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Abstract

A stochastic dynamical context is developed for Bookstein's shape theory. It is shown how Bookstein's shape space for planar triangles arises naturally when the landmarks are moved around by a special Brownian motion on the general linear group of invertible (2×2) real matrices. Asymptotics for the Brownian transition density are used to suggest an exponential family of distributions which is analogous to the von Mises-Fisher spherical distribution and which has already been studied in [23]. The computer algebra implementation *Itovsn3* [34] of stochastic calculus is used to perform the calculations (some of which actually date back to work by Dyson on eigenvalues of random matrices and by Dynkin on Brownian motion on ellipsoids). An interesting feature of these calculations is that they include the first application (to the author's knowledge) of the Gröbner basis algorithm in a stochastic calculus context.

KEYWORDS: Bookstein shape, Brownian motion, computer algebra, D.G. Kendall shape, von Mises-Fisher distribution, Gröbner basis algorithm, holomorphic correspondence, hyperbolic plane, mean shape, Minakshisundaram-Pleijel recursion formulae, statistical shape, symbolic Itô calculus.

1 Two different shapes for planar triangles

David Kendall [25, 26, 27, 28, 29] has shown that the shape of a triangle of three landmark points in the plane is naturally parametrized by a (D.G. Kendall shape-) point on a sphere Σ_2^3 of radius $1/2$.

Justifications for this include the following:

(i) An analysis of a procrustean metric for shapes, which delivers exactly this metric structure. See [26];

(ii) A symmetry argument about the result of "mixing" the three planar landmark points of the triangle using $\text{SO}(6)$ acting on $\mathbb{R}^{(3\times 2)}$) (this is the appropriate symmetry if the points are random, independent, identically distributed with circularly symmetric Gaussian distribution), involving reference to the famous *Hopf fibration* of complex projective spaces: $\mathbb{C}P^2 \to \mathbb{C}P^1 = S^2(\text{ radius } 1/2)$ [7, page 235];

(iii) If the three landmark points move independently on the underlying Euclidean plane, either by Brownian motion or by Ornstein-Uhlenbeck process, then the shape moves according to a two-dimensional random process. If the size is measured by the sum of squares of sides then a random time-change τ based only

on size (itself given by an autonomous squared Bessel process, if the underlying process is the Ornstein-Uhlenbeck process) turns the shape process into a diffusion; consideration of its intrinsic geometry shows that this *shape diffusion* is naturally regarded as a Brownian motion on the sphere of radius $1/2$. See the work of David Kendall [25] and also generalizations to higher dimensions covered by myself [31, 32, 34], Le [41], and Carne [9].

Of course these three justifications for the spherical geometry of Σ_2^3 are closely related. They identify a shape geometry which is appropriate when (in some sense) the landmark points of the configuration have only a weak interdependence, as might be relevant when considering shapes formed by a point process (see for example the original application to archaeology in [8, 30]: see also [13]).

Notice also the following: while in most applied contexts one does not suppose the points move in time, nevertheless the time-change variable τ in the transition kernel for shape diffusion in (iii) can be viewed as a dispersion parameter, and the Markov property then converts into a convolution relationship between distributions given by the transition kernel. It is also possible to use the original time parameter t (scaled by the size of the initial triangle) as dispersion parameter, and one then obtains the delightfully simple *Mardia-Dryden* family of distributions [45], though the convolution property is then lost.

Independently Bookstein has developed a notion of shape based mainly on biological applications (see [4, 6] for reviews and [5] for more recent work), in cases where it is *not* appropriate to assume the inter-point dependence is only weak. In fact Bookstein derives *two* notions of shape. One is based on an idea of ratios of strain, is principally to do with triangles, and is what we shall discuss here. The other, which we do not discuss, is relevant for configurations of more than three points and is based on the theory of elasticity of thin plates.

Bookstein's idea is to consider the strains inherent in distorting an initial configuration of three points into a new configuration. The resulting parametrization delivers a (Bookstein shape-) point in the half-plane and the implicit geometry is now *hyperbolic* (constant negative curvature). Distortion of a non-collinear configuration into a collinear configuration is an extreme case, and corresponds to moving the corresponding shape point out to the boundary: indeed to be absolutely precise one should represent Bookstein shape space by *two* hyperbolic planes (the shape represented by points on the one half-plane corresponding to mirror images of shapes represented by points on the other), and regard shapes which are mutual reflections as infinitely distant from each other. We shall confine our attention to just one half-plane, corresponding to shapes which can be obtained by continuously distorting a reference shape without passing through collinearity. This is a natural restriction in the biological context!

(An alternative, though less exact, point of view regards Bookstein shape as *reflection shape*: invariant under translation, rotation, scaling, and reflection.)

In the discussion of [4], D.G. Kendall indicates a connection between Bookstein shape space and a tangent plane to D.G. Kendall shape space. Small [55] compares Bookstein shape with D.G. Kendall shape and suggests that it would be desirable further to delineate the statistical assumptions underlying Bookstein shape for triangles. This paper responds to Small's suggestion by showing how to relate Bookstein triangle shape to a suitable random dynamics for three points on the plane. It thus provides a justification for the underlying hyperbolic geometry in a manner similar to that of (iii) above in the case of D.G. Kendall shape.

The paper is divided into 6 sections: after this introductory section, Section 2 describes how the symbolic Itô calculus of *Itovsn3* can be used to derive Bookstein's shape space geometry from a global stochastic dynamical model. Section 3 continues this theme by using *Itovsn3* to obtain a holomorphic mapping from Bookstein's shape space to D.G. Kendall's shape space. The geometrical setting of Bookstein's shape space is then used in Section 4 to develop asymptotic approximations for the (Brownian) shape-density, resulting in an analogue of the von Mises-Fisher distribution on the sphere. Section 5 sketches an application to estimation of mean shape which demonstrates the amenability of the resulting shape distribution. Section 6 presents a final discussion and indicates possible avenues of future research.

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2 A stochastic calculus model for Bookstein's shape

The main purpose of this paper is to set down the fact that Bookstein's shape space (together with a metric of constant negative curvature) arises naturally from a simple and natural random dynamics induced by a randomly evolving global transformation, and then to indicate how this may be exploited in shape analysis. The underlying strategy is the same as was used to study diffusion of D.G. Kendall shape [31, 32, 34]: compute the characteristics of the shape diffusion in a computationally convenient set of coordinates and then identify the underlying Riemannian metric structure which turns the diffusion into a Riemannian Brownian motion (intuitively speaking, an infinitesimal unbiased random walk with step-size dependent on direction and location) modified by a drift (for an exposition of this see for example [22, §V.4] or [54, §V.34.93]). As in the treatment of D.G. Kendall shape diffusion [31, 32, 34], it is helpful to use computer algebra for *both* these steps: better still a computer algebra implementation of stochastic calculus such as my own *Itovsn3* (at the time of writing implementations of *Itovsn3* are available in the computer algebra packages `REDUCE` [34] and *Mathematica* [35], and others are being developed for `MAPLE` and the innovative new computer algebra system `AXIOM`).

The random global transformation which we will study is the simplest non-trivial random transformation which might be useful for studies in shape theory: the special "Brownian motion on the general linear group $\mathrm{GL}^+(2,\mathbb{R})$" defined in Definition 2.2 below.

First we recall some notation from matrix group theory.

Definition 2.1 *(a)* $\mathrm{GL}(2,\mathbb{R})$ *denotes the group of invertible real* (2×2) *matrices;*

(b) $\mathrm{GL}^+(2,\mathbb{R})$ *denotes the subgroup of* $\mathrm{GL}(2,\mathbb{R})$ *formed by* (2×2) *matrices having positive determinant;*

(c) $(2,\mathbb{R})$ *denotes the subgroup of* $\mathrm{GL}^+(2,\mathbb{R})$ *formed by* (2×2) *matrices having unit determinant;*

(d) $\mathrm{SO}(2)$ *denotes the subgroup of* $(2,\mathbb{R})$ *formed by special orthogonal* (2×2) *matrices.*

Now we use Stratonovich differential calculus formalism to define the required Brownian motion.

Definition 2.2 *A general (right-invariant-) Brownian motion on* $\mathrm{GL}^+(2,\mathbb{R})$ *is a* $\mathrm{GL}^+(2,\mathbb{R})$*-valued diffusion* $G = \{G(t) : t \geq 0\}$ *which satisfies the following Stratonovich stochastic differential equation:*

$$\begin{aligned} d_S\, G &= (d_S\, B)\, G \\ G(0) &= g_0 \end{aligned} \tag{1}$$

where the initial state g_0 *belongs to* $\mathrm{GL}^+(2,\mathbb{R})$ *(a consequence of this is that* G *stays in the* $\mathrm{GL}^+(2,\mathbb{R})$ *component for ever) and* B *is a linear transformation of standard four-dimensional Brownian motion BM*$(\mathbb{R}^4)$*, with coordinates rearranged to form a* (2×2) *matrix. Suppose that the statistics of the vectorized version of the process* B *are those of BM*$(\mathbb{R}^4)$ *itself. Then we say that* G *is a special Brownian motion on* $\mathrm{GL}^+(2,\mathbb{R})$.

This is a natural candidate for a diffusion to underly the theory of Bookstein's triangle shapes. The configuration of three points determined by the matrix g is continually being altered by infinitesimal perturbations acting as linear transformations on the ambient plane.

Note that Equation (1) is right-invariant under the action of $\mathrm{GL}(2,\mathbb{R})$; thus if G is a (perhaps special) Brownian motion on $\mathrm{GL}^+(2,\mathbb{R})$ then so is $G\hat{G}$ for any fixed $\hat{G} \in \mathrm{GL}(2,\mathbb{R})$.

There is an entirely similar definition of Brownian motions and special Brownian motions on $(2,\mathbb{R})$, except that the (2×2) matrix process B is replaced by the traceless process $B - {}^1\!/_2\,\mathrm{trace}(B)\mathbb{I}_2$, for $\mathbb{I}_2$ the (2×2) identity matrix. In fact if G is a special Brownian motion on $\mathrm{GL}(2,\mathbb{R})$ then $G/\sqrt{\det(G)}$ is a special Brownian motion on $(2,\mathbb{R})$. Special Brownian motions on the semi-simple Lie group $(2,\mathbb{R})$ can be related to its Killing form, and are called *canonical Brownian motions* by J.C. Taylor [58].

The following fact is immediate from basic considerations of stochastic calculus: if G is a special Brownian motion on $\mathrm{GL}^+(2,\mathbb{R})$ then so is RG, for any fixed rotation $R \in \mathrm{SO}(2)$. (However this does *not* characterize special Brownian motions amongst Brownian motions on $\mathrm{GL}^+(2,\mathbb{R})$.)

Given that we are interested in shape, hence in rotational invariants of configurations (x_1, x_2, x_3), it is therefore reasonable to consider the random process of shapes induced by (Gx_1, Gx_2, Gx_3) for G a special Brownian motion on $\mathrm{GL}^+(2,\mathbb{R})$. For, by the above fact, the law of the shape of (Gx_1, Gx_2, Gx_3) then depends only on the shape of (x_1, x_2, x_3). We now identify the distribution of this shape process.

Theorem 1 *Consider three landmarks* X_1*,* X_2*,* X_3 *in the Euclidean plane* $\mathbb{R}^2$*. Suppose that they move in the following manner:*

$$X_i(t) = G(t)x_i \tag{2}$$

for a fixed reference configuration (x_1, x_2, x_3)*, where* $\{G(t) : t \geq 0\}$ *is a special Brownian motion on the general linear group* $\mathrm{GL}^+(2,\mathbb{R})$*. To avoid degeneracy, suppose that the reference configuration* (x_1, x_2, x_3) *is affinely independent. Consider the shape* $\sigma(t)$ *of the triad* $\{X_1(t), X_2(t), X_3(t)\}$*, which is to say its* equivalence class *under the equivalence relation determined by ignoring location, scale and rotation. Then* σ *is a diffusion (no time-change necessary!) whose state-space has intrinsic geometry making* σ *into Brownian motion on the* 2*-dimensional hyperbolic plane* $\mathbb{H}(-2)$*, with constant curvature* -2*. Furthermore, geodesic polar coordinates* (r,θ) *of the hyperbolic plane, centred on the shape of* $\{x_1, x_2, x_3\}$*, can be related to the shape* σ via *the* *transformation G as follows:*

$$\begin{aligned}
\det(G)^{-1}G^TG &= \begin{bmatrix} \xi & \zeta \\ \zeta & \eta \end{bmatrix}, \\
\sqrt{2}r &= {}^1\!/_2\text{arccosh}\left({}^1\!/_2(\xi+\eta)^2-1\right) \\
&= {}^1\!/_2\,\text{arccosh}\left({}^1\!/_2(\det(G)^{-1}\,\text{trace}\,G^TG)^2-1\right) \\
&= \log(\lambda_1/\lambda_2)\,, \qquad (3)
\end{aligned}$$

$$\begin{aligned}
{}^1\!/_2\sin\theta &= \frac{\zeta}{\sqrt{(\xi+\eta)^2-4}} = \frac{\zeta}{\sqrt{(\det(G)^{-1}\,\text{trace}\,G^TG)^2-4}} \\
&= \frac{\zeta}{(\lambda_1/\lambda_2-\lambda_2/\lambda_1)}\,. \qquad (4)
\end{aligned}$$

Here $\lambda_1 \geq \lambda_2$ are the non-negative square roots of the eigenvalues of G^TG. We use the non-negative branch of arccosh*.*

Analysis shows that r vanishes exactly when trace $G^TG = 2\det(G)$, which occurs exactly when the two eigenvalues of G^TG coincide. Using the singular-value decomposition, we see that this happens if and only if G is a multiple of a rotation matrix. So the above geodesic polar coordinates are indeed centred on the shape $\{x_1, x_2, x_3\}$.

Note that the shape σ is coordinatized by $\det(G)^{-1}G^TG$ and hence by (r, θ). The angle θ is not continuously defined at $\theta = \pm{}^\pi\!/_2$; however this can be dealt with by rotating the reference shape $\{x_1, x_2, x_3\}$ (corresponding to rotating the coordinate system at twice the speed) and using the overlap of the two charts.

Proof: The main concepts in this proof date back to pioneering work by Dyson [15] on eigenvalues of random matrices and by Dynkin [14] and Orihara [48] on Brownian motion on ellipsoids. This corresponds to the case of special Brownian motion on $\text{GL}(n, \mathbb{R})$. Norris, Rogers and Williams [46] describe a stochastic calculus approach to the n-dimensional situation, and Rogers and Williams [54] give a description specialized to our $n = 2$ case and sketch a relationship to the hyperbolic plane. In the following we indicate the steps of a proof using *Itovsn3* to carry out the stochastic calculus calculations in the REDUCE computer algebra package. Detailed scripts and related software are available on request from the author.

The first step is to check that if G is special Brownian motion on $\text{GL}(2, \mathbb{R})$ then $\tilde{G} = G/\sqrt{\det(G)}$ is special Brownian motion on $(2, \mathbb{R})$. This rather easy exercise is done using *Itovsn3* procedures to introduce the various components of the (2×2) matrix G, REDUCE matrix manipulation to compute the determinant, then *Itovsn3* procedures again to compute the semimartingale characteristics of the entries forming the matrix $G/\sqrt{\det(G)}$.

The second step again uses *Itovsn3* and the matrix algebra capabilities of REDUCE to build $\tilde{G} = G/\sqrt{\det(G)} \in (2, \mathbb{R})$ as a matrix of semimartingales. We then compute ξ and ζ, where as above (ξ, ζ) is the top row of the product $\tilde{G}^T\tilde{G}$ (by the $\det(\tilde{G}) = 1$ condition these two quantities parametrize the shape random process) and use the Gröbner basis algorithms of REDUCE to find convenient re-expressions of their semimartingale characteristics. In passing, to my current knowledge this is the first application of Gröbner basis algorithms in the context of computer algebra in stochastic calculus, though [49] describes their application in parts of applied statistics. For example they allow one to reduce a given polynomial expression using nonlinear polynomial side relations such as the requirement $\det(\tilde{G}) = 1$. As a simple example, the REDUCE command

```
dt*GREDUCE(<<(d xx)*(d yy)>>/dt, {DET(G)=1,x=xx,y=yy}),
```

when applied to expressions `xx`, `yy` representing ξ, η (and `G` representing the corresponding matrix G), yields

```
2*dt*z^2 - 2*dt.
```

Incidentally it is necessary here to divide by `dt` before applying `GREDUCE` to the differential `(d xx)*(d yy)` since `GREDUCE` assumes its first argument has the algebraic properties of a polynomial and therefore will fail if applied to a stochastic differential. (This is because the ring of stochastic differentials has "zero-divisors" arising from the "Itô multiplication rules" $dt^2 = 0$, $dt\,dB = 0$, etc.)

Briefly, the Gröbner basis algorithm shows how to reduce a given multivariate polynomial into the most "elegant" equivalent form, where the equivalence is defined by listing a collection of polynomials which vanish identically (for example $\texttt{DET}(\texttt{G}) - \texttt{1} = \xi\eta - \zeta^2 - 1$ in the above). Here there is no natural notion of "elegance" (except in the univariate case, where one could use the degree of the polynomial) and instead one must choose arbitrarily, using for example an ordering of monomials based on lexicographic ordering within degree. However given this choice the algorithm is well-specified, has been implemented in a wide variety of computer algebra packages, and allows one automatically to reduce a multivariate polynomial in the presence of side-relations. (For further details of the use of Gröbner basis algorithms in computer algebra, see [20, 12, 43].)

As a result we find that ξ and ζ satisfy the stochastic differential equations

$$\begin{aligned}
(d\,\xi)^2 &= 2\xi^2\,dt\,,\\
(d\,\zeta)^2 &= 2(\zeta^2+1)\,dt\,,\\
(d\,\xi)\times(d\,\zeta) &= 2\xi\zeta\,dt\,,\\
\texttt{Drift}\,d\,\xi &= 2\xi\,dt\,,\\
\texttt{Drift}\,d\,\zeta &= 2\zeta\,dt\,.
\end{aligned} \tag{5}$$

Thus the shape process (ξ,ζ) is a diffusion – no time-change is required! It is helpful for later purposes to add in the lower-right entry η of $\tilde{G}^T G$: we have

$$\begin{aligned}
(d\,\eta)^2 &= 2\eta^2\,dt\,,\\
(d\,\xi)\times(d\,\eta) &= 2(\zeta^2-1)\,dt \quad = \quad 2(\eta\xi-2)\,dt\,,\\
(d\,\eta)\times(d\,\zeta) &= 2\eta\zeta\,dt\,,\\
\texttt{Drift}\,d\,\eta &= 2\eta\,dt\,.
\end{aligned} \tag{6}$$

(It turns out to be better still to use the second of the equivalent forms for $(d\,\xi)\times(d\,\eta)$.)

The third step formulates η, ξ, ζ directly as basic semimartingales and computes the intrinsic geometry of the shape diffusion (ξ,ζ). Computing such invariants of Riemannian geometry is involved but routine, and is a facility of *Itovsn3* which can be invoked with a single command:

```
Compute!_Geometry("Bookstein triangle shape",{x,z}).
```

The automatic computation shows that the state-space has intrinsic geometry of constant negative curvature -2. With respect to this geometry the shape diffusion (ξ, ζ) is a Riemannian Brownian motion with no intrinsic drift.

The final step computes geodesic polar coordinates for (ξ, ζ) under this metric, again using *Itovsn3*. The procedure is first to find a homogeneous quadratic w in ξ and ζ such that $(d\,w)^2$ and `Drift` $d\,w$ can be expressed in terms of w alone. Again the Gröbner basis package is of use here as it allows one to identify cleanly the terms which must vanish for the above to be true. One then computes a nonlinear transformation $r = f(w)$ such that $(d\,r)^2 = dt$ (a simple matter of integration) and checks that `Drift` $d\,r$ satisfies the equation required of the radial part of Brownian motion in a space of constant negative curvature -2:

$$\texttt{Drift}\,d\,r \quad = \quad {}^1\!/_2 \left(\sqrt{2}\coth(\sqrt{2}r)\right)\,dt\,. \tag{7}$$

Having found that, one searches for an expression α in ξ and ζ such that $(d\,\alpha)(d\,w) = 0$. A suitable expression is $\zeta/\sqrt{(\xi+\eta)^2-4}$ as given in equation (4): however it was less straightforward to find this as (at least at first glance) it involves ratios of polynomials for which the Gröbner basis algorithm is less accessible.

Finally one finds a nonlinear transformation $\theta = a(\alpha)$ such that `Drift` $d\,\theta = 0$, and checks that $(d\,\theta)^2$ depends on r in the way required of the angular part of Brownian motion in a space of constant negative curvature -2:

$$(d\,\theta)^2 \quad = \quad \frac{2dt}{(\sinh(\sqrt{2}r))^2}\,. \tag{8}$$

The Gröbner basis algorithm has no direct application here, because we have to search for a *ratio* of polynomials. Consequently the desired expression was found in a more *ad hoc* way, by analyzing the spectral decomposition of $G^T G$.

These calculations lead to the equations (3,4) for (r, θ).

These four computer algebra steps constitute the bulk of the proof of the Theorem. It remains only to observe that ξ and ζ can vary so as to cover the whole plane of negative curvature (this follows by checking that all values of (r, θ) can be obtained, subject to the above remarks concerning choice of charts and $\theta = \pm{}^\pi\!/_2$). □

The behaviour of Brownian motion on the hyperbolic plane has been thoroughly studied: in [40, 50] it is established that such Brownian motions (to be precise, Brownian motions on simply-connected manifolds of pinched negative curvature) drift off to infinity at linear rate (so do not reach infinity in finite time!) and settle into (random) limiting directions. Correspondingly the Bookstein shape diffusion discussed above will tend towards a specific collinear shape, but will not reach it in finite time.

3 Relating Bookstein shape to D.G. Kendall shape

We now need to relate the two notions of shape in a way that takes account of the relevant diffusions and their geometry.

First consider the way in which the definitions of D.G. Kendall shape, as given in [26], are expressed in the notation established above. The D.G. Kendall shape for the triad $\{x_1, x_2, x_3\}$ is obtained in terms of

$$u \quad = \quad \frac{x_2 - x_1}{\sqrt{2}}\,, \qquad v \quad = \quad \frac{2x_3 - x_2 - x_1}{\sqrt{6}} \tag{9}$$

(see [26, equation (1)]) as follows. Arrange the two vectors u, v in a (2×2) partitioned matrix as

$$\tilde{w} \quad = \quad [u|v] \tag{10}$$

and normalize to obtain the *pre-shape*

$$w \quad = \quad \frac{\tilde{w}}{\sqrt{\text{trace}\, \tilde{w}^T \tilde{w}}}\,. \tag{11}$$

The D.G. Kendall shape is the equivalence class of w under left-multiplication by $\mathrm{SO}(2)$, and can be parametrized by $w^T w$ and (the sign of) $\det(w)$.

The (procrustean) distance ρ between shapes represented by pre-shapes w and w_0 is given by ([26, equation (23)])

$$\rho(w, w_0) \quad = \quad \arccos\left(\text{trace}\sqrt{w {w_0}^T w_0 w^T} - 2\alpha s\right) \tag{12}$$

where s is the smallest eigenvalue of $\sqrt{w {w_0}^T w_0 w^T}$ and $\alpha = 1$ if $\det(w {w_0}^T)$ is negative, otherwise $\alpha = 0$. It is an easy exercise to show that $\rho(w, w_0)$ depends only on the shapes represented by w, w_0.

Let $U(t)$, $V(t)$, $\tilde{W}(t) = [U(t)|V(t)]$, $W(t) = \tilde{W}(t)/\sqrt{\text{trace}(\tilde{W}(t)^T \tilde{W}(t))}$ be the corresponding quantities for the triad $\{X_1(t), X_2(t), X_3(t)\}$ evolving as in equation (2) above, so $X_i(t) = G(t)x_i$ for G a special Brownian motion on $\mathrm{GL}^+(2,\mathbb{R})$. We can then compare normal polar coordinate systems for the two kinds of shapes: D.G. Kendall shape, $(\rho(W(t), w_0), \phi)$ and Bookstein shape with the normal polar coordinates (r, θ) obtained in equations (3,4) in the previous section.

Remarkably, there turns out to be a holomorphic (that is to say, complex-analytic) correspondence between the two shape structures. To understand this, which is the content of our next theorem, note that the hyperbolic plane $\mathbb{H}(-2)$ can be viewed as a unit disc $\{z \in \mathbb{C} : |z| < 1\}$ in the complex plane (this is the *Poincaré model*) using the map which sends $(s, \theta) \in \{z \in \mathbb{C} : |z| < 1\}$ to $(\log(\frac{1+s}{1-s})/\sqrt{2}, \theta) \in \mathbb{H}(-2)$ (polar coordinates in both cases). This produces a conformal change of metric (from $ds^2 + s^2 d\theta^2$ to $dr^2 + {}^1\!/_2 \sinh(\sqrt{2}r)^2 d\theta^2$) and thus ($a$) maps complex Brownian motion to a time-changed Brownian motion on $\mathbb{H}(-2)$, and (b) furnishes $\mathbb{H}(-2)$ with a complex structure.

Similarly the sphere S^2 can be given a complex structure by mapping it onto the extended complex plane using projection from the north pole onto a plane tangent to the south pole. This also converts Brownian motion on S^2 into a time-changed complex Brownian motion.

Thus it makes sense to ask whether the canonical mapping between the two shape spaces is holomorphic (complex-analytic).

Theorem 2 *Suppose that $W(t)$ is the pre-shape corresponding to the triad $\{X_1(t), X_2(t), X_3(t)\}$ as described above. Let $(\rho(W(t), w), \phi(W(t)))$ be normal polar coordinates for D.G. Kendall shape, centred at an equilateral triangle pre-shape w with positive $\det(w)$. Suppose further that $(r(W(t)), \theta(W(t)))$ is normal polar coordinates for Bookstein shape as given in the previous section in equation (3,4), based on an equilateral triangle $\{x_1, x_2, x_3\}$. The two systems of coordinates are connected by the equations*

$$\begin{aligned} \phi \quad &= \quad \theta + \text{constant}\,, \\ \sin(2\rho) \quad &= \quad \tanh(\sqrt{2}r)\,. \end{aligned} \tag{13}$$

Moreover this correspondence gives a holomorphic diffeomorphism between Bookstein's hyperbolic shape space and the upper hemisphere of D.G. Kendall's shape space Σ_2^3: the Bookstein shape diffusion is carried by this diffeomorphism into the D.G. Kendall shape diffusion (described in (iii) in Section 1) subject to a random time-change given by

$$d\tilde{\tau} \quad = \quad \frac{dt}{2\cosh(\sqrt{2}r)^2}\,. \tag{14}$$

Proof: We deal first with the angles θ and ϕ. If $G(t)$ is the general linear transformation sending $\{x_1, x_2, x_3\}$ into $\{X_1(t), X_2(t), X_3(t)\}$ then linearity shows that

$$\tilde{W}(t) \quad = \quad [U(t)|V(t)] \quad = \quad G(t)[u|v] \quad = \quad G(t)\tilde{w}\,.$$

Consequently the pre-shape $W(t)$ is given by

$$W(t) \quad = \quad \frac{G(t)\tilde{w}}{\sqrt{\text{trace}\,(G(t)\tilde{w})^T G(t)\tilde{w}}} \quad = \quad \frac{G(t)}{\sqrt{\text{trace}\,G(t)^T G(t)}} \tag{15}$$

where we have used the fact that $\tilde{w}$ is proportional to a rotation matrix, so that ww^T is a multiple of the identity matrix.

Since in addition we know $G(t) \in \text{GL}^+(2,\mathbb{R})$ it therefore follows that $\det(W(t))$ is always positive. Consequently the D.G. Kendall shape is parametrized by the expression $G(t)^T G(t)/\text{trace}\,G(t)^T G(t)$. Now the conjugation action of SO(2) isometries on this matrix is exactly the same as in the Bookstein parametrization $G(t)^T G(t)/\det(G(t))$. It follows by symmetry arguments that angular coordinates ϕ, θ differ only by a constant.

We have seen in equation (3) that the radial distance r is related to the eigenvalues $\lambda_1^2 \geq \lambda_2^2$ of $G(t)^T G(t)$ by

$$\begin{aligned} \sqrt{2}r \quad &= \quad {}^1\!/\!{}_2\,\text{arccosh}\Big(\frac{(\lambda_1/\lambda_2 + \lambda_2/\lambda_1)^2}{2} - 1\Big) \\ &= \quad \log(\lambda_1/\lambda_2)\,. \end{aligned} \tag{16}$$

On the other hand the radial distance ρ is related to the eigenvalues $\lambda_1^2 \geq \lambda_2^2$ of $G(t)^T G(t)$ by

$$\begin{aligned} \cos\rho(W(t), w) \quad &= \quad \text{trace}\,\sqrt{W(t)w^T w W(t)^T} \\ &= \quad \frac{\lambda_1 + \lambda_2}{\sqrt{2}\sqrt{\lambda_1^2 + \lambda_2^2}} \\ &= \quad \frac{\lambda_1/\lambda_2 + 1}{\sqrt{2}\sqrt{(\lambda_1/\lambda_2)^2 + 1}} \end{aligned} \tag{17}$$

where the first step follows from equation (12) because the relevant determinant is positive for all time t, and the second because the equilateral shape w is $\mathbb{I}_2/\sqrt{2}$. Elementary trigonometry now shows that

$$\sin(2\rho) \quad = \quad \frac{(\lambda_1/\lambda_2)^2 - 1}{(\lambda_1/\lambda_2)^2 + 1}\,. \tag{18}$$

It follows directly from equations (16), (18) that $\sin(2\rho) = \tanh(\sqrt{2}r)$ as required.

Finally we have to check that the correspondence is holomorphic, and we have to compute the time-change involved. Again *Itovsn3* is useful here. To prove the correspondence to be holomorphic, it suffices to consider the complex semimartingale obtained by mapping the Bookstein shape diffusion to the sphere and then to the complex plane by projection from the north pole to a plane tangent to the south pole. This semimartingale is given by

$$Z \quad = \quad {}^1\!/_2 \exp(i\theta) \coth(r/\sqrt{2})\,. \tag{19}$$

Both $\texttt{Drift}\, dZ$ and $\texttt{Drift}\, d(Z^2)$ vanish, so Z is a conformal martingale (see [52]). This means the corresponding map from Bookstein hyperbolic shape space to the complex plane is either holomorphic or anti-holomorphic. A check of the orientation shows it is holomorphic. Since the projection from the sphere to the plane is a holomorphic diffeomorphism (except for the singular point at the north pole) we see that the correspondence between Bookstein and D.G. Kendall shape spaces is holomorphic, as required.

Finally, Lévy's celebrated theorem tells us that holomorphic images of complex Brownian motion are time-changed complex Brownian motions. (This is usually stated for the complex plane, see [52], but applies equally to two-dimensional hyperbolic planes.) It remains only to compute the time-change, which can be done in *Itovsn3* by the formula

$$d\tilde{\tau} \quad = \quad (d\rho)^2/dt \tag{20}$$

and gives the required result. □

As far as I know the above is the first example of the use of computer algebra to perform *complex* symbolic Itô calculus. Interest also attaches to the way in which stochastic calculus is used as a computational tool to find out about the map from Bookstein to D.G. Kendall shape space.

Note that a calculation (which is rather laborious even when making careful use of *Itovsn3*) shows that the above result does not hold at the level of pre-shapes. That is to say, the Bookstein pre-shape diffusion $W(t)$ is *not* a random time-change of the D.G. Kendall pre-shape diffusion (which is Brownian motion on the unit 3-sphere). This can be seen by computing the characteristics of the semimartingale S which is the distance of $W(t)$ from a specified point: we find

$$\frac{\texttt{Drift}\, S}{(dS)^2} \quad \neq \quad \cot(S)\,;$$

were S to be a time-change of 3-sphere Brownian motion then we would have equality.

4 Asymptotic approximations for the shape-density

It is natural to ask whether there is a useful analogue of the Mardia-Dryden distribution [45], which is a closed-form expression for the density of the *D.G. Kendall* shape formed by the independent Brownian points (started at different locations) after a fixed time t. In our context this resolves to the query, whether there is a useful form for the Brownian probability transition kernel (equivalently, the heat density kernel) on the hyperbolic plane. Unfortunately there is no expression in terms of familiar functions: explicit expressions typically involve at least an integral which cannot be evaluated in closed form, such as

$$p_t(x,y) \quad = \quad \frac{e^{-t/4}}{(2\pi t)^{3/2}} \int_{\mathrm{dist}(x,y)}^{\infty} \frac{\psi\ \exp(-\psi^2/(2t))}{\sqrt{\cosh(\sqrt{2}\psi) - \cosh(\sqrt{2}\,\mathrm{dist}(x,y))}}\, d\psi$$

(this is the case of curvature -2: it can be obtained using a rescaling argument from for example [19, 57] for the case of curvature -1, or [11, page 246] for the heat kernel form). Frustratingly, there *is* a closed form for the transition kernel for hyperbolic space of dimension 3 (and all odd dimensions), but this is of no use to us here.

However for the purposes of statistical shape theory it is sufficient to find an amenable asymptotic form for the low-dispersion case, and this *is* available. A start is made by considering the Minakshisundaram-Pleijel recursion formulae for a series solution to the heat kernel for a general Riemannian manifold (see for example [11, page 148]). We illustrate the computational power of the *Itovsn3* machinery by indicating how these recursion formulae may be computed using *Itovsn3*.

Define R the radial part of Brownian motion on the hyperbolic plane of curvature -2. This is determined by the requirements

$$\begin{aligned} (dR)^2 \quad &= \quad dt\,, \\ \texttt{Drift}\, dR \quad &= \quad {}^1\!/\!_2 \sqrt{2}\coth(\sqrt{2}R)\, dt \end{aligned} \tag{21}$$

(compare the discussion around Equation (7)). If $p_t(r) = p_t(x,y)$ is the Brownian transition kernel between two points x and y with $r = \mathrm{dist}(x,y)$, then a backwards differential equation argument shows that $p_{T-t}(R_t)$ is a martingale. The idea is to search for an expression of $p_t(r)$ as a small-time perturbation of the Euclidean Brownian transition kernel:

$$p_t(r) \quad = \quad \frac{1}{2\pi t}\exp\left(-\frac{r^2}{2t}\right) \times \sum_j t^j u_j(r) \tag{22}$$

for appropriate functions u_j. Following the thought that the drift of an approximation to $p_{T-t}(R_t)$ should be small for small $T-t$, we require that

$$\begin{aligned} &\texttt{Drift}\left(\frac{1}{2\pi(T-t)}\exp\left(-\frac{R_t^2}{2(T-t)}\right) \times \sum_{j=0}^{N}(T-t)^j u_j(R_t)\right) \\ &\quad = \quad \frac{1}{2\pi t}\exp\left(-\frac{R_t^2}{2(T-t)}\right)(T-t)^N \times \Big(\texttt{Drift}\, u_N(R_t)\Big) \end{aligned} \tag{23}$$

together with the initial condition $u_0(0) = 1$.

These equations resolve into a recursive sequence of *ordinary* differential equations for the u_j (since the second-order derivatives of u_N cancel), which can then be solved using integrating factors. Using an *Itovsn3* script to implement the above, and to solve the resulting differential equations, in the case of the hyperbolic plane the initial approximation turns out to be

$$p_t^{(0)}(r) \quad = \quad \frac{1}{2\pi t}\exp\left(-\frac{r^2}{2t}\right)u_0(r) \quad = \quad \frac{1}{2\pi t}\sqrt{\frac{\sqrt{2}r}{\sinh(\sqrt{2}r)}}\exp\left(-\frac{r^2}{2t}\right) \tag{24}$$

(higher-order expressions are much less tidy!).

This is of course a well-known computation: see for example the reference in [19, page 59] where the above (for the case of curvature -1) is presented as the asymptotic formula for the transition kernel when r is held fixed and $t \to 0$: and this is the low-dispersion asymptotics which we require.

Of course this asymptotic form is still not very convenient, since it produces a family of probability densities

$$\left\{ p_t^{(0)}(\text{dist}(x,y)) \;:\; y \text{ a point in the hyperbolic plane} \right\} \tag{25}$$

which is not an exponential family. We can improve matters a little by considering the simplification which occurs if $t \to 0$ while $\text{dist}(x,y)^2/t = r^2/t$ is bounded, which yields the well-known transition kernel asymptotics for Brownian motion on a two-dimensional manifold:

$$p_t(x,y) \quad \sim \quad \frac{1}{2\pi t} \exp\left(-\frac{\text{dist}(x,y)^2}{2t} \right) . \tag{26}$$

However a more amenable approximation for this regime arises if we note that

$$\text{dist}(x,y)^2/(2t) \quad \sim \quad (\cosh(\sqrt{2}\,\text{dist}(x,y)) - 1)/(2t) \,, \tag{27}$$

since we obtain

$$p_t(x,y) \quad \sim \quad q_t(x,y) \quad = \quad \frac{1}{2\pi t} \exp\left(-\frac{\cosh(\sqrt{2}\,\text{dist}(x,y)) - 1}{2t} \right) . \tag{28}$$

In polar coordinates the area element for the hyperbolic plane of curvature -2 is

$$\frac{\sinh(\sqrt{2}r)}{\sqrt{2}} \; dr \, d\theta \, .$$

Since $q_t(\cdot, y)$ integrates to unit total mass against this area element it is an exact probability density (contrast the asymptotic form for $p_t(x,y)$ given by (26), which does *not* integrate to unity against the hyperbolic area element). In the next section we explain why this is a more amenable approximation, and why in particular $\{q_t(x,y) : y \text{ a point in the hyperbolic plane}\}$ is an exponential family.

5 Application to the statistics of shape

To clarify applications to the statistics of shape, we need a special representation of hyperbolic space known as the *hyperboloid model*, or the *Beltrami model*. The following summary is derived from the description in [18, Ch. V Section 1.1], though the ideas are common currency in textbooks on geometry (see for example [51, Part III]). The initial discussion is carried through for the case of general n, as nothing is to be gained from specializing to the hyperbolic plane.

The hyperboloid model for n-dimensional hyperbolic space is based on the locus $\mathcal{H}$ in $\mathbb{R} \oplus \mathbb{R}^n$ of $Q(x,x) = 1$, where $Q(x,y)$ is the indefinite inner product

$$Q(x,y) \quad = \quad x_0 y_0 - \langle x_+, y_+ \rangle \tag{29}$$

and $x = (x_0, x_+)$, $y = (y_0, y_+)$ are decompositions conforming to the splitting $\mathbb{R} \oplus \mathbb{R}^n$. The geometrical structure of $\mathcal{H}$ is largely determined by the specification that its symmetry group be the group $\mathcal{G}$ of all invertible $(n+1) \times (n+1)$ matrices preserving the inner product Q. Clearly rotations of the R^n coordinate belong to $\mathcal{G}$: so do matrices such as

$$\begin{bmatrix} \begin{matrix} \cosh(u), & \sinh(u) \\ \sinh(u), & \cosh(u) \end{matrix} & 0 \\ 0, & \mathbb{I} \end{bmatrix}$$

(where $\mathbb{I}$ is the $(n-1) \times (n-1)$ identity matrix).

It is an exercise to show that if $Q(x, x) = Q(y, y) = 1$, so both x and y lie in $\mathcal{H}$, then

$$\cosh(\sqrt{2}\rho(x, y)) \quad = \quad x_0 y_0 - \langle x_+, y_+ \rangle \tag{30}$$

defines a metric $\rho(x, y)$ on $\mathcal{H}$ which is $\mathcal{G}$-invariant. We insert the $\sqrt{2}$ because computation then shows that this metric turns $\mathcal{H}$ into the hyperbolic space of curvature -2. This is most easily seen by considering polar coordinates: in dimension $n = 2$ the key calculation is

$$\begin{aligned} x &= (\cosh(\sqrt{2}r), \sinh(\sqrt{2}r), 0)\,, \\ y &= (\cosh(\sqrt{2}r), \cos(\theta)\sinh(\sqrt{2}r), \sin(\theta)\sinh(\sqrt{2}r))\,. \end{aligned} \tag{31}$$

For small θ the distance ρ between x and y is given by

$$\cosh(\sqrt{2}\rho) \quad = \quad \cosh^2(\sqrt{2}r) - \cos(\theta)\sinh^2(\sqrt{2}r)$$

and this delivers an induced Riemannian metric

$$d\rho^2 \quad = \quad dr^2 + \frac{\sinh^2(\sqrt{2}r)}{2}\, d\theta^2\,. \tag{32}$$

Integration recovers the original metric, which is thus identified as the Riemannian metric as required. Alternatively one can apply the hyperbolic cosine formula [51, Part III].

The family of densities identified in the previous section can now be written in the hyperboloid representation as

$$q_t(x, y) \quad = \quad \frac{1}{2\pi t} \exp\left(-\frac{x_0 y_0 - x_1 y_1 - x_2 y_2 - 1}{2t} \right) \tag{33}$$

so clearly is an exponential family of densities in the hyperbolic plane. (Notice that Equation (31) for the coordinates of y, together with r and θ as determined by Equation (3,4) in Theorem 1, allow us to pass between the hyperboloid model and the matrix model for Bookstein shape space.) If $X^{(1)}, \ldots, X^{(k)}$ are independently distributed as $q_t(\cdot, y)$ for some fixed t and y then a set of sufficient statistics for y is given by $\sum_i X_0^{(i)}, \sum_i X_1^{(i)}, \sum_i X_2^{(i)} = \sum_i \sqrt{(1 - (X_1^{(i)})^2 + (X_2^{(i)})^2)}$.

Indeed it is now clear that $q_t(\cdot, y)$ is the hyperbolic analogue of the von Mises-Fisher density on the sphere, which is used in directional statistics ([44, page 232]: see also [53]) and in statistical shape theory as a convenient proxy for a Brownian or Brownian-derived transition density [45]. The statistical properties of this hyperbolic von Mises-Fisher distribution have been studied in detail in [23]: here we summarize some basic aspects.

The densities $q_t(\cdot, y)$ provide particularly amenable likelihoods. Suppose for example we observe k shapes $X^{(1)}, \ldots, X^{(k)}$, drawn independently from the shape density $q_t(\cdot, y)$, for unknown "mean shape" y and unknown but shared dispersion parameter t. The maximum likelihood estimate for y is obtained by maximizing

$$L(y : X^{(1)}, \ldots, X^{(k)}) \quad = \quad \prod_{i=1}^{k} \frac{1}{2\pi t} \exp\left(-\frac{Q(X^{(i)}, y) - 1}{2t}\right) \tag{34}$$

(where we view $X^{(i)}$, y as points in the hyperboloid representation above) and this is equivalent to minimizing

$$\sum_{i=1}^{k} Q(X^{(i)}, y)\,. \tag{35}$$

Exploiting the invariance under the group $\mathcal{G}$, we may rotate the configuration $X^{(1)}$, $\ldots, X^{(k)}$ by a $\mathcal{G}$-matrix M so that the Euclidean mean of the configuration is located on the x_0-axis, that is to say $\sum_{i=1}^{k} X_+^{(i)} = 0$. But the linearity of $Q(\cdot, y)$ then implies that the above quantity (35) is given by

$$\sum_{i=1}^{k} Q(X^{(i)}, y) \quad = \quad \sum_{i=1}^{k} \left(X_0^{(i)} y_0 \; - \; X_+^{(i)} y_+\right) \quad = \quad \left(\sum_{i=1}^{k} X_0^{(i)}\right) y_0$$

and is therefore minimized (uniquely) at $y = (1, 0, 0)^T$. Hence the maximum likelihood estimate for y is given by $M^{-1}(1, 0, 0)^T$, where M is the symmetry above. Thus maximum likelihood estimates can be calculated exactly: in fact the maximum-likelihood estimator estimate for $y = (y_0, y_1, y_2)$ is simply that normalization of the sample mean of the X-vectors which lies on the hyperboloid:

$$\hat{y} \quad = \quad \frac{\left(\sum_i X_0^{(i)}, \sum_i X_1^{(i)}, \sum_i X_2^{(i)}\right)}{\sqrt{(\sum_i X_0^{(i)})^2 - (\sum_i X_1^{(i)})^2 - (\sum_i X_2^{(i)})^2}}\,. \tag{36}$$

Note that the term inside the square root is positive (unless the X-vectors all agree, when it is zero; but then inference on y is unnecessary!) because of convexity of the hyperboloid.

We should however note the less desirable feature, that the approximation of $p_t(x, y)$ by $q_t(x, y)$ leads to greater sensitivity to outliers (since r^2 in the exponential is replaced by $\cosh(\sqrt{2}r)$). If this is felt undesirable then $\hat{y}$ can be used as an initial value for an iterative algorithm using a likelihood based on the first-order Minakshisundaram-Pleijel approximation (24). For this we also need an initial estimate for t (since we can no longer estimate y and t separately): simple algebra shows the estimate of t based on the exponential family (33) is given by

$$\hat{t} \quad = \quad {}^1\!/\!_2 \left(1 - \frac{1}{k}\sqrt{(\sum_i X_0^{(i)})^2 - (\sum_i X_1^{(i)})^2 - (\sum_i X_2^{(i)})^2}\right) \tag{37}$$

and this could serve as an initial estimate for iterative work. However for many purposes it may be preferable to work directly with the statistical model (33), because of its greater simplicity.

The exponential family approach is closely related to the treatment of mean values for D.G. Kendall shape spaces in [42]: the above procedure actually finds the unique minimizer y of

$$^1/_2 \int \cosh(\sqrt{2}\,\text{dist}(x, y))\, \mu(dx) \tag{38}$$

for μ a measure placing mass $1/k$ on each of $x^{(1)}, \ldots, x^{(k)}$. The corresponding problem for D.G. Kendall shape space Σ^3_2 seeks to minimize

$$^1/_2 \int \cos(2\,\text{dist}(x, y))\, \mu(dx) \tag{39}$$

and has a similar closed-form solution (but note that (a) the solution is no longer unique, though for Σ^3_2 it is easy to show that there is just one minimizing solution for μ not concentrated on an equator [33, §9] (and the case of Σ^m_2 is described in [38, 37]), and (b) the work of [42] deals with general shape spaces of several points in many dimensions, which is beyond the current scope of our approach). Indeed from the approximation (26) it is clear that for small dispersion t the minimizers (38), (39) are similar, which of course we would expect on geometric grounds (see also comment 2 of [37, §10.2.7]). Arguments from hyperbolic geometry make it clear that, for figures with a tendency towards collinearity, the Bookstein-space estimator based on (38) will be more "equilateral" than the D.G. Kendall-estimator based on (39): it would be most interesting to see how this works out for real data.

The general idea of finding Riemannian centres of mass goes back to Cartan [10] and Fréchet [17]; a detailed geometrical study is to be found in [24], while other applications to statistics, probability and stochastic analysis can be found for example in [16, 59, 32, 36, 47].

6 Conclusions

Theorem 1 mirrors the connection of D.G. Kendall shape to Euclidean Brownian motion, both in its statement and also in the proof by computer algebra. Various questions and observations present themselves, to suggest future directions for research.

- There is a similarity between this derivation of hyperbolic geometry for Bookstein shape space and justification (ii) for the geometry of D.G. Kendall shape space. In fact the stochastic calculus aspects of the above argument can be peeled away, so that for example Theorem 2 can be viewed as a special case of the holomorphic realization (well-known to differential geometers) of a non-compact Hermitian symmetric space as an open subset of its compact dual. See [21, chapter 8]. (I am grateful to Fran Burstall for pointing me to this reference!)

- It is noteworthy that it is unnecessary to time-change out the effect of size. Because we work in $\text{GL}(2, \mathbb{R})$ and $(2, \mathbb{R})$ it is to be expected that any time-change would be based on area rather than sum-of-squared-sides: however the need for a time-change is eliminated by the multiplicative nature of the noise term in the basic stochastic differential system (1). Of course there is a time-change required when moving from Bookstein hyperbolic shape space to D.G. Kendall shape space, but this is not based on size.

- Theorem 2 shows that there is another dynamical context for Bookstein shape. It can arise when the three points are moving independently by identical Brownian motions or by identical Ornstein-Uhlenbeck processes, but are subject to a time-change based on intrinsic shearing derived from equation (14). The resulting shape process can be turned into the Bookstein shape diffusion by a size-based time-change. However this construction is far less natural than the one described in Section 2. Moreover calculations concerning pre-shapes, reported at the end of Section 3, show that the underlying time-change does not relate the two constructions at the pre-shape level.

- For applications the significant question is, whether it is possible to generalize this to (for example) the case of $k > 3$ points on the plane? Clearly there is no simple generalization, both because the $\mathrm{GL}(2, \mathbb{R})$-action would then degenerate and because Bookstein's treatment of shape differentiates between the linear part (essentially as described above) and the non-linear part, which is dealt with using thin-plate spline theory. It is possible a clue may be found in recent work by Kent and Mardia [39], and this will be followed up, as will an alternative approach described by Small and Lewis [57], where again one has to differentiate between two different kinds of shape-change (deviation from conformality and nonhomogeneous scaling). A good prospect for progress is to replace the global random transformation by a randomly evolving diffeomorphism. Fortunately there is already a strong theoretical framework for such entities: see for example Baxendale's work [2, 3].

- It is also natural to ask what the above approach offers for the case of shapes of landmarks in higher dimensional space, particularly 3-space. Small has studied the geometry of the natural generalization of Bookstein's shape to the case of $m + 1$ points in m-space [56, §3.6]; unfortunately this geometry is less pleasant if $m > 2$ and in particular does not have constant curvature (work of HuiLing Le noted in [56, §3.8]). In principle the computer algebra and stochastic calculus approach described above will extend, and this will be followed up in future work; however it is clear the answer will not be so simple.

- In conclusion, some particular questions are raised by the part played by computer algebra in the above investigation. As with the earliest application [31] of computer algebra in this field, the computations are straightforward enough that they can be undertaken by hand without much difficulty (except for rather excruciating calculations to check that there is not a time-change relating Bookstein and D.G. Kendall pre-shape diffusions). However the general features (particularly the application of Gröbner bases) can be expected to carry through to much more demanding problems. This has certainly happened with the earliest application, the techniques of which recently led to a success in the theory of coupling of random processes [1] which would definitely not have been susceptible to efforts without the help of computer algebra. The intervention of the Gröbner basis algorithm raises the intriguing challenge of systematizing its application in this sort of problem in stochastic calculus.

  It has already been noted that a novel part of this work is the use of *Itovsn3* to deal with complex-valued semimartingales, in particular to establish the holomorphic nature of the correspondence between the two shape spaces. The symbolic Itô calculus environment makes this calculation delightfully easy!

The above work has also turned up a requirement to be able to specify matrix- or vector-valued semimartingale diffusions within *Itovsn3* simply by declaring their defining system of stochastic differential equations. A facility to do this already exists for scalar semimartingale diffusions: the appropriate extension will be provided in the planned AXIOM implementation, as the innovative object-oriented and category-theoretic features of AXIOM are ideally suited for such requirements.

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