Advances in Computational Mathematics **17:** 369–383, 2002.

Hermite interpolation by rotation-invariant spatial Pythagorean-hodograph curves

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Received 28 September 2001; accepted 3 December 2001
Communicated by C.A. Micchelli

The interpolation of first-order Hermite data by spatial Pythagorean-hodograph curves that exhibit closure under arbitrary 3-dimensional rotations is addressed. The hodographs of such curves correspond to certain combinations of four polynomials, given by Dietz et al. [4], that admit compact descriptions in terms of quaternions – an instance of the "PH representation map" proposed by Choi et al. [2]. The lowest-order PH curves that interpolate arbitrary first-order spatial Hermite data are quintics. It is shown that, with PH quintics, the quaternion representation yields a reduction of the Hermite interpolation problem to three "simple" quadratic equations in three quaternion unknowns. This system admits a closed-form solution, expressing all PH quintic interpolants to given spatial Hermite data as a two-parameter family. An integral shape measure is invoked to fix these two free parameters.

Keywords: Pythagorean-hodograph curves, Hermite interpolation, quaternions

1. Introduction

Pythagorean-hodograph (PH) space curves are polynomial parametric curves $\mathbf{r}(t) = (x(t), y(t), z(t))$ with the distinguishing property that their derivatives or *hodographs* $\mathbf{r}'(t) = (x'(t), y'(t), z'(t))$ satisfy the Pythagorean condition

$$x'^2(t) + y'^2(t) + z'^2(t) = \sigma^2(t), \tag{1}$$

where $\sigma(t)$ is a polynomial. This feature ensures that PH space curves admit *exact* measurement of arc length – a fact that is especially advantageous in the formulation of real-time interpolators to drive multi-axis CNC machines along curved paths at fixed or variable feedrates [9,12,17].

The formulation of algorithms to construct and manipulate PH curves is a basic necessity for their adoption in design and manufacturing applications. Hermite interpolation – i.e., the construction of smooth curve segments that match given end points and derivatives – is a common approach to satisfying this requirement. The first-order Hermite interpolation problem for *planar* PH quintics has been thoroughly studied [10,15] using the complex-variable model [5], which greatly facilitates both the construction and shape analysis of interpolants. The extension to C^2 PH splines interpolating a sequence of points is described in [1,8] and Jüttler [13] has also studied the interpolation of second-order "geometric" Hermite data by planar PH curves.

Spatial PH curves were first investigated in [11], using the form

$$\begin{aligned} x'(t) &= u^2(t) - v^2(t) - w^2(t), \\ y'(t) &= 2u(t)v(t), \\ z'(t) &= 2u(t)w(t), \\ \sigma(t) &= u^2(t) + v^2(t) + w^2(t), \end{aligned} \tag{2}$$

in terms of *three* polynomials $u(t)$, $v(t)$, $w(t)$ as a sufficient condition for the satisfaction of (1). Solutions of the Hermite interpolation problem, in terms of these curves, were also presented in [11] – as with the planar case, there are four solutions, among which the "good" interpolant must be identified by means of various shape measures. As only a *sufficient* condition for a spatial Pythagorean hodograph, however, the form (2) has a fundamental defect – it is not invariant under arbitrary 3-dimensional rotations.

A sufficient-and-necessary condition for satisfaction of (1) was identified by Dietz et al. [4] – namely, the hodograph components must be expressible in terms of *four* polynomials $u(t)$, $v(t)$, $p(t)$, $q(t)$ in the form

$$\begin{aligned} x'(t) &= u^2(t) + v^2(t) - p^2(t) - q^2(t), \\ y'(t) &= 2\big[u(t)q(t) + v(t)p(t)\big], \\ z'(t) &= 2\big[v(t)q(t) - u(t)p(t)\big], \\ \sigma(t) &= u^2(t) + v^2(t) + p^2(t) + q^2(t). \end{aligned} \tag{3}$$

Subsequently, Choi et al. [2] gave an elegant characterization of this form in terms of quaternions. This interpretation is invaluable in demonstrating [7] the rotation-invariance of (3) – namely, given a hodograph $\mathbf{r}'(t)$ defined by (3) and the axis $\mathbf{n}$ and angle θ of a spatial rotation, we can obtain four new polynomials $\tilde{u}(t)$, $\tilde{v}(t)$, $\tilde{p}(t)$, $\tilde{q}(t)$ that define the rotated hodograph $\tilde{\mathbf{r}}'(t)$.

Our present goal is to solve the Hermite interpolation problem using the quaternion representation for spatial PH curves with hodographs of the form (3). We shall find that, as with the complex-variable model for planar PH curves, this more sophisticated representation greatly facilitates the solution procedure and analysis of the resulting interpolants. Our plan is as follows. In section 2 we formulate the first-order Hermite interpolation for PH quintic space curves in scalar form. We then proceed to the quaternion formulation in section 3, where we solve the problem of characterizing the set of spatial rotations that map one unit vector into another, and apply this solution to the construction of spatial PH quintic Hermite interpolants. The question of the rotation invariance of these interpolants is then addressed in section 4. In section 5 we consider the treatment of certain degrees of freedom that arise in the solution and present some examples. Finally, section 6 summarizes our present results and make some concluding remarks.

2. Hermite interpolation

To define a PH quintic, we insert quadratic Bernstein–form polynomials

$$\begin{aligned}
u(t) &= u_0(1-t)^2 + u_1 2(1-t)t + u_2 t^2,\\
v(t) &= v_0(1-t)^2 + v_1 2(1-t)t + v_2 t^2,\\
p(t) &= p_0(1-t)^2 + p_1 2(1-t)t + p_2 t^2,\\
q(t) &= q_0(1-t)^2 + q_1 2(1-t)t + q_2 t^2,
\end{aligned}$$

into (3) and integrate. If the resulting curve is expressed in Bézier form

$$\mathbf{r}(t) = \sum_{k=0}^{5} \mathbf{p}_k \binom{5}{k} (1-t)^{5-k} t^k, \tag{4}$$

with $\mathbf{p}_0 = (x_0, y_0, z_0)$ being an arbitrary integration constant, the remaining control points $\mathbf{p}_k = (x_k, y_k, z_k)$ for $k = 1, \ldots, 5$ are given by the expressions

$$\begin{aligned}
x_1 &= x_0 + \frac{1}{5}\bigl(u_0^2 + v_0^2 - p_0^2 - q_0^2\bigr),\\
x_2 &= x_1 + \frac{1}{5}(u_0u_1 + v_0v_1 - p_0p_1 - q_0q_1),\\
x_3 &= x_2 + \frac{1}{15}\bigl(2u_1^2 + u_0u_2 + 2v_1^2 + v_0v_2 - 2p_1^2 - p_0p_2 - 2q_1^2 - q_0q_2\bigr),\\
x_4 &= x_3 + \frac{1}{5}(u_1u_2 + v_1v_2 - p_1p_2 - q_1q_2),\\
x_5 &= x_4 + \frac{1}{5}\bigl(u_2^2 + v_2^2 - p_2^2 - q_2^2\bigr),
\end{aligned} \tag{5}$$

$$\begin{aligned}
y_1 &= y_0 + \frac{2}{5}(u_0q_0 + v_0p_0),\\
y_2 &= y_1 + \frac{1}{5}(u_0q_1 + u_1q_0 + v_0p_1 + v_1p_0),\\
y_3 &= y_2 + \frac{1}{15}(u_0q_2 + 4u_1q_1 + u_2q_0 + v_0p_2 + 4v_1p_1 + v_2p_0),\\
y_4 &= y_3 + \frac{1}{5}(u_1q_2 + u_2q_1 + v_1p_2 + v_2p_1),\\
y_5 &= y_4 + \frac{2}{5}(u_2q_2 + v_2p_2),
\end{aligned} \tag{6}$$

$$z_1 = z_0 + \frac{2}{5}(v_0q_0 - u_0p_0),$$

$$
\begin{aligned}
z_2 &= z_1 + \frac{1}{5}(v_0 q_1 + v_1 q_0 - u_0 p_1 - u_1 p_0),\\
z_3 &= z_2 + \frac{1}{15}(v_0 q_2 + 4v_1 q_1 + v_2 q_0 - u_0 p_2 - 4u_1 p_1 - u_2 p_0),\\
z_4 &= z_3 + \frac{1}{5}(v_1 q_2 + v_2 q_1 - u_1 p_2 - u_2 p_1),\\
z_5 &= z_4 + \frac{2}{5}(v_2 q_2 - u_2 p_2).
\end{aligned}
\tag{7}
$$

In general, the spatial PH quintic defined by (5)–(7) can satisfy 15 (scalar) interpolation conditions, since it is defined by 15 variables – the coefficients of $u(t)$, $v(t)$, $p(t)$, $q(t)$ and the initial point $\mathbf{p}_0 = (x_0, y_0, z_0)$. We consider the interpolation of Hermite data of the form

$$
\mathbf{p}_\mathrm{i} = \mathbf{r}(0), \qquad \mathbf{d}_\mathrm{i} = \mathbf{r}'(0) \quad \text{and} \quad \mathbf{p}_\mathrm{f} = \mathbf{r}(1), \qquad \mathbf{d}_\mathrm{f} = \mathbf{r}'(1),
$$

i.e., initial and final points and derivatives, $\mathbf{p}_\mathrm{i} = (x_\mathrm{i}, y_\mathrm{i}, z_\mathrm{i})$, $\mathbf{d}_\mathrm{i} = (d_{\mathrm{i}x}, d_{\mathrm{i}y}, d_{\mathrm{i}z})$ and $\mathbf{p}_\mathrm{f} = (x_\mathrm{f}, y_\mathrm{f}, z_\mathrm{f})$, $\mathbf{d}_\mathrm{f} = (d_{\mathrm{f}x}, d_{\mathrm{f}y}, d_{\mathrm{f}z})$. Interpolating the initial and final derivatives gives the systems of equations

$$
\begin{aligned}
u_0^2 + v_0^2 - p_0^2 - q_0^2 &= d_{\mathrm{i}x},\\
2(u_0 q_0 + v_0 p_0) &= d_{\mathrm{i}y},\\
2(v_0 q_0 - u_0 p_0) &= d_{\mathrm{i}z},
\end{aligned}
\tag{8}
$$

$$
\begin{aligned}
u_2^2 + v_2^2 - p_2^2 - q_2^2 &= d_{\mathrm{f}x},\\
2(u_2 q_2 + v_2 p_2) &= d_{\mathrm{f}y},\\
2(v_2 q_2 - u_2 p_2) &= d_{\mathrm{f}z}.
\end{aligned}
\tag{9}
$$

Furthermore, integrating the hodograph from $t = 0$ to $t = 1$ gives

$$
\begin{aligned}
&3(u_0 u_1 + v_0 v_1 - p_0 p_1 - q_0 q_1)\\
&\quad + (2u_1^2 + 2v_1^2 - 2p_1^2 - 2q_1^2 + u_0 u_2 + v_0 v_2 - p_0 p_2 - q_0 q_2)\\
&\quad + 3(u_1 u_2 + v_1 v_2 - p_1 p_2 - q_1 q_2) = 15(x_\mathrm{f} - x_\mathrm{i}) - 3(d_{\mathrm{i}x} + d_{\mathrm{f}x}),
\end{aligned}
\tag{10}
$$

$$
\begin{aligned}
&3(u_0 q_1 + u_1 q_0 + v_0 p_1 + v_1 p_0)\\
&\quad + (u_0 q_2 + 4u_1 q_1 + u_2 q_0 + v_0 p_2 + 4v_1 p_1 + v_2 p_0)\\
&\quad + 3(u_1 q_2 + u_2 q_1 + v_1 p_2 + v_2 p_1) = 15(y_\mathrm{f} - y_\mathrm{i}) - 3(d_{\mathrm{i}y} + d_{\mathrm{f}y}),
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
&3(v_0 q_1 + v_1 q_0 - u_0 p_1 - u_1 p_0)\\
&\quad + (v_0 q_2 + 4v_1 q_1 + v_2 q_0 - u_0 p_2 - 4u_1 p_1 - u_2 p_0)\\
&\quad + 3(v_1 q_2 + v_2 q_1 - u_1 p_2 - u_2 p_1) = 15(z_\mathrm{f} - z_\mathrm{i}) - 3(d_{\mathrm{i}z} + d_{\mathrm{f}z}).
\end{aligned}
\tag{12}
$$

Conditions (8)–(12) amount to a system of nine coupled quadratic equations for twelve real unknowns.

3. Solution using quaternion representation

The system of equations (8)–(12) is rather cumbersome. We now present the quaternion representation, which yields a more compact and elegant system, and offers better geometrical insight into the solution procedure.

3.1. Basics of quaternion algebra

Quaternions are "four-dimensional numbers" of the form

$$\mathcal{A} = a + a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k} \quad \text{and} \quad \mathcal{B} = b + b_x\mathbf{i} + b_y\mathbf{j} + b_z\mathbf{k}, \tag{13}$$

where the "basis elements" 1, $\mathbf{i}, \mathbf{j}, \mathbf{k}$ satisfy the relations

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{i}\,\mathbf{j}\,\mathbf{k} = -1.$$

Here 1 is the usual real unit; its product with $\mathbf{i}, \mathbf{j}, \mathbf{k}$ leaves them unchanged. Preserving the order of terms in products, we deduce from the above that

$$\mathbf{i}\,\mathbf{j} = -\mathbf{j}\,\mathbf{i} = \mathbf{k}, \qquad \mathbf{j}\,\mathbf{k} = -\mathbf{k}\,\mathbf{j} = \mathbf{i}, \qquad \mathbf{k}\,\mathbf{i} = -\mathbf{i}\,\mathbf{k} = \mathbf{j}. \tag{14}$$

Thus, since the products of the basis elements are noncommutative, we have $\mathcal{AB} \neq \mathcal{BA}$ in general. Quaternion multiplication is associative, however – so that $(\mathcal{AB})\mathcal{C} = \mathcal{A}(\mathcal{BC})$ for any three quaternions $\mathcal{A}, \mathcal{B}, \mathcal{C}$.

The sum of the two quaternions (13) is simply

$$\mathcal{A} + \mathcal{B} = (a + b) + (a_x + b_x)\,\mathbf{i} + (a_y + b_y)\,\mathbf{j} + (a_z + b_z)\,\mathbf{k}, \tag{15}$$

and using relations (14), the product is given by

$$\begin{aligned} \mathcal{AB} = {} & (ab - a_xb_x - a_yb_y - a_zb_z) + (ab_x + ba_x + a_yb_z - a_zb_y)\,\mathbf{i} \\ & + (ab_y + ba_y + a_zb_x - a_xb_z)\,\mathbf{j} + (ab_z + ba_z + a_xb_y - a_yb_x)\,\mathbf{k}. \end{aligned} \tag{16}$$

The notations of 3-dimensional vector analysis furnish a useful shorthand for quaternion operations.[1] Regarding $\mathbf{i}, \mathbf{j}, \mathbf{k}$ as unit vectors in a Cartesian coordinate system, we interpret $\mathcal{A}$ as comprising "scalar" and "vector" parts,[2] a and $\mathbf{a} = a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}$, and we write $\mathcal{A} = (a, \mathbf{a})$. All real numbers and 3-dimensional vectors are subsumed as "pure scalar" and "pure vector" quaternions, of the form $(a, \mathbf{0})$ and $(0, \mathbf{a})$, respectively – for brevity, we often denote such quaternions as simply a and $\mathbf{a}$.

Writing $\mathcal{A} = (a, \mathbf{a})$ and $\mathcal{B} = (b, \mathbf{b})$ in lieu of (13), the sum (15) and the product (16) may be more compactly expressed [16] as

$$\begin{aligned} \mathcal{A} + \mathcal{B} &= (a + b, \mathbf{a} + \mathbf{b}), \\ \mathcal{AB} &= (ab - \mathbf{a}\cdot\mathbf{b}, a\mathbf{b} + b\mathbf{a} + \mathbf{a}\times\mathbf{b}), \end{aligned}$$

[1] Historically, dot products and cross products of vectors were extracted from the theory of quaternions, rather than being used as tools in the development of that theory [3].

[2] Also known as the "real" and "imaginary" parts – the square of a "pure imaginary" quaternion is always a negative real number.

where the usual rules for vector sums and dot and cross products are invoked. Every quaternion $\mathcal{A} = (a, \mathbf{a})$ has a *conjugate*, $\mathcal{A}^* = (a, -\mathbf{a})$, and a *magnitude* equal to the non-negative real number $|\mathcal{A}|$ defined by

$$|\mathcal{A}|^2 = \mathcal{A}^*\mathcal{A} = \mathcal{A}\mathcal{A}^* = a^2 + |\mathbf{a}|^2. \tag{17}$$

One can readily verify that the conjugates of products satisfy the rule

$$(\mathcal{A}\mathcal{B})^* = \mathcal{B}^*\mathcal{A}^*. \tag{18}$$

If $|\mathcal{A}| = 1$, we say that $\mathcal{A}$ is a *unit* quaternion. The unit quaternions form a (non–commutative) *group* under multiplication, since the product of two unit quaternions is always a unit quaternion. Unit quaternions are necessarily of the form $\mathcal{U} = (\cos\frac{1}{2}\theta, \sin\frac{1}{2}\theta\mathbf{n})$ for some angle θ and unit vector $\mathbf{n}$.

For any pure vector quaternion $\mathbf{v}$ and unit quaternion $\mathcal{U}$, the quaternion product $\mathcal{U}\,\mathbf{v}\,\mathcal{U}^*$ always yields a pure vector quaternion, that corresponds to a rotation of $\mathbf{v}$ through angle θ about the axis defined by $\mathbf{n}$ [16]. Note also that the unit quaternion $-\mathcal{U} = (-\cos\frac{1}{2}\theta, -\sin\frac{1}{2}\theta\mathbf{n})$ specifies a rotation through $2\pi - \theta$ about $-\mathbf{n}$, and thus has the same effect as $\mathcal{U} = (\cos\frac{1}{2}\theta, \sin\frac{1}{2}\theta\mathbf{n})$.

3.2. *Solution of the equation* $\mathcal{A}\,\mathbf{i}\,\mathcal{A}^* = \mathbf{c}$

In the Hermite interpolation problem, we are often concerned with quaternion solutions $\mathcal{A} = a_0 + a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}$ to equations of the form

$$\mathcal{A}\,\mathbf{i}\,\mathcal{A}^* = \mathbf{c}, \tag{19}$$

where $\mathbf{c} = c_x\mathbf{i} + c_y\mathbf{j} + c_z\mathbf{k}$ is a given vector.[3] This is equivalent to the system

$$\begin{aligned} a_0^2 + a_x^2 - a_y^2 - a_z^2 &= c_x, \\ 2(a_0a_z + a_xa_y) &= c_y, \\ 2(a_xa_z - a_0a_y) &= c_z. \end{aligned}$$

Since we have *three* equations in *four* unknowns, the solutions to (19) exhibit one degree of freedom. Now let $\mathbf{v} = \mathbf{c}/|\mathbf{c}| = (\lambda, \mu, \nu)$ be a unit vector in the direction of $\mathbf{c}$. Then a particular solution, with $a_0 = 0$, is easily seen to be

$$\mathcal{A} = \pm\sqrt{\tfrac{1}{2}(1+\lambda)|\mathbf{c}|}\left(\mathbf{i} + \frac{\mu}{1+\lambda}\,\mathbf{j} + \frac{\nu}{1+\lambda}\,\mathbf{k}\right). \tag{20}$$

Moreover, if $\mathcal{Q}$ is any quaternion satisfying the equation

$$\mathcal{Q}\,\mathbf{i}\,\mathcal{Q}^* = \mathbf{i}, \tag{21}$$

then $\mathcal{A}\mathcal{Q}$ must also be a solution of (19). Since the quaternions that satisfy (21) are [7] of the form

$$\mathcal{Q} = \cos\phi + \sin\phi\,\mathbf{i},$$

[3] Note that the left-hand side of (19) is necessarily a pure vector quaternion.

the most general solution[4] to equation (19) can be parameterized in terms of an angular variable ϕ as

$$\mathcal{A}(\phi) = \sqrt{\tfrac{1}{2}(1+\lambda)|\mathbf{c}|}\bigg(-\sin\phi + \cos\phi\,\mathbf{i} + \frac{\mu\cos\phi + \nu\sin\phi}{1+\lambda}\mathbf{j} + \frac{\nu\cos\phi - \mu\sin\phi}{1+\lambda}\mathbf{k}\bigg). \tag{22}$$

Since $\sin(\phi+\pi) = -\sin\phi$ and $\cos(\phi+\pi) = -\cos\phi$, the above embodies the sign ambiguity in (20). Thus, upon proceeding from the special solution (20) to the general solution (22), we may omit the $\pm$ sign.

Now writing $\mathcal{A} = \sqrt{|\mathbf{c}|}\,\mathcal{U}$, where $\mathcal{U} = (\cos\frac{1}{2}\theta, \sin\frac{1}{2}\theta\mathbf{n})$ is a unit quaternion specifying a spatial rotation, we may interpret these results geometrically as follows. Under this scaling, equation (19) becomes

$$\mathcal{U}\,\mathbf{i}\,\mathcal{U}^* = \mathbf{v}, \tag{23}$$

which amounts to asking: *which spatial rotations, specified by unit quaterions $\mathcal{U}$, map the unit axis vector* **i** *onto a given unit vector* **v**? In terms of θ and the components (n_x, n_y, n_z) of **n**, equation (23) is equivalent to the system

$$\begin{aligned} n_x^2(1-\cos\theta) + \cos\theta &= \lambda, \\ n_x n_y(1-\cos\theta) + n_z\sin\theta &= \mu, \\ n_z n_x(1-\cos\theta) - n_y\sin\theta &= \nu. \end{aligned}$$

Writing $\alpha = \cos^{-1}\lambda$, this has (for $\alpha \le \theta \le 2\pi - \alpha$) the general solution

$$\begin{aligned} n_x &= \frac{\sqrt{\cos^2\frac{1}{2}\alpha - \cos^2\frac{1}{2}\theta}}{\sin\frac{1}{2}\theta}, \\ n_y &= \frac{\mu\sqrt{\cos^2\frac{1}{2}\alpha - \cos^2\frac{1}{2}\theta} - \nu\cos\frac{1}{2}\theta}{(1+\lambda)\sin\frac{1}{2}\theta}, \\ n_z &= \frac{\mu\cos\frac{1}{2}\theta + \nu\sqrt{\cos^2\frac{1}{2}\alpha - \cos^2\frac{1}{2}\theta}}{(1+\lambda)\sin\frac{1}{2}\theta}. \end{aligned}$$

Thus, there is *a one-parameter family of spatial rotations* that map **i** to **v**.

Geometrically, we can interpret the vectors **i** and **v** as points on the unit sphere. Consider the great circle that is orthogonal to the great circle passing through these points and bisecting the angle between them. This great circle defines the set of rotation axes $\mathbf{n} = (n_x, n_y, n_z)$ specified above. In particular, for the cases $\theta = \alpha$ and $2\pi - \alpha$, the axis **n** is orthogonal to the plane defined by **i** and **v**, and the motion of **i** into **v** is along the great circle through these points. For any other θ, however, the motion of **i** into **v** is

[4] The proper limit of expression (22) must be used when $(\lambda, \mu, \nu) \to (-1, 0, 0)$.

along a small circle of the sphere, orthogonal to the corresponding $\mathbf{n}$. When $\theta = \pi$, for example, the axis $\mathbf{n}$ is midway (along a great circle) between $\mathbf{i}$ and $\mathbf{v}$.

By comparing expression (22) with the solution just derived, of the form

$$\mathcal{A}(\theta) = \sqrt{|\mathbf{c}|}\left[\cos\tfrac{1}{2}\theta + \sin\tfrac{1}{2}\theta(n_x\mathbf{i} + n_y\mathbf{j} + n_z\mathbf{k})\right],$$

we find the relationship between the angular variables ϕ and θ to be

$$\phi = -\tan^{-1}\frac{\cos\frac{1}{2}\theta}{\sqrt{\cos^2\frac{1}{2}\alpha - \cos^2\frac{1}{2}\theta}} \in \left[-\tfrac{1}{2}\pi, +\tfrac{1}{2}\pi\right] \quad \text{for } \theta \in [\alpha, 2\pi - \alpha].$$

Although the parameter θ has a clearer geometrical interpretation (the angle of rotation from $\mathbf{i}$ to $\mathbf{v}$ about the corresponding axis $\mathbf{n}$), the parameterization (22) in terms of ϕ is simpler and thus easier to use in practice. We note that the minimum-angle rotation of $\mathbf{i}$ into $\mathbf{v}$ corresponds to the case $\phi = -\frac{1}{2}\pi$, in which case (22) specializes to

$$\mathcal{A} = \sqrt{\tfrac{1}{2}(1+\lambda)|\mathbf{c}|}\left(1 - \frac{\nu}{1+\lambda}\mathbf{j} + \frac{\mu}{1+\lambda}\mathbf{k}\right). \tag{24}$$

3.3. Construction of Hermite interpolants

Consider now the quadratic polynomial

$$\mathcal{A}(t) = \mathcal{A}_0(1-t)^2 + \mathcal{A}_1 2(1-t)t + \mathcal{A}_2 t^2, \tag{25}$$

with quaternion coefficients

$$\mathcal{A}_r = u_r + v_r\mathbf{i} + p_r\mathbf{j} + q_r\mathbf{k}, \quad r = 0, 1, 2. \tag{26}$$

In quaternion form, the spatial Pythagorean hodograph

$$\begin{aligned}\mathbf{r}'(t) = {} & \left[u^2(t) + v^2(t) - p^2(t) - q^2(t)\right]\mathbf{i} \\ & + 2\left[u(t)q(t) + v(t)p(t)\right]\mathbf{j} + 2\left[v(t)q(t) - u(t)p(t)\right]\mathbf{k}\end{aligned}$$

can be expressed [2] in terms of $\mathcal{A}(t)$ as

$$\mathbf{r}'(t) = \mathcal{A}(t)\,\mathbf{i}\,\mathcal{A}^*(t). \tag{27}$$

The coefficients (26) are to be determined by solving a Hermite interpolation problem. Once $\mathcal{A}_0, \mathcal{A}_1, \mathcal{A}_2$ are known, the control points of the interpolant (4) are given, in quaternion form $\mathbf{p}_r = x_r\mathbf{i} + y_r\mathbf{j} + z_r\mathbf{k}$, by the formulae

$$\begin{aligned}\mathbf{p}_1 &= \mathbf{p}_0 + \frac{1}{5}\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_0^*, \\ \mathbf{p}_2 &= \mathbf{p}_1 + \frac{1}{10}\left(\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_1^* + \mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_0^*\right), \\ \mathbf{p}_3 &= \mathbf{p}_2 + \frac{1}{30}\left(\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^* + 4\mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_1^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^*\right),\end{aligned} \tag{28}$$

$$\mathbf{p}_4 = \mathbf{p}_3 + \frac{1}{10}\big(\mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_2^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_1^*\big),$$
$$\mathbf{p}_5 = \mathbf{p}_4 + \frac{1}{5}\mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_2^*,$$

where we set $\mathbf{p}_0 = \mathbf{p}_\mathrm{i}$ (and $\mathbf{p}_5 = \mathbf{p}_\mathrm{f}$ by construction). This is the quaternion form of expressions (5)–(7), with $\mathcal{A}_r$ for $r = 0, 1, 2$ as in (26).

To solve the Hermite interpolation problem, we begin by expressing the data as "pure vector" quaternions – i.e., we write

$$\mathbf{p}_\mathrm{i} = x_\mathrm{i}\mathbf{i} + y_\mathrm{i}\mathbf{j} + z_\mathrm{i}\mathbf{k}, \qquad \mathbf{d}_\mathrm{i} = d_{\mathrm{i}x}\mathbf{i} + d_{\mathrm{i}y}\mathbf{j} + d_{\mathrm{i}z}\mathbf{k},$$
$$\mathbf{p}_\mathrm{f} = x_\mathrm{f}\mathbf{i} + y_\mathrm{f}\mathbf{j} + z_\mathrm{f}\mathbf{k}, \qquad \mathbf{d}_\mathrm{f} = d_{\mathrm{f}x}\mathbf{i} + d_{\mathrm{f}y}\mathbf{j} + d_{\mathrm{f}z}\mathbf{k}.$$

Interpolation of the end-derivatives then yields the equations

$$\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_0^* = \mathbf{d}_\mathrm{i} \quad \text{and} \quad \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_2^* = \mathbf{d}_\mathrm{f} \tag{29}$$

for $\mathcal{A}_0$ and $\mathcal{A}_2$. Moreover, with $\mathbf{p}_\mathrm{i}$ as an integration constant, interpolation of the end points gives the condition

$$\begin{aligned}\int_0^1 \mathcal{A}(t)\,\mathbf{i}\,\mathcal{A}^*(t)\,\mathrm{d}t &= \mathbf{p}_\mathrm{f} - \mathbf{p}_\mathrm{i}\\ &= \frac{1}{5}\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_0^* + \frac{1}{10}\big(\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_1^* + \mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_0^*\big)\\ &\quad + \frac{1}{30}\big(\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^* + 4\mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_1^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^*\big)\\ &\quad + \frac{1}{10}\big(\mathcal{A}_1\,\mathbf{i}\,\mathcal{A}_2^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_1^*\big) + \frac{1}{5}\mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_2^*.\end{aligned} \tag{30}$$

Since equations (29) are of the form (19), they can be solved directly to give $\mathcal{A}_0$ and $\mathcal{A}_2$ as

$$\begin{aligned}\mathcal{A}_0 = \sqrt{\tfrac{1}{2}(1+\lambda_\mathrm{i})|\mathbf{d}_\mathrm{i}|}\bigg(&-\sin\phi_0 + \cos\phi_0\,\mathbf{i} + \frac{\mu_\mathrm{i}\cos\phi_0 + \nu_\mathrm{i}\sin\phi_0}{1+\lambda_\mathrm{i}}\mathbf{j}\\ &+ \frac{\nu_\mathrm{i}\cos\phi_0 - \mu_\mathrm{i}\sin\phi_0}{1+\lambda_\mathrm{i}}\mathbf{k}\bigg),\end{aligned} \tag{31}$$

$$\begin{aligned}\mathcal{A}_2 = \sqrt{\tfrac{1}{2}(1+\lambda_\mathrm{f})|\mathbf{d}_\mathrm{f}|}\bigg(&-\sin\phi_2 + \cos\phi_2\mathbf{i} + \frac{\mu_\mathrm{f}\cos\phi_2 + \nu_\mathrm{f}\sin\phi_2}{1+\lambda_\mathrm{f}}\mathbf{j}\\ &+ \frac{\nu_\mathrm{f}\cos\phi_2 - \mu_\mathrm{f}\sin\phi_2}{1+\lambda_\mathrm{f}}\mathbf{k}\bigg),\end{aligned} \tag{32}$$

where $(\lambda_\mathrm{i}, \mu_\mathrm{i}, \nu_\mathrm{i})$ and $(\lambda_\mathrm{f}, \mu_\mathrm{f}, \nu_\mathrm{f})$ are the direction cosines of $\mathbf{d}_\mathrm{i}$ and $\mathbf{d}_\mathrm{f}$, and ϕ_0, ϕ_2 are free angular variables. Knowing $\mathcal{A}_0$ and $\mathcal{A}_2$, the solution of (30) for $\mathcal{A}_1$ appears, at first sight, to be more difficult. By use of (29) and appropriate re-arrangements, however, this equation can be written as

$$\begin{aligned}&(3\mathcal{A}_0 + 4\mathcal{A}_1 + 3\mathcal{A}_2)\,\mathbf{i}\,(3\mathcal{A}_0 + 4\mathcal{A}_1 + 3\mathcal{A}_2)^*\\ &\quad = 120(\mathbf{p}_\mathrm{f} - \mathbf{p}_\mathrm{i}) - 15(\mathbf{d}_\mathrm{i} + \mathbf{d}_\mathrm{f}) + 5\big(\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^*\big),\end{aligned} \tag{33}$$

which has the form (19) with $\mathcal{A} = 3\mathcal{A}_0 + 4\mathcal{A}_1 + 3\mathcal{A}_2$. Note that the quantity on the right-hand side of (33) is a known pure vector: since $\mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^* = (\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^*)^*$, $\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^*$ is twice the vector part of $\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^*$. From (31) and (32) we may write

$$\mathcal{A}_0\,\mathbf{i}\,\mathcal{A}_2^* + \mathcal{A}_2\,\mathbf{i}\,\mathcal{A}_0^* = \sqrt{(1+\lambda_\mathrm{i})|\mathbf{d}_\mathrm{i}|(1+\lambda_\mathrm{f})|\mathbf{d}_\mathrm{f}|}\,(a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}),$$

where

$$\begin{aligned}
a_x &= \cos(\phi_2-\phi_0) - \frac{(\mu_\mathrm{i}\mu_\mathrm{f} + \nu_\mathrm{i}\nu_\mathrm{f})\cos(\phi_2-\phi_0) + (\mu_\mathrm{i}\nu_\mathrm{f} - \mu_\mathrm{f}\nu_\mathrm{i})\sin(\phi_2-\phi_0)}{(1+\lambda_\mathrm{i})(1+\lambda_\mathrm{f})},\\
a_y &= \frac{\mu_\mathrm{i}\cos(\phi_2-\phi_0) - \nu_\mathrm{i}\sin(\phi_2-\phi_0)}{1+\lambda_\mathrm{i}} + \frac{\mu_\mathrm{f}\cos(\phi_2-\phi_0) + \nu_\mathrm{f}\sin(\phi_2-\phi_0)}{1+\lambda_\mathrm{f}},\\
a_z &= \frac{\nu_\mathrm{i}\cos(\phi_2-\phi_0) + \mu_\mathrm{i}\sin(\phi_2-\phi_0)}{1+\lambda_\mathrm{i}} + \frac{\nu_\mathrm{f}\cos(\phi_2-\phi_0) - \mu_\mathrm{f}\sin(\phi_2-\phi_0)}{1+\lambda_\mathrm{f}}.
\end{aligned}$$

Writing $\mathbf{c} = c_x\mathbf{i} + c_y\mathbf{j} + c_z\mathbf{k}$ for the right-hand side of (33), we deduce from (19) the solution

$$\begin{aligned}
\mathcal{A}_1 = -\frac{3}{4}(\mathcal{A}_0 + \mathcal{A}_2) + \frac{\sqrt{\frac{1}{2}(1+\lambda)|\mathbf{c}|}}{4}\bigg(&-\sin\phi_1 + \cos\phi_1\,\mathbf{i}\\
&+ \frac{\mu\cos\phi_1 + \nu\sin\phi_1}{1+\lambda}\mathbf{j} + \frac{\nu\cos\phi_1 - \mu\sin\phi_1}{1+\lambda}\mathbf{k}\bigg),
\end{aligned} \tag{34}$$

where (λ, μ, ν) are the direction cosines of $\mathbf{c}$, and ϕ_1 is another free angular variable. Note that $\mathcal{A}_1$ depends on ϕ_0, ϕ_2 as well as ϕ_1, due to the dependence of $\mathcal{A}_0$, $\mathcal{A}_2$, λ, μ, ν, $|\mathbf{c}|$ on those variables.

4. Rotation invariance of interpolants

The quaternion formulation (27) for spatial Pythagorean hodographs has the important feature that it admits a simple, explicit demonstration of rotation invariance [7]. Namely, if

$$\mathcal{U} = \cos\tfrac{1}{2}\theta + \sin\tfrac{1}{2}\theta\,\mathbf{n} \tag{35}$$

is the unit quaternion specifying a rotation by angle θ about the unit vector $\mathbf{n} = n_x\mathbf{i} + n_y\mathbf{j} + n_z\mathbf{k}$, then the rotated hodograph can be written in the form

$$\tilde{\mathbf{r}}'(t) = \tilde{\mathcal{A}}(t)\,\mathbf{i}\,\tilde{\mathcal{A}}^*(t),$$

where we define $\tilde{\mathcal{A}}(t) = \mathcal{U}\mathcal{A}(t)$. When $\mathcal{A}(t)$ is the quadratic (25), for example, $\tilde{\mathcal{A}}(t)$ has the Bernstein coefficients $\tilde{\mathcal{A}}_\mathrm{i} = \mathcal{U}\mathcal{A}_\mathrm{i}$ for $i = 0, 1, 2$.

In this connection a subtle issue arises concerning the role of the ϕ_0, ϕ_1, ϕ_2 parameters in the Hermite interpolation algorithm. Consider the pure vector quaternion $\mathbf{c}$ – under the rotation (35), it is mapped [16] to the vector

$$\tilde{\mathbf{c}} = \mathcal{U}\,\mathbf{c}\,\mathcal{U}^*.$$

Now suppose we rotate the Hermite data $\mathbf{p}_\mathrm{i}$, $\mathbf{d}_\mathrm{i}$ and $\mathbf{p}_\mathrm{f}$, $\mathbf{d}_\mathrm{f}$ to obtain

$$\tilde{\mathbf{p}}_\mathrm{i} = \mathcal{U}\,\mathbf{p}_\mathrm{i}\mathcal{U}^*, \qquad \tilde{\mathbf{d}}_\mathrm{i} = \mathcal{U}\,\mathbf{d}_\mathrm{i}\mathcal{U}^* \quad \text{and} \quad \tilde{\mathbf{p}}_\mathrm{f} = \mathcal{U}\,\mathbf{p}_\mathrm{f}\mathcal{U}^*, \qquad \tilde{\mathbf{d}}_\mathrm{f} = \mathcal{U}\,\mathbf{d}_\mathrm{f}\mathcal{U}^*.$$

One can easily verify that, if $\mathcal{A}_0$, $\mathcal{A}_1$, $\mathcal{A}_2$ are a solution to the Hermite system (29)–(30), then the quaternions

$$\tilde{\mathcal{A}}_0 = \mathcal{U}\mathcal{A}_0, \qquad \tilde{\mathcal{A}}_1 = \mathcal{U}\mathcal{A}_1, \qquad \tilde{\mathcal{A}}_2 = \mathcal{U}\mathcal{A}_2 \tag{36}$$

solve the system (29)–(30) with $\tilde{\mathbf{p}}_\mathrm{i}$, $\tilde{\mathbf{d}}_\mathrm{i}$, $\tilde{\mathbf{p}}_\mathrm{f}$, $\tilde{\mathbf{d}}_\mathrm{f}$ substituted for $\mathbf{p}_\mathrm{i}$, $\mathbf{d}_\mathrm{i}$, $\mathbf{p}_\mathrm{f}$, $\mathbf{d}_\mathrm{f}$. The PH quintic Hermite interpolant defined by (36) is precisely the image of the original interpolant, under a rotation by angle θ about $\mathbf{n}$.

However, the quaternions (36) do *not* correspond to solving the Hermite interpolation problem for the rotated data, using the same ϕ_0, ϕ_1, ϕ_2 values in the algorithm of section 3: *different* values $\tilde{\phi}_0$, $\tilde{\phi}_1$, $\tilde{\phi}_2$ must be invoked in the algorithm to obtain the solution (36). Consider, for example, the choice $\phi_0 = \phi_1 = \phi_2 = 0$ in expressions (31), (32), (34) – this yields pure vector quaternions for *any* given Hermite data, but the quaternions (36) are not, in general, pure vectors when θ is not an integer multiple of π.

To find the correspondence between ϕ_0, ϕ_1, ϕ_2 and $\tilde{\phi}_0$, $\tilde{\phi}_1$, $\tilde{\phi}_2$ that ensures rotation invariance of the interpalation algorithm (i.e., that the interpolant to rotated Hermite data coincides precisely with the rotated copy of the original interpolant), we recall from section 3 the general solution

$$\mathcal{A} = \sqrt{\tfrac{1}{2}(1+\lambda)|\mathbf{c}|}\left(\mathbf{i} + \frac{\mu}{1+\lambda}\mathbf{j} + \frac{\nu}{1+\lambda}\mathbf{k}\right)(\cos\phi + \sin\phi\,\mathbf{i}),$$

where $\mathbf{c}$ is a vector with direction cosines (λ, μ, ν), to equation (19). Setting $\mathcal{Q}(\phi) = \cos\phi + \sin\phi\,\mathbf{i}$, we can write $\mathcal{A}$ in the form

$$\mathcal{A} = \sqrt{|\mathbf{c}|}\,\frac{\mathbf{i}+\mathbf{v}}{|\mathbf{i}+\mathbf{v}|}\,\mathcal{Q}(\phi),$$

$\mathbf{v} = \lambda\,\mathbf{i} + \mu\,\mathbf{j} + \nu\,\mathbf{k}$ being the unit vector in the direction of $\mathbf{c}$. Correspondingly, if the rotated vector $\tilde{\mathbf{c}} = \mathcal{U}\,\mathbf{c}\,\mathcal{U}^*$ has direction cosines $(\tilde{\lambda}, \tilde{\mu}, \tilde{\nu})$, solutions to

$$\tilde{\mathcal{A}}\,\mathbf{i}\,\tilde{\mathcal{A}}^* = \tilde{\mathbf{c}}$$

can be expressed in terms of the unit vector $\tilde{\mathbf{v}} = \tilde{\lambda}\,\mathbf{i} + \tilde{\mu}\,\mathbf{j} + \tilde{\nu}\,\mathbf{k}$ as

$$\tilde{\mathcal{A}} = \sqrt{|\tilde{\mathbf{c}}|}\,\frac{\mathbf{i}+\tilde{\mathbf{v}}}{|\mathbf{i}+\tilde{\mathbf{v}}|}\,\mathcal{Q}(\tilde{\phi}).$$

The correspondence between the free parameters ϕ and $\tilde{\phi}$ is then established by the requirement that $\tilde{\mathcal{A}} = \mathcal{U}\mathcal{A}$. Since $|\tilde{\mathbf{c}}| = |\mathbf{c}|$, this furnishes (after some elementary manipulations) the equation

$$\mathcal{Q}(\tilde{\phi})\,\mathcal{Q}^*(\phi) = \cos\left(\tilde{\phi}-\phi\right) + \sin\left(\tilde{\phi}-\phi\right)\mathbf{i} = \frac{(\mathbf{i}+\tilde{\mathbf{v}})^*\mathcal{U}(\mathbf{i}+\mathbf{v})}{|\mathbf{i}+\tilde{\mathbf{v}}|\;|\mathbf{i}+\mathbf{v}|}.$$

The expression on the right-hand side is necessarily a unit quaternion with zero $\mathbf{j}$ and $\mathbf{k}$ components. By evaluating it, we can unambiguously deduce the difference $\tilde{\phi} - \phi$ for a given rotation $\mathcal{U}$. Since all the equations we encounter in the Hermite interpolation problem are of the form (19), this approach can be applied to determine each of $\tilde{\phi}_0$, $\tilde{\phi}_1$, $\tilde{\phi}_2$.

Because of the complicated nature of the relationships among $\tilde{\phi}_0$, $\tilde{\phi}_1$, $\tilde{\phi}_2$ and ϕ_0, ϕ_1, ϕ_2, the preferred means of rotating Hermite interpolants is clearly to first perform the interpolation for data in a "canonical" orientation, and then effect the rotation by pre-multiplying $\mathcal{A}_0$, $\mathcal{A}_1$, $\mathcal{A}_2$ with $\mathcal{U}$. This ensures rotation-invariance without consideration of the appropriate $\tilde{\phi}_0$, $\tilde{\phi}_1$, $\tilde{\phi}_2$ values that arises when the Hermite data is rotated *prior* to interpolation.

5. Fixing the ϕ_0, ϕ_1, ϕ_2 degrees of freedom

As noted in section 3, the parameters ϕ_0, ϕ_1, ϕ_2 are chosen from the interval $[-\frac{1}{2}\pi, +\frac{1}{2}\pi]$. Now as far as the shape of the interpolants is concerned, these degrees of freedom are not independent. We can demonstrate this as follows. The control points (28) depend only on products of the form

$$\mathcal{P}_{rs} = \mathcal{A}_r\,\mathbf{i}\,\mathcal{A}_s^* \quad \text{for } r, s \in \{0, 1, 2\}. \tag{37}$$

Since $\mathcal{A}_r = \mathcal{A}_r(0)(\cos\phi_r + \sin\phi_r\,\mathbf{i})$, with $\mathcal{A}_r(0)$ being the value of $\mathcal{A}_r$ when $\phi_r = 0$, and likewise for $\mathcal{A}_s$, the quantities (37) can be written in the form

$$\begin{aligned}
\mathcal{P}_{rs} &= \big[\mathcal{A}_r(0)(\cos\phi_r + \sin\phi_r\,\mathbf{i})\big]\,\mathbf{i}\,\big[\mathcal{A}_s(0)(\cos\phi_s + \sin\phi_s\,\mathbf{i})\big]^* \\
&= \mathcal{A}_r(0)\big[(\cos\phi_r + \sin\phi_r\,\mathbf{i})\,\mathbf{i}\,(\cos\phi_s - \sin\phi_s\mathbf{i})\big]\,\mathcal{A}_s^*(0) \\
&= \mathcal{A}_r(0)\big[\sin(\phi_s - \phi_r) + \cos(\phi_s - \phi_r)\,\mathbf{i}\big]\,\mathcal{A}_s^*(0),
\end{aligned}$$

from which it is apparent that they depend only on *differences* of the angles ϕ_0, ϕ_1, ϕ_2. Hence we may, without loss of generality, assume that $\phi_1 = -\frac{1}{2}\pi$ and specialize (34) to

$$\mathcal{A}_1 = -\frac{3}{4}(\mathcal{A}_0 + \mathcal{A}_2) + \frac{\sqrt{\frac{1}{2}(1+\lambda)|\mathbf{c}|}}{4}\left(1 - \frac{\nu}{1+\lambda}\mathbf{j} + \frac{\mu}{1+\lambda}\mathbf{k}\right). \tag{38}$$

With this choice for ϕ_1, substituting expressions (31), (32), (38) into (28) yields a two-parameter family of solutions to the problem of interpolating first-order Hermite data $\mathbf{p}_{\mathrm{i}}$, $\mathbf{d}_{\mathrm{i}}$ and $\mathbf{p}_{\mathrm{f}}$, $\mathbf{d}_{\mathrm{f}}$ by PH quintics with hodographs of the form (3). Although they all match the prescribed end-point data, the shape of these interpolants also depends on the two free parameters ϕ_0, ϕ_2. As we exercise these degrees of freedom, the first and last two control points $\mathbf{p}_0$, $\mathbf{p}_1$ and $\mathbf{p}_4$, $\mathbf{p}_5$ will remain fixed, while $\mathbf{p}_2$, $\mathbf{p}_3$ vary.

We might, in principle, seek to employ these remaining degrees of freedom to satisfy two additional (scalar) interpolation conditions. For example, we might attempt to interpolate end-point curvatures, but in three dimensions this is of questionable value without being able to specify the corresponding principal normals (osculating planes).

We propose instead to select ϕ_0, ϕ_2 so as to ensure desirable overall shape properties of the curves.

Because of the highly nonlinear nature of their dependence on ϕ_0, ϕ_2 the formal optimization of a suitable "shape integral" for the PH quintic Hermite interpolants with respect to these parameters is intractable. We rely instead on an empirical investigation of the behavior of such shape measures. Recall that the *Frenet frame* of a space curve – comprising the tangent **t**, principal normal **n**, and binormal **b** – is defined [14] by

$$\mathbf{t} = \frac{\mathbf{r}'}{|\mathbf{r}'|}, \qquad \mathbf{n} = \frac{\mathbf{r}' \times \mathbf{r}''}{|\mathbf{r}' \times \mathbf{r}''|} \times \mathbf{t}, \qquad \mathbf{b} = \mathbf{t} \times \mathbf{n}.$$

The variation of the Frenet frame with respect to arc length s along the curve is described by the equations

$$\frac{\mathrm{d}\,\mathbf{t}}{\mathrm{d}s} = \mathbf{d} \times \mathbf{t}, \qquad \frac{\mathrm{d}\,\mathbf{n}}{\mathrm{d}s} = \mathbf{d} \times \mathbf{n}, \qquad \frac{\mathrm{d}\,\mathbf{b}}{\mathrm{d}s} = \mathbf{d} \times \mathbf{b}, \tag{39}$$

where the *Darboux vector*

$$\mathbf{d} = \tau \mathbf{t} + \kappa \mathbf{b}$$

is defined in terms of the curvature and torsion, given by

$$\kappa = \frac{|\mathbf{r}' \times \mathbf{r}''|}{|\mathbf{r}'|^3} \quad \text{and} \quad \tau = \frac{(\mathbf{r}' \times \mathbf{r}'') \cdot \mathbf{r}'''}{|\mathbf{r}' \times \mathbf{r}''|^2}. \tag{40}$$

Equations (39) characterize the instantaneous variation of the Frenet frame as a rotation about the vector **d**, at a rate given by the "total curvature"

$$\omega = |\mathbf{d}| = \sqrt{\kappa^2 + \tau^2}. \tag{41}$$

Note that, in terms of the quaternion representation, the first, second, and third curve derivatives required in (40) and (41) can be expressed as

$$\begin{aligned}
\mathbf{r}' &= \mathcal{A}\,\mathbf{i}\,\mathcal{A}^*, \\
\mathbf{r}'' &= \mathcal{A}'\,\mathbf{i}\,\mathcal{A}^* + \mathcal{A}\,\mathbf{i}\,\mathcal{A}'^*, \\
\mathbf{r}''' &= \mathcal{A}''\,\mathbf{i}\,\mathcal{A}^* + 2\mathcal{A}'\,\mathbf{i}\,\mathcal{A}'^* + \mathcal{A}\,\mathbf{i}\,\mathcal{A}''^*.
\end{aligned}$$

In general, large values of the total curvature are incompatible with the desire for a smooth curve. Thus, we adopt minimization of the shape measure

$$\mathcal{E} = \int_0^1 \omega^2 \big|\mathbf{r}'\big|\,\mathrm{d}t \tag{42}$$

as our criterion for choosing appropriate ϕ_0, ϕ_2 values. In the case of a plane curve ($\tau \equiv 0$), this reduces to the usual elastic bending energy [6]. We have observed empirically from many examples that the choice[5] $\phi_0 = \phi_1 = \phi_2 = -\frac{1}{2}\pi$ gives the least (or

[5] Actually, it is sufficient to have ϕ_0, ϕ_1, ϕ_2 equal to some arbitrary value – since, as noted above, only the *differences* between the angles affect the shape of the interpolants.

Table 1
The energy integral (42) for PH quintic interpolants to Hermite data $\mathbf{p}_\mathrm{i} = (0, 0, 0)$, $\mathbf{d}_\mathrm{i} = (1, 0, 1)$ and $\mathbf{p}_\mathrm{f} = (1, 1, 1)$, $\mathbf{d}_\mathrm{f} = (0, 1, 1)$, using various choices for the free parameters ϕ_0, ϕ_2 and the fixed value $\phi_1 = -(1/2)\pi$.

	$\phi_0 = -\pi/2$	$\phi_0 = -\pi/4$	$\phi_0 = 0$	$\phi_0 = +\pi/4$	$\phi_0 = +\pi/2$
$\phi_2 = -\pi/2$	3.38	6.36	32.49	172.31	3351.54
$\phi_2 = -\pi/4$	6.92	15.32	40.44	282.94	8516.21
$\phi_2 = 0$	26.65	46.38	76.16	296.64	5210.33
$\phi_2 = +\pi/4$	156.19	267.88	340.16	443.74	3599.70
$\phi_2 = +\pi/2$	4148.60	1757.13	1151.00	1520.08	4012.95

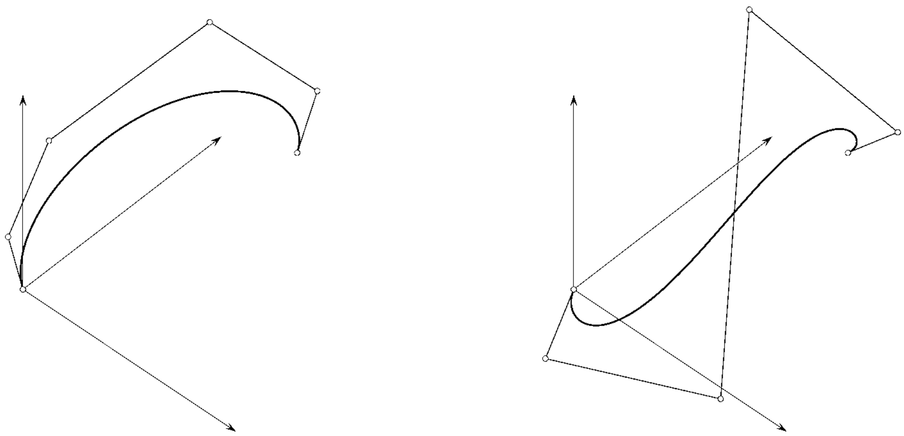

Figure 1. Examples of rotation-invariant PH quintic space curves with end points $\mathbf{p}_\mathrm{i} = (0, 0, 0)$, $\mathbf{p}_\mathrm{f} = (1, 1, 1)$ and end derivatives $\mathbf{d}_\mathrm{i} = (-0.8, 0.3, 1.2)$, $\mathbf{d}_\mathrm{f} = (0.5, -1.3, -1.0)$ and $\mathbf{d}_\mathrm{i} = (0.4, -1.5, -1.2)$, $\mathbf{d}_\mathrm{f} = (-1.2, -0.6, -1.2)$ on the left and the right. Both curves employ the choice $\phi_0 = \phi_1 = \phi_2 = -(1/2)\pi$.

close to the least) value for the integral (42). Table 1 gives $\mathcal{E}$ values for a representative example, in which we fix $\phi_1 = -\frac{1}{2}\pi$ and increase ϕ_0, ϕ_2 in $\frac{1}{4}\pi$ increments.

Figure 1 shows some examples of rotation–invariant spatial PH quintics, together with their Bézier control polygons, constructed from given Hermite data through the methods described above. Both curves correspond to the "canonical" choice $\phi_0 = \phi_1 = \phi_2 = -\frac{1}{2}\pi$ of the free parameters in (31), (32), (34) and have eminently pleasing shapes, consistent with the given data.

6. Closure

Spatial Pythagorean-hodograph curves that exhibit invariance under general 3-dimensional rotations are characterized by certain combinations of four polynomials, which admit an elegant characterization in terms of quaternions. In terms of this representation, the first-order Hermite interpolation problem allows a simple reduction to a system of three quadratic equations in three quaternion unknowns. Two scalar degrees of freedom remain on solving this system, for which we suggest "canonical" values based on the behavior of an energy integral characterizing the smoothness of the interpolants.

We conclude by remarking that the quaternion solution of the first-order Hermite interpolation problem presented here admits a natural extension to the construction of spatial C^2 PH quintic splines, interpolating a sequence of points $\mathbf{p}_0, \ldots, \mathbf{p}_N$ in space with prescribed end conditions. This gives rise to a "tridiagonal" system of N quadratic equations in N quaternion unknowns, which may be solved by suitable adaptation of the complex-variable methods described in [1,8] for planar C^2 PH splines (with due allowance for the noncommutative nature of quaternion multiplication).

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