46. The Role of Computers in Exploration Geochemistry

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ABSTRACT

The role that computing has assumed in exploration geochemistry for the period 1977 to 1987 has been assessed on the basis of a literature review, and to a lesser extent the personal experiences of the author. In the last decade, major changes have occurred in the computing environment. Microcomputers are now widely used in both the office and field. This has resulted in a significant increase in interactive computing, often accompanied with graphical capabilities, which has permitted geochemists to work more closely with their data. At the opposite extreme, supercomputers are becoming available to geochemists so that modeling and simulation problems previously considered intractable can now be solved. The new realm of expert systems and artificial intelligence is just beginning to be investigated in the context of exploration geochemistry. These techniques hold considerable promise as so many of the practical applications in mineral exploration are based on accumulated knowledge, "lore", and empirical or heuristic rules. The review concludes with a look forward to the next decade and identifies some areas where significant progress is likely.

INTRODUCTION

The period 1977 to 1987 has seen a rapid growth in the application of mathematical, statistical, and graphical procedures using computers to a variety of exploration geochemistry tasks and problems. The groundwork for much of this had taken place during the previous decade in research groups. The almost explosive growth of computer applications in the last decade has been largely due to availability of affordable computing power and better, more friendly and easy to use, software.

In 1977, the first microcomputers became available, the following year Apple introduced its model I machine, a little later machines using the generic CP/M operating system were widely available, and in 1982, IBM introduced its PC machine using the MS/DOS operating system. With that last event, half way through the decade we are considering, microcomputing became fully acceptable. The year 1978 was also marked by the introduction of the VAX 11/780 super–minicomputer by Digital Equipment Corporation. This machine, and similar ones supplied by other vendors, gave traditional large mainframe computing power to users at minicomputer prices. Much of the growth in acceptance of computing by exploration geochemists is due to the availability of cheap computational power available through the generation of hardware introduced in the late 1970s. Over the longer period of 25 years since computers have been used by exploration geochemists, the cost of the same computing power has dropped three orders of magnitude, from four million dollars to four thousand dollars.

The subsequent sections consider exploration geochemistry computing activities under several topics, these are: data acquisition and data base activities, survey design and quality control, univariate statistics, mapping and spatial data presentation, multivariate data analysis, classification, resource appraisal studies, artificial intelligence, modeling, and microcomputers for geochemical data analysis. Finally, on the basis of the last decade's progress and today's computing technologies, some conclusions and thoughts are presented on where important advances may occur in the next decade.

Since the previous decennial review by Howarth and Martin (1979), several other books and papers of a review nature have been published. Readers may find these of interest in determining the role that computers have taken in assisting exploration geochemists over the last decade; Garrett, Kane, and Zeigler (1980), Cameron (1983), K. Campbell (1983), Garrett (1983a), Howarth (1983b), De Vletter (1983), Howarth (1984), Garrett (1985), Howarth and Garrett (1986), Hanley and Merriam (1986), and Siriunas (1987). Additionally, Howarth and Turner (1987) have published a revealing study of the use and misuse of graphical procedures in geochemistry.

DATA ACQUISITION AND DATA BASE ACTIVITY

Currently, computers are still dominantly being used for laboratory data acquisition rather than field data acquisition. Rugged microcomputers have been developed for field data acquisition in geochemical and soil surveys in Sweden and the U.K. (Clarke *et al.* 1986; Lundholm *et al.* 1986); however, their use does not seem to be widespread. More commonly computer and communications technology has been used in geochemical laboratories to automate data acquisition, track samples, assist in quality control procedures and compile data for geochemical samples derived by different analytical procedures. Little has been written concerning this work; however, in North America many large commercial and government geochemical laboratories use systems based on minicomputers. One commercial laboratory example

has been described by Blok (1986). An example of a low cost microcomputer based system, GLADD was developed in the early 1980s at the Geological Survey of Canada, Ottawa. GLADD uses a network of inexpensive CP/M based machines attached to analytical instrumentation that feeds data to a larger CP/M machine where quality control and data compilation is undertaken.

The availability of digital data has made it feasible for users to directly obtain their geochemical data from the laboratories where they are being generated by transmission over telephone lines. S.C. Smith *et al.* (1983) described such a system named CRAG. The growth in computer usage and advances in communications technology and computer networking are such that within the decennial review period digital communication of this type has gone from being a rarity to being routine.

Data bases in the 1960s and 1970s were usually considered to be major institutional resources. That has changed and now geochemists have access to sophisticated data base management packages, e.g. dBase III, Rbase System V and Oracle, on the microcomputers in their offices. Networks of data bases are emerging that are maintained to meet institutional and corporate objectives. The institutional data base is typified by the U.S. Geological Survey's RASS system (van Trump and Miesch 1977), and others have been described by Ferguson *et al.* (1977), Garrett, Kane, and Zeigler (1980), and Bliss (1986). A review of data base requirements for exploration geochemistry has been presented by Mattiske (1983), and proposals for some standardization, particularly appropriate for those working on international cooperative studies, have been made by Grandclaude (1979). Often data bases are developed for a specific project by a small group of geoscientists. One such example which has been described as a case history concerns geological and geochemical data acquired for a project in Ethiopia (Davidson and Moore 1978).

Although geochemical data bases almost always include sample location coordinates, these are usually not manipulated at any other than a simple level, e.g. retrieve all samples that fall within defined limits. A new breed of specialized data bases known as geographic information systems (GISs) are now available. However, they are large and expensive, and all but a few require at least a minicomputer. Such information as maps may be stored in a GIS and retrievals such as: find all samples that are within 2 km of rhyolite–andesite contacts, are possible. Olson (1986) has described such a system running on a microcomputer, and several major geoscience institutions are purchasing or considering the purchase of such systems.

SURVEY DESIGN AND QUALITY CONTROL

The design of geochemical sampling procedures, i.e. the selection of sample densities, is not a topic that has drawn much attention. Various aspects of design selection criteria have been reviewed by Garrett (1983b), and a study by Garrett and Sinding–Larsen (1984) proposed criteria for the preparation of composite samples. In the latter study, it was demonstrated that cost considerations were more important in selecting composite sample sizes than statistical concerns in most instances. In an interesting paper by Shulman (1988), the problems of optimizing the entire exploration process are studied. The objective being to determine the optimal allocation of resources between geological, geochemical, geophysical, and other surveys.

Quality control procedures for geochemical analytical work have received far more attention. Of particular note is the graphical procedure developed by Thompson and Howarth (Thompson 1978; Thompson and Howarth 1978; Thompson 1983a, 1983b) and also described by Fletcher (1981). This procedure, based on plotting differences between duplicate analyses against the duplicate mean on a log–log display, is easy to implement and the display can be continuously updated in the laboratory so that any procedural problems can be rapidly detected and action taken. The simple model of a linear dependence of analytical error on concentration assumed by Thompson and Howarth may not always be true, as pointed out by Ottesen *et al.* (1983). This is due to changes in solute concentration or spectral line performance in the total range of concentrations being studied, brought about by the need for solute dilutions or line changes due to self absorbance phenomena. In such cases, several control charts can be prepared, one for each homogeneous concentration range.

The subject of reproducibility of geochemical surveys and the apportionment of variability between true geochemical, sampling and analytical factors has not received much interest. The reasons are most likely that, firstly, most mineral explorationists believe they are looking for "anomalies" that are so large they will be detected anyway, and secondly, they are not prepared to bear the cost of the additional sampling and analysis required to quantify the variability. An effective and economic method for determining survey variability was described by Garrett and Goss (1979) who employed an unbalanced sampling design for studying lake sediment survey data. In an attempt to determine after the event how effective a geochemical survey may have been at detecting patterns related to mineral deposits, Garrett and Goss (1980) employed the variability measures to modify the estimates of probability of intersecting

a pattern of known size based on geometric probability. The empirical model performed acceptably and was used to determine the probable effectiveness of the lake sediment surveys of Canada's Uranium Reconnaissance Programme. James and Radford (1980) described a simple procedure employing duplicate sampling and analysis to determine the relative magnitude of sampling and analytical variability in relation to total survey variability. They concluded, as many others have done, that today in most instances sampling variability is of far more concern than analytical variability.

UNIVARIATE STATISTICS

In reviewing activities over the last decade, one might be led to believe that little progress has been made. However, although relatively few papers have been published compared to those dealing with mapping and multivariate techniques, some are important contributions. The following section is divided into three topics, data transformations, anomaly recognition, and miscellaneous.

Transforming data to normality so that the assumptions of a variety of statistical methods might be met received a lot of attention in the early part of the decade. Kane (1979) proposed the use of a three–parameter lognormal distribution, where in addition to the mean and variance a shift parameter, α, was applied to the data. Thus a value x was replaced by $x + \alpha$, and α was estimated using a maximum likelihood procedure. As the value of α approaches zero, the familiar two–parameter lognormal distribution is obtained. Almost simultaneously, Howarth and Earle (1979) introduced the Box–Cox generalized power transform into geochemical use. Here the value of a parameter, λ, is estimated for a transformation, $z = ((x+\alpha)^{\lambda} - 1)/\lambda$, such that the skewness of the transformed variable z is minimized. The shift parameter α is chosen so that $x + \alpha$ is always positive; if x is never negative, α is set to zero. The values of λ may assume a continuum, e.g. -1, representing $1/x$, through zero where $z = \log x$ to 0.5 corresponding to $\sqrt{x}$ and 1 where z represents x and finally to 2 where z represents x^2. This method is extremely powerful and examples of its use are provided by Howarth and Martin (1979) and Mancey and Howarth (1980), both in the context of multivariate data analysis procedures. However, if this procedure is applied routinely, problems can arise. For instance, if a data set is in fact drawn from an underlying normal distribution but also contains some erratically high values drawn from some other distribution(s), i.e. potential geochemical anomalies, the Box–Cox generalized power transform in attempting to consider the data as being drawn from a single distribution will generate a value of λ indicating a positively skewed, possibly lognormal, distribution. In the light of our *a priori* knowledge, this is clearly not correct and herein lies the problem with routine use of such powerful transformation procedures. In recent years, it has become more common to use robust statistical procedures and select a model, e.g. normal or lognormal, on *a priori* geochemical grounds. Robust statistical procedures (e.g. Garrett *et al.* 1980; Campbell 1984) give less weight to outlying members of the data set and base the parameter, i.e. mean and variance, estimation on the core data. A clear trend over the decade has been a decreased use of means and standard deviations due to the conceptual problems over distribution models and multiple populations. In their place, medians and various percentiles are being used, having the advantage that they are distribution–free. Additionally, the median is a stable resistant estimator for the central tendency of data. Although percentiles are more tedious to estimate as the data have to be sorted, this is no longer a problem now that computers are widely available. However, for very large data sets special algorithms are required (Howell 1983).

The prime task in geochemical data interpretation still remains anomaly recognition and threshold selection. This topic has continued to be one of major interest and discussion (e.g. Garrett 1984). The procedure for cumulative frequency plot decomposition forwarded by Sinclair in the 1970s was "computerized" by Bridges and McCammon (1980). The great advantage of this was that the user could quickly try out a number of decompositions and observe the effects of any changes in input parameters, or number of populations, on the ultimate outcome in an interactive computer graphics environment. A limitation of the Sinclair, and Bridges and McCammon procedures is that only a single distributional type can be worked with at a time, e.g. all normal or lognormal subpopulations. Additionally, Campbell (1984) had pointed out and demonstrated the problems that can arise with numerical solutions to frequency decomposition when outliers are present, and proposed the use of robust procedures to solve this problem. Bjorklund (1983) demonstrated a number of situations where the anomalous population was more likely to be exponential, and discussed the impact of this on decomposition procedures. The impact of very skewed distributions on anomaly recognition procedures has also been discussed by Ingamells (1981). Ingamells demonstrated the impact of the nugget effect giving rise to a relatively small number of extremely high values for elements dispersed in discrete element–rich mineral grains and how this in part could be due to sample preparation variability.

An alternative procedure has been investigated by Miesch (1981) and Stanley and Sinclair (1987b). Instead of focussing on linear sections of a probability plot, the transition regions of sparser data density between the linear sections are studied. A gap test was proposed to determine if the data were sparse enough to be the upper and lower tail area of two

distributions. If such was the case, the data could be subdivided and the two populations interpreted in the light of local geological and geochemical knowledge. The method may be thought of as a one–dimensional cluster analysis, and would seem to be particularly appropriate where there is limited overlap between adjacent populations. Cole and Rose (1984) proposed the use of a Student's t–test to determine whether two identified groups of data could in fact be considered as drawn from two populations, or should be considered as a single population.

Li (1984, 1985) took a different approach by simultaneously taking spatial information into account in an analysis procedure developed to subdivide data sets into their component parts. The result of this approach is that when a post–analysis map of the populations is prepared, it is "cleaner", border line cases being grouped into the population which is locally dominant. Page and Young (1981) have used spatial clustering to determine the significance of "anomalous" samples. If a threshold is set that identifies the top 5 percent of the data and the "anomalies" were just high level background samples, one would expect them to be scattered randomly over the survey area. The probability of these anomalies lying together as contiguous groups can be determined for various group sizes. Intuitively, the larger the group the less likely this is due to chance alone and the more likely the group is related to a discrete geochemical cause. Page and Young's approach is based on binomial theory and therefore has the attraction of being assumption free concerning the underlying geochemical distributions.

Several other papers are of note. Cameron (1983) and Sinclair (1983) both provided useful reviews of univariate statistical procedures applied to exploration geochemistry. In a recent paper, Stanley and Sinclair (1988) discussed the bridge between univariate and multivariate procedures. Often this involves using a multivariate procedure to determine a univariate measure related to the process under study, and then using univariate procedures on that derived measure. Andrew (1984) provided examples of univariate procedures in anomaly recognition, extending into the bivariate and multivariate realms, emphasizing the multivariate nature of most geochemical data. Finally, although geochemists usually collect field data at the sample site, traditionally used to reconstruct the sample site environment during detailed interpretation, rarely have the field data been subjected to detailed analysis. However, Matysek *et al.* (1983) analyzed field data from a British Columbia stream sediment survey and showed the results to be consistent with the geochemical data and useful in support of data interpretation.

MAPPING AND SPATIAL DATA PRESENTATION

The geochemical map is a fundamental tool to the exploration geochemist; the past decade has seen a continued growth of computer use to aid map preparation, and more importantly the adoption of new procedures, e.g. image analysis systems. The subject will be reviewed in three sections concerning contouring and interpolation algorithms, the application of image analysis approaches, and miscellaneous new developments and the use of colour. Additionally, Howarth (1983a) has reviewed mapping and data presentation techniques.

One of the first computer procedures used by geochemists to prepare contoured maps in the 1960s was polynomial surface fitting, often called trend surface analysis. The procedure is still being used, for example in papers by Chapman (1978), Ganicott *et al.* (1979), Mercready *et al.* (1979), Yu (1981), Pride and Hasenhohr (1983), and Roy (1983). However, with time these techniques seem to be used less and less. An interesting variant has been described by Bezvoda *et al.* (1986) who used a fitted Fourier model to describe the spatial variability of soil geochemical data. Most contouring today is undertaken using local fitting or filtering, and these techniques break down into two groups: firstly *a priori* based procedures, e.g. inverse squared distance weighting, or secondly, data–based local weighting, e.g. kriging based on autocorrelation (variogram) studies or some similar procedure. Howarth *et al.* (1980), Sarma and Koch (1981), and Chork and Cruikshank (1984) have shown that by fine tuning filters applied to spatial data different features can be highlighted to advantage. An interesting study by Myers *et al.* (1982) and Kane *et al.* (1982) compared a procedure for determining the optimum parameters of a filter, i.e. the power applied to the spatial distance measure and the search radius, with an autocorrelation study. By comparing interpolated results at validation points with observed data, they determined that, for their particular geochemical groundwater data set, kriging generally provided an inferior map to that obtained using optimal inverse distance weighting model. This conclusion may be due to non–stationarity in the regional data set. This property of the data is likely a reality in regional geochemistry, and may be the reason that kriging does not always provide acceptable regional geochemical maps. Unfortunately, testing for and handling non–stationarity is difficult (Henley 1981). Bonham–Carter and Goodfellow (1984) undertook an autocorrelation study of regional stream sediment survey data from the Northern Canadian Cordillera. In this work, they demonstrated that the spatial correlation in the data was due to the geology of the area, and that if the data were adjusted for local geologically controlled geochemical background, they were not

significantly spatially correlated. As a general rule, it seems likely that for large regional geochemical survey data sets with broad sample spacings spatial correlation is more closely related to differences in local lithology and the autocorrelation due to the geometry of the geological units than to any internal spatial variation patterns within lithologies. It is interesting to speculate as to whether this observation will hold true on the scale of continental geochemical map compilations where major crustal scale phenomena may exert a control on regional geochemical background in a systematic way.

Kriging procedures have been used to prepare regional geochemical maps, e.g. Armour-Brown *et al.* (1983), Bonham-Carter and Chung (1983), Lindquist *et al.* (1987), Muge *et al.* (1987), Sandjivy (1987), and Wackernagel and Butenuth (1987), or as an intermediate step in moving from an irregular pattern of geochemical data sites to a regular grid as required by an image analysis system, e.g. Bolivar *et al.* (1983). However, more commonly autocorrelation studies and Kriged maps have been applied on a local scale where the true distance related spatial variability in the data is not overwhelmed by differences related to lithologically controlled backgrounds. Examples of the more local studies, often applied in the multivariate context can be found in the work of Royer (1984, 1988), Sandjivy (1984, 1987), and Grunsky and Agterberg (in press). The proximity analysis approach of Royer is a logical extension to the formal inclusion of spatial information in a statistical analysis framework.

It has been long recognized that numerical interpolation and contouring procedures have caused problems when applied to drainage basin samples on a local scale. Quite simply, the coordinate stored is that of the sample site, not the centre of the area that the geochemist considers the sample to represent. Earle (1978) made an attempt to solve this problem by associating each stream drainage site with a sector of defined radius, orientation, and arc. In retrospect, Earle was ahead of his day as graphical data-acquisition procedures of that time rendered the procedure of academic interest only. The availability of optical scanners has made it possible to directly capture the geographic coordinates defining the boundary of a drainage catchment basin (Ellwood *et al.* 1986; Aronof *et al.* 1986; Los Alamos National Laboratory *et al.* 1987). With the digital cartography and image analysis procedures now available, a totally new approach can be taken to geochemical map presentation, as colour or a grey-scale coded polygon can be used to indicate the actual area represented by each geochemical sample.

The impact of image analysis systems is now beginning to be felt, especially as lower-cost microcomputer-based workstations are becoming available. The power of an image analysis system lies in its ability to manipulate maps as digital images. In addition to geochemical maps, they may include satellite imagery (e.g. Aronof *et al.* 1986), geological maps (e.g. Bolivar *et al.* 1983), and geophysical maps (e.g. Guiness *et al.* 1984). It is the data integration aspect that makes image analysis so attractive, and there are now many examples of this. The first attempts at data integration included work that was not carried out on a true image analysis system, e.g. Bonham-Carter and Chung (1983), followed shortly by the more elegant colour-based systems, e.g. Green (1984), Leymarie and Durandau (1985), Fettes *et al.* (1986), Aronof *et al.* (1986), Plant *et al.* (1986), Maassen and Bolivar (1987), and Lasserre *et al.* (1987). Perhaps one of the most interesting of these is the work of Aronof *et al.* (1986) where stream sediment and water data and geological information were combined to undertake a tungsten mineral resource appraisal. Other noteworthy work is that by Plant *et al.* (1986) where clarification of a number of outstanding problems in Scottish geology has been obtained from geochemical mapping. An interesting alternative has been pursued by Bolivar *et al.* (1983) and Freeman *et al.* (1983) where they used multivariate procedures to combine the geochemical data into new variables prior to integrating it with the geological data using an image analysis system.

Due to the availability of colour devices in both large and small formats for computers, the use of colour is becoming more widespread. However, much of this use is during data interpretation and is never published due to high printing costs, though it is noticeable that journals are more willing to publish colour figures now than 10 years ago. The paper by Reid (1987) on primary tin dispersion provides an example of colour graphics in the interpretation role. Colour maps are now being published at either page size, e.g. Friske (1985), Bjorklund and Gustavsson (1987), and Maassen and Bolivar (1987), or in larger formats in geochemical Atlases, e.g. Webb *et al.* (1978), Weaver *et al.* (1983), Bolviken *et al.* (1986), and Los Alamos National Laboratory *et al.* (1987).

There have been a number of proposals for new methods of mapped data presentation in addition to those described above. Fortescue (1981, 1983) and Fortescue *et al.* (1982) proposed a greater use of maps where the data is ratioed against a crustal abundance estimate, e.g. the Clarke. These maps have particular appeal to health and environmental studies, where the maps are being used in epidemiological studies. In such cases, users are not interested in absolute values but differences from a norm, mainly for spatial correlation with areas where population statistics indicate increased longevity or mortality. Bjorklund and Gustavsson (1987) discussed methodology behind certain of the maps used in the Geochemical Atlas of Fennoscandia (Bolviken *et al.* 1986). In light of a recent proposal to the International Geological Correlation Programme

that geochemists cooperate internationally to prepare a global geochemical map series, their introduction of moving median maps as the best stable measure of regional background geochemistry may have particular importance.

MULTIVARIATE DATA ANALYSIS

In comparison with other branches of geoscience, exploration geochemistry has been a centre of multivariate data analysis, no doubt due to the abundance of multi–element survey data. To aid discussion of the large body of literature generated in the last decade, the review is divided into seven topics as follows: closed numbers, bivariate procedures, clustering, regression, principal component and correspondence analysis, discriminant analysis, and miscellaneous topics of interest. Underlying many of the applications of multivariate statistics to exploration has been a desire to classify individual samples, or at least identify those that may be considered "anomalous", on the basis of some objective criteria (Garrett 1984; Mellinger *et al.* 1984). During the review decade, several papers have been published which treat the role and potential of multivariate data analysis from a more general point of view, i.e. Chapman (1978), N.A. Campbell (1983), Garrett (1983a), Howarth and Sinding–Larsen (1983), Howarth and Garrett (1986), and Mellinger (1987a).

Exploration geochemists working with whole–rock data and petrochemists have long been aware of the problems arising from the fact that major element analyses sum to a constant, 100 percent. Therefore, as a major component increases, say silica, other components necessarily decrease, and studies of intercomponent variability using correlation measures have not always been satisfactory. Trace–element geochemists have been far less concerned with these problems, and it is now known on theoretical grounds that the commonly used log–log plots of trace elements are not affected by the closure problem. Hohn and Nuhfer (1980) proposed a procedure for computing true correlation coefficients uneffected by closure through the use of ratios involving the major component. For example, instead of computing the correlation of Fe and K, the correlation of Fe and K/(100 – Si) was computed; and for K and Fe, the correlation of K and Fe/(100 – Si) was derived. The problem with this procedure is that the correlation of K with Fe is not the same as Fe with K, and where the range of a variable is large, e.g. Si, the correlation of Si with Si/(100 – Si) may not be equal to 1, which is intuitively unsettling. The breakthrough in this area was made by Aitchison (1981), and in two later papers (Aitchison 1984a, 1984b), when he proposed the use of the logistic transform, all this work is reported in Aitchison (1986). If there are $d + 1$ components that sum to a constant, e.g. 1 or 100, each of the d values are divided by the $(d + 1)$–th and logs are taken. The new transformed variables do not exhibit the closure effect and any correlations between them reflect true correlations due to geochemical processes. The selection of the $(d + 1)$–th component is not critical, and therefore with whole–rock geochemical data oxides such TiO_2 or ZrO_2 are often chosen on the basis of common petrochemical practice. Therefore, the plotting of K_2O/TiO_2 versus Fe_2O_3/TiO_2 on a log–log scale reveals correlations that are truly geochemical. This does not mean that the old Harker diagram approach of direct elemental plots is obsolete; they are useful in the study of classification due to the enormous mass of historical data so plotted; however, they have no place in the study of geochemical processes. Butler (1981) carried out studies along a different line, however, Woronow and Butler (1986) later adopted Aitchison's logistic transform and published computer software for testing for the presence of true independence in close arrays. Royer (1983) proposed the use of correspondence analysis as a solution to the closed number problem, and the relative merits of correspondence and principal components—factor analysis will be discussed in a later section.

The simplest form of multivariate data are bivariate data sets, or true multivariate data treated pairwise. Two different approaches have been taken with pairwise data to reduce the effect of outlying individuals which influence the estimation of lines–of–fit or correlation coefficients. Rock (1986) and Rock and Duffy (1986) have encouraged the use of non–parametric or assumption–free methodologies. In contrast, others, e.g. Zhou (1987), Wurzer (1988), and a procedure described by Rock and Duffy (1986), have preferred to remain with the more common parametric procedures and modify them to downweight the influence of outlying individuals. Wurzer (1988) proposed the use of influence functions displayed directly on bivariate plots to assist in the identification of outliers that might effect the statistical estimators. Examples of bivariate data analyses are found in the work of Gibbs (1982) to study Cu versus Fe or Mn in tropical stream sediments; Garrett (1983a) to investigate Zn–Fe relationships in temperate zone stream sediments; Andrew (1984) used bivariate plots to aid in anomaly recognition; and Drew *et al.* (1985) studied a variety of combinations of Cu–Ni data to differentiate between stratigraphic zones in the Stillwater ultramafic complex.

Cluster analysis procedures offer a very useful tool with which to commence the investigation of large or complex data sets in order to disaggregate the mass of data into several smaller more tractable subsets. These subsets are likely to be composed of individuals dominated by particular geological or geochemical processes, perhaps even related to a mineralization process, and may then be further

treated by the most appropriate methods. There are two specific approaches to cluster analysis, one is hierarchical and commonly uses dendrograms, and the other is non–hierarchical and often referred to as a *k*–means or partitioning method (Howarth and Sinding–Larsen 1983). Examples of the use of dendrograms may be found in Ayalon *et al.* (1981), Roy (1981), Yu and Xie (1985), and Hoffman *et al.* (1987). The work by Yu and Xie (1985) is particularly interesting as they take account of the "fuzziness", i.e. uncertainty, due to natural and measurement variability in their analysis. Jambu (1981) proposed an interesting heirarchial procedure for use with large data sets, however, Mancey (1982) in a review of clustering procedures for large geochemical data sets states a preference for non–heirarchical methods. Examples of these may be found in the work of Lefebvre and David (1977), Dumitriu *et al.* (1980), Mancey (1982), Garrett (1983a), Granath (1984), Chork and Govett (1985), Grunsky (1986), Kurzl (1987), and Shepherd *et al.* (1987). Garrett (1983a), Chork and Govett (1985), and Kurzl (1987) used assumption–free planing or non–linear mapping procedures. Gustavsson (1980, 1983) also made use of a graphical clustering procedure, the Andrew's plot. In these graphical procedures, the user makes the partition on an *x*–*y* plot of the multidimensional data, rather than relying on a partitioning algorithm, which commonly breaks down when single outliers are encountered. Both Lefebvre and David (1977), and Grunsky (1986) have used a procedure known as dynamic cluster analysis to advantage with petrochemical data. By employing the concept of clouds of points, the aspect of data fuzziness is introduced where a group of data is not characterized by a single so–called "typical" sample, or a "typical" composition not reflected in any individual, but by the statistical properties of all the individuals in the group. A particularly interesting facet of this procedure is the method used to determine the true number of clusters in a data set and how after repeated trials persistent sets of data groupings are identified. Granath (1984) proposed a *k*–means procedure which also takes data fuzziness into account; this method is potentially very powerful but has the drawback of being computationally intensive. However, with new computing tools this drawback will disappear. One drawback with cluster analysis procedures is that they usually illustrate the data variability in either the variable space (*R*–mode) or sample space (*Q*–mode). Therefore, one can determine which samples are similar but not why, i.e. which variables provide them with a unique fingerprint. One of the few procedures that can achieve this are Kleiner–Hartigan trees, these were used by Garrett (1983a) and indicated the complexity that even a small data set can attain. Like the planning and non–linear mapping procedures, it is the user who groups the trees into "groves" of similar morphology and/or size. As a generalization, it would appear that partitioning procedures, whether algorithmic like *k*–means or graphical, are becoming the methods of choice in exploration geochemistry in preference to dendrograms.

Regression analysis has a long history of application to geochemical exploration data back to the 1960s. The objective in these studies has been to develop models of trace–element background in terms of other trace elements, the major elements dominating geochemical composition, and geology. The inclusion of geological information in regression analysis has commonly been via 0 – 1 dummy variables indicating the presence or absence of the lithologies or formations of interest, e.g. Whitney (1981), Bonham–Carter and Goodfellow (1986), and Bonham–Carter *et al.* (1987), or by subdividing the data into subsets on the basis of geology, e.g. Koch *et al.* (1981). Of note recently has been the use of the actual proportion of a geological unit comprising a drainage catchment basin by Bonham–Carter and his co–workers; however, Bonham–Carter *et al.* (1987) still recorded the presence of geological contacts considered important in the analysis with 0 – 1 dummy variables. The very outliers being sought when regression models are being used to identify them can distort the analysis and render it ineffective. Therefore, a number of workers have used robust and/or iterative procedures to remove the influence of the outliers and so generate improved geochemical background estimates. Garrett *et al.* (1982) and Zhou (1985, 1987) both used robust estimators for the means and covariances required by the regression analysis, whereas, Malmqvist (1978) and Stanley and Sinclair (1987a) both used iterative procedures to eliminate influential outliers from their analyses. Other examples of the application of regression procedures can be found in the work of Price and Ferguson (1980), de Vivo *et al.* (1981), Capaldi *et al.* (1982), Bonham–Carter and Chung (1983), Howarth *et al.* (1981), Dubov (1983), Rose *et al.* (1983), Selinus (1983b), and Wynne and Strong (1984). An interesting variant for estimating local backgrounds in large multivariate data sets probably drawn from multiple populations is presented by Roquin and Zeegers (1987). Instead of using the total data set to estimate the expected value for an individual under study, they used only a subset of data from the multivariate data space close to the individual to be estimated. This means that as many regression models have to be computed as there are individuals in the data base. Although several years ago this would have been a daunting task, with today's computing power, either a supercomputer in seconds or geochemists' microcomputer running overnight, it no longer poses a problem.

For some 20 years it is reasonable to say that principal components–based approaches, joined by correspondence analysis about 14 years ago, have been the most popular multivariate data analysis techniques. Their lure is in their ability to re–express

the data variability in terms of geological or geochemical process rather than raw elemental compositions. Like cluster analysis, principal components and factor analysis may be undertaken in either the *R*– or *Q*–mode. Since the implementation of the *RQ* transform procedure in the early 1970s, the analyses have become interchangeable; there does however appear to be a preference for using *R*–mode scores rather than *Q*–mode loadings due to users preference for interpreting the *R*–mode inter-variable loadings in terms of geochemical processes. Correspondence analysis has always been carried out in the *RQ* domain. A brief note must be made concerning principal components and factor analysis as the terms are used interchangeably by many. In practice, both are usually carried out on the data correlation matrix, however, the assumptions are different and in a practical sense a user commits to a factor analysis once a rotation procedure, e.g. using the Varimax criterion, is undertaken. In components analysis, the new axes are computed to explain a maximum amount of the original variance, in factor analysis the new axes maximize the correlation of the variables. Useful discussions of this with illuminating examples may be found in Chayes and Trochimcyzk (1978), Trochimcyzk and Chayes (1978), and Miesch (1980). A similarly very useful paper focussing on the differences between principal components and factor analysis on one hand and correspondence analysis on the other has been presented by Zhou *et al.* (1983). In the past decade, there have been two reviews of multivariate procedures in exploration geochemistry which discuss these procedures in some detail, Chapman (1978), and Howarth and Sinding–Larsen (1983). The examples of the use of *R*–mode principal components and factor analysis by geochemists are many, and include Barbier and Wilhelm (1978), Santos–Oliviera (1978), Olade *et al.* (1979), Tripathi (1979), Leach *et al.* (1980), Ajayi (1981), Dunn (1981), Selinus (1981), de Vivo *et al.* (1981), Capaldi *et al.* (1982), Imeokparia (1982), Bolivar *et al.* (1983), K. Campbell (1983), Davenport *et al.* (1983), Selinus (1983a), Olorunfemi (1984), de Vivo *et al.* (1984), Eleuze and Olade (1985), Nurmi (1985), Vriend *et al.* (1985), Bezvoda *et al.* (1986), McConnell and Batterson (1987), Sharp and Nardi (1987), and Smith *et al.* (1987). All of these workers have used *R*–mode analysis procedures to support their interpretations, in some cases the results are used to confirm an already developed interpretation, and in others the analysis plays a more important role. A number of other authors have proposed new or modified procedures of more interest. The most frequently used rotation procedure applied during *R*–mode analysis is the Varimax, which is an orthogonal rotation and leaves the factors uncorrelated. Leymarie and Frossard (1983) proposed an oblique rotation for use with petrochemical data and found it aided their interpretation. Olesen and Armour–Brown (1984) used *R*–mode residual scores to identify individuals whose variability could not be explained by the *R*–mode factors they selected as representative of the major controlling geological–lithological processes; a generally similar approach has also been employed by Esbensen and Steenfelt (1987). These are elegant procedures and can be likened to focussing on individuals that exhibit large regression residuals from a satisfactory background model. Both Zhou (1985, 1987) and Wurzer (1988) have proposed using robust estimates of the data set means and covariances (correlations) as a starting point for analysis. The resulting downweighting of outliers leads to a far better estimation of factor loadings reflecting the background geochemical processes, and the better resolution of background models itself leads to an easier recognition of "anomalies" different from the background(s). Lindqvist *et al.* (1987) presented work on a procedure named SIMCA which includes a partial least square approach where different variable sets, e.g. major and trace elements, or trace–element and geophysical parameters, are separately analyzed in *R*–mode and then related to each other in order to identify common factors controlling the variable sets. This procedure has been particularly useful in integrating data sets concerning the same individuals but of disparate nature, e.g. geochemistry, geophysics, mineralogy, etc. Finally, in *R*–mode analysis Royer (1984, 1988) and Sandjivy (1984) have both attempted to take the spatial context of data into account during factor analysis. Sandjivy (1984) proposed a procedure called factorial kriging analysis, the main drawback is that for large data sets it is extremely computationally intensive. Royer (1984, 1988) proposed an alternative, proximity analysis, which he states to be less of a computational task. However, with reference to both techniques, the interpretation of the results is more complex than in the routine *R*–mode procedures now so widely available in computational packages. On this basis, widespread application of these spatial techniques is unlikely in the near future.

Q–mode approaches are now rare, the most notable work has been by Miesch (1979) in interpreting petrochemical data in terms of sample vectors representing specific mineralogical compositions. This permits the results of the analysis to be interpreted as petrological mixing models. Correspondence analysis is routinely used in a similar fashion to *Q*–mode factor analysis, as evidenced by the plots of individual samples in the factor space. Much has been made by some workers of the ability to plot the variables on these same diagrams. However, this is not unique to correspondence analysis and biplotting has been available through the commonly used *RQ* transform procedure since the early 1970s. In a series of papers by Valenchon (1982, 1983) and Miesch (1983), various aspects of the factor analysis–correspondence analysis relationship are discussed. In a paper by Grunsky (1986) where corre-

spondence analysis is used to study petrochemical data, the author also discussed the relative merits of the two procedures; and Zhou *et al.* (1983), as mentioned earlier, discussed the mathematical relationships. Examples of the application of correspondence analysis to geochemical problems have been published by Dumitriu *et al.* (1979) and by Mellinger (1984, 1986, 1987b, 1987c) in addition to the previously cited authors. In the author's opinion, the strength of correspondence analysis is its ability to handle binary, e.g. presence–absence, data (Mellinger 1984; Mellinger *et al.* 1984). Correspondence analysis requires that the data be regarded as a contingency table or probability distribution, many geochemists are not particularly comfortable with this assumption. It seems to the author that now the closed number (constant sum) problem has been solved and that correlation matrices may be computed that reflect the true underlying geochemical processes that *RQ* factor analysis procedures have a lot to offer where constant sum geochemical data are being analyzed.

Factor scores, however computed, have the attraction that they combine data for multiple elements and re–express them in a manner that is more process than response related. If only a small proportion of the data is related to a particular process, as with mineralization processes in a regional reconnaissance survey, it may not be reflected well in a formal "factor" analysis. Several workers have used multi–element scoring procedures to aid in focussing attention on individuals associated with particular trace–element patterns, often selected due to an association with a particular mineral deposit type. Some procedures lead to an "empirical factor score", e.g. the weighted sums of Garrett *et al.* (1980), whilst others lead to a simple additive score, e.g. Smith and Perdrix (1983). In addition to the above two papers, examples may be found in the work of Marsh and Cathrall (1981), and Chaffee (1983). A slightly different approach has been proposed by Mellinger (1983) in a procedure he calls "Tails Analysis", the work of Skvortsov *et al.* (1982) appears to also follow a similar thrust, and Baird and Dennen (1985) offer an alternative procedure with a similar objective of focussing on "anomalous" multi–element patterns. Finally, it may be noted that the image analysis procedure used by Aronof *et al.* (1986) to generate a tungsten mineral potential map can be viewed as a graphical image combinatorial analogue of the numerical scores. These heuristic procedures may lack the formalism of a *RQ* mathematical procedure, but they gain by their direct geochemical motivation, in which lies their strength.

CLASSIFICATION

Traditionally, exploration geochemists have used various forms of linear discriminant analysis to classify unknown individuals into one or more populations. However, in the last decade other techniques have become available based on slightly different approaches. Two are of particular note, firstly, logistic regression, and secondly probabilistic modeling. Logistic regression is a particular regression procedure where the dependent variable is set to 0 or 1 for two data sets, e.g. background and mineralization associations. Maximum likelihood procedures are used to determine the coefficients of the independent (geochemical) variables in the regression model. The major advantages are two–fold, there are no assumptions of multivariate normality and homogeneity of covariance for the two data sets, and the results, i.e. estimated values of the dependent variable, are directly interpretable as pseudo–probabilities of group (data set) membership. The problem of homogeneity of covariance is often neglected by non–statisticians, however, homogeneity is an assumption of the simple linear discriminant method. In many cases in exploration geochemistry the assumption is probably not warranted. For example, in a background area Pb might be negatively correlated with Zn due to a negative correlation of feldspathic (Pb richer) minerals with dark (Zn richer) minerals, but be positively correlated in a mineralized zone due to the presence of sulphides. In such a case, the assumption of homogeneity of covariance is clearly not warranted. Probabilistic modeling can be likened to a multivariate probability plot where an individual is viewed in the light of one or more control populations. The individual's probability of group membership in that group is determined via its Mahalanobis distance, which can be regarded as a multivariate analogue of the familiar univariate standard normal deviate (N.A. Campbell 1983; Garrett 1987). This procedure has an advantage in regional surveys where very often although background populations are abundantly represented, the "anomalous" ones of interest are not. Therefore it is a useful strategy to characterize the background population(s) reliably and look for individuals that do not fit (c.f. Olesen and Armour–Brown, 1984). During the last decade two reviews of a more general nature have been published that discuss classification procedures and/or discriminant analysis, Chapman (1978), and Howarth and Sinding–Larsen (1983). Simple linear discriminants have been used by Santos–Oliviera (1979), Marcotte and David (1981), Pirie and Nichol (1981), Amor and Nichol (1983), Brabec (1983), Selinus (1983a), Andrew (1984), Wynne and Strong (1984), Chork and Govett (1985), and Shepherd *et al.* (1987). A common problem encountered in discriminant analysis studies is the selection of the most appropriate variables. One may rely on geochemical common sense and select ones known *a priori* from previous work to be good discriminators; use various exploratory data analysis approaches; use factor scores which are linear combinations of the elemental data, selecting the factors that contribute most useful information to the prob-

lem (c.f. Selinus 1983a); or use a stepwise variable selection procedure. The stepwise procedure has been used in studies by Beauchamp *et al.* (1980), Fedikow and Turek (1981), Clausen and Harpoth (1983), and R.E. Smith *et al.* (1983, 1984). Certainly some procedure should be used, because the presence of non–contributing variables in a "discriminant" analysis can greatly reduce its efficiency, although the superiority of any one procedure is not clear. Three of these papers are of particular note as they discuss the problems of homogeneity of covariance, which as pointed out earlier, is a concern often ignored, Beauchamp *et al.* (1980), Clausen and Harpoth (1983), and Chork and Govett (1985). A more nearly assumption–free approach named empirical discriminant analysis is based on kernel estimation, and by direct density estimation avoids the problems of multivariate normality and homogeneity of covariance. Examples or a discussion of this procedure may be found in Gustavsson (1980), Van den Boom *et al.* (1980), Gustavsson (1983), Rehder and Van den Boom (1983), and Armour–Brown and Olesen (1984). Some workers have used multiple discriminant procedures where more than two end–members are considered. In this method, new axes are derived that maximize the differences between groups and the data are usually plotted against the discriminant coordinates, sometimes referred to as canonical variates. However, this nomenclature can be confusing as canonical variates are also used to describe the new linear combinations arising from a canonical correlation study. R.E. Smith *et al.* (1983, 1984) have extensively used discriminant coordinates in their studies of pisolitic laterites of Western Australia to display their geochemical variability and how this relates to provenance. The probabilistic approach based on the computation of Mahalanobis distances has been used by Beauchamp *et al.* (1980), and R.E. Smith *et al.* (1983, 1984) to assist in classifying or allocating new individuals into a pre–established framework. The work of R.E. Smith *et al.* (1983, 1984) is particular interesting as it touches on the problems of allocation procedure and because robust methods are used to compute the means and covariances essential to the method, thus leading to an improved statistical definition of background. Lastly, logistic regression as a discriminant tool has been little–used to date, probably due to the paucity of software to undertake the procedure and the complexity of the computations relative to linear discriminant analysis. However, Bonham–Carter and Chung (1983) described a comparative study where stepwise and multiple regression, and logistic regression, were used with geochemical data to estimate uranium resources.

RESOURCE APPRAISAL STUDIES

Resource appraisal can be differentiated from classical geochemical exploration in that it is used to make statements concerning areas rather than individual sample sites. Resource appraisals attempt to quantify expected mineral resources in an area or region without being specific as to where those resources may be found. Within the field of resource assessment studies, there exists a technique referred to as the geochemical abundance model which relates crustal abundances to mass of element in a particular resource category (Garrett 1978, 1986; Harris 1984, 1988). A different approach is based on a log–binomial model where in a simulation a mass of crustal material of some average composition is subdivided into smaller and smaller blocks by a binary process, and with each subdivision the element is either concentrated into, or depleted from, the prior blocks subject to the constraint of mass conservation. The limit of this procedure is a lognormal distribution and the upper tail of this defines blocks of ore–grade (Harris 1984, 1988; Garrett 1986). The problem with this procedure, which is usually carried out on global, continental, or national scales, is with regard to its validity as smaller and smaller regions are studied. Garrett (1986) proposed a modeling procedure based on training areas of known mineral endowment as a potential solution to this problem.

Other resource appraisal procedures are based on subdividing the region to be studied into regular cells. Characteristic analysis, which has its roots in principal component analysis, was proposed as a technique for use in such studies (Botbol *et al.* 1978; and McCammon *et al.* 1983). Characteristic analysis involves coding the cells into –1, 0, +1 scale for the attributes, geochemical or otherwise, being used in the resource appraisal, the values indicate "response unfavourable", "not known", and "response favourable". To assist in this task, software has been published by Bridges *et al.* (1985). Regression approaches have also been used to forecast if a particular cell or area has a favourable mineral potential, e.g. Koch *et al.* (1981), and Bonham–Carter and Chung (1983). In fact once the departure from cell to area has been made it takes but little extension to proceed to geochemical drainage catchment basins, although this is getting closer to mineral exploration than resource appraisal (c.f. Aronof *et al.* 1986). However, this clearly demonstrates the continuum between regional resource appraisal and mineral exploration.

ARTIFICIAL INTELLIGENCE

To date, artificial intelligence, and in particular expert systems, have had little impact on exploration geochemistry. However, there have been some applications in mineral exploration that involve geochemical knowledge. The best known example is PROSPECTOR developed at Stanford Research Institute as part of a U.S. Geological Survey project (Hart *et al.* 1978, 1979; Campbell *et al.* 1982; and Maslyn 1986). PROSPECTOR involves deposit models and uses the presence or absence of particular trace element patterns associated with those de-

posit models as part of its decision–making process. The only example of a truly geochemical expert system for which some details have been published that the author is aware of is SERGE (Bonnefoy *et al.* 1987). SERGE incorporates the knowledge obtained by Bureau de Recherches Géologiques et Minières staff members in interpreting geochemical mapping data from Brittany, France. Through a question–and–answer session, or direct interrogation of the data, SERGE classifies geochemical anomalies as to whether they are likely anthropogenic or geological, and if geological it attempts to classify the anomaly and assess its significance. It is likely that work is being undertaken on geochemical expert systems by others, but at this time little information is in the public domain.

COMPUTER MODELING

The availability of increased computing power and improved mathematical procedures have permitted geochemists to mathematically model many of the processes they hypothesize control the distribution of elements and minerals we observe today. The greatest amount of this work has concerned water–rock interactions, although other interesting studies have been made. In the field of water–rock and water–overburden reactions, the studies may be conveniently divided into two groups, firstly, those concerning mineral deposit formation and therefore what elements and minerals may be left by the path of mineralizing fluids; and secondly, those concerning the dispersal of elements in groundwaters from previously formed mineral deposits. All these studies are based on an important series of papers concerning thermodynamic modeling in the geological environment, including, Plummer *et al.* (1978), Parkhurst *et al.* (1980), Reed (1982), Parkhurst *et al.* (1982), Plummer *et al.* (1983), Flowers (1986), Perkins *et al.* (1986), and Deloule and Gaillard (1986) who consider the graphical presentation of the modeling results. Nordstrom *et al.* (1979) published the results of a major collaborative effort to assess the relative merits of the various aqueous systems modeling procedures, and it was from this that much of the development this decade stemmed. Studies involving ore–mineral deposition have been dominated by water–rock interaction modeling, these include work by Langmuir (1978), Sopuck and Lehto (1979), Runnels *et al.* (1980), and more recently with the shift of interest from U to Au and Ag, Cole and Drummond (1986) and Loucks (1986). In contrast, studies of ore–mineral dissolution and trace–element dispersion in groundwaters have been undertaken by Langmuir and Chatham (1980), Runnels and Lindberg (1981), Deering *et al.* (1983), Mann (1983), Rose *et al.* (1983), Smee (1983), and Lueck *et al.* (1978). The work concerning hydrogeochemical surveys has demonstrated very clearly the necessity of studying the trace–element composition of waters in the light of their total chemistry, and in particular the role of the saturation index as computed for each sample site in such studies (Langmuir and Chatham 1980; Rose *et al.* 1983). A number of other studies have modeled various aspects of groundwater flow and chemistry of interest to the mineral explorationist, e.g. White (1979), Kimball (1981), Hull (1984), Montgomery *et al.* (1987), and Harris *et al.* (1987). All the previous work has concerned aqueous or ionic transport; two papers by Ruan, Hale, and Howarth (1985) and Ruan, Howarth, and Hale (1985) considered gaseous transport through overburden, and as such are similar in motivation to Smee's (1983) studies of ionic transport in overburden, both being concerned with the generation of geochemical anomalies at surface. Lastly, Donker (1987) has modeled various aspects of surface run–off and groundwater charge with respect to rainfall which has importance when modeling weathering processes and *in situ* geochemical anomaly development.

MICROCOMPUTERS AND GEOCHEMICAL DATA ANALYSIS

The availability of microcomputers and associated software has had a major impact on the way exploration geochemists work. Some software, e.g. the U.S. Geological Survey's GRASP and STATPAC data file management and data analysis programs, is available at nominal costs through the open file mechanism, whilst other software is in the commercial and consulting domains and has to be purchased. With reference to the U.S. Geological Survey, Dodd (1982) provided a catalog of available pre–1982 computer programs. Later packages such as the MIRA geochemical data analysis system (Hanley and Schruben, 1983) are also available. Specific microcomputer systems, some of which are available commercially, have been described by Lavin and Nichol (1981), Hoffman and Mitchell (1984), Koch (1986), and Lundholm *et al.* (1986). Several commercial geochemical data processing packages are available from companies in Europe and North America, but have not been described in the technical literature.

CONCLUSIONS

That the role of computers in exploration geochemistry is an important one is a fact as established by the wide diversity of published activity over the last decade. The published papers probably reflect the true diversity in all the fields discussed here, except probably artificial intelligence which is still in its infancy for exploration geochemistry. However, the number of research papers underestimates the volume of production work involving the use of computers, certainly the application of simpler statistical procedures that are used on a routine basis in many mineral industry and government surveys. This is partly due to the widespread availability of computing power in mini and microcomputers, but more

importantly to the availability of software packages and the acceptance of computer methods as routine tools. Much of the routine use of computing is with "canned" programs, bringing with it problems as well as benefits. Firstly, although it is easy to enter data into these software packages and obtain results, the user may not be fully aware of the assumptional rules of the methods being used, leading to disastrous interpretations. Secondly, the majority of the popular statistical packages that are in use were not written for geological users, e.g. BMDP, MiniTab, SAS, and SPSS on mainframe computers, and these and others such as Statgraphics and Systat available for microcomputers. Therefore, they are not always well adapted to geochemical practice and there is a lag between the development and publication of new procedures and their implementation in easy–to–use well–documented software packages. However, this is changing as more specifically geochemical software packages become available, although in general these are expensive in comparison with the widely used statistical packages due to their smaller market.

Geochemical data processing is mainly multivariate, and this situation will not change as improved analytical chemical procedures produce progressively more elemental analyses per sample at low cost. It is not surprising that over the last decade much of the published work has focussed on the recognition of patterns and outliers in multivariate datasets. Over the decade a new approach to multivariate data analysis and synthesis has become available through the use of image analysis systems. These have opened up a variety of new ways of viewing geochemical data and permit relationships with spatial features to be studied, whereas previously this was difficult and time consuming. The modeling work of today is multivariate in that many species and minerals may be considered simultaneously. The kind of approaches that these procedures make possible have had an enormous impact on hydrogeochemistry and the quality of data interpretation in that field. The modeling is both making it clear why we find the elements in abundance where we find them, and conversely allowing us to recognize what environments have been like in the past on the basis of the observed geochemical distributions. Modeling is playing an important role in changing exploration geochemistry from an observational science to a predictive one.

An important trend that has picked up momentum in the last decade has been the use of assumption– and distribution–free methods on one hand, and robust estimators on the other. Both of these approaches are resistant to statistical outliers, potentially the true geochemical anomalies being sought, but which can distort the procedures being used to detect them, resulting in poor definitions of background and therefore a reduced ability to recognize anomalies.

Very importantly there has been a complete change in attitude to computer–assisted interpretation over the past 20 years. Largely due to today's interactive and graphical computing environment, it is possible to carry out computer–assisted interpretations the way we would by hand if we ever had sufficient time. In an interpretation, geochemists partition data into groups on the basis of spatial or geochemical characteristics and provide each response group with a set of plausible geological and geochemical controlling processes, e.g. background lithological population or a mixture of lithological "end–members", secondary environmental modification, mineralization process, etc. The computer approach is to subdivide the data, preferrably using interactive graphics, into subsets and then use whatever tool, graphical or statistical, is most appropriate to discover or confirm the processes associated with the response group. Thus many workers at the leading edge are developing what might be described as geochemist's interpretational tool–kits which combine a variety of data base (relational and/or geographic), graphical, statistical, and image analysis procedures into integrated systems which can be used in the intuitive ways of the geochemist. Interpretation can be likened to peeling an onion, one strips off data layer by layer, interpreting the layer(s) stripped at one stage using whatever tools are most appropriate; and then returning to the onion to strip off further layers, again using the most appropriate tool(s). This continues until the job is complete,and the necessary summaries, maps and graphics are prepared to convince an audience that the proposed interpretation is reasonable and complete.

THE NEXT DECADE

Crystal–ball gazing can be hazardous; in 1977 who would have realized that the computer power we have today would be so available on the geochemist's desk at such low prices. A remarkable spectrum of low cost hardware (computers, graphics devices, etc.) is now available and will become more powerful and cheaper in the future. What is missing is appropriate software embodying the best of the advances discovered by methodology developers in a way that makes them usable and, most importantly, helps the user employ them in a correct way. This will lead to a series of specialized workstation environments, some strong on computational power for modeling, others on graphics, and general purpose compromises, where geochemists can work with their data to achieve their particular objectives. Probably most of the techniques required to make competent interpretations already exist in data analysis, graphical methods, and image analysis. It is likely that important advances will be made in the sphere of algorithms for interpetation. Simply, how to approach a problem and knowing which tools are most likely to help solve the specific task at hand.

The next decade will see major advances in the use of geographic information systems (GIS), both at the institutional data base and individual project levels. Currently, the digital capture of thematic maps is a bottleneck, however, progress in raster scanning technology and the associated editing tasks will overcome this problem. This, coupled with reduced computer hardware and software costs will lead to a wide acceptance and use of GISs in exploration geochemistry and data integration studies. Advantages offered by this technology include a flexible electronic light-table approach which permits the evaluation of geochemical data and anomalies in the light of geological, geophysical, and other geoscience data, and the ability to produce maps which display only the features relevant to the particular problem under investigation.

In modeling exercises, increased computer power and improved methods will make it feasible to tackle ever more complex problems, and so realistically model the geochemical reality. A major benefit of these studies will be when practical rules can be developed for use in the field to recognize specific environments and their place in the overall scheme of element dispersion in the crust. Clearly, a part of this model is the processes and environments characteristic of element accumulation to form mineral deposits, and the later processes involved in their destruction and the dispersion of elements away from them.

All these activities involve knowledge. For instance, the design of geochemical exploration programs is largely heuristic and experience based, and much of this work is undertaken by mineral explorationists. There will be major attempts in the coming decade to try and organize the rules used by experienced geochemists in planning, managing, and interpreting geochemical surveys and other related activities into expert systems (Garrett and Leymarie, in press). If these are successful, they will have a major impact by improving the effectiveness of geochemical surveys in mineral exploration, which is surely our ultimate objective.

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