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Geoscience after IT: Part G

Familiarization with spatial analysis

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Abstract - Spatial pattern is crucial to geoscience. It enables us to compare the observed properties of objects and explain their spatial relationships, correlation and distribution in terms of the geological circumstances and processes that formed them. Digital cartography and the spatial model provide computer support for looking at objects and properties in their spatial context. Transformations enable us to move and shape the objects for better visualization and analysis. Spatial statistics can quantify configuration for analysis of form and structure. The fractal model reminds us of the divergence between our models and reality.

Key Words - Digital cartography, spatial relationships, spatial models, spatial transformations, fractals.

1. Digital cartography

A vector (x_{i1}, x_{i2}) can represent a point in two dimensions, and a vector (x_{i1}, x_{i2}, x_{i3}) can represent a point in three dimensions. A straight line joining two points is also a vector in the geometric sense (it has length, orientation and direction). A string of vectors, joined end to end, linking a set of points, can represent a curved line on a map. A set of lines joined end to end can delimit a closed area on the map, sometimes referred to as a **polygon**. The point, line and area are sometimes known in digital cartography as a **vertex**, **edge** and **face**.

Computer systems for drawing maps may be specifically developed for cartography, or could be computer-aided design systems, adapted for cartographic purposes. Areas can be filled with a selected color or ornament, and symbols and text positioned at points selected by the user. Fig. 1 for example shows a diagrammatic geological map prepared on a desktop computer. Other cartographic representations show, for example, a vertical section of beds measured at an exposure or from a borehole (Fig. 2), or a fence diagram (Fig. 3) showing the variation in thickness of each of a sequence of beds across a number of measurement sites. Symbol maps of various kinds can show the spatial variation of one or more variables. Programs for a personal computer are available at reasonable cost to support a range of these tasks.

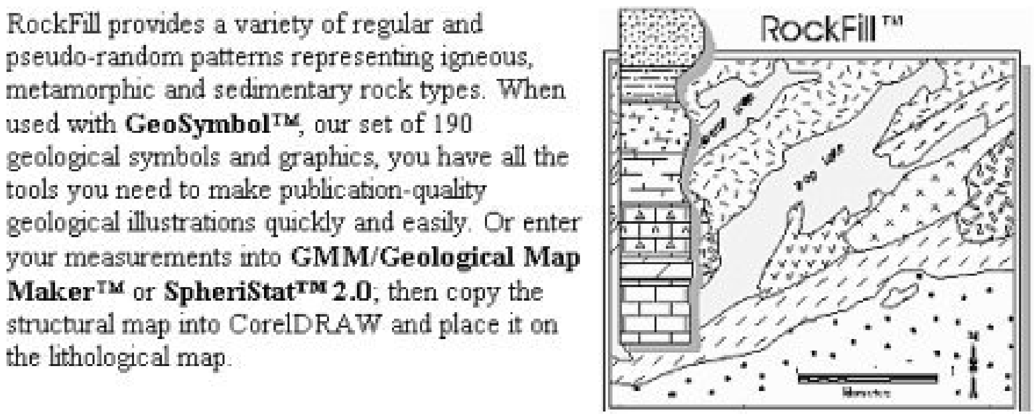

Fig. 1. Diagrammatic geological map. Example of a diagram prepared on a desktop computer. Reproduced by permission of Rockware. More at http://www.rockware.com/

See next page for Fig 2.

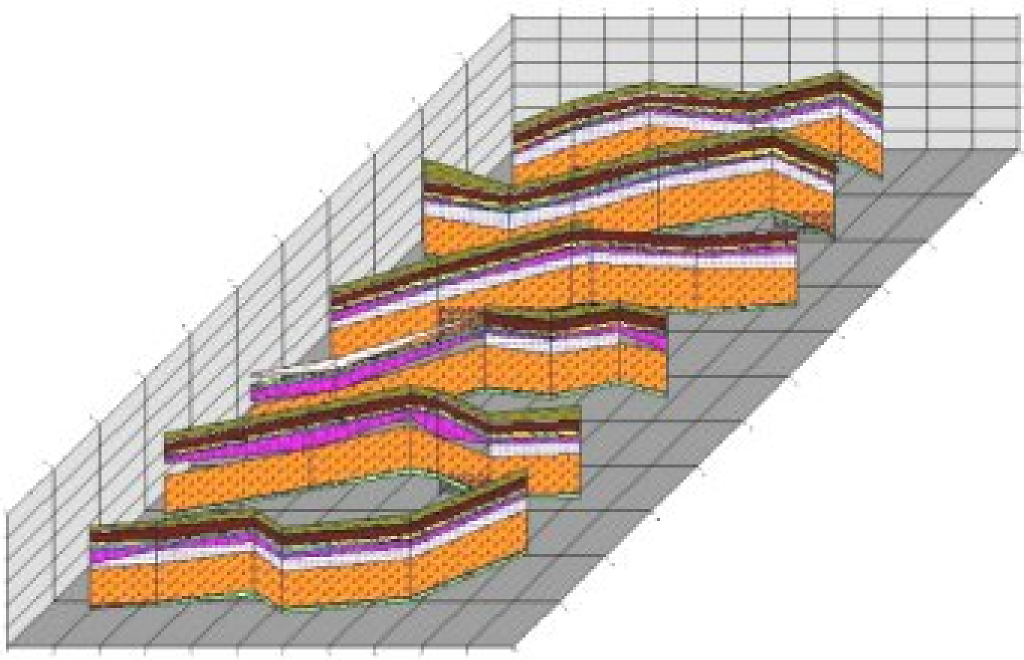

Fig. 3. Fence diagram. Example of diagram prepared on a dektop computer. Reproduced by permission of Rockware. More on http://www.rockware.com/

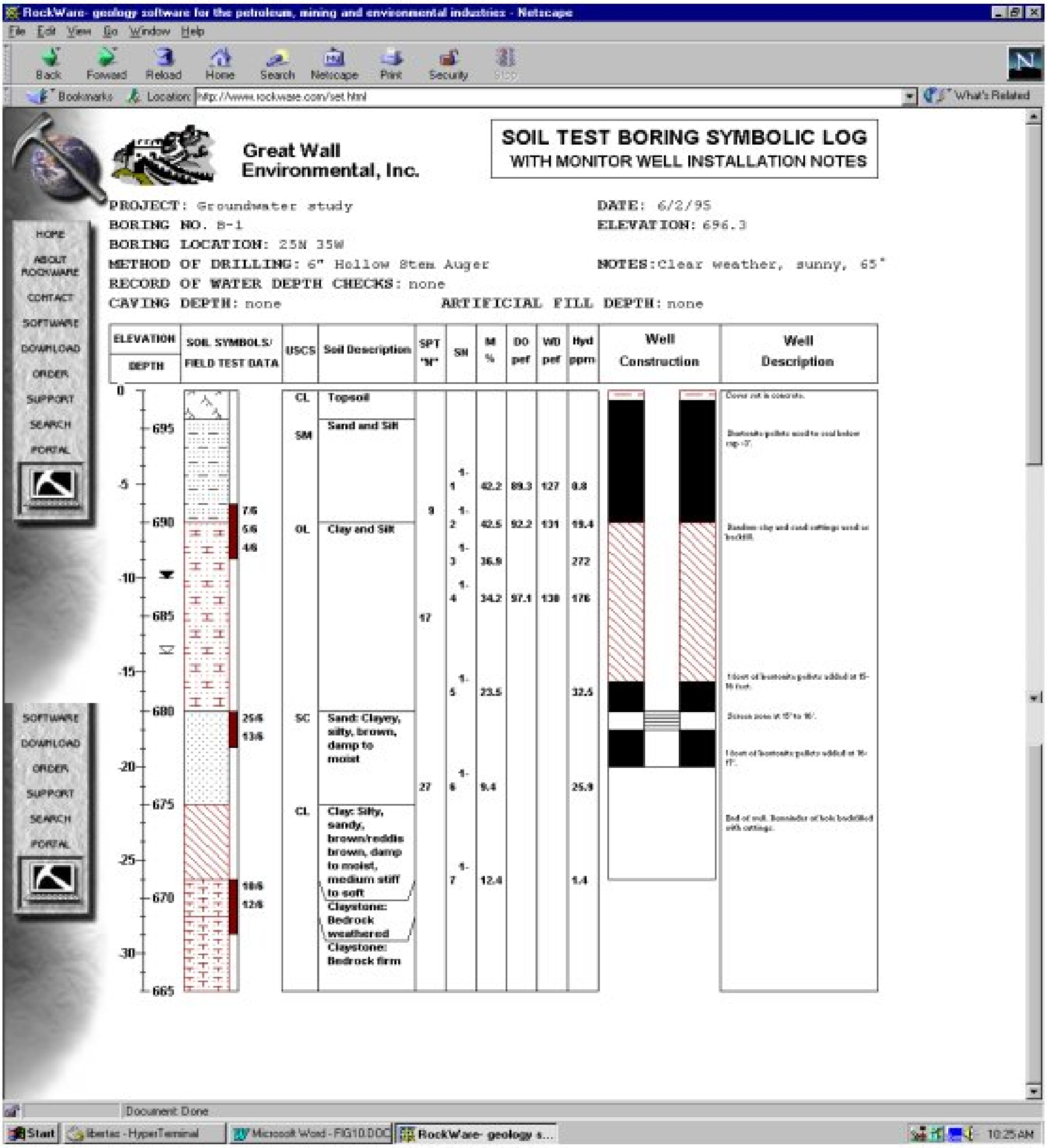

Fig. 2. Log of vertical section. Example of diagram prepared on a desktop computer. Reproduced by permission of Rockware. More at http://www.rockware.com/

Existing maps can be digitized by clicking on selected points. A sequence of points can be digitized to record a line, and a sequence of lines to enclose an area. Because the short lines joining points are vectors, this is known as vector digitizing, and generates a **vector format**. Another way to capture existing images is with a scanner. This creates a **raster format**, in which the image is made up of a rectangular grid of small cells (picture elements, picture cells, or **pixels**). The scanner assigns a value to each pixel to indicate the color at that point. The computer stores the values for the array of pixels. A minimum of one bit records each pixel in a monochrome image, but up to 24 bits or more may be used to store the proportions of red, green and blue in a pixel of a color image.

The raster format is an effective and efficient means of recording and storing complex images, such as air photographs, satellite imagery or “busy” topographic maps. Vector representation is more flexible and efficient where there are relatively few lines, as in a geological map. It has the advantage that individual lines and areas can be referred to and processed separately. Thus, one could select all the areas enclosed by the Cretaceous boundary, and find specimens within it by a **points-in-polygon** process.

Raster and vector methods are frequently used together. For example, a topographic map might be scanned and displayed as a raster image on the screen. Points and lines of geological significance could then be traced by moving a cursor on the screen and recorded in vector mode. This is a widely used procedure for digitizing geological maps, having the advantage of providing separate but linked representation of the topography and the geology in exact register. The two layers can be overlain when required and displayed together. Each is also available separately in its most useful format. Conversion from one format to the other is possible when required, and vector format is generally rasterized before it is displayed on the screen or printed. Many rasters, however, such as satellite images, could not be represented satisfactorily by vectors.

2. The spatial model

Ideas about how quantitative methods fit into broader schemes of investigation are taken up later (part L, section 6.3). Meanwhile, we may note that most quantitative work in geoscience arises in geophysics and other subjects where instruments provide much of the raw data. Examples from geophysics include gravity, aeromagnetic or exploration seismic surveys, geomagnetism and global seismology. Other examples can be found in some geochemical and oceanographic surveys, aerial photography and satellite imagery. The initial data processing may be concerned more with correcting and clarifying the instrumental records than in exploring geological ideas. The mathematical models may be specific to the tools used in probing the properties of the Earth. The consistency of well-calibrated instruments, and the ability to correct for extraneous effects, are powerful features of these methods. Standardization makes it possible to conduct surveys over large regions or of global extent. Conclusions are not limited by local circumstances.

The significance of the results is not likely to lie in a single measurement at one point, but rather in the regional spatial patterns, and their correlation with spatial patterns from other types of survey. Integration of the ideas from the various topics could proceed through examination and comparison of maps showing the final interpretations of the topic experts. However, **digital spatial models** (computer representations of objects and their properties in geographic space) offer more powerful methods of representing, analyzing, comparing and displaying the data. Spatial data, such as measurements of gravity, or formation elevations determined from downhole logs, may be recorded as part of a general database system, and still be part of the spatial model.

Traditional geological maps, showing the distribution of formations and other features at or near the ground surface, are now generally prepared by digital cartography (G 1). Contour maps, showing the variation of properties across an area, may also be drawn by computer (see Watson, 1992). The case for digital methods usually refers to long-term cost savings, flexibility, rapid production and ease of editing and updating. However, the longer-term benefits may depend on end products beyond the published map. The map, after all, is no more than an illustration of the underlying concepts (B 4.1). IT offers the prospect of expressing the latest conceptual model more comprehensively, and linking it to the quantitative surveys mentioned in F 5 (Förster and Merriam, 1996, Grunsky et al., 1996). The model can thus include three-dimensional rock bodies, their disposition and configuration, their composition and properties, their changes through geological time, the evidence and confidence in the conclusions (M 2.3). There is a prospect of freeing spatial information from the limitations of the paper map (B 4), and integrating it within the computer model (L 4). The ability to integrate concepts, and therefore the scope of the spatial model, is determined by the human interpreter, not by the capabilities of the software. Ultimately, therefore, the model reaches out beyond the computer with links to the scientists' unstated knowledge.

The computer spatial model, unconstrained by cartographic limitations, can express the conceptual model more fully. More of the ideas in the minds of the surveyors can be recorded and become the shared resource of the community. Maps can then be seen as ephemeral documents to assist visualization, illustrating selected two-dimensional projections of the model (see MacEachern, 1998 and the special issue of the International Journal of Geographical Information Science introduced by Kraak, 1999). The collection and archiving of spatial data are freed from the limitations of the map. Users would choose their own map content and display, after interacting with the model to clarify the availability of information and to select from it to meet their requirements. Comparison and correlation with other models, such as topography, land-use, or patterns of mineral deficiency in livestock, could be based on the models themselves, not on their cartographic representation. These future prospects are discussed in L 4 and M 2. The objective at this point is to look at the methods of handling data in the context of a spatial model.

A geological map enables the user to find (in the map key) a list of the things of interest (objects), such as stratigraphic units, displayed on the map. The map shows the location of the objects, related to topography and to a geographic grid or latitude and longitude. It gives an indication of the pattern and form of the objects. Contour maps may show, for example, chemical composition or engineering properties, and their spatial variation. The digital spatial model should combine these tasks and perform them more effectively. Like the map key, the metadata (D 3) associated with the model should identify the objects, perhaps grouping them within object classes or topics that might correspond to projects or to types of map, such as geology, geophysics or topography.

The location of data must obviously be recorded in the model. The configurations of objects and their distribution patterns and correlations may be investigated numerically, but are more likely to be examined by eye. The data must be displayable on a computer screen or printed as a map, and this involves transforming their three-dimensional locations to appropriate positions on the display. The transformation must preserve significant relationships among the data. We therefore look next at what these relationships are, how the transformations can be carried out, and which quantitative methods might be appropriate for the spatial data.

3. Spatial relationships

Spatial relationships can be important to the interpretation of a geological map, such as a formation boundary veeing upstream or a fossil being collected from a particular rock unit. They fall into two main categories - topological and geometric. **Topological relationships** are those that are unchanged by rubber-sheet deformations. If you imagine a map drawn on a thin elastic sheet, the sheet could be distorted by stretching and the relative position of points altered. Straight lines could become curved, angles between them altered, distances changed. Topological relationships are **invariant** (unaltered) during these distortions. Examples are: a point lying on a line; points, lines or areas coinciding or contained inside an area; lines touching, branching or intersecting; lines bounding an area; and their opposites, such as a point lying outside an area.

Geometric relationships on the other hand, require a consistent **metric**, that is, distance and direction must be measured consistently throughout the space. Geometric relationships include: above, near, adjacent to, farther from, parallel to, converging with, at right angles to, interdigitated with, larger than, and their opposites and approximations. Unlike topological relationships, geometric relationships can generally be quantified, as in: twice as large, 234 meters from, converging at 20^{o}.

Some relationships may be obvious in the field, such as an outcrop being on the north side of a river below a road bridge. The relationship might be shown with some difficulty on a map, but is liable to be lost if the map is generalized for scale change. A printed geological map may be locked into a specific base map by overprinting. The spatial model seeks the flexibility of allowing each topic and each project to be managed separately, preferably meeting standards (L 4) that allow easy interchange of data. As this allows datasets to change independently, important relationships between them should be recorded explicitly. If need be, the short section of river and road bridge might be digitized and made available permanently within the geological model. It can then be compared with the same fragment of river on the topographic model during display, and any necessary adjustments made.

Spatial information can be transformed in various ways, altering the geometric relationships between objects. The transformations are an important part of computer graphics and essential for manipulating and visualizing the spatial model. They must be used with care to avoid accidentally distorting patterns or altering spatial relationships. For example, different map projections alter the size, shape and location of areas and cause difficulty in overlaying maps. Spatial transformations are also used in recreating surfaces from point data and in multivariate statistics. Understanding their effects is useful background.

4. Spatial transformations

Spatial transformations of a geoscience model generally alter geometry rather than topology. However, it is possible that, say, two separate lines would coincide on the display when the scale is reduced. On a printed map, a cartographic draftsman might move the lines apart, to preserve the relationship at the expense of accurate positioning. On an interactive system, the ability to zoom in and clarify the relationships makes this unnecessary, and the true positions of the lines could be preserved.

For display purposes, a simple set of geometric transformations is available (Foley, 1994). **Translation** is bodily movement of an object relative to the origin. **Rotation** involves the object being turned about an axis. They are both **rigid-body** transformations that do not alter the size or shape of an object. **Stretching** changes the length of an object along an axis, thus changing its shape and altering distances and angles, except in the special case of **enlargement** where scaling is the same in all directions, and only the size and distances are altered. **Projection** involves reducing the number of dimensions, as when a three-dimensional body is projected on a two-dimensional screen. The linear transformations just mentioned are known as **affine** transformations. **Perspective** change gives a more lifelike appearance to the projection of an object by including perspective effects, such as apparent size diminishing with distance and parallel lines converging.

These transformations, which are illustrated in Fig. 4, are carried out on the computer by matrix multiplication (F 4). For display purposes, a sequence of transformations may be called for, such as rotate about the x-axis by 30^{o}, dilate to twice the length along the new y-axis, then rotate back by -30^{o} about the x-axis. This can be represented by a sequence of matrices, which could be applied in turn. It is more efficient, however, to multiply the transformation matrices together to obtain a composite matrix of the same size representing the entire sequence of transformations. The composite matrix is then applied to each of the original data points.

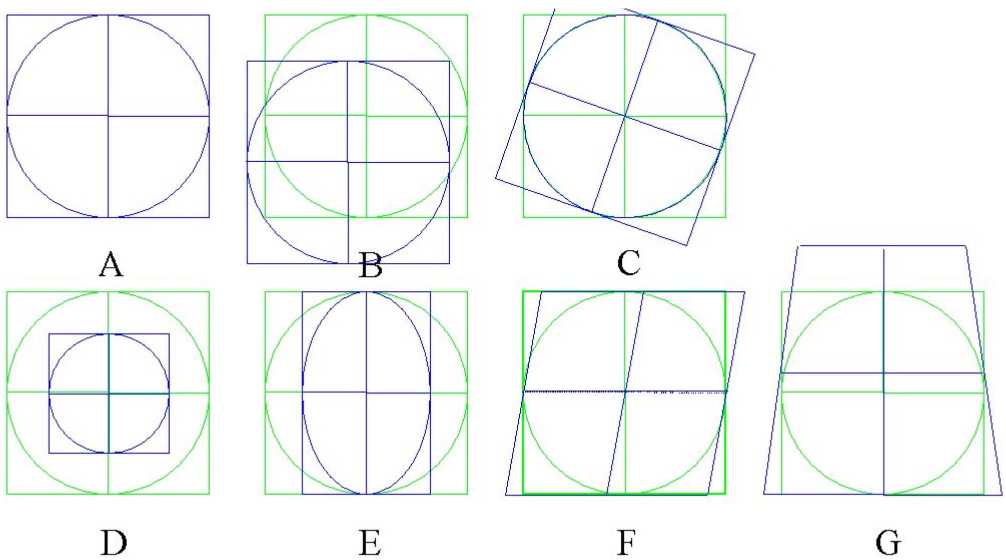

Fig. 4. Some geometric transformations. The figure at A is translated in B and rotated in C. The scale is changed in D, and the figure is stretched in E, with only the horizontal scale being altered. The figure is sheared in F. There are obvious three-dimensional equivalents. More complex transformations include perspective projections (G) in which the change of scale varies across the figure.

The transformation matrix is a square matrix, with two rows and two columns (2x2) for transformations in two dimensions, 3x3 for three dimensions and so on. The transformations, and the matrix multiplications, must be carried out in the correct order. Translation involves addition, rather than multiplication, but can be included in the multiplication by adding an extra dimension. The three-dimensional data are transformed in four dimensions. The extra dimension is also needed for perspective transformations.

The main application of these spatial transformations is for graphical display and manipulation, such as projection of three-dimensional objects onto two-dimensional paper or a computer screen. They also play a part in structural geology, process modeling, and such areas as multivariate statistics, surface interpolation and shape analysis.

An image can be subdivided into small patches. Each patch can be transformed separately, while forcing continuity across patches by modifying the transformations to ensure that the patches meet smoothly at the edges, by methods comparable to blending functions (G 5). The process is sometimes known as rubber sheeting. **Distorted** images such as oblique air photographs can be corrected. For example, points could be selected on the distorted photograph as landmarks for which exact coordinates could be found on a map. The distorted image could then be corrected by joining adjacent landmarks by lines and transforming the patches between them to conform to the map coordinates.

Spatial transformations also arise in **map projections**, which offer solutions to the problem of projecting an irregular oblate spheroid (the surface of the Earth) onto two-dimensional paper. The transformations are generally more complex than those just described. Different projections maintain different aspects of the original geometry. Areas, angles, distances and continuity cannot all be preserved when part of the surface of a sphere is distorted for representation in two dimensions. Aspects that can be neglected on the screen are important on printed maps. For instance, the user is likely to expect roads to meet across sheet boundaries without sharp breaks in direction.

Continuity from area to area raises problems as even the coordinate system, based on latitude and longitude, has local variations. The Earth is irregular, and mathematical approximations must be used for such concepts as the **datum** (the origin of the local coordinate system including mean sea level) and the **geoid** (a mathematical surface approximating, at least locally, to the shape of the earth). Different geoids and datums have been used at different times and in different places. Map coordinates and projections are a subject in their own right (see, for example, Snyder, 1987). However, if you combine spatial data from different sources, you should at least be aware of this potential source of error.

5. Spatial statistics and surface fitting

The statistical methods described in F 5 apply to properties measured at points in space. In geoscience, spatial patterns and spatial correlations are often crucial. Statistical methods describe the observed patterns quantitatively, guide interpolation between sampled points, and measure spatial correlations. The patterns are likely to reflect underlying geological processes that have influenced many measurable variables. Possible aims are to put individual points in context by fitting them to a surface, then to compare and correlate surfaces from the same area to learn more of the environment in which they developed, the formative processes and their effects. Specific tasks might be to estimate the elevation of a formation at a drilling location, the amount of ore in a mineral deposit, or the amount of folding across a cross-section.

As always, the validity of conclusions depends on appropriate sampling techniques (D 4). The sample should be random, in the sense that each item in the population has an equal chance of being included in the sample. You might try to obtain a representative sample of the lithologies in a rock body by selecting collection points as near as possible to, say, random points on a map grid, or every 25 paces along a traverse. The sample would be unrepresentative, however, if hard sandstones formed outcrops, with interbedded soft shales covered by soil and vegetation. If you were studying the relationship between, say, petrography and geochemistry, then spatial randomization could be misleading. It might be better to ensure that every petrographic composition of interest had an equal chance of selection. We should continually review our raw material and ask how appropriate our models are, and whether it is possible to improve their correspondence to reality.

A surface is most readily analyzed if the data points are evenly spaced on a rectangular grid. But most data are positioned for reasons unconnected with surface analysis. Uneven clusters of points are found in oilfields, or soil samples from a housing development. Sampling points may lie along lines, such as geophysical traverses, geotechnical measurements along a new highway, or geochemical analyses of samples along streams. But even if the sampling pattern rules out statistical conclusions, quantitative methods may still be of value.

Time series, sequences of measurements at successive times, have been widely studied in statistics. In geoscience, time series arise in geophysics, hydrology, oceanography and other subjects. Similar methods can be applied to sequences along a line in space, and some can be extended to two or more dimensions. Regression techniques are one way to relate the variation of a property to its position in time or space. For example, the grain size (p) of samples could be related to distance (x) above the base of a vertical section, by the equation:

$$p = a + bx$$

The straight line which this represents is unlikely to show the variation adequately, and more terms from a power series or a trigonometric series can be added (see F 5):

$$p = a + bx + cx^2 + dx^3 + \ldots + mx^n$$

or:

$$p = a + b\sin x + c\sin 2x + d\sin 3x + \ldots + m\sin nx$$

In two dimensions (x and y) the equations represent **surfaces** and are slightly more complicated. For example, they might refer to the top of a formation based on its elevation (p) as measured at wells:

$$p = a + bx + cy + dx^2 + exy + fy^2 + gx^3 + \ldots + my^n$$

or:

$$p = a + b\sin x + c\sin y + d\sin 2x + e\sin x.\sin y + f\sin 2x + \ldots + m\sin ny$$

The regression equations are calculated as in F 5 to minimize the sum of squares of deviations between the measured and calculated values of *p*. An excellent mathematical introduction is provided by Lancaster and Salkauskas (1986).

Let us take as an example the elevations of the top of the Cretaceous as known from fifty wells over the flank of a depositional basin. One possibility would be to fit a regression equation of fifty terms. As this equals the number of wells, it would fit the values perfectly, and the sum of squares of deviations would be zero. The position of contours on the quantitative surface could be calculated and drawn as a contour map. There is little reason to suppose, however, that the mathematical surface would match the geology. There is no obvious reason why geological processes would produce forms shaped like polynomial curves (F Fig. 4), and the result will be greatly influenced by the spatial distribution of data points, which were almost certainly not positioned with this type of analysis in mind.

A better approach would be to fit a simpler third-order regression surface to the data, that is, an equation with terms up to the third power of *x* and *y*. The result would be a smooth surface that was less sensitive to the point distribution. It shows slow systematic change and is known as a **trend surface**. The **residuals**, that is the deviations between the data points and the fitted surface, can be displayed and mapped separately. Variations at different scales have been separated. The trend might be the result of regional tilting, subsidence and folding, the residuals the result of depositional and erosional features. By mapping the residuals separately, features might be noticed which were not apparent on the original map. Attempts at a rigorous mathematical justification for such conclusions tend to be rather unconvincing, but are unnecessary if the results can be justified by geological reasoning.

In order to arrive at a unique surface, the least-squares criterion can be applied (F 5), minimizing the sum of squares of deviations of data points from the fitted surface. An alternative is to fit **spline surfaces** (Lancaster and Salkauskas, 1986) that minimize the tension, or more strictly, the strain energy, in the surface (thinking of the surface as a flexible sheet). This model can give a good fit to some types of geological surface, and might, for example, mimic the shape of a folded surface.

For geophysicists, the use of periodic functions needs no introduction. The seismologist, for example, deals with shock waves generated by earthquake or explosion, and their modification by the rocks through which they pass. Waves, by definition, have a repetitive form and this may readily be described by fitting a function of sines and cosines (see F 5), a process known as **harmonic** or **Fourier** analysis. Rather than characterizing the wave by values at successive moments of time, a static view of the **power spectrum**, or relative importance of components of different wavelength, can be calculated. The values in the spectrum relate to the constants, *a, b, c, . . .* in the sine-wave equation. The power spectrum incorporates a great deal of information about the form of the wave, and makes it possible to compare the amplitude of different wavelengths (spectral analysis) as a separate issue from their time of arrival or position in space.

Fourier analysis has benefited from the existence of many accurate time series collected digitally, and from the development of the Fast Fourier Transform (FFT), an efficient algorithm that reduces the computing load. Although the main applications are in seismic work, geomagnetism and gravity studies also study periodicity with Fourier transforms. Methods such as the fast Fourier transform can be applied to large digital datasets such as satellite imagery and downhole logs. With imagery, they can give information about the texture and its variation that may be related to changing geology.

For a geologist, the value of spectral analysis is less clear. The notion of treating distance from the origin as an angle may seem bizarre, but poses no mathematical problem. More fundamental is the relevance to the geological model. The periodicity of deposition of sediment, for example, might be related to geological time, with distance from the base of the section an inadequate substitute. Random events during deposition are likely to throw subsequent periodicity out of phase with that below. Similar comments could be made about variation in two dimensions, on a geological surface.

One way around this difficulty is to look at the relationship of each point to the adjacent points, as this is less affected by phase shifts. A mathematical function can be fitted **globally**, that is to the entire sequence or surface of interest, or **piecewise**, that is to a small number of adjacent measurements at a time (see Watson, 1992, Houlding, 1994). Piecewise fitting involves treating small parts of the section, or small patches of the surface, separately, and aggregating the results. The patches can be selected in many ways, preferably in some coherent and unambiguous manner. One way of creating surface patches is with Delauney triangles (see Bonham-Carter, 1994), a unique set of evenly shaped triangular facets with a data point at each apex.

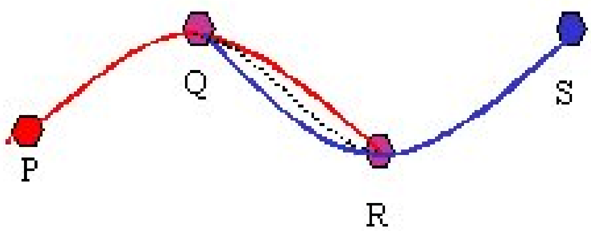

Fig. 5. Blending functions. Separate curves are fitted through the points P, Q, R and Q, R, S. They can be blended into one another where they overlap by the dotted curve, which is a weighted combination of the other two. The weight that the blending function gives to the curve PQR varies gradually from 1 at Q to 0 at R, while the weight given to QRS varies from 0 at Q to 1 at R. Blending functions can also smooth transitions between surface patches.

A polynomial function can be fitted separately to each triangle. The simplest would be a flat plane. The planar facets would meet at the edges of the triangles, but the abrupt breaks in slope would be distracting to the eye, and would have no geological significance (section 6). A cubic function could therefore be fitted to each patch, and a **blending function** (see Watson, 1992, Foley, 1994) applied at each vertex to ensure continuity from one patch to the next (Fig. 5). This is one approach used in computer contouring and in computer graphics and visualization. The **finite element methods** used by engineers for representing complex shapes adopt a similar approach, also including four-sided shapes (Lancaster and Salkauskas, 1986, or Buchanan, 1995). Functions known as **wavelets** (Graps (1995; Strang, 1994) can similarly be fitted to small patches. They lead to an interesting analysis by measuring the fit of wavelets to the surface while altering their position, amplitude and scale. There are occasions when local and regional variations are both of interest, as in trend-surface analysis, where local fitting methods can be applied to the residuals from the global trend. Piecewise fitting provides more detail where more is known, thus partly overcoming the sampling problem.

Many algorithms work best with data spaced on a regular grid. Therefore, one method may be used to interpolate from the raw data to grid points, and a different method to analyze and visualize the surface based on the grid points. The drawback is that one artifact is then being applied to another, obscuring the link between model and reality.

Other approaches are mentioned in G 7. Principal component analysis or PCA (F 5) can be applied to spatial data, including satellite images. Where quantitative information is available for each dot on the image (pixel) from each of a number of bands of the electromagnetic spectrum, PCA can distribute this information across a smaller number of principal components that can be mapped separately. They may be more readily interpreted than the original. PCA can also be applied to measurements of a suite of downhole logs, but is less likely to be successful. Since each of the logging tools, such as the microlog and the laterolog, are measuring properties of different volumes of rock, the results are not comparing like with like. It would not be clear what each of the principal components could be referring to, and the geologist's insights, which stem from an understanding of the strata and the tool, would be lost.

6. The fractal model

A computer program can define a sequence of mathematical operations. It enables the scientist to express a conceptual model of a geological process. This is particularly satisfying where theoretical ideas of the process match the fitted function. Not infrequently, however, it turns out that the conceptual model and reality differ in important ways. For example, we may visualize geological boundaries as smooth surfaces, even when we know from field observation that this is not so. Aided and abetted by the cartographer, we simplify by smoothing. It is inevitable that our records reflect our mental images, but smooth models can mislead and we should be aware of their divergence from the real world (J 2.3).

Mandelbrot (1982) takes as an example the question: How long is the coastline of Great Britain? Faced with the question, many of us visualize a map, maybe even wondering what scale is appropriate. Few think of the coast itself, with its headlands, beaches, boulders and breaking waves. We know that the answer must depend on a conceptual model, and we simplify reality in order to think about it. The more detailed our model, the longer the coastline seems to become. The length of a line joining the main headlands might give a first approximation (see Fig. 9). However, the line becomes longer without limit as we extend it to give the outline of each bay; the detail of each small irregularity; the outline of each sand grain; the microscopic and atomic structure of the interface. The question has no single number for an answer, but leads to an interesting discussion of measurement techniques. A precisely defined conceptual model can define the distance. There is no uniquely appropriate model, however, and none that matches reality in every respect.

Mandelbrot pointed out that continuity, which is an essential feature of most of our models, is not typical of natural phenomena, which tend to be discontinuous at all scales. **Continuity** refers to the characteristic of a mathematical function of having the possibility of creating a very small zone about a point, within which the value of the function does not significantly change. On a geological surface, for example, continuity may refer to elevation, slope (rate of change of elevation), curvature (rate of change of slope), and so on (Fig. 6).

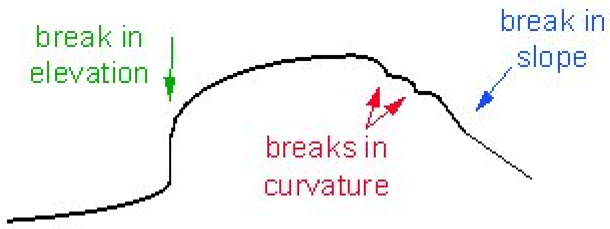

Fig. 6. Continuity of elevation, slope and curvature. Large and sudden changes in elevation, such as cliff faces, are obvious when looking at a landscape. Elevations on either side of the break differ, with no gradual transition. Large breaks in slope and curvature (the first and second derivatives of elevation) may also be apparent. Close inspection reveals similar breaks at all levels of detail.

In the natural world, we can seldom demonstrate mathematical continuity at any level. It must therefore be a feature of our perception. When we look at the distant outline of a mountain ridge, the small-scale variation is blurred, and we see an apparently smooth edge against the sky. As we examine the edge, the changes in direction, breaks in slope and even changing curvature catch our eye. In preparing maps and models, we therefore avoid such breaks if we know they have no geological significance. For the same reason, flat triangular facets joining data points are generally an unsatisfactory representation of a geological surface. The discontinuities of slope between facets draw the eye to the sampling pattern and obscure the underlying geology.

The approach taken by Mandelbrot is to study a number of mathematical functions that he terms fractals (Fig. 7). As well as lack of continuity, they exhibit another feature of interest to geoscience. They show **self-similarity**, that is, the pattern created by the function looks the same if we enlarge a small part of the original (Fig. 8). The concept is familiar to the geologist. Microfolds can mimic regional structure, and trickles of water on a mud bank may form a delta like a scaled-down Mississippi. He extends this to self-affinity, where vertical exaggeration or other affine transformations (G 4) alter the pattern. Manipulations of the fractals can produce images uncannily like real islands, mountains and clouds. The functions that generate them, however, are not obviously related to geological processes.

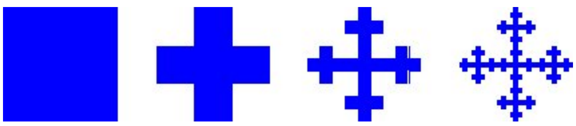

Fig. 7. Example of fractal function. Starting on the left of the diagram, a simple square is the initial object (initiator). The object is copied and attached to the north, east, south and west sides to form a new object, here reduced in scale. The same simple process (generator) is repeated, going from left to right, to give ever more complex objects. Reproduced by permission of David G. Green. More at http://life.csu.edu.au/complex/tutorials/tutorial3.html

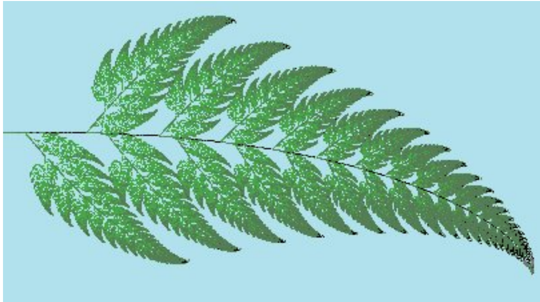

Fig. 8. Self-similarity of fractal. Enlarging one of the segments of this fractal fern would create another image similar to this frond, and so on. Many fractal functions show this property of self-similarity over a range of scales, as do the results of many geological processes. Reproduced by permission of David G. Green. More at http://life.csu.edu.au/complex/tutorials/tutorial3.html

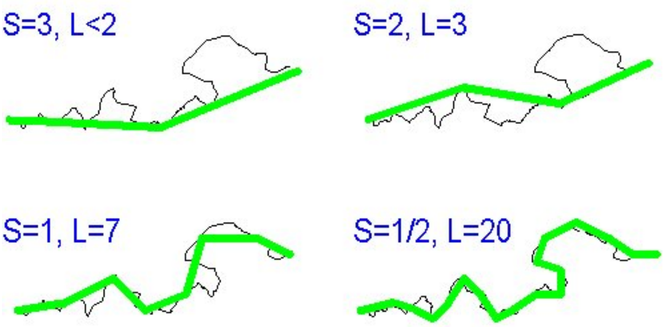

Fig. 9. Coastline and yardstick length. As the length S of the yardstick (or the span of a pair of dividers) decreases, the apparent length (S × L) of the coastline increases. Reproduced by permission of David G. Green. More at http://life.csu.edu.au/complex/tutorials/tutorial3.html

In studying fractals, we can visualize the length of a coastline being measured by a hypothetical set of dividers. We measure the length of the coast by stepping the giant pair of dividers around it. The apparent total length increases as the span of the dividers diminishes (Fig. 9). We can plot the resulting calculated length against the length of the measuring device. The plot throws some light on the intricacy of the convolutions at various resolutions. The overall slope of the plotted curve has a bearing on a property (the fractal dimension) of the configuration of the coastline as a whole. Accounts of the numerous applications of fractals in geoscience can be found in journals such as *Computers & Geoscience* (Agterberg and Cheng, 1999) and textbooks such as those by Turcotte (1992) and Barton and La Pointe (1995).

7. Spatial configuration

We have looked in section 5 at the **disposition** of a property, at ways of describing the distribution in space of its values. An obvious next step is look at the **configuration**, that is, the spatial form and structure of the values. An important insight that geologists bring to spatial data is their expectation of how knowledge of nearby values might influence prediction. The distribution of commercially exploitable minerals in the Earth's crust, for example, is obviously uneven. Experience and concepts of formative processes guide geological expectations of their distribution. The study of **geostatistics** (for an introduction, see Isaaks and Srivastava, 1989) attempts to formalize and quantify this knowledge, and then to use it with available data to predict unknown values. Its roots lie in mining geology, where it offers techniques, for example, for estimating ore reserves from core sample data. The methods apply to estimating values at points, and also to estimating large volumes from small volumes, such as ore reserves from core samples or comparing readings from a laterolog and a microlog.

An obvious approach to describing the configuration is to compare values at different distances apart. One can then draw a graph of distance versus the similarity of values. The results are not tied to one location, but make a general statement about spatial correlation within the dataset. The power spectrum (section 5) takes this approach, as does the correlogram, which shows correlation coefficients between data points at a given distance apart, plotted against that separation distance.

Geostatistics also considers the amount of change to be expected between values at various distances apart. For each separation distance, one can sample the difference in values, calculate the variance and plot it against the separation distance in a so-called **semi-variogram** (Fig. 10). Subsequently, one can estimate the value of an unsampled point on the basis of surrounding data points weighted according to the semi-variogram. This process is referred to as **kriging**. It can take direction as well as distance into account, as ore bodies, say, may be elongated, with greater variation in one direction than another. Not surprisingly, nearby points predict unknown values better than those farther away. Thus, tightly clustered data points are all to some extent providing the same predictive information. Kriging therefore gives them less weight than more isolated data points.

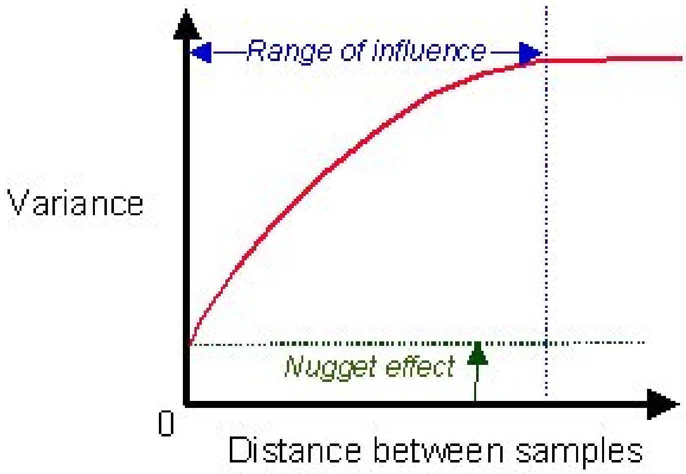

Fig. 10. Variogram. A geological property varies from place to place. Its values are likely to be more similar at nearby points than at those further apart, at least over a limited range of influence. This pattern can be quantified in a variogram, which plots the geographical distance between samples against the mean squared difference of their values. Samples taken at the same point may not give identical results, and rapid change can occur over short distances (the nugget effect).

There is a major advantage in looking at the general configuration separately from the individual values. The general summary is not totally dependent on the sample. The sample gives an indication of the likely form of the semi-variogram, but conclusions about the population require geological inference. One can select a general curve that is compatible with the sample but takes experience of other similar situations into account.

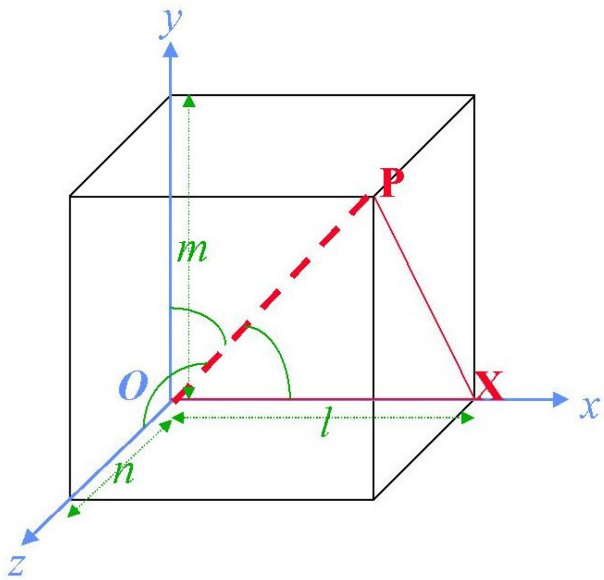

Fig. 11. Direction cosines. The line from the origin O to the point P is of unit length. It represents the orientation of a line parallel to OP or the pole to a plane perpendicular to OP. The cosines of the angles which OP makes with the x, y and z axes give the direction cosines l, m and n. Using Pythagoras' theorem, it can be shown that $l^2 + m^2 + n^2 = OP^2 = 1$. The direction cosines can be treated as lengths when applying geometrical transformations, but rescaling will then be needed to ensure that their sum of squares is again 1.

Structural geologists and geomorphologists may prefer to think of change between values at various distances apart in terms of slopes rather than differences in height. Slopes are easier to measure, are invariant under translation, are not limited to a single surface, and relate more obviously to their conceptual model. For computer processing, slopes in two, three or more dimensions can be conveniently represented by **direction cosines** (Fig. 11) for manipulation and analysis. The subject of **differential geometry** (Kreyszig, 1991) is concerned with the intrinsic geometric properties of surfaces, such as principal axes and lines of greatest and least curvature. It offers a mathematically rigorous account of geometric features that resemble geological features such as fold axes. It is relevant to considerations of shape and form as opposed to size and position.

These various methods can take into account detailed information from past and present studies. They do not however supplant the geologist's insight into the geological setting, the processes and complex relationships. Already some spatial modeling programs enable geologists to input additional information about, say, the position of faults. To benefit fully from the capabilities of both the computer and the human brain, interactive methods must be the way ahead. This will require the development of computer processes that accept interactive control by users who can formulate their background information in appropriate terms. In turn, this will need greater appreciation by geologists of the underlying mathematical concepts.

There are many instances where it is difficult for geologists to convey their ideas with a conventional contour map. A buried landscape might be sculpted with a pattern of river valleys. One cannot place the valleys accurately on the map if elevations are known only at widely spaced boreholes. There are two choices. One could contour a smooth surface showing the most likely elevation of the surface based on known data, but giving no indication of the detailed form of the surface. Alternatively, one could draw an illustrative surface, matching the data points and between them showing the nature of the surface and hence its likely origin, but with the features in arbitrary and possibly misleading positions. In computer graphics, the process of superimposing texture on a surface to make it looks more realistic is known as **rendering**. A computer system should offer the flexibility of separating likely position from likely form and shape.

Another issue arises with positioning, say, the edge of a steep-sided carbonate reef or a vertical fault. One might know the overall geometry, but not the position of the feature, which might lie anywhere between two widely spaced wells. Hand contouring could lead to arbitrary positioning of the feature. Computer contouring could lead to a smooth slope between the wells. But this is not realistic for a vertical feature, like betting that a coin will land on its edge because heads and tails are equally probable. The solution requires a clearer perception of probabilities. Probabilities cause problems in hand contouring but are well suited to computer calculation. Many contouring programs can provide probability envelopes, in effect indicating the most likely value of a surface, and bands on either side where it is decreasingly likely to occur. Near the steep feature and between the two widely spaced wells, there are two likely positions of the surface, separated by an improbable zone. The problem is not calculating the positions but in providing a comprehensible display. An exact definition of what the contours represent, such as most likely position or most likely shape, and different displays showing different aspects, can make the situation clearer.

Surfaces that repeat as with a thrust fault, or roll over as with a recumbent fold, are again difficult to contour manually. The computer contouring procedures described earlier are also unable to handle them. The computer graphics solution uses parametric coordinates *s* and *t* (Rogers and Adams, 1976), which are drawn on the surface itself, and related to the conventional coordinates (x, y and z) by polynomial equations. Visualization of the results may require a block diagram rather than a conventional contour map.

It is clearly necessary to have a wide choice of methods available for handling spatial data. There is no single method appropriate to all circumstances. Geostatistics and spectral analysis inevitably provide different solutions to the same problem. To find the best solution, the geologist must combine wide background knowledge with some understanding of the computer techniques.

In order to provide adequate flexibility, the computer system must offer a wide range of processes that one can apply to the data. The data, and the general supporting information, must be managed within a flexible framework that makes it readily available as and when it is required for any process. Information management is the topic of part H.

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