(x,y,z) = [f_1(u,v), f_2(u,v), f_3(u,v)]$$

In order that adjacent cells match with appropriate continuity across their mutual boundaries, the form of f_{1-3} is circumscribed. The most common form is due to Coons (see Forrest, 1972), but a development using B-splines appears to be more practical. Required boundary conditions include the coordinates of a set of points which can be arranged into a network topologically equivalent to a planar rectangular grid, and (for the Coons formulation) the surface slope and twist at each data point.

Trend surface, bicubic spline, and CAD modelling methods have been applied in the classical areas of geology—stratigraphy and structural geology, sedimentology, paleontology, and geomorphology. In fields such as geophysics and hydrogeology that have greater mathematical underpinning, surface modelling has developed differently. The mathematical form of surfaces in these disciplines such as the piezometric surface of an artesian aquifer often can be derived theoretically. Under steady-state conditions the surface often follows Poisson's equation

$$\nabla^2 \phi = f(x,y)$$

Surfaces must be considered whose forms are time-dependent, such as the transient form of a water table during pumping. Provided that suitable boundary conditions are specified, each of the relevant equations can in theory be solved, although an analytical solution is rarely possible except in the simplest of circumstances. Mechanical and electrical analogs often are used to give approximate solutions (Prickett, 1975), but numerical methods now predominate.

Until recently, finite-difference methods have been in wide use (Remson, Hornberger, and Molz, 1971). In these, the differential equations for the surface are reduced to discrete form to simplify their solution. Currently, finite-element methods are in vogue (Pinder and Gray, 1977); these replace the continuous surface by a connected set of local elements, each of simple form and each contributing to the total solution. For transient models, combination finite-difference/finite-element methods may be used.

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GLOSSARY

This glossary is far from exhaustive, but includes many of the terms that are used in the analysis of time- and space-dependent data in the geological sciences. The definitions are only those relevant to this particular subject area; many of the terms have alternative meanings in other contexts. Terms or definitions from regionalized variable theory are indicated by the symbol .

- Aliasing Incorporation of variance from frequencies higher than the sampling rate into lower frequencies.
- Analysis of variance Separation of total variation in a data set into components attributed to different sources.
- Anisotropy Having properties which differ according to direction; possessing a grain or preferred fabric.
- Anomaly A marked deviation from the local average; in geophysics, a small area possessing unusually high or low values of a property.
- Autocorrelation A standardized measure of the relationship between observations in an ordered series expressed as a function of the interval between observations. See correlation coefficient.
- Autocovariance The covariance measured between pairs of observations in an ordered series, expressed as a function of the interval between observations. See covariance.
- B-spline A continuous, smooth approximation of a curve or surface known only at discrete points. The B-spline is composed of n-k+1 segments or patches which blend into each other with specified continuity, where n = number of points on curve or surface, k = degree of spline function.
- Bicubic spline A continuous, smooth approximation of a surface known only at discrete points by a series of second-order polynomial patches. Adjacent patches are constrained to be uniform in slope across their common boundary.
- **Block diagram** A three-dimensional representation of a part of the Earth's crust shown as a perspective or isometric projection.
- Boundaries Apparently abrupt discontinuities separating distinguishable classes, either two-dimensional (soil boundaries or geologic contacts shown on a map) or three-dimensional (formation boundaries).
- **Boundary conditions** Mathematical requirements set for the behavior of a function at control points on the surface being evaluated.
- CAD See computer-aided design.
- Canonical correlation An eigenvector technique related to both factor analysis and regression analysis. Two sets of variables are transformed into linear combinations so that within each set combinations are uncorrelated but each combination in one set is correlated with a combination in the other.
- Cartesian coordinates Measurements in a plane made with respect to two orthogonal reference

- axes, or in solid space with respect to three orthogonal reference axes.
- Chi-square A statistic distributed as the sum of squares of an independent normal variate; commonly used in tests of goodness-of-fit and of independence in cross-tabulated data.
- Choropleth map A map divided into distinct regions on the basis of the average value of some property within each region. An example is a map in which classes are based on mineral worth per square mile.
- Cluster analysis Arrangement of a collection of observations into groups that are relatively homogeneous and distinct. Some cluster techniques also impose a hierarchical ordering on the groups.
- Cokriging Estimation of one spatially distributed variable from values of another, related variable.
- Conditional simulation Creation of partially random functions which have the same geostatistical properties and the same values at control points as the phenomenon being modelled.
 - Computer-aided design Modelling of three-dimensional objects by fitting of mathematical forms to known points on the surface of the objects.
 - Contouring Construction of isolines which show the three-dimensional form of a real or conceptual surface. Contouring usually involves the fitting of local, mathematically defined surfaces to data points.
 - Coons patch A continuous, smooth approximation of a surface known only at discrete points by a series of mathematically defined patches or splines. Unlike other spline methods, Coons patches are defined in terms of nonorthogonal coordinates on the surface itself rather than by Cartesian coordinates.
 - Correlation coefficient A measure of interdependence between two variables, expressed as a unitless number between +1 (perfect relationship) and -1 (perfect inverse relationship).
 - Covariance A measure of joint variation of two variables, measured on the same objects, around their common mean. It is expressed as the average cross-product of deviations from the means.
 - Cross-correlation A standardized measure of correspondence between elements in two different ordered series. See autocorrelation.
 - DIME Acronym for Dual Independent Map Encoding, a scheme widely used in cartographic data bases to store digitized lines.
 - Data bank Informal term referring to a large computer data file or organized collection of files on a particular topic.

- Degrees of freedom The number of independent items of information available for calculation of a statistic; usually, the number of observations minus the number of parameters already estimated from the data.
- Digitizing Process of converting graphic information such as lines on maps and charts into numerical coordinates that can be processed by computer.
- Directional analysis Analysis of variation in data that consist of angular measurements, either two-dimensional (circular) or three-dimensional (spherical).
- Dispersion The directional equivalence of variance; the scatter of angles about a preferred or mean direction.
- Double Fourier surface A two-dimensional mathematical surface defined as the sum of two orthogonal sets of sine waves. A form of trend surface analysis in which a series of sine and cosine terms are fitted by least squares.
- Drift The local expected value of a variable within a neighborhood. It is a smoothed approximation of the regionalized variable itself, somewhat analogous to a trend surface; a two- or three-dimensional weighted moving average. If the drift is correctly determined the residuals from the drift will be stationary.
 - Embedded Markov chain A Markov chain in which the probability that a state will succeed itself must be zero.
 - Ergodicity A property of a time series population, in which statistics such as the mean and autocorrelations computed for any segment are, on average, equal to those of all other segments.
 - Estimation error Standard error of estimation, or expected squared difference between an estimate based on samples and the true value of the variable.
 - Fence diagram Three-dimensional representation of a segment of the Earth's crust, shown as a series of interconnected vertical panels or cross-sections.
 - Filter A series of weights applied as a moving average to a time series. The weights are designed so that certain characteristics are emphasized.
 - Fourier analysis Transformation of a time series from the time or space domain into the frequency domain. It involves resolving the time series into a series of orthogonal components or harmonics, each of the form a sin X + b cos X.
 - Frequency analysis See Fourier analysis.
 - Generalization Simplification of line detail or shape, necessary when reproducing a map at a scale smaller than that of the original.
- Geometric support A description of the physical size, shape, separation, and arrangement of samples in two or three dimensions.

- Geostatistics 1. The application of statistics to geologic problems. 2. Analysis of space-varying natural phenomena.
- Global fit Fitting a single function, usually by least squares, to all observations of a spatially distributed property, as in a trend surface.
- Grid A regular two-dimensional array of interpolated points created as an intermediate step in the automated contouring of irregularly arranged observations.
- Harmonic analysis See Fourier analysis.
- Histogram A diagram in which the frequencies of occurrence of observations within successive intervals are shown as bars whose heights or areas are proportional to the frequencies.
- Independent events Occurrences in time or space that are independent of all other occurrences regardless of the duration or spacing between them.
- Instantaneous events Occurrences in time of such short duration that they are considered to be instantaneous. An example is a volcanic eruption considered on the scale of geologic time.
- Interactive A computer program which allows for user intervention during its execution, usually by dialogue through a terminal.
- Intra-class correlation A measure of similarity between members within a single class or group, in contrast to that between members of several groups.
- Intrinsic hypothesis An assumption that the residuals or deviations from the drift of an observed property are stationary, even though the property itself may not be.
 - Isoline A contour line, or line of equal value.
 - Isopach map A contour map showing changes in thickness of a stratigraphic interval. An abbreviation of isopachous, from iso = equal and pachous = thickness.
- Kriging A distance-weighted moving average estimation procedure that uses the semivariogram to determine optimal weights. If the semivariogram is known, kriging is a best linear unbiased estimator.
 - Least squares Fitting a function to observations so that the sum of the squares of deviations of the observations from the function is a minimum.
 - Linear estimators Weighted averages; estimates made by weighting observations and summing them.
 - Linear interpolation Straight-line interpolation; a point located intermediately between two others is assigned a value proportionally intermediate between their values.
 - Local fit method Fitting a function, usually by least squares, to a small, spatially limited subset of observations. The process is repeated until the entire map area is covered with a set of local functions. Examples of local fit methods are contouring algorithms and spline curves.

- Logit map A contour map of logit scores, which are a transformation of frequencies of occurrence such that the estimated probabilities are constrained to the range 0 to 1.
- Map units Distinct bounded areas shown on maps. Examples include formations on a geologic map or soil types on a soils map.
- Markov chain A sequence of states, such as stratigraphic lithologies, in which the probability that one state succeeds another is less than 1 but more than 0, and does not change throughout the sequence; a semi-deterministic succession of states.
- Model A mathematical representation of a natural object, property, or process.
- Monte Carlo simulation Methods of approximating solutions of problems by sampling from simulated random processes.
- Multiple regression A statistical technique in which the variation in a dependent variable is expressed as a linear function of a number of independent variables.
- Neighborhood An area or volume within which all points are related to some degree.
 - Nonparametric Statistical tests which do not depend upon the assumption of a population having specified parameters, such as the normal distribution; distribution-free statistical procedures.
 - Nyquist frequency The highest frequency detectable in a discrete time series sampled at regular intervals. The wavelength of the Nyquist frequency is twice the spacing between observations.
 - Octant search A constrained search around a point, such that a specified number of nearest observations are found within each of eight 45-degree sectors.
 - Optimal zonation Separation of an ordered sequence, such as a stratigraphic succession, into a specified number of contiguous categories so that the ratio of between-categories to within-category variances is the maximum possible.
 - Orientation The angle of a line in two- or threedimensional space with respect to a coordinate system. An oriented line does not possess a sense of direction, so orientation may be specified as either of two complementary measures.
 - Parametric Statistical tests which assume that samples are drawn from a population with known characteristics, such as a normal distribution.
 - Pattern recognition A branch of applied statistics primarily concerned with the interpretation of two-dimensional images.
 - Point process A time series consisting of events which occur at points in time, in contrast to ordinary time series which consist of observations taken at fixed intervals.
 - Poisson process A continuous random process through time, in which the probability of occurrence of events is proportional to the length of time between them, the probability of two events occurring simultaneously is zero, and intervals

- between events are independent. A process describing the occurrence of rare random events.
- **Polynomial** Linear function of the form $Y = b_0 + b_1 X + b_2 X^2 + \dots + b_k X^k$. Trend surfaces are polynomial functions of two geographic coordinates.
- Power spectrum Plot of "power" or variance versus frequency. In Fourier analysis, a time series is resolved into a series of sinusoidal components of different frequencies. The variance of each of the sinusoids is equal to the square of its amplitude.
- Principal components In multivariate analysis, a set of linear combinations of original variables which form a set of new transformed variables that are independent and which account in turn for as much of the total variation in the data set as possible. The eigenvectors of a covariance matrix.
- Probability 1. The probability of an event is the proportion of times the event will occur in the long run (relative frequency definition). 2. A measure of the strength of a person's belief concerning the occurrence of events (subjective definition).
- Quadrant search A constrained search around a point, such that a specified number of nearest observations are found within each of four 90-degree sectors.
- Random process A process which is governed at least in part by some chance mechanism. That is, only probabilistic predictions of the future state of the process can be made; exact predictions are not possible.
- Range Distance at which observations are essentially independent of one another, or at which the semivariance becomes equal to the variance.
- Regionalized variable Functions describing natural phenomena that have spatial or geographic distributions, such as the elevation of the ground surface or the grade of ore in a mine. Unlike random variables, regionalized variables have continuity from point to point, but are so complex that they cannot be described by any tractable deterministic function. They have properties intermediate between a random function and a deterministic function.
 - **Regression** Statistical method in which observations of a dependent variable Y_i are expressed as a function of one or more independent variables X_i , plus a random component \mathcal{E}_i .
 - Renewal process Process leading to a time series in which the intervals between events are independent and identically distributed.
 - Residual map A map of the deviations of observations from a fitted trend surface, usually made by contouring the original data, then subtracting the trend surface from the contour map.

- Rose diagram A circular histogram, showing the frequencies of directions within specified angular intervals.
- Sampling density Number of observations per unit area or per unit time.
- Schmidt net In petrofabric analysis, an equal-area projection of a lower hemisphere used for the plotting of directions and poles to planes. A Lambert equal-area polar projection.
- Semivariance One-half the variance of differences between pairs of observations spaced a specified distance apart.
- Semivariogram A plot of semivariance versus distance between pairs of observations.
 - Serial correlation Correlation between observations in a time series and those observations a fixed distance behind or ahead. Autocorrelation.
 - Series of events A time series produced by a point process.
 - Signal theory A body of mathematical, statistical, and computer techniques for analysis of time series generated by automated instruments such as remote sensing scanners. The objective is to eliminate random "noise" and other unwanted components from the signal. Also called communications theory.
- Sill The part of a semivariogram which is approximately flat, at a value equal to the variance.

 The sill lies beyond the range.
 - Spatially filtered map A contour map which has been processed to remove certain spatial frequencies, either by manipulation of its Fourier spectrum or more commonly by smoothing using a weighted moving average filter.
 - Spectral analysis See Fourier analysis.
 - Standard deviation Square root of the variance. A measure of dispersion about the mean, given in the same units as the observations.
 - Stationary A time series is said to be stationary if its statistical characteristics remain unchanged with time.
 - Stochastic Containing a random component. Used often as a synonym for random.
 - Stretch coefficient Amount of expansion or contraction necessary to bring two stratigraphic sections into coincidence or geologic correlation.
- Structural analysis Determination of an appropriate model for the semivariogram, or for the drift and semivariogram of residuals from the drift.
 - Time series A sequence of observations ordered in time or space.

- Transients Sudden, extremely rare or unique events in a time series, such as a spike or single aberrant value, or an abrupt change in mean value.
- Trend surface A global-fit surface in which a mapped variable is expressed as a function (usually a polynomial) of geographic coordinates. A trend surface is fitted by least squares, so is a smoothed approximation of the observations. The mapped variable is partitioned into the trend and the deviations or residuals. Depending upon the application, either the trend or the residuals may be of primary interest.
- Triangulation The construction of a network of triangles over a map, such that an observation lies at the vertex of every triangle. An initial step in some methods of contouring.
- Uniform distribution All possible values of a variable are equally probable; a rectangular probability distribution.
- Universal kriging An extension of the kriging estimation procedure which allows unbiased estimates to be made even with certain types of nonstationarity. It requires estimation of the form of the drift and a model for the semi-variogram.
 - Weighted average An average of a set of observations, in which each observation has been weighted or multiplied by some factor reflecting its importance.
 - Weighting function In local fit mapping procedures, the influence of control points is weighted according to their distance away from the point being estimated. A plot of weight versus distance is the weighting function.
 - Wiener filter A weighted least squares moving average applied to a time series used for signal enhancement.
 - Window The span or number of points included within a weighted moving average applied to a time series.
 - Wulff net In crystallography, an equal-angle projection of a lower hemisphere, used for plotting axes, poles, and crystallographic planes. A polar stereographic projection.
 - Zone of influence 1. Area around a point within which there is a partial dependency with values at other locations. 2. Area around a drill hole which can be regarded as "tested" with respect to probable occurrence of an oil pool or ore body of specified dimensions.



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