SCIENCE

CURRENT PROBLEMS IN RESEARCH

The Computer in Geology

Quantification and the advent of the computer open new vistas in a science traditionally qualitative.

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Under the stimulus of increasing amounts of numerical data and the wide availability of high-speed computers, geologists have begun to look into problems of automatic data processing. Automatic data acquisition by means of sensing devices, or automatic methods of rock analysis, represents one aspect of the problem. Data storage and retrieval, with punched cards or magnetic tape, are aspects that include design of storage systems and establishment of geological data centers. Data analysis includes routine treatment of large masses of data for purposes of summarization, as well as analysis of limited amounts of data by more complicated computational methods. The problem of assembling a library of computer programs especially adapted to geological data is an important facet of data analysis. Automatic presentation of computer output, another aspect of data handling, includes devices for direct plotting of scatter diagrams, regression lines, contour-type maps, and other kinds of visual machine output. Interpretation of computational results is a feature of data handling normally performed by the geologist, but "decision criteria" can be prepared for the computer, leading to automatic interpretation, as illustrated by automatic classification of sedimentary rocks as marine or nonmarine by means of programmed criteria.

Automatic data acquisition raises an interesting challenge in geology: to what extent, and in which domains of geology, can automatic data acquisition be achieved most effectively, by such procedures as digitization of subsurface records from exploratory boreholes, or of records from remote sensing equipment, such as airborne radiation detectors? Even more challenging are the implications of "decision functions" that transfer the interpretation of geological data from man to machine. If such transfers can be made successfully, what do they imply for the development of geology? Is it conceivable that the computer may become part of an automatic system that will, in some problems, completely replace the geologist in functions that go all the way from data acquisition, through data processing, to final interpretation of the results?

These questions cannot be answered today. At present we cannot say with fairness that all or even many geologists are directly concerned with computer applications. Most nongeologists are surprised that the computer enters the science at all. It is the major purpose of this article, in fact, to induce more geologists to look into the subject, as well as to acquaint nongeologists with some "fringe activities" in the science, carried on mainly by individuals or small groups in universities, governmental agencies, and research institutes.

Although all of the several aspects of data processing are of equal importance in the further development of automatic procedures in geology, this article is confined to some features of data analysis within the framework of the kinds of studies made in geology, the kinds of data available to geologists, and the sorts of data-processing problems encountered. It will be apparent that some geological problems—especially those that involve empirical data —can be organized in more than one way, and that this, in turn, permits use of a diversity of models for essentially the same sets of data.

Numbers in Geology

Geology is basically a qualitative science, but geologists have long used numerical data. Areal geology maps, that show the distribution of rocks on the surface of the earth's crust, are constructed from field observations that include many measurements of dip and strike of beds as well as measurements of thicknesses of rock layers. The map printed on a topographic base is a quantitative device from which cross sections can be made, and from which, within limits, the areal distribution and thicknesses of buried rocks in the subsurface may be predicted. The qualitative content of these maps (involving subjective assessment) lies in the definition of the stratigraphic units used for mapping and in the interpretation of complex field relations among the rock bodies observed.

It is only relatively recently that numerical measurements have begun to match in volume the body of qualitative observation in the science. Today numbers pour in from geochemical study of rocks; from geophysical measurements of gravitational and magnetic features of the solid earth; from oceanographic and marine geological expeditions; from controlled laboratory experiments on geological processes; and as a great quantity of stratigraphic data from the many and various mechanically recorded well logs obtained during exploration for oil and gas. Geological field studies on rock outcrops and landforms each year become more quantitative as previously qualitative concepts are transformed into numbers.

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Quantification in Geology

The influx of numbers into geology does not necessarily mean that the science is becoming wholly quantitative. Numerical data thus far have sharpened and refined the core of qualitative reasoning based on the method of "multiple working hypotheses," introduced in 1897 by T. C. Chamberlin (1). In his qualitative evaluation of multivariate phenomena by this method the geologist selects and integrates from innumerable details those factors or components that appear to have controlled a given geological situation. The internal consistency of the data, and the "weighing" of several lines of evidence simultaneously, commonly provide a basis for selecting some single set of conditions that most satisfactorily accounts for the phenomenon.

Quantification carries its own problems with it. The development of measurement procedures requires the setting up of operational definitions that express the concept or attribute as a number on the nominal, ordinal, interval, or ratio scale. These numbers lead a life of their own; they are endowed with properties that depend on the measuring process, and these properties determine to some degree the meaningfulness of the numbers in geology, as well as what can be done with them after they are obtained.

A second problem raised by quantification pervades all of geology. This problem involves making a distinction between those parts of the science that can best be treated wholly on a quantitative basis and those that may actually be weakened by overquantification. An example is stratigraphic correlation, where strong qualitative (and subjective) considerations as well as numerical data enter into the problem of subdividing the stratigraphic column into workable units. These units are then correlated stratigraphically from place to place and used to prepare geological maps. The great influx of mechanically recorded well logs from explorations for oil and gas has made it possible for stratigraphic subdivision and correlation to be performed automatically by computers operating with numerical data obtained from the logging devices. What are the implications of such procedures, in techniques of exploration for economic deposits as well as in more academic pursuits? What are the long-term implications for the science in removing from this basic part of

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geology the subjective assessment and "mental integration" of many purely qualitative considerations?

A third problem raised by quantification relates to the selection or design of models appropriate to specific geological problems. Models-in the sense of devices for organizing data-have long been used in geology, and their use is implied in Chamberlin's principle of multiple working hypotheses. For some classes of geological problems involving numerical data the appropriate model appears to be an empirical one that "sorts out" a number of complexly interlocked variables, as in statistical correlations between trace elements in rocks; for others, such as problems involving heat flow or fluid flow through rocks, the physical situation is well enough understood to permit use of models based on differential equations.

Once a model is formally stated, it becomes a guide in data acquisition and analysis. Some geological studies can be organized—"structured"—in any of several ways, as already mentioned, and it is not always immediately apparent what the optimum model is, at least in empirical studies. What kinds of models are used for structuring data and what kinds of computer programs are required for their analysis obviously depends in part on the kinds of data available.

The Nature of Geological Data

The data of geology may be classified into three main groups. The first group represents qualitative observations or statements regarding natural objects or events as they are examined in the field or in the geologist's measurement laboratory, and the second represents numerical measurements on these natural objects or events. The third group constitutes quantitative measurement data arising under specified and controlled conditions in an experimental laboratory. The first two groups are called, for convenience, the observational data of geology, in contrast to the third, the experimental data of geology.

The measurement laboratory in this specific context provides an opportunity to examine in detail samples or speciments collected in the field. The experimental laboratory is used for studies of mineral origin, or of sedimentary particle movement in a flume, conducted under specified and controlled conditions. The data that arise in the experimental laboratory are the data of an experimental science, in distinction to the data of an observational science.

Some differences between observational and experimental data in geology are shown in Table 1, where the brief statements perhaps need qualification. Things are not quite as bad on the observational side, or quite as good on the experimental side, as Table 1 may imply. However, the distinction is real in many geological problems, especially when it comes to handling empirical data in terms of specific models for analysis and interpretation.

In his day-to-day work the geologist is much more concerned with observational data than with experimental data. Geological processes examined in the field (such as stream action, wave action, and volcanic eruptions) and their end products—rocks, fossils, landforms, and geologic structures—all yield data on the "Observational" side of Table 1. Field observations contain both qualitative and quantitative items, and the study of samples or specimens in the measurement laboratory tends to swell the proportion of numerical data in the total set of observations.

Table 2 lists geological studies that vield data of an observational kind. Many field projects include several of the items and are supplemented by measurement-laboratory data. This is especially true in studies of relations among geological processes and the deposits associated with them. Field study of a sedimentary environment may include observations on the process elements-waves, currents, tidal effects -and on the response elements, represented by the texture and composition of the bottom deposits, commonly in terms of their patterns of areal distribution over the sedimentary environment.

In ancient rocks, the formative geological agents have long since vanished and only the response elements are left. Emphasis is thus placed on studies of rock texture, composition, areal distribution of properties, and relations among adjoining rock bodies. The objectives of these studies may be to develop rock classifications; to reconstruct the conditions of rock origin (that is, to infer what process elements were present); to understand the geological history of the area; or to locate natural resources associated with the rocks.

Two kinds of "field study" are listed under the measurement-laboratory studies as the last items in Table 2. These include the mapping of buried rocks as they are disclosed in boreholes, as well as integration of geological and geophysical data. These rocks may not be exposed at the earth's surface at all, but contour-type maps showing structural attitude, thickness, areal extent, and composition of the rock bodies can be constructed from data available in some regions. It is likely that more subsurface maps than surface maps are being made today, in North America at least.

As Table 2 indicates, some studies in the measurement laboratory involve experimentation with natural objects under controlled statistical conditions. Experimental designs based on analysis of variance for comparison of measurement methods, and of operators or analysts performing the measurements, are examples. A case in point is the comparison of methods for measuring the shapes of pebbles in terms of objectivity, precision, cost, and so on.

Analytical and Statistical Models

The observational data that arise from geological studies as listed in Table 2 have many features in common, even though the geological objects or events that are measured differ from one study to another. Thus, geological studies (or the sets of observational data arising from them) may also be grouped according to the kinds of models appropriate for their analysis.

It is significant that the characteristics of observational data in geology, as listed in Table 1, are in large part the characteristics of statistical data in general. When phenomena are encountered in which numerous variables act simultaneously, where man's control may be limited or lacking, and where reliance must be placed on part of the whole phenomenon (samples) rather than on all of it, the appropriate framework for analysis is statistical.

Not all geological problems are statistical, not even all problems based mainly on observational data. For example, the question of whether or not a rock layer has been overturned during structural deformation can be ascertained by study of sedimentary features such as cross bedding and graded bedding. If such features can be found, they answer the question directly. Similarly, cross cutting among igneous dikes can be established directly, to determine relative times of intrusion.

Where the physical and chemical

Table 1. A comparison of observational and experimental data in geology.

Observational data	Experimental data		
Numerous variables operate simultaneously in a complexly interlocked manner	Selected variables are "permitted to oper- ate" one or several at a time; interactions can generally be controlled		
Data tend to be "noisy" because of local geographic and temporal variations in the operative processes	Measurement error and "unexplained varia- bility" can be kept very small; experi- mental results are independent of geo- graphic location or time of experiment		
Variables are not controlled by man	Experiment is performed as completely as possible under man's control		
Observations can be made only where natural phenomena occur or can be reached by probes	Essentially all of a given phenomenon can be studied within the range of experi- mental conditions		
Heavy reliance is placed on sample ob- servations, sometimes greatly limited by lack of access to points of observations	Measurements ("samples") can be taken at will, essentially continuously if desired		
Many observations are not yet quantifiable, thus full numerical analysis is limited	Experiments can be deliberately confined to measurable processes and responses		

processes in a geological phenomenon are well understood, or where aspects of a problem can be related to an underlying differential equation, an analytical model may be used. Such a model may treat small-scale geographic or temporal fluctuations as part of the "noise" that partially obscures the systematic effects of main interest. Generalizations or predictions that arise from analysis are evaluated in terms of the agreement between the model and the phenomena under investigation. Studies of process and response elements, mentioned earlier, thus give rise to process-response models, which for some studies (as of ancient rocks) may be stated separately as process models and response models.

Even where the physical and chemical processes are not well understood, an empirical "analytical model" may be used to search for relations among a number of measured variables. These empirical models commonly are based on a straight-forward least-squares approach, and they may discard as "noise" some small-scale fluctuations that actually contain geological signals. Empirical analytical models have wide use in geology, and they are a preliminary step toward development of process-response models by their sorting out of interlocked data.

A statistical model may have the same initial form as an analytical model in that it specifies process and response elements; or it may be empirical in seeking for relationships among geological phenomena. The statistical model explicitly specifies the geological populations involved; it includes a formal

Table 2. Some examples of geological studies.

Field studies

Definition, description, and field correlation of stratigraphic units

Mapping of rock occurrences for areal geology maps

Mapping of surface structural features

Mapping of detailed relations within a rock body, including associated ore bodies

Geomorphological studies (landform analysis)

Field studies of geological processes (streams, groundwater, waves and shore currents, etc.) and their associated deposits

Measurement-laboratory or office studies

Chemical, textural, and other kinds of rock analyses, in part to supplement the data from field studies

Development of methods for measuring properties of rocks and the fluids they contain

Analysis of variance studies on measurement methods, on the subjective effects of analysts, etc. Analytical and statistical study of relations among measurable properties of rocks or of fossils

Development of classifications of rocks, fossils, landforms, etc.

Integration of field and laboratory data for interpretation of depositional environments, paleogeography, paleotectonics, etc.

Preparation of subsurface contour-type maps from borehole cores, rock cuttings, and various kinds of well logs

Interpretation of subsurface structure and stratigraphy from geophysical data, including gravity, magnetics, seismic records, etc.

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Table 3. Examples of geological data-analysis categories (se	see text)	(see	categories	data-analysis	geological	of	Examples	Table 3.	
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<i>1. Classification</i> Systematic grouping of fossils, rocks, minerals, stratigraphic units, landforms, etc.
2. Process and response Analysis of statistical or functional relations between geologically important, identifiabl dependent and independent variables in the observational data
3. Areal variation (map analysis) Gradients and trends in mappable data treated as functions of geographic coordinates
4. Associations among variables Analysis of statistical correlations in sets of observational data, to identify interlocke variables, especially where geologically important dependency relations may not be clearl discernible
5. Data evaluation
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Preliminary analysis of sets of data for noise content, for data redundancy, for data interlocking, for "sporadic items," and as a guide to choice of more specific models

plan of probability sampling; it identifies the several sources of variability in the data (including variability attributable to small-scale geographic and temporal fluctuations); and it includes procedures for drawing statistical inferences about the populations from the sample observations, with provisions for setting confidence limits on all estimates. In short, the statistical model uses the sample data to learn something about the population, and then uses the inferred population characteristics as its basis for generalizations and predictions.

Statistical models have been applied extensively in the measurement laboratory, as several items in Table 2 indicate. Here are included a large variety of analysis-of-variance models, including randomized blocks, Latin squares,

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factorial designs, "nested" designs, and so on (2). Many of these are now handled by means of standard computer library programs.

Application of statistical models in field studies is sometimes limited by severe sampling restrictions. Rock exposures and subsurface data may be so sparse that the geologist must take his data as they come, and he may prefer purposive selection of "typical specimens," in terms of an empirical analytical model, rather than the use of a formal statistical model that specifies a sampled population which may represent only a negligible part of some large but inaccessible target population (3). For studies with these limitations, a model of the data evaluation type, mentioned later, is sometimes appropriate, at least for pilot studies.



Fig. 1. Cross-section of stratigraphically correlated shale and sand unit (hypothetical) observed in boreholes on inset map. Dots are control points; distance represented by length of map, about 12 miles.

Geological Data Analysis

One way of looking at the analysis of geological data is in terms of the objectives of the study, or of the kinds of problems encountered in connection with observational data arising from the studies listed in Table 2. This approach is a continuation of the topic of models, though emphasis moves to the kinds of models—whether statistical or analytical—that are appropriate to machine processing of observational data.

Table 3 lists several data-analysis categories that apply in geology (4). Classification (category 1) is interwoven with many specific studies. Some aspects of classification can be handled by the computer. Thus, it is possible to evaluate classifications based on substantive judgment according to their success in yielding operationally meaningful classes. The computer can also be used to develop classifications with maximum similarity of attributes within classes and maximum differences between classes. Little has been published on this problem in geology, but it offers many interesting possibilities.

The second category in Table 3 includes a large class of geological studies in which dependent and independent variables can be defined, as in the geological experimental laboratory. A field example is the study of the angle of slope and the particle size distribution of sand on a foreshore as they respond to changing conditions of wave height, wave period, and wave length Many measurement-laboratory (5).studies can be included here, such as the study of rock permeability with respect to fluids in terms of particle size, shape, packing, and other attributes of the rock aggregate.

Studies of areal variation in geological phenomena, the third category of Table 3, have many academic aspects and many applications. Systematic changes of one kind or another (physical or chemical, gross or detailed) are commonplace in rocks, assemblages of fossils, sedimentary environments, and stratigraphic units, over their areas of occurrence. These areal changes may occur on several geographic scales, and commonly it is possible to discern an underlying large-scale trend in the data, on which may be superimposed smallerscale, seemingly nonsystematic, fluctuations. The computer can be used to separate the trend from the residuals on the trend. In some studies the trend is of major importance; in others the



Fig. 2. Contour maps of rock thicknesses in stratigraphic unit of Fig. 1. The shale has a pronounced linear trend, whereas the sand varies irregularly from about 75 to 85 feet. Statistical correlation between sand and shale in these open data: r = +0.0130.

small-scale fluctuations may be associated with economic deposits that occur where local changes in the pattern of variation produce special conditions favorable for the accumulation of oil, gas, or ore. Trend analysis has been applied to a variety of geological map problems, most commonly by fitting polynomial surfaces to the data (6).

The fourth category of Table 3, that of detecting and evaluating associations among variables (statistical correlation), is involved in almost all geological studies. The particular class of problem emphasized in Table 3, however, is an assemblage of data in which there may be no obvious basis for specifying dependent and independent variables in a physical or chemical sense. An example is the assemblage of trace elements or of minerals in rocks (7). Interest may focus on identifying those that "go together," as against those that seem antipathetic. In such studies a major problem is the distinction (normally made on a substantive basis) between fortuitous correlations and geochemically meaningful relations. An additional problem in evaluating associations arises when the data are "closed" -that is, when the variables measured on the samples add up to a constant sum (8). Observational data on the mineralogical composition of rocks, which must add up to 100 percent, are

closed systems. One may close data initially "open" by converting them to percentages. Closed systems have builtin statistical correlations that depend on the relative magnitude of the variances associated with the several variables.

A more general class of models for data analysis is indicated as the last item in Table 3. In this category a set of observations is examined in an empirical least-squares fashion in terms of its noise content, data redundancy, and other attributes. Data evaluation programs of this sort can play an important part in sorting out geological variables interlocked in complex ways. Especially needed are "map-screening' methods for examining a set of mappable variables to detect interrelationships and for predicting which maps will give most information in terms of the objectives of the map study and of its cost.

The preceding statement can be illustrated by an example. In subsurface stratigraphic mapping the data include measurements of thickness, structural attitude, and composition of the stratigraphic unit under study. A structure map and a thickness map are made as a matter of course, but the composition can be shown in a wide variety of lithofacies maps, and a decision is required as to which will be most useful for the objectives of the study. Stratigraphic data on thicknesses of rock types in boreholes are open, but a common procedure is to close them by computing percentage compositions. This procedure may change the resulting map patterns markedly.

The most obvious illustration of these changes is in two-component systems. Figure 1 shows a stratigraphic cross section with sandstone of uniform thickness at the base of a shale body increasing in thickness to the right. Figure 2 shows each component mapped directly as thickness in feet, a dominantly linear trend in shale thickness being assumed. The sandstone map is "spotty," owing to minor changes in thickness, but it displays no trend in any direction. Figure 3 shows the same data mapped as percentages of total rock thickness. The shale map is little changed in its pattern, whereas the sandstone map is now strongly "locked in," with a linear trend opposite to that of the shale, because of the built-in negative linear correlation in a two-component percentage system.

The relations in a two-component closed system are well known--they



Fig. 3. Contour maps of shale and sand percentages computed from rock thicknesses in Figs. 1 and 2. The sand now has a pronounced linear trend, and r in this closed system is -0.9995

are in fact mathematically trivial-but as the number of components increases, and especially if correlations or trends are present in the initially open data, the interlock may become quite complicated when the system is closed. Yet percentage maps play an important role in some stratigraphic problems, and map-screening and data-evaluation procedures can be of considerable aid in bringing to light the changed relations that occur when the map data are transformed either by taking percentages or by using ratios of the thickness of one rock type to that of another. In these circumstances the map maker has a much better basis for his interpretations and decisions if the interrelationships among the map variables have been first looked into.

Diversity of Models in Geology

I mentioned earlier that many geological studies can be organized in more than one way. For those problems which are approached primarily in an empirical manner—and this may include examples under each heading in Table 3—the geologist commonly has a choice of models. Thus, in process and response problems the model chosen may be an analytical model based on a differential equation that establishes a functional relation between the variables investigated. On the other hand,

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a multiple regression model may be used to determine which of several process elements appears to control some given response most strongly.

As a result of this variety of ways for organizing data, geologists interested in computer applications are experimenting with a wide range of methods for analyzing observational data. It is evident even at this relatively early stage in the use of computers in geology that numerous conventional ways for treating interlocked data are being looked into. These include factor analysis, component analysis, multiple regression analysis, multiple correlation analysis, the use of discriminant functions, and a wide range of standard analysis-of-variance models (9). If the scope of this article were enlarged to embrace computer applications in all the earth sciences-oceanography, atmospheric sciences, solid-earth geophysics, the growing domain of geochemistry, and so on-the number of applications discussed would be enormously increased, and there would be much more emphasis on analytical models arising from differential equations. Similarly, in economic applications of geology and geophysics in the search for oil and ore, application of systems analysis, linear programming, decision theory, and operations research to combinations of geologic and economic data directed toward exploration problems appears to be well under way. As for the academic aspects of geology, the present stage is largely one of presentation, before scientific societies, of papers and symposia (10), from which ultimately a body of literature will grow.

Particularly important for increased use of computers in geology is the fact that some of the methods of analysis indicated above—factor analysis is one —can be used for combinations of quantitative and qualitative observation. It is not necessary, therefore (and it may not be desirable), for every variable included in analysis to be expressible as a measurable quantity.

It is significant in the growth of geology as a science that increased use of quantification and computer techniques commonly directs the geologist's attention back to the field—to the outcrops and borings from which his data come. The occurrence of unexpected deviations or seeming inconsistencies in the analyzed data may suggest that some features merely recorded in passing in observing an outcrop need to be examined more carefully as an important part of the larger problem.

As is evident, this article covers only a very small part of the general subject of the computer in geology and its content is biased by emphasis on considerations arising from personal experience with digital computers. The whole domain of the analog computer, important as it is in many fields of geology, has been omitted. Despite the restricted area of discussion, however, I hope that enough has been brought out to show that geology is in a very challenging stage of development-or that at least some aspects of it are. Forty years ago, when new kinds of numerical data began to appear in geology in relative abundance, it was hardly feasible to handle a dozen variables simultaneously. Geologists as a group were not strongly inclined toward mathematics, and many advances in mathematical statistics bearing on problems of sampling, analysis of variance, and statistical inference were still beyond the horizon. The high-speed computer, of course, was even farther off.

Perhaps it is too early to suggest that the advent of the computer, with its capability for processing qualitative as well as quantitative data, may pave the way for broadened use of the method of multiple working hypotheses, this time on an even more comprehensive basis, by means of formal models adapted to a wide variety of geological problems. In this framework the computer becomes an essential part in a sequence of acquisition, storage, retrieval, and analysis that makes possible the assimilation into geology of the continually increasing flood of observational and experimental data.

The present dominantly empirical aspect of much data analysis in geology is not disturbing in a science where much effort, both qualitative and quantitative, must still be directed toward a search for controls and responses in a web of intricately interlocked data. Out of these methods will arise an understanding of functional relationships that can be used in developing more analytical models that increasingly reflect the "real-life" world of geological phenomena.

References and Notes

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- 4. An alternative tabulation to that in Table 3 emphasizes statistical problems in geology rather than the more general categories of Table 3. The alternative subheadings would be (i) estimation of mean values and degrees of variability of measurable properties of a geological population; (ii) estimation of degrees of association (correlation and regression) among measurable properties of geological populations (iii) detection and evaluation of areal patterns of variation (trends) in the mappable attributes of geological populations; and (iv) detection of geologically important differences between measured properties of geological populations,
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- At the time of writing, a symposium entitled "Geology Enters the Computer Age" is planned for the San Francisco meeting (March 1962) of the American Association of Petroleum Geologists.