ELSEVIER

Earth-Science Reviews 57 (2002) 211–253

EARTH-SCIENCE REVIEWS

www.elsevier.com/locate/earscirev

# Quantitative analysis of detrital modes: statistically rigorous confidence regions in ternary diagrams and their use in sedimentary petrology

Gert Jan Weltje*

*Delft University of Technology, Department of Applied Earth Sciences, PO Box 5028, NL-2600 GA Delft, The Netherlands*
*Netherlands Institute of Applied Geosciences TNO~National Geological Survey, Department of Geo-Energy, PO Box 80015, NL-3508 TA Utrecht, The Netherlands*

Received 14 July 2000; accepted 12 June 2001

**Abstract**

Detrital modes are the basic type of quantitative data used in sedimentary petrology. They represent estimates of the petrographic framework composition of sand or sandstone obtained by point counting of thin sections. At present, geological inferences from analysis of these numerical data are semi-quantitative only, because many of the data-processing methods employed in sedimentary petrology lack a firm theoretical basis. A review of existing methods reveals a number of fundamental statistical problems associated with the use of univariate statistics and the construction of so-called hexagonal fields of compositional variation. It is shown that these problems can be overcome by using multivariate methods that honour the non-negativity and unit-sum constraints on compositional data, and incorporate the covariance structure. Spread in compositional data can be modelled on two levels: (1) by regarding the grain as unit of observation, and the total point count as a sample from a multinomial distribution; (2) by regarding the total count as unit of observation, and a set of counts as a sample from an additive logistic normal distribution. Numerical methods are presented for constructing statistically rigorous confidence regions in ternary diagrams by inversion of significance tests for these two distributions. Statistical analyses of the framework composition and heavy-mineral assemblages of modern beach and river sands illustrate their use. The case histories are followed by a brief overview of popular multivariate methods for reconstructing sediment provenance. 

*Keywords:* sediment provenance; compositional data; ternary diagrams; confidence regions; multivariate statistics

> "*First shalt thou take out the holy pin Then shalt thou count to three — No more, no less Three shall be the number thou shalt count, And the number of the counting shall be three Four shalt thou not count, neither shalt thou count two, Excepting that thou then proceed to three*"
>
> The Book of Armaments (Monty Python and the Holy Grail, 1975)

## 1. Introduction

Quantitative estimation of detrital modes of sand and sandstone is traditionally performed by point counting. At present, geological inferences from

* Delft University of Technology, Department of Applied Earth Sciences, PO Box 5028, 2600 GA Delft, The Netherlands.
*E-mail address:* g.j.weltje@citg.tudelft.nl (G.J. Weltje).

0012-8252/02/$ - see front matter 
PII: S0012-8252(01)00076-9

analysis of these numerical data are semi-quantitative only, because many of the data-processing methods employed in sedimentary petrology lack a firm theoretical basis. Most sands and sandstones contain many different types of grains, indicating that their compositional variation can only be properly characterised by multivariate statistical methods. However, sedimentary petrologists have traditionally limited themselves to the analysis of ternary (sub)compositions that can be displayed in ternary diagrams. The prime example of the use of ternary diagrams in sedimentary petrology is the inference of plate-tectonic setting of sedimentary basins from sandstone composition (Dickinson, 1985, 1988).

The introductory section of this article discusses the procedures by which detrital modes are obtained. The main body of this review is devoted to theory and application of statistical analysis of ternary compositions. It concludes with a brief section on the use of multivariate methods of compositional data analysis in sedimentary petrology.

## 2. Point counting in sedimentary petrography

### *2.1. Classification schemes*

Following standard practice in sedimentary petrology, the framework composition of sandstone is estimated by counting a certain number of points in thin section (usually between 300 and 600) according to the Glagolev–Chayes method (Chayes, 1949, 1956; Galehouse, 1971). Each grain beneath the crosshair is assigned to a category within the petrographic classification system used. The petrographic modal composition of sands and sandstones may be regarded as a mineralogical mode augmented by information about composition and texture of polycrystalline grains. The latter is of considerable importance for sedimentary provenance studies, because it provides a direct link with parent-rock assemblages in the source area.

Two schools of sedimentary petrographers have evolved, which use different classification schemes to quantify sandstone framework composition: the Indiana method and the Gazzi–Dickinson method. The principal difference between these methods is the way in which coarse-crystalline (phaneritic) polymineralic grains are classified. Relative strengths and weaknesses of both schemes have been discussed by Ingersoll et al. (1984, 1985a,b), Suttner and Basu (1985), Decker and Helmold (1985) and Zuffa (1980, 1985). Classification criteria for monocrystalline grains, fine-grained (aphanitic) polymineralic grains and quartz varieties are common to both methods. Operational definitions for these framework categories have been presented by Gazzi (1966), Dickinson (1970), Wolf (1971), Basu et al. (1975), Graham et al. (1976), Basu (1985), Dorsey (1988), Johnsson (1990), Valloni (1985; in Ibbeken and Schleyer, 1991), Garzanti (1991), and Di Giulio and Valloni (1992). Standardised definitions of non-framework categories are not yet available. A synthesis of various schemes in current use has been published by Mijnlieff et al. (1999).

### *2.2. The traditional or Indiana method*

The ‘Indiana school’ regards the framework composition of sandstone as a function of provenance, transport history and post-depositional modifications (Suttner, 1974; Suttner et al., 1981). The Indiana point-counting method is essentially based on formalisation of traditional sedimentary–petrographic classification criteria. Ternary framework compositions are commonly expressed in terms of quartz, feldspar and rock-fragment percentages (QFR%). A rock fragment is defined as a grain consisting of two or more phases or crystals, fulfilling at least one of the following criteria:

- No single phase occupies more than 90% of the total area of the grain as observed in a thin section (commonly applicable to very fine or fine sand grains);
- The two phases or crystals are both larger than 0.0625 mm in size (commonly applicable to medium or coarse sand grains).

An exception to this rule is made for polycrystalline quartz varieties, which are regarded as monomineralic rock fragments (Suttner et al., 1981). Carbonate fragments do not readily fit into this scheme.

The Indiana point-counting method has been designed to detect changes in sandstone composition resulting from weathering and transport. Grain-size reduction is invariably accompanied by compositional modification, because the operational definition of rock fragments is sensitive to grain size. Therefore,

a narrow size range must be selected for point counting to ensure compatibility of different data sets.

The results obtained by the Indiana method may be illustrated by considering the compositional evolution of coarse-grained granite detritus, initially consisting of sub-equal proportions of monocrystalline quartz, monocrystalline feldspar and quartzo-feldspathic rock fragments. Compositional evolution in the early stages of weathering is governed by disaggregation of quartzo-feldspathic rock fragments along crystal interfaces, which produces Q and F grains of medium and fine-sand size. Hence, slightly weathered granite detritus could be classified according to the Indiana method as ranging from lithic to arkosic, depending on the proportion of R. The proportion of R is expected to vary not only with the extent of weathering, but also across size classes at any given time.

### 2.3. The Gazzi–Dickinson method

The 'Dickinson school' emphasises the use of petrographic techniques for the reconstruction of plate-tectonic settings of sedimentary basins (Dickinson, 1985, 1988). The Gazzi–Dickinson point-counting method was developed independently by Gazzi (1966) and Dickinson (1970) to minimise the effects of grain-size variations on sandstone composition. Ternary framework compositions are commonly expressed as quartz, feldspar and lithic percentages (QFL%). The Gazzi–Dickinson method differs from the Indiana method because sand-sized monomineralic grains or crystals (phaneritic grains: crystal size exceeding 0.0625 mm) forming part of a larger polymineralic grain are classified as phanerites instead of polymineralic grains. Only fine-grained polymineralic fragments (aphanitic grains: crystal size less than 0.0625 mm) are classified as lithics, because such grains can be recognised throughout the sand-size range (Boggs, 1968). Again, carbonate fragments do not fit easily into this scheme. In the absence of other criteria, such grains are labelled 'lime clasts'.

The results obtained by the Gazzi–Dickinson method may be illustrated by considering the compositional evolution of granite detritus expressed in terms of QFL instead of QFR units. If the ratio of sand-size quartz and feldspar crystals in the phanerites is similar to that of the monocrystalline Q and F grains, the proportions of Q and F would not change by breakage of coarse-grained (phaneritic) rock fragments into monomineralic grains of medium and fine-sand size. Note that the proportion of L is expected to be very small, due to the large crystal size of the average granite. Hence, granite detritus would be classified as arkosic according to the Gazzi–Dickinson method, regardless of the extent of weathering and size class considered.

### 2.4. The Gazzi–Zuffa method: a synthesis

Zuffa (1980, 1985, 1987, 1991), building on the work of Gazzi (1966), developed a classification scheme encompassing all grain types occurring in sand and sandstone. In addition to the non-carbonate extrabasinal (NCE) grains commonly considered in provenance studies, this extended classification scheme also includes detailed subdivisions for other categories of framework elements: carbonate extrabasinal (CE), non-carbonate intrabasinal (NCI), and carbonate intrabasinal (CI) grains. The extended scheme was developed to enable analysis of spatial and temporal relations between grains in mixed siliciclastic-carbonate sands (e.g., Fontana et al., 1989; Garzanti, 1991). It can be used in conjunction with both point-counting methods.

Compatibility between the Indiana and Gazzi–Dickinson methods is achieved by subdividing each category of phanerites into a category comprising monocrystalline grains and several categories of sand-size crystals within larger rock fragments, as originally proposed by Gazzi (1966). For instance, Qm may be defined as a monocrystalline quartz grain, Qrp as a quartz crystal within a plutonic rock fragment, and Qrm as quartz crystal within a meta-sedimentary rock fragment, etc.

### 2.5. Spread and uncertainty in point-count data

A brief note on terminology is required to facilitate subsequent discussions. The term *sample* may have different meanings, depending on the geological or statistical context, so a formal distinction is in order. A *statistical sample* refers to randomly collected observations of certain properties of a population. A *geological sample* is more loosely defined as a finite quantity of rock or unconsolidated sediment, sampled (at random) from (the accessible part of) a rock or sediment body. The possibility of confusion between the two meanings of the term sample is minimised by referring to a geo-

logical sample as a *specimen* (Rock, 1988), so that the term sample is used exclusively in the statistical sense.

Composition estimates obtained by point counting are subject to uncertainty, which results from the sampling scheme used in the field, the preparation of thin sections and the counting procedure itself. The uncertainty is largely determined by the following factors (for general overviews see Griffiths, 1967; Kelley, 1971; Frangipane and Schmid, 1974; Neilson and Brockman, 1977):

- Selection of sampling sites in the field. Sediments tend to be compositionally heterogeneous on a large (inter-specimen) scale, owing to processes such as mixing, weathering and diagenesis. Ideally, the localities where hand specimens are collected should be selected according to a sampling scheme aimed at capturing the spatial compositional variation in a lithosome (e.g., Whitten, 1961; Griffiths, 1967).
- Preparation of thin sections from hand specimens. Heterogeneity within a hand specimen contributes to the uncertainty of the composition estimate. This factor is negligible if the specimen is completely homogeneous, which is unlikely because sediments are in general laminated. It is recommended to cut thin sections perpendicular to laminae or bedding planes, in such a way that the areal proportions of the laminae in thin section equal the volumetric proportions in the rock (Chayes, 1956).
- Selection of the inter-point distance (grid size) to be used in counting. In detrital sediments, where adjacent grains may be safely regarded as independent, the best results are obtained by selecting an inter-point distance larger than the maximum grain size in thin section. Smaller distances reduce the amount of information in the analysis because adjacent observations may fall on the same grain, which inflates the uncertainty (Van der Plas and Tobi, 1965; Manetti and Turi, 1969; Neilson and Brockman, 1977).
- Selection of the total number of points to be counted. Counts of individual components follow a binomial distribution under the appropriate sampling conditions (i.e., randomly chosen points from a homogeneous thin section), implying that component standard deviations are proportional inversely to the square root of the number of points counted (Dryden, 1931; Chayes, 1956; Van der Plas and Tobi, 1965).
- Random operator error, resulting from occasional misidentification of components. For practical purposes, it can be regarded as a kind of sampling error that tends to inflate the spread of the estimates.
- Systematic operator error, resulting from systematic misidentification of certain components relative to a standard classification scheme. Systematic deviations from the 'true' composition arise if probabilities of misidentification are unequal for different grain types. Systematic operator error may thus be thought of as the application of different classification schemes to the same (suite of) specimens. Posterior adjustment of composition estimates is possible in the unlikely event that probabilities of misidentification can be estimated (Demirmen, 1972). In practice, the magnitude of operator error depends on the type of rock and the degree of training of the analyst, so that it can only be assessed successfully by replicate analyses involving multiple operators. Careful evaluation of operator error is required in cases where data produced by multiple analysts have been lumped to generate large data sets for statistical analysis.

### *2.6. Thin-section grain-size analysis*

Point counting has also been applied in sedimentary petrography to estimate grain-size distributions of consolidated sediments from measurements of apparent grain size in thin section. Conversion from number-frequency distribution of apparent diameters into weight-frequency distribution of 'true' diameters is a difficult problem. Theoretical conversion equations have been designed for idealised particles, such as spheres, spheroids, or ellipsoids following specific spatial distribution functions (Ripley, 1981). Their applicability to sands and sandstones appears to be limited. Moreover, the uncertainties associated with the thin-section measurements should also be taken into account in the estimation procedure. Many researchers have attempted to bypass these problems by developing empirical conversion equations (Rosenfeld et al., 1953; Friedman, 1958, 1962, 1996; Griffiths and Ondrick, 1969; Adams, 1977; Harrell and Eriksson, 1979; Johnson, 1994, 1996). The theoretical conversion problem belongs to the field of geometric probability theory known as stereology. As an exhaustive discussion of this subject is far beyond the scope of this review, the interested reader is referred to Ripley (1981). Textoris (1971), Kellerhals et al. (1975) and Johnson (1994) discuss

thin-section grain-size analysis of sandstones in some detail.

### 2.7. Conversion between modes and norms

Detrital modes of sands and sandstones are usually regarded as the most informative compositional description for a wide range of sedimentary–petrologic applications. However, it may be required to convert a detrital mode into a chemical composition, or it may be desirable to cast the results of chemical analyses in mineralogical terms. The latter conversion is known as normative analysis and has a long history in petrology, starting with the classic work of Cross et al. (1902). Most efforts in this field have concentrated on normative partitioning of chemical elements between (hypothetical) minerals (Rock, 1988; Weltje, 1997). While this approach has been successful in igneous and metamorphic petrology, where mineral assemblages can be assumed to be in equilibrium with specific physicochemical conditions, it has been far more difficult to develop a useful normative partitioning approach to detrital sediments. Two obvious reasons for the lack of success are that a considerable proportion of sand-size grains is of polymineralic composition, and the concept of an equilibrium assemblage cannot be applied. Reed and Condie (1987) discussed the problem of reconstructing original detrital composition of graywacke from chemical analysis of the pseudo-matrix. Bangs Rooney and Basu (1994) proposed integration of optical and X-ray techniques to infer detrital precursors of clay-size materials in sandstone, in order to reconstruct mineralogical modes of muddy sandstones. Recent advances in normative partitioning have resulted in the development of general-purpose computer codes (De Caritat et al., 1994). Friedman (1960), Root (1978) and Usdansky (1985) have presented methods to predict chemical composition from mineralogical modes obtained by point counting of igneous and metamorphic rocks.

## 3. Analysis of ternary compositions: a brief history

### 3.1. Compositional data

Compositions are the principal data used in sedimentary petrology. Such data are commonly expressed as proportions, percentages, or parts per million, and thus sum to a constant value $C$ (equal to 1, 100, or $10^6$, respectively):

$$\sum_{i=1}^{k} x_i = C, \text{ where } x_i \geq 0 \quad (1)$$

Because all component abundances $x_i$ are non-negative by definition, the value of the $k$-th component in a composition of $k$ parts is automatically fixed by the sum of the other $k-1$ values. This inevitable physical limitation implies that compositional data are constrained in the sense that they are not free to take on any value or to vary independently. Consequently, they are not amenable to analysis by common statistical methods designed for use with unconstrained data (Chayes, 1960; Aitchison, 1986).

The difficulty of interpreting compositional data is well illustrated by the following trivial example: '...If one analyses the contents of a jar half-filled with sand and finds, by a random sample, that it contained (by volume) about 20% quartz, 30% feldspar, 40% rock fragments, and 10% miscellaneous constituents, then, if the volume of the jar were doubled by addition of grains of pure quartz, a second random sample would reveal that the jar contains 60% quartz, 15% feldspar, 20% rock fragments, and 5% miscellaneous. Feldspar, rock fragments, and miscellaneous constituents appear pair-wise positively correlated and all three appear negatively correlated with the quartz abundance. Also, all four components have shifted mean values despite the fact that only the quartz content of the jar changed...' (Woronow, 1991).

Although the interdependency of compositional variables has been recognised for over a century (Pearson, 1897), appropriate statistical methods for analysing such data have been extremely slow to emerge. Researchers who recognised the problems associated with statistical analysis of compositions were unable to provide feasible solutions (e.g., Chayes, 1960; Butler, 1979). Many scientists therefore decided to abandon statistical analysis of compositions altogether. Others wished away or ignored the awkward constraints on compositions to justify the use of standard statistical methods for compositional data analysis (Aitchison, 1986).

### 3.2. Ternary diagrams

Ternary diagrams have been used widely in the earth sciences to visualise numerical data that can be expressed in terms of ratios of three components (ternary percentages or proportions). The first of these diagrams appeared in the geological literature around the end of the nineteenth century (Becke, 1897). Examples of the use of ternary diagrams can be found in geochemistry, sedimentology and palaeontology, but they have been especially popular in various branches of petrology. The following discussion largely concentrates on sedimentary petrology, but many of the concepts are equally relevant to other disciplines in which use is made of ternary diagrams.

Ternary compositions play a central role in classification schemes and provenance models of sand and sandstone. A typical sedimentary provenance analysis proceeds as follows: Raw point-count data or subsets thereof, are amalgamated to form three groups, whose totals are normalised to yield ternary percentages or proportions. The data points or their arithmetic means may then be displayed in a ternary diagram, at which stage most petrographic analyses are considered complete. Dissatisfaction with this purely descriptive approach has led many petrographers to take one further step by constructing so-called *fields of compositional variation*. The objective of these fields is to capture the scatter of data points in ternary diagrams using summary statistics like the sample means and standard deviations of the data. Ongoing discussion about the preferred method of construction and statistical interpretation of such fields (Philip et al., 1987; Howard, 1993, 1994) may be due to the fact that their theoretical basis has not been fully examined.

The ideal field of variation corresponds to a statistically rigorous *confidence region* or *predictive region* that adequately captures the distribution of data points in a ternary diagram. A fundamental property of such regions is that they define an area in which the true values of the population parameters are located with some fixed probability. This implies that their boundaries must be defined by equal probability contours. The probability associated with a confidence region is termed the *confidence level* or simply the *content*, usually expressed as $(1-\alpha)$ or $100(1-\alpha)\%$, where $\alpha$ is defined as the *significance level*. Such regions could be used to predict the range of variation of the entire population, or the range of variation of the population mean.

The capability to construct predictive regions of compositional variation is essential to quantitative sedimentary petrography, because it enables one to assess the significance of compositional differences between (sets of) rock specimens in an objective and reproducible way. It also allows quantitative predictions to be made based on observations, which should increase the usefulness of petrographic techniques in provenance studies, hydrocarbon exploration and sedimentological reservoir characterisation, because it opens the way to stochastic simulation of sediment composition across a basin (Woronow, 1993). Moving from the current, largely descriptive methods towards a statistically rigorous approach is a prerequisite for elevating the status of sedimentary petrology to that of a widely applicable quantitative tool for basin analysis.

The fundamental problems associated with the various methods put forward thus far are discussed below to provide a starting point for alternative approaches. Two well-established multivariate statistical models will be adapted to the task of visualising the range of variation in a series of ternary composition estimates, and the uncertainty associated with a single composition estimate from point-count data. The statistical theory and numerical implementation of the methods will be exposed in some detail, followed by a few applications to practical problems.

### 3.3. Non-statistical approaches

The simplest method for capturing patterns of compositional variation in ternary diagrams is to trace the outline of a cluster of data points by a smooth hand-drawn line (e.g., Dickinson and Rich, 1972; Fontana et al., 1989; Valloni *in* Ibbeken and Schleyer, 1991). A variation on this theme is ‘eyeball fitting’ of regular geometric shapes, usually ellipses, to clusters of data points. The mere intention of these methods is to facilitate qualitative assessments of the data. A quantitative non-statistical approach to characterise compositional variation in ternary diagrams was proposed by Philip and Watson (1988) and Watson and Philip (1989). The essence of their method is local-density estimation and contouring on the basis of a

tessellation of ternary compositional space. This computationally intensive method does not allow any straightforward inference such as statistical testing of compositional homogeneity of multiple samples. Moreover, the validity of the assumptions underlying this method has been strongly debated (Aitchison, 1990, 1991a,b, 1992; Watson, 1990, 1991).

### 3.4. Univariate normal approximation for multiple compositions

The most popular statistical model in the sedimentary–petrologic literature has been the univariate normal or Gaussian distribution. The conventional approach to statistical analysis in sedimentary petrography may be introduced by considering a typical data set consisting of ternary composition estimates. The data are assumed to have been obtained from point counting a series of thin sections, each derived from a different specimen. The sample size $n$ is thus equal to the number of specimens. This data set is usually processed by calculating the *arithmetic sample mean*:

$$m_x = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{2}$$

and the *sample standard deviation*:

$$s_x = \sqrt{\frac{\sum_{i=1}^{n}(x_i - m_x)^2}{n-1}} \tag{3}$$

of each component separately, under the implicit assumption that component proportions follow a univariate normal distribution. In the 'Dickinsonian' approach to provenance analysis, each sample standard deviation must be divided by the square root of the sample size to obtain the *standard error of the mean*:

$$e_x = \frac{s_x}{\sqrt{n}} \tag{4}$$

The next step is to convert the measures of spread (Eqs. (3) and (4)) to confidence limits. Proper application of the univariate normal distribution requires that each of the standard deviations (or standard errors) be multiplied by a value of Student's $t$ with $df = n - 1$ degrees of freedom, corresponding to a desired significance level $\alpha$. The $(1-\alpha)$ confidence limits of $x$ in the population of interest are defined as:

$$\mathrm{CL_d} = m_x \pm s_x t_{(df;\alpha/2)} \tag{5}$$

In addition, the $(1-\alpha)$ confidence limits of the population mean $m$ are defined as:

$$\mathrm{CL}_m = m_x \pm e_x t_{(df;\alpha/2)} \tag{6}$$

The results of the univariate statistical analysis are summarised in statements such as: The (mean) quartz content of this type of sandstone is $Q\% \pm \Delta Q\%$, the (mean) feldspar content is $F\% \pm \Delta F\%$, and the (mean) lithic content is $L\% \pm \Delta L\%$, at a confidence level $(1-\alpha)$.

### 3.5. Univariate normal approximation for a single composition

A similar approach was adopted in igneous and metamorphic petrology (Chayes, 1949, 1956; Chayes and Fairbairn, 1951; Van der Plas and Tobi, 1965), to quantify the uncertainty in estimates of mineral composition obtained by point counting. In this field of petrology, the univariate normal distribution plays a central role as a large-sample approximation to the binomial distribution. A typical application involves the counts obtained from a single thin section (specimen). Note that the term sample in this context refers to the count length $N$. The number of points falling on the $i$-th component is defined as $n_i$ and the observed component proportions $\hat{p}_i$ are obtained from the relation:

$$\hat{p}_i = n_i/N \tag{7}$$

According to statistical theory, the observed component proportions $\hat{p}_i$ are the best estimate of the corresponding population values $p_i$, allowing use of the population standard deviation of the binomial distribution to estimate the standard deviation of the observed proportions. The normal approximation to

the binomial standard deviation of the estimated proportion is defined as:

$$s_{\hat{p}} = \sqrt{\frac{\hat{p}_i(1-\hat{p}_i)}{N}} \tag{8}$$

The confidence limits for the estimated proportions are defined analogously to those above:

$$\mathrm{CL}_{\hat{p}} = \hat{p}_i \pm s_{\hat{p}} t_{(df;\alpha/2)} \tag{9}$$

where $df = N - 1$ and $\alpha$ is the desired significance level.

Van der Plas and Tobi (1965) used a similar method for constructing their widely used nomogram. The same large-sample approximation was proposed earlier in sedimentary petrology for assessing the uncertainty associated with counting of heavy minerals in slides (Dryden, 1931). It leads to statements about compositional variability similar to the one given above.

### 3.6. Validity of univariate normal approximations

The above methods are valid only in cases where the proportions of each component can be reasonably well approximated by a normal distribution. In addition, the univariate approach carries the implicit assumption that the proportions of each component are independent of those of the other components. Let us examine if these assumptions are reasonable in the simplest of cases, i.e., a single thin section cut from a specimen made up of two components only. The binomial distribution is appropriate for characterising the uncertainty associated with counting a finite number of points which may fall into one of two classes (a classic example is the number of heads or tails in a coin-tossing experiment). The counts follow a binomial distribution if we make the additional assumption that successive observations (points) are independent and the rock is homogeneous on the scale of the thin section.

Fig. 1 shows the normal approximation (Eq. (9)) of the 90%, 95% and 99% confidence limits on three proportions (0.5, 0.2 and 0.05). If the proportions of the two minerals in the rock are sub-equal, i.e. each close to 0.5 (Fig. 1A), their binomial distributions are symmetric and can be well approximated by a normal distribution. However, for small samples ($N < 12$), the normal approximation to the 99% confidence limits predicts values less than zero and greater than unity, for which there can be no physical explanation. One should realise that even a predicted value of exactly zero is impossible, because it implies that the observed

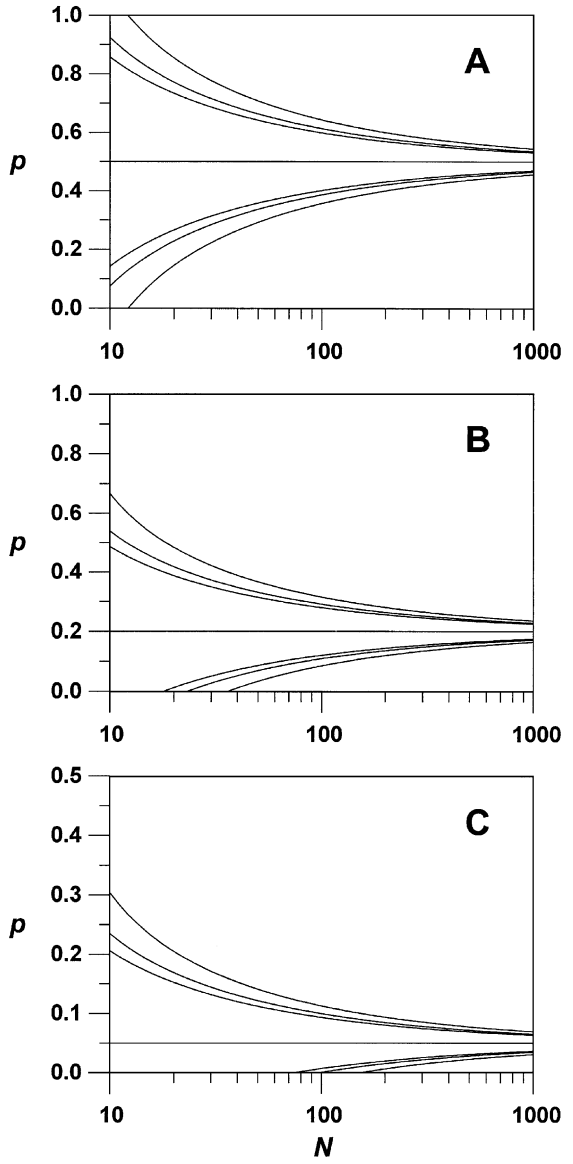


Fig. 1. Univariate normal approximations to binomial confidence limits of proportions ($p$) as a function of count length ($N$). (A) $p = 0.5$; (B) $p = 0.2$; (C) $p = 0.05$. Confidence limits are 90%, 95% and 99%. Predictions extending into the realm of negative proportions indicate that the statistical model is not valid across the full range of $p$ and $N$.

component is not represented in the population under consideration, so that it could never have been observed (similar logic applies to a predicted value of exactly unity). The validity of the normal approximation is questionable for proportions that deviate considerably from 0.5 (Fig. 1B and C), because the binomial distributions of such rare components are markedly skewed. The inadequacy of the normal approximation is apparent for lower confidence limits, which predict negative proportions even for large sample sizes (99% lower confidence limits are negative for $N<40$ and $N<150$, respectively). The symmetry of lower and upper confidence limits about the observed proportions indicates that the same applies to predicted upper confidence limits on dominant components (0.8 and 0.95, the exact mirror images of Fig. 1B and C), which may exceed unity.

Extension of this discussion to a rock with three (or more) components leads to similar conclusions about the validity of the normal approximation. It gives reasonable results for large samples of component distributions near the centre of the ternary diagram (1/3,1/3,1/3), but fails for small samples and proportions close to the edges because there is no guarantee that predicted component ranges fall within the interval $\langle 0;1\rangle$. The reason for this undesirable result is that the normal distribution is a rather poor model for compositional data, because it can produce any value between $[-\infty;+\infty]$ and often fails to yield good approximations. Van der Plas and Tobi (1965) correctly stated that their nomogram, which is based on the above approximation, should not be used for rare components.

It is clear that the second (implicit) assumption of independence of proportions is fundamentally incorrect. The lack of independence between proportions is an intrinsic property of compositional data, which arises from the non-negativity and constant-sum constraints listed above. We know that in the case of a two-component rock, the sum of the two proportions equals unity by definition, implying that one proportion fully defines a binary composition. The two components thus show a perfect negative correlation (Pearson's correlation coefficient $r=-1.0$). In this particular case, the univariate description of one component happens to provide an exhaustive description of the rock's composition, because there are only two components. However, the univariate description exemplified by the statement given above does not honour this constraint, as shown by a simple stochastic simulation experiment. One cannot select at random two values from the permissible ranges of uncertainty specified for each of the two components (cf. Eq. (9)) without violating the constant-sum constraint. Instead, one should choose a value from the permissible range of uncertainty of one component and deduce the value of the second from the relation $p_2=1-p_1$. This still does not eliminate the problem of spurious negative proportions resulting from the normal approximation.

In rocks made up of more than two components, it is no longer possible to uniquely define compositional variability by means of univariate statistics. Again, the simplest way to check this is to use the conventional summaries of compositional variability in ternary systems as a basis for conducting stochastic simulations. One cannot select three arbitrary values from the permissible ranges of uncertainty in each component (cf. Eq. (9)) without violating the constant-sum constraint, owing to the lack of independence of component proportions. The only way to obtain a physically meaningful composition would be to select at random two out of three values, and impose $p_3=1-p_1-p_2$. Randomly selecting two out of three proportions implies that two out of three proportions are statistically independent. This arbitrary decision forces the third proportion to be negatively correlated with the other two (Chayes, 1960). Which of the three proportions (if any) should fulfil this role is not clear, again indicating that information is missing from the univariate description. If we add to this the possibility of obtaining negative values, as discussed above, we are compelled to conclude that conventional univariate statements do not allow a valid characterisation of compositional variation in systems of three or more components.

### 3.7. Other univariate approaches

The binomial and univariate normal distributions are by no means the only statistical models applied to point-count data. More sophisticated univariate models have been developed by several workers in igneous, metamorphic and sedimentary petrology to deal with specific sampling schemes and scales of compositional heterogeneity. The interested reader is referred to Chayes (1949, 1956), Griffiths and Rosenfeld (1954), Shaw and Harrison (1955), Bayly (1960a,b, 1965),

Griffiths (1960, 1962, 1967), Hasofer (1963), Solomon (1963), Chatterjee (1965), Schryver (1968), Manetti and Turi (1969), Guasparri and Sabatini (1970), Demirmen (1971, 1972), Frangipane and Schmid (1974), Neilson and Brockman (1977) and Bardsley (1983). Without exception, the methods proposed by these authors aim at establishing suitable frequency distributions of proportions of individual minerals. Although some of the above models will undoubtedly be more appropriate in specific cases than the binomial or normal distributions, they do not eliminate the fundamental problems of a univariate approach. In view of the unit-sum constraint on proportions, univariate methods are at most capable of characterising compositional variability in a two-component system. They cannot be used as a general tool for characterising compositional variation of sediments comprising more than two components.

### 3.8. Hexagonal fields of variation

The well-known hexagonal fields of compositional variation in ternary diagrams were introduced independently in various fields of the earth sciences (e.g., Stevens et al., 1956) as a logical extension of the use of univariate normal approximations. The papers by Guasparri and Sabatini (1970) and Ingersoll (1978) provide early examples of their use in igneous and sedimentary petrology, respectively. A hexagonal field of variation is usually constructed by plotting each measure of spread, calculated by means of normal approximation (Eqs. (2)–(6)), as a pair of lines about the arithmetic sample mean (Philip et al., 1987; Howard, 1994). The orientation of each pair of lines is parallel to the side of the diagram that is opposite to the component's vertex. The desired hexagon corresponds to the area of intersection of the three bands that define each component's range. The procedure is illustrated by labelling the predicted lower and upper confidence limits of each component (Eqs. (5) and (6)) with subscripts L and U, to give the following range of possible values for the component proportions in a ternary QFR system:

$$Q_L \le Q \le Q_U$$

$$F_L \le F \le F_U$$

$$R_L \le R \le R_U \tag{10}$$

From these limits, a set of six ternary compositions is constructed to define the hexagon:

$$\begin{bmatrix} C-F_L-R_U & F_L & R_U \\ Q_L & C-Q_L-R_U & R_U \\ Q_L & F_U & C-Q_L-F_U \\ C-F_U-R_L & F_U & R_L \\ Q_U & C-Q_U-R_L & R_L \\ Q_U & F_L & C-Q_U-F_L \end{bmatrix}, \tag{11}$$

where $C$ is the constant-sum value defined in Eq. (1).

At first glance, the hexagonal fields of variation appear to be a straightforward graphic translation of the statement about compositional variability in the QFR system given above. However, closer examination reveals three important differences.

The first difference may be illustrated by considering a bivariate normal population with zero covariance. We expect the correlation coefficient of a random sample from this distribution to be close to zero, indicating near independence of the two variables (Fig. 2A). Application of the conventional univariate statistical methods (Eqs. (5) and (6)) allows one to calculate the confidence ranges of each of the variables separately. It is well known from statistical theory that the equal probability contours of a bivariate normal distribution are elliptical (Morrison, 1976; Davis, 1986; Press et al., 1994). Fig. 2A shows the 90%, 95% and 99% confidence ellipses (equal probability contours) for the sample, calculated according to the method given in Appendix B.2. The meaning of equal probability contours is most easily understood in terms of sampling from the bivariate normal distribution. Specimens sampled at random from this distribution have a probability equal to $(1-\alpha)$ of being enclosed by a $(1-\alpha)$ ellipse, and therefore a probability equal to $\alpha$ of falling outside this region. It is clear that data points with both $(x,y)$ values equal to the lower and/or upper limit of each variable's range are considerably less likely to be observed, because such data points fall outside the ellipse. In other words, there is no statistically meaningful way to construct a 'confidence box' or 'rectangular field of variation' around the data points by means of univariate statistics, even in cases where two variables are uncorrelated. Boundaries of hexagonal fields in ternary diagrams are constructed according

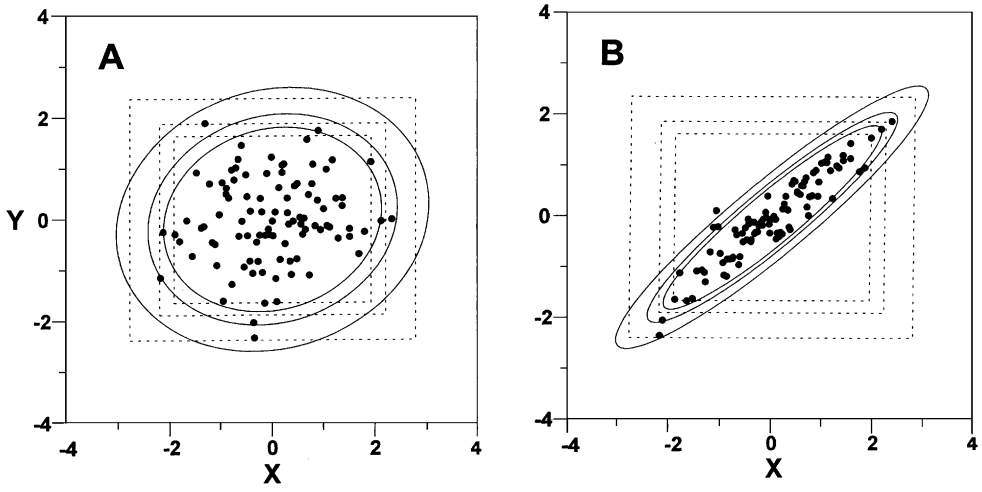


Fig. 2. (A) Bivariate normal distribution with zero correlation between attributes, showing univariate ranges at 90%, 95% and 99% confidence levels in the form of horizontal and vertical bars. Each confidence region is represented by an ellipse with principal axes subparallel to *X*- and *Y*-axes. Also shown is a 'rectangular field of compositional variation' constructed from univariate ranges. (B) Bivariate normal distribution with univariate summary statistics identical to (A), but displaying strong positive correlation between attributes. Each confidence region is represented by an elongated ellipse with principal axes oblique to *X*- and *Y*-axes. Also shown is a 'rectangular field of compositional variation' constructed from univariate ranges. Note the lack of fit due to nonzero correlation.

to the same principle: They enclose the area of intersection of three independently calculated univariate ranges, and therefore are the ternary equivalent of the 'rectangular field of variation.' It follows that the outline of the hexagon cannot possibly represent an equal probability contour.

The other two differences between the numerical and graphic representations are related to the method of constructing the hexagon, which enforces the two fundamental constraints on compositional data. The unit-sum constraint is automatically implemented because all points in the ternary diagram are located on the constant-sum plane passing through the points ($C$,0,0), (0,$C$,0) and (0,0,$C$), as shown in Eq. (11). Simply deleting those parts of the hexagon extending beyond the triangular boundaries of the diagram ensures non-negativity. The fundamental flaws of the univariate normal approximation are thus hidden from view.

### *3.9. The missing covariance structure*

In many sedimentary–petrologic applications, the objective is to model the spread of ternary composition estimates from a series of genetically related specimens. The univariate approach is even less appropriate if compositional variation reflects specific geological processes, instead of some random sampling error. Examples of geological processes that generate characteristic patterns of compositional variation in sediments are (Weltje, 1995, 1998; Weltje et al., 1998):

- Mixing of different sediment populations (feeder systems);
- Selective depletion/enrichment of components due to weathering and/or diagenesis;
- Selective entrainment, transport and deposition related to variations in size, shape and density of grains.

Each of these processes is likely to be associated with a characteristic covariance structure of component proportions. The pattern of compositional variability obtained by random sampling of grains from a fixed population is expected to differ from patterns in natural sediments, because the population is fixed and the underlying process is non-selective. Because complete independence of component proportions is impossible owing to the unit-sum constraint, the covariance structure of composition estimates associ-

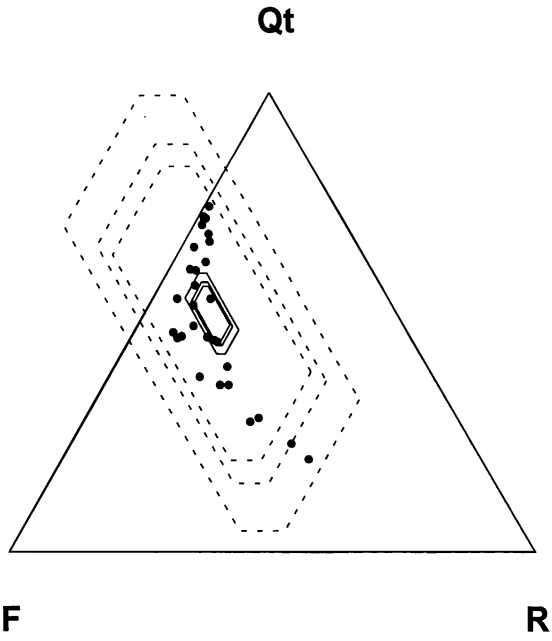


Fig. 3. Hexagonal fields of variation constructed from univariate summary statistics of the data in Table 1. Solid line: confidence regions of the population mean; dashed line: confidence regions of the entire population. Confidence limits are 90%, 95% and 99%. The curved pattern of compositional variation resulting from selective compositional modification cannot be captured by a hexagon, resulting in a clear lack of fit. Also note the predictions extending beyond the limits of compositional space.

ated with random counting errors provides the closest possible analogue of the familiar concept of uncorrelated random errors in unconstrained variables.

A sample from a bivariate normal distribution with means and standard deviations identical to the sample shown in Fig. 2A is depicted in Fig. 2B. The 'rectangular field of variation' or 'confidence box' constructed from univariate summary statistics of this sample is therefore identical to the one in Fig. 2A. However, the two variables in our second sample from a bivariate normal distribution display a strong positive correlation. This is reflected in the elongated 90%, 95% and 99% confidence ellipses shown in Fig. 2B. The shortcomings of the univariate approach are even more conspicuous in the presence of inter-component correlation, as the rectangle completely fails to capture the shape of the cloud of data points. Use of the 'rectangular field of variation' thus leads to extremely poor predictions. The similarities and differences between Fig. 2A and B clearly illustrate the incompleteness of a univariate description that provides no information about the covariance structure of the data.

Similar problems with the univariate approach can be shown to exist in the ternary case. Fig. 3 shows hexagonal fields of variation of a synthetic data set listed in Table 1. The data can be thought of as a series of specimens obtained from different depths of a weathering profile, which covers the full range of compositional modification from a saprolith to a mature soil. They illustrate the compositional trend expected from mechanical and chemical weathering of sand-sized granite detritus (Nesbitt et al., 1997), if detrital modes are obtained by the Indiana point-counting

Table 1
Synthetic point-count data (Indiana method) constructed to emulate a pattern of compositional variation attributable to selective modification (mechanical and chemical weathering of granitic detritus)

| Label | Qt | F | R |
|---|---|---|---|
| G-01 | 102 | 164 | 234 |
| G-02 | 119 | 172 | 209 |
| G-03 | 143 | 199 | 158 |
| G-04 | 147 | 189 | 164 |
| G-05 | 183 | 207 | 110 |
| G-06 | 183 | 199 | 118 |
| G-07 | 192 | 222 | 86 |
| G-08 | 203 | 190 | 107 |
| G-09 | 230 | 186 | 84 |
| G-10 | 232 | 188 | 80 |
| G-11 | 234 | 222 | 44 |
| G-12 | 235 | 193 | 72 |
| G-13 | 236 | 217 | 47 |
| G-14 | 240 | 223 | 37 |
| G-15 | 247 | 200 | 53 |
| G-16 | 269 | 189 | 42 |
| G-17 | 276 | 201 | 23 |
| G-18 | 276 | 169 | 55 |
| G-19 | 290 | 177 | 33 |
| G-20 | 306 | 168 | 26 |
| G-21 | 307 | 173 | 20 |
| G-22 | 315 | 154 | 31 |
| G-23 | 331 | 157 | 12 |
| G-24 | 337 | 139 | 24 |
| G-25 | 345 | 136 | 19 |
| G-26 | 355 | 137 | 8 |
| G-27 | 361 | 132 | 7 |
| G-28 | 362 | 130 | 8 |
| G-29 | 364 | 131 | 5 |
| G-30 | 375 | 120 | 5 |

Qt = total quartz, F = feldspar, R = rock fragments. Sample size $n = 30$.

method (Weltje, 1995, 1998; Weltje et al., 1998). The main effect of mechanical weathering, the dominant process in the initial stages of compositional modification, is to produce monocrystalline Q and F from disaggregation of R. The effect of chemical weathering, which becomes the dominant process after most of R has been removed, results in the depletion of F relative to Q. The combined effect of these weathering trends is expressed as a curved pattern in ternary QFR space. The mismatch between the predicted range of variation (the hexagons) and the data indicates that such patterns of compositional variation cannot be captured by a set of univariate normal approximations, as observed by several authors (Philip et al., 1987; Philip and Watson, 1988; Aitchison, 1989).

### 3.10. Concluding remarks

The fundamental problems associated with the use of univariate statistics and the construction of 'hexagonal fields of variation' can be summarised as follows:

- The assumption that the distribution of component proportions can be adequately approximated by a normal distribution is not generally valid, especially in cases of small samples and/or (average) proportions close to zero or unity, because it leads to predictions extending beyond $\langle 0;1 \rangle$, the physical limits on proportions.
- Hexagonal fields of variation that have been calculated from univariate summary statistics show a distinct lack of fit to the data in cases where the pattern of compositional variability results from selective modification. All information about the covariance structure of the data is lost if a univariate method is applied. The implicit assumption that component proportions are independent, which is necessary for justifying a univariate approach to compositional data, is incorrect.
- Hexagonal boundaries in ternary diagrams do not represent equal probability contours, but actually consist of the area of intersection of three independently calculated univariate ranges. The points raised above indicate that hexagonal fields of variation must be regarded as mere graphic constructs that are not supported by a viable statistical model, and thus cannot be used as predictive tools. It is also clear that any appropriate method for constructing statistically rigorous confidence regions in ternary diagrams should honour the two fundamental constraints on compositional data (Eq. (1)). This automatically leads to the use of multivariate methods that treat the composition as a whole and enable one to take into account the covariance structure of the data. Two multivariate statistical models applicable to a wide range of practical problems encountered by sedimentary petrologists are discussed below.

## 4. Statistical models: concepts and definitions

### 4.1. Introduction

The uncertainties of composition estimates based on point counts can be described on two levels:

- Model A: The point (grain) is regarded as the basic unit of observation, and the count (composition) as a sample.
- Model B: The count (composition) is regarded as the basic unit of observation, and a series of counts as a sample.

### 4.2. Model A: the grain as unit of observation

During point counting, each point or observation is classified into one of a number of mutually exclusive categories. All categories together should represent an exhaustive description of the rock. This is usually accomplished by introducing a class of points labelled 'other' or 'rest' to ensure that all observed points can indeed be classified.

The uncertainty associated with such composition estimates obtained by point counting of a single thin section under ideal conditions can be predicted from statistical theory. The following conditions define this so-called Bernouilli sampling process:

- Homogeneity: the probability of observing a grain of a given type is a fixed quantity throughout the thin section;
- Independence: the probability of observing a grain of a given type is independent of the result of the previous observation.

Loosely speaking, the first assumption is justifiable if a thin section is visually homogeneous, implying that

components are randomly distributed throughout the thin section. Sediments that are laminated on a scale smaller than the dimensions of a thin section cannot be considered as homogeneous. The condition of independence of successive observations is fulfilled if sampling points are chosen at random (Chayes, 1956; Demirmen, 1971; Neilson and Brockman, 1977; Bardsley, 1983). This condition is difficult to reconcile with the use of a rectangular sampling grid, because all points are fixed after the first grid point has been chosen. However, stochastic independence of observations can be safely assumed if the grid size (point distance) is greater than the maximum grain size, because adjacent observations do not fall on the same grain (Van der Plas and Tobi, 1965; Manetti and Turi, 1969; Galehouse, 1971), and adjacent framework grains in detrital sediments are independent by definition.

Under the above conditions, the proportions of each component follow a binomial distribution. The composition of the specimen as a whole, i.e., the joint distribution of component proportions, can be described by a multivariate generalisation of the binomial called the *multinomial distribution*. Eisenhart (1935a,b) implicitly referred to the multinomial by advocating the use of a $\chi^2$ test to quantify the degree of compositional similarity between heavy-mineral counts. Griffiths (1960, 1967) was the first to explicitly mention the multinomial distribution as a suitable statistical model for sedimentary–petrologic data. Kelley (1971) should be credited for providing the first examples of its application, and for discussing the problem of spurious correlations between proportions induced by the unit-sum and non-negativity constraints (Eq. (1)).

According to this model, each point represents an independent observation. A composition estimate obtained by counting a series of $N$ points in thin section is thus regarded as a statistical sample of size $N$. Composition estimates are usually regarded as representative samples of thin sections, which in turn are assumed to be representative of the hand specimens from which they were cut. Statistical inferences about the population of interest thus refer to the specimens. The condition of homogeneity implies that component proportions in the population are fixed quantities. The only source of variation pertains to a random sampling error associated with the finite number of points counted, with a precision proportional to the square root of sample size $N$. This model allows one to describe the uncertainty in the estimated composition of a rock as a whole by calculation of $(1-\alpha)$ confidence regions of the population composition. Hence, multinomial confidence regions calculated from point-counted thin sections that were cut from different specimens may be used to determine if the rock unit from which these specimens were derived is compositionally homogeneous. Sources of compositional variation other than a random sampling error must be present if the point counts differ significantly, indicating that the sediment is not of uniform composition. Because the population concept in this model is tied to a random sampling error only, the conclusion in the latter case should be that the point counts are unlikely to represent samples from a single population. The multinomial can also be applied to analysis of operator error, by comparing composition estimates obtained from the same thin section by different analysts.

Model A cannot be applied if assumptions of independence or homogeneity do not hold. Manetti and Turi (1969) and Demirmen (1971) experimentally showed the effects of violating the independence assumption. A lack of independence is obvious if the size of the counting grid approaches the grain size of sediments. The multinomial distribution is also inadequate in cases where stochastic independence of adjacent observations cannot be safely assumed, as in many crystalline rocks (Whitten and Dacey, 1975; Neilson and Brockman, 1977; Vistelius and Harbaugh, 1980). The problems associated with violation of the homogeneity assumption have been addressed mainly in the context of quantifying the composition of strongly foliated metamorphic rocks (Shaw and Harrison, 1955; Chayes, 1956). Griffiths (1960, 1967) pointed out that they are equally relevant to the analysis of laminated sediments. A practical solution to the problem of estimating the uncertainty of point-count data in such cases is to perform a series of replicate analyses, as advocated by Chayes (1949, 1956), Griffiths (1960, 1967), Demirmen (1971), Neilson and Brockman (1977) and Bardsley (1983). Essentially the same approach may be used to investigate the effects of operator error. Statistical analysis of such replicates may be performed with Model B.

### 4.3. Model B: the composition as unit of observation

An alternative view is that a series of points counted in thin section forms a single multivariate observation (Imbrie and Van Andel, 1964; Aitchison, 1986, 1989; Aitchison and Shen, 1984; Weltje, 1995, 1997, 1998). A series of $n$ composition estimates thus constitutes a sample of size $n$. The population concept employed in Model B is much more flexible than the fixed population employed in Model A. Composition estimates obtained by point counting are considered replicates, whose pattern of variation reflects the covariance of component proportions in the population. The operational definition of the population of interest depends on the experimental layout. If the thin sections were cut from specimens derived from a single rock unit, the population is that unit. It is also conceivable that the thin sections were derived from specimens belonging to different rock units within a basin, in which case the entire basin fill may be considered as the population of interest.

This conceptual model is formalised by use of the multivariate *additive logistic normal distribution* (Aitchison, 1986). Stattegger and Morton (1992), Prins and Weltje (1999a) and Garzanti et al. (2000) have used ternary confidence regions for petrographic data based on this model. Application of the logistic normal distribution allows the calculation of two types of $(1-\alpha)$ confidence regions for a series of $n$ compositions:

- Confidence regions of the entire population, which may be used to predict the range of variation in observations;
- Confidence regions of the population mean, which are useful for deciding if samples differ significantly from one another.

Confidence regions calculated with this model show the combined effects of all sources of variation, including the sampling error as defined above. The number of points counted to arrive at each composition estimate is not taken into account in Model B. The uncertainty associated with sampling of a few hundred points (cf. Model A) is typically small relative to the spread of the entire population, because sediments tend to be heterogeneous on a large (inter-specimen) scale. Hence, individual composition estimates within a sample are expected to differ significantly from each other according to Model A if the spatial extent of the population of interest exceeds the scale of a thin section.

## 5. Construction of confidence regions

### 5.1. General properties

The construction of confidence regions for population parameters is complementary to common significance tests. The purpose of such tests is to determine if parameter values estimated from a sample are consistent with known population parameters. A well-known univariate test of this type is the one-sample Student's $t$-test (e.g., Davis, 1986; Rock, 1988; Press et al., 1994). Student's $t$, the test statistic, provides a measure of discrepancy between population and sample means that can be interpreted in probabilistic terms by comparing its value to a 'critical' value of $t$ corresponding to a given $\alpha$. The sample mean is considered consistent with a population mean if the calculated $t$ is less than or equal to the 'critical' $t$. This procedure may be inverted to calculate 'critical' population means from a sample mean and a 'critical' $t$. The result is a $(1-\alpha)$ confidence interval of the population mean (Eq. (6)). Multivariate extensions of the above approach result in confidence regions instead of confidence intervals.

A confidence region associated with a multivariate sample contains all combinations of population parameters that are consistent with the corresponding parameter values estimated from the sample. The boundary of the confidence region represents the set of population parameters corresponding to the critical value of the test statistic at the desired significance level $\alpha$. The confidence region thus contains all sets of population parameters for which the significance test gives levels equal to or greater than $\alpha$ for the sample under consideration.

Three commonly adopted significance levels $\alpha$ for constructing confidence regions are 0.10, 0.05 and 0.01. The corresponding $(1-\alpha)$ confidence levels 0.90, 0.95 and 0.99 can be thought of as representing the probability of covering the true values of the set of parameters, or simply as the content of the region. In other words, if we could take an infinitely large

number of independent samples from a given multivariate distribution and we would calculate a $(1-\alpha)$ confidence region from each sample, we would expect a proportion of $(1-\alpha)$ confidence regions to contain the true population parameters. For instance, a 90% confidence region about the multivariate sample mean has an associated 0.90 probability of containing the population mean. A 95% confidence region of the same set of parameters must cover a larger portion of the parameter space. The 95% confidence region thus fully encloses the 90% confidence region, and the 99% confidence region encloses both the 95% and 90% regions. The canonical 90%, 95% and 99% confidence levels are also considered reasonable in most geological applications. Confidence levels below 90% have little practical use, because the associated probability of attributing statistical significance to chance variations is greater than 0.10, which is hardly a sound basis for geological inferences. Confidence levels exceeding 99% are unlikely to be useful in practice, given the relatively small number of observations available in most petrographic studies.

### 5.2. Treatment of zeros

A composition estimate based on point-count data may contain several zero values. Faced with such compositions, one may argue that the presence of zero values indicates the absence of certain components in the specimen under study. However, it is quite plausible that one or more components are present in trace amounts only and have not been encountered during point counting. In the latter case, the absence of components in a sample of finite size is attributable to sampling error. The fundamental difference between these two interpretations of zero values can be illustrated with the help of a ternary diagram.

The vertices of a ternary QFL diagram commonly used in sedimentary petrology can be thought of as representing hypothetical end-member sands consisting of pure quartz (Q), feldspar (F) and lithic fragments (L). The three edges of the diagram represent binary mixtures of these three end members, and the area inside the diagram covers the set of all possible ternary mixtures. Thus, if $k$ is defined as the number of components present in the populations under consideration, $k=1$ for the vertices, $k=2$ for the edges, and $k=3$ for the inside of the diagram. These three fixed end members and their four associated mixing spaces (three binary spaces and one ternary space) have different dimensions, $k-1$. Consequently, if one or more components are regarded as truly absent in the populations from which the samples were drawn, then these populations belong to different spaces and cannot be compared directly.

This leads to the conclusion that the ternary compositional space of the *populations* under consideration does not include the edges and vertices of the ternary diagram. We could use an appropriate significance test to calculate the parameter values of samples from any given ternary population associated with a fixed confidence level $(1-\alpha)$. Some of these parameter values could be equal to zero, especially if one or more components are present in small amounts. Hence, sampling from such ternary populations will occasionally give rise to *observations* located on the edges and vertices of the diagram.

The problem facing us when we attempt to use significance tests in inverse mode is that the range of 'critical' population parameters must fully enclose the parameter values estimated from a sample. The unknowns, i.e., the 'critical' values of the ternary population parameters are constrained to the interval $\langle 0,1\rangle$, and cannot be equal to zero or unity. A population parameter equal to zero implies that the corresponding component cannot possibly be observed, indicating that $k<3$. A ternary population parameter equal to one implies that the other two parameters must be equal to zero (indicating that $k=1$). This population, located at one of the vertices of the ternary diagram cannot be a composition, as it consists of one component only and does not represent a multivariate entity. It follows that any sample with one or more estimated parameter values equal to zero cannot possibly be enclosed within a ternary confidence region for compositional data. A meaningful comparison between ternary compositions thus requires that all observed zero values are attributed to sampling error, i.e., they are assumed to reflect the low probability of encountering certain rare components in a sample of finite size. Therefore, the statistical methods discussed below require that observed zero values are replaced by statistically acceptable positive values.

Techniques for eliminating zeros in a matrix of compositions are, in increasing order of sophistication:

- Formation of subcompositions by deletion of rows (observations) or columns (components), followed by recalculation to unit sum;
- Amalgamation of columns (components) assumed to have the same genetic significance;
- Replacement of zeros by (statistically acceptable) small positive values, followed by recalculation to unit sum.

The first two techniques are self-explanatory. The third has been applied chiefly in geochemistry, where components present in small amounts may not be recorded if their concentration approaches the lower detection limit of the measurement device. The usual practice is to replace zeros by a positive value corresponding to the detection limit, the maximum round-off error, or the data precision (Aitchison, 1986). A straightforward method for point-count data is to replace all recorded zeros with 0.5 point (maximum round-off error) or 1.0 point (detection limit), after which the constant-sum constraint may be imposed on the counts or any ternary subset thereof.

### 5.3. Interpolation of discrete numerical solutions

An immediate consequence of the constrained nature of ternary compositions is that the sum of two components provides full knowledge of the third. Two co-ordinates thus uniquely define each point in a ternary diagram. The construction of a ternary confidence region may thus be reduced to a bivariate problem, whose numerical solution consists of a series of boundary points $(b_1,b_2)$. The confidence regions described below generally possess smooth, convex boundaries in two-parameter space. Approximation of such continuous boundaries by cubic spline interpolation (Davis, 1986; Press et al., 1994) of at least 40 points gives good results, provided that the points are approximately equally spaced along the perimeter of the confidence region. The points must of course be in the correct order for interpolation, and the first point must be identical to the last to allow closure of the boundary. Interpolation of the discrete solution is preceded by transformation from bivariate boundary points to ternary co-ordinates if the boundaries of confidence regions must be displayed in a ternary diagram. The discrete solution may thus be defined as a set of 41 boundary points in ternary co-ordinates, collected in the array $B$. This array is submitted to a graphics software package with a cubic spline interpolation option. The following sections discuss the methods for obtaining discrete numerical solutions for various types of confidence regions.

## 6. A confidence region for a single composition

### 6.1. A goodness-of-fit measure for the multinomial distribution

A classical goodness-of-fit measure for data that are assumed to follow a multinomial distribution is Pearson's chi-squared statistic (PXS). This measure of discrepancy between data and model is a member of the class of so-called power-divergence statistics, which encompasses all commonly used goodness-of-fit statistics for categorical data. The behaviour of all power-divergence statistics has been shown to converge to that of the PXS statistic in the case of large samples (Cressie and Read, 1984; Read and Cressie, 1988; Medak and Cressie, 1991). The PXS statistic is defined as:

$$\mathrm{PXS} = \sum_{i=1}^{k} \frac{(n_i - Np_i)^2}{Np_i} \tag{12}$$

where $p_i > 0$, $\Sigma_{i=1}^{k} p_i = 1$ and $\Sigma_{i=1}^{k} n_i = N$

The total number of petrographic classes is defined as $k$ and the total number of points counted in $k$ classes (i.e., the sample size) as $N$. The number of points falling on the $i$-th component is defined as $n_i$ and the component proportions in the population are defined as $p_i$. The estimated component proportions $\hat{p}_i$ are obtained from Eq. (7).

The PXS statistic is approximately distributed as $\chi^2$ with $df = k - 1$ under the null hypothesis. A compositional difference between a specified population and an estimated composition is considered significant at a level $\alpha$ if:

$$\mathrm{PXS} \geq \chi^2_{(1-\alpha;k-1)} \tag{13}$$

The boundary of the $(1-\alpha)$ confidence region of an estimated composition may be calculated by inversion

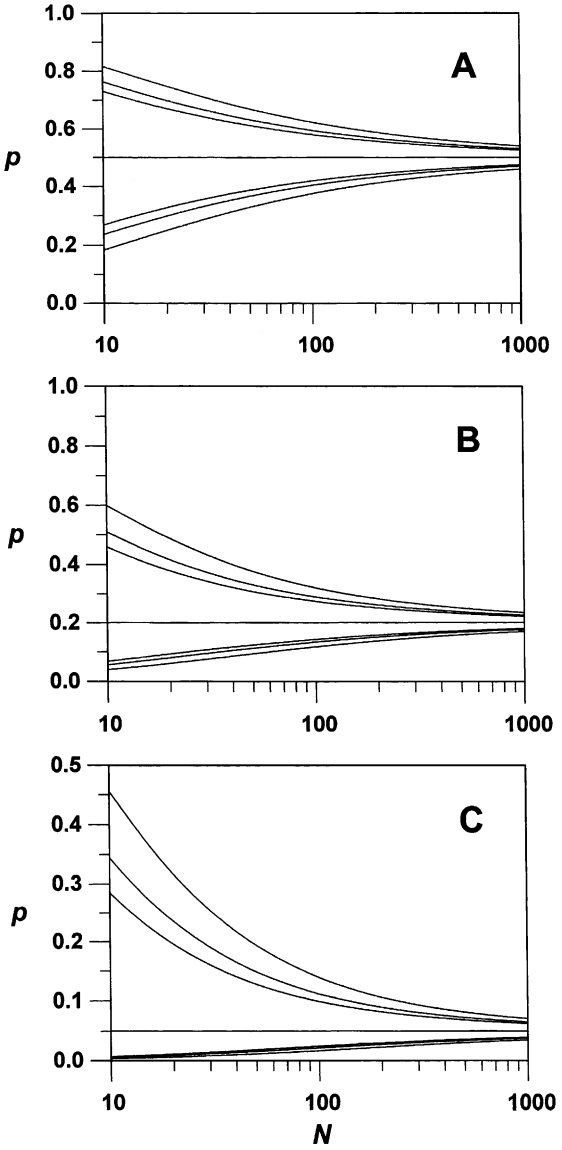


Fig. 4. Pearson's $\chi^2$ approximations to binomial confidence limits of proportions ($p$) as a function of count length ($N$). (A) $p=0.5$; (B) $p=0.2$; (C) $p=0.05$. Confidence limits are 90%, 95% and 99%. Predictions stay within the physical limits on proportions, resulting in asymmetric confidence limits (compare to Fig. 1).

of this test, i.e., by solving for the range of permissible population parameters $p_i$ (Watson and Nguyen, 1985; Watson, 1987; Medak and Cressie, 1991). The equation to be solved is obtained by substituting the estimated proportions for the observed number of points (Eq. (7)) and the critical value of $\chi^2$ for PXS (Eq. (13)), giving:

$$\sum_{i=1}^{k} \frac{(\hat{p}_i - p_i)^2}{p_i} = \frac{\chi^2_{(1-\alpha;k-1)}}{N} \tag{14}$$

The numerical solution of this equation for binary and ternary compositions is given in Appendix A. The binary case will not be discussed in detail, as the main topic of this paper is analysis of ternary compositions. The confidence limits obtained by using the PXS approximation to component proportions of binary compositions are shown in Fig. 4, which may be directly compared with Fig. 1. The superiority of the PXS approximation is obvious in cases where $p_i$ is close to zero or unity and $N$ relatively small. The marked asymmetry of the lower and upper confidence limits on proportions deviating considerably from 0.5 is a consequence of the fact that estimates are constrained to the interval $\langle 0,1 \rangle$.

## 7. Confidence regions for multiple compositions

### 7.1. The additive logistic normal model

Many patterns of compositional variation can be described by additive logistic normal distributions (Aitchison, 1986). This class of statistical models is based on the logratio transformation, which removes the non-negativity and constant-sum constraints on compositional variables (Eq. (1)). Let $x_i$ represent the relative abundances of components in a composition made up of $k$ constituents ($1 \le i \le k$). The $k$-th component $x_k$, whose value is fully specified by the sum of the other $k-1$ values, is used as a common denominator to form a series of $k-1$ ratios of component abundances. The logarithms of these ratios are defined as the set of logratios $y_i$:

$$y_i = \log\left(\frac{x_i}{x_k}\right) = \log x_i - \log x_k, \quad \text{where } i = 1,2,\ldots,k-1 \tag{15}$$

Logratios are amenable to rigorous statistical analysis, unlike the constrained compositional variables. They are unconstrained in the sense that they can take on any value between $[-\infty;+\infty]$, and their values can be modified without automatically forcing a response

of the other logratios formed from the same composition. Moreover, the outcomes of logratio statistical analysis are permutation invariant, i.e., unaffected by the choice of common denominator. The logratio transformation thus provides a unique specification of the covariance structure of compositional data (Aitchison, 1986).

By definition, compositional data follow an additive logistic normal distribution if their logratios are multivariate normally distributed. The requirement of additive logistic normality appears to be fulfilled by many types of compositional data. A well-known example is the approximately lognormal distribution of many trace elements in rocks, which has been empirically established in geochemistry. If we consider the rock as a binary system, made up of a trace element $t$ and the rest, comprising $(1-t)$ of the total mass, we can write for the distribution of $t$:

$$\mathbf{N}\left\{\log\left(\frac{t}{1-t}\right)\right\} = \mathbf{N}\{\log(t) - \log(1-t)\}$$
$$\approx \mathbf{N}\{\log(t) - 0\} = \mathbf{N}\{\log(t)\} = \mathbf{L}\{t\},$$

where **N** and **L** are defined as normal and lognormal distributions. In other words, $t$ is lognormally distributed because $(1-t)$ is close to one, implying that its logarithm is practically equal to zero.

Statistical models for ternary compositions ($x_1$, $x_2$, $x_3$) are thus preferentially constructed under the assumption of a bivariate normal distribution of the corresponding set of logratios ($y_1, y_2$). The results of logratio statistical analysis may be mapped back onto the compositional plane for display in a ternary diagram. Mapping is accomplished by the inverse logratio transformation, which comprises the following steps. The logistic transformation reimposes the non-negativity constraint:

$$z_i = \begin{cases} \mathrm{e}^{y_i} & \text{for } i = 1,2,\ldots,k-1 \\ 1 & \text{for } i = k \end{cases} \quad (16)$$

After which the constant sum $C$ is restored:

$$x_i = \frac{Cz_i}{\sum_{i=1}^{k} z_i} \quad (17)$$

For example, the arithmetic mean of a set of compositions in logratio space corresponds to the geometric mean of the raw data, if both are recalculated to unit sum (cf. Eqs. (16) and (17)). The geometric mean is a much more flexible measure of central tendency than the traditional arithmetic mean calculated from untransformed data. The latter may be very atypical of data sets that display curved patterns in ternary diagrams (Philip and Watson, 1988; Aitchison, 1989).

The logratio transformation is a powerful tool that enables the use of standard multivariate statistical methods based on the assumption of multivariate normality. Actually testing this assumption is beyond the scope of this article (for an overview of tests of multivariate normality, see Aitchison, 1986). A powerful bivariate normality test applicable to logratio-transformed ternary compositional data is given by Press et al. (1994). Other data transformations, in conjunction with methods of outlier detection, should be used in cases where data do not fit this model (see Barceló et al., 1996).

Until now, applications of the logratio transformation to petrographic data have been relatively scarce. Butler and Woronow (1986) analysed the data set of Dickinson and Suczek (1979) for the presence of spurious correlations induced by the constant-sum constraint. Their results suggest that the compositional trend within the 'magmatic arc' field of Dickinson and Suczek (1979) can also be produced by imposing the constant-sum constraint on a set of independent variables, which may indicate that it has no geological meaning.

A fundamental problem of compositional data analysis that cannot be resolved by mathematical manipulations, is the fact that the behaviour of a single variable cannot be studied in 'isolation'. Techniques have been developed, based on the methodology of Aitchison (op. cit.) to identify the source of compositional shifts across data suites (Woronow, 1990; Woronow and Love, 1990). Systematic comparison of all logratios that can be formed from two sets of compositions allows the identification of logratios whose means display identical trends, i.e., increase, equality or decrease from one data set to another. A similar two-sample test was used by Weltje et al. (1996) to investigate shifts in sandstone composition associated with variations in the rate of sediment supply in an Eocene fan-delta system in the Spanish Pyrenees.

### 7.2. A goodness-of-fit measure for the multivariate normal distribution

Confidence regions of the multivariate normal distribution are obtained by inverting the multivariate equivalent of the familiar one-sample Student's *t*-test. This test may be used to quantify the probability that a random sample has been drawn from a univariate normal population with specified mean and unknown variance. The appropriate test statistic for the multivariate case is Hotelling's $T^2$, which is defined as (Morrison, 1976; Davis, 1986):

$$T^2 = n[\overline{\boldsymbol{Y}} - \boldsymbol{Y}]^{\mathrm{T}} \boldsymbol{S}^{-1} [\overline{\boldsymbol{Y}} - \boldsymbol{Y}] \tag{18}$$

Where $n$ is the sample size, $\overline{\boldsymbol{Y}}$ is a column vector of sample means, $\boldsymbol{Y}$ is the specified column vector of population means, and $\boldsymbol{S}$ is the sample covariance matrix (superscripts T and $-1$ denote transpose and inverse, respectively).

A difference between the multivariate sample mean and a specified multivariate population mean is considered significant at a level $\alpha$ if:

$$T^2 \geq \frac{m(n-1)}{n-m} F_{(1-\alpha;\, df_1;\, df_2)} \tag{19}$$

The above formula shows how the calculated values of Hotelling's $T^2$ may be compared to critical values of the $F$-statistic for a $(1-\alpha)$ confidence level. The number of degrees of freedom are equal to $df_1 = m$ and $df_2 = n - m$, where $m$ is defined as the number of variables (two in case of logratio-transformed ternary compositions). The boundary of the confidence region for the population mean may be calculated by inversion of this test, i.e., by solving:

$$[\overline{\boldsymbol{Y}} - \boldsymbol{Y}]^{\mathrm{T}} \boldsymbol{S}^{-1} [\overline{\boldsymbol{Y}} - \boldsymbol{Y}] = \frac{m(n-1)}{n(n-m)} F_{(1-\alpha;\, df_1;\, df_2)} \tag{20}$$

for the range of permissible population parameters $\boldsymbol{Y}$. The solution is represented by an $m$-axial ellipsoid centred about the sample mean $\overline{\boldsymbol{Y}}$, with a set of principal axes whose orientation and relative lengths are determined by the properties of $\boldsymbol{S}$ (Morrison, 1976; Aitchison and Shen, 1984). The sample size and choice of confidence levels determine the absolute lengths of the principal axes.

A similar ellipsoidal region may be constructed to show the range of compositional variation of a given proportion $(1-\alpha)$ of the population, which may be used to predict the range of variation of individual observations (specimens). Such a region is termed a predictive region of content $(1-\alpha)$ (Aitchison, 1986). The equation for the boundary of this region expressed in terms of the $F$-statistic is identical to the above equation, apart from the multiplication factor $(n+1)$ on the right-hand side:

$$[\overline{\boldsymbol{Y}} - \boldsymbol{Y}]^{\mathrm{T}} \boldsymbol{S}^{-1} [\overline{\boldsymbol{Y}} - \boldsymbol{Y}] = \frac{m(n-1)(n+1)}{n(n-m)} F_{(1-\alpha;\, df_1;\, df_2)} \tag{21}$$

The numerical solution of Eqs. (20) and (21) is outlined in Appendix B.2.

### 7.3. Additional comments on bivariate normal confidence regions

Fig. 5 shows additive logistic normal confidence regions of the synthetic data listed in Table 1. The elliptic boundaries calculated in bivariate $y$-space (Fig. 5A) map onto a far less regular region in ternary $x$-space, that need not be convex (Fig. 5B). However, the essential properties of the regions are preserved. In both spaces, a series of six concentric 'confidence shells' is encountered when moving outward from the sample mean, which corresponds to the centre of the distribution. The first three are 90%, 95% and 99% confidence regions of the population mean. These are followed by 90%, 95% and 99% confidence regions of the entire population, i.e., regions expected to contain 90%, 95%, and 99% of the observations drawn from the population of interest. The size of the confidence region of the mean is a factor $\sqrt{n+1}$ smaller than the size of the region of the entire population. Note that the additive logistic normal confidence regions, which do not extend beyond the boundaries of the ternary diagram, adequately capture the curved pattern of compositional variation. The difference between Figs. 3 and 5 highlights the superiority of the additive logistic normal regions over the hexagonal fields of variation calculated from the same data.

The sizes of the two types of elliptical regions as a function of the sample size are illustrated in Fig. 6, which shows a plot of $\sqrt{h_k}$ (a measure of the size of the confidence region, defined in Eq. (B-3), Appendix

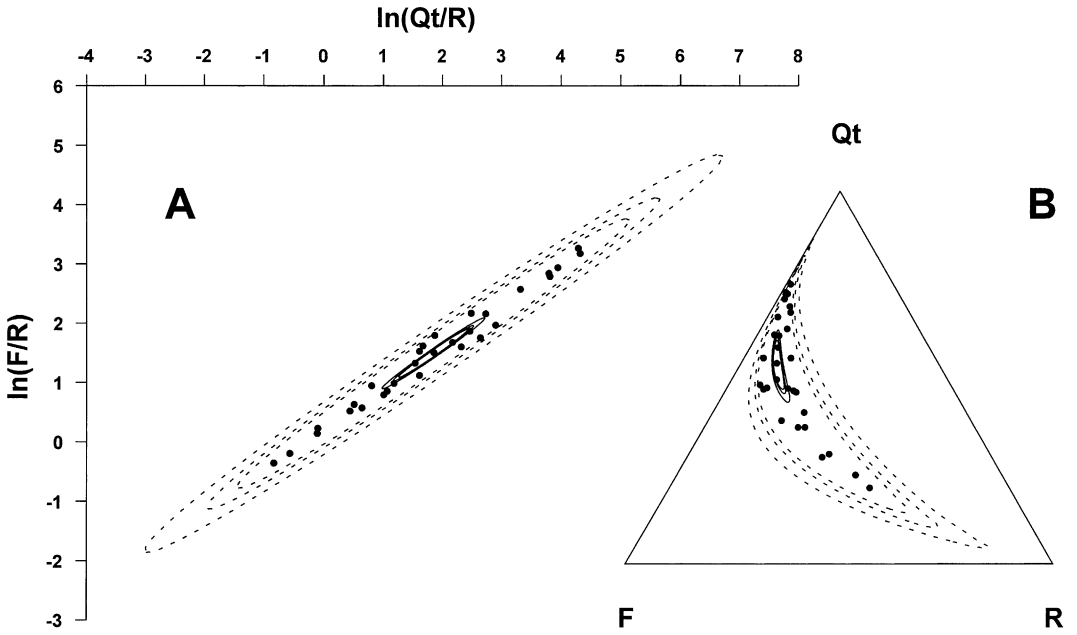


Fig. 5. Additive logistic normal confidence regions constructed from bivariate logratio distributions of the data in Table 1. Solid line: confidence regions of the population mean; dashed line: confidence regions of the entire population. Confidence limits are 90%, 95% and 99%. (A) Elliptic confidence regions in logratio space reflect the shape of the bivariate normal distribution. (B) The non-linear inverse logratio transformation produces a crescent-shaped region in ternary compositional space, corresponding to an additive logistic normal distribution. Curved pattern associated with selective compositional modification is adequately captured (compare to Fig. 3).

B.2) vs. $n$ for the three confidence levels used in this article. For very small samples ($3 \leq n \leq 5$), both types of regions are similar in size. The size of predictive regions of the entire distribution decreases rapidly with increasing sample size up to $n$ 24 30, but it is nearly independent of sample size for $n > 30$. At $n = 30$, confidence regions of the population mean are almost one order of magnitude smaller than the regions of the entire distribution (Fig. 5A). Further increase of the sample size is accompanied by an exponential decrease in size of the confidence region for the population mean, shown in Fig. 6 as a linear decrease on the logarithmic scales. The size of this region is inversely proportional to the resolution of the statistical model, i.e., the precision with which the population mean can be estimated.

A point that is often missed is that two or more samples differ significantly if the confidence regions of the population means (corresponding to a common significance level) do not overlap one another, *regardless of the extent of overlap of the population confidence regions*. Fig. 6 shows that the capability to detect subtle differences between partly overlapping populations increases with sample size, which is intuitively obvious. In general, samples of size $n = 30$ should suffice for discriminating between overlapping populations, unless the differences in means are extremely small relative to the population standard deviations. Detecting more subtle differences by means of point counting is generally not feasible in view of the limited amount of data available in most studies.

The conventional test for differences in means of multivariate data is based on the assumption that the variation within a series of samples can be represented by a common covariance matrix (Morrison, 1976; Davis, 1986). Tests for significant differences among multivariate means should therefore be preceded by tests for significant differences among sample covariance matrices (Morrison, 1976; Davis, 1986). If at least one of the covariance matrices differs significantly from the rest, the results of the means test cannot be trusted. The ‘graphic significance test for multivariate means’ formed by examining the degree

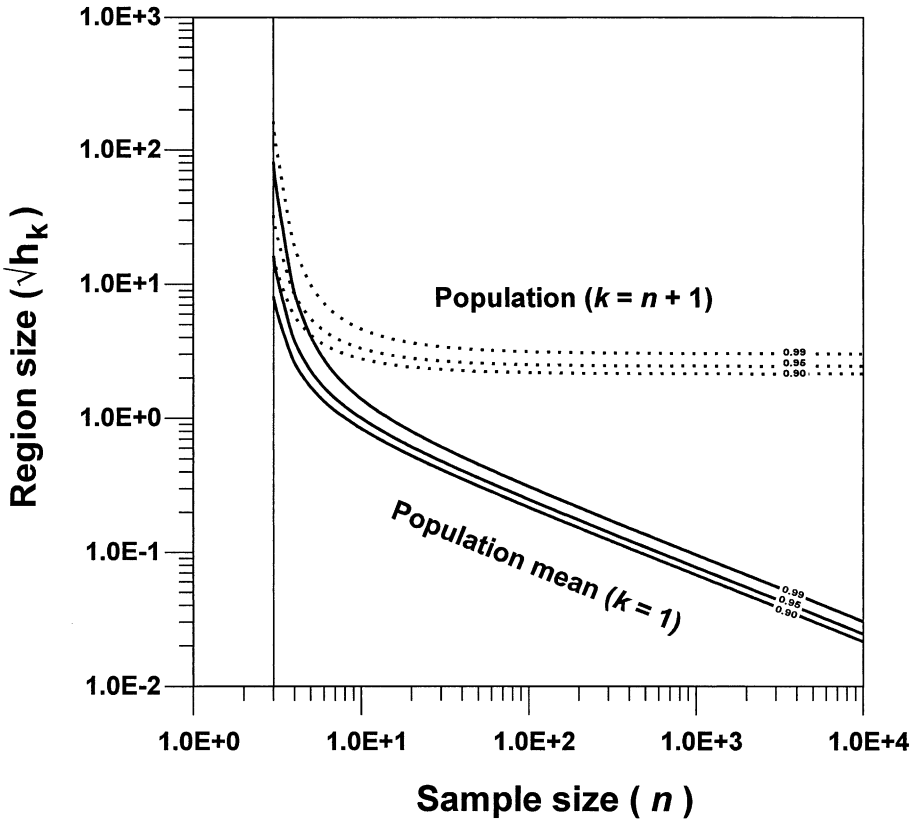


Fig. 6. Sizes of additive logistic normal regions as a function of sample size ($n$).

of overlap between confidence regions of population means in a ternary diagram does not suffer from this problem, because confidence regions are calculated from the mean vector and covariance matrix of each sample separately.

## 8. Example 1: modern beach sands (Italy)

### *8.1. Data*

Compositional data acquired in the course of a systematic sampling programme of modern beach sands (Aiello et al., 1978) will be used to illustrate the above techniques. Two sets of specimens were collected from sections dug on the berms of Tyrrhenian beaches near the Cecina River mouth (about 30 km south of Livorno, Italy). Sections X and Y are located 7.5 km north and 1.0 km south of the river mouth, respectively. Four specimens were sampled in each section at different depths below the surface. All specimens were split into halves. One set of 'subspecimens' of each section was mixed, homogenised and again split to obtain four replicates. Statistical analysis of this set of so-called 'mixture replicates' thus permits an assessment of compositional variation attributable to analytical procedures alone. In contrast, compositional variation between the original specimens within a single section reflects the combination of local sedimentary processes (selective sorting according to size, shape, and density of grains) and analytical procedures.

Each of the original specimens and mixture replicates was sieved into three size fractions (fine: $\varphi = \{4,2\}$; medium: $\varphi = \{2,0\}$; coarse: $\varphi = \{0,-2\}$). The fine fractions were subdivided into light and heavy minerals by means of gravimetric separation. The

framework composition was estimated by counting 350 (coarse fraction) to 500 (fine and medium fraction) grains by the Indiana method. The composition of the heavy-mineral assemblage was estimated by counting 300 grains. The relation between the original counts and the compositional classes used in this exercise is defined in Table 2. Ternary framework compositions were defined as {Qt, F, Rns}. Sedimentary rock fragments, bioclasts, micas, and chlorites were excluded from the analysis (the group labelled 'rest'). Ternary heavy-mineral compositions were produced by amalgamation of pyroxenes, epidote, and zoisite into a single class of transparent heavy minerals, and by excluding micas, chlorites, and carbonates. Composition estimates in these ternary systems are based on approximately 225 framework grains and 250 heavy-mineral grains. A part of this data set, including the framework composition of the medium-sized fractions and the composition of the heavy-mineral assemblages is presented in Table 3.

Table 2
Relation between the compositional classes of published data and the classes used in this study. Numbers in brackets indicate that the categories were not reported separately

| Grain types | | ABP (1978) | RJ (1997) |
|---|---|---|---|
| Qm | Mono-x quartz | + (1) | + |
| Qp | Poly-x quartz | + | + |
| Qc | Chert | + (1) | – |
| Fk | K-feldspar | + (2) | + |
| Fp | Plagioclase | + (2) | + |
| Rm | Metasedimentary RF | + | + |
| Ri | Igneous RF | + | – |
| Rs | Siliciclastic RF | + (3) | + |
| Rc | Carbonate RF | + (3) | + |
| Ro | Other RF | – | + |
| Bi | Bioclasts | + (3) | + |
| A | Alterites | – | + |
| M | Micas and Chlorite | + | – |
| Qt | Qm + Qp + Qc | | |
| F | Fk + Fp | | |
| Rns | Rm + Ri + Ro | | |
| Rnc | Rns + Rs | | |
| Opq | Opaque HM | + | – |
| Alt | Alterite HM | + | – |
| Px | Pyroxene | + | – |
| EZ | Epidote and Zoisite | + | – |
| MC | Micas and Chlorite | + | – |
| C | Carbonate | + | – |
| Trn | Px + EZ | | |

ABP (1978) = Aiello et al. (1978); RJ (1997) = Robinson and Johnsson (1997).

Table 3
Compositional data of modern beach sands from Tuscany, Italy (Aiello et al., 1978)
Numbers in the table are the actual numbers of points/grains counted. See Table 2 for additional explanation.

| Label | Qt | F | Rns | Rest | Label | Opq | Alt | Trn | Rest |
|---|---|---|---|---|---|---|---|---|---|
| X-A-1-m | 13 | 19 | 148 | 320 | X-A-1-h | 148 | 37 | 46 | 69 |
| X-A-2-m | 5 | 18 | 218 | 259 | X-A-2-h | 110 | 68 | 87 | 35 |
| X-A-3-m | 47 | 39 | 110 | 304 | X-A-3-h | 139 | 40 | 69 | 52 |
| X-A-4-m | 67 | 15 | 224 | 194 | X-A-4-h | 150 | 51 | 58 | 41 |
| X-B-1-m | 16 | 32 | 180 | 272 | X-B-1-h | 155 | 46 | 43 | 56 |
| X-B-2-m | 24 | 35 | 150 | 291 | X-B-2-h | 157 | 51 | 38 | 54 |
| X-B-3-m | 47 | 18 | 139 | 296 | X-B-3-h | 170 | 51 | 32 | 47 |
| X-B-4-m | 32 | 18 | 146 | 304 | X-B-4-h | 168 | 43 | 35 | 54 |
| Y-A-1-m | 71 | 7 | 70 | 352 | Y-A-1-h | 203 | 32 | 37 | 28 |
| Y-A-2-m | 44 | 45 | 157 | 254 | Y-A-2-h | 180 | 37 | 56 | 27 |
| Y-A-3-m | 81 | 8 | 96 | 315 | Y-A-3-h | 163 | 55 | 53 | 29 |
| Y-A-4-m | 62 | 13 | 194 | 231 | Y-A-4-h | 89 | 90 | 25 | 96 |
| Y-B-1-m | 25 | 17 | 149 | 309 | Y-B-1-h | 175 | 52 | 48 | 25 |
| Y-B-2-m | 116 | 9 | 115 | 260 | Y-B-2-h | 165 | 49 | 54 | 32 |
| Y-B-3-m | 99 | 5 | 58 | 338 | Y-B-3-h | 174 | 48 | 45 | 33 |
| Y-B-4-m | 97 | 7 | 105 | 291 | Y-B-4-h | 169 | 49 | 45 | 37 |

Specimen labels are coded as follows: section ID (X or Y), subspecimen set (A or B), number (1 to 4), fraction (m = framework components, medium sand size; h = heavy minerals, fine sand size).

### 8.2. Multinomial regions

Confidence regions for each estimated composition in the data set may be constructed with the multinomial model. Differences among the estimated compositions are not statistically significant if these regions overlap one another, as would be expected in cases where random sampling error is the only source of compositional differences among point counts. In geological terms, such a lack of significant differences strongly suggests that the sections are compositionally homogeneous.

The multinomial confidence regions of the heavy-mineral assemblages of sections X and Y are shown in Figs. 7 and 8. One specimen from section X differs significantly from the other three at a 95% confidence level (Fig. 7A). In section Y, one specimen differs significantly from the other three at a level exceeding 99% (Fig. 8A). The other specimens of sections X and Y cluster together, indicating a general lack of significant compositional variation within the sections. The mixture replicates from both sections are of virtually identical composition (Figs. 7B and 8B), as demonstrated by the nearly complete overlap of their

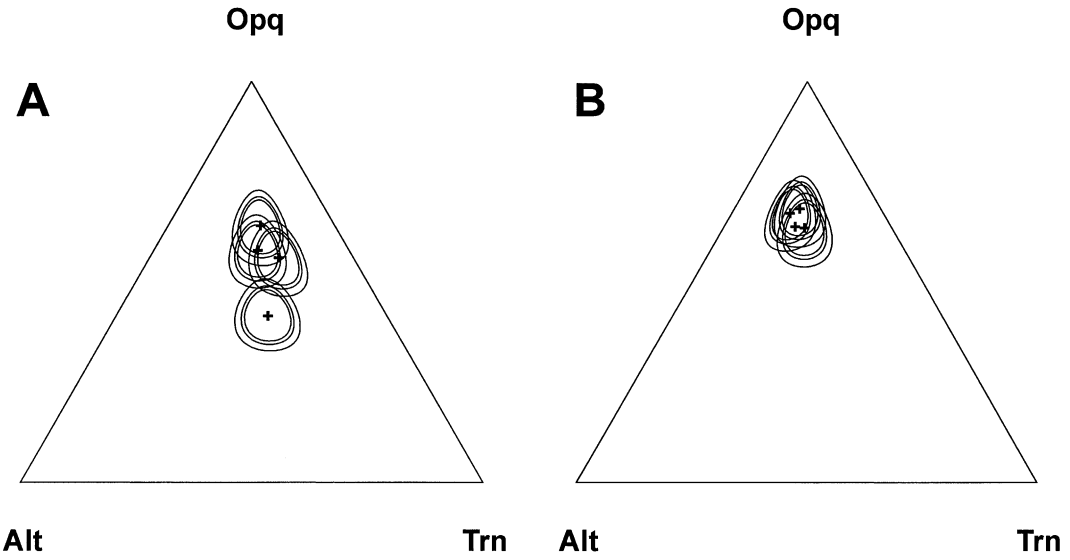


Fig. 7. Multinomial confidence regions of heavy-mineral compositions from section X. Confidence limits are 90%, 95% and 99%. (A) Original specimens; (B) mixture replicates. See Table 2 for additional explanation.

confidence regions. Compositional variation among the original specimens thus exclusively reflects transport-related selection in the beach environment. The mixing-and-splitting strategy is an effective method for reducing the small-scale compositional variation of heavy-mineral assemblages, because compositional variation cannot be attributed to the analytical procedures used.

The multinomial confidence regions of the framework components are shown in Figs. 9 and 10. Compositional variation of framework components in sections X and Y is more conspicuous than that

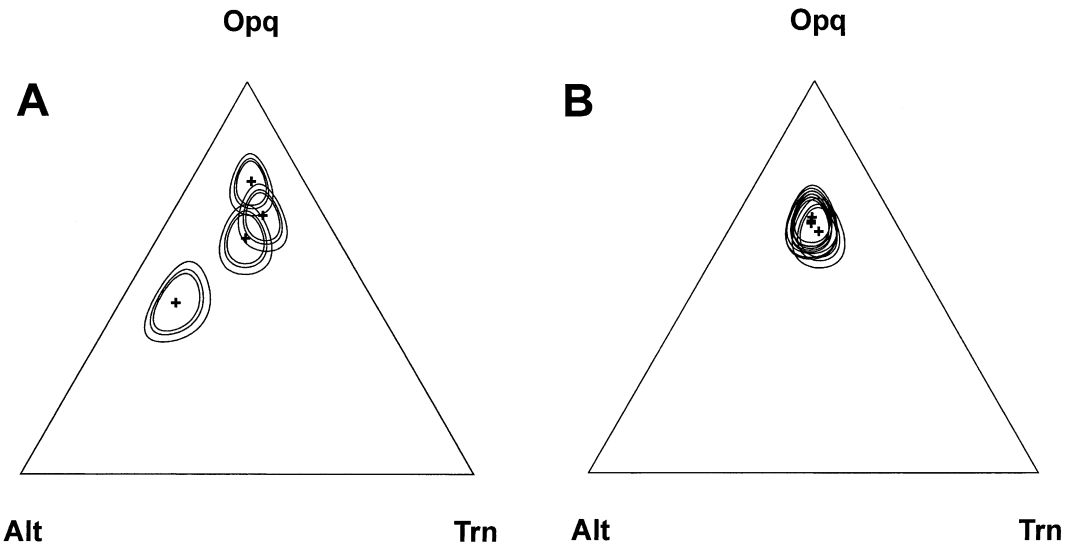


Fig. 8. Multinomial confidence regions of heavy-mineral compositions from section Y. Confidence limits are 90%, 95% and 99%. (A) Original specimens; (B) mixture replicates. See Table 2 for additional explanation.

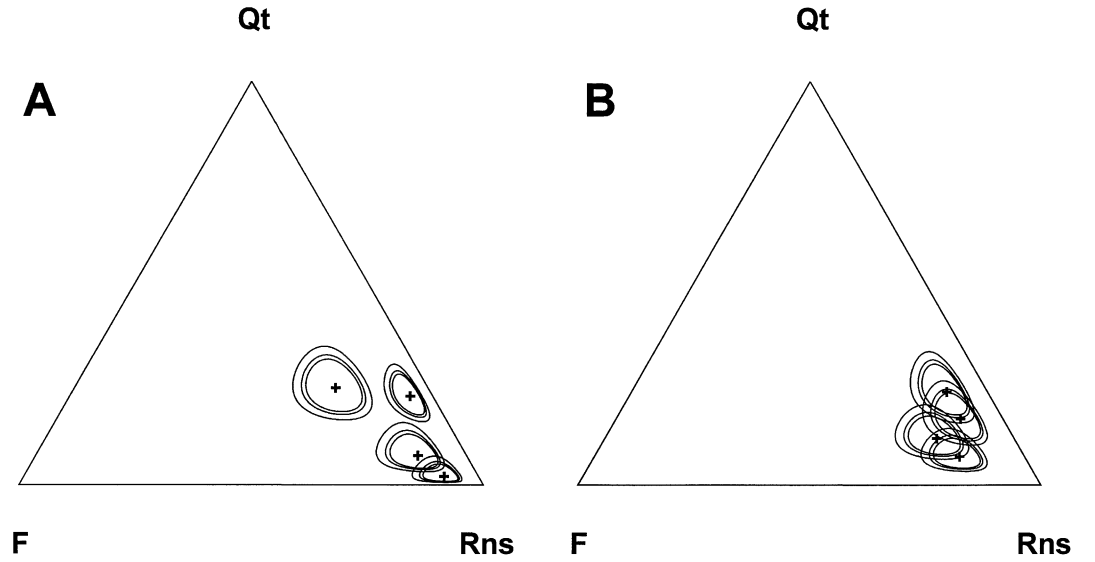


Fig. 9. Multinomial confidence regions of framework compositions from section X. Confidence limits are 90%, 95% and 99%. (A) Original specimens; (B) mixture replicates. See Table 2 for additional explanation.

of the heavy minerals. In fact, only two out of four specimens from each section show a lack of significant compositional differences (Figs. 9A and 10A). Reduction of the compositional variation by the mixing-and-splitting strategy appears to have been moderately successful in case of the specimens from section X (Fig. 9B), but it failed completely for section Y (Fig. 10B). The overall similarity in spread of original specimens and mixture replicates indicates that the recorded variation of framework composition is largely attributable to analytical procedures. The information presented by Aiello et al. (1978) does not

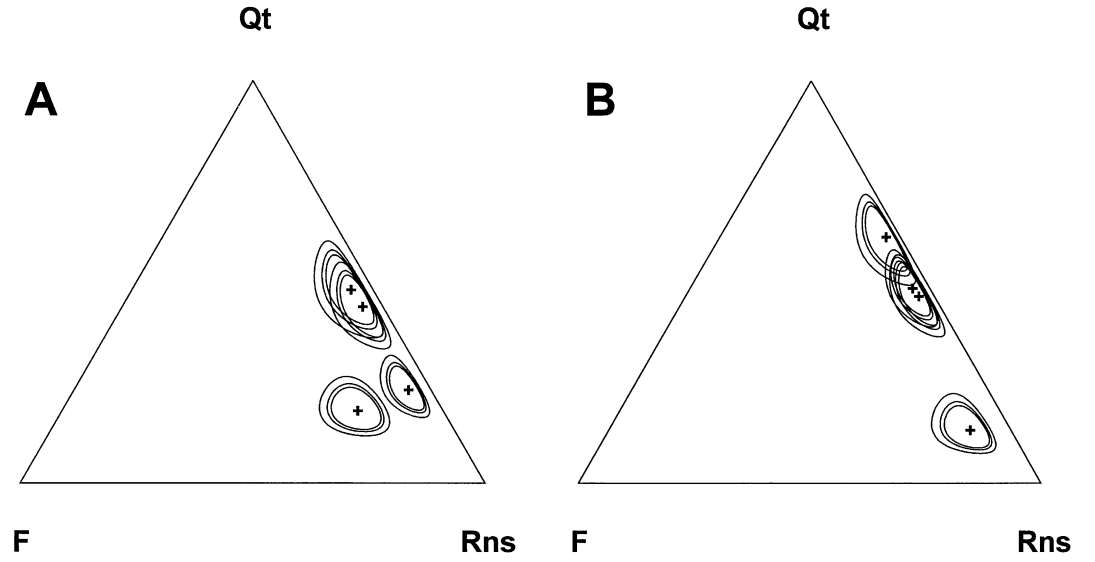


Fig. 10. Multinomial confidence regions of framework compositions from section Y. Confidence limits are 90%, 95% and 99%. (A) Original specimens; (B) mixture replicates. See Table 2 for additional explanation.

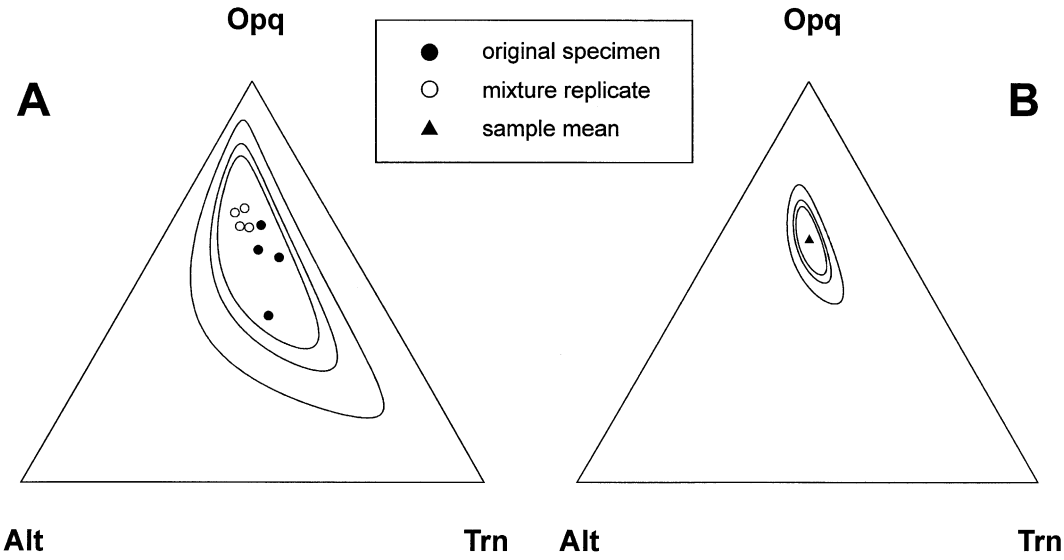


Fig. 11. Additive logistic normal regions of the heavy-mineral association in section X. Confidence limits are 90%, 95% and 99%. (A) Predictive regions of the data points; (B) confidence regions of the population mean. See Table 2 for additional explanation.

suggest any particular reason for the unusually wide scatter of framework compositions. Two possible explanations for the apparent compositional variation between mixture replicates are:

• The assemblage of framework grains is highly sensitive to selection, implying that many of the original specimens and mixture replicates are in fact of significantly different composition. This suggests that mechanical selection took place during splitting of the specimens.

• The original specimens and mixture replicates are in fact of identical composition. In that case, the

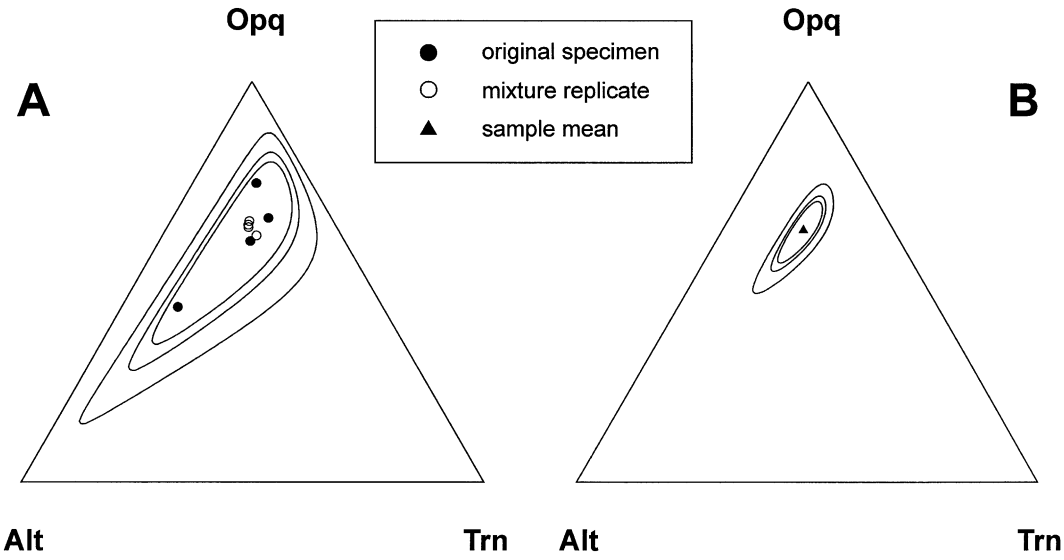


Fig. 12. Additive logistic normal regions of the heavy-mineral association in section Y. Confidence limits are 90%, 95% and 99%. (A) Predictive regions of the data points; (B) confidence regions of the population mean. See Table 2 for additional explanation.

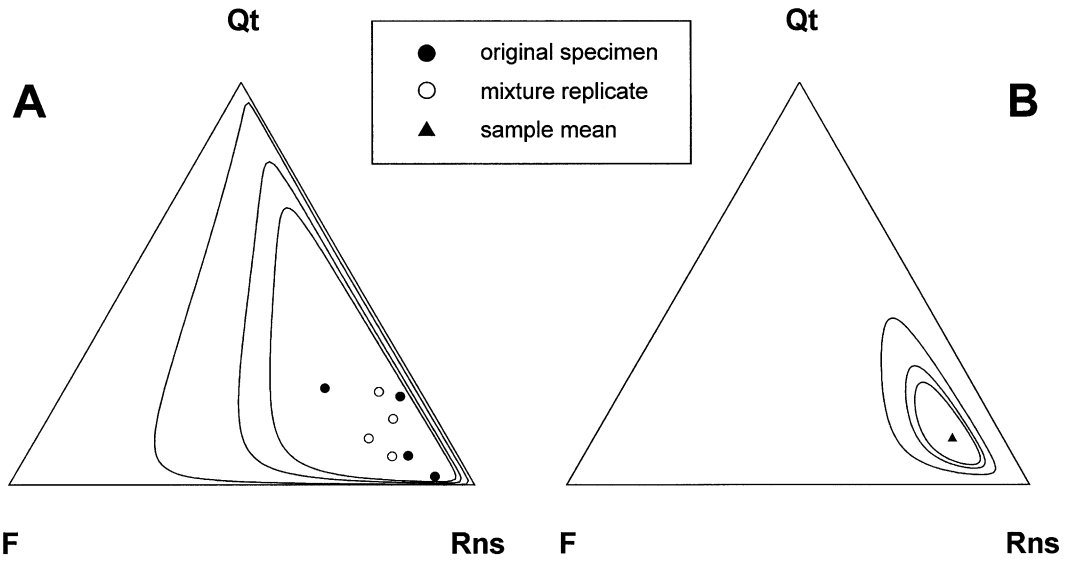


Fig. 13. Additive logistic normal regions of the framework association in section X. Confidence limits are 90%, 95% and 99%. (A) Predictive regions of the data points; (B) confidence regions of the population mean. See Table 2 for additional explanation.

formation of replicates would have been successful, but the compositional variation would have been fabricated during counting of the grain mounts. This suggests a significant influence of random operator error.

### 8.3. Logistic normal regions

A more flexible population concept is desirable in many geological applications, for instance in the present case where we would like to define the ‘local

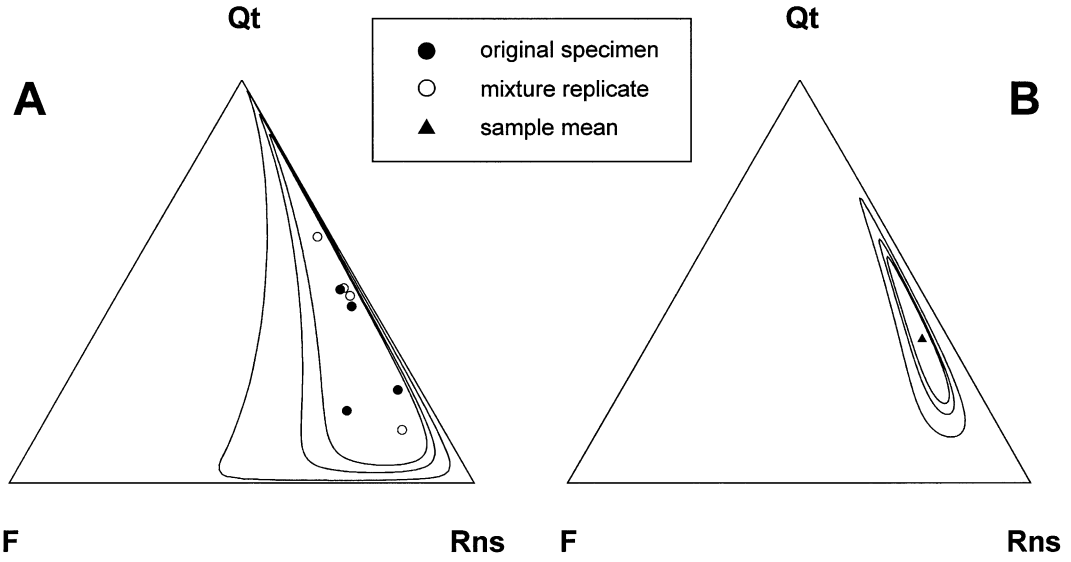


Fig. 14. Additive logistic normal regions of the framework association in section Y. Confidence limits are 90%, 95% and 99%. (A) predictive regions of the data points; (B) confidence regions of the population mean. See Table 2 for additional explanation.

beach sand' as the population of interest. Invoking the second model allows a quantitative characterisation of this population. In this model, the point counts are treated as replicates, i.e., a series of random realisations whose spread reflects the properties of the population. The shape of the population of interest can be inferred from the covariance structure of the data because it is assumed that an appropriate class of distribution functions has been specified. Predictive regions of the populations and confidence regions of the population means are shown to illustrate the characterisation of compositional variation with this model.

Confidence regions based on the additive logistic normal distribution are shown in Figs. 11–14. For the purpose of this exercise, sample sizes were artificially increased by regarding all eight specimens from each section as a single sample. Although incorrect from a methodological point of view, it was considered necessary because the statistical uncertainty associated with the small samples would have inflated the regions to such an extent that few geological inferences could have been made otherwise (see Fig. 6). This negation of the careful sampling design of Aiello et al. (1978) results in an underestimation of the compositional variability of the heavy-mineral assemblages, because the spread of the mixture replicates is significantly smaller than that of the original specimens. However, it is unlikely to affect the inferences from statistical analysis of the framework components, because the patterns of compositional variation displayed by the original specimens and mixture replicates are similar.

Confidence regions of the entire distribution may be used to predict the range of compositional variation of specimens from the same locality. The shapes of these regions (Figs. 11A–14A) accurately capture the sample distributions, suggesting that the assumption of additive logistic normality is reasonable. The confidence regions of the population means may be used to decide if two samples are likely to have been drawn from the same population. The considerable overlap in confidence regions of the heavy-mineral population means (Figs. 11B and 12B) provides no reason to assume that the two samples are derived from different populations. In fact, the sizes of the confidence regions have been underestimated by treating the four original observations and the four mixture replicates as a single sample. The confidence regions of the framework population means (Figs. 13B and 14B) also overlap one another, but the considerable difference in location of the regions suggests that two framework populations could have been distinguished if the samples would have been twice as large (see Fig. 6).

## 9. Example 2: modern fluvial sands (Alaska)

### 9.1. Data

Point-count data of sands from the Sagavanirktok river, Alaska (Robinson and Johnsson, 1997) will be used to illustrate the flexibility of the additive logistic normal distribution (Model B) for characterising compositional variability in a system dominated by chemical and mechanical weathering. The results obtained by applying Model B to the data will be compared to the use of hexagons constructed from univariate normal approximations. The data consist of 19 specimens of medium-sized sand, whose compositions were quanti-

Table 4
Point-count data of medium-sized sands from the Sagavanirktok river basin, North Slope, Alaska (Robinson and Johnsson, 1997). Numbers in the table are the actual numbers of points counted

| Label | DE | Qt | Rnc | Rc | Rest |
|---|---|---|---|---|---|
| S-01 | A | 54 | 246 | 0 | 0 |
| S-02 | A | 42 | 256 | 0 | 2 |
| S-03 | A | 61 | 61 | 172 | 6 |
| S-04 | A | 46 | 77 | 177 | 0 |
| S-05 | A | 50 | 88 | 154 | 8 |
| S-06 | A | 30 | 156 | 109 | 5 |
| S-07 | B | 59 | 141 | 93 | 7 |
| S-08 | B | 58 | 112 | 122 | 8 |
| S-09 | B | 51 | 95 | 136 | 18 |
| S-10 | C | 228 | 58 | 10 | 4 |
| S-11 | C | 205 | 75 | 14 | 6 |
| S-12 | C | 184 | 93 | 16 | 7 |
| S-13 | C | 172 | 92 | 30 | 6 |
| S-14 | C | 139 | 119 | 35 | 7 |
| S-15 | C | 144 | 128 | 16 | 12 |
| S-16 | B | 103 | 135 | 57 | 5 |
| S-17 | B | 107 | 139 | 49 | 5 |
| S-18 | B | 69 | 180 | 43 | 8 |
| S-19 | B | 92 | 181 | 23 | 4 |

DE = depositional environments; DE codes: A = mountain range, B = foothills, C = coastal plain. See Table 2 for additional explanation.

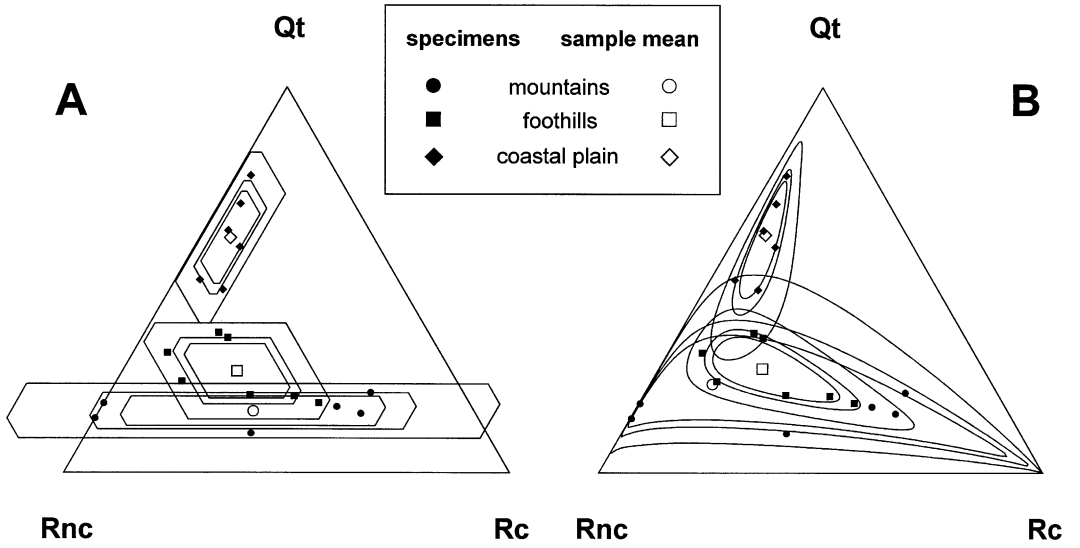


Fig. 15. Predictions of subpopulation means of the Sagavanirktok river sands. Subpopulations correspond to different environments within the alluvial system. Confidence limits are 90%, 95% and 99%. (A) Hexagonal fields of variation; (B) additive logistic normal confidence regions. See Table 2 for additional explanation.

fied by counting 300 points in thin section according to the Indiana method. Robinson and Johnsson (1997) distinguished three subpopulations of sands on the basis of a threefold subdivision of depositional environments within the alluvial system. From source to basin, the subpopulations are: mountain-range specimens ($n = 6$),

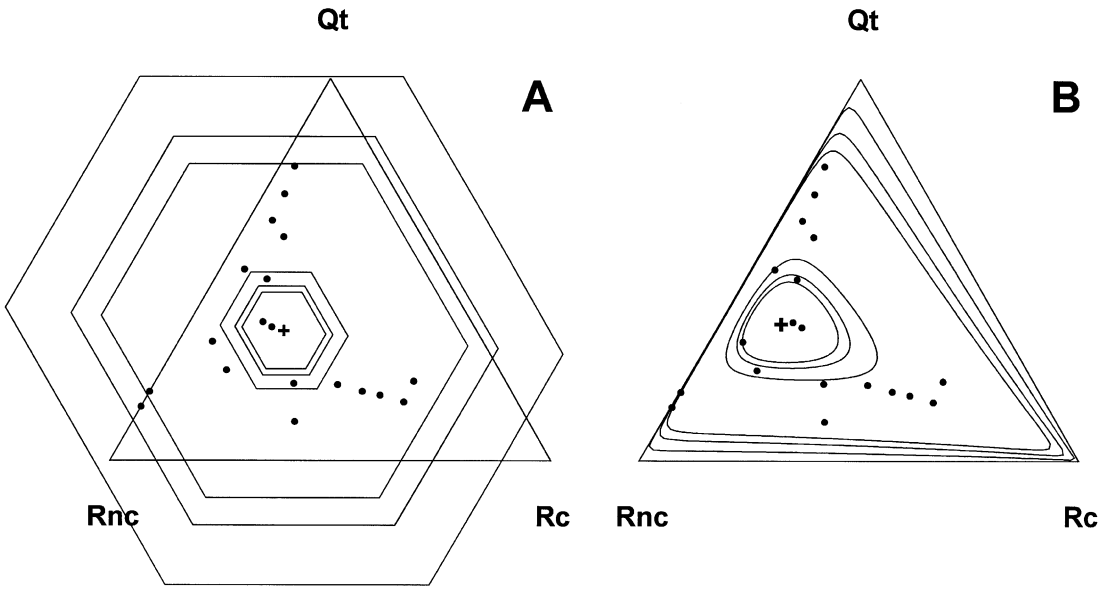


Fig. 16. Predictions of population means and the range of variation of the entire population of the Sagavanirktok river sands. All specimens have been treated as a single sample to characterise the overall compositional variation within the alluvial system. Confidence limits are 90%, 95% and 99%. (A) Hexagonal fields of variation; (B) additive logistic normal confidence regions corresponding to Fig. 17A. See Table 2 for additional explanation.

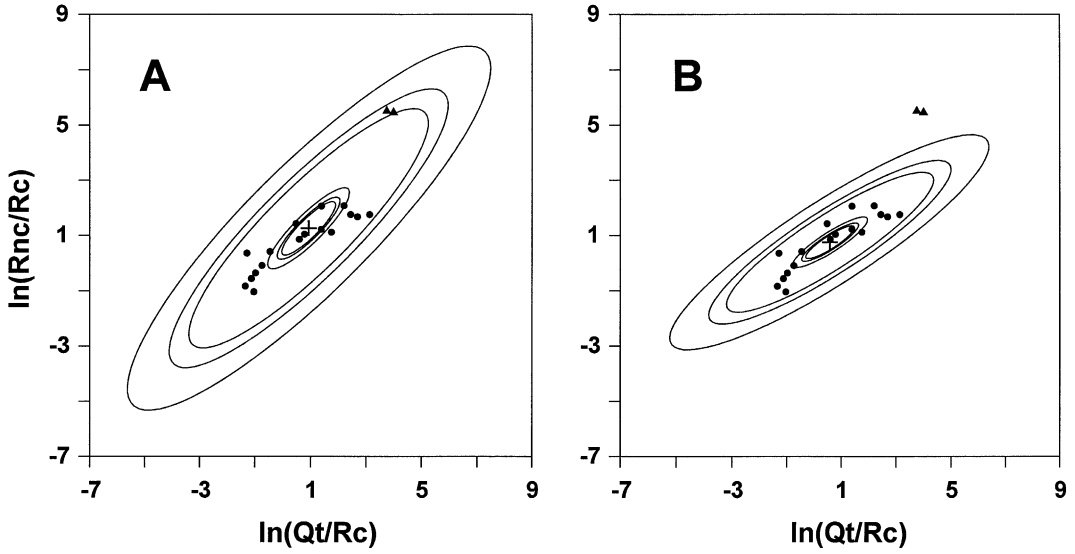


Fig. 17. Bivariate normal confidence ellipses of the Sagavanirktok river sands in logratio space. The two anomalous specimens S-01 and S-02 are represented by triangles. (A) Model based on all data points ($n=19$); (B) revised model obtained by exclusion of anomalous specimens ($n=17$). See Table 2 for additional explanation.

foothill specimens ($n=7$) and coastal-plain specimens ($n=6$). Because these environments are part of a single system, the compositional variability of the population as a whole has also been characterised. The relation between the original point-count categories and the ternary projections discussed in this paper are defined in Table 2. Ternary framework compositions were formed by {Qt, Rnc, Rc}. Other categories present in

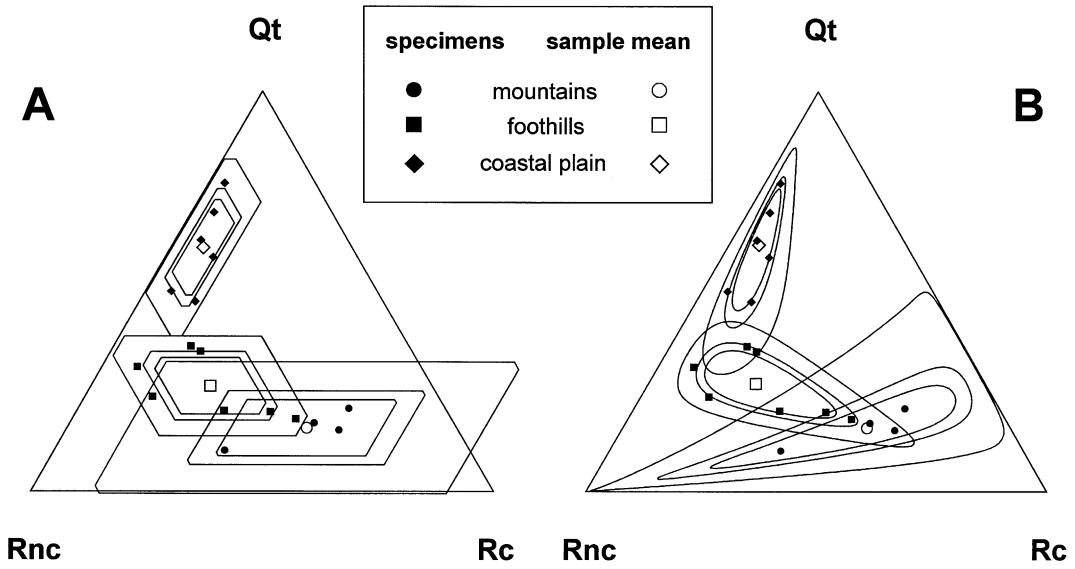


Fig. 18. Predictions of subpopulation means of the Sagavanirktok river sands after exclusion of specimens S-01 and S-02. Subpopulations correspond to different environments within the alluvial system. Confidence limits are 90%, 95% and 99%. (A) Hexagonal fields of variation; (B) additive logistic normal confidence regions. See Table 2 for additional explanation.

small proportions were excluded from the analysis (group labelled 'rest'). The reconstructed counts are shown in Table 4.

### 9.2. Comparison of hexagons and Model B

Fig. 15 shows the hexagonal fields of variation (Fig. 15A) and the logistic normal confidence regions (Fig. 15B) of the subpopulation means. The hexagonal fields of variation of the population mean are plotted together with the hexagonal field predicting the range of variation of individual specimens in Fig. 16A. The logistic normal confidence regions of the population mean and the entire population are shown in Fig. 16B. A comparison of the hexagonal fields with the logistic normal fields clearly brings out the fundamental flaws in the former. For instance, the hexagonal field of variation of the mean of the mountain-range subpopulation extends beyond the boundaries of the ternary diagram (Fig. 15A), which expresses the belief that the subpopulation mean is expected to be characterised by a negative proportion of either Rc or Rnc grains. Similar predictions of negative proportions, in conjunction with a severe mismatch between the shape of the 'data cloud' and the shape of the predicted population, can be observed in Fig. 16A. The corresponding logistic normal confidence regions do not show such mismatches, apart from the region depicting the mean of the mountain-range subpopulation (Fig. 15B).

### 9.3. Outlier detection and model revision

The confidence region of the mean of the mountain-range subpopulation (Fig. 15B) is unusually large and its shape does not properly mimic the distribution of data points in the ternary diagram. The reason for this seems to be the presence of two anomalous data points on the left-hand side of the ternary diagram (specimens S-01 and S-02). A similar phenomenon can be observed in the logistic normal regions of Fig. 16B, where the same two data points are located on the outer edge of the predicted region of the entire population, whereas the other data points are much closer to the centre of the region. In other words, these two anomalous observations can only be explained by a logistic normal distribution whose confidence region fills almost the entire area of the ternary diagram. The

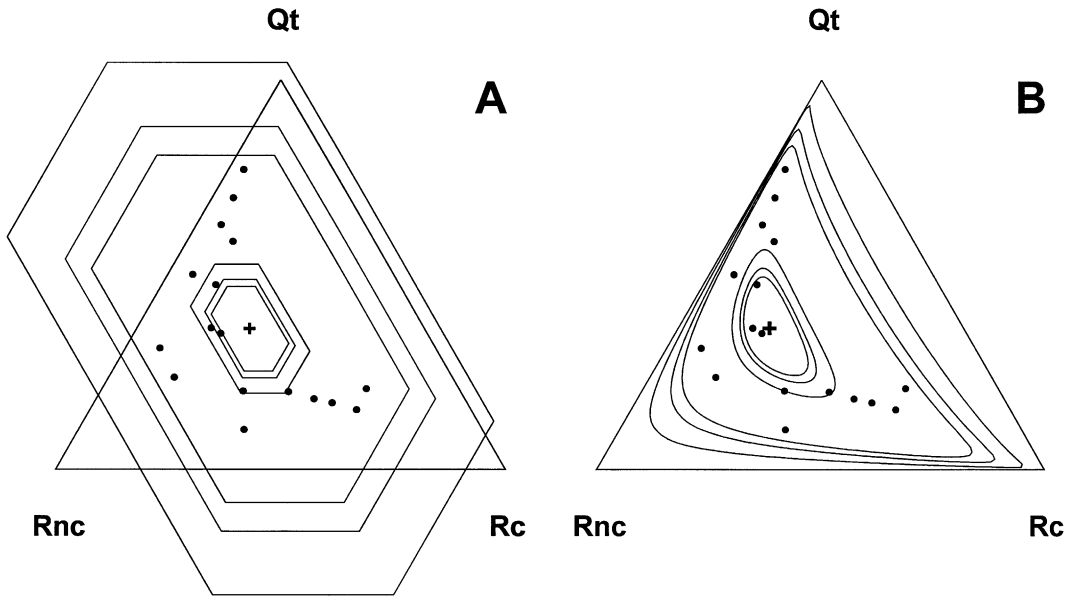


Fig. 19. Predictions of population means and the range of variation of the entire population of the Sagavanirktok river sands after exclusion of specimens S-01 and S-02. All specimens have been treated as a single sample to characterise overall compositional variation within the alluvial system. Confidence limits are 90%, 95% and 99%. (A) Hexagonal fields of variation; (B) additive logistic normal confidence regions corresponding to Fig. 17B. See Table 2 for additional explanation.

suggestion that specimens S-01 and S-02 represent outliers is supported by Robinson and Johnsson (1997) who state that all other specimens belonging to the mountain-range subpopulation are rich in carbonate. The two anomalous specimens represent sands derived from portions of the hinterland without carbonate outcrops.

Examination of the distribution of data points in bivariate logratio space highlights the atypicality of the two specimens (Fig. 17). Fig. 17A shows the 90–95–99% confidence regions of the entire population that were used to construct the ternary confidence regions of Fig. 16B. A revised estimate of the bivariate normal distribution of logratios was obtained by excluding the two specimens, giving the result shown in Fig. 17B. This distribution is much more compact and better fits the remaining 17 data points. Figs. 18 and 19 show the hexagonal fields and confidence regions obtained after exclusion of the two observations from the analysis. Exclusion of the two anomalous specimens has some effect on the hexagonal fields of variation of the mountain-range subpopulation mean, but the prediction still extends beyond the boundary of the ternary space (Fig. 18A). The hexagonal fields of the entire population and its mean have been somewhat reduced in size (Fig. 19A). However, the logistic normal regions of the mountain-range subpopulation in Fig. 18B and the confidence regions in Fig. 19B differ conspicuously from those of Figs. 15B and 16B. The curved pattern of data points in the ternary diagram of Fig. 19B has now been adequately captured.

The shape of the confidence regions of the entire population confirms the dominant controls of mechanical and chemical weathering on compositional variation in the Sagavanirktok river basin inferred by Robinson and Johnsson (1997). The curved shape probably represents the dissolution of carbonate rock fragments (Rc) during the initial stage of weathering, followed by disaggregation of non-carbonate rock fragments (Rnc) during later stages, when most of the carbonate has been removed. This pattern of variation is analogous to the chemical weathering trend in the synthetic data set of Table 1 (Fig. 5). Variation in the proportion of carbonate rock fragments (Rc) supplied by the lower-order drainage basins is likely to have overprinted this weathering trend. The overall pattern in the Sagavanirktok sands may thus be interpreted as a chemical weathering trend that is slightly overprinted by mixing of sediments along the transport pathway (cf. Weltje et al., 1996). Such patterns can only persist if the rate of chemical weathering is significantly higher than the rate of homogenisation through exchange of bedload and sediments in temporary storage (Weltje, 1995, 1998).

## 10. Alternative approaches

### *10.1. Introduction*

A basic assumption for constructing confidence regions is that a set of observed compositions represents a sample from a single population. This may be reasonable in many cases, but is unlikely to cover all possible situations. For instance, sediment properties often display systematic spatial variations caused by mixing of detritus from multiple feeder systems, varying degrees of intrabasinal weathering, and variations in diagenetic history across a basin. In such cases, where the presence of several populations is suspected, other approaches to characterisation and prediction may be more appropriate. Many different multivariate statistical tools are available (e.g., Morrison, 1976; Davis, 1986; Rock, 1988). The methods most widely used in sedimentary petrology are briefly discussed below. They are seldom applied to ternary systems because of their capability to handle many variables simultaneously, allowing use to be made of all the information in the data. This approach must be considered superior to the data reduction a priori that takes place when multivariate data are compressed into a three-component system before statistical analysis.

### *10.2. Discrete groups: empirical classification and assignment*

Classification and assignment are useful if meaningful (genetic) groups can be recognised within the data. The presence of multiple types of sand in a basin fill may be detected by means of cluster analysis of petrographic data (e.g., Fay, 1982; Cavazza, 1989; Stattegger and Morton, 1992). Cluster analysis is usually employed as an exploratory tool, because the statistical significance of the clustering cannot be evaluated. Many different methods are available (e.g.,

Bezdek et al., 1984; Davis, 1986; Rock, 1988; Gordon, 1999). Because all cluster analyses are based on some measure of similarity between specimens, the results are also influenced by the sampling distributions of the components (Gordon, 1999). A permutation test for interpreting the results of cluster analysis in a statistical sense was proposed by Jerram and Cheadle (2000). It is based on Monte Carlo simulation of random uniform distributions with the same range of variation as the data. Clustering of these benchmark distributions allows one to examine the degree of clustering attributable to random variation only.

Discriminant function analysis may be used to assign new specimens to predefined compositional classes. This method has enjoyed substantial use in provenance studies (e.g., Middleton, 1962; Kelley and Whetten, 1969; Davies and Ethridge, 1975; Pingitore and Shotwell, 1976; Ingersoll, 1978, 1990; Potter, 1978; Pirkle et al., 1985; Gergen and Ingersoll, 1986; Packer and Ingersoll, 1986; Darby, 1990; Molinaroli et al., 1991; Stattegger and Morton, 1992). Most versions of discriminant function analysis require that the compositional variables follow a multivariate normal distribution. Because compositional data fail to meet this requirement, the results of discriminant function analysis should be interpreted with great caution (Butler, 1982; Aitchison, 1986; Rock, 1988; Barceló-Vidal et al., 1999). A practical solution, discussed above, is to apply a form of logratio transformation (Aitchison, op. cit.).

### *10.3. Continuous variation: end-member modelling*

Classification and assignment procedures are based on the assumption that several distinct groups of specimens are present in a data set. This assumption may not be valid in certain cases, because transitions from one type of sand to another are expected to occur given the fact that the factors that control sediment composition may vary continuously in space or time. Methods that can cope with continuous compositional variation as well as the presence of discrete groups are known as ordination techniques. In sedimentary petrology, principal components analysis and factor analysis have been occasionally used for this purpose (Griffiths, 1966; Griffiths and Ondrick, 1969).

Continuous compositional variation of sediments is often attributed to physical mixing of sediments from multiple sources, which has been recognised as one of the central problems in sedimentary provenance analysis. "... In its broadest aspect, the problem of provenance can be considered as a problem of accounting–making an inventory of the different types of grains contributed by different source rocks. To this, one should add the problem of the same kinds of grains coming from different source rocks ..." (Pettijohn et al., 1987).

Various attempts have been made to predict the mixing coefficients of known parent-rock types from detrital modes, or to predict detrital modes from assumed mixing proportions of known parent rocks (Graham et al., 1986; DeCelles, 1988; Pivnik, 1990; DeCelles et al., 1991; Ibbeken and Schleyer, 1991; Molinaroli and Basu, 1993). However, detailed information about the parent-rock assemblages forming the end members of a series of observed mixtures is not commonly available, and the primary objective of a provenance analysis is to identify likely end members.

In the absence of prior knowledge, a suite of sandstone specimens from a single sedimentary basin may be regarded as a series of mixtures of sediments supplied by an unknown number of sources with unknown compositional characteristics. A provenance reconstruction thus requires an assessment of the number of sediment sources and their compositional signatures, before each specimen can be expressed as a mixture. The development of multivariate models aimed at explaining compositional variation in terms of mixing of fixed end members was initiated in the early 1960s and continues to this day (Manson and Imbrie, 1964; Klovan and Imbrie, 1971; Klovan and Miesch, 1976; Miesch, 1976, 1981; Full et al., 1981, 1982; Renner, 1993, 1995; Van der Ark, 1999; Weltje, 1997, 1998, in press). In the earth sciences, this form of analysis has been historically conceived as unmixing, but the term *end-member modelling* is considered more appropriate (Weltje, 1995, 1997). Early versions of end-member modelling algorithms have been applied to heavy-mineral assemblages by Imbrie and Van Andel (1964), Pigorini (1968), Flores and Shideler (1978), Fay (1982), Bahk and Chough (1983), Stattegger (1987), Clemens and Komar (1988), Mezzadri and Saccani (1989) and Mezzadri and Valloni (in Ibbeken and Schleyer, 1991).

Weltje (1995), Weltje et al. (1996), Prins and Weltje (1999a,b), Prins et al. (2000) and Stuut et al. (in press)

have presented applications of a recent end-member-modelling algorithm. Numerical experiments with this algorithm as well as validation of modelling results by means of independent data on 'true' end-member compositions have clearly established its usefulness for unravelling contributions of sediments from multiple sources in the absence of prior knowledge.

## 11. Discussion and conclusions

### *11.1. Compositional hierarchy*

Compositional data used in sedimentary petrology represent different levels of information within a compositional hierarchy. Compositional elements at a given level may be expressed as linear combinations (mixtures) of elements at a lower level. For detrital modes of sands and sandstones, this hierarchy can be represented by:

- Grain assemblages (sediment sources),
- Mineral assemblages (polymineralic grains),
- Minerals (monomineralic grains),
- Chemical elements.

The compositional hierarchy provides a useful frame of reference for data acquisition and analysis, because many problems in sedimentary provenance studies are related to the 'conversion' of information from a lower to a higher level (or vice versa). For instance, low-level characterisation of sediment composition can be routinely performed by means of chemical analysis, but these data cannot be routinely converted into detrital modes, as discussed in the section on normative analysis. In contrast, the high-level information obtained by a careful examination of polymineralic fragments in thin section potentially allows for detailed provenance interpretations in terms of individual parent lithologies, but it implies a time-consuming analysis that cannot be easily automated. Successful application of quantitative sedimentary petrology to the field of basin analysis requires some form of compromise between these two extremes, based on the trade-off between the desire for high-level information on the one hand, and ease of (automated) data acquisition on the other hand.

Genetic interpretations of compositional heterogeneity other than the 'single population concepts' underlying the use of confidence regions should be based on a quantitative description of sediment composition on the highest level within the hierarchy presented above, that is in terms of grain assemblages. According to this view, the objective of quantitative sedimentary provenance studies is to infer the mixing structure of a basin fill, i.e. to translate the spatio-temporal distribution of grain types into proportional contributions of fixed grain assemblages. Such end-member assemblages may have been supplied by a single source at different times, or shed by different sediment sources at the same time.

### *11.2. Conclusions*

Current developments in sedimentary petrology focus primarily on the improvement of data-acquisition techniques. The development of appropriate numerical and statistical techniques for extracting genetic information from petrographic data has received far less attention. The focus on acquisition methodology suggests a widespread conviction that many problems encountered in provenance studies cannot be resolved by analysis of petrographic data gathered by 'conventional' methods such as point counting. Unfortunately, the current state of affairs in quantitative sedimentary–petrologic data processing tends to reinforce such beliefs. Disappointing results from petrographic data analysis are to be expected if nonrigorous or inappropriate procedures are used, that fail to provide theoretically sound inferences about the nature of compositional variation in sediments.

Many of the current problems in statistical characterisation and prediction of sediment composition can be overcome by using appropriate multivariate methods that honour the intrinsic properties of compositional data. The use of statistically rigorous confidence regions in ternary diagrams is a first step in this direction. Their advantages over the conventional hexagons have been illustrated by analysing the compositional variability of modern sands. In cases where the observed variation among specimens cannot be satisfactorily explained in terms of sampling from a single population, more sophisticated multivariate procedures should be used. Some of the multi-

variate tools that have been regularly applied in sedimentary provenance studies have been briefly discussed, and suggestions have been made as to their proper application. The need for a well chosen physically based statistical model to characterise basin fills is of paramount importance for prediction of sediment composition across a reservoir or basin (Giles, 1997). The examples presented in this review highlight the added value of appropriate multivariate statistical models, that can be coupled with stochastic simulation tools for compositional data (Woronow, 1993) to provide such predictions. The next step along this line of quantitative sedimentary petrology is the development of process-based models of sediment production, which predict sediment composition and texture (Weltje et al., 1998).

As shown in this study, much of the valuable information that could be gained from quantitative analysis of sedimentary–petrographic data is lost forever if one attempts to 'summarise' the results of one's painstaking labour in the form of univariate statistics. This common practice has not been beneficial to the development of sedimentary provenance studies and related fields of sedimentary petrology. Fortunately, it has become standard practice to publish raw point-count data in digital format, so that other researchers can re-analyse the data with different models, or test other hypotheses. There are no compelling reasons to assume that pattern recognition in petrographic data will become easier if larger data sets are available. On the contrary, problems of provenance interpretation tend to increase with larger data sets, as shown by Ibbeken and Schleyer (1991). In view of the increasing sophistication of data-acquisition technology, the development of a theoretical framework and appropriate quantitative models for deductive reasoning and testing of hypotheses becomes ever more important. The development of more sophisticated data processing and modelling techniques forms an essential part of provenance studies, because it enables sedimentary geologists to fully enjoy the benefit of current developments in data-acquisition technology.

## Acknowledgements

Raymond V. Ingersoll and Jeffrey L. Howard reviewed an earlier version of this manuscript and made many suggestions for improvement. The final version also benefited from the comments of ESR reviewers Alex Woronow and Gerald M. Friedman. I have many people to thank for sharpening my view on the nature of compositional variation in sediments, but above all I am grateful to John Aitchison for his unwavering encouragement and stimulating interest in all matters compositional. Computer programmes for constructing statistically rigorous confidence regions in ternary diagrams according to the procedures in Appendices A and B are available on request from the author (g.j.weltje@citg.tudelft.nl).

## Appendix A. Multinomial confidence regions

### *A.1. Binary composition (binomial model)*

Critical values of $\chi^2$ in the binary case ($k=2$, hence $df=1$) are equal to 2.71, 3.84 and 6.63, for the usual $(1-\alpha)$ confidence regions of content 0.90, 0.95, and 0.99, respectively (Davis, 1986). The problem to be solved is explicitly:

$$\chi^2_{(1-\alpha)} = \frac{(n_1 - Np_1)^2}{Np_1} + \frac{(n_2 - Np_2)^2}{Np_2} \tag{A-1}$$

By taking into account that $\Sigma_{i=1}^2\ p_i = 1$ and $\Sigma_{i=1}^2\ \hat{p}_i = 1$, this equation is simplified to:

$$1 + \frac{\chi^2_{(1-\alpha)}}{N} = \frac{\hat{p}_1^2}{p_1} + \frac{\hat{p}_2^2}{(1-p_1)} \tag{A-2}$$

Solving for $p_1$ results in a quadratic equation of standard form: $ap_1^2 + bp_1 + c = 0$, where

$$\begin{cases} a = -N - \chi^2_{(1-\alpha)} \\ b = \chi^2_{(1-\alpha)} + 2N\hat{p}_1 \\ c = -N\hat{p}_1^2 \end{cases} \tag{A-3}$$

The quadratic equation has two roots for each value of $p_1$:

$$p_1 = \frac{-b \pm \sqrt{D}}{2a}, \text{ where } D = b^2 - 4ac \tag{A-4}$$

The solution consists of two pairs $(p_1,p_2)$ given by:

$$\begin{cases} p_1 = \dfrac{\chi^2_{(1-\alpha)} + 2N\hat{p}_1 \pm \sqrt{\chi^2_{(1-\alpha)}\{\chi^2_{(1-\alpha)} + 4N\hat{p}_1(1-\hat{p}_1)\}}}{2N + 2\chi^2_{(1-\alpha)}} \\ p_2 = 1 - p_1 \end{cases} \tag{A-5}$$

*A.2. Ternary composition (trinomial model)*

Critical values of $\chi^2$ in the ternary case ($k=3$, hence $df=2$) are equal to 4.61, 5.99, and 9.21, for the usual $(1-\alpha)$ confidence regions of content 0.90, 0.95, and 0.99, respectively (Davis, 1986). The problem to be solved is explicitly:

$$\chi^2_{(1-\alpha)} = \frac{(n_1 - Np_1)^2}{Np_1} + \frac{(n_2 - Np_2)^2}{Np_2} + \frac{(n_3 - Np_3)^2}{Np_3} \tag{A-6}$$

By taking into account that $\Sigma_{i=1}^3 p_i = 1$ and $\Sigma_{i=1}^3 \hat{p}_i = 1$, this equation is simplified to:

$$1 + \frac{\chi^2_{(1-\alpha)}}{N} = \frac{\hat{p}_1^2}{p_1} + \frac{\hat{p}_2^2}{p_2} + \frac{\hat{p}_3^2}{(1-p_1-p_2)} \tag{A-7}$$

Numerical solution of this equation is accomplished by calculation of a series of discrete points $(p_1,p_2)$. Solving for one of the two unknowns, in this case $p_1$, results in a quadratic equation of standard form: $ap_1^2 + bp_1 + c = 0$, where:

$$\begin{aligned} a &= -N\hat{p}_2^2 + Np_2 + \chi^2_{(1-\alpha)}p_2 \\ b &= Np_2(p_2 - 2\hat{p}_1 - 2\hat{p}_2 - 2\hat{p}_1\hat{p}_2) \\ &\quad + \chi^2_{(1-\alpha)}p_2(p_2 - 1) + N\hat{p}_2^2 \\ c &= N\hat{p}_1^2 p_2(1-p_2) \end{aligned} \tag{A-8}$$

The roots of the quadratic equation are given by Eq. (A-4). A quadratic equation has two roots for positive values of $D$, and one root if $D$ is equal to zero. The minimum and maximum values of $p_2$, $\min(p_2)$ and $\max(p_2)$, are thus found by solving the equation $D=0$. A convenient strategy for obtaining these values is to use bracketing and bisection (e.g., Press et al., 1994).

The equation for $D$ is a fourth-degree polynomial in $p_2$. Some care is required in the estimation of $\min(p_2)$, because a singular point exists for small values of $p_2$ (i.e., the coefficient of the quadratic equation $a=0$). This point is defined as:

$$\tilde{p}_2 = \frac{N\hat{p}_2}{N + \chi^2_{(1-\alpha)}} \tag{A-9}$$

The desired value of $\min(p_2)$ is located somewhere in the interval $(\tilde{p}_2, \hat{p}_2)$ and the value of $\max(p_2)$ in the interval $(\hat{p}_2,1)$. In the bracketing phase, the value of $D$ is calculated iteratively for different trial values of $p_2$, starting at $p_2 = \hat{p}_2$. Progressively smaller or larger trial values of $p_2$ are substituted until $D$ becomes negative, indicating that current and previous estimates of $p_2$ bracket the desired $\min(p_2)$ or $\max(p_2)$. In the bisection phase, the intervals containing the desired values of $p_2$ are narrowed until an approximation criterion is satisfied (i.e., $D$ should be sufficiently close to zero). The range of admissible values of $p_2$ has now been defined.

The following procedure has been developed for calculating 40 approximately equally spaced boundary points and placing them in the correct order in an array:

- Define the array index: $1 \le j \le 40$.
- The values of $p_1$ corresponding to $\min(p_2)$ and $\max(p_2)$ are calculated from the relation:

$$p_1 = \frac{-b}{2a}, \tag{A-10}$$

  where $a$ and $b$ are defined as in Eq. (A-8).
- Put the two points $(p_1,p_2)$ in array locations $\{j=40\}$ and $\{j=20\}$.
- The remaining 38 boundary points are calculated pairwise, as the value of $D$ is positive throughout the range of $p_2$. Define a loop index for calculation of 19 successive pairs as: $i = 1 \rightarrow 19$. Then, for each $i$:
- Calculate the value of $p_2$ as:

$$p_2 = \min(p_2) + \frac{1}{2}\{\cos(\beta) + 1\}\{\max(p_2) - \min(p_2)\} \tag{A-11}$$

  where $\beta = \pi - (i\pi/20)$

- Calculate the two values of $p_1$ corresponding to each $p_2$, using the above equation for the roots of the standard quadratic (Eq. (A-4)) or the equivalent expression given by Press et al. (1994).
- Put the point $(p_1, p_2)$ with the smallest value of $p_1$ in array location $\{j = i\}$, and the other point in array location $\{j = 40 - i\}$.
- If $i < 19$ loop back for the next $i$.
- The transformation to ternary coordinates is performed by generating the values of $p_3$ from the relation:

$$p_3 = 1 - p_1 - p_2 \tag{A-12}$$

## Appendix B. Logistic normal confidence regions

### B.1. Binary compositions (univariate normal model)

Logratio transformation of binary compositions leads to a univariate normal distribution of observations, whose parameters may be estimated with the help of the univariate Eqs. (2)–(6). The fundamental difference between application of these equations to raw compositions of the form $(x_1, x_2)$ and a logratio $y$ is the unconstrained nature of the latter. Hence, one is free to use all of these equations if the appropriate logratio transformation has been applied (cf. Eq. (15)), which in this case is defined by:

$$y = \ln\left(\frac{x_1}{x_2}\right) = \ln\left(\frac{x_1}{1 - x_1}\right) \tag{B-1}$$

After the desired calculations have been completed, the results can be transformed back to conventional binary coordinates by applying:

$$\begin{cases} x_1 = \dfrac{\mathrm{e}^{y}}{1 + \mathrm{e}^{y}} \\ x_2 = 1 - x_1 \end{cases} \tag{B-2}$$

which is the binary equivalent of Eqs. (16) and (17).

### B.2. Ternary compositions (bivariate normal model)

The boundaries of the ellipsoidal confidence regions are constructed as follows. Firstly, the right-hand side of Eqs. (20) and (21) is simplified for notational convenience by defining:

$$h_k = \frac{km(n-1)}{n(n-m)} F_{(1-\alpha; df_1; df_2)} \tag{B-3}$$

where $k$ equals one of two possible values: $k = 1$ for a confidence region of the population mean; $k = n + 1$ for a confidence region of the entire population.

Secondly, the singular value decomposition of the inverted sample covariance matrix $\boldsymbol{S}^{-1}$ is introduced to obtain a more convenient expression for subsequent calculations. The singular value decomposition of a square symmetric matrix (e.g., Press et al., 1994) is defined as:

$$\boldsymbol{S} = \boldsymbol{V}\boldsymbol{W}^2\boldsymbol{V}^{\mathrm{T}} \tag{B-4}$$

and its inverse is given by:

$$\boldsymbol{S}^{-1} = \boldsymbol{V}[\boldsymbol{W}^2]^{-1}\boldsymbol{V}^{\mathrm{T}} \tag{B-5}$$

The matrix $\boldsymbol{V}$ contains the set of columnwise orthonormal eigenvectors of the data matrix, which represent the principal axes of the confidence ellipsoid. The elements of the diagonal matrix $[\boldsymbol{W}^2]^{-1}$ are simply the reciprocals of the eigenvalues of the data matrix $\boldsymbol{W}^2$, which may be thought of as scaling factors for the relative lengths of the principal axes.

After substitution of Eqs. (B-3) and (B-5) into Eqs. (20) or (21), the equation to be solved is written as:

$$[\overline{\boldsymbol{Y}} - \boldsymbol{Y}]^{\mathrm{T}}\boldsymbol{V}[\boldsymbol{W}^2]^{-1}\boldsymbol{V}^{\mathrm{T}}[\overline{\boldsymbol{Y}} - \boldsymbol{Y}] = h_k \tag{B-6}$$

A coordinate transformation involving translation and rotation is applied to facilitate the numerical solution of this equation. The problem is put into standard form by defining the vector $\boldsymbol{G}$ as:

$$\boldsymbol{G} = \boldsymbol{V}^{\mathrm{T}}[\overline{\boldsymbol{Y}} - \boldsymbol{Y}] \tag{B-7}$$

The centre of the ellipsoid in $g$-space now coincides with the origin of the $g$-coordinate system, and the principal axes of the ellipsoid are parallel to the $g$-axes. The equation to be solved simplifies to:

$$\boldsymbol{G}^{\mathrm{T}}[\boldsymbol{W}^2]^{-1}\boldsymbol{G} = h_k \tag{B-8}$$

Logratio transformation of ternary compositions leads to a bivariate version of the above equation. The equation for the bivariate case is obtained by writing

out Eq. (B-8) for the case $m=2$, giving the standard ellipse:

$$\left(\frac{g_1}{w_1\sqrt{h_k}}\right)^2+\left(\frac{g_2}{w_2\sqrt{h_k}}\right)^2=1 \tag{B-9}$$

The eigenvalues and eigenvectors of a bivariate covariance matrix can be found by a simple algorithm (e.g., Fisher et al., 1993). If the sample covariance matrix $\boldsymbol{S}$ is defined as:

$$\boldsymbol{S}=\begin{bmatrix} A & B \\ B & C \end{bmatrix} \tag{B-10}$$

and the matrix of eigenvectors $\boldsymbol{V}$ as:

$$\boldsymbol{V}=\begin{bmatrix} a & -b \\ b & a \end{bmatrix} \tag{B-11}$$

Then:

$$\begin{cases} a=\dfrac{\beta}{\sqrt{\beta+1}} \\ b=\dfrac{1}{\sqrt{\beta+1}} \end{cases}, \tag{B-12}$$

where $\beta=\dfrac{A-C}{2B}+\sqrt{\left(\dfrac{A-C}{2B}\right)^2+1}$. The elements of the diagonal matrix of eigenvalues:

$$\boldsymbol{W}^2=\begin{bmatrix} w_1^2 & 0 \\ 0 & w_2^2 \end{bmatrix} \tag{B-13}$$

are given by:

$$\begin{cases} w_1=+\sqrt{a^2A+2abB+b^2C} \\ w_2=+\sqrt{b^2A-2abB+a^2C} \end{cases} \tag{B-14}$$

The desired solution consists of a series of 40 approximately equally spaced pairs $(g_1,g_2)$ located on the boundary of the elliptical confidence region. These are calculated as follows:

- Start by defining a loop index as: $i=1\rightarrow 40$. Then, for each $i$:
- Calculate a boundary point $(g_1,g_2)$ in polar coordinates as:

$$\begin{cases} g_1=w_1\sqrt{h_k}\cos\beta \\ g_2=w_2\sqrt{h_k}\sin\beta, \end{cases} \tag{B-15}$$

  where $\beta=(i\pi/20)$
- Put the pair $(g_1,g_2)$ in array location $\{i\}$
- If $i<40$, loop back for the next $i$.

After the above equation has been solved, the location of the boundary points in $y$-space is obtained by applying the inverse coordinate transformation (Eq. (B-7)). The ellipse is symmetrical about the origin in $g$-space, indicating that the inverse transform may be defined as:

$$\boldsymbol{Y}=\boldsymbol{V}\boldsymbol{G}+\overline{\boldsymbol{Y}} \tag{B-16}$$

In other words, the 40 pairs $(g_1,g_2)$ are premultiplied with $\boldsymbol{V}$ (the inverse rotation), after which the vector of sample means is added to each point (the inverse translation). Finally, the inverse logratio transformation (Eqs. (16) and (17)) is applied to obtain the ternary coordinates of the array of boundary points $\frac{\boldsymbol{B}}{\boldsymbol{N}}$.

## References


Adams, J., 1977. Sieve size statistics from grain measurement. J. Geol. 85, 209–227.

Aiello, E., Bartolini, C., Pranzini, E., 1978. Testing the reliability of beach sand samples. Mem. Soc. Geol. Ital. 18, 171–183.

Aitchison, J., 1986. The Statistical Analysis of Compositional Data. Chapman & Hall, London, 416 pp.

Aitchison, J., 1989. Measures of location of compositional data sets. J. Math. Geol. 21, 787–790.

Aitchison, J., 1990. Comment on "Measures of variability for geological data" by D.F. Watson and G.M. Philip. J. Math. Geol. 22, 223–226.

Aitchison, J., 1991a. Delusions of uniqueness and ineluctability. J. Math. Geol. 23, 275–277.

Aitchison, J., 1991b. A plea for precision in Mathematical Geology. J. Math. Geol. 23, 1081–1083.

Aitchison, J., 1992. On criteria for measures of compositional difference. J. Math. Geol. 24, 365–379.

Aitchison, J., Shen, S.M., 1984. Measurement error in compositional data. J. Math. Geol. 16, 637–650.

Bahk, K.S., Chough, S.K., 1983. Provenance of turbidites in the Ulleung (Tsushima) back-arc basin, East Sea (Sea of Japan). J. Sediment. Petrol. 53, 1331–1336.

Bangs Rooney, C., Basu, A., 1994. Provenance analysis of muddy sandstones. J. Sediment. Res. 64, 2–7.
Barceló, C., Pawlowsky, V., Grunsky, E., 1996. Some aspects of transformations of compositional data and the identification of outliers. J. Math. Geol. 28, 501–518.
Barceló-Vidal, C., Martín-Fernández, J.A., Pawlowsky-Glahn, V., 1999. Comment on "Singularity and nonnormality in the classification of compositional data" by C.G. Bohling, J.C. Davis, R.A. Olea, J. Harff. J. Math. Geol. 31, 581–585.
Bardsley, W.E., 1983. Random error in point counting. J. Math. Geol. 15, 469–475.
Basu, A., 1985. Reading provenance from detrital quartz. In: Zuffa, G.G. (Ed.), Provenance of Arenites. NATO ASI Ser., Ser. C, Reidel Publ., Dordrecht, pp. 231–247.
Basu, A., Young, S.W., Suttner, L.J., James, W.C., Mack, G.H., 1975. Re-evaluation of the use of undulatory extinction and polycrystallinity in detrital quartz for provenance interpretation. J. Sediment. Petrol. 45, 873–882.
Bayly, M.B., 1960a. Errors in point-counter analysis. Am. Mineral. 45, 447–449.
Bayly, M.B., 1960b. Modal analysis by point counter — the choice of sample area. J. Geol. Soc. Aust. 6, 119–129.
Bayly, M.B., 1965. The sampling error in modal analysis. Am. Mineral. 50, 196–211.
Becke, F., 1897. Gesteine des columbretes. Tschermak's Mineral. Petrogr. Mitt. 16, 308–336.
Bezdek, J.C., Ehrlich, R., Full, W.E., 1984. FCM: the fuzzy c-means clustering algorithm. Comput. Geosci. 10, 191–204, and 11, 660 (Erratum).
Boggs Jr., S., 1968. Experimental study of rock fragments. J. Sediment. Petrol. 38, 1326–1339.
Butler, J.C., 1979. Trends in ternary petrologic variation diagrams-fact or fantasy? Am. Mineral. 64, 1115–1121.
Butler, J.C., 1982. The closure problem as reflected in discriminant function analysis. Chem. Geol. 37, 367–375.
Butler, J.C., Woronow, A., 1986. Extracting genetic information from coarse clastic modes. Comput. Geosci. 12, 643–652.
Cavazza, W., 1989. Detrital modes and provenance of the Stilo–Capo d'Orlando Formation (Miocene), southern Italy. Sedimentology 36, 1077–1090.
Chatterjee, P.K., 1965. On the applicability of the Solomon–Hasofer relationship for estimating the counting and sampling error in the modal analysis of natural rocks. Bull. Geol. Soc. India 2, 36–39.
Chayes, F., 1949. A simple point counter for thin-section analysis. Am. Mineral. 34, 1–11.
Chayes, F., 1956. Petrographic Modal Analysis. Wiley, New York, 113 pp.
Chayes, F., 1960. On correlation between variables of constant sum. J. Geophys. Res. 65, 4185–4193.
Chayes, F., Fairbairn, H.W., 1951. A test of the precision of thin-section analysis by point counter. Am. Mineral. 36, 704–712.
Clemens, K.E., Komar, P.D., 1988. Oregon beach-sand compositions produced by the mixing of sediments under a transgressing sea. J. Sediment. Petrol. 58, 519–529.
Cressie, N., Read, T.R.C., 1984. Multinomial goodness-of-fit tests. J. R. Stat. Soc., Ser. B 46, 440–464.
Cross, W., Iddings, J.P., Pirsson, L.V., Washington, H.S., 1902. A quantitative chemico-mineralogical classification and nomenclature of igneous rocks. J. Geol. 10, 555–690.
Darby, D.A., 1990. Evidence for the Hudson River as the dominant source of sand on the US Atlantic shelf. Nature 346, 828–831.
Davis, J.C., 1986. Statistics and Data Analysis in Geology, 2nd edn. Wiley, New York, 646 pp.
Davies, D.K., Ethridge, F.G., 1975. Sandstone composition and depositional environment. Am. Assoc. Pet. Geol. Bull. 59, 239–264.
De Caritat, P., Bloch, J., Hutcheon, I., 1994. LPNORM: a linear programming normative analysis code. Comput. Geosci. 20, 313–347.
DeCelles, P.G., 1988. Lithologic provenance modeling applied to the Late Cretaceous synorogenic Echo Canyon conglomerate, Utah: a case of multiple source areas. Geology 16, 1039–1043.
DeCelles, P.G., Gray, M.B., Ridgway, K.D., Cole, R.B., Srivastava, P., Pequera, N., Pivnik, D.A., 1991. Kinematic history of a foreland uplift from Paleocene synorogenic conglomerate, Beartooth Range, Wyoming and Montana. Geol. Soc. Am. Bull. 103, 1458–1475.
Decker, J., Helmold, K.P., 1985. The effect of grain size on detrital modes: a test of the Gazzi–Dickinson point-counting method—Discussion. J. Sediment. Petrol. 55, 618–620.
Demirmen, F., 1971. Counting error in petrographic point-count analysis: a theoretical and experimental study. J. Math. Geol. 3, 15–41.
Demirmen, F., 1972. Operator error in petrographic point-count analysis: a theoretical approach. J. Math. Geol. 4, 35–43.
Di Giulio, A., Valloni, R., 1992. Analisi microscopica delle areniti terrigene: parametri petrologici e composizioni modali. Acta Nat. Ateneo Parmense 28, 55–101.
Dickinson, W.R., 1970. Interpreting detrital modes of graywacke and arkose. J. Sediment. Petrol. 40, 695–707.
Dickinson, W.R., 1985. Interpreting provenance relations from detrital modes of sandstones. In: Zuffa, G.G. (Ed.), Provenance of Arenites. NATO ASI Ser., Ser. C, Reidel Publ., Dordrecht, pp. 333–361.
Dickinson, W.R., 1988. Provenance and sediment dispersal in relation to paleotectonics and paleogeography of sedimentary basins. In: Kleinspehn, K.L., Paola, C. (Eds.), New Perspectives in Basin Analysis. Springer-Verlag, New York, pp. 3–25.
Dickinson, W.R., Rich, E.I., 1972. Petrologic intervals and petrofacies in the Great Valley sequence, Sacramento Valley, California. Geol. Soc. Am. Bull. 83, 3007–3024.
Dickinson, W.R., Suczek, C., 1979. Plate tectonics and sandstone compositions. Am. Assoc. Pet. Geol. Bull. 63, 2164–2182.
Dorsey, R.J., 1988. Provenance evolution and unroofing history of a modern arc–continent collision: evidence from petrography of Plio–Pleistocene sandstones, eastern Taiwan. J. Sediment. Petrol. 58, 208–218.
Dryden, A.L., 1931. Accuracy in percentage representation of heavy mineral frequencies. Proc. Natl. Acad. Sci. U. S. A. 17, 233–238.
Eisenhart, C., 1935a. A note on a statistical method for the comparison of heavy mineral suites. Am. J. Sci. 30, 549–553.
Eisenhart, C., 1935b. A test for the significance of lithological variations. J. Sediment. Petrol. 5, 137–145.

Fay, M., 1982. Die marinen Sande des nordwestdeutschen Paläogens: Schwerminerale, Liefergebiete, Verbreitung, Gliederungsmöglichkeiten. Berl. Geowiss. Abh., Reihe A 38, 55–144.

Fisher, N.I., Lewis, T., Embleton, B.J.J., 1993. Statistical Analysis of Spherical Data. University Press, Cambridge, 329 pp.

Flores, R.M., Shideler, G.L., 1978. Factors controlling heavy-mineral variations on the South Texas outer continental shelf, Gulf of Mexico. J. Sediment. Petrol. 48, 269–280.

Fontana, D., Zuffa, G.G., Garzanti, E., 1989. The interaction of eustacy and tectonism from provenance studies of the Eocene Hecho Group turbidite complex (South-Central Pyrenees, Spain). Basin Res. 2, 223–237.

Frangipane, M., Schmid, R., 1974. Point counting and its errors: a review. Schweiz. Mineral. Petrogr. Mitt. 54, 19–31.

Friedman, G.M., 1958. Determination of sieve-size distribution from thin-section data for sedimentary petrological studies. J. Geol. 66, 394–416.

Friedman, G.M., 1960. Chemical analyses of rocks with the petrographic microscope. Am. Mineral. 45, 69–78.

Friedman, G.M., 1962. Comparison of moment measures for sieving and thin-section data for sedimentary petrological studies. J. Sediment. Petrol. 32, 15–25.

Friedman, G.M., 1996. Discussion: thin section grain size analysis revisited. Sedimentology 43, 189.

Full, W.E., Ehrlich, R., Klovan, J.E., 1981. EXTENDED QMODEL — Objective definition of external end members in the analysis of mixtures. J. Math. Geol. 13, 331–344.

Full, W.E., Ehrlich, R., Bezdek, J.C., 1982. FUZZY QMODEL — A new approach for linear unmixing. J. Math. Geol. 14, 259–270.

Galehouse, J.S., 1971. Point counting. In: Carver, R.E. (Ed.), Procedures in Sedimentary Petrology. Wiley-Interscience, New York, pp. 385–407.

Garzanti, E., 1991. Non-carbonate intrabasinal grains in arenites: their recognition, significance, and relationship to eustatic cycles and tectonic setting. J. Sediment. Petrol. 61, 959–975.

Garzanti, E., Andó, S., Scutella, M., 2000. Actualistic ophiolite provenance: the Cyprus case. J. Geol. 108, 199–218.

Gazzi, P., 1966. Le arenarie del flysch sopracretaceo dell'Appennino modenese; correlazioni con il flysch di Monghidoro. Mineral. Petrogr. Acta 12, 69–97.

Gergen, L.D., Ingersoll, R.V., 1986. Petrology and provenance of Deep Sea Drilling Project sand and sandstone from the North Pacific Ocean and the Bering Sea. Sediment. Geol. 51, 29–56.

Giles, M.R., 1997. Diagenesis: A Quantitative Perspective — Implications for Basin Modelling and Rock Property Prediction. Kluwer Academic Publishing, Dordrecht, 526 pp.

Gordon, A.D., 1999. Classification. 2nd edn. Chapman & Hall/CRC, Boca Raton, 256 pp.

Graham, S.A., Ingersoll, R.V., Dickinson, W.R., 1976. Common provenance for lithic grains in Carboniferous sandstones from Ouachita mountains and Black Warrior basin. J. Sediment. Petrol. 46, 620–632.

Graham, S.A., Tolson, R.B., DeCelles, P.G., Ingersoll, R.V., Bargar, E., Caldwell, M., Cavazza, W., Edwards, D.P., Follo, M.F., Handschy, J.F., Lemke, L., Moxon, I., Rice, R., Smith, G.A., White, J., 1986. Provenance modelling as a technique for analysing source terrane evolution and controls on foreland sedimentation. In: Allen, P.A., Homewood, P. (Eds.), Foreland Basins. Spec. Publ. Int. Assoc. Sedimentol., vol. 8, pp. 425–436.

Griffiths, J.C., 1960. Modal analysis of sediments. Rev. Geogr. Phys. Geol. Dyn. 3, 29–48.

Griffiths, J.C., 1962. Statistical methods in sedimentary petrography. In: Milner, H.B. (Ed.), Sedimentary Petrography, 4th edn., Volume I: Methods in Sedimentary Petrography. Allen and Unwin, London, pp. 565–617.

Griffiths, J.C., 1966. A genetic model for the interpretive petrology of detrital sediments. J. Geol. 74, 655–672.

Griffiths, J.C., 1967. Scientific Method in Analysis of Sediments. McGraw-Hill, New York, 508 pp.

Griffiths, J.C., Ondrick, C.W., 1969. Modelling the petrology of detrital sediments. In: Merriam, D.F. (Ed.), Computer Applications in the Earth Sciences: An International Symposium. Plenum, New York, pp. 73–97.

Griffiths, J.C., Rosenfeld, M.A., 1954. Operator variation in experimental research. J. Geol. 62, 74–91.

Guasparri, G., Sabatini, G., 1970. Studio metodologico per l'analisi modale al contatore di punti: risultati di ricerche su rocce magmatiche della Sardegna centro-settentrionale. Rend. Soc. Ital. Mineral. Petrol. 26, 147–178.

Harrell, J.A., Eriksson, K.A., 1979. Empirical conversion equations for thin-section and sieve derived size distribution parameters. J. Sediment. Petrol. 49, 273–280.

Hasofer, A.M., 1963. On the reliability of the point-counter method in petrography. Aust. J. Appl. Sci. 14, 168–179.

Howard, J.L., 1993. The statistics of counting clasts in rudites: a review, with examples from the upper Palaeogene of southern California, USA. Sedimentology 40, 157–174.

Howard, J.L., 1994. A note on the use of statistics in reporting detrital clastic compositions. Sedimentology 41, 747–754.

Ibbeken, H., Schleyer, R., 1991. Source and Sediment: A Case Study of Provenance and Mass Balance at an Active Plate Margin (Calabria, southern Italy). Springer-Verlag, Berlin, 286 pp.

Imbrie, J., Van Andel, T.H., 1964. Vector analysis of heavy mineral-data. Geol. Soc. Am. Bull. 75, 1131–1156.

Ingersoll, R.V., 1978. Petrofacies and petrologic evolution of the Late Cretaceous fore-arc basin, northern and central California. J. Geol. 86, 335–352.

Ingersoll, R.V., 1990. Actualistic sandstone petrofacies: discriminating modern and ancient source rocks. Geology 18, 733–736.

Ingersoll, R.V., Bullard, T.F., Ford, R.L., Grimm, J.P., Pickle, J.D., Sares, S.W., 1984. The effect of grain size on detrital modes: a test of the Gazzi–Dickinson point-counting method. J. Sediment. Petrol. 54, 103–116.

Ingersoll, R.V., Bullard, T.F., Ford, R.L., Pickle, J.D., 1985a. The effect of grain size on detrital modes: a test of the Gazzi–Dickinson point-counting method — reply to discussion of Lee J. Suttner and Abhijit Basu. J. Sediment. Petrol. 55, 617–618.

Ingersoll, R.V., Bullard, T.F., Ford, R.L., Pickle, J.D., 1985b. The effect of grain size on detrital modes: a test of the Gazzi–Dickinson point-counting method — reply to discussion of John Decker and Kenneth P. Helmold. J. Sediment. Petrol. 55, 620–621.

Jerram, D.A., Cheadle, M.J., 2000. On the cluster analysis of grains and crystals in rocks. Am. Mineral. 85, 47–67.

Johnson, M.R., 1994. Thin section grain size analysis revisited. Sedimentology 41, 985–999.
Johnson, M.R., 1996. Reply: thin section grain-size analysis revisited. Sedimentology 43, 190–191.
Johnsson, M.J., 1990. Overlooked sedimentary particles from tropical weathering environments. Geology 18, 107–110.
Kellerhals, R., Shaw, J., Arora, V.K., 1975. On grain size from thin sections. J. Geol. 83, 79–96.
Kelley, J.C., 1971. Mathematical analysis of point count data. In: Carver, R.E. (Ed.), Procedures in Sedimentary Petrology. Wiley-Interscience, New York, pp. 409–425.
Kelley, J.C., Whetten, J.T., 1969. Quantitative statistical analyses of Columbia River sediment samples. J. Sediment. Petrol. 39, 1167–1173.
Klovan, J.E., Imbrie, J., 1971. An algorithm and FORTRAN-IV program for large-scale Q-mode factor analysis and calculation of factor scores. J. Math. Geol. 3, 61–77.
Klovan, J.E., Miesch, A.T., 1976. Extended CABFAC and QMODEL computer programs for Q-mode factor analysis of compositional data. Comput. Geosci. 1, 161–178.
Manetti, P., Turi, A., 1969. L'analisi modale col contatore di punti come metodo di campionamento. Atti Soc. Toscana Sci. Nat., Mem., Ser. A 76, 361–402.
Manson, V., Imbrie, J., 1964. FORTRAN program for factor and vector analysis of geologic data using an IBM 7090 or 7094/1401 computer system. Kans. Geol. Surv. Spec. Distrib. Publ. 13, 46 pp.
Medak, F., Cressie, N., 1991. Confidence regions in ternary diagrams based on the power-divergence statistics. J. Math. Geol. 23, 1045–1057.
Mezzadri, G., Saccani, E., 1989. Heavy mineral distribution in late Quaternary sediments of the southern Aegean Sea: implications for provenance and sediment dispersal in sedimentary basins along active margins. J. Sediment. Petrol. 59, 412–422.
Middleton, G.V., 1962. A multivariate statistical technique applied to the study of sandstone composition. Trans. R. Soc. Can. 56, 119–126.
Miesch, A.T., 1976. Q-mode factor analysis of compositional data. Comput. Geosci. 1, 147–159.
Miesch, A.T., 1981. Computer methods for geochemical and petrologic mixing problems. In: Merriam, D.F. (Ed.), Computer Applications in the Earth Sciences, an Update of the 70s. Plenum, New York, pp. 243–265.
Mijnlieff, H.F., Reijers, T.J.A., Dronkert, H., Kouwe, W.P.F., Van De Bilt, G.P., Kelly, S.B., Van Den Heuvel, P.B.J., Weltje, G.J., 1999. The Petrographic Description System of clastic sedimentary rocks: a proposal for standardised petrographic data storage. Meded. Ned. Inst. Toegepaste Geowetenschappen TNO 62, 30 pp.
Molinaroli, E., Basu, A., 1993. Toward quantitative provenance analysis: a brief review and case study. In: Johnsson, M.J., Basu, A. (Eds.), Processes Controlling the Composition of Clastic Sediments. Geol. Soc. Am. Spec. Pap. vol. 284, pp. 323–333.
Molinaroli, E., Blom, M., Basu, A., 1991. Methods of provenance determination tested with discriminant function analysis. J. Sediment. Petrol. 61, 900–908.
Morrison, D.F., 1976. Multivariate Statistical Methods, 2nd edn. McGraw-Hill Kogakusha, Tokyo, 415 pp.
Neilson, M.J., Brockman, G.F., 1977. The error associated with point-counting. Am. Mineral. 62, 1238–1244.
Nesbitt, H.W., Fedo, C.M., Young, G.M., 1997. Quartz and feldspar stability, steady and non-steady-state weathering, and petrogenesis of siliciclastic sands and muds. J. Geol. 105, 173–191.
Packer, B.M., Ingersoll, R.V., 1986. Provenance and petrology of Deep Sea Drilling Project sands and sandstones from the Japan and Mariana forearc and backarc regions. Sediment. Geol. 51, 5–28.
Pearson, K., 1897. Mathematical contributions to the theory of evolution – On a form of spurious correlation which may arise when indices are used in the measurement of organs. Proc. R. Soc., London 60, 489–502.
Pettijohn, F.J., Potter, P.E., Siever, R., 1987. Sand and Sandstone, 2nd edn. Springer-Verlag, New York, 553 pp.
Philip, G.M., Watson, D.F., 1988. Determining the representative composition of a set of sandstone samples. Geol. Mag. 125, 267–272.
Philip, G.M., Skilbeck, C.G., Watson, D.F., 1987. Algebraic dispersion fields on ternary diagrams. J. Math. Geol. 19, 171–181.
Pigorini, B., 1968. Sources and dispersion of recent sediments of the Adriatic Sea. Mar. Geol. 6, 187–229.
Pingitore Jr., N.E., Shotwell, J. 1976. Composition of sand released from three source areas under humid, low relief weathering in the North Carolina piedmont: a discussion. J. Sediment. Petrol. 46, 1041–1047.
Pirkle, F.L., Pirkle, E.C., Pirkle, W.A., Dicks, S.E., 1985. Evaluation through correlation and principal component analysis of a delta origin for the Hawthorne and Citronelle sediments of peninsular Florida. J. Geol. 93, 493–501.
Pivnik, D.A., 1990. Thrust-generated fan-delta deposition: little Muddy Creek conglomerate, SW Wyoming. J. Sediment. Petrol. 60, 489–503.
Potter, P.E., 1978. Petrology and chemistry of modern big river sands. J. Geol. 86, 423–449.
Press, W.H., Teukolsky, S.A., Vetterling, W.T., Flannery, B.P., 1994. Numerical Recipes in Fortran: the Art of Scientific Computing. 2nd. edn. Univ. Press, Cambridge, 963 pp.
Prins, M.A., Weltje, G.J., 1999a. End-member modeling of siliciclastic grain-size distributions: the late Quaternary record of eolian and fluvial sediment supply to the Arabian Sea and its paleoclimatic significance. In: Harbaugh, J.W., Watney, L., Rankey, E.C., Slingerland, R., Goldstein, R.H., Franseen, E.K. (Eds.), Numerical Experiments in Stratigraphy: Recent Advances in Stratigraphic/Sedimentologic Computer Simulations. SEPM Spec. Publ., vol. 62, pp. 91–111.
Prins, M.A., Weltje, G.J., 1999b. End-member modelling of grain-size distributions of sediment mixtures. In: Prins, M.A. (Ed.), Pelagic, hemipelagic and turbidite deposition in the Arabian Sea during the late Quaternary. Geol. Ultraiectina, vol. 168, pp. 47–68 [PhD Thesis, Utrecht University].
Prins, M.A., Postma, G., Weltje, G.J., 2000. Controls on terrigenous sediment supply to the Arabian Sea during the late Quaternary: the Makran continental slope. Mar. Geol. 169, 351–371.
Read, T.R.C., Cressie, N., 1988. Goodness-of-Fit Statistics for Discrete Multivariate Data. Springer-Verlag, New York, 211 pp.
Reed, J.R., Condie, K.C., 1987. Geochemical constraints on the

composition of sandstone matrix and the interpretation of detrital modes. Geol. Mijnbouw 66, 327–332.
Renner, R.M., 1993. The resolution of a compositional data set into mixtures of fixed source compositions. Appl. Stat., J. R. Stat. Soc., Ser. C 42, 615–631.
Renner, R.M., 1995. The construction of extreme compositions. J. Math. Geol. 27, 485–497.
Ripley, B.D., 1981. Spatial Statistics. Wiley, New York, 252 pp.
Robinson, R.S., Johnsson, M.J., 1997. Chemical and physical weathering of fluvial sands in an arctic environment: sands of the Sagavanirktok river, North slope, Alaska. J. Sediment. Res. 67, 560–570.
Rock, N.M.S., 1988. Numerical geology: a source guide, glossary and selective bibliography to geological uses of computers and statistics. Lect. Notes Earth Sci., vol. 18. Springer-Verlag, Berlin, 427 pp.
Root, M.R., 1978. BULK: a computer program for calculating bulk chemical analyses from mineral phases observed in thin section. Comput. Geosci. 4, 199–204.
Rosenfeld, M.A., Jacobsen, L., Ferm, J.C., 1953. A comparison of sieve and thin-section technique for size analysis. J. Geol. 61, 114–132.
Schryver, K., 1968. Precision and components of variance in the modal analysis of coarse-grained augen gneiss. Am. Mineral. 53, 2036–2046.
Shaw, D.M., Harrison, W.D., 1955. Determination of the mode of a metamorphic rock. Am. Mineral. 40, 614–623.
Solomon, M., 1963. Counting and sampling errors in modal analysis by point counter. J. Petrol. 4, 367–382.
Stattegger, K., 1987. Heavy minerals and provenance of sands: modeling of lithological end members from river sands of northern Austria and from sandstones of the austroalpine Gosau formation (Late Cretaceous). J. Sediment. Petrol. 57, 301–310.
Stattegger, K., Morton, A.C., 1992. Statistical analysis of garnet compositions and lithostratigraphic correlation: Brent Group sandstones of the Oseberg field, northern North Sea. In: Morton, A.C., Haszeldine, R.S., Giles, M.R., Brown, S. (Eds.), Geology of the Brent Group. Geol. Soc. Spec. Publ., vol. 61, pp. 245–262.
Stevens, N.P., Bray, E.E., Davis, E.D., 1956. Hydrocarbons in sediments of Gulf of Mexico. Am. Assoc. Pet. Geol. Bull. 40, 975–983.
Stuut, J.B.W., Prins, M.A., Schneider, R.R., Weltje, G.J., Jansen, J.H.F., Postma, G., 2001. A 300 kyr record of aridity and wind strength in southwestern Africa: inferences from grain-size distributions of sediments on Walvis Ridge, SE Atlantic. Mar. Geol. (in press).
Suttner, L.J., 1974. Sedimentary petrographic provinces: an evaluation. In: Ross, C.A. (Ed.), Paleogeographic Provinces and Provinciality. SEPM Spec. Publ., vol. 21, pp. 75–84.
Suttner, L.J., Basu, A., 1985. The effect of grain size on detrital modes: a test of the Gazzi–Dickinson point-counting method—Discussion. J. Sediment. Petrol. 55, 616–617.
Suttner, L.J., Basu, A., Mack, G.H., 1981. Climate and the origin of quartz arenites. J. Sediment. Petrol. 51, 1235–1246.
Textoris, D.A., 1971. Grain-size measurement in thin section. In: Carver, R.E. (Ed.), Procedures in Sedimentary Petrology. Wiley-Interscience, New York, pp. 95–107.
Usdansky, S., 1985. GRCHEM: a BASIC program to calculate granite chemistry from modal mineralogy. Comput. Geosci. 11, 229–234.
Valloni, R., 1985. Reading provenance from modern marine sands. In: Zuffa, G.G. (Ed.), Provenance of Arenites. NATO-ASI Ser., Ser. C, Reidel Publ., Dordrecht, pp. 309–332.
Van der Ark, L.A., 1999. Contributions to Latent Budget Analysis: a Tool for the Analysis of Compositional Data. DSWO Press, Leiden [PhD Thesis, Utrecht University], 221 pp.
Van der Plas, L., Tobi, A.C., 1965. A chart for judging the reliability of point counting results. Am. J. Sci. 263, 87–90.
Vistelius, A.B., Harbaugh, J.W., 1980. Granitic rocks of Yosemite Valley and an ideal granite model. J. Math. Geol. 12, 1–24.
Watson, G.S., 1987. Confidence regions in ternary diagrams 2. J. Math. Geol. 19, 347–348.
Watson, D.F., 1990. Reply to comment on "Measures of variability for geological data" by D.F. Watson and G.M. Philip. J. Math. Geol. 22, 227–231.
Watson, D.F., 1991. Reply to "Delusions of uniqueness and ineluctability" by J. Aitchison. J. Math. Geol. 23, 278.
Watson, G.S., Nguyen, H., 1985. A confidence region in a ternary diagram from point counts. J. Math. Geol. 17, 209–213.
Watson, D.F., Philip, G.M., 1989. Measures of variability for geological data. J. Math. Geol. 21, 233–254.
Weltje, G.J., 1995. Unravelling mixed provenance of coastal sands: the Po delta and adjacent beaches of the northern Adriatic sea as a test case. In: Oti, M.A., Postma, G. (Eds.), Geology of Deltas. Balkema, Rotterdam, pp. 181–202.
Weltje, G.J., 1997. End-member modeling of compositional data: numerical–statistical algorithms for solving the explicit mixing problem. J. Math. Geol. 29, 503–549.
Weltje, G.J., 1998. Compositional and textural heterogeneity of detrital sediments: towards a quantitative framework for sedimentary petrology. In: Buccianti, A., Nardi, G., Potenza, R. (Eds.), Proceedings of IAMG '98 — 4th Annual Conference of the International Association for Mathematical Geology, vol. 1. De Frede Editore, Napoli, pp. 65–70.
Weltje, G.J., 2001. Decomposing compositions: minimum chi-squared reduced-rank approximations on the simplex. Proceedings of IAMG2001 — 6th Annual Conference of the International Association for Mathematical Geology. (in press).
Weltje, G.J., Van Ansenwoude, S.O.K.J., De Boer, P.L., 1996. High-frequency detrital signals in Eocene fan-delta sandstones of mixed parentage (south-central Pyrenees, Spain): a reconstruction of chemical weathering in transit. J. Sediment. Res. 66, 119–131.
Weltje, G.J., Meijer, X.D., De Boer, P.L., 1998. Stratigraphic inversion of siliciclastic basin fills: a note on the distinction between supply signals resulting from tectonic and climatic forcing. In: Hovius, N., Leeder, M. (Eds.), Thematic Set on Sediment Supply to Basins. Basin Res. 10, pp. 129–153.
Whitten, E.H.T., 1961. Quantitative area modal analysis of granite complexes. Geol. Soc. Am. Bull. 72, 1331–1360.
Whitten, E.H.T., Dacey, M.F., 1975. On the significance of certain Markovian features in granitic textures. J. Petrol. 16, 429–453.
Wolf, K.H., 1971. Textural and compositional transitional stages

between various lithic grain types (with a comment on "Interpreting detrital modes of graywacke and arkose"). J. Sediment. Petrol. 41, 328–332.
Woronow, A., 1990. Methods for quantifying, statistically testing, and graphically displaying shifts in compositional abundances across data suites. Comput. Geosci. 16, 1209–1233.
Woronow, A., 1991. Enigmas and solutions in the analysis of compositional data. J. Geol. Educ. 39, 299–302.
Woronow, A., 1993. Generating random numbers on a simplex. Comput. Geosci. 19, 81–88.
Woronow, A., Love, K.M., 1990. Quantifying and testing differences among means of compositional data suites. J. Math. Geol. 22, 837–852.
Zuffa, G.G., 1980. Hybrid arenites: their composition and classification. J. Sediment. Petrol. 50, 21–29.
Zuffa, G.G., 1985. Optical analyses of arenites: influence of methodology on compositional results. In: Zuffa, G.G. (Ed.), Provenance of Arenites. NATO-ASI Ser., Ser. C, Reidel Publ., Dordrecht, pp. 165–189.
Zuffa, G.G., 1987. Unravelling hinterland and offshore palaeogeography from deep-water arenites. In: Leggett, J.K., Zuffa, G.G. (Eds.), Marine Clastic Sedimentology. Graham and Trotman, London, pp. 39–61.
Zuffa, G.G., 1991. On the use of turbidite arenites in provenance studies: critical remarks. In: Morton, A.C. (Ed.), Developments in Sedimentary Provenance Studies. Geol. Soc. Spec. Publ., vol. 57, pp. 23–29.

**Gert Jan Weltje** (1962) is assistant professor of applied clastic sedimentology and mathematical geology at Delft University of Technology. He obtained a MSc in natural sciences (1988) and a PhD in earth sciences (1994) at Utrecht University, The Netherlands. Between 1994 and 1997 he carried out postdoctoral research in applied nuclear physics and sedimentary geology, and worked as a statistical-sedimentological consultant for the oil industry. From 1997 to 2000 he was employed as a researcher at TNO-NITG, the National Geological Survey. He received the 1997 Vistelius Research award of the International Association for Mathematical Geology, of which he is presently a council member. His research focuses on process-response simulation for predictive reservoir modelling, and on inversion of geological data.