From graphical display to dynamic model: mathematical geology in the Earth sciences in the nineteenth and twentieth centuries

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Abstract: Graphical displays were used early in geophysics and crystallography, mineralogy, petrology and structural geology by the early 1800s, but nineteenth-century geology obstinately remained mainly descriptive. Charles Lyell's quantitative classification of the Tertiary Sub-Era in 1828 was a notable exception. Nevertheless, by 1920 the quantitative approach had become established. W. C. Krumbein, who introduced the computer into geology in 1958, encouraged use of probabilistic sampling and process-response models. Early work focused on databases, statistical data analysis and display. By the 1970s, stochastic simulation, deterministic modelling and spatial 'geostatistics' (pioneered by Matheron and his co-workers), were of growing importance. The introduction of the personal computer and the graphical user interface in the 1980s brought well-proven quantitative methods out of the research environment onto the workbench and into the field. Since the mid-1980s, the analysis, display and modelling of behaviour in three dimensions, underpinned by spatial statistics, computational fluid-flow, visualization technology, etc., has proved of economic benefit to mining, petroleum geology and hydrogeology. Other, computationally intensive, methods likely to be of importance in the Earth sciences are the application of 'robust' statistical methods, increasing use of Bayesian methods in uncertainty (risk) estimation (as a result of a renewed interest in statistical intervals and forecasting), and computational mineralogy.

Although the quantitative display and analysis of Earth science data can be traced back to the measurement of magnetic declination and inclination and, later, gravity (from pendulum observations) in the seventeenth and eighteenth centuries, the concern here is with the history of mathematical geology. This subject includes the application of mathematics, classical statistics and, since the late 1960s, spatial statistics, to assist the interpretation of geological data and the modelling of geological phenomena as an aid both to understanding, and to forecasting, in fields such as resource assessment, petroleum geology and hydrogeology. However, a vital part of all these techniques is the graphical display of either raw (or, in more recent times, perhaps smoothed) data values, to assist interpretation, or the presentation of the results of some modelling process.

The visual language inherent in such displays is now taken for granted to such an extent that it is difficult to imagine that even as late as the 1850s, there was a body of opinion among those in the then newly emerging science of statistics arguing against the 'inexactness' of graphical displays and that it was far preferable to record results solely in the form of tables (Funkhouser 1938, pp. 293, 295). Editors and publishers may have tacitly gone along with this view owing to the high cost of preparing the plates of illustrations.

The appearance of graphical displays of geological data and related thematic maps in publications gradually became more widespread during the last half of the nineteenth century (see Fig. 1), but because the history of this development is little-known today, it is touched on here in order to describe their role at the beginning of the use of quantitative methods in the geological sciences.

The emergence of statistical graphics

Isoline maps

The concept of a line of equal value (isoline or isopleth) as a cartographic tool has a long and complex history. Bathymetric maps of limited parts of rivers and harbours, such as that by the geologist Auguste Bravais (1811–1863) showing the topography of the underwater delta front formed by the river Aar, the third largest river in Switzerland, where it flows into Lake Brienz (in Martins 1844), are known from the sixteenth century onwards (Robinson 1982, p. 211). However, the first published topographic contour map was J. Dupain-Triel's (1722–1805) map of France (Dupain-Triel 1798–1799).

From: OLDROYD, D. R. (ed.) 2002. The Earth Inside and Out: Some Major Contributions to Geology in the Twentieth Century. Geological Society, London, Special Publications, **192**, 59–97. 0305-8719/02/\$15.00 © The Geological Society of London 2002.

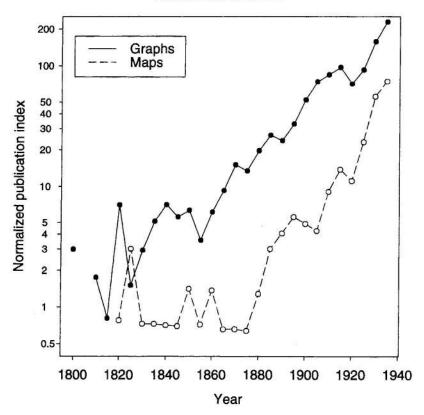


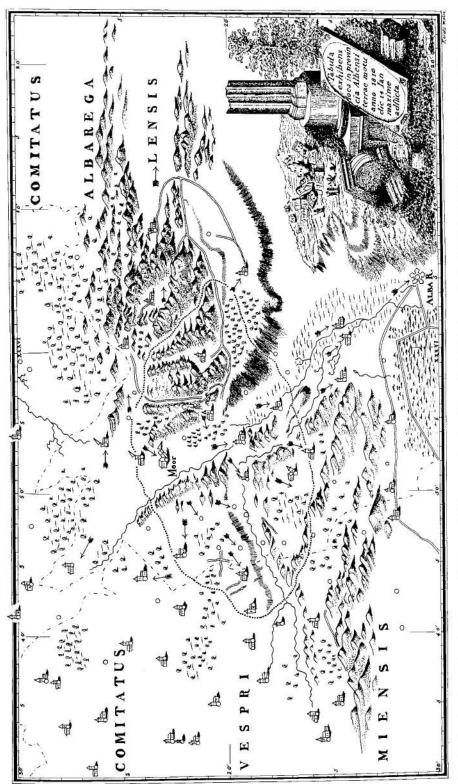
Fig. 1. Count of numbers of statistical graphs and thematic maps per five-year interval (1801–1805, 1806–1810, etc.) in articles on geological subjects in a total of 103 serial publications which existed during the period 1800–1935. Counts (totalling 1942 statistical graphs and 236 thematic maps) have been normalized by dividing through by values of Table 2 (in Appendix). Index is zero where no symbols are shown.

Edmond Halley's (1656–1742) chart of magnetic declination for the North Atlantic (Halley 1701) was the earliest map to show isolines of an observed non-topographic phenomenon, but with the failure of magnetic declination to provide the solution to determining longitude at sea, it had little lasting impact. It was the later publication of a map of temperature distribution for the northern hemisphere by the German explorer, naturalist and geologist Alexander von Humboldt (1769–1859) (1817a,b) which, on account of his scientific reputation, really excited interest in the thematic mapping of the values of relatively abstract phenomena.

Interest in delineation of the effects of earthquakes prompted some of the earliest isoline maps in the geological sciences. The earliest known map (Fig. 2) was drawn up by two Hungarian academics, Pál Kitaibel (1757–1817) and Ádám Tomtsányi (1755–1831), following an earthquake which occurred on 14 January 1810,

whose effects were felt as far away as Prague and Vienna. The map (Kitaibel & Tomtsanyi 1814, pl. ff., p. 110) includes a single, closed, isointensity curve which outlines the area of major damage surrounding the village of Mór, near Székesfehérvár in western Hungary. However, the earliest map to use a definite intensity scale, depicted by multiple isoseismal lines, was drawn by the German geographer and cartographer Auguste Petermann (1822-1878) (in Volger 1856) on the basis of information supplied by Georg H. O. Volger (fl. 1822-1897), a student of Swiss earthquakes. By 1862, in a map of the destruction following the Neapolitan earthquake of 16 December 1857, the Irish engineer and seismologist Robert Mallet (1810-1881) included proportional-sized symbols, to indicate intensity at particular localities, as well as isoseismal lines (Mallet 1862, map A, pp. 252-254).

The construction of structure contour maps, which show the subsurface depth to a given





stratigraphic horizon, began with the work of the American geologist Benjamin Lyman (1835–1920), in a report to the Public Works Department of the Indian government on the oil prospects of the Punjab (Lyman 1870). An example of one of his maps (reproduced in Owen 1975, fig. 4-2) shows 100 ft (30.5 m) structure contours on the top of the 'oil bearing bed' for an area of c. 230 m² of anticlinal folding surrounding an oil seep near Bara Katta, Bannu District, Punjab. Lyman apparently had tried the idea of using 'underground contour lines to give the shape of rock beds' while working on coal, lead and iron deposits in Virginia in 1866 and 1867 (Lyman 1873), but did not publish anything until his report on his work in the Punjab. In Europe, structure contour mapping was used by the geologist Albert De Lapparent (1839-1908) to delineate the top surface of the Gault Clay under the English Channel between Dover and Calais in a report (De Lapparent & Potier 1877) following the second submarine geological survey, conducted in 1875 and 1876, as part of a feasibility study for the first bored Channel Tunnel. In 1885, Gustave F. Dollfus (1850-1931) exhibited structure contour maps for the top of the Gault and Chalk (Fig. 3) in the region around Paris (Dollfus 1888). The earliest structure contour map to be published by the US Geological Survey was a regional map (Orton 1889, pl. LV) showing the top of the Trenton Limestone in western Ohio and eastern Indiana, made by the geologist Edward Orton (1829-1899). Towards the end of the nineteenth century, structure contour maps were regularly appearing in geological reports on coal fields, mineral deposits, and oil and gas fields, and were taken for granted by the time Emmons' (1921) textbook on petroleum geology was published.

By the 1850s, there was growing concern in improving the quality of water supply to cities. In England, the geologist Joseph Lucas (1846–1926) drew the earliest 'hydrogeological' map to show 'contours of the upper surface of water in the Chalk' in a privately published book (Lucas 1874, cited in Mather 1998). This was followed by an isoline map covering an area of c. 500 km² (Lucas 1877) for an area of the Chalk lying SE of London, and this eventually led to the publication of the earliest true hydrogeological maps in 1878 (Mather 1998). By the turn of the century, such maps were becoming relatively commonplace elsewhere (Linstow 1905; Veatch 1906).

Point-symbol maps

The idea of a map in which a specific symbol indicates the value of a mapped attribute at a

given location was current in structural geology by the 1820s, when Carl F. Naumann (1797-1873) used small, locality-specific, strikebar symbols in his mapping of gneisses in southern Norway (Naumann 1824, vol. 1, plate III, fig. 4). However, maps in which the area of a symbol at a locality is proportional to the value of a quantity only seem to have begun when British army officer, Henry Harness a (1804–1883), used proportional circles in a map of the population of Ireland which he drew up in 1837 (Robinson 1982, p. 205). The idea of proportional symbols was popularized in continental Europe by the work of Petermann and a French engineer Charles J. Minard (1781–1870) in the 1850s (Robinson 1982, p. 205). Minard (1862) also published the first memoir to be devoted to the graphic method. The American geologist James D. Dana (1813-1895) used strike-bar symbols in which the length of the 'stem of the T' was proportional to the amount of dip (Dana 1880), but this idea was largely ignored by others. Other examples of early maps to use point-symbols in the geological literature include mineral production in Russia (Keppen 1894) using proportional squares, and a regional map of heavy-mineral distribution in Quaternary sands of the Netherlands in which the intensity of constant-size circles was made proportional to concentration (Schroeder van der Kolk 1896). The latter style of presentation eventually became widely used in exploration geochemistry following the work of Webb et al. (1964).

Proportional line widths were rarely used until they were taken up in the 1950s to show element concentration in segments of stream drainage networks in reconnaissance geochemical-mapping applications (Webb 1958). An exception was a map in an early report on the lignites of Bohemia (Lallemand 1881) showing the volume of lignite transported by water and rail during the year 1879. The style of Lallemand's map was similar to that of maps of traffic flow independently produced by Harness in 1837, and by Minard in 1845 (Funkhouser 1938, p. 301). See Robinson (1982, p. 209) and Tufte (1983, pp. 25, 177) for other examples.

An isolated 'time-lapse' map occurs in Schmidt (1874) and shows the gradually increasing extent of lava flows around the volcanic isle of Santorini (Thíra), in the Aegean, north of Crete, during a series of eruptions which occurred between February 1866 and June 1870. In each of twelve panels, Schmidt showed the area occupied by a new flow (or flows) in red, contrasting with the greenish colour of the rest of the landmass. The series of maps clearly

FROM GRAPHICAL DISPLAY TO DYNAMIC MODEL

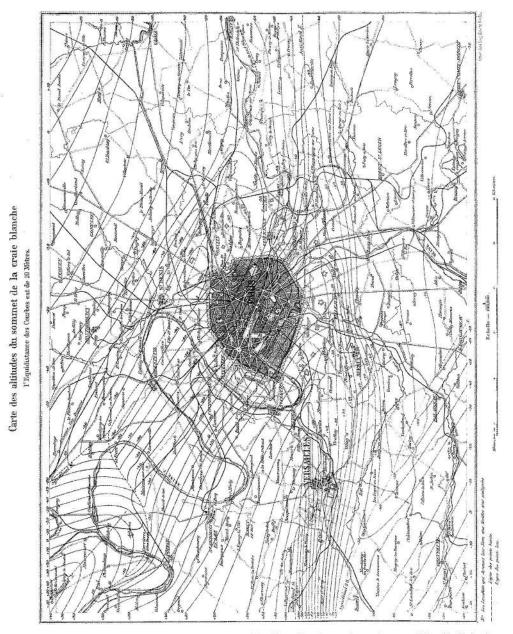


Fig. 3. Structure contours (solid lines, shown red in original) at 10 m intervals on the top of the Chalk in the region of Paris, France. Dashed and pecked lines mark axial lines of anticlines and synclines respectively. Reproduced from Dollfus (1888, unnumbered plate).

shows the emergence and gradual coalescence of flows from two separate vents.

Graphs

The earliest record of the commercial production of printed graph-paper occurs in 1686 (Gunther 1939). It was made by a London scientific instrument-maker, John Warner, in the year following Robert Plot's (1640–1696) ground-breaking publication (Plot 1685) in the *Philosophical Transactions of the Royal Society*, London, of a graph of daily barometric pressure. By the late eighteenth century, graphical displays had begun to come into their own, with the portrayal of experimental and non-meteorological scientific data pioneered by physicists such as Johann H. Lambert (1728–1777) (Lambert 1765); the introduction of line-graphs, bar-graphs and proportional-sized circles to illustrate econometric data by William Playfair (1759–1823) (Playfair 1798, 1801, 1805), younger brother of the Edinburgh mathematician, and Huttonian geologist, John Playfair (1748–1819); and the use of subdivided bar-graphs and proportional squares popularized by the work of Humboldt (1811–1812). Examples of W. Playfair's work are reproduced in Tufte (1983, pp. 32–34, 44, 64–65, 73, 91–92; 1990, p. 107).

Although William Playfair attributed his original interest in graphs to his brother, who had apparently taught him, when they were children, how to make a chart showing daily temperature variations (Funkhouser 1938, p. 289), J. Playfair's own graphical work (e.g. Playfair 1812, plate X, fig. 3) followed firmly in the style current in mathematical publications since the seventeenth century (e.g., Halley 1686) in resembling geometrical figures, without scales or axis annotation. They completely lacked the flair of his younger brother's work. Particularly surprising is the fact that, even in a publication on meteorology, J. Playfair (1805) exhibited his own data in tabular, rather than graphical, form. Funkhouser (1938, p. 289) has suggested that it may have been his younger brother's period of work (c. 1780) as an engineering draftsman for James Watt which helped to form his innovative graphic style. Possibly because he became a political exile in France (as a result of debts and his radical political views), W. Playfair's work was ignored in England but it inspired great interest in France and Germany. This eventually led to the appearance of a number of books devoted to the 'graphical method' between the years 1845 and 1854, and by 1890 graphs were regularly appearing in government publications and had become commonplace in most scientific meetings (Funkhouser 1938, pp. 300-330).

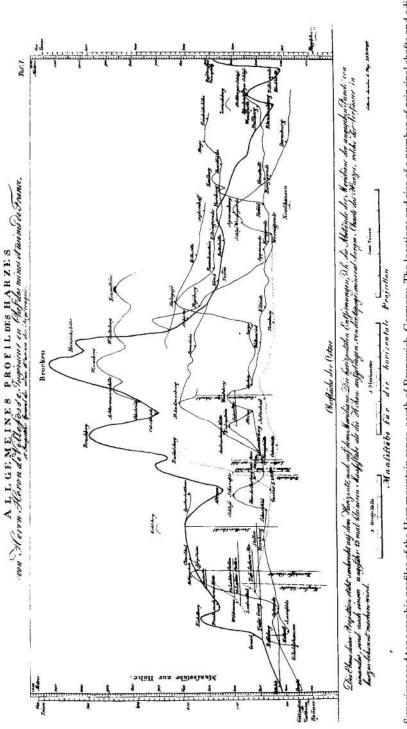
Line-graphs

From today's perspective, in which the bivariate scatter-plot (i.e. a graph in which a point corresponding to a particular sample or specimen is plotted on the basis of a grid of $\{x, y\}$ co-ordinates which lie at right angles to each other) is ubiquitous, it may come as a surprise to learn that the scatter-plot *per se* made a relatively late appearance in the geological literature. It was far more usual to have line-graphs, in which the *x*-axis corresponded to distance or (particularly in economic geology) time, the ordinate y-axis to the attribute in question, and the ordered data points (which usually were not distinguished individually) were joined by a continuous line. An early example (see Fig. 4), drawn by the French engineer and inspector of mines Antoine M. Héron de Villefosse (1774-1852), shows a series of overlaid topographic profiles across the Harz mountain range, south of Brunswick, Germany. The locations and size of a number of principal shafts and adits are also shown (Héron de Villefosse 1808). The British bookseller and geologist William Phillips (1775-1828) published schematized 'scenic views' showing comparative heights of mountains (Phillips 1815, frontispiece), but they became more popular following their use by Humboldt (1825, 1855). This form of illustration became a standard feature of geographical atlases following their incorporation in the magnificent Physical Atlas of Natural Phenomena (Johnson & Johnson 1856, plates 2, 9, 11).

Line-graphs also were used by investigators with an interest in hydrology. Examples include a graphical time-series of water levels in the Nile (Girard 1819) drawn by the French engineer Pierre Girard (1765–1836) from observations made when he accompanied Napoleon III's expedition to Egypt. Girard's fellow-countryman, the engineer Benjamin Dausse (1801-1890), drew an elegant composite diagram (Fig. 5) to show the mean height of the River Seine in Paris per month during the period from 1777 until 1836 together with frequency distributions of the water level per month for the same period (reproduced in Élie de Beaumont 1849, plate III, fig. 2).

An early example from mineralogy comes from the work of the British mathematician, physicist and astronomer Sir John F. W. Herschel (1792-1871) who drew a set of graphs to illustrate the absorption of polarized light as a function of wavelength in crystals of the mineral apophyllite (Herschel 1822). Herschel's graphs were drawn in the classical 'mathematical' style and consequently lacked axes, but by the time the French structural geologist, petrologist and mineralogist, Auguste Michel Lévy (1844-1911), published a review paper on the optical determination of minerals in thin section (Michel Lévy 1877), his graphs (Michel Lévy 1877, plates VIII, IX) at least had scaled axes, and their annotation was improved further in Michel Lévy & Lacroix's (1888) textbook.

By the late 1800s, the systematic study of igneous geochemistry was giving rise to the first 'variation diagrams' in which major element oxide compositions (typically Al_2O_3 , FeO,





RICHARD J. HOWARTH

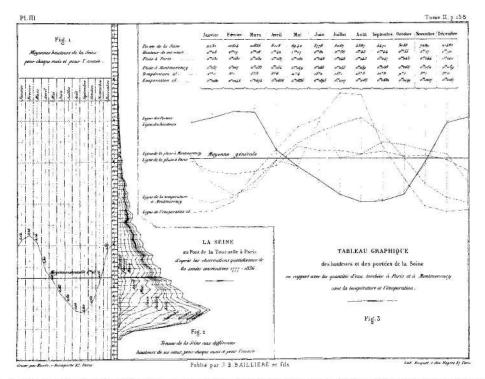


Fig. 5. Line-graphs showing: 'Fig. 1' mean monthly height (m) for the years 1777 to 1836 of the River Seine at the Tournelle Bridge, Paris, France; 'Fig. 2' superimposed frequency distributions for river height (m) per month from 1777 to 1836; 'Fig. 3' a graph and table ('graphic table') of the span and height (m) of water in the Seine, depth of rain fallen in Paris (m) and depth of rain, temperature and evaporation at Montmorency (c. 15 km north of the centre of Paris). Reproduced from drawings by Benjamin Dausse in: Élie de Beaumont (1849, plate III).

Fe₂O₃, CaO, MgO, K₂O and Na₂O) were plotted as line-graphs, as a function of increasing SiO₂ concentration, in the same diagram. In early examples of this type of plot, the increasing SiO₂ was shown implicitly (by appropriate ordering of the rock-types), as in the work of the Austrian igneous petrologist Eduard Reyer (1849–1914) (Reyer 1877, plates I, II); or explicitly, by a labelled axis, as was the situation in the work (Iddings 1892) of the American geologist and igneous petrologist Joseph P. Iddings (1857–1920).

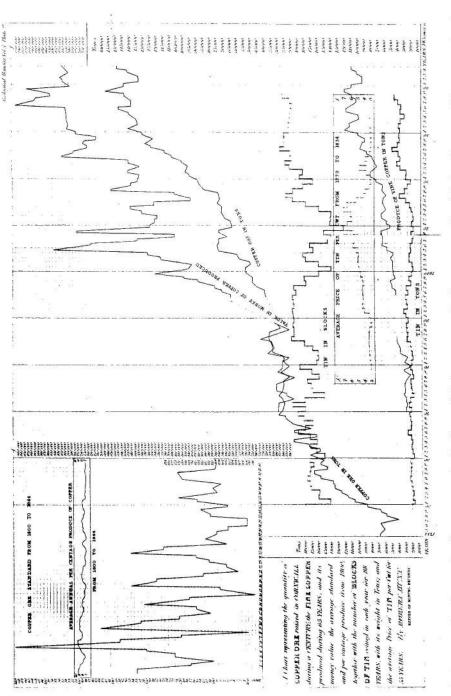
The British surgeon and vertebrate paleontologist, George Busk (1807–1886), also used multiple-line plots, which he termed 'odontograms,' to assist the classification of vertebrate remains on the basis of their dentition: the measured characteristics of each tooth were plotted as a function of tooth position in the jaw (Busk 1870). He later used this method to illustrate his identification of teeth found in Brixham Cave, Torquay, Devon, as Ursus priscus (in Prestwich et al. 1873, pp. 540–548). Two-dimensional polar co-ordinates were occasionally used in the early literature, e.g. mineralogical applications by the French physicist Jean B. Biot (1774–1862) (Biot 1817) and the British chemist William Ramsay (1852–1916) (Ramsay 1888), but the majority of such plots were related to orientation statistics.

With the opening up of gold mines in the Transvaal, South Africa, by the 1890s, keen attention was being paid to the problems of sampling such a rare and irregularly dispersed oremineral and line-graphs began to be used (De Launay 1896; Wybergh 1897) to illustrate the variations in ore-grade along sampling traverses as a guide to improved exploitation.

Rather surprisingly, econometric time-series formed the majority of line-graphs published in the early geological literature, illustrating timetrends of production for the commodity in question. Notable early examples include graphs showing the annual production of copper and tin from mines in Cornwall, England, from 1744 to 1845 (Fig. 6) (Hunt 1846); of silver in the

average standard and per centage produce from 1800; together with the number of blocks of tin coined in each year for 88 years; with its weight in toms; and the Fig. 6. 'A chart representing the quantity of copper ore raised in Cornwall during a century: the fine copper produced during 65 years; and its money value the average price of tin per cwt. for 55 years', reproduced from Hunt (1846, plate 9).





Frieberg mining-district, Germany, from 1524 to 1847 (Herder & Gäßfchmann 1849); of coal in northern England from 1821 to 1888, together with the price at Manchester, miners' wages and the number of accidents, and the total number of employees (Knowles 1890); and the production of crude oil from 1859 to 1893 in states of Pennsylvania and New York, and the total United States, together with the price of production (Cadell 1898).

One curious, rather later, example is a paper (Bailly 1905) in which an attempt was made to predict the time-span of future production of sedimentary iron-ore from Luxembourg, France and Germany. In each instance, an exponential growth-curve was fitted to the production rate from 1853 to 1905 in order to predict the year of expected maximum production and, using an estimate of the total reserves, an exponential decline-curve then was applied to obtain the expected production life. Bailly's model predicted that ore supplies would be exhausted in Luxembourg by 1943, Germany by 1953, and France by 2023. His predictions were reprinted in the Zeitschrift für praktische Geologie together with an assessment which concluded (Anon. 1910) that the sedimentary iron-ore supplies of Germany, Luxembourg and Italy would be exhausted within 30 years, whereas those of Russia, Sweden and France had expectations of 75, 100 and 700 years, respectively. It would be interesting to know whether this publication helped to influence opinion in pre-war Germany regarding the necessity to obtain additional (external) sources of ore-supply.

Time-series also began to be used in hydrogeology, where plots of groundwater level as a function of time proved to be a useful monitoring tool (Keilhak 1913).

Scatter-plots

Prior to 1900, bivariate 'scatter-plots' (which are sometimes referred to as 'cross-plots') were unusual in Earth science literature. Early examples in non-geophysical publications include a graph by Mallet (1873) showing the increase in volume of slags as a function of temperature. The French mineralogist Julien Thoulet (fl. 1843-1922) plotted laboratory experimental data on sedimentation rates (see Fig. 7) (Thoulet 1891, plate I); and both Michel Lévy (1897a,b) and Iddings (1898a,b) began to use the scatter-plot as an interpretational tool in igneous geochemistry. Although the scatter-plot was subsequently used particularly widely in geochemical applications, in the 1920s it also began to be taken up (together with line-graphs)

by palaeontologists as an aid to morphometric distinction between species (e.g. Swinnerton 1921; Arkell 1926; Davies & Trueman 1927).

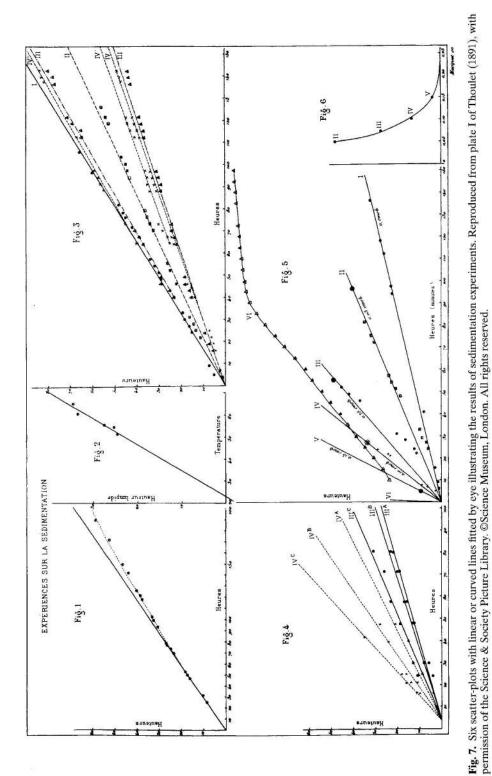
Ternary and tetrahedral diagrams

The earliest ternary diagrams (in which composition, in terms of three components, is represented by their relative proportions plotted on the basis of a triangular grid) made their first appearance in papers by Michel Lévy (1897a,b)and the German mineralogist, Carl Osann (1859-1923) (Osann 1900). The origins and usage of the ternary diagram are more fully discussed by Howarth (1996) and Sabine & Howarth (1998). Tetrahedrons were also widely used in mineralogy and geochemistry to display the relationships between four variables, following their introduction by the German geologist and mineralogist, Hellmut von Philipsborn (1928). A similar idea was later used by the American sedimentologist and mathematical geologist, William ('Bill') C. Krumbein (1902-1979), for the classification of sedimentary lithofacies for mapping purposes, e.g. based on the relative thicknesses of limestone, sandstone, shale and evaporite at different localities in the same formation (Krumbein 1954a).

From time-line to bar-chart

Funkhouser (1938, pp. 279–280) attributes W. Playfair's invention of the comparative device of the bar-chart to his awareness of the time-line, a graphical device introduced in 1765 by the British chemist Joseph Priestley (1733–1804), in which the length of an individual's life is shown by a line drawn parallel to the time-axis of a graph, beginning and ending at the years of birth and death of the subject. Exactly the same style applies to the simplest form of a taxonomic range-chart, as used by the British naturalist Samuel Woodward (1821–1865) (Woodward 1854, pp. 414–415) and the geologist Hugh Miller (1802–1856) (Miller 1857, p. 8).

It was the British geologist, Sir Charles Lyell (1797–1875) who, in the third volume of the first edition of his *Principles of Geology* (Lyell 1830–1833) was the earliest to use a 'statistical' count of the relative abundances of extant and extinct species to distinguish between the Eocene, Miocene and Pliocene Series of the Tertiary Sub-Era (see Rudwick (1978) for further discussion of Lyell's approach), but he presented his results simply as tables. The French geologist Joachim Barrande (1799–1883) later used proportional-width lines to indicate the relative abundance of different genera of trilobites in



each stratigraphic division of the Silurian Period rocks of Bohemia (Barrande 1852). Many authors subsequently adopted the inclusion of frequency information in taxonomic range charts. By the 1920s, this form of presentation was regularly used to illustrate micropalaeontological or micropalynological results in the form of range-charts for the purposes of biostratigraphic correlation (Goudkoff 1926; Driver 1928; Wray *et al.* 1931). The idea of the time-line also became enshrined in petrology in the form of the mineral paragenesis diagram, first introduced by the Austrian mineralogist Gustav Tschermak (1836–1927) to illustrate the evolution of granites (Tschermak 1863).

In addition to tabular summaries, in his book Life on the Earth Phillips (1860, p. 63) used proportional-length bars and proportional-width time-lines (Phillips 1860, p. 80), to illustrate the change in composition of 'marine invertebrata' throughout the 'Lower Palaeozoic' of England and Wales. In the frontispiece to the book, he also showed the relative proportions of eight classes of 'marine invertebral life' in each Period of the Phanerozoic, as constant-length bars subdivided according to the relative proportions of each class (see Fig. 8). A similar presentation was used subsequently by Reyer (1888, p. 215) to compare the major-element oxide compositions of suites of igneous rocks. Proportional-length rectangles (Greenleaf 1896), squares (Ahlburg 1907) and bars (Umpleby 1917) were occasionally used, particularly in publications related to economic geology. In an early paper on stratigraphic correlation using heavy minerals, the German petroleum geologist, Hubert Becker (b. 1903) used a range-chart with proportionallength bars to illustrate progressive stratigraphic change in the mineral suite (Becker 1931), but the 'graphic log', based on the proportions of different lithologies in the well-cuttings and drawn as a multiple line-graph, had already been introduced by the American petroleum geologist Earl A. Trager (1920).

Pie diagrams

The division of a circle into proportional-arc sectors to form a 'pie diagram' dates back to the work of W. Playfair (1801) and was used as a cartographic symbol by Minard in 1859 (see Robinson 1982, p. 207). However, apart from occasional applications comparing the composition of fresh with altered rock as a result of mineralization (Lacroix 1899; Leith 1907) or the relative production of metals or coal (Anon. 1907; Butler *et al.* 1920), it was little used by geologists.

Multivariate symbols

Between 1897 and 1909, there was a short-lived enthusiasm for comparison of the majorelement composition of igneous rocks using a variety of symbols based mainly on graphic styles which resemble the modern 'star plot' in which the length of each arm is proportional to the amount of each component present in a sample (Fig. 9). The earliest of these was devised by Michel Lévy (1897a) but it was Iddings (1903, 1909, pp. 8-22, plates 1, 2) who was a determined advocate for this type of presentation (and for the use of graphical methods in igneous petrology in general). However, the tedium of multivariate symbol construction by hand ultimately prevented the widespread take-up of these methods. For example, although their use was advocated in a 1926 article 'Calculations in petrology: a study for students' by the American geologist Frank F. Grout (b. 1880), they were not mentioned in the influential textbook Petrographic Methods and Calculations by the British geologist Arthur Holmes (1890-1965), published in 1921 (in which he restricted his discussion to variation and ternary diagrams) Similar multivariate graphical techniques, such as the well-known Stiff (1951) diagram for water composition, were later introduced for comparison of hydrogeochemical data. (For further information, see Howarth (1998) on igneous and metamorphic petrology, and Zaporozec (1972) on hydrogeochemistry.) However, the usage of multivariate symbols did not really revive until it was eased by computer graphics in the 1960s. Figure 10 summarizes the relative frequency of all types of statistical graphs and maps from 1750 to 1935, based on a systematic scan of 116 geological serial publications, plus book collections. Apart from crystallographic applications (which were often undertaken by physicists or other non-geologists), major growth in usage and graphic innovation essentially began in the 1890s.

The rise of statistical thinking

The time-series describing commodity production in economic geology, discussed previously, typify the nineteenth century view of 'statistics' as 'a collection of numerical facts'. Lyell's subdivision of the Tertiary Sub-Era on the basis of faunal counts in 1829 (Lyell 1830–1833) conformed to this somewhat simplistic view, although it is believed that he hoped to verify a general method, a '*statistical* paleontology' (Rudwick 1978, p. 236), which he could apply to earlier parts of the succession. The rapidly

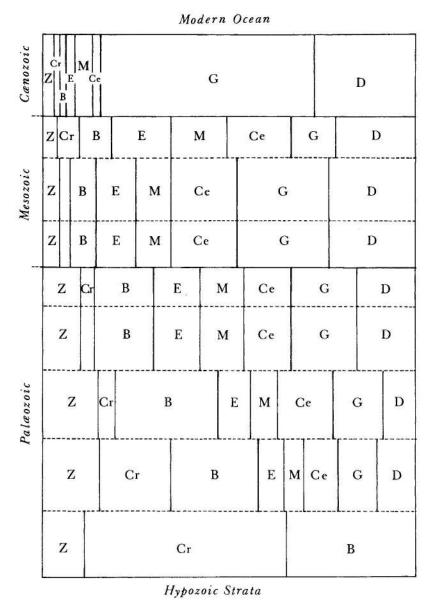


Fig. 8. Divided bar-chart showing 'successive systems of marine invertebral life': Z, Zoophyta; Cr, Crustacea; B, Brachiopoda; E, Echinodermata; M, Monomysaria; Ce, Cephalopoda; G, Gasteropoda; and D, Dimyaria. Redrawn from Phillips (1860, frontispiece).

growing body of mathematical publications on the 'theory of errors' and the method of 'least squares' published in the wake of the pioneering work of the mathematicians Adrien M. Legendre (1752–1833) in 1805 and Carl F. Gauss (1777–1855) in 1809, had little appeal outside the circle of mathematicians and astronomers involved in its development. However, the Belgian astronomer and statistician, Adolphe Quetelet (1796–1874) wrote, in a more approachable manner, on the normal distribution and used statistical maps, in his writings on the 'social statistics' of population, definition of the characteristics of the 'average man,' and

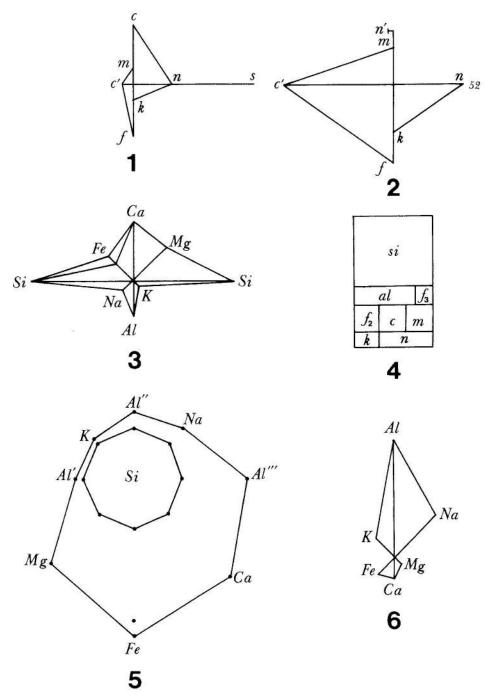
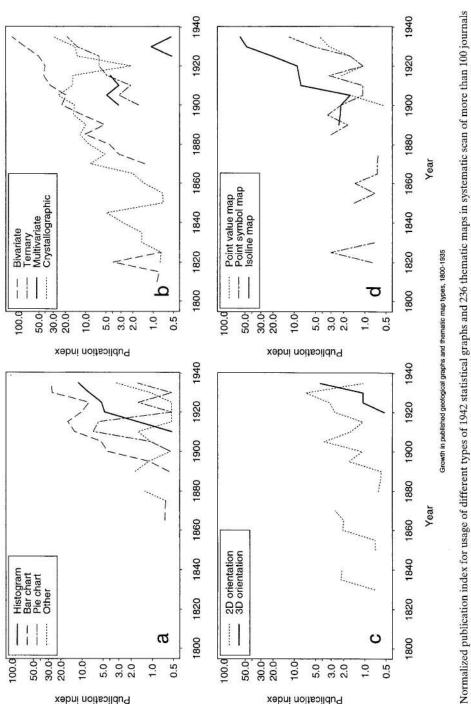


Fig. 9. Different styles of multivariate graphics used to illustrate major element sample composition: 1, Michel Lévy (1897b); 2, Michel Lévy (1897a); 3, Brøgger (1898); 4, Loewinson-Lessing (1899); 5, Mügge (1900); 6, Iddings (1903). Reproduced from fig. 5 of Howarth, R. J. 1998. Graphical methods in mineralogy and igneous petrology (1800–1935). *In*: Fritscher, B. & Henderson, F. (eds) *Toward a History of Mineralogy, Petrology, and Geochemistry. Proceedings of the International Symposium on the History of Mineralogy, Petrology, and Geochemistry, Munich, March 8–9, 1996*, pp. 281–307, with permission of the Institut für Geschichte der Naturwissenschaften der Universität München. All rights reserved.





the statistics of crime (Quetelet 1827, 1836, 1869). As a result, Quetelet's work proved to be enormously influential, and raised widespread interest in the use of both frequency distributions and statistical maps.

In geology, this interest soon manifested itself in the earthquake catalogues of the Belgian scientist Alexis Perrey (1807-1822), who followed Quetelet's advice (Perrey 1845, p. 110) and from 1845 onwards used line-graphs (drawn in exactly the same style as used by Quetelet in his own work) in his earthquake catalogues to illustrate the monthly frequency and direction of earthquake shocks. Other early examples of earthquake frequency polygons occur in Volger (1856). The use of maps showing the frequency of earthquake shocks occurring in a given timeperiod for different parts of a region was pioneered by the British seismologist John Milne (1850–1913) and his colleagues in Japan (Milne 1882; Sekiya 1887).

In structural geology, attempts to represent two-dimensional directional orientation distributions began in the 1830s, although use of an explicit frequency distribution based on circular co-ordinates only became widespread following the work (Haughton 1864) of the Irish geologist Samuel Haughton (1821-1897). The more specialized study of the three-dimensional orientation distributions did not begin until the 1920s with the work of the Austrian mineralogist Walter Schmidt (1885-1945) and his colleague, the geologist Bruno Sander (1884-1979) who began petrofabric studies of metamorphic rocks. Their work introduced use of the Lambert equal-area projection of the sphere to plot both individual orientation data and isoline plots of point-density. A simpler method of representation, using polar co-ordinate paper, was introduced by Krumbein (1939) to plot the results of three-dimensional fabric analyses of clasts in sedimentary rocks, such as tills. (See Howarth (1999) and Pollard (2000) for further discussion of aspects of the history of structural geology.)

Some early enthusiastic efforts to apply the properties of Quetelet's 'binomial curve' (his approximation of the normal distribution using a large-sample binomial distribution) were misdirected, for example Tylor's (1868, p. 395) attempt to match hill-profiles to its shape. Nevertheless, by the turn of the century, Thomas C. Chamberlin (1843–1928) in America was advocating the use of 'multiple working hypotheses' when attempting to explain complex geological phenomena (Chamberlin 1897) and Henry Sorby (1826–1908) in England was demonstrating the utility of quantitative methods (including model experiments) to gaining a better understanding of sedimentation processes (Sorby 1908).

Nevertheless, statistical applications tended to remain mainly descriptive, characterized by the increasing use of frequency distributions. Examples include morphometric applications in palaeontology (Cumins 1902; Alkins 1920) and igneous petrology (Harker 1909; Robinson 1916; Richardson & Sneesby 1922; Richardson 1923). However, it was the British mineralogist and petrologist William A. Richardson who first made real use of the theoretical properties of the normal distribution. Using the 'method of moments' (Pearson 1893, 1894), which had been developed by the British statistician Karl Pearson (1857-1936), Richardson (1923) successfully resolved the bimodal frequency distribution of SiO₂ wt% in 5159 igneous rocks into two, normally distributed, acid and basic subpopulations and was able to demonstrate their significance in the genesis of igneous rocks.

Another area in which frequency distributions soon grew to play an essential role was in sedimentological applications. Systematic investigation of size-distributions using elutriation and mechanical analysis developed in the second half of the nineteenth century (Krumbein 1932). A grade-scale, based on sieves with mesh sizes increasing in powers of two, was introduced in America by Johan A. Udden (1859–1932) in 1898 (see also Udden 1914; Hansen 1985) and was modified subsequently by Chester K. Wentworth (b. 1891) to the size-grade divisions 1/1024, 1/512, 1/256, ..., 8, 16, 32 mm (Wentworth 1922). Cumulative size-grade curves began to be used in the 1920s (Baker 1920), and both Wentworth and Parker D. Trask (b. 1899) tried to use statistical measures, such as quartiles, to describe their attributes (Wentworth 1929, 1931; Trask 1932).

Krumbein had acquired statistical training while gaining his first degree in business management, before turning to geology. This led to his interest in quantifying the degree of uncertainty inherent in sedimentological measurement (Krumbein 1934) and enabled him to demonstrate, using normal probability plots (Krumbein 1938), the broadly lognormal nature of the size distributions and that statistical parameters were therefore best calculated following logtransformation of the sizes. This led to the introduction of the 'phi scale' (given by base-2 logarithms of the size-grades) which eliminated the problems caused by the unequal class intervals in the metric scale. Parameters based on moment measures were eventually augmented by Inman's (1952) introduction of graphical analogues, such as the phi skewness measure.

It soon became apparent that a manual of laboratory methods concerned with all aspects of the size, shape and compositional analysis of sediments was needed. Krumbein collaborated with his former PhD supervisor at the University of Chicago, Francis J. Pettijohn (1904–1999), to produce the Manual of Sedimentary Petrography (Krumbein & Pettijohn 1938). In this text, Krumbein described the chi-squared goodnessof-fit test for the similarity of two distributions (Pearson 1900; Fisher 1925), which had been recently introduced into the geological literature (Eisenhart 1935) by the American statistician Churchill Eisenhart (1913-1994). However, although Krumbein discussed the computation of Pearson's (1896) linear correlation coefficient, he rather surprisingly made no mention of fitting even linear functions to data using regression analysis, treating the matter entirely in graphical terms (Krumbein & Pettijohn 1938, pp. 205-211).

The use of bivariate regression analysis in geology began in the 1920s, in palaeontology (Alkins 1920; Stuart 1927; Brinkmann 1929; Waddington 1929), and in geochemistry (Eriksson 1929). The use of other statistical methods was also becoming more widespread, championed, for example, during the 1930s by Krumbein in the United States, and in the 1940s by the British sedimentologist Percival Allen (b. 1917), and by Andrei Vistelius (1915-1995) in Russia (Allen 1944; Vistelius 1944; see also selected collected papers (1946-1965) in Vistelius 1967). The foundations of multivariate statistical methods, such as multiple regression analysis and discriminant function analysis (used to assign an unknown specimen on the basis of its measured characteristics to one of two, or more, pre-defined populations), had been laid previously by the British statistician Sir Ronald Aylmer Fisher (1890-1962, Kt., 1952) (Fisher 1922, 1925, 1936). Although these techniques began to make an appearance in geological applications (Leitch 1940; Burma 1949; Vistelius 1950; Emery & Griffiths 1954), with the odd exception - Vistelius apparently carried out a factor analysis by hand in 1948 (Dvali et al. 1970, p. 3) – their use was restricted by the tedious nature of the hand-calculations. For example, Vistelius recalls undertaking Monte Carlo (probabilistic) modelling of sulphate deposition in a sedimentary carbonate sequence by hand in 1949, a process (described in Vistelius 1967, p. 78) which 'required several months of tedious work' (Vistelius 1967, p. 34). In the main, geological application of more computationally demanding statistical methods had to await the arrival of the computer.

The roots of mathematical modelling

As Merriam (1981) has noted, mathematicians and physicists have a history of early involvement in the development of theories to explain Earth science phenomena and have underpinned the emergence of geometrical and physical crystallography (Lima-de-Faria 1990). Although in many instances their primary focus was on geophysics, geological phenomena were not excluded from consideration. For example, Italian mathematician the Paolo Frisi (1728–1784) made an early quantitative study of stream transport (Frisi 1762). In the nineteenth century, J. Playfair (1812) applied mathematical modelling to questions such as the thermal regime in the body of the Earth, but he also calculated the vector mean of dip directions measured in the field (Playfair 1802, fn., pp. 236–237); the British mathematician and geologist William Hopkins (1793-1866), who had Stokes, Kelvin, Maxwell, Galton and Todhunter as his Cambridge mathematical tutees, developed mathematical theories to explain the presence and orientation of 'systems of fissures' and ore-veins (Hopkins 1838), glacier motion and the transport of erratic rocks (Hopkins 1845, 1849a), the nature of slaty cleavage (Hopkins 1849b); and the British geophysicist the Reverend Osmond Fisher (1817-1914) provided mathematical reasoning to explain volcanic phenomena in his textbook Physics of the Earth's Crust as well as discussion of the nature of the Earth's interior (Fisher 1881).

As the use of chemical analysis of igneous and metamorphic rocks increased, petrochemical calculations began to be used both to assist the classification of rocks on the basis of their chemical composition and to understand their genesis. This type of study essentially began with the 'CIPW' norm (named after the authors Cross, Iddings, Pirsson and Washington, 1902, 1912) which was used to re-express the chemical composition of an igneous rock in terms of standard 'normative' mineral molecules instead of the major-element oxides.

Another area in which quantitative numerical methods were becoming increasingly important was hydrogeology. Hydrogeological applications in Britain date back to the work of William Smith at the beginning of the nineteenth century (Biswas 1970). Following experiments carried out in 1855 and 1856, the French engineer Henry Darcy (1803–1858) discovered the relationship which now has his name (Darcy 1856, pp. 590–594). He concluded that 'for identical sands, one can assume that the discharge is directly proportional to the [hydraulic] head and inversely proportional to the thickness of the layer traversed' (quoted in Freeze 1994, p. 24). Although Darcy used a physical rather than a mathematical model to determine his law (measuring flow through a sand-filled tube), this can be regarded as the earliest groundwater model study. Thirty years later, Chamberlin (1885) published his classic investigation of artesian flow, which marked the beginning of groundwater hydrology in the United States. The first memoir of the British Geological Survey on underground water supply was published soon afterwards (Whittaker & Reid 1899).

Following the appointment of the American hydrogeologist Oscar E. Meinzer (1876-1948) as chief of the groundwater division of the United States Geological Survey in 1912, quantitative methods to describe the storage and transmission characteristics of aquifers advanced considerably. Meinzer himself laid the foundations with publication of his PhD dissertation as a US Geological Survey water supply paper (Meinzer 1923). Early applications had to make do with steady-state theory for groundwater flow, which only applies after wells have been pumped for a long time. Charles V. Theis (1900-1987) then derived an equation to describe unsteady-state flow conditions (Theis 1935) using an analogy with heatflow in solids. This enabled the 'formation constants' of an aquifer to be determined from the results of pumping tests. His achievement has been described as 'the greatest single contribution to the science of groundwater hydraulics in this century' (Moore & Hanshaw 1987, pp. 317). Theis (1940) then explained the mechanisms controlling the cone of depression which develops as water is pumped from a well. His work enabled hydrologists to predict well vield and to determine their effects in time and space.

That same year, M. King Hubbert (1903–1989) discussed groundwater flow in the context of petroleum geology (Hubbert 1940). By the 1950s, physical models used a porous medium such as sand (as had Darcy in the 1850s), or stretched membranes, to mimic piezometric surfaces, and analytical solutions were being applied to two-dimensional steady-state flow in a homogeneous flow system However, these analytical methods proved inadequate to solve complex transport problems. The possibility of using electrical analogue models (based on resistor-capacitor networks) in transient-flow problems was investigated first by H. E. Skibitzke and G. M. Robinson at the US Geological Survey in 1954 (Moore & Hanshaw 1987, p. 318). Their work eventually led to the establishment of an analogue-model laboratory at Phoenix, Arizona, in 1960 (Walton & Prickett 1963; Moore & Wood 1965) and more than 100 different models were run by 1975 (Moore & Hanshaw 1987). The use of graphical displays in hydrogeology is discussed in detail in Zaporozec (1972).

The arrival of the digital computer

By the early 1950s, in the United States and Britain, digital computers had begun to emerge from wartime military usage and to be employed in major industries such as petroleum, and in the universities. At first, these computers had to be painstakingly programmed in a low-level machine language. Consequently, it must have come as a considerable relief to users when International Business Machines' Mathematical FORmula TRANslating system (the FORTRAN programming language) was first released in 1957, for the IBM 704 computer (Knuth & Pardo 1980), as FORTRAN had been designed to facilitate programming for scientific applications. Computer facilities did not become available to geologists in Russia until the early 1960s (Vistelius 1967, pp. 29-40), and in China until the 1970s (Liu & Li 1983).

The earliest publication to use results obtained from a digital computer application in the Earth sciences is believed to be Steven Simpson Jr's program for the WHIRLWIND I computer at the Massachusetts Institute of Technology, Cambridge, Massachusetts. His program was essentially a multivariate polynomial regression in which the spatial co-ordinates, and their powers and cross-products, were used as the predictors to fit second- to fourth-order non-orthogonal polynomials to residual gravity data. This type of application later became known as 'trend-surface analysis' (Krumbein 1956; Miller 1956). Simpson presented his results in the form of isoline maps, which had to be contoured by hand on the basis of a 'grid' of values printed out on a large sheet of paper by the computer's Flexowriter (Simpson 1954, fig. 8). However, Simpson also used the computer's oscilloscope display to produce a 'density plot' in which a variable-density dot-matrix provided a greyscale image showing the topography of the surface formed by the computed regression residuals. This display was then photographed to provide the final 'map' (Simpson 1954, fig. 9).

Nevertheless, it was Krumbein who mainly pioneered the application of the computer in geological applications. Following a short period after World War II working in a research group at the Gulf Oil Company, he developed a strong interest in quantitative lithofacies mapping (Pettijohn 1984, p. 176), the data being mainly derived from well-logs (Krumbein 1952, 1954*a*, 1956). This interest soon led Krumbein and the stratigrapher Lawrence L. Sloss (1913–1996), based at Northwestern University (Evanston, Illinois), to write a machine-language program for the IBM 650 computer to compute clastic and sand-shale ratios in a succession based on the thicknesses of three or four designated endmembers. A flowchart and program listings are given in Krumbein & Sloss (1958, fig. 8, tables 2, 3). The data were both input and output via punched cards, the final ratios being obtained from a listing of the output card deck.

Krumbein was interested in being able to differentiate quantitatively between large-scale systematic regional trends and essentially nonsystematic local effects, in order to enhance the rigour of the interpretation of facies, isopachous and structural maps. This led him, in 1957, to write a machine-language program for the IBM 650 to fit trend-surfaces (Whitten *et al.* 1965, iii). It was not long before the release of the FORTRAN II programming language made such tasks easier.

In 1963, two British geologists who had emigrated to the United States, Donald B. McIntyre (b. 1923) at Pomona College, Claremont, California, and E. H. Timothy Whitten (b. 1927), who was working with Krumbein at Northwestern University, both published trend-surface programs programmed in FORTRAN (Whitten 1963; McIntyre 1963a) and in Russia, Vistelius was also using computer-calculated trend-surfaces in a study of the regional distribution of heavy minerals (Vistelius & Yanovskaya 1963; Vistelius & Romanova 1964).

More routine calculations, such as sediment size-grade parameters (Creager *et al.* 1962), geochemical norms (McIntyre 1963b) and the statistical calibrations which underpinned the adaptation of new analytical techniques, such as X-ray fluorescence analysis (Leake *et al.* 1970), to geochemical laboratory usage, were all greatly facilitated.

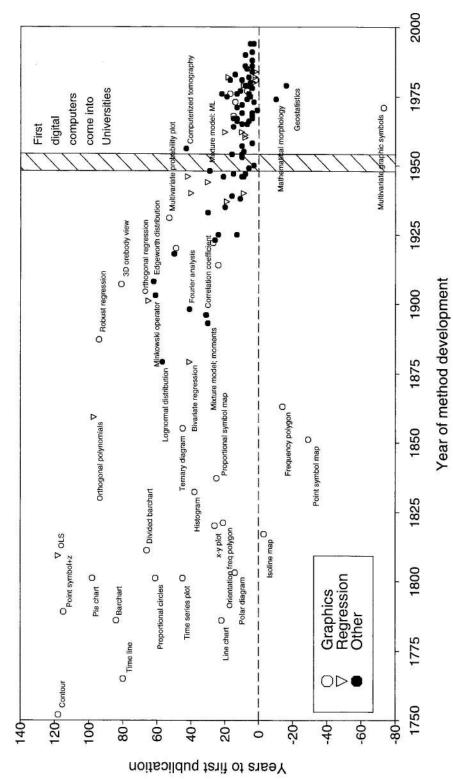
However, it was the rapid development of algorithms enabling the implementation of complex statistical and numerical techniques which perhaps made the most impression on the geological community, as they demonstrated in an unmistakable manner that computers could enable them to apply methods which had hitherto seemed impractical. Examples of early computer-based statistical applications in the west included the following.

(i) The use of stepwise multiple regression (Efroymson 1960) to determine the optimum number of predictors required to form an effective prediction equation (Miesch & Connor 1968).

- (ii) The methods of principal components and factor analysis (Spearman 1904; Thurstone 1931; Catell 1952) which were developed to compress the information inherent in a large number of variables into a smaller number which are linear functions of the original set, in order to aid interpretation of the behaviour of the multivariate data and to enable its more efficient representation. The concept was extended, by the American geologist John Imbrie (b. 1925), to represent the compositions of a large number of samples in terms of a smaller number of end-members (Imbrie & Purdy 1962; Imbrie 1963; Imbrie & van Andel 1964; McCammon 1966) and proved to be a useful interpretational tool.
- (iii) Hierarchical cluster-analysis methods, originally developed to aid numerical taxonomists (Sokal & Sneath 1963), proved extremely helpful in grouping samples on the basis of their petrographical or chemical composition (Bonham-Carter 1965; Valentine & Peddicord 1967).
- (iv) Application of the Fast Fourier Transform (FFT; Cooley & Tukey 1965; Gentleman & Sande 1966) to filtering time series and spatial data (Robinson 1969).

Figure 11 shows the approximate time of the earliest publication in the Earth sciences of a wide range of statistical graphics and other statistical methods imported from work outside the Earth sciences (as well as the relatively few examples known to the author in which the geological community seem to have been the first to have developed a method). Note the sharp decrease in the time-lag after the introduction of computers into the universities at the end of World War II, presumably as a result of improved ease of implementation and increasingly rapid information exchange as a result of an exponentially increasing number of serial publications.

In the early years, the dissemination of computer applications in the Earth sciences was immensely helped by the work of the geologist Daniel Merriam (b. 1927), at the Kansas Geological Survey, later assisted by John Davis (b. 1938), through the dissemination of computer programs and other publications on mathematical geology. These initially appeared as occasional issues of the Special Distribution Publications of the Survey, and then as the Kansas Geological Survey Computer Contributions series, which ran to 50 issues between





1966 and 1970. By the end of 1967, Computer Contributions were being distributed, virtually free, to workers across the United States and in 30 foreign countries (Merriam 1999). The Kansas Geological Survey sponsored eight colloquia on mathematical geology between 1966 and 1970.

The International Association for Mathematical Geology (IAMG) was founded in 1968 at the International Geological Congress in Prague, brought to an abrupt end by the chaos of the Warsaw Pact occupation of Czechoslovakia. Syracuse University and the IAMG then sponsored annual meetings ('Geochautauquas') from 1972 to 1997 and Merriam became the first editor-in-chief for the two key journals in the field: *Mathematical Geology*, the official journal of the IAMG (1968–1976 and 1994–1997), and *Computers & Geosciences* (1975–1995).

Sedimentological and stratigraphic applications continued to motivate statistical applications during the 1960s. Krumbein had earlier drawn attention to the importance of experimental design, sampling strategy and of establishing uncertainty ('error') magnitudes (Krumbein & Rasmussen 1941; Krumbein 1953, 1954b, 1955; Krumbein & Miller 1953; Krumbein & Tukey 1956); and the work of the émigré British sedimentary petrographer and mathematical geologist John C. Griffiths (1912-1992) reinforced this view (Griffiths 1953, 1962). Following a PhD in petrology from the University of Wales and a PhD in petrography from the University of London, Griffiths worked for an oil company before moving to Pennsylvania State University in 1947, where he remained until his retirement in 1977. An inspirational teacher, administrator and lecturer, he is now perhaps best known for his pioneering studies in the application of search theory (Koopman 1956-1957) to exploration strategies and quantitative mineral- and petroleum-resource assessment (Griffiths 1966a,b, 1967; Griffiths & Drew 1964, 1973; Griffiths & Singer 1970). The legacy of the work of Griffiths and his students can be seen in the account by Lawrence J. Drew (who was one of them), of the petroleum-resource appraisal studies carried out by the United States Geological Survey (Drew 1990).

Krumbein also introduced the idea of the conceptual process-response model (Krumbein 1963; Krumbein & Sloss 1963, chapter 7) which attempts to express in quantitative terms a set of processes involved in a given geological phenomenon and the responses to that process. Krumbein's earliest example formalized the interaction in a beach environment, showing how factors affecting the beach (energy factors:

characteristics of waves, tides, currents, etc.; material factors: sediment-size grades, composition, moisture content, etc.; and shore geometry) were reflected in the response elements (beach geometry, beach materials) and he suggested ways by which such a conceptual model could be translated into a simplified statistically based predictive model (Krumbein 1963). Reflecting Chamberlin's (1897) idea of using multiple working hypotheses in a petrogenetic context, Whitten (1964) suggested that the characteristics of the response model might be used to dispetrogenetic tinguish between different hypotheses resulting from different conceptual process models. Whitten & Boyer (1964) used this approach in an examination of the petrology of the San Isabel Granite, Colorado, but determined that unequivocal discrimination between the alternative models was more difficult than anticipated.

At this time there was also renewed interest in the statistics of orientation data arising from both sedimentological applications (Agterberg & Briggs 1963; Jones 1968) and petrofabric work in structural geology (see Howarth (1999) and Pollard (2000) for further historical discussion).

The Australian statistician Geoffrey S. Watson (1921-1998), who had emigrated to North America in 1959, published a landmark paper reviewing modern methods for the analysis of two- and three-dimensional orientation data (Watson 1966) in a special supplement of the Journal of Geology which was devoted to applications of statistics in geology. This issue of the journal also contained papers in several areas which would assume considerable future importance: the multivariate analysis of majorelement compositional data and the apparently intractable problems posed by its inherent percentaged nature (Chayes & Kruskal 1966; Miesch et al. 1966), stochastic (probabilistic) simulation (Jizba 1966), and Markov schemes (Agterberg 1966). The American petrologist Felix Chayes (1916–1993) made valiant efforts to solve the statistical problems posed by percentaged data, which also were inherent in petrographic modal analysis, a topic with which he was closely associated for many years (Chayes 1956, 1971; Chayes & Kruskal 1966). A solution was ultimately provided by another British émigré, the statistician John Aitchison (b. 1926), then working at the University of Hong Kong, in the form of the 'logratio transformation': y_i $\leftarrow \log(x_i/x_n)$, where the index *i* refers to each of the first to the (n-1)th of the *n* components, while x_n forms the 'basis', e.g. SiO₂ in the case of percentaged major oxide composition (Aitchison 1981, 1982).

A series of observations is said to possess the Markov property if the behaviour of any observation can be predicted solely on the basis of the behaviour of the observations which precede it. Such behaviour may be characterized using a transition probability matrix, which summarizes the probability of any given state switching to another (Allégre 1964). Empirical switching probabilities for the transition from one lithological state to another, e.g. sandstone \Leftrightarrow shale \Leftrightarrow siltstone \Leftrightarrow lignite (data of Wolfgang Scherer, quoted in Krumbein & Dacy 1969), are derived from observations, made at equal intervals along measured stratigraphic sections or well-logs, recording which of a given set of lithologies is present at each position. Although originally pioneered by Vistelius (1949), such applications only came into prominence in the 1960s. This was mainly as a result of renewed interest in cyclic sedimentation, aided by the possibility of using the computer to simulate similar stratigraphic processes (Krumbein 1967). Workers such as Walther Schwarzacher (b. 1925), at the University of Belfast (Northern Ireland) and Krumbein concentrated on lithostratigraphic data (Schwarzacher 1967; Krumbein 1968; Krumbein & Dacy 1969). The Dutch mathematical geologist Frederik ('Frits') P. Agterberg (b. 1936), who had recently joined the Geological Survey of Canada following a postdoctoral year (1961-1962) at the University of Wisconsin, considered the more general situation of multicomponent geochemical trends (Agterberg 1966). Vistelius undertook a longterm study of the significance of grain-to-grain transition probabilities in the textures of 'ideal' granites and how they change in conditions of metasomatic alteration (Vistelius 1964, revisited in Vistelius et al. 1983), although Whitten & Dacey (1975) raised some doubts about the utility of his approach.

The conventional techniques of time-series analysis, as used in geophysics (i.e. power-spectral analysis, enabled by the FFT), also have been applied to sequences of stratigraphic-thickness data as an alternative to the Markov chain approach (Anderson & Koopmans 1963; Schwarzacher 1964; Agterberg & Banerjee 1969). In recent years, increasing interest in the influences of orbital variations on sedimentary processes (on Milankovich cyclicity; see Imbrie & Imbrie 1979, 1980; Schwarzacher & Fischer 1982; Imbrie 1985; and Terra Nova 1989, Special Issue 1, pp. 402-480) has resulted in new techniques being applied to stratigraphic time series analysis, such as the use of Walsh power spectra (Weedon 1989) and wavelet analysis (Prokoph & Barthelmes 1996) which provides not only information regarding the amplitudes (or power) at different frequencies, but also information about their time dependence.

An important application area, in which the role of time is implicit, is that of quantitative biostratigraphy and related methods of stratigraphic correlation. The American palaeontologist Alan B. Shaw first developed the technique of 'graphic correlation', based on correlating the first and last appearances of a series of key taxa in two or more surface- and/or well-sections, while working for the Shell Oil Company in 1958 (Shaw 1995) and, as a result of its simplicity and efficacy, the method is still widely used (Mann & Lane 1995). Quantitative methods for faunal comparison, and seriation of samples based on such information to produce a pseudo-stratigraphy, an approach initially founded on techniques developed in archaeology (Petrie 1899), also began to develop in the 1950s, and the numbers of publications on quantitative stratigraphy increased steadily, until levelling off in the 1980s (Thomas et al. 1988; CQS 1988-1997). Since 1972, much of this work has been conducted under the auspices of the International Geological Correlation Programme (IGCP) Project 148 (Evaluation and Development of Quantitative Stratigraphic Correlation Techniques). This was initiated in 1976 as a project on quantitative biostratigraphic correlation under James C. Brower (Syracuse University, New York). Later the same year, its scope was broadened to include equivalent aspects of lithostratigraphic correlation under the leadership of the British geologist John M. Cubitt (at that time also at Syracuse). In 1979 Agterberg took over as project leader and aspects of chronostratigraphic correlation were added in 1981, so that the project then embraced all aspects of quantitative stratigraphic correlation. By the time the project terminated in 1986, some 150 participants in 25 countries had contributed to the research effort. Broadly speaking, the emphasis was on method development to 1981 and applications thereafter. Following cessation of the IGCP project, activities have been co-ordinated by the International Commission of Stratigraphy Committee for Quantitative Stratigraphy, again under the chairmanship of Agterberg. The types of methods and applications covered in the course of this work are discussed in Cubitt (1978), Cubitt & Reyment (1982), Gradstein et al. (1985), Agterberg & Gradstein (1988) and Agterberg (1990). See Doveton (1994, chapters 6, 7) for a review of recent lithostratigraphic correlation techniques and the application of artificial intelligence techniques to well-log interpretation.

81

Computer-based models

Computer simulation has already been mentioned. Early applications were concerned with purely statistical investigations, such as comparison of sampling strategies (Griffiths & Drew 1964; Miesch *et al.* 1964), but computer modelling also afforded an opportunity to gain an improved understanding of a wide variety of natural mechanisms. With the passage of time, and the vast increases in hardware capacity and computational speed, computer-based simulation has become an indispensable tool, underpinning both stochastic methods (Ripley 1987; Efron & Tibshirani 1993) and complex numerical modelling.

Particularly impressive among the early applications were those by the American palaeontologist David M. Raup (b. 1933), of mechanisms governing the geometry of shell coiling and the trace-fossil patterns resulting from different foraging behaviours by organisms on the sea floor (Raup 1966; Raup & Seilacher 1969); Louis I. Briggs and H. N. Pollack's (1967) model for evaporite deposition; and the beginning of John W. Harbaugh's (b. 1926) long-running investigations of marine sedimentation and basin development (Harbaugh 1966; Harbaugh & Bonham-Carter 1970), which became an integral part of the ongoing geomathematics programme at Stanford University (Harbaugh 1999).

Numerical models have also become crucial in underpinning applications involving fluid-flow, a topic of particular relevance to hydrogeology, petroleum geology and, latterly, nuclear and other contaminant transport problems. The use of analogue models in hydrogeology has already been mentioned. Although effective, they were time-consuming to set up and each hard-wired model was problem-specific. The digital computer provided a more flexible solution. Finitedifference methods (in which the user establishes a regular grid for the model area, subdivides it into a number of subregions and assigns constant system parameters to each cell) were used initially (Ramson et al. 1965; Pinder 1968; Pinder & Bredehoeft 1968) but these gradually gave way to the use of finite-element models, in which the flow equations are approximated by integration rather than differentiation, as used in the finite-difference models (see Spitz & Moreno (1996) for a detailed review of these techniques).

Although both types of model can provide similar solutions in terms of their accuracy, finite-element models had the advantage of allowing the use of irregular meshes which could be tailored to any specific application, required a smaller number of nodes and enabled better treatment of boundary conditions and anisotropic media. They were introduced first into groundwater applications by Javandrel & Witherspoon (1969). With increasing interest in problems of environmental contamination, the first chemical-transport model was developed by Anderson (1979). Stochastic (random-walk) 'particle-in-cell' methods were subsequently used to assist visualization of contaminant concentration in flow models: the flow system 'transports' numerical 'particles' throughout the model domain. Plots of the particle locations at successive time-steps gave a good idea of how a concentration field developed (Prickett et al. 1981). Spitz & Moreno (1996, table 9.1, pp. 280–294) give a comprehensive summary of recent groundwater flow and transport models.

The use of physical analogues to model rock deformation in structural geology was supplemented in the late 1960s by the introduction of numerical models. Dieterich (1969; Dieterich & Carter 1969) used an approach rather similar to that of the finite-element flow models, discussed previously, to model the development of folds in a single bed (treated as a viscous layer imbedded in a less viscous medium) when subjected to lateral compressive stress. In more recent times, the development of kinematic models has underpinned the application of balanced crosssections to fold and thrust belt tectonites (Mitra 1992).

Models in which both finite-element and stochastic simulation techniques are applied have become increasingly important. For example, Bitzer & Harbaugh (1987) and Bitzer (1999) have developed realistic basin-simulation models which include processes such as block fault movement, isostatic response, fluid flow, sediment consolidation, compaction, heat flow, and solute transport. Long-term forward-forecasts are required in the consideration of risk which nuclear waste-disposal requires. William Glassley and his colleagues at the Lawrence Livermore National Laboratory, California, are currently trying to develop a reliable model to evaluate the 10 000-year risk of contaminant leakage from the site of the potential Yucca Mountain high-level nuclear waste repository, 160 km NW of Las Vegas, Nevada. This ongoing project uses 1400 microprocessors controlled by a Blue Pacific supercomputer, and the threedimensional model combines elements of both thermally induced rock deformation and flow modelling (O'Hanlon 2000). In a less computationally demanding groundwater flow problem, Yu (1998) reported significant reductions in processing time for two- and three-dimensional solutions using a Cray Y-MP supercomputer.

The emergence of (Matheronian) 'geostatistics'

Because of their dependence on computer processing, many of the previous applications were first developed in the United States, partly as a product of their relatively easier access to major computing facilities when mainframe machines tended to predominate prior to the mid-1980s. However, what has come to be recognized as one of the most important developments in mathematical geology originated in France. While working with the Algerian Geological Survey in the 1950s, the recently deceased French mining engineer, Georges Matheron (1930-2000), first became aware of publications by the South African mining engineer, Daniel ('Danie') G. Krige (b. 1919), who was then working on the problems of evaluation of goldmining properties (Krige 1975). When Matheron returned to France he continued to work on problems of ore-reserve evaluation. The term géostatistique (geostatistics)¹ which Matheron defined as 'the application of the formalism of random functions to the reconnaissance and estimation of natural phenomena' (quoted in Journel & Huijbregts 1978, p. 1) first appeared in his work in 1955 (unpublished material listed in bibliography of Matheron's work; M. Armstrong, pers. comm. 2000). It came to be synonymous with the term krigeage, introduced by Matheron in 1960 (M. Armstrong, pers. comm. 2000) in honour of Krige's pioneering work using weighted moving-average surface-fitting (see Krige (1970) for the history of this work), or kriging as it has come to be known in the English-language literature. Implicit in all these terms is the analysis of spatially distributed data.

The techniques served two purposes. Firstly, they provided an optimum three-dimensional spatial interpolation method to assist oredeposit evaluation, with the initial data generally being obtained by grid-drilling the ore-body at the appraisal stage, or through a combination of drilling and chip sampling in an active mine. The key departure from assessment methods used up to that time was Matheron's estimation procedure (Matheron 1957, 1962–1963, 1963, 1965, 1969). Central to this was the idea of fitting a mathematical model which characterized the spatial correlation between ore grades at different locations in the deposit as a function of their distance apart. This function (the experimental variogram) was fitted to the means of the differences in concentration values in all pairs of samples separated by given distance (d) taken in a fixed direction (generally defined with regard to the orientation of the deposit as a whole), as a function of d. Knowledge of this behaviour then enabled an optimum estimate of the grade at the centre of each ore-block to be made, together with the uncertainty of this estimate (no other spatial interpolation method could provide an uncertainty value). In addition, the directional semivariograms enabled computer simulation techniques to provide models of the ore-deposit which reflected the actual spatial structure of the variation in the ore grades. Based on these simulated realizations, greatly improved estimates of the variation which could be expected in a deposit when mined could be obtained.

Acceptance of this radical new approach to mineral appraisal was not without its difficulties. The work of Matheron and his colleagues at the Centre de Géostatistique (established by Matheron in 1968), Fontainebleau, France, 'encountered no serious problems of acceptance in the Latin-speaking countries of Europe and South America nor in Eastern Europe but at times had stormy receptions from the English-speaking mining countries around the world' (Krige 1977). Such complications gradually eased, following the move to North America of two civil mining engineer graduates of the Ecole des Mines, Nancy: Michel David (1945-2000) went to the École Polytechnique, Montreal, c. 1968, and André Journel (b. 1944) to Stanford University, California, in 1977. Both had taken Matheron's probability class in 1963, and they persuaded him to start a formal geostatistics programme the following year. Matheron did so, and it was initially taught by Phillipe Formery (A. Journel, pers. comm. 2000). David and Journel soon proved themselves to be able ambassadors for the geostatistical method, both through their Englishlanguage publications (David 1977; Journel & Huijbregts 1978), which were more approachable in style for the average geologist than the more formidable mathematical formalism in which Matheron's own work was couched, and through industrial consultancy.

With the passage of time, the geostatisticsbased simulation methods originally developed for mine evaluation have come to play an essential role in reservoir characterization in the

¹ Somewhat confusingly, the term 'geostatistics' was independently adopted, particularly in North America, simply to denote the application of statistical methods in geology.

	M G	C & G	
Publication time-span	1969-99	1975-99	
No. of papers on geology-related topics	1416	1264	
Topic			
Statistics	85.4	28.1	
Spatial statistics	37.8	8.7	
Matheronian geostatistics	26.5	5.7	
Mathematical methods		14.7	
Petrological and mineralogical calculations		13.3	
Data management		12.0	
Graphics		11.7	
Cartographic methods		10.4	
Resource estimation and appraisal	9.9	9.6	
Geochemistry	6.1		
Mathematical models	5.6		
Simulation (excluding geostatistics usage)	5.4	8.7	
Cluster and principal components analysis, etc.		7.6	
Image analysis, image processing		6.2	
Orientation statistics		5.5	
Laboratory and field instrumentation		5.4	

Table 1. Percentage of papers in Mathematical Geology and Computers & Geosciences by non-exclusive topic

Non-geological papers and topics with under 5% frequency of occurrence are excluded

petroleum industry (Yarus & Chambers 1994) and risking of environmental contamination problems in hydrogeology (Gotway 1994; Fraser & Davis 1998). Furthermore, the practice of geostatistics has attracted the interest and participation of leading statisticians, such as Brian D. Ripley in Britain (Ripley 1981), and Noel A. C. Cressie, formerly in Australia and now in the United States (Cressie 1991). As a result, the use of such methods has now become firmly established as a tool in fields as diverse as climatology, hydrology, environmental monitoring and epidemiology.

Current trends

The spread of geostatistics (in its Matheronian sense), whose development has been driven by mining engineers and statisticians rather than geologists, characterizes a trend evident in the last 30 years from the pages of the leading journals *Mathematical Geology* (which has tended to publish the more theoretical papers) and *Computers & Geosciences*, which took over from the Kansas Geological Survey as major outlets for computer-oriented publications in the field of mathematical geology. Table 1 summarizes the overall most important topics of papers published in the two journals.

A classification of the type of authors contributing papers to these journals (see Fig. 12) shows that from the 1970s until the mid-1980s there was an overall decline in the number of 'geological' authors per publication and, particularly noticeable in *Mathematical Geology*, a corresponding increase in the contributions of mathematicians, statisticians, computer scientists, and mining and other engineers, all of whom will have had a strong mathematical training. This change in authorship should not be too surprising: even in nineteenth century Europe, mining engineers generally had a more rigorous mathematical education than geologists (Smyth 1854).

A literature database search (see Fig. 13) shows that although mathematical and stochastic modelling techniques have played the most important role since the 1960s (particularly in areas such as the characterization of fluid-, heat- and rock-flow, the study of pressure and stress regimes, geochemical modelling of solute transport), the use of physical models has remained relatively constant since the 1980s. It looks as though usage of simulation-based models is beginning to overtake that of purely mathematical models.

These trends reflect a broad change in the interests and requirements of the community engaged in mathematical geology (see Fig. 14). Early topics of interest, such as trend-surface analysis, Markov chains, and the application of multivariate statistics, have given way to geostatistical applications. More recent entrants to the field are fractal and chaotic processes which

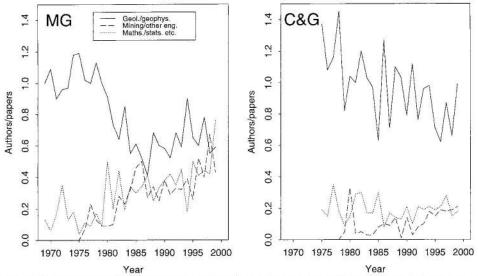


Fig. 12. Ratio of numbers of authors of various types (geologists and geophysicists; mining, hydrological, civil and environmental engineers; mathematicians, statisticians, computer scientists) to number of papers published in *Mathematical Geology* (MG; 1416 non-geophysics articles) and *Computers & Geosciences* (C&G; 1264) from earliest publication to end 1999. Other types of author (e.g. oceanographers, geographers, environmental scientists, etc. not shown).

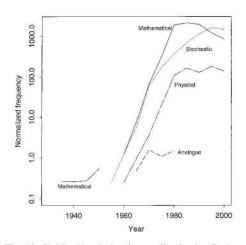


Fig. 13. Publication index (normalized using factors in Table 2, Appendix) for papers in the $GeoRef^{TM}$ bibliographic database (as distributed by the SilverPlatter knowledge-provider), from 1935 to June 2000, with key words: mathematical models (total 40030), physical models (3561), stochastic models (65) and analogue models (23).

describe the behaviour of scale-invariant phenomena. Such processes typically describe the size-frequency distributions of phenomena which range in magnitude from the porosity distribution within a rock to the sizes of oil fields (Barton & La Pointe 1995; Tourcotte 1997) and are beginning to be incorporated in geostatistical simulations (Yarus & Chambers 1994). This has happened mainly as a result of the attention gained by the pioneering work of the mathematician Benoit B. Mandelbrot (1962, 1967, 1982).

Image-processing techniques have become increasingly important in the Earth sciences since the late 1960s, driven mainly by the impact of remote-sensing of the Earth and other planetary imagery (Nathan 1966; Rindfleisch et al. 1971; Nagy 1972; Viljoen et al. 1975), and now are taken for granted, although spatial filtering techniques derived from image-processing have proved useful in other geological contexts, such as geochemical map analysis (Howarth et al. 1980). A different image-related area of application has been the development of mathematical morphology by Matheron and his colleague, the civil engineer and philosopher Jean Serra (b. 1940). This grew out of petrographic applications of sedimentary iron ores undertaken by Serra in 1964 and 1965 and their applications now underpin the software routinely used in Leitz and other texture-analysis instrumentation (Matheron & Serra 2001). Computergenerated images have also proved invaluable in enabling the visualization of complex threedimensional, or occasionally higher, relationships which may arise from something as relatively simple as serial-sectioning of a

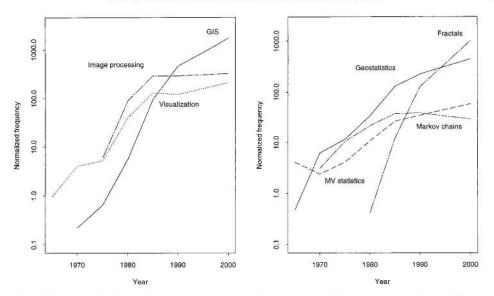


Fig. 14. Publication index (normalized using factors in Table 2, Appendix) for papers in the *GeoRef*TM bibliographic databases, from 1935 to 2000, with the following strings in title or keywords: image processing (total 6094), visualization (2813), geographic information system (GIS; 2692), multivariate (MV) statistics (777), Markov chains (779), geostatistics (4285), and fractals (3437).

fossil-bearing rock (Marschallinger 1998); to fault and other subsurface geometry (Houlding 1994; Renard & Courrioux 1994) and viewing the results of geostatistical simulations (Yarus & Chambers 1994; Fraser & Davis 1998), both of which are crucial in reservoir characterization and mining and environmental geology; or examining the results of integration of topographical, geological, geophysical, and other data by geographical information systems (Bonham-Carter 1994; Maceachren & Kraak 1997; Fuhrmann *et al.* 2000).

The development of computer-intensive methods in statistics, such as the resampling ('bootstrap') techniques of Efron & Tibshirani (1993), for assessing uncertainty in parameter estimates, evidently have considerable potential (Joy & Chatterjee 1998), but may need to be used with care with spatially correlated data (Solow 1985). Similarly, 'robust' methods for parameter estimation and related regression techniques (Huber 1964; Rousseeuw 1983, 1984), which provide the means to obtain reliable regression models even in the presence of outliers in the data, are proving extremely effective (e.g. Cressie & Hawkins 1980; Garrett *et al.* 1982; Powell 1985; Genton 1998).

There is also growing interest in the application of the Bayesian 'degree-of-belief' philosophy as an alternative to the classical 'frequentist' or 'long-run relative frequency' view. In its simplest form, the Bayesian approach could be described as a way of implementing the scientific method in which you state a hypothesis by a prior distribution, collect and summarize relevant data, and then revise your opinion by application of the Bayes rule. This is named for a principle first stated by the British cleric and mathematician Thomas Bayes (c. 1701–1761), in a posthumous publication in 1764. It was later discovered independently by the French mathematician Pierre-Simon Laplace (1749–1827) in 1774 (see Stigler (1986) and Hald (1998) for further discussion). Bayes' rule can be expressed as: the probability of a stated hypothesis being true, given the data and prior information, is proportional to the probability of the observed data values occurring given the hypothesis is true and the prior information, multiplied by the probability that the hypothesis is true given only the prior information. In practice, implementation of Bayesian inference is often computer-intensive for reasons which become apparent from the article by Smith & Gelfand (1992). It is true to say that the application of Bayesian statistics is somewhat controversial (see, for example, the arguments advanced for and against the use of Bayesian methods in the 1997 collection of papers in The American Statistician, 51,

241-274). The relatively few geological applications in which Bayesian inference has been used include biostratigraphy (Strauss & Sadler 1989), hydrogeology (Eslinger & Sagar 1989; Freeze et al. 1990), resource estimation (Stone 1990), hydrogeochemistry (Crawford et al. 1992), geological risk assessment at the Yucca Mountain high-level nuclear waste repository site (Ho 1992), analysis of the time evolution of earthquakes (Peruggia & Santner 1996), and spatial interpolation (Christakos & Li 1998). Bayesian methods are also used in archaeology in connection with radiocarbon dating (Christen & Buck 1998), classification of Neolithic tools (Dellaportas 1998), and archaeological stratigraphic analysis (Allum et al. 1999), all of which have obvious geological analogues. There seems to be considerable scope for further use of Bayesian methods in geological applications.

Computational mineralogy is another area which is making rapid strides as a result of advances in processing power. Price & Vocadlo (1996; Vocadlo & Price 1999) believe that before long computational mineralogists will be able to 'simulate entirely from first principles the most complex mineral phases undergoing complicated processes at extreme conditions of pressure and temperature' such as exist within the Earth's deep interior. The results obtained would be used to interpret or extend understanding of laboratory results.

As has been remarked, geostatistical and fluid-transport studies currently are providing some of the most challenging and computationally intensive applications. New techniques being applied include simulated annealing (Deutsch & Journel 1992; Carle 1997), Markov chain Monte Carlo (Oliver *et al.* 1997) and Bayesian maximum entropy (Christakos & Li 1998). Results of recent research are described in Gómez-Hernández & Deutsch (1999).

Conclusion

This account began with the slow growth, during the nineteenth century, of awareness of the utility of hand-drawn graphics as an efficient way to encapsulate information and to convey ideas through the visual medium. The next 50 years saw the beginning of the application of statistical (mainly univariate) and mathematical methods to geological problems. With the spread of computers into civilian use after the end of World War II, the average time-lag of statistical method development (or adaptation) in the geological sciences, compared to its earliest use outside the field, dropped from around 40 years to ten, and since 1985 it has been of the order of one to two years (Fig. 11). Method development time has continued to shorten rapidly as improved computer hardware has become available, both in terms of raw computing power and portability. The increasing dissemination of ideas through journal and book publication and, in the last few years, media such as the Internet, has also improved dramatically the ease of co-working.

application of computer-intensive The methods, coupled with computer-aided visualization, is revolutionizing our capability in fields such as metalliferous mining and reservoir characterization, but the ability to deal effectively with problems involving fluid flow has already had a profound impact in hydrogeological, environmental geology, and environmental contamination applications. The experimental Yucca Mountain nuclear-waste repository study, based as it is on massively parallel processing, is pointing the way towards obtaining significantly improved long-term forecasts of behaviour, as well as better hindcasting. To achieve such goals will, in general, require well-integrated teams of geologists with mathematicians, statisticians and mining engineers. Figure 12 suggests that such team-work is already happening, but the mathematical and statistical skills of many geologists may need to be strengthened if we are to capitalize fully on the opportunity presented by the ongoing technological revolution.

I am grateful to F. Agterberg, G. Bonham-Carter, J. Brodholt, B. Garrett, C. Gotway Crawford, C. Griffiths, E. Grunsky, S. Henley, T. Jones, G. Koch, D. Krige, A. Lord, R. Olea, D. Price, J. Schuenemeyer, S. Treagus and T. Whitten, who all answered my enquiry as to what they thought the five most important innovations in mathematical geology might have been. The resulting diversity was so immense that I have been forced to try to narrow the spectrum to some kind of commonality (or else this article would have grown to book length). In doing so, many interesting ideas have had to fall by the wayside, but nevertheless all their suggestions have been immensely useful. My thanks also go to M. Armstrong and J. Serra for giving me information regarding Georges Matheron's early career, and to G. Bonham-Carter, D. Pollard, D. Price and J. Serra for sending me preprints of papers in press at the time of writing this article. It is some fifteen years since I read Karl Pearson's History of Statistics in the Seventeenth & Eighteenth Centuries (ed. E. Pearson 1978). In the Introduction to this text, based on lectures which he gave in the 1920s, Pearson wrote 'I do feel how very wrongful it was to work for so many years at statistics and neglect its history, and that is why I want to interest you in this matter'. This struck a distinct chord, as I was then in exactly the same position, having been teaching statistics and quantitative geology in the Department of Geology at Imperial College, London, for many years. I have been trying to explate my guilt ever since! I am extremely grateful to the librarians at what was formerly the Department of Geology in the Royal School of Mines (now, sadly, subsumed into the all-embracing Huxley School of Environment, Earth Science and Engineering), Imperial College, The Science Reference Library, the D. M. S. Watson Library, University College London, and The Geological Society, London, throughout the years, without whose assistance in locating dusty volumes from their stack rooms my research would have been impossible to undertake. Photographic work over this time has been carried out by A. Cash and N. Morton (Imperial College), M. Grey (University College), and the Science Museum Library (now the Science Reference Library), and their help is also gratefully acknowledged. I am also grateful to D. Merriam for his referee's comments.

Appendix

An index for the geoscience publication rate from 1700 to 2000 has been derived by comparison of counts of journal holdings in the Geological Society of London with the articles and books recorded in the $GeoRef^{TM}$ bibliographic database (as distributed by the Silver-Platter knowledge-provider). Undercount of the latter, pre-1936, has been corrected using robust regression analysis of the $GeoRef^{TM}$ counts on the Geological Society journal holdings. Undercount post-1989 has been corrected by extrapolation from the immediately preceding trend for 1982 to 1987. Taking base-10 logarithms of the regression-predicted counts per five-year period yields the final index values of Table 2, which have been used for normalization of Figures 1, 10, 13 and 14.

Year	1700	1800	1900	2000	
0	0.30	1.35	3.86	5.00	
5	0.30	1.52	3.87		
10	0.30	1.56	3.90		
15	0.30	1.68	3.90		
20	0.41	1.79	3.88		
25	0.55	1.90	3.92		
30	0.70	2.05	3.91		
35	0.70	2.19	3.90		
40	0.70	2.36	3.90		
45	0.70	2.48	3.69		
50	0.70	2.60	3.78		
55	0.70	2.82	3.96		
60	0.76	3.00	4.04		
65	0.78	3.14	4.15		
70	0.83	3.28	4.51		
75	0.90	3.44	4.67		
80	1.03	3.61	4.74		
85	1.12	3.68	4.84		
90	1.21	3.77	4.87		
95	1.28	3.83	4.93		

Table 2. Publication index: 1700-2000

Italicized entries based on extrapolated values

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