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A Survey of the Statistical Theory of Shape

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Abstract. This is a review of the current state of the "theory of shape" introduced by the author in 1977. It starts with a definition of "shape" for a set of k points in m dimensions. The first task is to identify the shape spaces in which such objects naturally live, and then to examine the probability structures induced on such a shape space by corresponding structures in $\mathbf{R}^m$. Against this theoretical background one formulates and solves statistical problems concerned with shape characteristics of empirical sets of points. Some applications (briefly sketched here) are to archeology, astronomy, geography and physical chemistry. We also outline more recent work on "size-and-shape," on shapes of sets of points in riemannian spaces, and on shape-theoretic aspects of random Delaunay tessellations.

Key words and phrases: Central place theory, convex polygon, Delaunay tessellation, galaxy, quasar, riemannian submersion, singular tessellation, spherical triangle, stochastic physical chemistry, void.

1. THE ORIGINS OF STATISTICAL SHAPE THEORY

First a few words about terminology. When I was working in Princeton in 1952–1953 someone (I think it was Hassler Whitney) posted a notice in Fine Hall listing a large number of four- and five-letter words not yet used as technical terms in pure mathematics. I do not remember whether "shape" was one of these, but about 1968, according to Borsuk (1975), it was duly appropriated for such a purpose by topologists, so now when we wish to write about the mathematics and statistics of *real* shapes we are required to add an explanatory adjective in order to make it clear that we do mean shape as ordinarily understood and not an arcane concept in topology. Oddly enough, as will shortly become apparent, some other branches of topology turn out to play an important role in our shape theory, but this has nothing to do with Whitney's list.

There are several different approaches to the *statistical analysis* of (real) shapes (see for example Kendall (1984) and the recent reviews of Bookstein (1986) and Small (1988)). There is an equal diversity of approaches to the *geometric description* of shape, but here I will only describe one that I have developed in a series of papers starting in 1977 (Kendall, 1977) and associated with what now seems a very premature attempt to study shape-valued stochastic processes. W. S. Kendall's most recent work on shape-diffusions (W. S. Kendall, 1988) substantiates and considerably generalizes that exploratory essay and links it with research in stochastic physical chemistry (Clifford, Green and Pilling, 1987).

My interest in shape theory was prompted by a statistical topic on the fringes of archeology. When one looks at Stonehenge one accepts the underlying circular structure without asking for statistical authentication, and the same is true of the underlying linear structures in the monuments of Carnac. Statistical tests here would be quite out of place. But there are other archeological situations in which a linear structure is accepted by some and dismissed by others. Thus the set of 52 standing stones near Land's End, Cornwall, studied by Broadbent (1980) yields $\binom{52}{3} =$ 22,100 triplets of stones, and there are those who say vaguely that "too many" of these are "too nearly" collinear, and who attribute this to deliberate planning, whereas others dismiss such claims as ridiculous. Who is right?

We can quantify "too nearly collinear" by interpreting this to mean "the obtuse angle of the triangle defined by the triplet differs from two right angles by less than (say) $\varepsilon = 0.5$ degrees." Figure 1 shows a map of the plan positions of the 52 stones. There are 81 such "nearly collinear" triplets. Figure 2 shows these by means of line segments drawn to join the extreme members of each such triplet.

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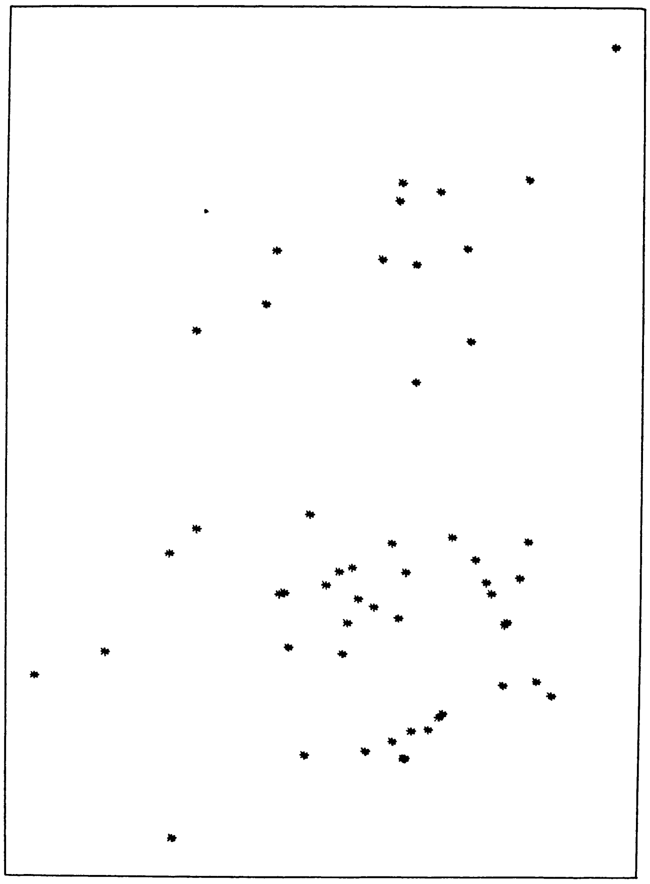

FIG. 1. *The plan positions for the 52 standing stones.* (*Data provided by S. R. Broadbent.*)

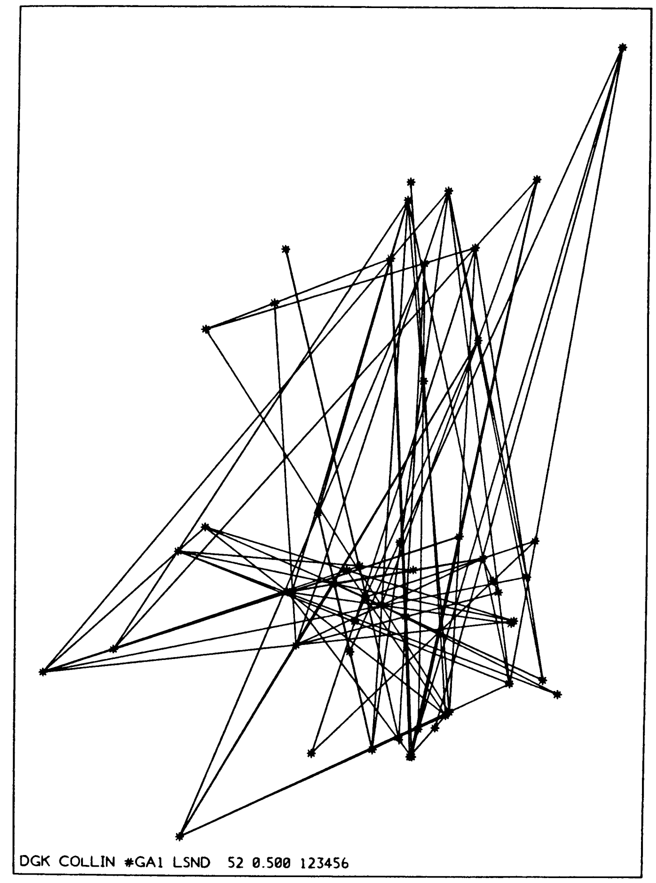

FIG. 2. *The 81* (*half-degree*) *collinearities.*

Is 81 "too many"? A model-based or data-based interpretation of "too many" is evidently called for.

One's first attempt at answering that question might be to pretend that the stones are independently uniformly distributed inside a rectangular frame whose length to breadth ratio is equal to the ratio of the component standard deviations of the configuration, and on that basis one finds that the expected number of triplets meeting the half-degree standard of near-collinearity is about 73, so that relative to approximately Poisson variations (here reasonable) the comment "too many" is unjustified. There is a small excess, but it could quite well be due to chance. I should add that it is preferable to avoid such artificial models and instead to devise a data-based simulation test *of the whole set of 52 sites* employing random lateral perturbations, as was done by W. S. Kendall and myself (Kendall and Kendall, 1980) in a study complementary to that of Broadbent and leading to the same conclusions. Our approach there also avoids the objectionable feature of fixing ε in advance; instead we set a rather broad tolerance region for ε. A detailed account of that and of the method of lateral perturbations would however take us too far from our present theme.

The scheme of our survey will be as follows. In Section 2 we introduce the shape space associated with k labeled points in $\mathbf{R}^m$ and discuss its local metric characteristics, and we illustrate the general discussion by fully identifying some of the simpler shape spaces. In Section 3 we organize the shape spaces in a two-dimensional array and use this to find weak but now global (homology) characteristics of all the shape spaces, with a precision sharp enough to distinguish any one space from all the others. In Section 4 we introduce probability distributions and densities for shape and illustrate this by a brief account of Huiling Le's recent determination of all shape densities for random triangles with vertices uniformly iid in arbitrary compact convex polygons. In Section 5 we turn to a brief account of size-and-shape spaces, and to the more general shape spaces associated with k labeled points in a riemannian manifold M relative to a nicely transitive group of symmetries $\mathscr{G}$. The latter very general situation is illustrated by a discussion of random spherical triangles (important in quasar astronomy). In Section 6 we discuss the size-and-shape problems associated with a random Delaunay tessellation. Finally in Section 7 we outline a few applications.

Much of the work covered by the present survey is still unpublished. It is intended to give a comprehensive account in the book by Carne, Kendall and Le now in preparation.

2. FINDING A NATURAL HOME FOR SHAPES

It was Broadbent's work on the 52 Land's End stones that made me ask the question: what is the natural mathematical home for the shape of a labeled set of k not totally coincident points in m dimensions? (We say labeled points because labels always exist explicitly or implicitly, for example in the form of reference numbers in the archeologist's notebook.) The idea is to filter out effects resulting from translations, changes of scale and rotations and to declare that shape is "what is left."

It is natural first to move the origin to the centroid G of the k points, and then to eliminate size we can compute $L = \sqrt{\sum_{j=1}^{k} GP_j^2}$ (where GP_j denotes the distance from G to P_j) and change the scale by making $L = 1$. This, to a statistician, is the most natural way to standardize for size, but it is not the only possible one, and as we shall see there are contexts in which a different standardization is worth consideration.

This leaves us with an $m \times k$ matrix of rank at most $k - 1$, and to clarify the rank situation we multiply the matrix on the right by a *fixed* element T of the orthogonal group $\mathrm{O}(k)$ that maps the column vector $(0, 0, \ldots, 0, 1)$ to a column vector all of whose elements are equal to $1/\sqrt{k}$. The new matrix will then have a final column of zeros. We omit that column, so that we are left with what is now an $m \times (k - 1)$ matrix the squares of whose elements sum to unity, and obviously we can identify this with a point on a sphere of unit radius and $m(k - 1) - 1$ dimensions. That sphere we shall call the sphere of preshapes. Each of its points is identified with an $m \times (k - 1)$ matrix on which the special orthogonal (rotation) group $\mathrm{SO}(m)$ acts from the left, and we define the shape space Σ_m^k to be the quotient of the preshape sphere by $\mathrm{SO}(m)$. Thus each $\mathrm{SO}(m)$ equivalence class in the preshape sphere is now viewed as a single point (by definition the shape of the original configuration) in this new space. Further details are given in Kendall (1984, 1985, 1986).

Notice that while the construction of the shape space depends on an arbitrary choice of T, the effect of varying that choice does no more than replace the first shape space by another isometric with it. Thus any such T in $\mathrm{O}(k)$ can be used, but must not thereafter be altered. A once for all choice is suggested in Kendall (1984).

It will be observed that it is in the process of standardization for size that we lose the opportunity to include the totally degenerate k-ad all of whose points are coincident. This does, of course, have a distinct shape, and we can if we wish adjoin it to the shape-space as a non-Hausdorff point. Normally the totally degenerate situation is ignored, but an exception is made when discussing the diffusion of size and shape; the non-Hausdorff point representing total degeneracy is then of importance as an entrance boundary. The true significance of this will become apparent when we extend our definition to cover size-and-shape spaces (for which see below).

Geometrically a maximal set of preshapes equivalent modulo $\mathrm{SO}(m)$ forms what is called a *fiber* in the sphere of preshapes, and two k-ads will be said to have the same shape if and only if they determine preshapes lying on the same fiber. It is customary to think of the preshape sphere as lying above the shape space, with the quotient-projection acting downward, so that the whole of each fiber can be thought of as lying above the shape(-point) to which it corresponds. Notice that these fibers do not intersect one another, so that we have a decomposition of the preshape sphere into nonoverlapping fibers. Thus we get the shape space by using the quotient operation that maps fibers *down* onto points (= shapes), and we then throw as much as we can of the natural structure of the preshape sphere down the projection into the shape space. Figure 3 gives a (drastically!) oversimplified sketch of the relationship between (i) the set of k points (here a triangle) in the ambient space (here $\mathbf{R}^2$), (ii) the preshapes and fibers in the preshape space (here a sphere $\mathbf{S}^3(1)$), and (iii) the shapes in the shape space (here a sphere $\mathbf{S}^2(\tfrac{1}{2})$).

That we can metrize a quotient space via the projection is well known, but we can do better. This is because (away from certain singularities when $m \geq 3$, to be discussed below) the projection that maps fibers to points is here what is called a *riemannian submersion* endowing the shape space with a natural smooth riemannian structure inherited from the ordinary riemannian structure of the preshape sphere in such a way that

> each pair of tangent vectors at any preshape on a given fiber, with the property of being orthogonal to the fiber, will map to a pair of tangent vectors at the image of the fiber in the shape space, *these last tangent vectors having the same inner product as the original "horizontal" pair.*

It is usual and helpful to think of the tangent space at a point on the preshape sphere as decomposed into two orthogonal complements: one contains the "vertical" tangents that are tangent to the fiber, whereas the other contains the "horizontal" tangents that are orthogonal to the fiber, so that the above statement is an assertion about pairs of horizontal tangent vectors at a point in the preshape space.

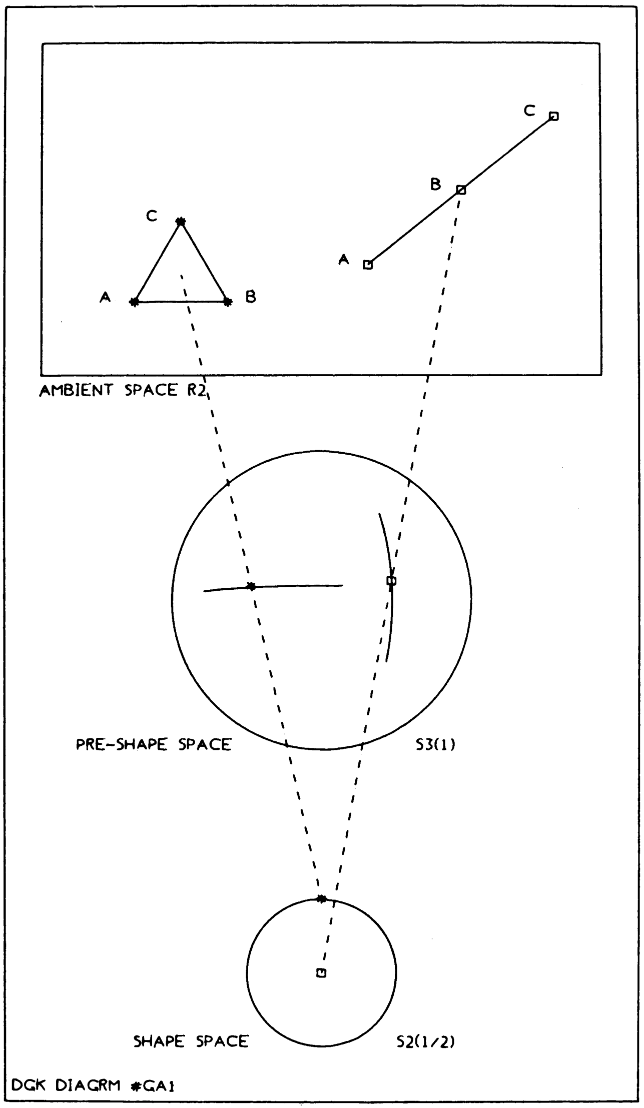

FIG. 3. *The ambient space, the preshape space and the shape space: an impressionistic sketch of the situation when $k = 3$ and $m = 2$.*

This inner product property holds everywhere outside the singular set and imposes a natural riemannian metric on Σ_m^k that has now been determined explicitly; it will be reported on in detail elsewhere. It is relevant that this method when fully implemented also tells us exactly which shapes are located in the singularity set.

Accordingly we immediately obtain local metrical information about the shape space, and obviously to gain a full geometric understanding we shall need to supplement this by other information of a more global character.

One way of meeting that need is to study the geodesics on the shape space. In such a situation as this it is known (O'Neill, 1966, 1967) that the geodesics in the shape space are exactly the projections of the horizontal geodesics (here horizontal great circles in the preshape sphere); moreover, these project with local preservation of arc length, so that the geodesic geometry of the shape space can be read off.

O'Neill has shown that for riemannian submersions one can greatly shorten the computation of sectional curvatures. Another important fact is that the relation between the riemannian structures associated with preshapes and shapes is such that it can also be used to relate diffusions in the two spaces. Here to avoid wearying the statistical reader with technicalities we omit the details.

We now summarize a few specific results for small values of k and m for which the corresponding shape spaces can be fully identified (that is, where they are known up to isometry). Many of these examples are of considerable practical importance.

For $m = 1$ the shape space is the sphere $\mathbf{S}^{k-2}(1)$, where 1 denotes the radius, and for $m = 2$ it is what is known as the complex projective space $\mathbf{C}P^{k-2}(4)$, where 4 denotes the (constant) holomorphic sectional curvature. For $m = 2$ and $k = 3$ we thus find that $\Sigma_2^3 = \mathbf{S}^2(\frac{1}{2})$ (here again the ½ denotes the radius). (This follows because $\mathbf{C}P^1(4) = \mathbf{S}^2(\frac{1}{2})$.) Accordingly $\mathbf{S}^2(\frac{1}{2})$ is the shape space for labeled triangles. It will be observed that the (constant) curvature of Σ_2^3 is equal to 4, although that of the preshape sphere was equal to 1. These facts illustrate a general principle established by O'Neill: this kind of mapping never decreases the curvature.

The singularities that arise when $m \geq 3$ correspond to the k-ads that lie in an $(m - 2)$-dimensional subspace. Thus the singular set is a projective image of Σ_{m-2}^k in Σ_m^k.

The natural generalization of the set of "collinear" labeled triangles in the plane is the set of $(m + 1)$-ads in $\mathbf{R}^m$ that happen to lie in an $(m - 1)$-dimensional subspace, and the corresponding set of shapes is a projective image Eq_m of Σ_{m-1}^{m+1} in Σ_m^{m+1}. In particular when $m = 2$ this tells us that the collinearity set Eq_2 is the projective image $\mathbf{S}^1(\frac{1}{2})$ of $\mathbf{S}^1(1)$ in $\mathbf{S}^2(\frac{1}{2})$, so that it is a special great circle in $\mathbf{S}^2(\frac{1}{2})$. We call this the *equator*, and it is useful to employ that terminology even when m is not equal to 2. It should by now be obvious to the reader that the study of near-collinearities for labeled triplets of points in two dimensions reduces to a study of the shape data in the vicinity of the equator on the shape space $\Sigma_2^3 = \mathbf{S}^2(\frac{1}{2})$. If we use a circularly symmetric gaussian model to describe the random distribution of the original points in $\mathbf{R}^2$ then it turns out that the corresponding distribution of the shape point is uniform on the surface of the spherical shape space. Thus the collinearity studies with which we started have been converted into an elementary exercise in spherical trigonometry.

The projective nestings of shape spaces in other shape spaces briefly illustrated above are very useful in other ways, and are possible because we have chosen to standardize the size measure L to a value (unity) that does not depend on k or m.

We have emphasized that a knowledge of the riemannian geometry of the shape space does not answer all the questions that one needs to ask, because some of those are essentially linked to the global rather than merely local geometrical situation. A complete elaboration of this point would be very technical, but we shall give a sketch of the possibilities in the next section. In preparation for this the reader might like to be reminded of the sort of tools that can be employed.

When one is confronted with a space (such as a shape space) and asks about its geometric structure, there is a hierarchy of levels at which one can operate. At the crudest level one might merely ask for the value of the Euler-Poincaré characteristic χ, probably familiar to all readers in the context of polyhedra in three dimensions. A useful fact to bear in mind is that for spheres this characteristic is equal to 2 when the dimension is even, and is zero when the dimension is odd, these facts holding for any space that is topologically equivalent to a sphere. (For polyhedra in 3 dimensions the dimension is 2, and as this is even the characteristic is also equal to 2.)

Now if one requires slightly more detailed information one can ask for the sequence of homology groups for the space, and here one can operate at three levels, using coefficients drawn from the additive group Z_2 of residues modulo 2, or the additive group Q of rational reals or the additive group Z of signed integers. The last of these three options yields the most detailed information.

After this one could proceed to cohomology, which is a theory dual to homology but with a more detailed structure related to naturally defined product operations, or beyond that to homotopy.

Even when all these possibilities are explored one may find that there is still some lack of detail; one will not necessarily have identified the space up to topological equivalence.

The metrical level at which we were working earlier in this section lies way beyond all the other approaches we have just mentioned, but if it happens to be accessible only in a local form then the additional global information supplied by the "weaker" methods can sometimes provide us with a much more satisfactory result. To illustrate this fact we recall that a complete n-dimensional riemannian manifold with $n \geq 2$ and with positive curvatures K such that $\frac{1}{4} + \varepsilon \leq K \leq 1$ must be a topological sphere $\mathbf{S}^n$ if it is known to be simply connected.

3. THE ARRAY OF SHAPE SPACES Σ_m^k

If we arrange the shape spaces in an array labeled by (k, m), where the number of points $k \geq 2$ increases down the columns and the dimension $m \geq 1$ increases along the rows, then all the spaces along the diagonal $m = k - 1$ are topological spheres (this important result was discovered by A. J. Casson). Clearly however they cannot be metric spheres when $m \geq 3$ because there are then singularities in the differentiable structure. Notice that these "diagonal" shape spaces are the ones needed for the discussion of the shapes of labeled simplexes. Their statistical importance is therefore considerable.

Beyond this diagonal, that is when $m > k - 1$, the shape spaces in the kth row are all metrically the same and topologically they can be identified with a "hemisphere" of the topological sphere Σ_{k-1}^k. (There are two such "hemispheres" in this topological "sphere" that are metrically congruent under a reflection operation and intersect in what we have called Eq_{k-1}.) The reflection referred to is that induced by a reflection of the original configuration in one of the coordinate planes of $\mathbf{R}^m$.

These "hemispheres" and "equators" play an important role when one studies the shape diffusion induced via a time change by a given k point diffusion in the ambient space $\mathbf{R}^m$. The paper by W. S. Kendall already mentioned starts with a brownian or an Ornstein-Uhlenbeck diffusion for a set of $k = 3$ points in $\mathbf{R}^m$, where $m = k - 1, k, k + 1, \ldots$, and then examines the corresponding time-changed diffusions in Σ_m^k as was done in a very tentative way in (Kendall, 1977). The first of these shape spaces is a topological sphere, and all the others are metric copies of one and the same "hemisphere" whose boundary is the "equator" defined above. But the successive diffusions in this "hemisphere" are not the same, and that fact leads to interesting and indeed surprising conclusions about the nature of the stochastic motion when the ambient dimension m tends to infinity.

There remains a triangular region of the array defined by the inequalities $m \geq 3$ and $m < k - 1$ about which we have so far said nothing, but I can now make a fairly complete statement concerning the homology-properties of the spaces in question. (i) None of these spaces is a sphere even in the crudest sense; i.e., none has the homology of a sphere. (ii) None is a topological manifold. (iii) All have torsion in homology. (iv) Any two such spaces are homologically distinct.

The details are long and complicated, but depend chiefly on the interesting fact that if we write

$$\Sigma_m^k \leq \Sigma_n^l$$

when both $k \leq l$ and $m \leq n$, then there is an elegant topological three-term recurrence that constructs Σ_m^k up to homeomorphy out of the topological spaces Σ_{m-1}^{k-1} and Σ_m^{k-1}, and so up to homeomorphy we can (in principle) construct all the shape spaces inductively, following the partial order and starting with the spaces at the margins of the array (for the nature of these is already known).

For the Euler-Poincaré characteristics χ_m^k we obtain a related two-dimensional numerical three-term recurrence that can be solved explicitly. We then find that the triangular region mentioned above contains some even-dimensioned spaces with $\chi = 2$ (as for even-dimensioned spheres) and some odd-dimensioned spaces with $\chi = 0$ (as for odd-dimensioned spheres). Nevertheless these are not topological spheres; for the proof of that we require the corresponding recurrence in homology.

In homology we get a short exact sequence that extends to a long exact sequence with homomorphisms whose action can be fully identified. In this way I have found the Z_2 homology explicitly for all the shape spaces Σ_m^k and a corresponding determination of the Q homology is in progress. Fitting these together via what is called the general coefficient theorem should yield the integer homology, but for our present purposes the Z_2 results suffice; in particular they immediately prove (i) and (iv) above.

One might expect that the shape spaces possessing singularities would prove to be of no practical interest, but that is not so. In fact the spaces Σ_3^k are precisely those that are important in the work of Clifford, Green and Pilling (1987) on stochastic problems in physical chemistry.

4. RANDOM SHAPES: CONVEX-POLYGONALLY GENERATED SHAPE DENSITIES

It might seem that the concentration on the geometry of shape spaces is excessive, but recent events have justified it in a striking way. When this program began in the 1970s, C. G. Small and I knew that a diffuse probability law $\mathscr{L}$ in $\mathbf{R}^m$ must determine in a natural way an induced law $\mathscr{L}^*$ on the shape space Σ_m^k, this being the law of distribution of the shape of a labeled k-ad of points each one of which is independently distributed with law $\mathscr{L}$, but we only knew one or two examples of such situations that we were able to study in explicit detail. It therefore seemed desirable to find a wide range of such explicit shape distributions, at least in the basically important case $k = 3$, $m = 2$. In particular we thought it would substantially remedy the situation if we could find the shape distribution for three points independently uniform in (i) a square and perhaps (ii) an equilateral triangle.

Unfortunately, what we thought a modest objective proved for 10 years unattainable, even in the "simple" cases just mentioned. To assist the mechanics of such calculations we used a stereographic projection of the sphere Σ_2^3, projecting it from the shape point where "$A = B \neq C$" onto the tangent plane at the shape point where "C is the midpoint of AB." This is a plane projection, and in the plane we took cartesian coordinates (x, y) such that the shape point where "$A = C \neq B$" had the coordinates $(-1/\sqrt{3}, 0)$, and the shape point where "$A \neq C = B$" had the coordinates $(+1/\sqrt{3}, 0)$. The occurrence here of $\sqrt{3}$ may seem peculiar, and some writers (e.g., Small, 1981, 1988) avoid it, but it is the kind of notational wrinkle that remains however much one pushes it under the carpet, and I prefer to accept it at this point for the sake of getting cleaner formulas elsewhere. With these coordinates we find that $y = 0$ is the locus of all collinearities apart from the one corresponding to the shape projected to the point at infinity. Thus, $y = 0$ together with the point at infinity is the stereographic version of Eq_2 and near-collinearity studies focus on its immediate neighborhood.

With these conventions it is natural to seek an explicit form for the shape density $m(x, y)$, that is the Radon-Nikodym derivative of the shape measure relative to the σ-finite measure $dxdy$. After many years of unsuccessful attempts by myself to find $m(x, y)$ in the two "simple" cases, the situation has changed dramatically with the work of the young Chinese mathematician Huiling Le, who succeeded in obtaining explicit formulas for the function $m(x, y)$ whenever the probability model is

three points A, B, and C are independently and uniformly distributed inside a compact convex polygon K.

Her solution (1987a, b; see also Kendall and Le, 1986, 1987a) is perfectly general, and covers all compact convex polygons K whatsoever.

What led to this remarkable achievement was the observation that for given K the function $m(x, y)$ is real-analytic inside each tile of a K-dependent "singular tessellation" $\mathscr{T}$ of the (x, y)-plane and jumps abruptly in analytic form when any edge of the tessellation is crossed. As there is a continuum of possible shapes for K, and so a continuum of possible tessellations, this seemed at first to make a complete solution even more unattainable, but the tradition of doing the geometry first, and then tackling the probability calculations when that was fully understood, turned out to be the key to the situation. The geometric dependence of $\mathscr{T}$ on the shape of K was fully investigated (Kendall and Le, 1987a, b), and once that was done the outline of what might be a possible way to a solution came into view, although many difficulties had to be overcome before this intuition was shown to be correct.

Next, the jump suffered on crossing any tile-edge of the tessellation was shown via an analytic continuation argument to be completely characterized by a real analytic *jump function* attached to that tile-edge and free of singularities in a two-dimensional open set containing the edge after removal of its end points. Thus, if one were given the function $m(x, y)$ in some "basic tile" and if also one knew all the jump functions, then it could in principle be extended by analytic continuation to an arbitrary "target" tile by a "stepping-stone" procedure following a sequence of pairwise contiguous tiles. Moreover, it was clear that if the argument could be pushed through then all such stepping-stone routes would provide equally good ways of arriving at a solution, although in practice one would expect some routes to be more convenient than others.

An equally vital and surprising step was Huiling Le's discovery that the problem can in fact be reduced to finite form. She followed this by finding explicitly (a) the function $m(x, y)$ in a particular so-called "basic" tile for all polygons K, and (b) the jump functions for all tile-edges of all tiles in the tessellations associated with all polygons K. Her solution has now been implemented in a computer-algebra language, although in practice the choice of the stepping stone route itself is best performed by eye after inspecting the tessellation. The successive contributions to the (finite) stepping-stone expansion of $m(x, y)$ can contain algebraic terms having singularities in the target tile, but the theory guarantees that in a computer-algebra implementation all such apparent singularities in the target tile will automatically cancel out when their sum is formed, to give a version of $m(x, y)$ that is real analytic inside that tile.

Figure 4 shows a typical tessellation; here K is an irregular pentagon. The shape density $m(x, y)$ is C^2 smooth save at the three shapes corresponding to coincidences among the triangle vertices, and the presence of the jump functions at the tile-edges is betrayed by jumps in the 3rd or 4th normal derivatives. It was indeed the detection of these (using central differences) in earlier numerical studies (Kendall and Le, 1986) that first gave us the necessity insights into the geometrical and analytical structure underlying the tessellations.

The reader may be curious to know whether it is possible to discern any systematic structure at all in Figure 4, and the following remarks are intended to reveal at least some of this; the whole story is a long one. On each edge of $\mathscr{T}$ each point is the shape of a triangle ABC such that two of A, B, and C lie at vertices of the polygon K, while the third lies on an edge of the polygon K, and conversely all such situations, with the triangle ABC arbitrarily labeled, will generate a shape on some linear or quadratic edge of $\mathscr{T}$. Figure 5 illustrates one possible situation, but of course there are many combinatorially distinct cases that have to be considered, and their classification yields further useful structural information concerning both $\mathscr{T}$ itself and the jump functions associated with it.

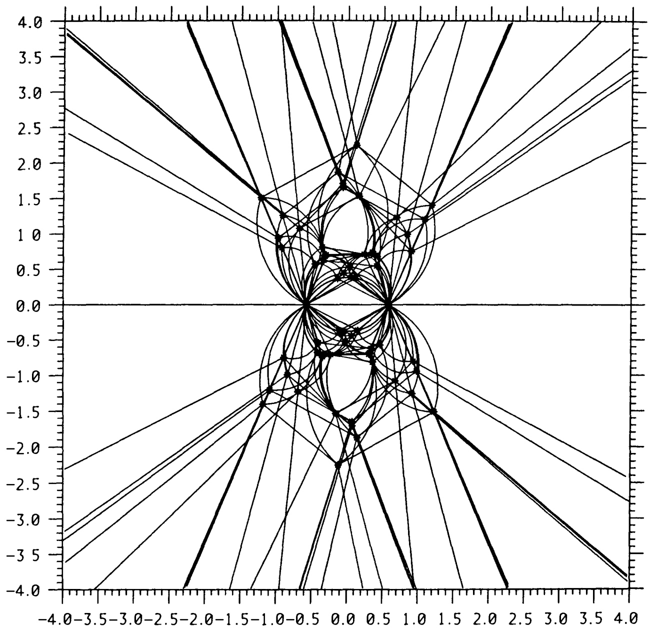

FIG. 4. *A singular tessellation for an irregular pentagon.* (*Reproduced by permission from Kendall and Le,* 1987*a.*)

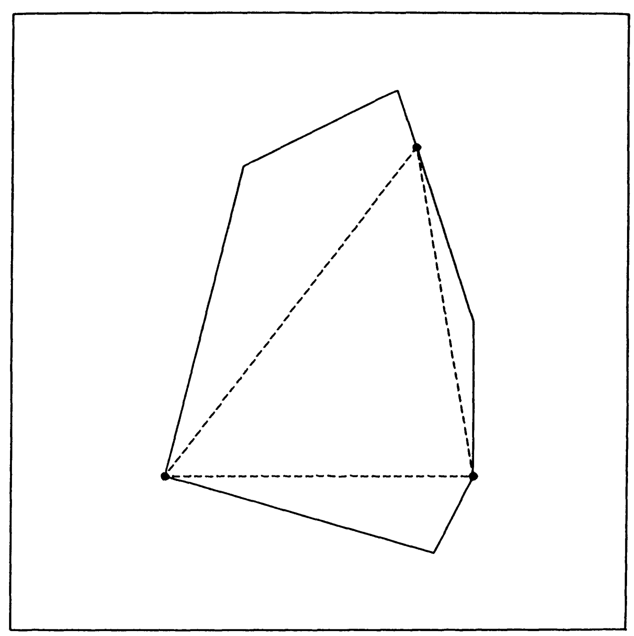

FIG. 5. *A configuration in the ambient space that projects to a shape lying on an edge of the singular tessellation.*

An interesting subsidiary question is: can we find the shape of K when the associated shape-density $m(x, y)$ is known? We can prove that the answer to this is affirmative if we exclude a nowhere-dense subset of the shape space $\Sigma_2^n = CP^{n-2}(4)$, where n is the number of vertices of K. The proof of this depends on the geometrical fact that the tessellation $\mathscr{T}$ is made up of three components: finite segments, semi-infinite half-lines and arcs of circles. If the semi-infinite half-lines and arcs of circles are removed, then what remains is the superposition of $n(n-1)$ scaled, rotated and shifted copies of K itself (built out of the finite segment components). The residual ambiguity is associated with the peeling apart of these $n(n-1)$ copies of K and can always be resolved if it is given in advance that the ratios of interpoint distances between all pairs of vertices of K are distinct.

This result contrasts surprisingly with a general result of Small (1981) telling us that the solution to the corresponding inversion problem can be non-unique when the common law $\mathscr{L}$ of the three triangle vertices is arbitrary (see also Small, 1988).

In this discussion of shape densities it has been supposed that the k original points $P_1, P_2, \ldots, P_k$ determining the shape are given a definite labeling, which could be either intrinsic or assigned at one's convenience. When as often happens the labeling is arbitrary, or of subsidiary importance, one is free to quotient out the permutation group on k letters to obtain a reduced shape space, but that is usually less well behaved, and such additional quotienting is normally avoided except in special circumstances. One such is the situation in which information about an unknown shape density $m(x, y)$ is to be obtained by simulating k-point configurations in m dimensions and then recording their shapes as a preliminary to plotting scatter diagrams, contour plots, etc. in the shape space or some transform of it. (Many examples of such plots will be found in Kendall, 1984.) In such circumstances an extra factor $k!$ in the effective size of the simulation can be gained by exploiting the relabeling group. Having established the result on the reduced shape space it will then often be convenient to construct its equivalents in the other $k! - 1$ permutation transforms in order to bring out more clearly the global structure that is being studied.

5. SIZE AND SHAPE SPACES AND THE SHAPES OF SPHERICAL TRIANGLES

Some of the above is now in a sense rather old work, because during the last 2 years interest in the Cambridge group has gradually shifted away from the shape spaces Σ_m^k toward the associated size and shape spaces here provisionally denoted by $\mathbf{S}\Sigma_m^k$, and also toward the shape spaces $\Sigma(M, \mathscr{G}, k)$ derived from an ambient space that is a riemannian manifold M (instead of $\mathbf{R}^m$) and an appropriate group $\mathscr{G}$ (instead of $SO(m)$) with respect to which the quotient operations take place. There is evidently a connection with the moduli spaces of the algebraic geometers, but this does not seem to lead to any further insights.

We note in passing that the size and shape space $\mathbf{S}\Sigma_m^k$ corresponding to Σ_m^k contains a point $*$ corresponding to the totally degenerate k-ad that was omitted from Σ_m^k itself; this is the point corresponding to size $L = 0$. In fact $\mathbf{S}\Sigma_m^k$ turns out to be a cone with a warped-product metric; the vertex of the cone is the point $*$, and each section of the cone is a scaled version of the shape space Σ_m^k. For m greater than unity $*$ is itself a singularity, and the remaining singularities are all the points on the rays meeting each section in a singularity of the shape space. The metrical theory for $\mathbf{S}\Sigma_m^k$ now follows immediately from these structural remarks, which have important implications for the applications to physical chemistry mentioned earlier.

An instructive example with a noneuclidean ambient space is $\Sigma(\mathbf{S}^2(1), SO(3), 3)$. This is the space of spherical triangles with labeled vertices, but it is not the space of spherical triangles that was studied by Grace Chisholm Young in her celebrated Göttingen doctoral thesis under Felix Klein in 1895. (She considered a triangle with sides that need not be minimal geodesics; also its sides were allowed to intersect at points other than the vertices.) Topologically our space is $\mathbf{S}^3$; this is easily demonstrated by a technique using the properties of identification topologies. But viewed within the differentiable category it possesses four point-singularities; one of these is the shape of total coincidence, whereas the other three correspond to the situations in which two of the vertices are coincident and the third is antipodal to them. Another interesting feature of this space is that it is in effect a size and shape space, because size for spherical triangles is just an aspect of shape. Moreover "location" is now irrelevant, because a change of location can be effected by using the group SO(3). A determined attack on this problem has been made during the last year by Carne, Huiling Le, and myself. We have now obtained (by three different methods, two involving computer-algebra) the riemannian structure, the sectional curvatures, the brownian differential generator, the geodesic geometry and the different but related metric that arises from a parallel procrustean study. We therefore now know almost as much about this shape space as we do about Σ_2^3. Still more recent investigations by Carne and by Huiling Le have extended many of these results to the shape space for k points in $\mathbf{S}^m$.

It is thus appropriate to turn to the statistical problem of finding interesting shape measures on $\Sigma(\mathbf{S}^2(1), SO(3), 3)$, and in the last few months Huiling Le has found the probability law for shapes of spherical triangles whose (labeled) vertices are independently uniform inside a spherical cap of angular radius α $(0 < \alpha \leq \frac{1}{2}\pi)$. (The upper bound on α is needed because otherwise it could happen that A and B lie in the cap although some part of the geodesic arc AB does not.) The whole bundle of these calculations taken together puts us in a position to resolve a problem of interest in quasar astronomy; this is, how should one analyze the claims that "too many" triplets of quasars lie on or suspiciously close to arcs of great circles on the celestial sphere. Or, to put it more roughly, how should one analyze the evidence for there being "too many" triplets of "nearly collinear" quasars. It is known that the effect of the curvature of the celestial sphere is not negligible here. We are now in a position to make an accurate assessment of it, by examining the above results for small α and comparing them with comparable results (again due to Huiling Le) for $\mathbf{S}\Sigma_2^3$. Note that size must come into this comparison, on the one hand because it is not separable from shape in the spherical triangle context, and on the other hand because in the collection of the astronomical data a selection for size will have been exercised.

6. RANDOM DELAUNAY TRIANGLES

Another problem in which size plays a significant role is that in which one studies the shapes of the simplexes that are the tiles of the Delaunay tessellation of a realization of an m-dimensional Poisson point process. We shall call these simplexes PDLY tiles, for short. The present account summarizes (Kendall, 1983, 1989) and adds some more recent results.

We first recall that the Delaunay tessellation of a (suitable) infinite set of distinct isolated points in $\mathbf{R}^m$ was introduced by the Soviet number theorist Boris Nikolaevitch Delone (1890–1980). The construction goes as follows. We look at each $(m + 1)$-ad of points in turn. If its circumsphere contains a point of the set in its interior we do nothing, but if its circumsphere is "empty" in that sense then we draw in the simplex determined by these $m + 1$ points. When all $(m + 1)$-ads have been examined in this way we obtain a nonoverlapping covering of $\mathbf{R}^m$, and that is the Delaunay tessellation, the component simplexes being the tiles thereof. We omit the necessary restrictions on the original set of points but remark that with probability one they will all be satisfied if we apply the construction to a realization of an m-dimensional Poisson process.

At first sight this looks like a problem involving Σ_m^{m+1}, but that turns out to be a partly misleading clue. Some years ago Miles (1970, 1974) proved that for PDLY tiles the circumradius R (which has a scaled χ^2 distribution) is statistically independent of the complete set of shape variables, so that *if* we use R as the measure of size, then size and shape will be independent. This suggests that the connection with Σ_m^{m+1} should be abandoned altogether, but that too would be a mistake. A more fruitful procedure is to compare

(i) the shape distribution for PDLY tiles, and
(ii) the shape distribution for a simplex with independent Gaussian vertices.

This gives us two shape measures μ_1 and μ_2, say. I have proved that the Radon-Nikodym density $d\mu_1/d\mu_2$ is of the form

$$c_m/\rho^{m^2},$$

where c_m is a known function of m only, and where $\rho = \underline{R/L}$ (note that this is a shape variable with $1/\sqrt{m+1}$ as its minimum value). It follows that on constructing by simulation an independent sequence of simplexes with independent Gaussian vertices, and at each step computing ρ and using the obvious acceptance-rejection rule based on

$$(\rho_{\min}/\rho)^{m^2},$$

then the resulting sequence of accepted simplexes will be a sequence of independent PDLY tiles.

In other words, we have found a way of creating "lone" PDLY tiles without doing any tessellating, with consequent immense gains in speed! This work is still in progress, but a few comments will illustrate what has so far been done.

First, the procedure just outlined works spectacularly well for dimensions m from 1 up to about 6 or 7. After that the random sample size obtained falls off drastically because the chance of acceptance (which is known exactly) tends rapidly to zero as m tends to infinity, and so eventually nearly all the Gaussian simulations are rejected. Recently Miles has pointed out to me that such "lone tile simulations" could also be carried out in another way; there μ_2 is to be replaced by μ_3, the shape measure for a simplex whose vertices are independently uniform on a unit sphere. A decomposition formula given by Miles (1974) then yields the Radon-Nikodym derivative, and thereafter one proceeds as before. It will be interesting to see how these two methods compare. I have also looked at the effect of replacing the acceptance/rejection rule by an importance-sampling procedure, the (normed) weights being proportional to the Radon-Nikodym derivatives. Here every simulation is retained, but the weights vary wildly because of their dependence on ρ, and so a suitable smoothing procedure has to be used. My experiments so far show that useful information on the distribution of shape can be obtained by this technique even when $m = 10$. This is remarkable when we consider that, from yet another formula established by Miles (1974), at dimension 10 the expected number of PDLY tiles having a given point as vertex is about

100 million. Thus at $m = 10$ we are working with a stochastic tessellation of PDLY tiles of fantastic complexity, even when viewed from such a narrowly local standpoint. It will be interesting to see how much more insight we can gain when trying new ways of studying this formidable stochastic object.

The main conclusions arrived at so far are that a typical PDLY tile is (1) more likely to be nearly regular (i.e., equilateral) and (2) less likely to be nearly degenerate than is the case for a typical Gaussian simplex. Figures 6 and 7 illustrate a few of the results that have been obtained in this way for $m = 2$, 3, and 6. I hope, by pushing the simulation technique out to higher dimensions, and by supplementary asymptotic calculations, to get some idea of what happens as $m \longrightarrow \infty$.

One would very much like to be able to make comparable statements about groups of "adjacent" tiles in the tessellation, but although some limited progress is possible, this problem seems to be exceedingly difficult. It will be observed that the whole tessellation could be thought of as a somewhat novel form of stochastic field. This remark does not appear to be very helpful, however.

A similar comment can be made about the analysis of the Land's End data. The locations of the 52 stones should strictly be regarded as identifying a single point in the enormous space Σ_2^{52}, and the associated

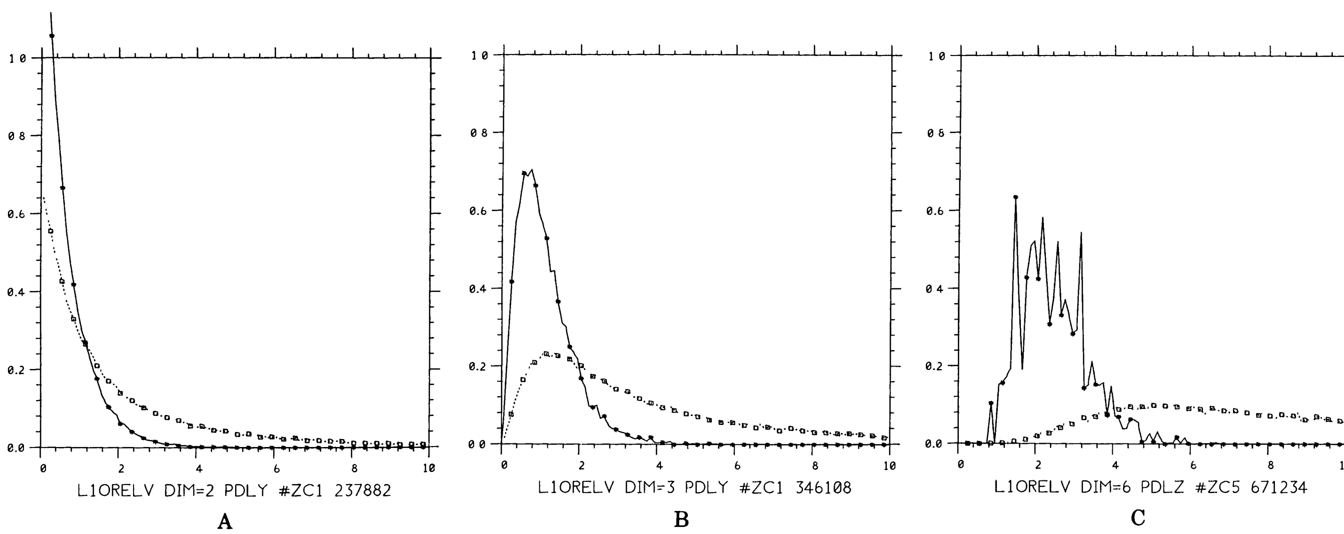

FIG. 6. *Distribution of* $\ln(V_{reg}/V)$. *Here V is the volume of the PDLY simplex and* V_{reg} *is the volume of a regular simplex of equal circumradius. Dotted line, Gaussian simplex; full line, PDLY simplex;* $m = 2, 3, 6$. *Equilaterals to the left of diagram, splinters to the right.*

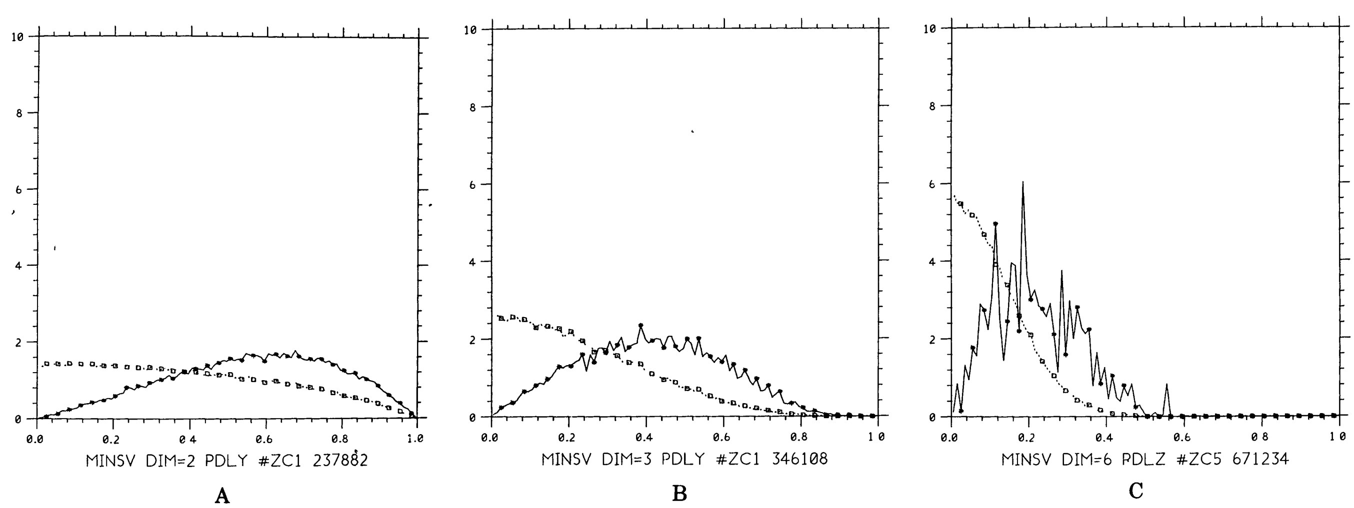

FIG. 7. *Distribution of* $\lambda\sqrt{m}$ (λ = *least singular value*). *Dotted line, Gaussian simplex; full line, PDLY simplex;* $m = 2, 3, 6$. *Equilaterals to the right of diagram, splinters to the left.*

stochastic field is then governed by the appropriate shape measure (given for a Gaussian model in Kendall, 1984) on that shape space.

7. SOME APPLICATIONS

I conclude with a few notes on applications.

It is well known that no classical test for two-dimensional stochastic point processes can match the performance of the human eye and brain in detecting the presence of improbably large holes in the realized pattern of points. This fact has generated a great deal of research in the last few years, especially in connection with the large "voids" and long "strings" that the eye sees (or declares that it sees) in maps of the Shane and Wirtanen catalogue of positions of galaxies (see for example Moody, Turner and Gott, 1983). Astronomers are interested in (i) whether these phenomena are sufficiently extreme to require explanation, and if so (ii) whether any of the various "model" universes now in vogue can be said to display them to just the same degree. Recently Icke and van de Weijgaert (1987) have suggested that useful progress might be made by studying the two- and three-dimensional Delaunay tessellations generated by the galaxy positions, and in particular by examining the observed distributions of various size and shape characteristics for the Delaunay triangles and tetrahedra. The investigation summarized in Section 6 was planned as a contribution to this enquiry.

There is another interesting application of the Poisson-Delaunay theory to geography. Geographers studying the spatial distribution of human settlements claim to see an underlying quasihexagonal structure and speak of "central-place theory." Some years ago Mardia, Edwards and Puri (1977) pointed out that this effect, if it exists, should increase the proportion of nearly equilateral Delaunay tiles. Now we have seen in Figures 6A and 7A that the Delaunay tessellation of a two-dimensional Poisson distribution will in any case contain a high proportion of nearly equilateral tiles, so that a small excess of this as the result of other causes might not be easy to detect.

In fact (Figures 8 and 9) there is indeed a striking number of nearly equilateral tiles in the Delaunay tessellation of 234 towns, villages and hamlets in Wisconsin, the other noticeable feature of that data set being a high proportion of thin splinter-shaped tiles round the edges of the region being tessellated. Of course these latter tiles are not true Delaunay tiles at all; they arise solely because their circumcircles lie mostly outside the region, and so they are "empty" in virtue of the cut-off at the edges.

Now central place theory also has something to say about distances. Thus one mechanism that has been invoked to explain central place effects in East Anglia is the tendency for neighboring market towns to be separated by the maximum distance over which one can drive sheep in a day. (I owe this remark to Dr. G. P. Hirsch.)

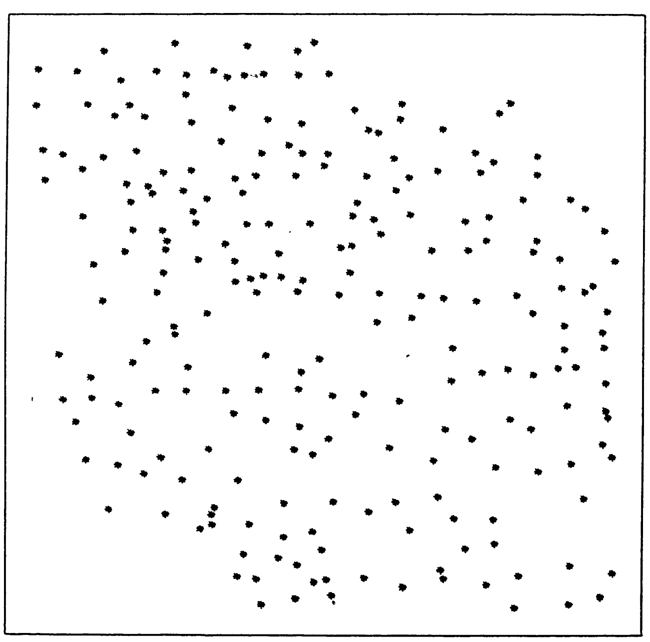

FIG. 8. *Locations of* 234 *settlements in Wisconsin.* (*Data provided by A. D. Cliff and based on Brush*, 1953.)

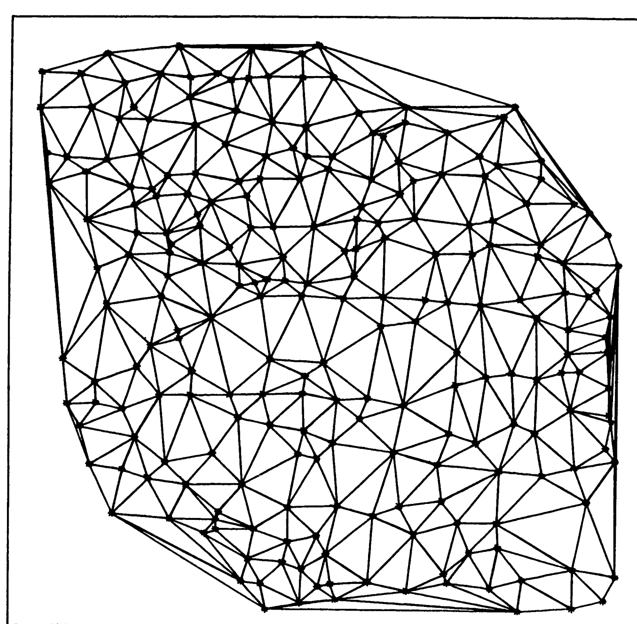

FIG. 9. *The Delaunay tessellation for the Wisconsin sites.*

Accordingly we ought to treat this as a problem that belongs to size and shape theory rather than to shape theory, and this presents no difficulties because for PDLY tiles in two dimensions the size (measured by the circumradius R) has a simple distribution; in fact R^2 has the law of a scaled χ_4^2, the scaling constant being known. The shape distribution in this situation is known from the work of Miles, and as remarked earlier size and shape are here statistically independent.

This suggests a new approach to such data, as follows. (i) Sort the tiles according to their shape, and select (a) those that by some convenient angular criterion are "nearly equilateral," then (b) those that are highly splinter-shaped and (c) the remainder. Then (ii) look at the distribution of circumradial size within the sets (a) and (c) and examine the departures from independence and from the theoretical χ^2 law.

This procedure has the attractive feature that it will not be seriously corrupted by the excess of splinter-shaped tiles that are associated with the edge effects. Normally in spatial statistics, edge effects are very difficult to deal with. Here we may be lucky!

Finally in Figure 10 we show the Delaunay tessellation for the 52 locations of the Land's End stones; the reader will perhaps find the comparison with Figure 2 instructive.

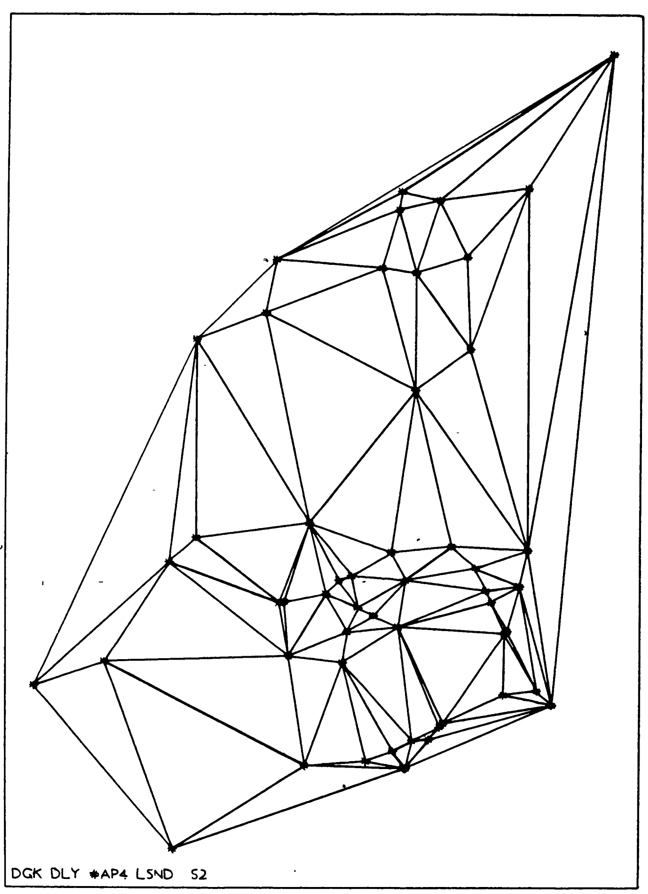

FIG. 10. *The Delaunay tessellation for the 52 Land's End sites.*

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Further references will be found in the survey papers by Bookstein (1986), Kendall (1984, 1986, 1989) and Small (1988).

Comment

Fred L. Bookstein

The elegant metric geometry of David Kendall's shape spaces Σ_m^k is inherited from the Euclidean metric of the spaces $\mathbf{R}^m$ containing the original point data. In the applications he has sketched here, the points in $\mathbf{R}^m$ are independent and identically distributed (iid) and the metric in shape space, in turn, is symmetric in the points, a sort of spherical distance. Point data generated in other disciplines, however, are not always iid; different metrics may be appropriate to those applications. In this comment I justify a certain analysis of small regions of Kendall's shape space by using a metric quite different from the usual Euclidean-derived version, depict its relation to Kendall's metric and indicate the sort of inquiries it permits.

Morphometrics is the quantitative description of biological form. Its data can often be usefully modeled as sets of labeled points, or landmarks, that correspond for biological reasons from organism to organism of a sample (Bookstein, 1986). We say that these points are biologically homologous among a series of forms: they have identities—names—as well as locations in some Cartesian coordinate system. Any set of landmark locations has a "size" and a "shape" that may be construed according to Kendall's definitions. But the biological relations among different instances of such configurations partake of a feature space not effectively represented by the metric inherited from $\mathbf{R}^2$ or $\mathbf{R}^3$.

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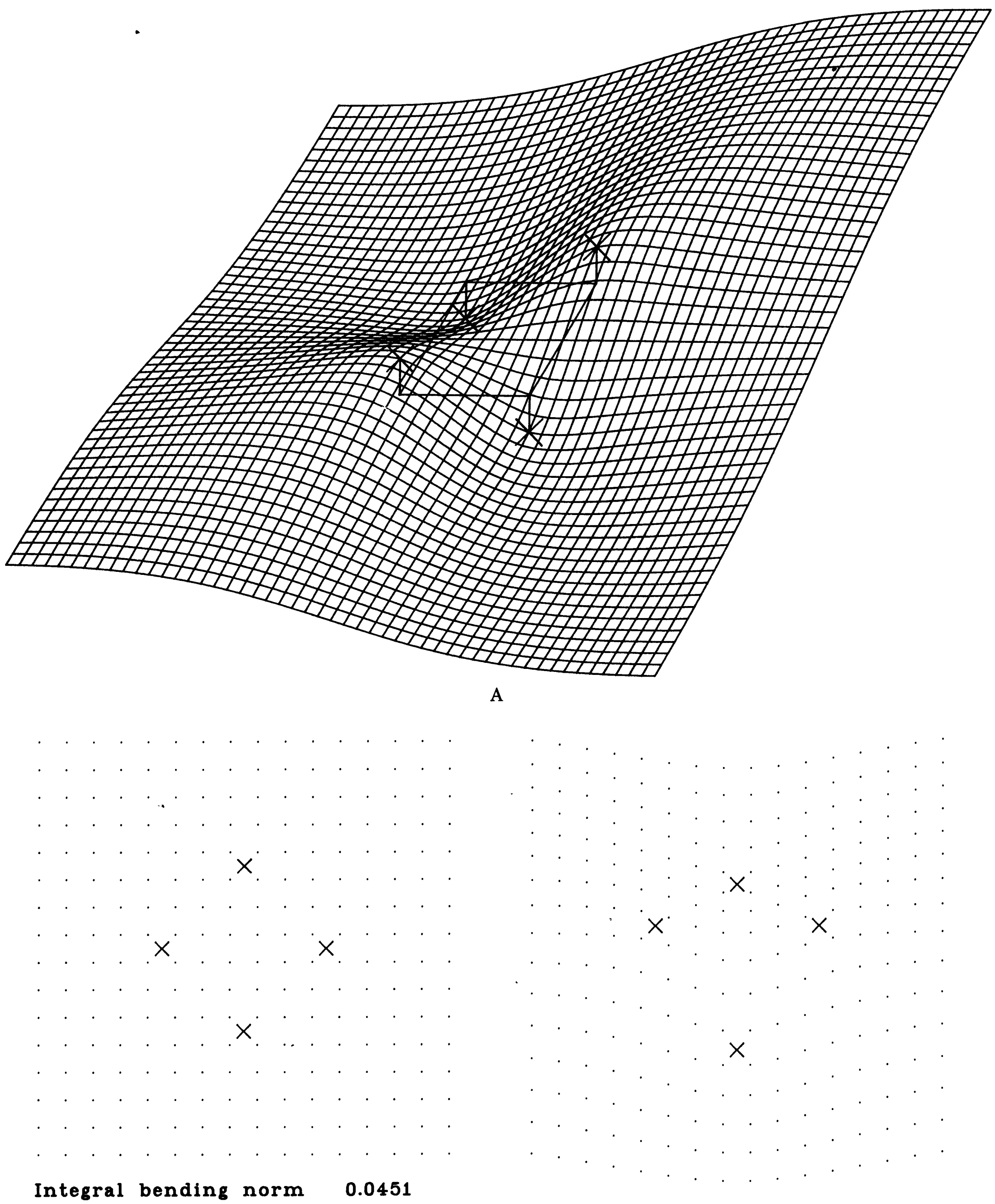
In the biological context, my style of statistical analysis of shapes proceeds, as Kendall pointed out in 1986, within a tangent space of his Σ_2^k or Σ_3^k in the vicinity of a sample "mean form." (Small (1988) has an interesting comment on this construction.) The questions that in Kendall's applications are asked of an entire shape space—questions about concentration upon the "collinearity set," and the like—are replaced in morphometric applications by the more familiar concerns of multivariate statistical analysis: differences of mean shape, covariances involving shape or factors that may underlie shape variation.

In the linearization of Kendall's shape space that applies to this tangent structure, the natural shape metric is an algebraic transformation of the "Procrustes metric," the ordinary summed squared Euclidean distance of two-point configurations after an appropriate optimizing rotation and scaling. But the Procrustes approach is not flexible enough fairly to represent biological structure within the context of multivariate statistical analysis. If two landmarks are typically close together, like the pupil of the eye and the outer corner, then we expect them to move together in their relation to more distant structures. The half-width and the orientation of the eye are more tightly controlled by diverse biological processes of regulation than is, say, the distance from the eye to the chin. These considerations lead one naturally to search out a shape metric that weights changes in small distances more heavily than changes in larger ones. In 1985, David Ragozin of the University of Washington suggested to me that the formalism of thin-plate splines be considered in this connection. The suggestion has kept me quite busy ever since.

Consider (Figure 1A) an infinite thin metal sheet, originally flat but now displaced perpendicularly to itself at a discrete set of points. In the figure, the points are displaced by a rigid armature in the form of a square (here viewed in perspective). The end points of one diagonal of the square are displaced by



B

FIG. 1. *Thin-plate splines. A, the shape of an infinite thin uniform metal plate originally level, then displaced (by the contrivance in the diagram) upward at the ends of one diagonal of a square, downward at the ends of the other diagonal. The plate takes a shape describable as a superposition of fundamental solutions* $U(r) = r^2 \log r^2$ *of its partial differential equation, as given in the text. B, reinterpretation of the same scene as a deformation. The vertical coordinate of frame (A) has been combined with the in-plane Cartesian coordinate along one diagonal. The square mesh of dots on the left is transformed by this deformation into the meshwork on the right. The "bending energy distance" between the shapes in (B) is taken to be the (idealized) physical bending energy of the equivalent displacement pattern in (A).*

equal distances upward with respect to the rest of the plate; those of the other, downward by the same distance.

Producing these displacements of the plate required that physical work be done in the course of bending. The configuration that the plate "actually" occupies has the minimum of bending energy consistent with the four-point constraint applied by the armature. Let us introduce the notation $U(r) = r^2 \log r^2$. This function satisfies the equation $(\partial^2/\partial x^2 + \partial^2/\partial y^2)^2 U \propto \delta_{0,0}$, the equation governing bending of the plate when the displacements are sufficiently small and elastic effects within the plane of the plate can be neglected. Under these assumptions, the formula for the final form of the plate can be written in terms of the function $U(r)$: the plate takes the shape

$$z(x,y) \propto U(\sqrt{\{x^2+[y-1]^2\}}) - U(\sqrt{\{[x+1]^2+y^2\}}) + U(\sqrt{\{x^2+[y+1]^2\}}) - U(\sqrt{\{[x-1]^2+y^2\}}).$$

The functions $U(r)$ based at each of the four corners of the square are taken with coefficients +1 for the ends of one diagonal, −1 for the ends of the other, just as were the displacements of the armature.

The metric I am suggesting for shape change is equivalent to the bending energy of configurations like these. We realize it in the context of morphometrics by conflating the z axis (the perpendicular to the plate) with one of the in-plane directions, for instance, that of one diagonal of the armature. There results (Figure 1B) a deformation throughout the plane of that starting square. Reversing this procedure, the shape difference of the two sets of points shown, the square (before "bending") and the kite (after "bending"), becomes the bending perpendicular to itself of the square in Figure 1A, and is assigned a shape "distance" representing the energy of that bending, the work required to attach the armature to the plate. For small changes of shape, this measure is symmetric.

The computation of this bending energy for more general starting configurations of points than squares proceeds along the following lines (Bookstein, 1988a, b, 1989). Let $P_1 = (x_1, y_1)$, $P_2 = (x_2, y_2)$, $\cdots$, $P_n = (x_n, y_n)$ be n points in the ordinary Euclidean plane according to any convenient Cartesian coordinate system. Write $r_{ij} = |P_i - P_j|$ for the distance between points i and j. Define matrices

$$K = \begin{bmatrix} 0 & U(r_{12}) & \cdots & U(r_{1n}) \\ U(r_{21}) & 0 & \cdots & U(r_{2n}) \\ \cdots & \cdots & \cdots & \cdots \\ U(r_{n1}) & U(r_{n2}) & \cdots & 0 \end{bmatrix}, \quad n \times n;$$

$$P = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \cdots & \cdots & \cdots \\ 1 & x_n & y_n \end{bmatrix}, \quad 3 \times n;$$

and

$$L = \left[\begin{array}{c|c} K & P \\ \hline P^T & 0 \end{array}\right], \quad (n+3) \times (n+3),$$

where ^{T} is the matrix transpose operator and 0 is a 3×3 matrix of 0's.

Let $V^T = (v_1, \cdots, v_n)$ be any n vector and write $Y^T = (V^T | 0\,0\,0)$. Define the vector $W^T = (w_1, \cdots, w_n)$ and the coefficients a_1, a_x, a_y by the equation

$$Y^T L^{-1} = (W^T | a_1\, a_x\, a_y).$$

Use the elements of $Y^T L^{-1}$ to define a function $f(x, y)$ everywhere in the plane

$$f(x,y) = a_1 + a_x x + a_y y + \sum_{i=1}^{n} w_i U(|P_i - (x,y)|).$$

Then the following three propositions hold:

1. $f(x_i, y_i) = v_i$, all i.
2. The function f minimizes the nonnegative quantity

$$I_f = \iint_{\mathbf{R}^2} \left(\left(\frac{\partial^2 f}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 + \left(\frac{\partial^2 f}{\partial y^2}\right)^2 \right)$$

over the class of such interpolants. This is a constant multiple of the physical bending energy referred to above.

3. The value of I_f is proportional to

$$W^T K W = V^T (L_n^{-1} K L_n^{-1}) V,$$

where L_n^{-1} is the upper left $n \times n$ subblock of L^{-1}. This form is zero only when all the components of W are zero: in this case, the computed map is $f(x, y) = a_1 + a_x x + a_y y$, a linear or uniform transformation.

In the present application we take V to be the $2 \times n$ matrix

$$V = \begin{bmatrix} x_1' & y_1' \\ x_2' & y_2' \\ \cdots & \cdots \\ x_n' & y_n' \end{bmatrix}$$

where each (x_i', y_i') is a point "homologous to" (x_i, y_i) in another copy of $\mathbf{R}^2$. The resulting function f now maps each point (x_i, y_i) to its homologue (x_i', y_i') and is least bent (according to the measure I_f, integral quadratic variation over all $\mathbf{R}^2$, computed separately for real and imaginary parts of f and summed) of all such functions.

In effect, our metric is the bending energy of a four-dimensional thin plate; two dimensions of plate displaced in two "other" perpendicular directions. A similar computation can be mounted in three dimensions, using the basis function $U_3(r) = |r|$, to represent the bending energy of a "six-dimensional thin plate." In one dimension, $U_1(r) = |r|^3$ gives the ordinary cubic spline.

The matrix $L_n^{-1}KL_n^{-1}$, which will be called the bending energy metric in the discussion to follow, is not of full rank. It annihilates affine transformations (uniform shears) of the landmark configuration as a whole. Physically, these play the role of vertical shifts and uniform tilts of the real metal plate; under our assumption of no in-plane elasticity terms, these "deformations" proceed without any energy cost. In the context of the biological applications driving this discussion, those transformations are the uniform transformations lacking any local features (gradients, growth centers or the like). The biological meaning of bending energy is thus a sort of measure of local information required to specify the landmark reconfiguration.

In the context of shape change, the Procrustes metric becomes the summed squared point displacement from one form to another, which is to say, the summed squared point displacements normal to the thin plate in the two "additional" (nonphysical) directions. Because of the annihilation of all shears, the metric geometry of shape space induced by bending energy is quite different from that driven by the Procrustes metric. (For instance, all parallelograms are at energy distance zero from each other.) We may summarize the differences by computing an eigenanalysis of the bending energy metric with respect to the Procrustes. This is just the ordinary eigendecomposition of $L_n^{-1}KL_n^{-1}$. The relative spectrum of the bending energy matrix always has three zero eigenvalues whose eigenvectors span the affine transformations. The remainder of the spectrum is a series of what I have named principal warps, normal modes of deformation that may be ordered by bending energy per unit Procrustes displacement.

An example of this spectrum is shown in Figure 2 for a configuration of seven landmarks drawn from a study in craniofacial syndromology (see Bookstein, 1989, Section 7.5). Frame (A) shows the mean configuration of these seven points in a (biologically) normal sample and in a sample of 14 cases of Apert Syndrome. The eigenvectors of bending energy may be shown all at once as distinctive patterns of simultaneous in-plane displacement of all the landmarks in parallel (the segments at intervals of 20° in frame (A)). Alternatively, they may be considered individual patterns of displacement perpendicular to the picture, as drawn in frames (B)–(E). Notice that the eigenvectors of higher eigenvalue look more bent per net (Procrustes) vertical displacement, and that the larger principal bending modes somewhat resemble that in Figure 1, the square-to-kite bend, at diverse scales.

The annihilation of those three degrees of freedom for the affine changes alters the metric geometry of shape space severely. The set of forms at constant bending energy distance from a fixed form is not a hypersphere but a hyperellipsoidal cylinder heading out to "infinity" in the tangent space. Figure 2, B–E, may be reinterpreted as the semiaxes of sections of this cylinder. The cylinder is not general: to each thin plate pictured there correspond two equal semiaxes representing the same in-plane displacements rotated by 90°. Thus the full constant-distance locus is the extended Cartesian product of an infinite flat hyperplane by a series of circles of different radii. The changes in Figure 2, B–E, are all (Procrusteanly) orthogonal to three dimensions of generators, the space of all the affine transformations, which have bending energy zero regardless of Procrustes length. If the mean configuration of landmarks were different, so, too, would be this pattern of axes, the geometry of "normal sections" of the cylinder.

The affine features of change annihilated by this shape metric can be restored by separately measuring that aspect using the Poincaré hyperbolic metric (see Bookstein, 1986, 1989). There results a joint feature space with the same dimensionality as Kendall's Σ_2^k, but with a metric now Galilean in the small (cf. Yaglom, 1979), so that there is no possibility of "rotation" between affine and bending parts; they are incommensurate. This is analogous to the treatment of real (physical) spacetime in Newtonian mechanics, for which space is measured in centimeters and time in seconds, with no possibility of interconversion by purely geometric maneuvers. Any relation between space and time is coded instead in a Newtonian velocity, a vector of change in space per change in time. That is, the net vector spline $L^{-1}Y$ has no unitary "length" or "direction." Rather, its affine part has a geometry that may usefully be taken as hyperbolic in the large (cf. Small, 1988), and its nonlinear part W has a geometry that is cylindrical Euclidean. These two conceptually independent aspects of measurement relate only by a joint distribution, such as a covariance structure.

With the help of the bending energy metric, we can refer to localization of biological variability and to the apparent physical scale of that variability. Neither of these is possible using the Procrustes metric. A useful first step is the relative eigenanalysis of the covariance matrix of the shape coordinates $(Z_k - Z_1)/(Z_2 - Z_1)$ with respect to the bending energy metric. Some delicacies of the computation are discussed in Bookstein (1989, Section 7.6).

For example, Figure 3 presents an analysis of the positions of eight cranial landmarks (frame (A)) in the skulls of 21 7-day-old male rats. (The data were originally drawn by Henning Vilmann, the landmarks digitized by Melvin Moss.) Our concern is with large-scale shape regulation in this diadem of sutures around the rapidly developing brain. Frame (B) indicates the five principal warps of this configuration of landmarks

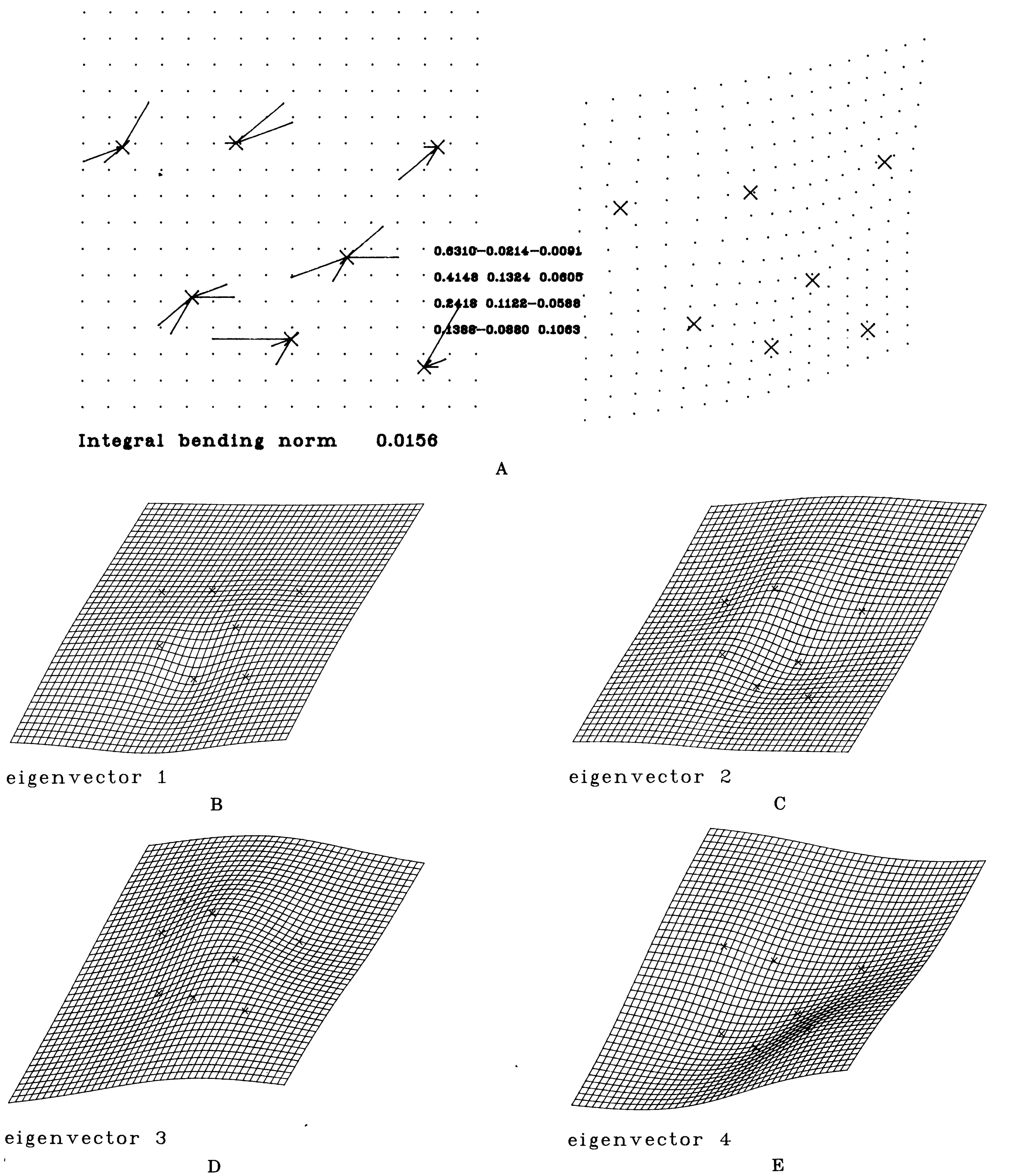


FIG. 2. *Spectrum of the bending energy with respect to the Procrustes metric. A, pattern of seven landmarks, and the four principal warps they generate, as described in the text. Segments along the horizontal: principal warp of largest bending energy,* 0.631 *(arbitrary units). At* 20° *counterclockwise of horizontal: eigenvector of second largest bending energy,* 0.415. *At* 40°: *third stiffest principal warp, eigenvector* 0.242. *At* 60° *counterclockwise of horizontal: eigenvector of smallest nonzero bending energy,* 0.139. *In the interpretation as deformation these multiply any two-vector to supply one displacement at each landmark. Also shown, by its effect upon the square grid at left, is the thin-plate spline mapping these seven landmarks to the homologous configuration on the right. The table in the center presents the loadings of the x- and y- components of this transformation upon each principal warp in turn: e.g., the y- component is mostly warp 4, the x- component the sum of warp 2 and warp 3. The data represent mean forms, as observed in lateral cephalograms, for a clinical sample of Apert Syndrome (right) and matched Ann Arbor normals (left). Landmarks, clockwise from upper left: sella, sphenoethmoid registration, nasion, anterior nasal spine, inferior zygoma, pterygomaxillary fissure (for definitions, see Riolo, Moyers, McNamara and Hunter,* 1974). *The "interior" landmark is orbitale. The transformation includes an affine component with strains of* 0.71 *along and* 0.93 *perpendicular to the direction at* 31° *counterclockwise of vertical on the left,* 37° *on the right. For the meaning of this example, see Bookstein* (1989, *Section* 7.5). *B–E, interpretation of each of the four eigenvectors as its own thin-plate spline: pairs of semiaxes of the bending energy cylinder.*

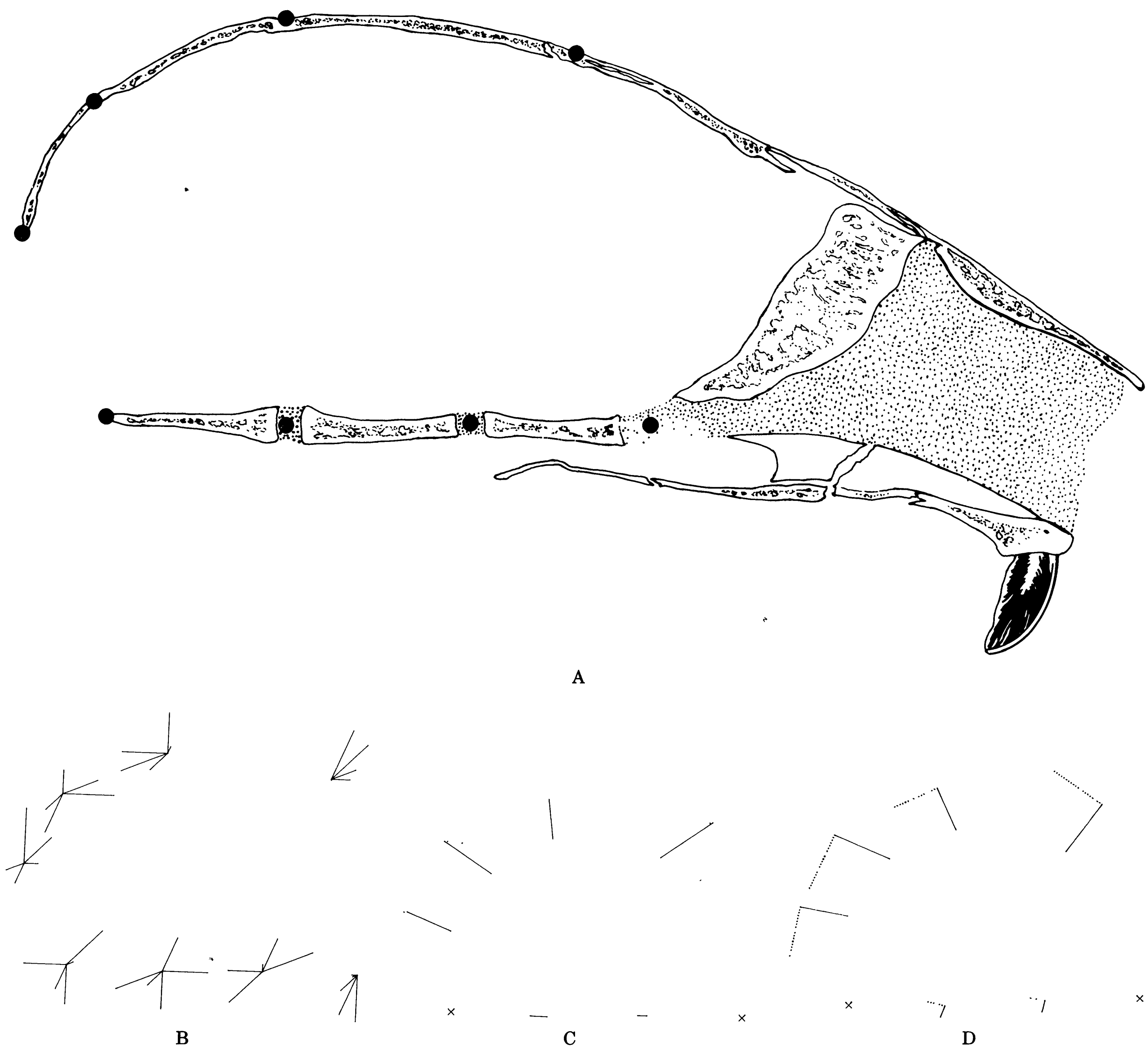


FIG. 3. *Relative bending energy component analysis of* 8 *cranial landmarks for* 21 *laboratory rats aged* 7 *days. A, midsagittal section: the landmarks* in situ. *B, the five principal warps, counterclockwise from the horizontal in decreasing order of bending energy (eigenvalues* 8.3, 6.2, 3.3, 1.8, *and* 1.1 *in arbitrary units). C, the last two principal warps as in-plane displacements in shape coordinate space (two landmarks fixed). Solid line, largest scale; dotted line, second largest scale. To each principal warp correspond two of these patterns, the one shown and its rotation by* 90° *at each landmark. D, the first and second relative eigenvectors of greatest sample variance relative to bending energy: the first and second components of scaled shape variance. Solid line, dominant relative eigenvector (eigenvalue* 0.0067*); dotted line, second relative eigenvector (eigenvalue* 0.0047*).*

after the fashion of Figure 2A, as parallel in-plane displacements, and frame (C) shows the last two of these (the bends of largest spatial scale) as in-plane displacements from the sample mean locations in shape coordinates (i.e., with two landmarks held fixed, as shown). The relative eigenanalysis of the sample shape coordinate covariance matrix with respect to bending energy has eigenvalues of 0.0067, 0.0047, 0.0003, · · ·, 0.0000. (There are ten in all, five principal warps times two Cartesian coordinates.) Figure 3D shows the first two of these relative eigenvectors (all others are trivial). The first of these connotes a generalized enlargement of upper cranial structures relative to the lower. The component is of highest relative eigenvalue in part because it has the lowest bending energy: compare the solid segments between frames (C) and (D). The second relative eigenvector, the dotted pattern in Figure 3D, represents rotation of the upper margin of the braincase with respect to the lower margin. It is not at all equivalent to the second weakest principal warp (dotted lines, frames (C) and (D)). The bending energy eigenanalysis has extracted these large scale patterns of shape covariance by explicitly weighting empirical covariance patterns inversely to geometric localizability. Other equally plausible geometric patterns, such as bending of the upper or lower structures, are not observed to bear any sample variance.

The example suggests the descriptive possibilities inherent in accommodating the metric geometry of Kendall's shape space to a biological subject matter. One can imagine other modifications of the metric in response to other contexts than the biometric. For instance, one can imagine the statistical study of the positions of a robot arm. When the state of the linkage is coded by the coordinates of its joints, then because certain parts of the robot are rigid, an appropriate measure of "distance" would be somewhat altered from the Procrustes. In another sort of constraint, certain "landmarks" might represent the loci of curves in the data—boundary arcs not otherwise labeled—and would thus be "deficient" by one coordinate; again the Procrustes metric needs to be modified. In a study of schools of fish, or flocks of birds, an appropriate shape metric might be the Cartesian product of a biological shape space by a hydro- or aerodynamic one (for the V of migrating geese, for instance). Yet other modifications would arise when the points of Kendall's space are "colored" in classes whose separate patterns cannot be usefully studied without reference to their interpenetration, as in problems of multispecies ecology. These and other possibilities represent an enrichment of the metric geometry of shape space within the global purview pursued so sparely and elegantly by David Kendall.

ACKNOWLEDGMENTS

Preparation of this comment was partially supported by Grant GM-37251 from the National Institutes of Health to F. L. Bookstein. Christopher Small commented usefully on an earlier draft. I and many of the rest of us in shape statistics are grateful to Colin Goodall for arranging a workshop around Kendall's Wilks Lectures, Princeton, May 1987. Part of this comment was presented at that workshop in even more preliminary form.

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Comment

Christopher G. Small

With a high standard of rigor David Kendall has given us an interesting survey of the theory of shape analysis that he has pioneered with the help of others over the last decade. This work is now of sufficient volume that the many topics discussed in this survey can be only briefly touched upon. I certainly hope that this paper is a stimulus to additional consideration of this topic by statisticians. It may well be that on future occasions the topologists will have to introduce their theory of shape with preparatory remarks to the effect that it is not to be confused with the growing statistical theory of shape.

At first glance, this paper might seem to have much in common with the differential geometric techniques in statistics that are associated with Amari (1985) and others. However, despite the abstraction of some of the theory, the methods of Kendall are essentially data analytic rather than model theoretic: the differential geometry is on the sample space not the parameter space. So how much differential geometry must the data analyst know in order to implement the techniques that are described in this paper? The answer is largely dependent on the amount of software

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that can be developed to analyze shapes, because the differential geometry need not be duplicated by the data analyst if it is built into the software. Software that is analogous to the techniques available for projection pursuit would be especially useful here because it is impossible for most of us to visualize global properties of shape manifolds. So it would be helpful to be able to search a shape space interactively through various two-dimensional (or even three-dimensional) projections. The appropriate tools would then be able to analyze shapes in much the same way that multivariate data sets can be analyzed by "Grand Tours." (See Buja and Asimov, 1985 and Hurley, 1987.)

It is the job of a discussant to provide a different perspective on a paper. As I have been involved in the work with D. G. Kendall this is not an easy task. Nevertheless, I would like to indicate why there is room for flexibility in the choice of geometries available to the statistician. Each geometry can be examined in light of criteria such as naturalness, computational convenience or graphical convenience, etc. Although among such geometries the shape space geometry of D. G. Kendall is by far the most developed, and perhaps the most important, other geometries deserve consideration.

Need the statistician consider geometry at all? The answer must be yes, because there is a natural interplay between geometrical and statistical considerations. Suppose for example we are to find a measure of location for a multivariate data set $\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_k$. A family of such measures based on minimum distance methods is given by using that point $\mathbf{x}$ which minimizes $\sum \rho(\mathbf{y}_i, \mathbf{x})$ where ρ is a metric that represents the geometry in use. If $\rho(\mathbf{y}, \mathbf{x}) = \| \mathbf{y} - \mathbf{x} \|^2$ then $\mathbf{x}$ is the centroid of the data set. However, the centroid is sensitive to outliers. So if a more robust measure of location is desired the metric $\rho(\mathbf{y}, \mathbf{x}) = \| \mathbf{y} - \mathbf{x} \|$ can be used. In this case $\mathbf{x}$ becomes the spatial median whose properties were investigated by Brown (1983). This example shows how a departure from the L_2 metric of "least squares" used in multivariate analysis leads to differing statistical properties in the resulting estimator.

To a statistician, the centroid of a data set is a sensible measure of location based upon the traditions of multivariate theory. Similarly, sums of squares are natural measures of scale. However, other geometries are worthy of consideration in contexts in which their properties are more useful than the standard geometry. Moreover, the assumption that there exists a unique natural geometry on the space of shapes presupposes that there exists a unique natural geometry on the space in which the observations lie. Yet different contexts seem to dictate different geometries, and differential geometric considerations only tell us how to transfer the geometry across from the space in which the observations lie to the shape space. A distinction must be made between the Euclidean space in which points lie (Kendall's $\mathbf{R}^m$) and the Euclidean space in which a data set is represented (Kendall's $\mathbf{R}^{m\times k}$). When $m \le 3$ the geometry of the former usually has a physical interpretation. The geometry of the latter is typically a mathematical construction.

The following example illustrates the point. Suppose X_1, X_2 and X_3 are three independent random variables that are uniformly distributed over some common interval, say $[0, 1]$. The shape σ of the three points is an element of a unit circle $S^1(1)$. If we compute the shape density on the unit circle, we find it to be analytic on six arcs that correspond to the $3! = 6$ possible rankings of the three variables. Alternatively, however, we could introduce the L_∞ norm on $\mathbf{R}^3$ by setting $\| \mathbf{x} \|_\infty = \max(|x_1|, |x_2|, |x_3|)$. The resulting induced metric on $\mathbf{R}^3$ can in turn be related to a metric space on equivalence classes of shapes. Let $x_{(i)}$ be the ith order statistic. Define $m = [x_{(1)} + x_{(3)}]/2$ and $r = [x_{(3)} - x_{(1)}]/2$. Then the point

$$\left[\frac{x_1 - m}{r}, \frac{x_2 - m}{r}, \frac{x_3 - m}{r}\right]$$

is a representation of the shape of the triplet (x_1, x_2, x_3) and lives on a closed path made of six line segments (i.e., a bent hexagon) that is the shape space in this case. The corners of the hexagon correspond to the places in the former shape space $S^1(1)$ where the shape density failed to be analytic. The bent hexagon can be described by removing two diametrically opposite vertices of a cube and joining the six remaining vertices with those edges connecting neighboring vertices among the six. The induced distribution on the hexagon can be seen to be uniform and therefore very easy to work with. Calculations are further simplified if the labels of the points are ignored in which case all shapes are represented on a single line segment that is the fundamental region on the hexagon. For a larger number k of points in dimension 1, the resulting shape space will be a continuous image of a sphere of dimension $k - 2$ lying within the boundary of a k dimensional hypercube. It will be made of the union of $k(k-1)$ hypercubes of dimension $k - 2$ attached at their boundaries. Once again, the induced distribution on the shape space will be uniform. The smoothness of the shape manifolds Σ_2^k is deceptive for the induced distributions of shapes of points uniformly distributed in a planar region. In such cases, the sets on which the shape density fails to be analytic are quite complex. Therefore a geometry in which the singularities are inherent in the shape space itself becomes plausible in light of the computational difficulty of such models on smooth manifolds.

The existence of numerous geometries for shapes does not give carte blanche to the researcher to use any geometric representation whatsoever. As always in data analysis, the geometry used must serve the goals of the statistical analysis if it is to be anything more than a mathematical theory. The use of a measure of distance between shapes (the "geometry") generates clustering and classification algorithms and test statistics based upon minimum distance methods. If the measure of distance used is artificial the resulting statistical analysis will surely not be any less so. Geometries give rise to statistical methods which can, in turn, be evaluated in the context of criteria for good inference or data analysis. This is as true for shape analysis as it is for multivariate analysis.

In defining metrics within the space $\mathbf{R}^{m\times k}$ or some subset of that space the nature of shape "kinematics" should be considered. Shape changes or shape differences can arise through perturbations of the individual k points. Alternatively, shape changes can arise through global transformations of the space $\mathbf{R}^m$ which a fortiori induce a change on the shape of the individual points of the data set. The usual Euclidean metric seems inappropriate for the latter case. For example, suppose we assume that changes in the shape of a data set arise from a global transformation T of $\mathbf{R}^{m\times k}$. We could measure the distance from one data set to another by means of a measure of distance of T from the identity transformation. The induced metrics on the space of shapes from these methods have a very different character from Kendall's geometry. For example, suppose $k=3$ and $m=2$. Any three points which are not collinear can be transformed to any other such set by composition of an affine transformation T. A measure of distance (in fact a pseudometric) of this transformation from the identity defined by Bookstein (1986) induces the riemannian geometry of the hyperbolic plane on the shape space in which Kendall's great circle of collinear shapes becomes the circle at infinity of the hyperbolic plane.

In his survey, D. G. Kendall has provided some interesting inversion results, showing that for three points independently and uniformly distributed in a compact convex set the induced distribution of shape determines the convex set modulo a shape preserving transformation. The argument, based upon the set where the shape density fails to be analytic, is quite delicate. Unfortunately we cannot expect to detect discontinuities in the higher derivatives of the shape density through statistical means. So the result does not transfer immediately into a statistical test although I expect that this could be done. The delicacy of the inversion is rather different from that of the inversion theorems that I have been working on over the last few years (Small, 1983, 1984, 1985) which are based upon transform techniques for larger sets of points.

Attention has recently been turned to the representation of shapes of objects more complex than finite sets of points. Bookstein has proposed that the shapes of objects can be studied by choosing a representative set of points (called "landmarks") on the object and studying the shape of this set of points. Although this works for biological structures in which there is some differentiation in terms of function of the various sites on the structure, the problem of representing complex shapes using finite sets of points is complicated in general by the lack of obvious landmarks. In such cases, multidimensional generalizations of Bernstein polynomials may be of value in representing complex shapes through finite sets of points. Note that the problem here is not simply to find a finite dimensional parametrization of complex shapes, but to ensure that there is a geometrical relationship between the coordinates of the parametrization and the shape itself. Thus, for example, the coefficients of a polynomial parametrize the shape of the polynomial but do not do so in such a way that there is a clear geometrical interpretation of the shape to be found within them. Let Δ^n be the n-dimensional simplex of all points $(p_1, \cdots, p_{n+1})$ such that $p_1, p_2, \cdots, p_{n+1} \ge 0$ and $\sum p_i = 1$. Suppose $\mathbf{g}(\mathbf{p}) = [g_1(\mathbf{p}), \cdots, g_m(\mathbf{p})]$ defines a continuous m-dimensional image $\mathbf{g}(\Delta^n)$ of the simplex. The image $\mathbf{g}(\Delta^n)$ can be approximated by a polynomial image $\mathbf{g}_j(\Delta^n)$ defined by

$$\mathbf{g}_j(p_1, \cdots, p_{n+1}) = E\left[\mathbf{g}\left(\frac{X_1}{j}, \cdots, \frac{X_{n+1}}{j}\right)\right]$$

where $X_1, \cdots, X_{n+1}$ have a multinomial distribution with $\sum X_i = j$ and $E(X_i) = jp_i$. Then $\mathbf{g}_j$ is a jth degree polynomial that uniformly approximates $\mathbf{g}$. The image $\mathbf{g}_j(\Delta^n)$ is determined by the set of points $\mathbf{g}(x_1/j, \cdots, x_{n+1}/j)$ where $0 \le x_i$ and $\sum x_i = j$. At this early stage I can only speculate as to the value of a theory of shape for random paths in applications such as dynamical systems.

The spaces that Kendall has called "size and shape spaces" may well turn out to be more useful than shape spaces themselves. Commonly in statistical problems it is impossible to ignore size variables without losing information that is important to the understanding of the data. The geometry of an object possessing no intrinsic position or orientation falls naturally into such a space. For cases where a group acts upon a riemannian manifold, the resulting quotient space is termed a "shape space" by Kendall. The generalization is an important one, although the terminology tends to separate the subject from an area that is well established in the statistical literature: the theory of maximal invariance. Thus a shape in this generalized sense is also a maximal invariant under the action of the group $\mathscr{G}$. Such maximal invariants for data on riemannian manifolds are not uncommon in statistics. For example, data in directional statistics live on a one- or two-dimensional sphere for which the most useful group to generate transformation models is the rotation group. For models in which the rotation group generates a nuisance parameter, questions involving the testing of a concentration parameter in the absence of knowledge of the nuisance parameter require the reduction to the maximal rotation invariant. Fraser (1968) has emphasized the importance of transformation models and the fibers of data sets equivalent under the action of a group. Some relationships with the statistics of shape are developed in Small (1983).

I would like to close these comments with some remarks of a more specialized technical nature. The elegance of D. G. Kendall's theory of shape is especially clear for data sets in dimensions 1 and 2. In higher dimensions, singularities start to emerge. Although these singularities are not obviously detrimental to a theory of shape, they do detract from the elegance of the representation. Even in dimensions 1 and 2, the shape spaces are more easily constructed and represented than the corresponding size and shape spaces. The reason for the elegance of the shape space for the cases where $m = 1, 2$ is that in these cases a shape preserving transformation can be uniquely decomposed into two transformations that correspond to multiplication and addition in the real line and complex plane for the respective dimensions. For both $m = 1$ and $m = 2$ the group of shape preserving transformations is a solvable group with a dimension (i.e., number of degrees of freedom), which is an integral multiple of m. But in dimension $m = 3$ this fails to be the case. The group of shape preserving transformations is of dimension 7, which is not a multiple of m.

Let me conclude my remarks by congratulating David Kendall on some very interesting work. The new directions that are sketched in this paper seem to be promising for the analysis of geometric data of various kinds and from various sources. I hope that much more is forthcoming.

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Comment: Some Contributions to Shape Analysis

Kanti V. Mardia

There are no words to express the profound depth of Kendall's work. I have been working in this area intermittently since 1976 and I believe his fundamental work (as well as Bookstein, 1986) has opened up the field.

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Bookstein (1986) has used the model for shape analysis assuming that the points are distributed independently as $N_2(\mu_i, \sigma^2\mathbf{I})$, $i = 1, 2, \cdots, p$. Consider $p = 3$. Let $\mathbf{x}$ be the point in Kendall's spherical shape space from these three points with ℓ representing the corresponding point in Kendall's space from μ_i's. Let $\bar{\mu}$ be their mean vector. Then using Mardia and Dryden (1989), it can be shown that the probability element of $\mathbf{x}$ is given by

$$\{1 + \varkappa(\ell'\mathbf{x} + 1)\}e^{\varkappa(\ell'\mathbf{x}-1)}dS, \quad \mathbf{x} \in S_2,$$

where $\varkappa \geq 0$, $\ell \in S_2$ and dS is the uniform measure on S_2. In fact, $\varkappa = \sum_{i=1}^{3} |\mu_i - \bar{\mu}|^2/(4\sigma^2)$ where $|\cdot|$ denotes the Euclidean norm. This distribution on Kendall's space will be written as $K(\ell, \varkappa)$. It has a mode at ℓ and for $\varkappa = 0$, it is uniform on S_2. Further, as $\varkappa \to \infty$, we have bivariate normality, and as $\varkappa \to 0$, we have uniformity. The distribution $K(\ell, \varkappa)$ is, of course, not the Fisher distribution $F(\ell^*, \varkappa^*)$, but it belongs to the class of rotationally symmetric distributions as one would have expected. On equating the first order moments, this distribution (see Figure 1), is found to be very similar to the Fisher distribution with $\ell^* = \ell$. As we would mostly expect large $\varkappa$ for biological shapes, it seems we can carry out inference for the triangle case using the Fisher distribution. Note that because $K(\ell, \varkappa)$ is not in the exponential family, inference is somewhat more complicated for this distribution than for the Fisher distribution. One possible advantage of this approach for $p = 3$ may be as follows. It can be shown that for the variables in Bookstein's space, the second moments are infinite (Mardia and Dryden, 1989), although here all the "moments" are finite. The statistical implication of this point needs closer examination but these two approaches, directional and multivariate, should prove complementary.

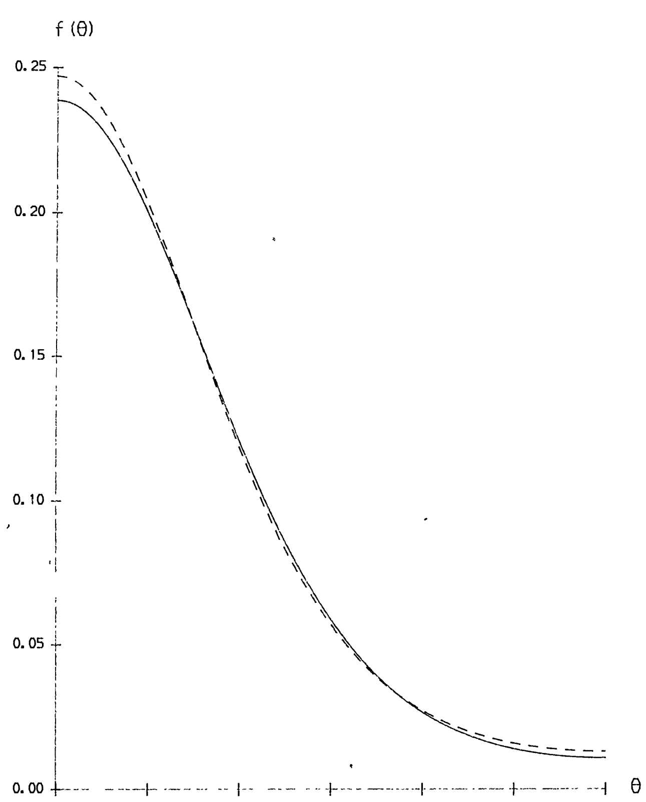

FIG. 1. *The profiles $f(\vartheta)$ of the two spherical distributions with $\ell'\mathbf{x} = \cos\vartheta$, $0° < \vartheta < 180°$. ——, exact distribution ($\varkappa = 1$); – – –, Fisher distribution ($\varkappa^* = 1.47$).*

Let α_1, α_2 and α_3 be the three angles of the triangle and suppose the "handedness" of the triangle is ignored. In passing, we note that Mardia (1980) obtained the p.d.f. of two angles α_1 and α_2 for $\sigma \to \infty$ (or μ_i's equal),

$$6S/\{\pi(3 - C)^2\}$$

with $S = \Sigma \sin 2\alpha_i$, $C = \Sigma \cos 2\alpha_i$ saying "it is uniform in a certain sense" but could not see its implication. Of course, it now dawns that this is uniform in Kendall's spherical space.

It has been assumed that the landmarks are known but in practice they may not be. The determination of biological landmarks relies on expert opinion in creating homologous points. However, we emphasize mathematical landmarks that are some extremal points on the outlines (e.g., points of maximum curvature). These points can also be obtained by fitting poly-lines recursively. For example, for the palm shape in Figure 2, using any standard algorithm, we get the landmarks $P_1, \cdots, P_8$ (not necessarily in that order) with base P_1P_2. How many landmarks one should take for a given shape depends on the problem. For discrimination, we can carry out tests of dimensionality on shape variables recursively to select the number of landmarks (see Mardia, 1986). However, there are many problems in making sure that there is correspondence of the landmarks within and between the groups. If the fingers are not abducted, only the point P_8 will be very unstable and it may be necessary to select the threshold to be large in the poly-lines fitting algorithm. In such cases, a suitable model for the points must be independent $N_2(\mu_i, \sigma_i^2\mathbf{I})$ where the σ_i's are not necessarily equal (see Mardia and Dryden,

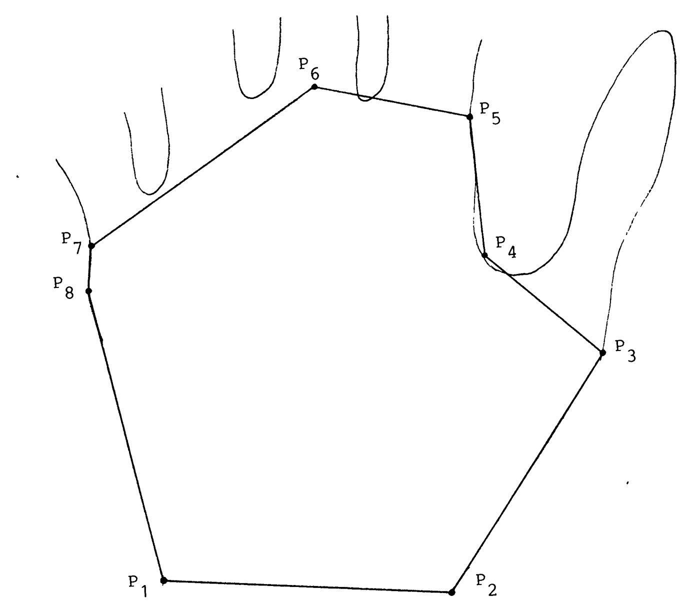

FIG. 2. *Landmarks estimation for a palm shape.*

1989). The problem of shape change seems to be more difficult.

Nowadays, one can work with video-digitized images and the outline in Figure 3A gives a digital reconstruction of a $T1$ mouse vertebra bone (see Johnson, O'Higgins, McAndrew, Adams and Flinn, 1985). An algorithm to estimate landmarks, developed jointly with Ian Dryden, works as follows. The digitized outline is represented by a set of points (here over 300 points) and the local absolute curvature maxima are found (about 30 points here). Then a poly-line fitting algorithm is applied to this subset of points and the vertices of the resulting polygon are taken as landmarks (which are the points $\circ$ of maximum curvature in Figure 3B). Some further landmarks are located at either side of each landmark, at points of low absolute curvature ($*$ in Figure 3B). We will call them pseudo-landmarks and they provide useful local shape information. Thus for the $T1$ vertebrae we obtain four landmarks and eight pseudo-landmarks as finally mapped onto the outline in Figure 3A. Consistency of the landmarks is verified by applying the algorithm to all the bones, and for the $T1$'s we have a reasonable correspondence both within and between the three groups. The algorithm is not straightforward for more complicated shapes like the $T2$ bone in Johnson, O'Higgins, McAndrew, Adams and Flinn (1985). It is expected that significant developments will take place in the estimation of landmarks, especially for shape change. Again, the work developed in the paper will play an important role.

Coming to the Central Place Theory application, Mardia (1977) also mentioned the use of the distribution of the circumradius R in addition to the shape variables when the size is relevant but now I am convinced by the practical reasons put forward here. I agree, the method of eliminating the edge effect is effective. Indeed, it was used in simulations for Mardia (1977). "One method of eliminating boundary effects is to neglect those triangles whose circumcircles are not wholly within the sampling window." (See Edwards, 1980, pages 107 and 108.) In particular, the table below shows for $n = 44$ (mimicking the Iowa data) for 1000 simulations, the effect of boundary on the area A of the shape of Delaunay triangles in a rectangle with sides in the ratio 1:2.

	Simulated	Corrected	Miles' Dist.
$E(A)$	1.52	1.57	1.57
$\mathrm{var}(A)$	0.46	0.45	0.45

As expected, the correction process throws out the long thin triangles with low values of A but in this case there is little effect. Even if we assume the independence of Delaunay's triangles, it has been pointed out that we will need a powerful test for the hypothesis of "equilateralness" under Delaunay's tesselations versus that under Central Place Theory. One new plausible approach is as follows. It can be shown that if we approximate Miles' density with $K(\ell, \varkappa)$ by equating the mode and the strength of the mode for the two distributions on the half-lune then $\ell' = (0, 0, 1)$, $\varkappa = 1.73 = \varkappa_0$, say. We can now test this null

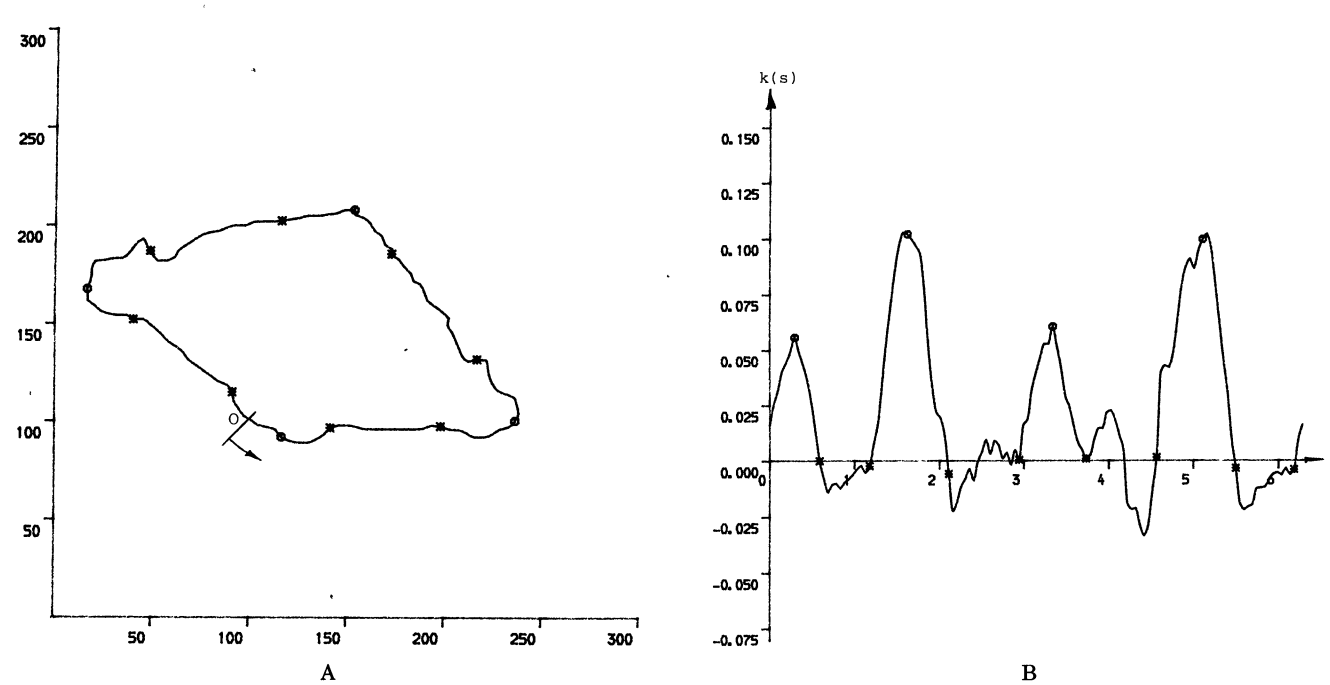

FIG. 3. *A, reconstructed T1 bone from video-digital image with estimated landmarks (°), psuedo-landmarks (*). O indicates the start point together with its direction for B. B, curvature k(s) versus arc length s for A, and the corresponding positions of estimated landmarks.*

hypothesis $\varkappa = \varkappa_0$ against $\varkappa > \varkappa_0$ because under Central Place Theory, $\varkappa$ will be very large under H_1. Note that under both hypotheses, we have $\ell' = (0, 0, 1)$.

Under the Fisher approximation to $K(\ell, \varkappa)$, we could use under H_0

$$2\gamma_0(n - \Sigma z_i) \sim \chi^2_{2n},\ \gamma_0^{-1} = \varkappa_0^{-1} - \frac{1}{5}\varkappa_0^{-3},$$

where (x_i, y_i, z_i), $i = 1, \cdots, n$, are the n spherical coordinates for Delaunay's triangles specified on the half-lune as in Kendall (1983). The critical region is the lower tail of the distribution. Note that in terms of Bookstein's shape variables for the triangles (Q_{1i}, Q_{2i}), $i = 1, \cdots, n$, we have

$$z_i = \sqrt{3}Q_{2i}/(Q_{1i}^2 + Q_{2i}^2 - Q_{1i} + 1).$$

There is considerable room to improve the test. For example, we could estimate the percentage points of the test by simulating the Poisson process. Also, we could carry out a test for the non-nested hypothesis of the Miles' distribution versus $K(\ell, \varkappa)$ without any approximation. All these ideas require further investigation. Another approach when the size of the triangles is important is to use the mean area of triangles like Mardia (1977) but now without normalizing to $R = 1$. Its mean and variance are known under the Miles' distribution and thus we can test the null hypothesis. Of course, testing H_0 is only a small part of the main problem; the shape and size summary statistics themselves are revealing, e.g., in investigating comparative evidence of Central Place Theory for various different data. It would be interesting to see a detailed analysis of the Wisconsin data along the lines given in the paper.

Finally, let me say that I found the paper very stimulating and look forward to reading the forthcoming book.

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Comment

Wilfrid S. Kendall

David Kendall has been my close collaborator from the very start of my scientific career, and so it gives me great pleasure to add to the discussion of this paper. I take as my theme the application of computer algebra in statistics and probability. As evidenced from the paper, some of the first instances of this have occurred in the statistical theory of shape. I shall make some remarks on the general application of computer algebra in statistical science, and then turn to the specific application (to the diffusion of shape) with which I have been involved recently.

1. COMPUTER ALGEBRA IN STATISTICS AND PROBABILITY

The reader will have noticed several references to the use of computer algebra (CA) in the investigations reported in the paper. To my knowledge this usage represents one of the first substantial applications of CA in the fields of statistics and probability. The others known to me are my own related work on shape diffusions (referred to in the paper as W. S. Kendall, 1988), which was encouraged by the success of CA in investigating the geometry of shape and is discussed further below; and the work on asymptotics in density estimation as described by Silverman and Young (1987). (I would be most grateful to hear of further instances.)

At present the use of CA in statistical science is in its infancy, although many exciting possibilities beckon. The emergence of readily available and powerful personal workstations gives reason to hope for rapid progress in the next few years. The wide screens, multiple tasking facilities and cut - and - paste editing of these workstations combine to yield a most productive environment for CA.

In what sort of areas might we anticipate CA's profitable employment? At the time of writing it seems

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to me that maximum benefits will derive in areas that not only require complicated calculations but also exhibit considerable structure. The theory of statistics of shape is a good example: the calculations comprising Le Huiling's magnificent determination of shape densities are undergirded by a profound appreciation of the tessellation structure hidden within the density, and I believe it is this structure that facilitates the implementation of an effective algorithm in CA. In this case manual calculations preceded the implementation, and so CA played a supportive role. But one can envisage a future in which the CA implementation of the structure develops at the same pace as one's theoretical understanding of the structure (and this was indeed the case in the work on diffusion of shape). Other possible applications are to the theory of asymptotic distributional approximations, and to the related field of differential geometry of statistical inference.

Where the underlying structure is not properly appreciated, naive use of CA can very easily lead to a kind of algebraic overflow. In the words of Hearn (1985) "... we attempt to solve more and more complicated problems and succeed only in producing larger and larger expressions." Hearn's point here (as author of a CA system) is the need for structure-detecting algorithms in CA systems; I believe that as users we should draw the moral that increasing usage of CA will force us to acquire ever deeper theoretical understanding in our search for useful and practicable ways to express the underlying structure. (Consider the mathematical demands made on the reader of Davenport (1981), which expounds a CA algorithm for solving indefinite integrals.)

It is of course a legitimate concern whether one can accept as valid an argument which depends on a CA package, whose correctness has not been mathematically established. Although a proper treatment requires more philosophical expertise on the nature of a valid proof than I can muster, the following remarks may be helpful. Firstly, we learn from the history of famous conjectures that (even when CA is not employed) it is a nontrivial matter to establish whether an argument is valid. At the very least, potential bugs in a CA package are rather more public than possible bugs in my head! Secondly, and related to this, convincing mathematical arguments derive from good exposition, which builds up a coherent and checkable mathematical world in which the target result appears as a natural result. In a similar way a good application of CA should clearly implement a mathematical structure, susceptible to interactive checking by sceptics. Thus the final CA program should serve as a kind of "active text"; if an opponent can legitimately manipulate it to derive (for example) a negative variance then the argument fails. These points provide further motivation to use CA to implement mathematical structure rather than merely to crunch large formulas.

As remarked above, the next few years should see rapid development in the application of CA to statistical science. The work surveyed in the paper is pioneering in this as well as in other respects.

2. DIFFUSION OF SHAPE

The investigations reported in W. S. Kendall (1988) were motivated by a desire to develop CA in application to statistics and probability. About two years ago I realized that the basic idea of stochastic calculus ("replace the square dB^2 of the Brownian path increment by the time increment dt") lent itself naturally to implementation as a substitution role in a CA language such as REDUCE. To my surprise I found this implementation could actually be used to provide a stochastic calculus proof of the remarkable Clifford-Green result reported in Clifford, Green and Pilling (1987), and this led naturally to determination of the statistics of shape diffusion for triads of points.

Here is a summary of the argument concerning diffusion of shapes of triads.

(a) The shape of a triangle formed by $k = 3$ points in m-space (for $m \geq 3$) is parametrized by the ratios of the squared side-lengths of the triangle (the so-called homogeneous shape coordinates).

(b) If the vertices of the triangle diffuse as Ornstein-Uhlenbeck processes then their equilibrium distribution is rotationally-symmetric Gaussian.

(c) Computer algebra allows the ready determination of the statistics of the induced random process of homogeneous shape coordinates, using the implementation of stochastic calculus described above.

(d) Further computer algebraic manipulation reveals: the natural geometry of the shape space (as suggested by the shape process) is that of ("northern") hemisphere of radius ½; and moreover a time change of the shape process is Brownian motion on this hemisphere modified by a drift directed toward the north pole of the hemisphere. The drift can of course be found explicitly!

(e) The equilibrium distribution of the shape diffusion (and thus the shape density for a rotationally symmetric Gaussian triangle) can then be found using diffusion theory arguments.

(f) The same picture arises (with minor technical modifications) if the vertices diffuse by Brownian motion.

In particular these results make it clear that in high dimensions a Brownian triangle spends most of the time in shapes that are close to equilateral. This is the surprising conclusion referred to in the paper—

surprise however is a relative concept and readers of McKean (1973) would not be surprised at all!

No doubt readers will see other ways of addressing these problems using perhaps stochastic calculus without benefit of CA or the theory of Wishart distributions (indeed Mr. James of Leeds University has shown me how to use Wishart matrix theory to establish the Clifford-Green result mentioned above). The main purpose of this work has been to initiate the development of CA as an effective tool in the study of random processes, rather than to develop new results. More recently, and with the same motivation, I have been working on the use of CA to derive the statistics of shape diffusions for k-ads with $k > 3$. Here the technical problem is to find effective ways of dealing with sums involving k summands, when k is not fixed beforehand but must be treated as a symbolic quantity. Some progress has been made, but work is not yet complete.

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Comment

Geoffrey S. Watson

In stochastic geometry as in number theory, it is easy to ask questions that the layman can understand but that the specialist can only answer with difficulty or not at all. Under the older name, geometrical probability, the subject is old, e.g., Buffon's famous problem was invented around the time Buffon was preparing a French version of Newton's "fluxions." I don't know of any ancient and unresolved conjectures like Fermat's but it is easy to give simple-sounding problems that are hard to solve, e.g., the motivating problem of Kendall's theory of shape. How do the shapes of triangles vary when their vertices are independently and uniformly distributed in a fixed rectangle? This problem arises from questions about whether there is too much "collinearity" in sets of points (see Figures 1 and 2). A recent and very readable survey of Kendall's theory has been given by Small (1988).

All but the most mathematically gifted readers will find this paper difficult. Rather more basic details are given in Kendall (1984), but this too is written for mathematicians. I hope the promised book (now in preparation) by Carne, Kendall and Le will make it clear to statisticians, because I'm sure that this is a fascinating area for research and applications. To support this belief I will give a brief summary of my own related efforts, sticking mainly to triangles. This is reasonable because most of the suggested applications use them and they are the simplest case.

The shape of Δ, a triangle P_1, P_2, P_3, with vertex angles α_1, α_2, α_3, could be defined as the pair (α_1, α_2). But for most problems this is not easy to work with, or to generalize to k labeled points in $\mathscr{R}^m$. There are lots of other ways to define the shape of a triangle. We may think of Δ as a 2×3 matrix $[z_1, z_2, z_3]$, where the column z_i has elements x_i, y_i, and denotes the position of the vertex P_i in the plane. Because we are only interested in the shape of Δ we may translate, dilate and rotate Δ without changing the shape of Δ, so we seek a "canonical" triangle. Kendall's approach is a variant of the following. Change the origin to the centroid of the triangle and consider the singular value decomposition of the new 2×3 matrix, $R\Lambda L'$, where R is a 2×2 rotation and so irrelevant. By scaling we could make $\lambda_1^2 + \lambda_2^2 = 1$. The remaining object defines the shape. See Mannion (1988) for a simple description—it is very similar to the next suggestion—and Small (1988).

I found Kendall's reduction hard to understand and considered (in Watson, 1986) two alternatives, which worked well in the simple planar problem I had posed. Move P_1 to the origin (0, 0), move P_2 to (0, 1), which uses up the available transformations, and denote P_3 by z, which then serves to define the shape of Δ. It is natural to take it as a point in the complex plane. The other alternative came from taking z_1, z_2, z_3 as

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complex numbers C, and letting them be the elements of a vector Z in C^3. With $\omega = \exp 2\pi i/3$, the vectors $(1, 1, 1)$, $(1, \omega, \omega^2)$, $(1, \omega^2, \omega)$, denoted by $\mathbf{1}$, $\mathbf{u}$ and $\bar{\mathbf{u}}$ are an orthogonal basis for C^3, so $Z = c_1\mathbf{1} + c_2\mathbf{u} + c_3\bar{\mathbf{u}}$ for complex numbers c_1, c_2, c_3. $\mathbf{1}$ denotes a degenerate triangle, and $\mathbf{u}$ and $\bar{\mathbf{u}}$ equilateral triangles with centroids at the origin. Clearly $c_1\mathbf{1}$ is of no interest $-$ $\mathbf{1}'Z/3$ is the centroid of Δ and so set $c_1 = 0$. Multiplying Z by a complex number is the same as dilating and rotating Δ. Thus my canonical version of Δ could be written as $u + b\bar{u}$, with b its "shape." I then complicated the problem by going on to ignore the labels on the vertices. Veitch and Watson (1986) used a generalization of this Fourier method for k-labeled points in m dimensions for a generalization of the problem that started me off: Go along side P_1P_2 a distance $S\,|P_1P_2|$ to a point Q_3, go along P_2P_3 a distance $S\,|P_2P_3|$ to a point Q_1, and along P_3P_1 a distance $S\,|P_3P_1|$ to get a point Q_2. Thus one gets a new triangle Q_1, Q_2, Q_3. Let $S_1, S_2, \cdots$ be iid on $[0, 1]$, and repeat this construction successively. Thus we get a random sequence of triangles and I was interested in the random sequence of shapes. Mannion (1988) studied a much more interesting and difficult problem. His sequence of triangles was obtained by successively picking 3 points, iid uniformly at random in the parent triangle to get a new triangle. The labeling of the vertices is irrelevant for Mannion as it was in my problem and in the next paragraph. As one can guess, his triangles tend to collinear triangles.

Yet another way to get random triangles is to imagine that the vertices represent the three solutions of a cubic equation with random coefficients, $P_3(Z) = a_0 + a_1z + a_2z^2 + a_3z^3 = 0$. Kac (1943) solved the problem of the distribution of the real roots of $P_{n-1}(z) = 0$ when the a_j's are iid $N(0, 1)$. This doesn't seem to be a very practical problem but it is intriguing and one wonders about the distribution of all the roots or the complex roots. It seems very hard to get nontrivial analytic answers. The number of roots inside any closed curve S in the complex plane is given by

$$\frac{1}{2\pi i}\int_S \frac{P_n'(z)}{P_n(z)}\,dz.$$

Hence one needs to find the expectation of $P_n'(z)/P_n(z)$ for various assumptions about the joint distribution of the a_j's, and then to integrate the result. As far as I can see no one has used this approach. Bharucha-Reid and Sambandham (1986) give many references and show simulations with $n = 30$.

Certainly one wants to start with the cubic. Appendix A of Watson (1986) relates the solution of cubics to the shape of the root triangle. With Javier Cabrera, of Rutgers University, I have been studying this case with National Science Foundation support (DMS-84-21301). We have many pictures of both the roots and the shapes of the triangles formed by these roots. Of course, when the coefficients are real, one must get isosceles or collinear triangles. The pictures, especially those for shape, are much more interesting when the coefficients are complex. But the trick is—how to explain the patterns we see!

The analytic behavior of the shape density $m(x, y)$ described in § 4 reminds me of ancient work (Watson, 1956) and references therein) on the joint distribution of the ratios

$$r = \frac{\mathbf{x}'\mathbf{A}\mathbf{x}}{\mathbf{x}'\mathbf{x}}, \quad s = \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}},$$

where $\mathbf{A}$ and $\mathbf{B}$ commute and $\mathbf{x} \sim N(\mathbf{0}, \mathbf{I})$. In canonical form they are

$$r = \frac{\sum \lambda_i \omega_i}{\sum \omega_i}, \quad s = \frac{\sum \mu_i \omega_i}{\sum \omega_i},$$

where the ω_i are independent gamma random variables. Thus (r, s) falls randomly in the convex hull of the points (λ_i, μ_i). Further their joint density changes its analytic form as (r, s) crosses joins of the points (λ_i, μ_i) and has alternative representations. I wonder if there are any connections?

Leaving triangles and returning to the original motivation of Kendall (whether there are too many collinear, or nearly so, points in a picture) we see this as but the first of a series of problems. Earth and planetary scientists often claim to see "lineaments" (linear and circular segments). Sometimes at the points of intersection there is oil or gold, *etc.*. The statistician is at a loss with this sort of data. The biostatistician faces similar problems, e.g., is a cluster of cancer deaths in a neighborhood indicative of a local problem? This public health issue and geology have recently come together in the radon problem (gas comes out from the interior of the earth through faults). The question (could some observed geometrical oddity be due to chance) will raise puzzles forever, I suspect.

In conclusion I would like to urge others in the United States to take an interest in stochastic geometry (at the moment it seems to be solely of interest to Europeans) and to congratulate David Kendall for his immense contributions to the whole field.

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Comment

Dietrich Stoyan

Professor Kendall's paper is an excellent survey on a very important topic and describes many deep and complicated results obtained by himself and his colleagues. It is a pleasure to congratulate him on this success and to wish him further progress. The publication in this journal will help to inform many statisticians of these ideas and methods and so lead to further interesting applications. Because my own work has had until now only weak connections to Professor Kendall's theory of shape (with the nice exception of being a coauthor of a book that contains a chapter on shape theory written by W. S. Kendall), I can give marginal comments only; I take the opportunity to ask some questions.

In my opinion, in some cases the original problem of finding collinearities in point patterns can be solved by means of methods of point process statistics. If the point pattern under study can be interpreted as a sample of a stationary point process, then the orientation analysis of Ohser and Stoyan (1981) can be used to detect orientations and collinearities; see also Stoyan, Kendall and Mecke (1987). More interesting is the case of motion-invariant point processes with "inner orientations"; a nice example is the pattern of self-intersection points of a motion-invariant planar line process. Hanisch and Stoyan (1984) suggested statistical characteristics that are based on third-order moment measures or two-point Palm distributions. An example is the mean number of points in a rhombus with vertices at the members of a "typical" point pair of the point process with distance r (see Figure 1). If the corresponding mean, for which an unbiased estimator was given, is clearly greater than "intensity × area of rhombus" for interesting values of r, then some form of collinearity in the point pattern is detected.

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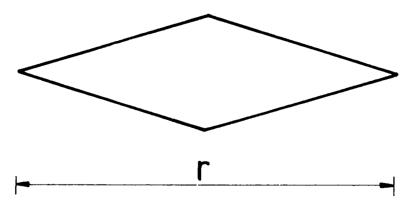

FIG. 1. *A rhombus with vertices of distance r. If the vertices are points of a point process and in the rhombus there are "many" other points of the point process, then this shows some inner orientation.*

Many statisticians and physicists, geographers (see the booklet by Boots, 1987) and others are very much interested in Dirichlet tessellations and the closely related Delaunay tessellations. Therefore the results on the Delaunay tessellation are of great value, both theoretically and practically. In particular, I like the elegant way of simulating "lone" Poisson Delaunay cells.

I think that a promising method for a "shape analysis" of tessellations could be based on the angles at vertices, if all vertices are Y-shaped, with three emanating edges. (This situation very often appears in practical problems, as physicists and materials scientists say.) Then each vertex corresponds to a triangle, which is similar to the Delaunay triangle if the tessellation under study is a Dirichlet tessellation with respect to a point pattern. Most empirical tessellations are not Dirichlet tessellations or, if their generating points are not given, the natural starting points for the shape analysis are the three angles. Therefore it would be helpful to transform shape theory results for triangles into angular coordinates, where, for example, a triangle is described by its maximal and minimal angles.

Perhaps it is of interest to mention a further (additionally to Professor Kendall's findings for PDLY tiles) interesting property of the Dirichlet tessellation, which in future may be better elucidated by the new simulation methods. Together with Dr. H. Hermann, I studied statistically simulated Poisson Dirichlet tessellations, in particular the point process of vertices of cells. Surprisingly we found that the corresponding second-order product density $\rho(r)$ has a striking form: it seems to be true that

$$\lim_{r \to 0} \rho(r) = \infty,$$

or, at least, $\rho(0)$ seems to be very great. Usually, such behavior of a product density is an indicator of a high degree of clustering. By visual inspection of some simulated tessellations we found that clusters of vertices in the usual sense of the word are not typical for these tessellations, but there appear frequently very short edges (of otherwise "normal" cells) or pairs of vertices very close together.

With respect to statistical shape problems related to "landmarks" in the sense of Bookstein (1978, 1986), I should like to ask the following question. Imagine three nonintersecting circles in the plane. Take a random point in each of the circles, for example uniformly or with respect to any distribution. Form the triangle having the three points as their vertices. Is it possible to give the corresponding shape density?

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Rejoinder

David G. Kendall

It is appropriate that Professor Bookstein should open this discussion in view of the importance of his work and the great influence that this has had through his own presentation in *Statistical Science* and his earlier 1978 monograph. I was already deeply involved in shape theory when I first read the latter, but did not at that time foresee how closely our two different and differently motivated approaches would converge. It is all the more valuable, therefore, that he has generously taken the time and trouble to survey their current interactions and differences of emphasis. His remarks will deserve careful study.

Professor Small's contribution is full of wise insights, and novel suggestions are made that I shall think about deeply. "Projection-pursuit" viewing of higher dimensional shape manifolds may well be a reality a few years from now. My current practice, not so technologically ambitious, is to try to understand these spaces as thoroughly as possible, and then to seek dimension-lowering projections that retain the important information and make it visible in a helpful way. One example of such a procedure will be found in my contribution to the discussion on Bookstein's 1986 paper referred to above. Of course I agree with the remarks that he and others have made about the advantages of having a variety of visual displays available. I recall that Kipling wrote a fine poem on a similar topic many years ago.

Professor Mardia's contribution was a shock to me because I did not expect to see so beautiful a solution as that found by Mardia and Dryden to the important problem they have studied. It makes one ask, why is it so beautiful? What has happened to all the horrible noncentral χ^2's? Of course the Gaussian distribution never ceases to spring surprises on us. I discussed Mardia's remarks with Wilfrid Kendall, and it occurred to us that a dynamic approach might at least "explain" what lies behind such a nice formula. So here are a few remarks intended only to illuminate the anatomy of the problem.

To start with it will be necessary to change the notation a little. We identify Mardia's κ with $s_0^2/(4c^2t)$, where c is a diffusion constant, t is the time elapsed during the interval considered and s_0 is a linear measure of the size of the triangle $\Delta_0 = (A_0, B_0, C_0)$ at the beginning of that time interval. The Mardia-Dryden formula then gives the law of distribution of the shape at the end of the time interval when we know what the shape was to start with. Notice that in this formulation it is no longer necessary to exclude $A_0 = B_0 = C_0$ as a possible initial shape, for then $s_0 = 0$, and this makes $\kappa = 0$, and then the Mardia-Dryden formula tells us that the distribution of size at the end of the interval is uniform over the sphere, as it ought to be.

More generally let us write $\zeta(t)$ for the shape of $\Delta_t = (A_t, B_t, C_t)$ at time t, this being undefined at

$t = 0$ if the size s_0 is then zero. We let the points A, B and C perform independent standard plane Brownian motions with no drift and with diffusion constant c, starting at A_0, B_0 and C_0, and we look at the situation after a positive time t has elapsed, when we have a new labeled triangle $\Delta_t = (A_t, B_t, C_t)$ with size $s(t)$ and shape $\zeta(t)$. Their problem was to find the law of distribution of $\zeta(t)$ for this given $t > 0$ when $\zeta(0)$ is given.

It is actually easier to think first about the stochastic motion performed by $(s(t), \zeta(t))$ on the size and shape space, which we know to be a cone with $\Sigma_2^3 = S^2(\frac{1}{2})$ as unit section. The vertex of the cone corresponds to the situation $A = B = C$ (almost surely only possible when $t = 0$). This combined size and shape process is known to be a diffusion, and it is a skew product factoring into a Bessel-type process on the generators (for size), and driftless spherical Brownian motion on the (spherical) cross sections (for shape), that spherical Brownian motion being described at a random rate $d\tau/dt$ inversely proportional to the current squared size s^2 of the triangle. This decomposition was hinted at in my 1977 note, and happily we now have a thorough analysis by W. S. Kendall (1988) in *Advances in Applied Probability*.

The formal solution to the dynamic form of the Mardia-Dryden problem is thus to write down the law of distribution of $\beta(\tau)$ for given $\tau > 0$, where β is spherical Brownian motion on the sphere Σ_2^3 starting at $\zeta(0)$, and then for given t to integrate out the dependence of $\beta(\tau(t))$ on the elapsed random-clock-time $\tau(t)$, using what we know about Bessel processes.

The result, for a fixed $t > 0$, ought to be the Mardia-Dryden law when reexpressed in the new notation. In fact it turns out that this diffusion approach really does work, and I have now pushed it through to get a stochastic calculus proof of the Mardia-Dryden result. Details will appear elsewhere, and perhaps will suggest higher dimensional generalizations.

I am grateful to Mardia for taking up my remarks about Central Place Theory (which, until the statisticians began to interfere, did not seem to have much theory in it). I hope that we can follow up some of his suggestions together.

I am delighted that one of my collaborators of long standing has chosen to write on the general philosophy of the use of computer algebra in stochastic science. I have found it helpful to match complicated calculations with parallel simulations, in order to cover the risk of not detecting gross errors (say extra factors of 2), and because such a practice can alert one to aspects of a problem that have been overlooked. With the arrival of computer algebra we have a second such "automatic colleague" skilled in the development of asymptotic formulae, able to tell at a "glance" whether two monstrous expressions are indeed equivalent, able also (with some persistent and inspired prodding) to "simplify" expressions and so forth. Wilfrid Kendall has now taken us a stage farther along that road, pointing out that computer algebra can be trained to be a good sniffer-out of unsuspected structures, although emphasizing that like all good colleagues it will make its most fruitful discoveries when supplied with well chosen hints. And if the hints turn out to have been unhelpful one can try again, knowing that computer algebra can wipe out the past at will, and so need not be prejudiced by false starts. What can be done when computer algebra is teamed up with a human expert is well shown in his research into shape diffusions, and we are lucky that he has documented the "learning" route with such helpful comments, and so supplemented in a most valuable way the necessarily terse style of the manuals.

Professor Watson rightly reminds us of the antiquity of geometrical stochastics in the sense that some specific problems ante-date its present general formulation. One needs to keep a sense of proportion when writing the history of a mathematical topic. Sometimes one is left wondering whether anything at all is really new. But this is an over-reaction; the problems have always been there, and have provoked reactions from time to time, but in most cases it has taken decades if not centuries for the language to have been developed in which to pose such questions in their natural form. Thus, Woolhouse in 1863 calculated for arbitrary a and b the chance that three points iid uniform in a rectangle of sides a and b will be the vertices of an acute-angled triangle. At first this seems like a demonstration that what we here call shape theory existed 125 years ago. But that this is a mistaken view is made clear when one notices that the article just quoted forms one of a series of papers by various writers including a "proof" that three points taken iid "uniformly in space" have a zero chance of forming an acute-angled triangle! Of the numerous valid variants of that improper problem today, the most attractive is: three Brownian particles set out at time $t = 0$ from a given point in the plane; show that at any given later time t there is a chance $\frac{1}{4}$ that they form the vertices of an acute-angled triangle. The proof takes just one line—but it makes use, implicitly or otherwise, of several branches of mathematics developed during the last century.

I am relieved that Watson finds shape theory difficult. So do I, and until his reassuring remarks I thought that this was merely a reflection of my own antiquity. He will be happy to learn that the first (a basic part) of the forthcoming book will be really elementary, being based on a lecture I have to give to school children later this year. (Of course "elementary" does not necessarily mean "uncomplicated.") I agree that it is helpful to have several different sets of shape coordinates, because different sets are convenient for different purposes. But two basic facts should not be forgotten. If we wish to keep to a metric directly related to the procrustean distance, then there is no question about it; we have to use the spherical representation for three points in two dimensions, and the appropriate complex projective representation for k points in two dimensions. If on the other hand we are primarily interested in (say) the possible occurrence of "hot spots" in the distribution on shape space, then we can use any convenient representation diffeomorphic (but not necessarily isometric) with the standard one provided that the "null" distribution as seen in a plotted simulation looks sufficiently nearly uniform in the relevant region. To indicate something of the variety of possible visual displays, here (Figure 1) is a collection of triangle shapes each one of which sits at its proper position on the sphere $S^2(\frac{1}{2})$, and here (Figure 2) is the distribution on that shape space of a large iid sample from a plane Gaussian law with $\sigma_2 = 5\sigma_1$. In each case the picture is to be interpreted as a three-dimensional one, and the viewer must bear in mind that, to the untutored eye, a uniform law on the surface of a sphere looks as if there were an enhanced density near the rim of the sphere. This reminds us that a proper education of the eye is essential to good practical geometric statistics. In this example the "hot belt" around the collinearity locus is easily recognizable, and is a genuine (and scarcely surprising) consequence of the fact that we made $\sigma_2/\sigma_1 = 5$.

I am fascinated by Watson's problem of the cubic with random complex coefficients $c_r = a_r + ib_r$ where all a's and b's are iid Gaussian. How about starting with a nice large simulation, the shape of each triangle-of-roots (z_1, z_2, z_3) being displayed on $S^2(\frac{1}{2})$ as above? It might be worth plotting separately those root triplets having different graded values of the size

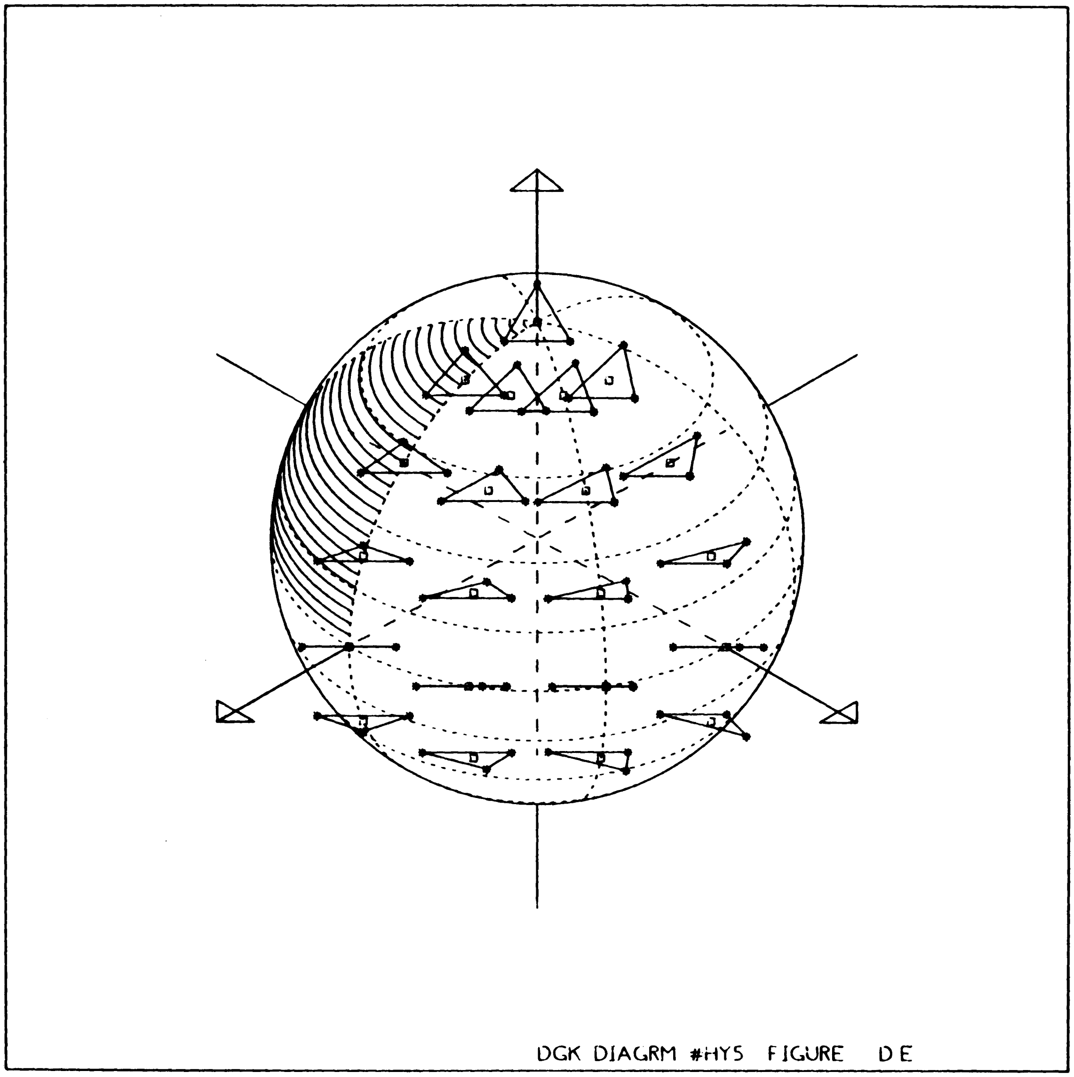

FIG. 1. *Some triangle shapes at home in the shape space. The shaded half-lune is the customary basic region.*

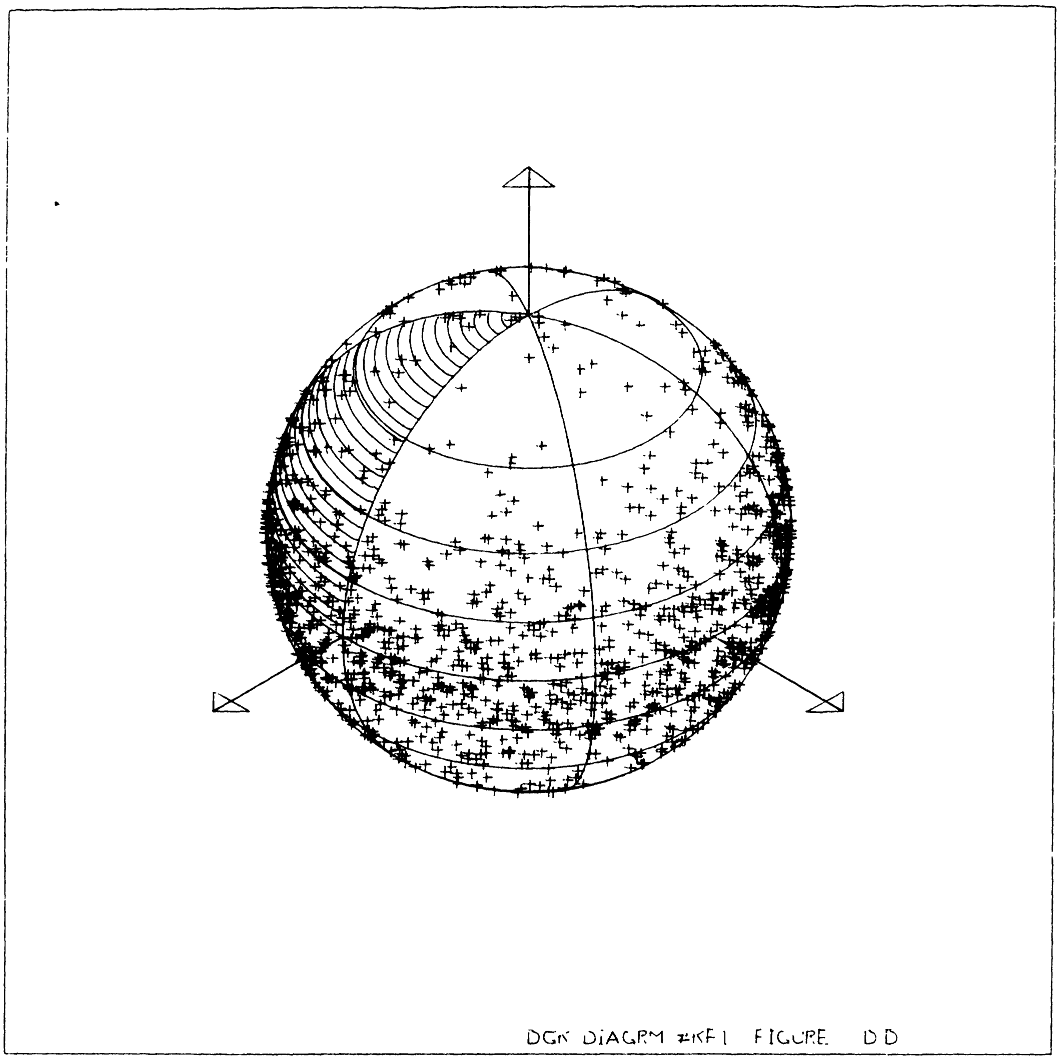

FIG. 2. *Shapes of triangles with iid vertices from $\mathcal{N}(0, 0; 1, 5)$.*

variable $\sqrt{\sum} \mid (z_j - \zeta) \mid^2$, where $\zeta = ⅓\sum z_j$. I look forward to seeing more of his work on this topic.

Dr. Stoyan has raised a large number of points and queries, and it will be impossible to deal with them all here, but I much value his interest both for its stimulating character and because his remarks illustrate well the splendid work in stochastic geometry by Stoyan and his colleagues in the DDR. Solutions to some of these problems using the powerful techniques of stationary point processes will certainly be useful, although we must of course remember that few things in life are really stationary. With regard to his suggestion about the rhomb, my preference is for a "trap" such as is shown in Figure 3. This is designed to catch near collinearities although excluding those that are better described as near coincidences (of two of the three vertices). It can conveniently be employed with the (x, y)-plots used by Huiling Le and myself, particularly because from her work we now know that the "uniform in a convex polygon" model tends to give an almost constant shape density (relative to $dxdy$) in such a rectangular trapping region.

I agree that "random Dirichlet cells" forms a rich topic. Formally this should be studied on CP^∞, but as a start, how do we modify that shape space so that it contains only the shapes of the convex labeled polygons? It seems worth remarking that the Dirichlet cell is more nearly dual to the whole collection of Delaunay cells that meet at a point—and as I have remarked in the paper, we know little about that at present. Another approach would be to condition the shape of the Dirichlet cell on the number of its vertices.

For the last problem proposed in Stoyan's contribution one should point to the work of Mardia and Dryden referred to elsewhere in the discussion and in this reply. It appears that the switch from disk distributions to Gaussian ones simplifies the question

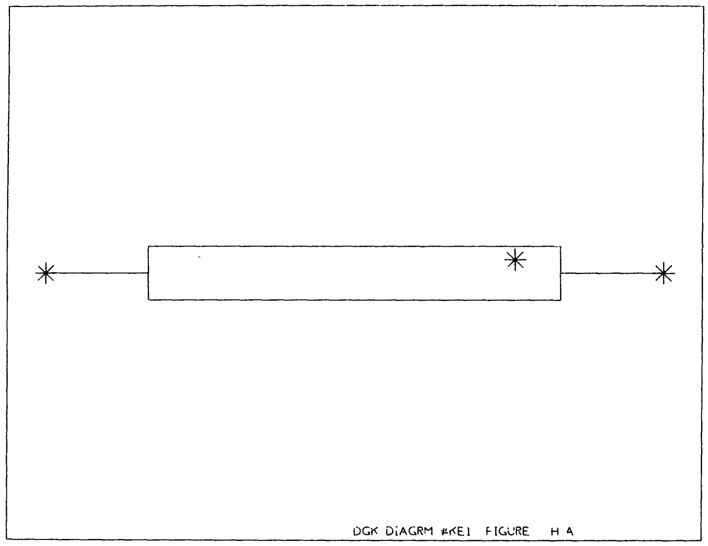

FIG. 3. *A trapping region for collinearity testing (not to scale).*

dramatically, and perhaps this alternative model would be equally appropriate for his purposes.

Finally I should like to add a special word of thanks to Morris DeGroot for his invitation to me to write this paper, and for his conviction, now splendidly vindicated, that it would generate a lively and interesting discussion.

ADDITIONAL REFERENCES

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