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Shapes of Quantum States

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Summary. The shape space of k labelled points on a plane can be identified with the space of pure quantum states of dimension $k-2$. Hence, the machinery of quantum mechanics can be applied to the statistical analysis of planar configurations of points. Various correspondences between point configurations and quantum states, such as linear superposition as well as unitary and stochastic evolution of shapes, are illustrated. In particular, a complete characterisation of shape eigenstates for an arbitrary number of points is given in terms of cyclotomic equations.

1. Statistical theory of shape

The idea of a shape-space Σ_m^k, whose elements are the shapes of k labelled points in $\mathbb{R}^m$, at least two being distinct, was introduced in a statistical context by Kendall (1984). Here, it is natural to identify shapes differing only by translations, rotations, and dilations in $\mathbb{R}^m$ (although there are situations of interest, not to be considered here, in which the scale is also relevant). However, this identification will not apply to reflections. Thus, the resulting shape space is the quotient

$$\Sigma_m^k = S^{m(k-1)-1}/SO(m)$$

of the sphere by the rotation group. This is the base space of a fibre bundle with total space $S^{m(k-1)-1}$ and fibre $SO(m)$. The former is naturally endowed with a uniform Riemannian metric, while the latter, being a compact Lie group, possesses an invariant metric.

The key observation of Kendall is that the metrical geometry of these quotient spaces, long studied by geometers, is precisely the required tool for the introduction of measures appropriate for the systematic comparison and classification of various shapes.

Now, for a planar distribution of points, with $m = 2$, the shape space Σ_2^k of k points is simply a complex projective space $\mathcal{P}^{k-2}$ of dimension $k-2$, with the Fubini-Study metric defining the geodesic distances between pairs of shapes. The vertices of a shape in $\mathbb{R}^2$ (viewed as a complex plane), with the centroid at the origin, determine the homogeneous coordinates of a point in $\mathcal{P}^{k-2}$. The permutation group $\Sigma(k)$ of order k interchanges homogeneous coordinates, and is therefore represented by projective unitary transformations of $\mathcal{P}^{k-2}$.

For three-point configurations, i.e. $k = 3$, the shape space is a complex projective line $\mathcal{P}^1$, which, viewed as a real manifold, is a two-sphere S^2. Hence, the natural shape space for triangles is essentially a Riemann sphere (Kendall 1985, Watson 1986).

2. Space of pure quantum states

A quantum state $|\psi\rangle$ of a physical system is represented by a vector in a complex Hilbert space $\mathcal{H}^{n+1}$ of dimension, say, $n+1$. Quantum states determine expectations of physical observables, that is, if X is a random variable, then its expectation in a given state $|\psi\rangle$ is determined, in the Dirac notation, by

$$\langle X\rangle = \frac{\langle\psi|X|\psi\rangle}{\langle\psi|\psi\rangle},$$

where $\langle\psi|$ denotes the complex conjugate of the vector $|\psi\rangle$. Notice that this expression is invariant under the complex scale change $|\psi\rangle \to \lambda|\psi\rangle$, where $\lambda \in \mathbb{C} - \{0\}$. Thus, a pure quantum state is an equivalence class of states, i.e. a ray through the origin of $\mathcal{H}^{n+1}$. This is just the complex projective space $\mathcal{P}^n$, with the Fubini-Study metric that determines transition probabilities. To see this, we recall that the transition probability between a pair of states $|\psi\rangle$ and $|\eta\rangle$ is given by

$$\cos^2 \tfrac{1}{2}\theta = \frac{\langle\psi|\eta\rangle\langle\eta|\psi\rangle}{\langle\psi|\psi\rangle\langle\eta|\eta\rangle}.$$

To recover the Fubini-Study metric we set $|\eta\rangle = |\psi\rangle + \mathrm{d}|\psi\rangle$ and $\theta = \mathrm{d}s$, and retain terms up to quadratic order (Hughston 1995, Brody & Hughston 2001). In particular, the maximum separation between a pair of states is given by $\theta = \pi$, whereas if the two states are equivalent in $\mathcal{P}^n$, then $\theta = 0$.

Therefore, a shape space of planar k-point configurations may be viewed as a pure quantum state space with $k-1$ generic energy levels. However, this correspondence applies only to planar configurations, and not those in higher dimensions. Nonetheless, all this suggests the possibility of applying quantum theoretical methods to the statistical theory of shapes, or conversely. I shall briefly outline some relevant ideas which might prove fruitful.

3. Triangles as spin-$\frac{1}{2}$ states

As noted above, the space of planar configurations of labelled triangles is $\mathcal{P}^1 \sim S^2$, or in quantum theory, the state space of a spin-$\frac{1}{2}$ particle. Specification of the Hamiltonian determines a pair of energy eigenstates, identifiable with the poles of the sphere.

As in quantum mechanics where any orthogonal pair of states can be the energy eigenstates, any pair of orthogonal triangles can form the poles of S^2. A natural symmetrical choice of the 'triangular eigenstates' would be as follows. Let z be a nontrivial cubic root of unity; this satisfies the cyclotomic equation $1 + z + z^2 = 0$, and the complex conjugate of z is z^2. Then the vectors

$$|\triangle\rangle = \frac{1}{\sqrt{3}}(1, z, z^2) \quad \text{and} \quad |\nabla\rangle = \frac{1}{\sqrt{3}}(z^2, z, 1)$$

could form two eigenstates. Thus, the corresponding shapes are two origin-centred equilateral triangles, differing only by two-vertex interchanges. See Fig. 1 (p. 118) in Kendall's Rejoinder (1989), displaying the triangles on S^2 corresponding to this choice of basis. The shape of an arbitrary triad of points can be expressed as a complex linear combination $\alpha|\triangle\rangle + \beta|\nabla\rangle$ of these two states such that $|\alpha|^2 + |\beta|^2 = 1$.

In many statistical problems, the labelling of the vertices has no significance, and we can work modulo permutations of points. As regards the representation of the permutation group $\Sigma(3)$ by transformations of S^2, we let the two-sphere be appropriately subdivided into six regions ('lunes' in Kendall's term) in a manner topologically equivalent to the subdivision of the surface of a cube into six faces. The projective unitary transformations induced by $\Sigma(3)$ then act in a manner that corresponds to the the permutations of the three oriented cartesian coordinate axes. The total group of rigid isomorphisms of the cube has 48 elements, i.e. the six permutations of the oriented coordinate axes, followed by any of the eight possible combinations of the reflections. In cases where the labelling of points is of no significance, the relevant state space is thus reduced to the 'spherical blackboard' of Kendall (1984).

4. Square and pentagon eigenstates

If z is a nontrivial quartic root of unity, so that the complex conjugate of z is z^3, then the most symmetrical choice for the square eigenstates consists of the two orthogonal states

$$|\Box_1\rangle = \tfrac{1}{2}(1, z, z^2, z^3) \quad \text{and} \quad |\Box_2\rangle = \tfrac{1}{2}(z^3, z^2, z, 1),$$

identifiable in quantum mechanical terms with the spin ± 1 eigenstates. The corresponding shapes are two regular origin-centred squares, differing by vertex interchanges. In this case, the third eigenstate (for spin-0) is the degenerate square, i.e. a line, given by

$$|-\rangle = \tfrac{1}{2}(1, -1, 1, -1),$$

and these three states form an orthonormal basis, so that any configuration of four points is linearly expressible in terms of these three states.

For pentagons, on the other hand, if z denotes a nontrivial fifth root of unity, satisfying the cyclotomic equation $1 + z + z^2 + z^3 + z^4 = 0$, with the complex conjugate of z given by z^4, then a symmetric basis consists of the four orthogonal states

$$\frac{1}{\sqrt{5}}(1, z, z^2, z^3, z^4), \ \frac{1}{\sqrt{5}}(1, z^2, z^4, z, z^3), \ \frac{1}{\sqrt{5}}(1, z^3, z, z^4, z^2), \ \text{and} \ \frac{1}{\sqrt{5}}(1, z^4, z^3, z^2, z)$$

of origin-centred regular pentagons. These states are identifiable with the eigenstates of a spin-$\frac{3}{2}$ particle in quantum mechanics.

5. Construction of general eigenshapes

In general, the projective space $\mathcal{P}^n$ corresponds to configurations of $n + 2$ points. In this case, the cyclotomic equation

$$1 + z + z^2 + \cdots + z^{n+1} = 0$$

indeed determines an orthonormal set of shape eigenstates. However, as I shall indicate below, if the number $N = n + 2$ of points is not a prime, then the most symmetrical choice of shape eigenstates, to be referred to as eigenshapes, will be degenerate in a sense analogous to that of the square eigenstates considered in the previous section. For example, in the case of six-point configurations, two of the eigenshapes are regular hexagons, two of the eigenshapes are equilateral triangles, and the fifth eigenshape is just a line. In particular, any sextet of points can be expressed as a linear combination of these five eigenshapes, and we do not require five hexagonal shapes to express an arbitrary configuration.

In order to construct general eigenshapes for an arbitrary number N of points, we let

$$z = \exp(2\pi i/N)$$

denote a nontrivial root of the cyclotomic equation. Then a generic eigenshape can be expressed in the form

$$|\omega_k\rangle = \frac{1}{\sqrt{N}}(z^{a_1}, z^{a_2}, \cdots, z^{a_N}),$$

where $\{a_j\}$ $(j = 1, 2, \ldots, N)$ is a set of integers between 0 and $N-1$, not all of which need be distinct. When they are distinct for a given N, the corresponding eigenshape $|\omega_k\rangle$ is nondegenerate.

For a general N-point configuration, there are $N-1$ eigenshapes $|\omega_1\rangle, |\omega_2\rangle, \cdots, |\omega_{N-1}\rangle$. These are given by the table below, specifying all the values of $\{a_k\}$ for an arbitrary N:

	a_1	a_2	a_3	a_4	$\cdots$	a_{N-2}	a_{N-1}	a_N
$\|\omega_1\rangle$	0	1	2	3	$\cdots$	$N-3$	$N-2$	$N-1$
$\|\omega_2\rangle$	0	2	4	6	$\cdots$	$N-6$	$N-4$	$N-2$
$\|\omega_3\rangle$	0	3	6	9	$\cdots$	$N-9$	$N-6$	$N-3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\|\omega_{N-2}\rangle$	0	$N-2$	$N-4$	$N-6$	$\cdots$	6	4	2
$\|\omega_{N-1}\rangle$	0	$N-1$	$N-2$	$N-3$	$\cdots$	3	2	1

Note that the numbers $0, 1, 2, \ldots, N-1$ successively appear in a cycle. Therefore, for example, if $N = 9$, then the value of a_4 in the eigenshape $|\omega_3\rangle$, which in this table is given by $a_4 = 9$, indicates the number following $N - 1 = 8$ in the cycle. In the present example, this is the number 0 rather than 9, so that the sequence represented by a_4 is $3, 6, 0, 3, 6, 0, 3, 6$.

This cyclic property clearly implies that if N is a prime number, then by following the sequence of numbers along any given row or column in this table, one never encounters any repetitions. Thus, the corresponding eigenshapes are all nondegenerate. Conversely, if N factors, then, by definition, repetitions will appear in some rows and columns, and consequently the corresponding shape becomes degenerate. Therefore, only if the number of points is a prime can regular polygons be chosen for all the corresponding eigenshapes.

Although all orthonormal bases are unitarily equivalent, the choice given here is preferred not only for aesthetic reasons but also for the practical purpose of systematically generating bases that are readily visualised. In a quantum mechanical problem, one begins by specifying the Hamiltonian. The eigenstates of the Hamiltonian constitute a naturally preferred basis. On the other hand, in a problem concerning statistical analysis of shape, there is no *a priori* preferred basis unless further conditions are specified. Consequently, for a given configuration with a large number of points, it has hitherto been unclear how one can systematically 'decompose' the configuration into a set of simple orthogonal components. The present scheme offers one possibility of achieving this task.

6. Separation and superposition of shapes

Given an arbitrary pair of $(n+2)$-point configurations in $\mathbb{R}^2$ we can determine the state vectors in the projective space $\mathcal{P}^n$ that correspond to these two configurations. Then, the separation of these two shapes (what Kendall calls the distance between two shapes) is determined by the transition probability between the two representative elements of $\mathcal{P}^n$.

The superposition of different shapes is also useful from the quantum mechanical point of view. In particular, the set of eigenshapes constructed in the previous section is complete in the sense that any shape can be expressed uniquely as a linear superposition of these eigenshapes. For example, superposition of a pair of orthogonal equilateral triangles, given by

$$|\triangleright\rangle = \cos\tfrac{1}{2}\theta|\triangle\rangle + \sin\tfrac{1}{2}\theta\, \mathrm{e}^{\mathrm{i}\phi}|\triangledown\rangle,$$

will generate all possible shapes associated with three points. In the special case where $\theta = \frac{1}{2}\pi$, all the collinear configurations of three points are obtained by varying the phase variable $\phi \in [0, 2\pi)$. Similarly, an arbitrary four-point shape can be expressed in the form

$$|\diamondsuit\rangle = \cos\tfrac{1}{2}\theta|-\rangle + \sin\tfrac{1}{2}\theta\cos\tfrac{1}{2}\eta\, \mathrm{e}^{\mathrm{i}\phi}|\Box_1\rangle + \sin\tfrac{1}{2}\theta\sin\tfrac{1}{2}\eta\, \mathrm{e}^{\mathrm{i}\psi}|\Box_2\rangle.$$

Thus, the decomposition scheme considered here allows us to recover simple parametric families of states that represent the totality of possible point configurations. It should be evident how these examples can be generalised to shapes with larger number of points.

7. Unitary evolution of shapes and geometric phases

For a given Hamiltonian, the unitary dynamics of a spin-$\frac{1}{2}$ quantum state corresponds to a rigid rotation of S^2 around the poles specified by the energy eigenstates. Thus, to study the unitary evolution of triangles, we must determine the infinitesimal deformations of a normalised triangle representing the direction orthogonal to that of a rotation about the origin.

After diagonalisation, the unitary evolution generated by the Hamiltonian consists in rotating the vertices of the triangle about the origin, but at generally different angular velocities. In general, if the angular velocities are commensurable, then the trajectory is closed in the projective space, but all the vertices of the triangle are hereby rotated through the same angle about the origin. This angle is just the geometric phase associated with the corresponding quantum state.

8. Quantum entanglement of shapes

Another interesting question in the present context is whether quantal notions such as entanglement could be relevant to statistical shape analysis. The entanglement concept arises when two or more physical systems are combined. If a system with m energy eigenstates (corresponding to an $(m+1)$-point shape space) and another with n energy eigenstates (an $(n+1)$-point shape space) are combined, one obtains the state space of an mn-eigenstate system (an $(mn+1)$-point shape space).

In particular, if the constituent subsystems are disentangled, then such states form an $(m+n-2)$-dimensional subspace $\mathcal{P}^{n-1} \times \mathcal{P}^{m-1}$ of the total space $\mathcal{P}^{nm-1}$. Thus, for example, if we combine a pair of triangles, we obtain a disentangled pair equivalent to a four-point configuration, while entangled states represent generic configurations of five points. More generally, when a pair of shapes are combined, then a generic shape that corresponds to a disentangled state will have four points that are collinear. The possible statistical significance of this situation constitutes an intriguing open question. Some examples of disentangled and entangled shape combinations are shown in the figure below.

9. Mixture of shapes

What would be quite relevant to the statistical analysis of shape is the notion of mixed states, i.e. distributions over the shape space $\mathcal{P}^n$. Often, in cases of interest, certain inter-

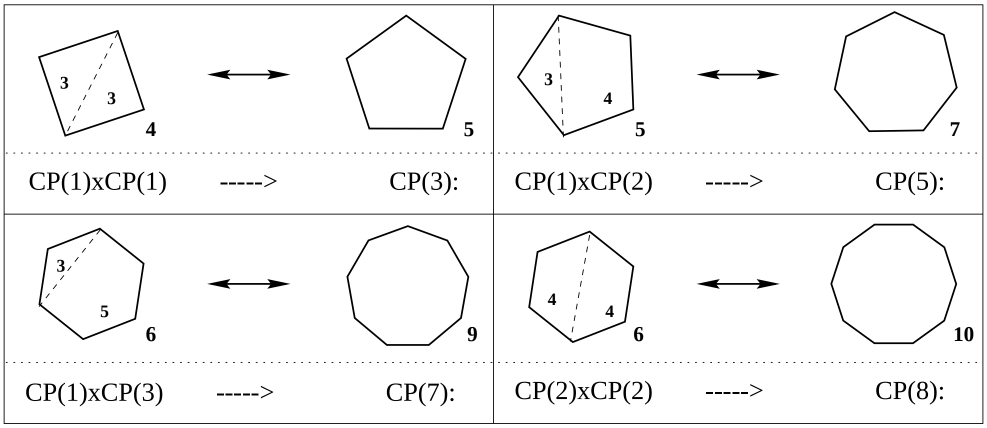

Fig. 1. Combination of shapes and their entangled configurations. When a pair of shapes are combined, the resulting shapes of the disentangled states have four points that are collinear, as indicated on the left-hand side. The right-hand side shapes correspond to entangled states. In general, entangled shapes have a larger number of points than the sum of the numbers of points associated with individual disentangled shapes.

actions or dynamics are associated with the points of the configurations under consideration. This permits one to define distributions of shapes. An example of this is the notion of a two-dimensional froth, which has important applications in biology (e.g., epithelial tissue growth). Each froth can be viewed as an irregular polygon, and the froth vertices where three polygonal edgesmeet (a vertex with higher incidence number is unstable) are the points of interest. For a given polygon, the number of edges can vary, although its expectation value, assuming we have a flat surface (i.e. zero curvature) and a large number of cells, must be 6 by virtue of Euler's relation (cf. Aste, *et al.* 1996). This is closely related to the fact that, for a wide range of interaction energies between point particles on a plane, the minimum energy configuration is typically given by a regular hexagonal lattice.

In the case of biological cells, for which divisions and disappearances occur, statistical analysis of the distribution and the dynamics of point configurations is important in understanding the properties of biological processes. More specifically, the statistical theory of shape is relevant here because the ability of a damaged tissue to restore its stable configuration can be explained by shape-dependent information stored in the cells, no further information being required (Dubertre, *et al.* 1998).

The problem of shape diffusion (cf. Kendall 1988), which would characterise the dynamical evolution of froths, can be formulated as a diffusion process for a single point in $\mathcal{P}^n$. In the quantum mechanical context this is known as the problem of quantum state diffusion. One special class of processes that has been studied extensively (when phrased in the shape-theoretic context) is as follows: given a set of eigenshapes that represent energy extremals, (that is, they are eigenstates of an energy operator), an arbitrary initial configuration will diffuse into one of the extremal eigenshapes in such a manner that the probability of terminating in such an eigenshape is given by the transition probability between the initial and final shapes. For such a process, an explicit solution to the diffusion equation is known (Brody & Hughston 2002) for an arbitrary number of points. These notions may be applicable to study diffusive dynamics of complex planar systems.

10. Discussion

Finally, I cite some recent developments in the study of point configurations (Atiyah & Sutcliffe 2002, Battye, *et al.* 2003). These investigations are motivated by the physical question of determining the minimum classical energy (i.e. most stable) configurations of point particles in two or three dimensions. Note, however, that their analysis does not exclude the possibility of all the points coinciding. Hence, the relevant shape spaces are slightly distinct from those investigated by Kendall. These studies, along with the above-mentioned quantum interpretation of shapes, might shed new light on statistical shape theory.

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