# Chapter 37
# Forward and Inverse Models Over 70 Years


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**Abstract** The transition over 70 years from qualitative rock description to attempted quantitative description of rocks and rock bodies (inverse modelling) and testing of process models with observation data (forward models) are outlined. Dramatic increases of readily measured variables, combined with almost unlimited computing power, yielded a plethora of varied inverse models, but limited attention has been given to critical sampling, variance, closure, 'black swan', and nonlinear issues; recent approaches to closure problems hold promise. Especially for plutonic rocks, paucity of quantitative process modelling left exciting forward-modelling opportunities neglected. Resulting challenges ahead are anticipated.

**Keywords** Sampling · Variance · Composition variability · Black swans Granite composition

## 37.1 Birth of IAMG in 1968

In many different ways, 1968 was an extraordinary year that rocked the world (cf., Kurlansky 2004). Some 20 enthusiasts gathered at the XXIII International Geological Congress in Prague's New Technical University, Czechoslovakia, to create the International Association for Mathematical Geology in exciting, but tragic, times. Soviet troops had occupied the city a couple of days previously; guns of encircling Soviet tanks pointed at the university, which was the centre for printing and disseminating news. Vistelius was elected first IAMG President and Krumbein 'Past President' (a designation he appreciated and found amusing!); both are fathers of geological models.

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At that meeting, dissimilar approaches came together, having evolved principally in the Soviet Union, Western Europe, and U.S.A. Vistelius championed the concept that Mathematical Geology is a separate branch of science based on testing geological hypotheses mathematically, and that this should be IAMG's primary focus (Whitten 2003; 2004, p. 384–5); for some years, he had contended it is not particularly important merely to manipulate geological data statistically. Dech and Henley (2003, p. 368) noted Vistelius (1991) considered that, if a science does not use mathematical modelling in constructing conclusions, "… it can be considered as belonging to the pre-Newtonian period, …. behind the present-day level of research by approximately 300 years."

## 37.2 In the Beginning (One Pre-1968 Experience)

Specializing in petrology in 1948, Hatch and Wells (1937) was my 'bible'. That descriptive, natural-history type, foundation meant it was thrilling in 1950 to visit Jacupiranga, the Brazilian jacupirangite type locality. For a Ph.D. project in 1948, it was recommended I look at 260 $km^2$ of coastal NW Ireland to see what is there; seventy years later, an unlikely method of identifying a thesis project. The area is red (granite) on the Geological Survey of Ireland 1:63,360 map (Hull et al. 1889).

A plan to record variability of granite across the area (including numerous islands in the Atlantic Ocean) was needed. Immediate problems in 1949 were devising (i) a scheme to collect representative samples, and (ii) realistic measurements (measurable in the field or laboratory) to reflect variability.

Unscientifically, a one-mile grid was oriented to maximize (by eye) grid nodes over outcrops (i.e., islands in the ocean and less peat-bog and drift-covered mainland areas). It was planned to collect samples (with hammer and chisel) at all nodes if possible. In the field, two compromises became necessary—using the nearest outcrop to nodes and accepting any hand-sample that could be hammered off.

Wet chemical analysis of numerous samples was beyond available resources; X-ray fluorescence analysis was then undeveloped. Point counting thin sections to determine mineral volume percentages with a Dollar (1937) mechanical stage was feasible, provided larger thin Sections. (3.3 × 2.3 cm) could be hand ground and stained with sodium cobaltinitrite—both challenging in 1949; this staining technique was described by Chayes (1952). Using a Chayes (1949) electrically-controlled stage improved point-counting accuracy. Studies of spacing and required number of counts (Chayes and Fairbairn 1951; Chayes 1954) suggested sufficiently large thin sections were being used. Manual contours for modal variables (e.g., K-feldspar volume percentage, colour index) at 44 grid nodes reflected considerable areal variation (Whitten 1957). Such contours were very controversial because they crossed ocean between islands and superficial deposits on land; also, no exposures occur in numerous grid squares. A senior reviewer deemed it impossible to draw contours across ocean (despite greater outcrop density with off-shore islands than on land with peat bogs, farming, etc.).

In 1958, I became a colleague at Northwestern University of W. C. Krumbein, who was pioneering quantitative description of sedimentary rocks. The University acquired an IBM360 mainframe computer; we used punch cards and wrote FORTRAN programs for statistical descriptors and surface-fitting algorithms for areally-distributed data (e.g., Whitten 1960, 1961). Analogous approaches began thriving at Kansas Geological Survey, Pennsylvania State University, etc. Krumbein developed the concept of descriptive, conceptual, and predictive models (Krumbein 1963; Krumbein and Graybill 1965, p. 13, *et seq*.; Whitten 1964). Driving to Leningrad to spend time at Vistelius' Institute for Mathematical Geology was a privilege in 1971.

## 37.3 Inverse and Forward Geology Problems

Vistelius (e.g., Vistelius 1977) differentiated *inverse* from *forward* problems. The objective with the former was describing the nature and variability of specified rocks, etc.; that is, with statistical or other techniques, formulating descriptive and/or genetic models for essentially arbitrary data for arbitrary variables. With forward problems, the objective was testing validity of genetic models (based on currently available information) for rocks, fold belts, etc. That is, testing whether a genetic model is supported or rejected by data for variables dictated by that model; many commonly measured variables are likely to be irrelevant for such testing (cf., Whitten 2005).

For sedimentary and metamorphic rocks inverse and forward problems present fewer difficulties. Thus, 'marine beach' can be defined descriptively by physical, chemical, and biological features that commonly enable marine-beach deposits to be recognised (e.g., in the stratigraphic column), or genetically by environmental conditions that result in beach formation (waves, currents, sediment transport, etc.). Similarly, as Bayly (1968) pointed out, metamorphic facies can be defined by presumed temperature and pressure during genesis (Eskola 1915, p. 114; Turner and Verhoogen 1951) or descriptively by diagnostic mineral assemblages (Fyfe et al. 1958). With igneous rocks (especially plutonic assemblages), geotectonics, etc., inter-relationships between the descriptive and genetic are commonly very debateable (Whitten et al. 1987a, p. 334).

## 37.4 Forward Models in Earth Sciences

Forward modelling is in its infancy and rare because, in most cases, little objective quantitative information is available about genetic factors, especially for plutonic rocks. Unlike many scientific fields, most earth-science domains do not permit *reproducible* experiment and testing. Vistelius (1972) used Tuttle and Bowen's (1958) experimental petrology to illustrate forward modelling of 'ideal granite',

extending his method[1] to Omsukchan Granite, SE Asia (Vistelius and Romanova 1972), Malsburg Granite, Germany (Choubert and Vistelius 1972), etc.

Over the past decade, numerous "forward models" appeared in geophysical studies (petroleum, mining, water, volcanic activity) for prediction and extrapolation based on measured variables (e.g., Geol Soc Amer Symposium 2002; Sui et al. 2012; Butler and Zhang 2016). Butler and Sinha (2012, p. 168) stated such forward modelling is useful for interpreting data. McInerney et al. (2007) compared gravity data computed for a 3D geological model with new Bouguer data to iteratively improve their geological model, calling this forward modelling. Comparable usage occurs in biology (e.g., Tolwinski-Ward 2012). In such studies, inverse models have been honed with new data for sundry variables, producing improved inverse models (cf., iterative forward modelling, Schlumberger Limited 2016). However, such "forward modelling", albeit useful, is wholly different from testing genetic models with new variables prescribed by those models. Different distinctive terminology would prevent confusion.

Vistelius' forward-model definition is retained in this paper.

## 37.5 Inverse Models in Earth Sciences

Inverse–models reach into many earth-science domains. Manual contours for variability of Donegal granite modes (Whitten 1957) represented an inverse-problem approach; more-sophisticated inverse models followed as computing power facilitated trend-surface map preparation (e.g., Whitten 1960). Computing power soon resulted in every available data set being processed by every available statistical artifice, to explore whether anything interesting (and publishable) emerged. Such research provoked Vistelius' strident remarks at the IAMG founding meeting.

Inverse problems fall into two categories:

(a) analysis and description of available (or readily measured) data for geological entities (e.g., colour index in granite plutons; grain-size skewness in silt samples), and
(b) use of data to predict

   (i) useful features (e.g., gold content and location; subsurface sedimentary rock permeability variation) as with kriging and so-called 'geostatistics'

[1]Numerous papers by Vistelius and coworkers used the important and challenging discovery that grain transitions along linear traverses of many granitic rocks possess the Markov property, to suggest testing or erecting genetic crystallization models can be based on grain-transition probabilities. However, Whitten and Dacey (1975) and Whitten et al. (1975) demonstrated Markov chains in actual mineral sequences in varied rocks (including a calc-silicate granulite) is insufficient for establishing validity of the granite crystallization model.

(cf., Krige 1964; David 1977; Journel and Huijbregts 1978), or flooding or other risks (e.g., Burke et al. 2016), or

(ii) petrogenetic processes (e.g., infra-crustal origins of *I*- and *S*-type granites within orogenic belts (e.g., White and Chappell 1983; Chappell 1984; Chappell and Stephens 1988).

Speculation about petrogenetic processes that produced described rock assemblages has always been common. Over a thousand high-quality chemical analyses of major and many trace elements for southeast Australian granites led to partitioning samples into *I*-type or *S*-type granitoids with dissimilar sub-crustal origins, and to the restite genetic model (e.g., Chappell et al. 1988, 1987; Chappell and Stephens 1988). Analogous methods were used elsewhere (e.g., North American Peninsula Ranges, Silver and Chappell 1987). Such inverse models could afford excellent forward-modelling bases, if prescribing new variables with which to support or negate the supposed genetic model/s.

However, such inverse models are fraught with difficulties (Whitten 1991, p. 121). Use of different variable sets from Chappell and colleagues' chemical analyses can partition samples into an almost infinite set of descriptive suites. It is unrealistic to enunciate genetic scenarios for one set of descriptive suites, without concomitantly embracing all other coexisting sets defined by using different variables, sets of variables, variable weightings, etc. (Whitten et al. 1987a, p. 341; 1987b). Again, if techniques like cluster analysis were used to partition hundreds of samples on the basis of 36 chemical variables, normalization (to give each variable equal weight) would commonly be used, despite no a priori reason for each element being equally important. Different clusters emerge if one (or more) variable receives different weighting, and when more or less variables are included (Whitten et al. 1987b, p. 69; Whitten 1991, p. 121). Also, standard cluster analysis (and similar partitioning techniques) yield questionable results when percentage and/or parts-per-million data are used (cf., Aitchison 1986, p. 300).

However, where components are conserved throughout crystallisation within certain basic igneous rocks, molar ratios with a common constant denominator were shown to display, accurately and unequivocally, the actual chemical variability (e.g., Nicholls 1988; Stanley and Russell 1989). Molar-ratio diagrams for some Australian *I*- and *S*-suites seem to show chemical variations accurately, permitting quantitative objective testing of, say, the restite model (Whitten 1996). This technique for avoiding daunting closed-data problems deserves further examination, although, for many granites, lack of component conservation during crystallization may introduce difficulties.

## 37.6 The Samples Analysed

Statistical or mathematical analyses of available data are the relatively easy part. Statistical manipulation (inverse modelling) describes characteristics and variation of particular data, but *not* necessarily characteristics and variation of those

variables in the rock samples from which the data were derived (or necessarily of variables of *petrogenetic* significance for forward modelling, or of direct *economic* importance).

Data come from samples (or geophysically-sampled rocks, etc.). It is important to assess how well available samples represent the *sampled population* of interest, and whether that sampled population permits realistic extrapolation to the *target population* of primary interest (cf. Whitten 1961). For example, where the objective is determining compositional variation of a pluton, the exposed surface is an arbitrary 2D section (or modestly 3D in mountainous terrain) through the original 3D mass, much of which is eroded away. Soil, vegetation, etc. always obscure major parts of 2D exposures; actual outcrops are disposed arbitrarily or preferentially, but not randomly. Analyses of those samples actually examined (samples collected from sampled outcrops) are necessarily used to estimate composition and variability of the sampled population, and subsequently the target population.

The significance of actual observed dependent data was reviewed by Whitten (2000, pp. 4 *et seq*.) who asserted that, in favourable circumstances, rigorous statistical inferences can be drawn about the sampled population on the basis of samples examined, and subsequently geologists can only use such inferences to make *subject-matter inferences* about the target population on the basis of previous geological experience (cf., Cochran et al. 1954, p. 19).

Unusually, such issues can be obvious. For example, road cuttings might expose significantly banded or layered rocks, but only some of those bands may be exposed in outcrops across neighbouring areas.

Serial thin sections from coarse-grained granite samples commonly yield modal values with considerable variance. Exposed igneous rocks may be porphyritic making collectable, representative, samples difficult to obtain. Commonly, samples of dissimilar size are required to estimate composition and variability of each variable. For variables measurable only by laboratory analyses (e.g., modal zircon percentage, trace-element weight percentages), an adequate sampling plan can be devised only following estimating the level of variance of each variable from analytical results. The classical example is Krumbein and Slack's (1956) determination that variance of their variable of interest within a black shale over many square kilometres of Illinois, USA, is greatest at their smallest level of sampling (thin-section level). Different rock types require dissimilar strategies (e.g., determining calcite volume percentage throughout a cratonic limestone requires a less-dense sampling plan than, say, assaying gold weight percentage within subsurface Witwatersrand conglomerates or apatite volume percentage in a granite).

For Rattlesnake Mountain Pluton, California (USA), Baird and Welday (1967) showed that, when variance of attributes is large at their smallest sampling level (hand-specimen level), adjacent samples yield dissimilar values and thus dissimilar areal-variability maps. For their monumental studies of Lachlan fold belt granitoids, Australia, Chappell and colleagues powdered very large samples (over a kilogram) from the mainly visually-homogeneous outcrops, with the intention of minimising major and trace-element variance at the sample level (e.g., White et al. 1977; Chappell 1978). Their sample size and reproducibility of their chemical analyses

yielded reliable data. In many regions, they collected a sample from virtually every outcrop protruding through arid rolling pasture. Areas between widely scattered outcrops (sometimes a kilometre apart) were necessarily un-sampled and unknown; it is appropriate to question whether extant outcrops exist because composed of rocks less susceptible to weathering (compositionally dissimilar to the majority).

Generalising, each variable commonly has dissimilar variance in samples of a specified size. Variance tends to be large between small samples, especially when grain size is large, and, as sample size increases, variance between samples decreases to a minimum, before increasing again for extremely large samples (cf, Whitten 1968; 2000, p. 6).

Such issues have long been recognized in mining exploration. Moving-average methods, developed by Krige (e.g., 1964) for South African gold-bearing conglomerates were extended and explicitly controlled (in what is known as 'geostatistics') by levels of variance of variable/s, as expressed by semi-variograms (e.g., David 1977; Journel and Huijbregts 1978); observed large outlier values are accommodated within the 'nugget' effect. 'Nugget' aptly reflects very sparse, larger gold particles within the conglomerates, which affect predicted profitability of subsequent mining; nuggets are represented only occasionally in actual samples and resulting assay values (Whitten 2010, p. 250).

It is not uncommon for it to be assumed that, provided sampling has been 'adequate', variables of interest follow standard frequency distributions (normal, lognormal, etc.). Many common statistical algorithms assume input data are normally distributed; frequently, packaged computer programs normalise input data automatically (often with unspecified algorithms) prior to effecting statistical analyses. However, different normalisation algorithms can produce dissimilar resulting analyses.

## 37.7 The Black Swan Effect

Throughout the earth sciences, sporadic sample measurements are wholly dissimilar to those for the majority of samples. Not infrequently, analyses lying on the extreme wings of distribution curves (normal, lognormal, etc.), or beyond the tails, are discarded; although such analyses might be attributable to analytical error, many are likely to be real and *very* meaningful. In studying the influence of the improbable in the earth sciences, Whitten (2010) demonstrated that real, localised, anomalous data can reflect features of significant genetic and/or economic importance; the 'black swan' effect (cf., Taleb 2007). That is, such data can reflect important factors not previously considered in models and theories—factors that, after recognition, are likely to be found highly significant.

Throughout geological time, all manner of events occurred that appear to be wholly arbitrary with respect to formation of lithology, structure, palaeontology, etc., of rock units. Impact of a meteor with the Earth is a good example, because it can apparently affect substantially both current organic evolutionary patterns and

ongoing physical processes (e.g., sedimentation). Consequently, some, but not necessarily all, dependent variables (with respect to space and time) might show anomalies reflected as outliers on a distribution curve (a nugget-like effect). Such phenomena reflect the operation of customary physico-chemical laws and the effects of irreducible elements of chance and indeterminism (Whitten 2010, pp. 250–1).

The traditional search for order and simplified description commonly deflects attention from important real black swans that require inclusion for realistic understanding of geological phenomena and natural hazards. Mandelbrot (1982) provided a beautiful introduction to fractal geometry in nature; more recently, fractal, chaos, and nonlinear approaches have helped expose basic characteristics of the physical world, whose fundamental significance throughout the earth sciences is rapidly becoming more clear. A report (Lovejoy et al. 2009) on 'geocomplexity' summarized the importance of nonlinear geophysical methods in elucidating rational bases for statistics and models of natural systems (including hazards), which previously were treated by ad hoc methods. That report reflected 15 authors' research ranging from earthquake dynamics, river-flood prediction, basalt columnar-joint formation, coastline topography, meteorological cloud models, and interaction of greenhouse gases and global warming. It concluded with a warning against (a) reliance on traditional state-of-the-art statistical techniques (and theories based on them) and (b) ignoring nonlinear methods which are often helpful for more-complete understanding of the natural world.

## 37.8 Concluding Thoughts

Throughout most geological domains, the qualitative-to-quantitative revolution via mathematical geology over the past half century has been awesome, made possible by numerical models and readily available data for greatly increased numbers of variables; all facilitated by hugely increased computing power. Investigations extend to variables whose variance cannot be estimated by eye (e.g., isotope ratios; electrical resistivity). The research is manifest in both IAMG Journals and other new approaches (e.g., 3-D visual digital models and virtual presentation of rocks and geological formations, De Paor 2016). Cataloguing, classifying, description, and presentation are often the useful goals, especially for economic geologists (e.g., oil-field research; kriging and 'geostatistics').

Pragmatic review emphasises that many basic (but apparently unexciting) problems enumerated five decades ago (e.g, variance; sampling), critical in inverse models for correctly portraying rock formations (rather than merely assembling data obtained from the rocks), have continued to receive little attention (Whitten 2003).

Birth, maturity, and old age characterise phases of all human endeavour. The past 50 years witnessed birth of IAMG and spreading of its influence throughout the earth sciences using inverse methods, but only initial recognition of the compelling importance of modelling forward problems (in Vistelius' meaning).

Inverse-problem studies will move into maturity as variance, sampling, and non-linear models underpin on-going research.

The challenging needs and goals of forward problems are reasonably obvious, but the complex issues involved have been addressed only occasionally (e.g., Vistelius and Romanova 1972; Maslov 2003). Commonly, forward problems will require non-linear process models (i.e., quantitative genetic models) that specify those variables required to test the hypothesis. The next 50 years await research towards that maturity in forward modelling. So-called forward models of recent geophysical studies must not obscure this challenge.

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