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## ■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... { Recall that $(u,v,w)^T$ is a normalized vector: $u^2+v^2+w^2=1$. }

• $\frac{1}{2}\left(1+c+(1-c)(u^2-v^2-w^2)\right)\cdot x$

$$= \tfrac{1}{2}\left(1+c+u^2-v^2-w^2-cu^2+cv^2+cw^2\right)\cdot x$$
$$= \tfrac{1}{2}\left(1+u^2-v^2-w^2+c(1-u^2+v^2+w^2)\right)\cdot x$$
$$= \tfrac{1}{2}\left(1+1-2v^2-2w^2+c(1+1-2u^2)\right)\cdot x$$
$$= \tfrac{1}{2}\left(2-2v^2-2w^2+c(2-2u^2)\right)\cdot x$$
$$= \left(1-v^2-w^2+c(1-u^2)\right)\cdot x$$
$$= \left(u^2+c(1-u^2)\right)\cdot x$$
$$= \left(u^2+c-cu^2\right)\cdot x = \left(u^2(1-c)+c\right)\cdot x$$

• $\frac{1}{2}\left(1+c+(1-c)(-u^2+v^2-w^2)\right)\cdot y$

$$= \tfrac{1}{2}\left(1+c-u^2+v^2-w^2+cu^2-cv^2+cw^2\right)\cdot y$$
$$= \ldots = \left(v^2+c(1-v^2)\right)\cdot y$$
$$= \left(v^2+c-cv^2\right)\cdot y = \left(v^2(1-c)+c\right)\cdot y$$

• $\frac{1}{2}\left(1+c+(1-c)(-u^2-v^2+w^2)\right)\cdot z$

$$= \tfrac{1}{2}\left(1+c-u^2-v^2+w^2+cu^2+cv^2-cw^2\right)\cdot z$$
$$= \ldots = \left(w^2+c(1-w^2)\right)\cdot z$$
$$= \left(w^2+c-cw^2\right)\cdot z = \left(w^2(1-c)+c\right)\cdot z$$

$$\Rightarrow x' = \left(u^2(1-c)+c\right)x + \left(uv(1-c)-ws\right)y + \left(uw(1-c)+vs\right)z;$$
$$y' = \left(uv(1-c)+ws\right)x + \left(v^2(1-c)+c\right)y + \left(vw(1-c)-us\right)z;$$
$$z' = \left(uw(1-c)-vs\right)x + \left(vw(1-c)+us\right)y + \left(w^2(1-c)+c\right)z.$$

$$\Rightarrow \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} u^2(1-c)+c & uv(1-c)-ws & uw(1-c)+vs \\ uv(1-c)+ws & v^2(1-c)+c & vw(1-c)-us \\ uw(1-c)-vs & vw(1-c)+us & w^2(1-c)+c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

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## ■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... It is now possible to compare this result obtained via quaternion multiplication with the result generated via "direct matrix multiplication," i.e., $\mathbf{x}' = \mathbf{R}\,\mathbf{x}$. The matrix $\mathbf{R}$ is the matrix defined on page 11 (12/2/2023). The comparison of the results confirms that quaternion multiplication and matrix multiplication are equivalent.

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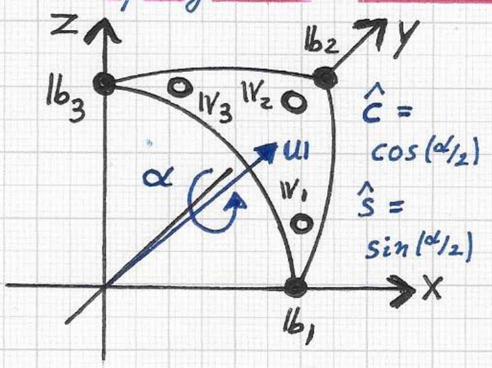
We are concerned with the optimal approximation of a given non-orthogonal basis (in 3D space) consisting of three normalized basis vectors by an orthonormal basis. Our goal is to achieve this goal via quaternions by minimization of a properly chosen error measure for approximation. We consider the numerical example illustrated on page 3 (11/3/2023). The left figure briefly




summarizes the essential data: points/positional vectors $\mathbb{b}_1 = (1,0,0)^T$, $\mathbb{b}_2 = (0,0,1)^T$ and $\mathbb{b}_3 = (0,0,1)^T$; three points $\mathbb{v}_1 = \sqrt{2}\,(2/3, 1/6, 1/6)^T$, $\mathbb{v}_2 = \sqrt{2}\,(1/6, 2/3, 1/6)^T$ and $\mathbb{v}_3 = \sqrt{2}\,(1/6, 1/6, 2/3)^T$ with non-orthogonal positional vectors and a rotation **axis** defined by the normalized direction vector $\mathbb{u} = \sqrt{3}\,(1/3, 1/3, 1/3)^T$.

...

## OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

• Laplacian eigenfunctions and neural networks:... We rotate the orthonormal basis vectors $\mathbb{b}_1$, $\mathbb{b}_2$ and $\mathbb{b}_3$ via quaternion algebra. The goal is the calculation of the optimal value of the unknown rotation angle $\alpha$ that — when used to rotate the basis $\{\mathbb{b}_i\}_{i=1}^{3}$ — would produce an orthonormal basis that approximates the normalized but non-orthogonal basis vectors $\mathbb{v}_1$, $\mathbb{v}_2$ and $\mathbb{v}_3$. Again, quaternion-based rotation combines/concatenates two rotations, each using the angle $\alpha/2$, to achieve the desired rotation by $\alpha$ via the (associative) multiplication

$$p'(\alpha) = q(\alpha/2)\cdot p\cdot \bar{q}(\alpha/2) = q\cdot p\cdot \bar{q} = \\ = (\hat{c} + (ui+vj+wk)\hat{s})\cdot p\cdot \\ \cdot(\hat{c} - (ui+vj+wk)\hat{s}),$$

where the x-, y- and z-coordinates of a specific basis vector $\mathbb{b}_i$ define the corresponding vector in quaternion representation, i.e., $p = 0 + xi + yj + zk$. Further, we use the pre-computed normalized **direction** vector $\mathbb{u} = (u,v,w)^T = \sqrt{3}\,(1/3, 1/3, 1/3)^T$ that specifies the rotation axis. We rotate the given orthonormal basis vectors, using $\alpha$ as variable, and subsequently calculate the optimal $\alpha$-value that leads to the minimal approximation error, i.e., the $\alpha$-value that defines the best approximation. We use the notation $\hat{c} = \cos(\alpha/2)$ and $\hat{s} = \sin(\alpha/2)$. ...

## ■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:... First, we compute the quaternion representation of the vector $\mathbb{b}_i$, $i = 1, 2, 3$, after a rotation by angle $\alpha$.

i) Mapping basis vector $\mathbb{b}_1$

$$b_1' = q \cdot p \cdot \bar{q} = \left( \hat{c} + \tfrac{\sqrt{3}}{3}\hat{s}\, i + \tfrac{\sqrt{3}}{3}\hat{s}\, j + \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \cdot$$

$$\cdot \left\{ \left( 0 + 1 i + 0 j + 0 k \right) \cdot \right.$$

$$\left. \cdot \left( \hat{c} - \tfrac{\sqrt{3}}{3}\hat{s}\, i - \tfrac{\sqrt{3}}{3}\hat{s}\, j - \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \right\}$$

$$= \ldots = \left( 0 + \left( \hat{c}^2 - \hat{s}^2/3 \right) i + \left( \tfrac{2}{3}\hat{s}^2 + \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) j + \left( \tfrac{2}{3}\hat{s}^2 - \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) k \right).$$

ii) Mapping basis vector $\mathbb{b}_2$

$$b_2' = q \cdot p \cdot \bar{q} = \left( \hat{c} + \tfrac{\sqrt{3}}{3}\hat{s}\, i + \tfrac{\sqrt{3}}{3}\hat{s}\, j + \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \cdot$$

$$\cdot \left\{ \left( 0 + 0 i + 1 j + 0 k \right) \cdot \right.$$

$$\left. \cdot \left( \hat{c} - \tfrac{\sqrt{3}}{3}\hat{s}\, i - \tfrac{\sqrt{3}}{3}\hat{s}\, j - \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \right\}$$

$$= \ldots = \left( 0 + \left( \tfrac{2}{3}\hat{s}^2 - \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) i + \left( \hat{c}^2 - \hat{s}^2/3 \right) j + \left( \tfrac{2}{3}\hat{s}^2 + \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) k \right).$$

iii) Mapping basis vector $\mathbb{b}_3$

$$b_3' = q \cdot p \cdot \bar{q} = \left( \hat{c} + \tfrac{\sqrt{3}}{3}\hat{s}\, i + \tfrac{\sqrt{3}}{3}\hat{s}\, j + \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \cdot$$

$$\cdot \left\{ \left( 0 + 0 i + 0 j + 1 k \right) \cdot \right.$$

$$\left. \cdot \left( \hat{c} - \tfrac{\sqrt{3}}{3}\hat{s}\, i - \tfrac{\sqrt{3}}{3}\hat{s}\, j - \tfrac{\sqrt{3}}{3}\hat{s}\, k \right) \right\}$$

$$= \ldots = \left( 0 + \left( \tfrac{2}{3}\hat{s}^2 + \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) i + \left( \tfrac{2}{3}\hat{s}^2 - \tfrac{2}{3}\sqrt{3}\,\hat{s}\hat{c} \right) j + \left( \hat{c}^2 - \hat{s}^2/3 \right) k \right).$$

$$\Rightarrow \mathbb{b}_1' = \begin{bmatrix} \hat{c}^2 - \hat{s}^2/3 \\ \frac{2}{3}\left( \hat{s}^2 + \sqrt{3}\,\hat{s}\hat{c} \right) \\ \frac{2}{3}\left( \hat{s}^2 - \sqrt{3}\,\hat{s}\hat{c} \right) \end{bmatrix}, \quad \mathbb{b}_2' = \begin{bmatrix} \frac{2}{3}\left( \hat{s}^2 - \sqrt{3}\,\hat{s}\hat{c} \right) \\ \hat{c}^2 - \hat{s}^2/3 \\ \frac{2}{3}\left( \hat{s}^2 + \sqrt{3}\,\hat{s}\hat{c} \right) \end{bmatrix}, \quad \mathbb{b}_3' = \begin{bmatrix} \frac{2}{3}\left( \hat{s}^2 + \sqrt{3}\,\hat{s}\hat{c} \right) \\ \frac{2}{3}\left( \hat{s}^2 - \sqrt{3}\,\hat{s}\hat{c} \right) \\ \hat{c}^2 - \hat{s}^2/3 \end{bmatrix}.$$

These rotated orthonormal basis vectors define the approximation error. •••

## OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- **Laplacian eigenfunctions and neural networks:...** Second, we define and minimize an error approximation function $E$ that depends only on the rotation angle $\alpha$.

i) Definition of error $E$

It is possible and appropriate to define $E$ as the sum of squared distances $d_i^2 = \| \mathbb{b}_i' - \mathbb{w}_i \|^2$, $i=1,2,3$. Thus, $E = \sum_{i=1}^{3} d_i^2$. A necessary condition for the minimization of $E$ is the requirement $d/d\alpha\, E(\alpha) = 0$ — and that $d^2/d\alpha^2\, E(\alpha) > 0$ for a local extremum of $E$ to be a minimum.

ii) Minimizing the error $E$

The value of $E$ is $E = \sum_{i=1}^{3} \| \mathbb{b}_i' - \mathbb{w}_i \|^2 =$

$$= 3 \cdot \left\{ \left(\hat{c}^2 - \hat{s}^2/3 - 2/3\sqrt{2}\right)^2 + \left(2/3\left(\hat{s}^2 + \sqrt{3}\,\hat{s}\hat{c}\right) - 1/6\sqrt{2}\right)^2 + \left(2/3\left(\hat{s}^2 - \sqrt{3}\,\hat{s}\hat{c}\right) - 1/6\sqrt{2}\right)^2 \right\}$$

{product rule: $\hat{s}\hat{c} = s(\alpha/2)\, c(\alpha/2) = 1/2\, s(\alpha) = s/2$.}

$$= 3 \cdot \left\{ \left(\hat{c}^2 - \hat{s}^2/3 - 2/3\sqrt{2}\right)^2 + \left(2/3\left(\hat{s}^2 + \sqrt{3}/2\, s\right) - 1/6\sqrt{2}\right)^2 + \left(2/3\left(\hat{s}^2 - \sqrt{3}/2\, s\right) - 1/6\sqrt{2}\right)^2 \right\}$$

$$= \ldots = 3\left(\hat{s}^4 + \hat{c}^4\right) + 3/2\, s^2 - 4\sqrt{2}\,\hat{c}^2 + 3$$

{power rules: $\hat{s}^4 = 1/8\left(3 - 4c(\alpha) + c(2\alpha)\right)$,
$\hat{c}^4 = 1/8\left(3 + 4c(\alpha) + c(2\alpha)\right)$;
$\Rightarrow \hat{s}^4 + \hat{c}^4 = 1/4\left(3 + \cos(2\alpha)\right) = 1/4(3 + \check{c})$.}

$$= 3/4\,(3 + \check{c}) + 3/2\, s^2 - 4\sqrt{2}\,\hat{c}^2 + 3$$

$$= \ldots = 21/4 + 3/4\cos(2\alpha) + 3/2\sin^2(\alpha) - 4\sqrt{2}\cos^2(\alpha/2)$$

$$\Rightarrow d/d\alpha\, E = -3/2\sin(2\alpha) + 3\sin(\alpha)\cos(\alpha) + 4\sqrt{2}\sin(\alpha/2)\cos(\alpha/2)$$

$$= \ldots = 2\sqrt{2}\sin(\alpha) \overset{!}{=} 0 \Rightarrow \alpha = n\cdot\pi,\ n = 0, 1, 2, \ldots$$

$$\Rightarrow d^2/d\alpha^2\, E = 2\sqrt{2}\cos(\alpha) \overset{!}{>} 0 \Rightarrow E \text{ MINIMAL}: \alpha = 2n\pi.$$

...