[American Journal of Science, Vol. 287, April, 1987, P. 332-352]

SUITES, SUBDIVISION OF BATHOLITHS, AND IGNEOUS-ROCK CLASSIFICATION: GEOLOGICAL AND MATHEMATICAL CONCEPTUALIZATION

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ABSTRACT. Methods proving the reality of named suites within an Australian batholith and of identifying similar mega-groups within new terrane are examined objectively. The work involves explicit differentiation between (1) suites defined genetically (in terms of conditions during formation and/or of distinctive parental material) and descriptively (in terms of current physical and chemical characteristics), and (2) igneous-rock categories based on true classification and on partitioning. A new mathematical basis for cluster analysis (used for partitioning) is presented. Being wholly dependent on the variables used to define them, descriptive suites are real but arbitrary (and thus of undetermined relevance to petrogenesis), unless the defining variables are prescribed by a genetic model. Available quantitative chemical variables do not permit retrieval of the Australian suites, whose genetic significance was recently described; these suites must either be abandoned or (preferably) be defined differently.

INTRODUCTION

Detailed chemical work in Australia (for example, Chappell and White, 1974; White and Chappell, 1983) focused interest on suites within granitoid batholiths and on I-, S-, and A-type granites (compare, Loiselle and Wones, 1979; Pitcher, 1982, 1983; Pitcher and others, 1985). It is natural to extend such thinking about natural groups within granitoid rocks to igneous rocks in general and thence to classification of igneous rocks as a whole.

The initial purpose of the present research was to address two apparently simple but important petrological *questions*:

1. Where granitoid suites have been described within a batholith (for example, O'Neill and Chappell, 1977; Chappell, 1978, 1984; Beams, ms) in terms of traditional geological field and laboratory descriptive variables, what objective quantitative tests based on existing or newly acquired data prove the reality or appropriateness of identified suites?

2. What objective quantitative criteria permit unequivocal identification of granitoid suites in new terrane?

Answering these two questions involves dealing with three complex *issues*, namely:

1. *Definitional issues.*—Because terminology, definitions, and concepts used currently in (1) discussion of suites and (2) igneous-rock classi-

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fication and partitioning are too imprecise for quantitative evaluations, they are clarified in part 1.

2. *Mathematical issues.*—In the geological sciences (from paleontology to petrology), cluster analysis is commonly used for "classifying" samples. Although an obvious tool for identifying granitoid suites, the underlying mathematical basis for cluster analysis has not been enunciated. In evaluating the two initial questions (in pt. 2), implications of new mathematical formulations for cluster analyses (provided in app. 1) are stressed.

Discriminant analysis has been used commonly to determine the efficiency with which a set of variables can partition samples into groups defined previously by other criteria. This method might seem appropriate for the first, but *not* for the second, question. However, discriminant analyses can support misleading conclusions (Whitten, 1985); in particular, if enough quantitative variables are available, purely arbitrary sample groups can be discriminated effectively (Li and others, in preparation). Whitten and others (1984, 1987) illustrated the value of Fisher's exact-test methods, and their results are important to geological arguments in part 2.

3. *Petrological issues.*—The preceding definitional and mathematical issues are integrated into answers to the two petrological questions in part 2, and they are pivotal to the petrological implications enunciated (pt. 3).

PART 1: DEFINITIONAL ISSUES

Suites: Genetic versus Descriptive

Harker (1909) introduced Pacific and Atlantic Suites for assemblages of dissimilar Tertiary and Holocene igneous rocks believed to have been developed under specific, dissimilar tectonic (genetic) conditions; Mediterranean Suite was used later in an analogous sense (Peacock, 1931). The term suite persists in genetic classification, Bayly (1968, p. 61) having defined it as ". . . a group of rocks whose field relations and composition characteristics make it appear that they have a common source." O'Neill and Chappell (1977) in work on oxygen- and hydrogen-isotope relationships in Berridale Batholith and Chappell (1978) in studying chemistry of New England Batholith used the term suite for assemblages of Australian granitoid rock units thought to be cogenetic. Elston and Bornhorst (1979) correlated Tertiary volcanic suites in New Mexico with tectonic (genetic) events at the American-plate margin. Rogers, Suayah, and Edwards (1984) used trace-element geochemistry and other geochemical and lithological features to characterize Sierra Nevadan volcanic suites developed in dissimilar tectonic environments. In numerous recent papers, Pitcher and coworkers (for example, Pitcher, 1984, p. 160) assigned Peruvian Coastal Batholith rocks to ". . . distinct time-separated plutonic units, consanguineous compositional sequences of which form clearly defined super-units (suites) . . . differences . . . are expressed in the terms of texture, fabric, mode . . . xenolith population and the composition of the time-associated dyke swarms . . . Appropriately each super-unit has its own geochemical signature . . ." (Pitcher and others, 1985, sheet 1).

Suites can be defined either

A. *descriptively* in terms of present known physical and chemical composition, characteristics, and spatial variability, or

B. *genetically* in terms of conditions during formation and/or of distinctive parental source material/s.

Symbolically, the types of suite are:

Types of suite ?

— **A** Descriptive
- — $\mathbf{A_1}$ Descriptive: based on variable/s **1**
- — $\mathbf{A_2}$ Descriptive: based on variable/s **2**
- — $\mathbf{A_3}$ Descriptive: based on variable/s **3**
- — •
- — •
- — $\mathbf{A_N}$ Descriptive: based on variable/s **N**

— **B** Genetic
- — $\mathbf{B_1}$ Genetic: different parental-source material
- $\mathbf{B_{1:2}}$ Genetic: different parent and process
- — $\mathbf{B_2}$ Genetic: different petrogenetic process

For example, "marine beach" can be defined descriptively by physical, chemical, and biological features that enable marine-beach deposits to be recognized by geologists (for example, in the stratigraphic column), or genetically by environmental (geographical or paleogeographical) conditions that result in beach formation (waves, currents, sediment transport, et cetera). Similarly, as pointed out by Bayly (1959), metamorphic facies can be defined in terms of presumed temperatures and pressures during genesis (as done originally by Eskola, 1915, p. 114; Turner and Verhoogen, 1951) or descriptively in terms of diagnostic mineral assemblages (Fyfe, Turner, and Verhoogen, 1958; Turner and Verhoogen, 1960, p. 503). With igneous rocks, the interrelationship between the descriptive and the genetic is commonly subject to debate.

Chappell, White, and coworkers used selected descriptive (petrographic and chemical) variables to define granitoid suites within Lachlan Fold Belt, southeastern Australia. On the assumption that these named (descriptive) suites are real, a genetic hypothesis (the restite model) was promulgated to explain their chemical and petrographic nature and their spatial distribution (White and Chappell, 1977). Thus, suites of type **A** (preceding chart) were defined initially, but later, following White and Chappell's (1977) genetic hypothesis, they were considered to be type-$\mathbf{B_1}$ suites. Figure 1 illustrates possible differences between types of genetic suite. If White and Chappell's restite model is relevant to southeastern Australia, then discrete descriptive suites within other batholiths throughout the world would be expected.

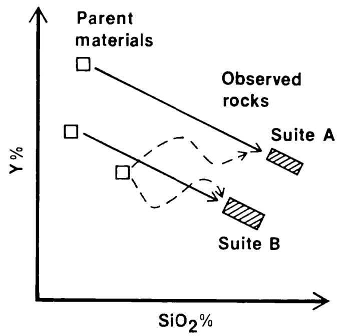


Fig. 1. Types of genetic suite; two-dimensional section through an n-space Harker diagram illustrating the hypothetical evolution of type of suite B_1 (solid lines) and type of suite B_2 (broken-line arrows). In both cases lines could be straight or curved, but Chappell and White's (1977) hypothesis involves straight lines and type B_1.

Unfortunately, identification of descriptive suites uniquely is problematical when numerous variables have been observed. Because a polynomial of degree n can always be found that fits exactly $(n+1)$ observed values with distinct abscissae (Vandermonde's Theorem, compare with Hamming, 1973, p. 230), it follows that, provided enough variables are measured for a population of samples, some variable, or set of variables, can always be found that will effectively discriminate between any truly-distinct pair of sets into which the samples are separated (compare with Li and others, in preparation). Hence, in general, one variable (or set of variables) can be expected to discriminate a different pair of groups (descriptive suites) of samples from groups discriminated by another variable (or set of variables). That is, within a batholith, variable **1** might identify descriptive suites $\mathbf{A}_1$, and variable **2** the different descriptive suites $\mathbf{A}_2$, and generally variable **N** the suites $\mathbf{A}_N$. Thus, different sets of descriptive suites occur within a batholith, their legitimacy depending on the variables used to identify (define) them.

If, and only if, all available measured variables identify (define) the same set of suites, would there be a single, unique set of suites (until additional variables are measured for the samples that do not conform, that is, do not define the same suites). If the alternate sentence "If, and only if, *all* available measured variables are used to define the suites are the suites identified meaningful (until additional variables require the suites to be modified)" were true, the described Australian suites would *not* be meaningful (that is, would not be real), because some measured variables are antipathetic to the described suites (compare with Li and others, in preparation). Additionally, gaining data for *all* the hundreds of measurable variables would be an impossible task. To assert that all available variables must be used simultaneously in defining a suite is untenable, because one petrologist may have modal and major-element chemical data, and another have these plus trace-element data, et cetera.

Conclusion.—Concentrating on descriptive, rather than genetic, definitions of suite, certain logical conclusions emerge. Suite, as a descriptive entity, has no meaning apart from the specified variable, or set of variables, by which it is defined. Different sets of (descriptive) suites (defined by different variable/s) coexist in the same assemblage of igneous rocks. It is unrealistic to enunciate a genetic scenario to account for one set of descriptive suites, without concomitantly embracing the other coexisting sets of descriptive suites (defined by different variables or sets of variables).

Igneous-rock Classification and Partitioning

In practical petrology and petrography, there have been varied approaches to classifying and partitioning igneous rocks. While sedimentary and metamorphic rocks are commonly classified on the bases of variables having genetic significance, igneous rocks have traditionally not been (compare with Shand, 1947, chap. XIII). Most traditional igneous rock nomenclatures (for example, Johannsen, 1931) and many modern publications (for example, Cox, Bell, and Pankhurst, 1979, fig. 2.2) used partitioning procedures that evolve arbitrary classes and terminology. Such classes may fortuitously have petrogenetical significance, but, in general, clustering procedures do not identify classes of petrogenetic significance. Some authors have extended partitioning of plutonic rocks by reference to assumed petrogenetic origins (Debon and LeFort, 1983).

In this paper, precise meanings are used to recognize the distinct differences between **classifying** igneous rocks and arbitrarily **partitioning**[1] them. The distinction, in mathematical terms, is between developing *canonical*, or natural, pattern classes and *conventional*, or symbolic, pattern classes, respectively (Jernigan and Srihari, 1983, p. 1112). This distinction is not generally recognized in igneous petrology and petrography.

In **classification** (identifying canonical or natural classes), variables (features) are chosen on the basis of real or supposed understanding of petrogenesis. Various classes are distinguished *a priori* (that is, based on previous knowledge or theory, rather than on observation or new experiment), so representative samples, defining variables, and/or defining-variable values are specified for each class; such criteria permit new samples to be classified within the scheme. Use of saturation of mineral phases with respect to SiO_2 (Shand, 1947), normative Q–Ab–Or–feldspathoid diagrams, and the basalt tetrahedron provide examples. Vistelius (for example, 1972) used mineral-grain transition probabilities to differentiate "ideal granites" from other granitoids; critical mineral-grain transition probabilities were based on experimental phase relationships established by Tuttle and Bowen (1958). Although not all petrologists accept this ideal-granite model, Vistelius' procedure, being based on an *a priori* petrogenetical concept, yields a canonical classification. For basaltic and andesitic lavas, correlation of observed tectonic setting with detailed trace-

[1] Partitioning is different from using discriminant functions, where a linear (or higher-degree) function is found to separate two predetermined sample groups in the space of variables for those samples. In partitioning, the task is to subdivide samples into groups, using only observed variables for each sample.

and major-element chemistry and with petrography (Pearce and Cann, 1973; Rogers, Suayah, and Edwards, 1984; Shervais and Kimbrough, 1985) permits classification on the basis of descriptive variables. Barker (1984) advocated recognition of genetically different F-, FA-, G-, I-, R-, and S-type granitoids but did not indicate what variables permit such conceptual groups to be discriminated.

In **partitioning** (identifying arbitrary conventional or symbolic classes), variables (features) are specified by class definitions that are uninfluenced by *a priori* considerations. This is clustering, that is empirical detection and description of natural groups or clusters in data for an unlabelled collection of samples (Jernigan and Srihari, 1983, p. 1112). New samples can be partitioned with respect to the empirical classes; this is the "classification procedure" of LeMaitre (1982, p. 170) in his numerical petrology text.

Since the earliest petrographic studies, petrologists and petrographers have tended to use a common set of variables for primary "classification" (that is, partitioning) of igneous rocks. Because it is the most abundant and has the largest variance of all chemical components, SiO_2 has been fundamental for subdividing igneous rocks and is commonly used with Na_2O, K_2O, Al_2O_3, and/or CaO, et cetera. The space of binary, ternary, and quaternary diagrams based on such variables or on modes (or their sums, ratios, et cetera) has commonly been subdivided arbitrarily with fundamental rock types named on the bases of such fields (Chayes, 1957; Streckeisen, 1976; Cox, Bell, and Pankhurst, 1979). Additional, or different, elements have been incorporated to subdivide particular groups of igneous rocks. If a different subset of elements (or function of elements) were used, a wholly dissimilar "classification" (that is, partitioning) would, in general, emerge. In this way, as many different partitionings ("classifications") as desired could be developed. Nomenclature systems (partitionings) based on, say, SiO_2 or MgO wt percentages, can inappropriately separate consanguineous (or allegedly consanguineous) rocks. Separation into classes based on fields defined by intersecting regression lines on Harker-type diagrams could be classification, rather than partitioning, if the intersection/s have genetic significance (compare with Peacock's, 1931, alkali-lime index); ratio-correlation problems compound interpretation problems.

Factors genetically significant for classification may not be intuitively obvious. SiO_2 wt percentage has fundamental importance for most nomenclature systems ("classifications"), but rocks with large SiO_2 range can evolve from a common parental source (for example, by fractional crystallization or partial melting). A natural classification differentiates genetically distinct igneous rocks; if separation into classes were based on arbitrary observational criteria that are independent of genetic differences, the resulting classification would almost certainly be obfuscatory. (Use of superficial similarities in paleontological and other biological classification, for example, would mask (distract from) a desired grouping based on phylogeny.)

Such arguments do not support classification of igneous rocks by genetic environment but favor classification based on petrographic and chemical descriptive parameters explicitly having genetic, rather than arbitrary, significance. This distinction has already been made by others for metamorphic rocks. Thus, original metamorphic facies were defined genetically (Eskola, 1915); subdivisions were based on assumed pressure and temperature during neocrystallization. Following Fyfe, Turner, and Verhoogen (1958, p. 9-10), metamorphic facies are now commonly defined by critical mineral assemblages that change as a function of pressure and temperature, thereby providing an objective basis for *classification*. Metamorphic rocks could readily be *partitioned* and named on the bases of chemical or mineral composition alone; however, such partitioning and nomenclature would not be useful, because materials of dissimilar petrogenesis would be associated together.

If Chappell and White (1974) and Pitcher (1982) were correct in recognizing two, fundamentally dissimilar, granitoid-rock types (I- and S-type granites, derived by partial melting from primary unweathered oceanic igneous crust and from cratonic crustal material reflecting at least one weathering cycle, respectively), a rational classification would separate rocks consanguineous with I-type granites from those of S-type lineage.

Pattern Recognition and Igneous Rocks

Many visual images of planets and their moons transmitted to Earth by space probes are blurred. Images can be sharpened by computer processing; algorithms use parameters deemed important by scientists for "true pattern" recognition (Duda and Hart, 1973). Similarly, with infrared photographic imagery used for military reconnaissance, pattern-recognition specialists filter and/or enhance digital images to detect, say, tank-like objects in imaged battle fields. Adjusting pattern-recognition parameters permits other items to be "enhanced" (recognized). If one knows what is being looked for, parameters can be selected to enhance (recognize) those features. Similarly with classifying animals, plants, or igneous rocks, if the desired result is specified, variables appropriate to the task can be chosen that effectively separate specimens into natural classes (for example, certain protein characteristics for zoological phylogenetical classification).

Figure 2A represents the pattern-recognition problem in remote sensing; in mathematical terms, reality — the sensed object/s — is "mapped" into the space of observed variables, which collectively comprise the visual image produced by remote sensing. This mapping involves information transfer, but, in the process, noise of various kinds is incorporated and entropy increases (that is, uncertainty about information content of the data increases). The pattern-recognition process involves interpretation of observations; in principle, this is an ill-posed problem because of dimensional changes involved in the mapping process and of entropy inherent in the data-acquisition process. Jernigan and Srihari (1983, p. 1112) recognized measurement (observation, enhancement, smoothing, et cetera of original data) and feature extraction (search for global and local char-

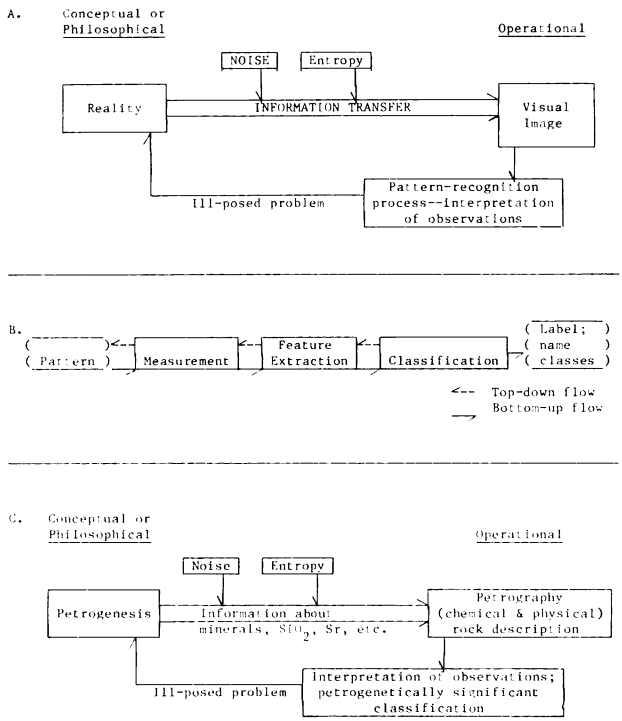


Fig. 2. Pattern recognition: (A) remote sensing; (B) stages in pattern-recognition system (after Jernigan and Srihari, 1983, fig. 1); (C) rock classification.

acteristics of refined measured data) as steps toward classification (see fig. 2B).

The parallel situation for igneous-rock classification is represented in figure 2C. Commonly, petrogenetic events are not directly observable. Interpretation of available observations to develop a chemically and petrographically significant classification is an ill-posed problem, rather than a well-posed problem characterized by the existence, uniqueness, and stability of the solution.

PART 2: MATHEMATICAL ISSUES AND THE TWO PETROLOGICAL QUESTIONS

The first of the two questions enunciated in the Introduction concerned quantitative tests to prove the reality or appropriateness of named descriptive granitoid suites. The second question involved objective criteria for suite recognition in new terrane. These questions are now addressed specifically.

Review of Previous Studies and Cluster Analysis

Not infrequently, petrologists (1) partition samples on the basis of field relationships, petrography, and analytical data, (2) examine the grouping with respect to relevant petrogenetic models, and then (3) classify the groups into genetic classes, suites, et cetera. Such procedures beg the first question posed in the Introduction, namely the identification of quantitative tests to prove the appropriateness of identified suites.

Cluster analyses (based on complete major- and trace-element chemical data for granitoid samples) appeared (Whitten and Chappell, 1984; Whitten, 1985) to lend credence to some previously named, chemically described, suites in Bega Batholith, southeastern Australia (White and Chappell, 1983; Chappell, 1984; Beams, White, and Chappell, in preparation). However, with large data sets (particularly those involving percentage data) results tend not to be stable, clusters varying with minor changes to the data set and with different data-weighting procedures, et cetera. In general, statisticians have been critical of cluster-analysis techniques that involve a heuristic method without (to the best of our knowledge) the benefit of rigorous mathematical foundations (Hartigan, 1975, chap. 6). Because of the potential usefulness of cluster analyses, a simplified outline of a reasonable and rigorous foundation providing the context for definitions and theorems is given in app. 1. Our Theorem 1 (app. 1) establishes the necessary and sufficient conditions for the *existence* of a suite-identifying (partitioning) function. This theorem is not constructive (that is, does not determine which samples should be grouped together). Our Theorem 2 is *constructive* and determines when a well-known clustering algorithm can partition an assemblage of samples uniquely; in addition to specific practical limitations, this theorem constructs only two suites under the hypothesis of sufficient separation. In a subsequent paper, we hope to describe an additional new procedure and theorem with higher cluster-resolving powers and flexibility to accommodate shapes more relevant than hyperspheres. If it could be stated *a priori* for a new set of samples that there is good separation into groups (suites), the practical exercise would be easy, but, in practice, this information is not known in advance.

A method based on Fisher's (1958) exact-test (randomization-test) approach, which allowed all possible partitionings of the original samples into groups (potential suites), has raised significant questions. For example, Whitten and others (1984, 1987) showed that some Bega Batholith suites are not the "best" pairs of groups of samples in terms of the analyzed chemical oxides. They concluded that the descriptive suites previously described in Bega Batholith are either (1) not real or (2) real provided that the variables Sr, Na_2O, and SiO_2 only, plus certain linear constraints, are prescribed as critical to definition of the term suite; other yet-unidentified variables may also be able to define critically the Bega Batholith suites.

Unfortunately, Whitten and others (1984, 1986) did not differentiate between genetic and descriptive suites. Chappell and coworkers (for example, Griffin, White, and Chappell, 1977; Chappell, 1978, 1984; Beams, ms; White and Chappell, 1983) identified the suites empirically on the bases of chemical and petrographic criteria; they relied heavily, but certainly *not* exclusively, on linear relationships of Na_2O and SiO_2 and of Sr and SiO_2 on Harker-type diagrams. Acceptance of the restite model

(White and Chappell, 1977) caused the original suites to assume genetic significance. The restite model assumes partial melting of crustal rocks at depth, which has two implications, namely that (1) all chemical components of the granitoid rocks participated in formation and definition of the descriptively identified suites[2], and (2) all chemical components of rocks comprising a suite are chemical signatures of crustal rocks at depth from which they evolved by partial or complete melting (for example, Chappell, 1984, p. 696). Indeed, B. W. Chappell, W. Compston, and A. J. R. White (personal commun., 1981) asserted that:

> Characterisation of a suite can be made using chemical and isotopic criteria and is achieved when all elements vary in concomitant fashion. Suites will normally encompass a range of chemical composition, but the specification of one element must define all others within the limits of sample variation of that suite.

If each suite within Bega Batholith is the product of dissimilar crustal material, this would be an appropriate *a priori* basis for natural classification of these I-type granitoids. Implicit would be that petrographically defined characteristics (chemical and physical variables of the granitoid rocks) permit classification of granitoids of Bega Batholith into suites.

Conclusion.—On the basis of part 1 of this paper, Whitten and others (1984, 1987) conclusion just cited above must be changed to: the suites are *either* (1) not real if considered to be genetically defined and products of the restite model, *or* (2) one of an almost infinite set of real suites, if defined wholly descriptively; different variables used to partition the samples into groups would identify other suites from an almost infinite set.

Descriptive Suites in Bega Batholith

Using only chemical analyses (32 elements) for every sample, we attempted to determine a partitioning model to retrieve five prominent descriptive suites in Bega Batholith, namely Bemboka, Candelo, Glenbog, Tonghi, and Why Worry Suites (Beams, ms; Chappell, 1984), for which analyses of 121 samples are available.

One could study the efficacy as a discriminant of each element used alone, each pair, each triplet, each group of four, ...; indeed, an immense array of possible discriminants. In principle, Fisher's exact-test approach (Whitten and others, 1984, 1987) could be used for each possible pair of suites for every pair of elements; this would involve an enormous amount of computation (that is, $5 \times 4 \times 32 \times 31 = 7{,}840$ runs of 20-min each on a UNIVAC 1100/81 Computer).

For economic convenience, library computer routine DISSPLA was used to draw two-dimensional scatter diagrams and regression lines for all 496 ($32 \times 31 \times 0.5$) pairs of elements for many pairs of the five suites and for all of the five suites together. If all points for each suite happen to be scattered along separate linear belts (with slopes of the same sign), suites can be differentiated clearly by eye; if the linear belts are close

[2] Such definition means that the descriptive suites exist discretely in the n-dimensional space defined by the n chemical components.

together or overlap, resort to the exact-test approach is necessary. Only SiO_2, K_2O, and/or Na_2O, Sr, and Cr proved to be realistic for identifying the five suites. Both K_2O and Na_2O correctly discriminate the suites, but K_2O is more efficient. The Cr *v.* Sr plot clearly identifies Candelo Suite rocks and is reasonably good at separating Why Worry Suite (fig. 3A). Bemboka, Glenbog, and Tonghi Suites cannot be recognized from a Cr *v.* Sr plot. On a Sr *v.* SiO_2 plot (fig. 3B), Candelo and Glenbog Suites are recognizable, but Bemboka, Tonghi, and Why Worry samples are mixed together. Thus, Bemboka and Tonghi samples overlap in Cr *v.* Sr and Sr *v.* SiO_2 spaces; in K_2O *v.* SiO_2 space, these two suites are clearly differentiated, although confused with samples of the other three suites (fig. 3C). We have not studied exhaustively every pair of the 32 elements, but other

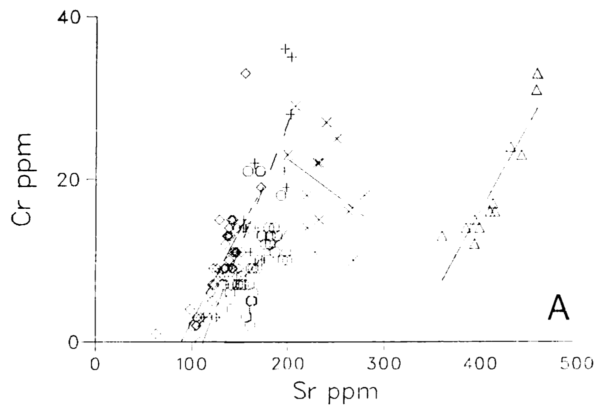
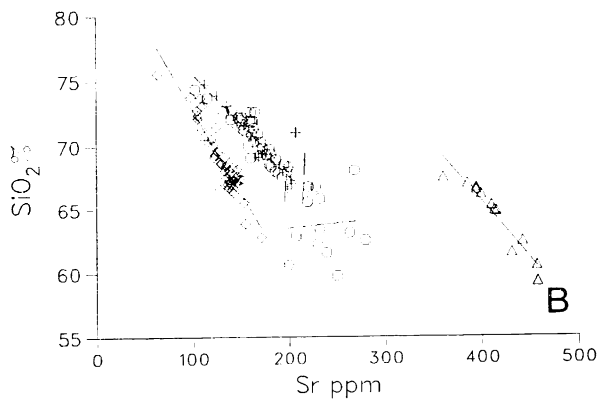


Fig. 3 (A) Harker-type diagram for Cr and Sr ppm with regression lines for Bemboka (○), Glenbog (diamonds), Tonghi (+), Candelo (triangles), and Why Worry (×) Suite rocks, Bega Batholith, southeastern Australia (Chappell's data).



(B) Harker-type diagram for Sr ppm and SiO_2 percent with regression lines for Bemboka (○), Glenbog (diamonds), Tonghi (+), Candelo (triangles), and Why Worry (×) Suite rocks, Bega Batholith, southeastern Australia (Chappell's data).

pairs of elements do not appear to facilitate separation of these suites. In other words, a stepwise process using Cr *v.* Sr, Sr *v.* SiO_2, and then K_2O *v.* SiO_2 permits retrieval of the five suites, but a single chemical criterion, applied to the whole 121-sample set, does not (seem to) retrieve these suites.

Because Cr, Sr, K_2O and/or Na_2O, and SiO_2 appear to be the only elements available for differentiating these suites on two-dimensional scatter diagrams, various combinations of them were used in cluster analyses (fig. 4). Sr, K_2O, and SiO_2 used together are almost completely successful in retrieving the five suites, especially if Tonghi Suite rocks are omitted. Inclusion of Cr does not improve the clustering, despite its value in figure 3A. We recognize that some additional variables (for example, modal constituents, textural features) may have been combined with SiO_2, Na_2O, and Sr by Chappell and coworkers in initially identifying their suites.

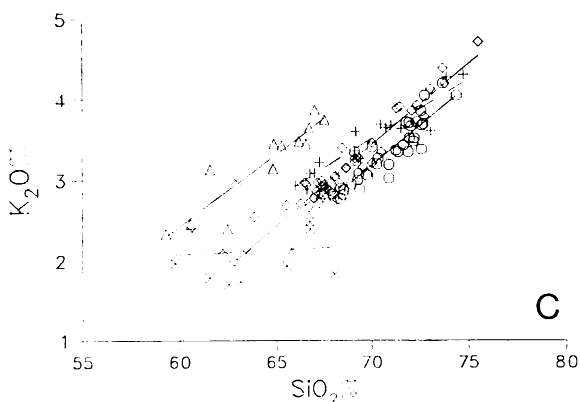
It seems clear from the large number of cluster analyses and other tests run that no set of the chemical variables available to us can retrieve all the named suites correctly and completely *without recourse to a different* ad hoc *step-wise succession of tests for each group of named suites.* It follows that

1. A wholly objective common set of criteria for identifying suites in southeastern Australia is not known to us (that is, a set of *n* chemical components that causes the suites to be discrete in *n*-space defined by those components is not known to us), and

2. Suites analogous to those named by Chappell and coworkers cannot be identified at present in other batholiths on the basis of the type of chemical data available for Bega Batholith alone.

PART 3: PETROLOGICAL ISSUES AND IMPLICATIONS

The *first* of the two questions was ". . . where granitoid suites have been described . . . in terms of traditional geological field and laboratory



(C) Harker-type diagram for K_2O and SiO_2 percent with regression lines for Bemboka (○), Glenbog (diamonds), Tonghi (+), Candelo (triangles), and Why Worry (×) Suite rocks, Bega Batholith, southeastern Australia (Chappell's data).

descriptive variables, what objective quantitative tests based on existing or newly acquired data prove the reality or appropriateness of identified suites?" From part 2, it is clear that, provided the same set of descriptive variables has been *consistently* used to partition all the sampled population of granitoids, comparable real descriptive suites will be identified;

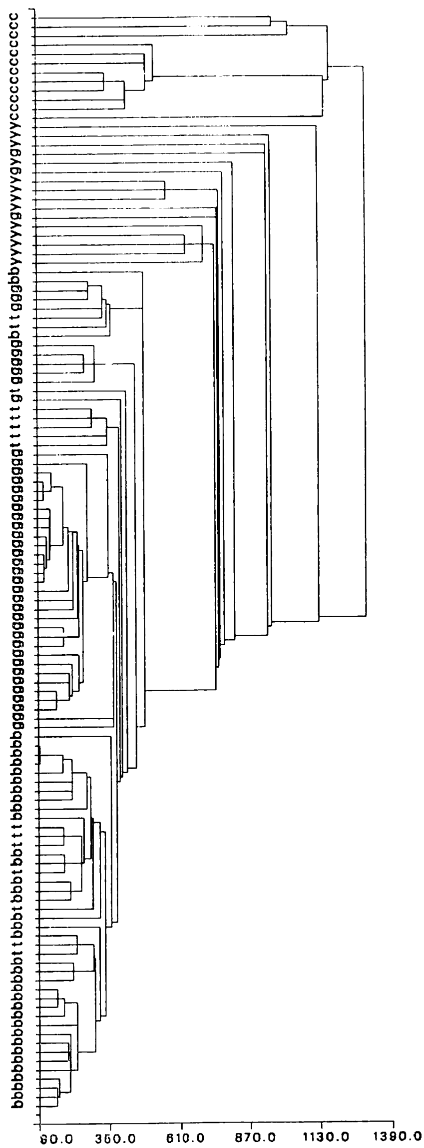


Fig. 4. Cluster analyses based on normalized SiO_2, K_2O, and Sr data for 121 samples from Bemboka (b), Glenbog (g), Tonghi (t), Candelo (c), and Why Worry (y) Suites.

problems would arise if some variables were used for some suites, and others for other suites. If the same partitioning model were used with additional (or different) variables, analogous, but *significantly different,* suites would be defined. New data (for the same variables) for a different set of samples from the same granitoid masses (for example, different sampled population) might also identify different suites because of the variance of some variables in replicate samples (although the Bega Batholith rocks appear to be unusually homogeneous compositionally at the local level).

If the same arbitrary partitioning rules are consistently reapplied, the same arbitrary suites will emerge and thus be real. However, in the original question, "prove the reality" implied more than being arbitrary. Problems arise if genetic significance is associated with suites or if suites are assumed to have been concomitantly defined genetically. Unless the original variables used for partitioning were prescribed by a genetic model, the suites remain arbitrary and, in general, of undetermined relevance to petrogenesis.

The *second question* concerned objective quantitative criteria that permit unequivocal identification of granitoid suites in new terrane. From the original context, this question relates to descriptive, rather than to genetic, suites. Consistent use of the same set of arbitrary variables with the same partitioning model will yield analogous arbitrary descriptive suites in a comparable new terrane (for example, in the Californian Sierra Nevada or the Okhotsk-Chuckchi volcanogenic belt of the Soviet Far East). Including geographical coordinates of sample locations as variables along with the petrographical and chemical variables will insure that samples in contiguous geographic areas are associated in the identified suites. In other words, the type of descriptive suites named in Bega Batholith will be found elsewhere, if the particular variables and the arbitrary partitioning model used by Chappell, White, and coworkers can be identified and used. These have not been fully documented. (Our study concerns objective identification and the reality of the Australian suites. However, if as some would argue, those suites are genetically defined by virtue of White and Chappell's, 1977, restite model, specific source materials are then implied if comparable suites are identified in other parts of the world. If *all n* variables are significant to definition of a set of suites, then those unique suites are discrete in *n*-dimensional space.)

Hence, the descriptive suites in Bega Batholith (being by implication defined by all chemical and isotopic chemical constituents in addition to some petrographic criteria) must *either* be abandoned *or* (preferably) be redefined as suites defined by Sr and other, yet-to-be-specified or yet-to-be-determined, variables. Field geologists will, probably correctly, claim that the Australian and other comparable suites can be recognized with relative ease. Experts commonly use characteristics easily observed and subjectively integrated (Pitcher and others, 1985) but rarely quantified or measured (for example, size, shape, orientation, and interrelationship of mineral grains; type and spatial variance of texture). If reproduceable objective, rather than subjective, quantitative and qualitative results are to be promulgated, there is urgent need for variables important to suite definition to be identified (and their mode of assessment to be standardized).

Although we have expressed concern about the current use of suite in petrology, the concept has potential as a true classification tool. In part 2, Chappell and White's (1974) and Pitcher's (1982) I- and S-granite work is recognized as a rational igneous-rock classification system available for objective testing. Unhappily, plutonic petrogenetic events are not directly observable, so proving the validity of significant classifications is commonly an ill-posed problem. Suites and classes of igneous rocks identified by partitioning based on an arbitrary set of specified variables can be useful for communication between geologists, but such rock groups may, in general, be irrelevant to petrogenesis. If some of the variables used by geologists in identifying groups are ill-defined or unquantified, extending the nomenclature types to other continents may be hazardous and imprecise.

White and Chappell's (1977) restite model appears to depend on the concomitant interaction of all major and minor chemical components being reflected in the chemistry and petrography of a suite; our results mean that such dependency raises severe questions about the applicability of this model to the Bega Batholith rocks. Hildreth (1981) also questioned the meaningfulness of "mixing" lines and source reconstruction as used by White and Chappell (1977).

ACKNOWLEDGMENTS

Special thanks are expressed to Dr. Bruce W. Chappell, who enabled one of us (E.H.T.W.) to gain first-hand knowledge of Lachlan Fold Belt in 1981 during sabbatical leave at Australian National University; he encouraged investigation of the statistical characteristics and significance of chemical analyses produced in his laboratory. Complete analytical data for 1000 Bega Batholith samples were made available on tape; these data were the bases for White and Chappell (1983) and Chappell (1984), many were listed by Beams (ms), but many remain unpublished (for example, Beams, Chappell, and White, in preparation). A travel grant (to E.H.T.W.) from the American Philosophical Society is acknowledged. Geologists Professors John C. Butler (Houston) and Wallace S. Pitcher (Liverpool) and Dr. Marc Loiselle (Maine), and mathematician Professor Donald Saari (Northwestern) kindly made useful detailed comments on early versions of this manuscript.

APPENDIX 1

A simplified formal statement of the problem

Suppose that, at the beginning, t_B, of a time interval of interest $[t_B,t_E]$, there are two parental magmas; for simplicity, assume evolution of both magmas is completed between times t_B tnd t_E. Again, for simplicity, suppose the only important factors are the relative weights $[a_1(t), b_1(t)]$ and $[a_2(t), b_2(t)]$ $(0 \leqslant a,b \leqslant 1)$ of two elements X and Y, respectively, in magmas 1 and 2 at time t. Let the vector-valued function f_X at time t be

$$f_X(t) = \begin{pmatrix} a_X(t) \\ b_X(t) \end{pmatrix},$$

where f_N is called the history of magma N. Thus, f_N maps time interval $[t_B,t_E]$ into the unit square

$$f_N : [t_B,t_E] \rightarrow [0,1] \times [0,1] .$$

(If the argument is extended to X, Y, Z, . . . measured variables, the unit square becomes a unit cube, unit hypercube, . . .) These histories for magma 1 may be graphed schematically as in figure 5.

Suppose four samples, S_P (P = 1, 2, 3, 4), are collected in the field from the final product at time t_E; let $S_P = (a_P, b_P)$, where a_P and b_P are relative weights of X and Y, respectively. These samples can be plotted on a Harker-type diagram for X and Y; there are three possible different ways of pairing up the points (fig. 6). If S_1 and S_3 evolved from magma 1 and S_2 and S_4 from magma 2, the "correct" pairing (that is, correct classification) is partitioning number 2 (fig. 6B); pair (S_1, S_3) may be called suite A and (S_2, S_4) suite B. A random partitioning would have a probability of success of 1/3 (one out of three times). The practical geological problem is to associate correctly the suites with the correct parental magma.

If suites were correctly identified by partitioning (probability 1/3), then random assignment of suites to parental magmas would have a probability of success of one out of two (or 1/2). Assuming independence of the two probabilities (1/3 and 1/2), the probability of successful assignment of the suites to parental magmas is the product of 1/2 and 1/3, or 1/6. As the numbers of samples and suites become large, the probability of random assignments being successful (correct) becomes vanishingly small.

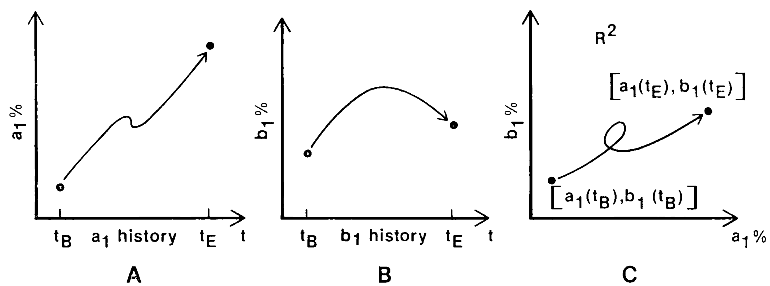


Fig. 5. Schematic history for hypothetical parental magma 1: $f_N(t) = \begin{pmatrix} a_N(t) \\ b_N(t) \end{pmatrix}$.

(A) and (B) History of change of elements a_1 and b_1, respectively, from time B to time E; (C) The magma-to-rock system 1 (time B to E) showing the history of elements a_1 and b_1 in the two-dimensional real-space (R^2) section through the hyperspace of all measured variables.

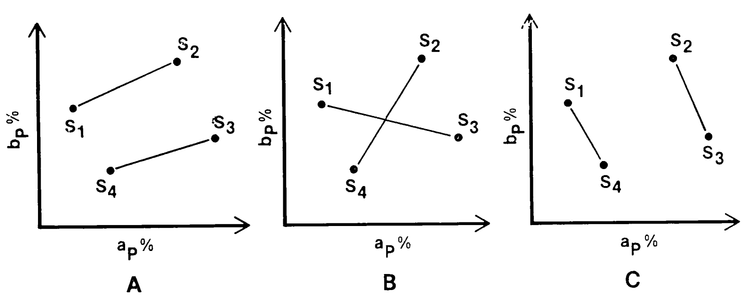


Fig. 6. The three (A, B, and C) possible ways of pairing up the samples $S_1, \ldots S_4$ by partitioning to form suites.

In summary, the petrogenetic (genesis-decision) problem, when M different parental magmas are involved, is posed as follows. Given a set of samples for which the measurements of the variables X, Y, Z, . . . are a, b, c, . . .

1. Correctly partition the data into M separate suites.
2. Correctly assign the M separate suites to M parental magmas.
3. Correctly decide from which of the M parental magmas any new sample located in (a, b, c, . . .) space evolved.

For the second proposition (2), it is appropriate to define a "family-naming function", N_f. As its argument, N_f takes the vector $(a(t_E),b(t_E),c(t_E), \ldots)$ of relative weights $(0 < a,b,c, \ldots \leqslant 1)$ of elements (X,Y,Z, . . .) in each rock sample from a supposed suite, and the value of N_f at this argument is the name, n, of the parental magma. That is, $N_f(a,b,c, \ldots) = n$, where n = 1 if the samples were derived from parental magma 1, n = 2 if derived from parental magma 2, et cetera.

A sufficient condition for definability of function N_f is that the histories of the two (or more) magmas be separable; here, separable means no overlap in the histories. For example, suppose the histories of parental magmas 1 and 2 lie entirely inside hyperspheres $\mathbf{H}_1$ and $\mathbf{H}_2$, respectively. If $\mathbf{H}_1 \cap \mathbf{H}_2 = 0$ (that is, if the intersection of the two hyperspheres is the empty set), then clearly a naming function can be defined (fig. 7). That is, if $(a,b,c, \ldots) \in \mathbf{H}_1$, then $N_f (a,b,c, \ldots) = 1$ and if $(a,b,c, \ldots) \in \mathbf{H}_2$, then $N_f (a,b,c, \ldots) = 2$. However, if $\mathbf{H}_1$ and $\mathbf{H}_2$ overlap (that is, $\mathbf{H}_1 \cap \mathbf{H}_2 \neq 0$), then it is not totally trivial to define N_f correctly in the region common to $\mathbf{H}_1$ and $\mathbf{H}_2$ (that is in $\mathbf{H}_1 \cap \mathbf{H}_2$). (For simplicity, hyperspheres are discussed, but a different shape could have been considered.) The existence of suites in D-dimensional space is based on the premise that parental material and derivative rocks for each suite are close together and contiguous in hyperspace. The following theorem establishes a sufficient condition for the existence of a family-naming function, N_f:

Theorem 1

Given two suites, S_1, S_2, in D-dimensional space, where for j = 1,2,

$$S_j = \{ \vec{a} \mid \vec{a} = (a_1, a_2, a_3, \ldots, a_D), \vec{a} \text{ is a vector of relative weights of a sample whose parent is } j \}.$$

Let $\mathbf{H}_1$ and $\mathbf{H}_2$ be a pair of D-dimensional hyperspheres, that is, for j = 1,2

$$\mathbf{H}_j = \{ \vec{a} \mid \| \vec{a} - \vec{c}_j \| < \mathbf{r}_j \} ,$$

where $\vec{c}_j$ and $\mathbf{r}_j$ are the center and radius of the hypersphere, respectively, and $\| \bullet \|$ is the standard Euclidean norm [that is, $\| \vec{a} - \vec{b} \| = \{(a_1 - b_1)^2 + (a_2 - b_2)^2 + \ldots + (a_D - b_D)^2\}^{1/2}$]. If there exist $\mathbf{H}_1$, $\mathbf{H}_2$, such that $\mathbf{S}_j \in \mathbf{H}_j$ for j = 1,2 and $\mathbf{H}_1 \cap \mathbf{H}_2 = 0$ (that is, $\mathbf{H}_1$ and $\mathbf{H}_2$ do not intersect), then there exists a family-naming function $\mathbf{N}_f$, such that, if $\vec{a} \in \mathbf{S}_j$, then $\mathbf{N}_f(\vec{a}) = j$.

Proof.—Let χ_j be the characteristic function of $\mathbf{H}_j$ for j = 1,2; that is, for j = 1,2,

$$\chi_j(\vec{a}) = \begin{cases} 1 \text{ if } \vec{a} \in \mathbf{H}_j \\ 0 \text{ if } \vec{a} \notin \mathbf{H}_j . \end{cases}$$

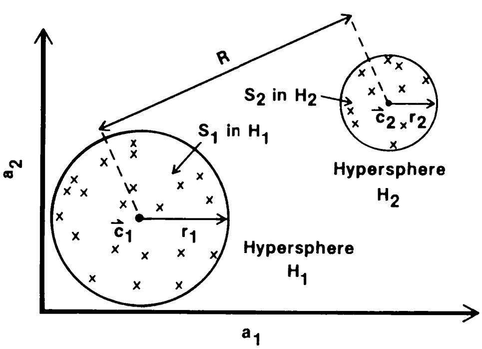


Fig. 7. Two hypothetical suites contained within hyperspheres S_1 and S_2 projected onto a Harker-type diagram showing their centers (c), radii (r), and separation (R); each x is the projection of an individual sample.

Now consider

$$N_f(\bar{a}) = \chi_1(\bar{a}) + 2\,\chi_2(\bar{a});$$

if $\bar{a} \in S_1$, then $N_f(\bar{a}) = 1$, and if $\bar{a} \in S_2$, then $N_f(\bar{a}) = 2$. Note that this definition works because $\mathbf{H}_1$ and $\mathbf{H}_2$ do not overlap. Q.E.D.

Remarks.—This theorem can be generalized for cases where $\mathbf{H}_j$ are arbitrary sets. A necessary condition for the existence of N_f is that nonoverlapping "family-history sets" $\mathbf{H}_1$ and $\mathbf{H}_2$ exist and $S_j \in \mathbf{H}_j$ for j = 1,2. Notice that the preceding theorem is not *constructive* (that is, does not determine which data points should be clustered together) but establishes the conditions for the *existence* of an appropriate partitioning.

From consideration of the probable parent/s and petrogeneses, it might be possible to estimate the centers and radii of hyperspheres containing the derivative rocks. If nonoverlapping $\mathbf{H}_1$ and $\mathbf{H}_2$ cannot be found, going to a higher dimension (that is, adding another variable a_{D+1}) might allow separation; new variables might be the relative weights of additional elements or be some other measured variables.

Construction of suites in hyperspace and use of cluster analysis

Theorem 1 is not constructive and therefore, from a practical, constructive point of view, it is not very useful. Constructive approaches can be considered. A commonly used algorithm in cluster analysis starts by identifying the two closest points and pairing them; for figure 8, this would erroneously pair points A and B. Although an algorithm that properly handles the configuration in figure 8 can be designed, almost any cluster-analysis algorithm could be fooled by sufficiently "pathological" examples. Duda and Hart (1973, chap. 6) and Hartigan (1975, chap. 6) provided good reviews and bibliographies of cluster analysis. Although they did not aim for high levels of rigor (in the interests of producing easily readable texts), they pointed out many weaknesses, pitfalls, and open questions involved in cluster analyses.

The question is how to construct the family-naming function, N_f. A commonly used method is based on **hierarchical cluster analysis by amalgamation** (Illingworth, 1983, p. 61), and we call the algorithm the H.A. algorithm. Assume that

$$S^{(d)} = \{\bar{a}_I \mid 1 \leqslant I \leqslant d, \quad \bar{a}_I \in \mathbf{R}^D\}$$

represents samples drawn from two different families F_1 and F_2. Let S_j be the subset of $S^{(d)}$ coming from family F_j, for j = 1,2. The first step is to find the (or a) nearest pair of samples in some norm; suppose that $\bar{a}_J$ and $\bar{a}_K$ are the two nearest points. For definiteness, the standard Euclidean or l_2 norm is chosen. The second step is to amalgamate (coalesce or cluster) these two points into a single point, $\bar{a}_L$, where $\bar{a}_L = (\bar{a}_J + \bar{a}_K)/2$. This reduces the cardinality of the data set by one; that is, $S^{(d)}$ is reduced to $S^{(d-1)}$; now, by repeating the first step with the new data set $S^{(d-1)}$, the data set is sequentially reduced to the two-point set, $S^{(2)}$.

For the purpose of stating the next theorem, let:

$$S_1 = \{\bar{a}_I \mid 1 \leqslant I \leqslant d_1\}\,,$$

and

$$S_2 = \{\bar{a}_I \mid d_1 + 1 \leqslant I \leqslant d_1 + d_2 = d\}\,.$$

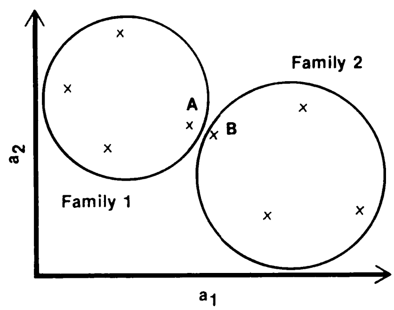


Fig. 8. Two hypothetical suites for which most cluster-analysis algorithms would erroneously put the closest pair of samples, A and B, into the same cluster (suite).

Theorem 2

Assume that both S_1 and S_2 contain at least one sample. Also assume S_1 is contained in hypersphere $\mathbf{H_1}$ with center

$$\vec{c}_1 = \sum_{I=1}^{d_1} \vec{a}_I/d_1 \text{ and radius } r_I = \max_{1 \leqslant I \leqslant d_1} \| \vec{a}_I - \vec{c}_1 \|,$$ and S_2 is contained in hypersphere $\mathbf{H_2}$,

with center $$\vec{c}_2 = \sum_{I=d_1+1}^{d} \vec{a}_I/d_2 \text{ and radius } r_2 = \max_{d_1+1 < I < d} \| \vec{a}_I - \vec{c}_2 \|.$$ Let the hypersphere

centers be separated by the distance $R = \| \vec{c}_1 - \vec{c}_2 \|$ (see fig. 7). A sufficient condition for the H.A. algorithm to cluster S_1 and S_2 correctly is

$$R - (r_1 + r_2) > 2 \{\max (r_1, r_2)\} . \qquad \text{(H.A.)}$$

Proof.—By induction. First, the case where $d = 2$ is apparent. Second, let the induction hyothesis $\mathbf{H}(d)$ be: The theorem is true for d. Consider $S^{(d+1)}$. Apply the H.A. algorithm. It will cluster a pair of points. The cluster is either in S_1 or S_2 because the (H.A.) hypothesis assures that the diameters of S_1 and S_2 are smaller than their separation distance. $S^{(d+1)}$ is thereby reduced to $S^{(d)}$. Apply the induction hypothesis $\mathbf{H}(d)$.

Q.E.D.

Remarks.—This theorem specifies when the H.A. algorithm can correctly partition the data; it constructs two suites under the hypothesis (H.A.) of sufficient separation. As Duda and Hart (1973, p. 230) pointed out, problems arise with clustering algorithms of this type, when the clusters are not compact, not well separated, or not basically hyperspherical. Other algorithms might resolve clusters S_1 and S_2 with a hypothesis weaker than (H.A.); that is, with S_1 and S_2 closer together. In a subsequent paper, we will prove that the least-mean-square Fisher exact test algorithm (LMSFET) based on Fisher's (1958) exact test (that is, minimize

$$\sum{}^2 = \sum_{\vec{a} \in S_1'} \| \vec{a} - \vec{c}_1 \|^2 + \sum_{\vec{a} \in S_2'} \| \vec{a} - \vec{c}_2 \|^2$$

over all possible partitions, $\{S_1', S_2'\}$, of the data set) provides higher resolution in the hyperspherical-cluster case and indicates how this procedure can be extended to non-hyperspherical clusters. Another severe problem that we will address is cluster validity (compare, Duda and Hart, 1973, p. 239), because it is unknown how many clusters are represented in a new data set. Duda and Hart (1973, p. 241) noted that ". . . the statistical problem of testing cluster validity is still essentially unsolved."

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