Quaternions

- Quaternions define a multiplication of 4D vectors, similar to how $\mathbb{C}$ defines a multiplication on $\mathbb{R}^2$.

Hamilton, 1805-1865

- Quaternions are defined as quantities $q = s + iv_1 + jv_2 + kv_3 \in \mathbb{H}$

real part

imaginary parts

where $i^2 = j^2 = k^2 = ijk = -1$.

- Convenient notation: $q = (s, \bar{v})$.

- Addition: $q_1 = (s_1, \bar{v}_1),\ q_2 = (s_2, \bar{v}_2) \Rightarrow q_1 + q_2 = (s_1 + s_2, \bar{v}_1 + \bar{v}_2)$ (ordinary addition in $\mathbb{R}^4$)

(contd.)

Quaternions

Not comutative! $q_1 \circ q_2 \neq q_2 \circ q_1$

- Quaternion multiplication: $q_1 \circ q_2 = (s_1 s_2 - \bar{v}_1^T \bar{v}_2,\ s_1 \bar{v}_2 + s_2 \bar{v}_1 + \bar{v}_1 \times \bar{v}_2)$

- Associativity: $(q_1 \circ q_2) \circ q_3 = q_1 \circ (q_2 \circ q_3)$

- No zero-divisors: $q_1 \circ q_2 = (0, \mathbf{0}) \Rightarrow q_1 = 0$ or $q_2 = 0$

- Existence of identity: $1 + i0 + j0 + k0 = (1, \mathbf{0})$ is unique with the property $1 \circ q = q \circ 1 = q \quad \forall q \in \mathbb{H}$

- Existence of inverse: If $q = (s, \bar{v}) \neq 0$, then $q^{-1} = \frac{1}{s^2 + \bar{v}^T \bar{v}} (s, -\bar{v})$

  has the property $q^{-1} \circ q = q \circ q^{-1} = 1$

  $q^{-1} \circ q = \frac{1}{s^2 + \bar{v}^T \bar{v}} (s, -\bar{v}) \circ (s, \bar{v}) = \frac{1}{s^2 + \bar{v}^T \bar{v}} (s^2 + \bar{v}^T \bar{v},\ s\bar{v} - s\bar{v} + \bar{v} \times \bar{v}) = (1, \mathbf{0}) = 1$

Quaternions as Rotations

$q^T q = \cos^2\frac{\alpha}{2} + \sin^2\frac{\alpha}{2}\,\underbrace{\hat{n}^T\hat{n}}_{=1} = 1$

- Unit quaternions: $S^3 = \{n \in \mathbb{R}^4 : n^T n = 1\}$ "unit sphere in $\mathbb{R}^4$"

  Any $q \in S^3$ can be written as $q(\alpha, \hat{n}) = q = (\cos\frac{\alpha}{2}, \hat{n}\sin\frac{\alpha}{2})$ for $\alpha \in \mathbb{R}$ and $\hat{n} \in \mathbb{R}^3$ with $\|\hat{n}\|^2 = 1$.

  Interpreted as a quaternion, rather than a vector in $\mathbb{R}^4$, $q \in S^3$ is a unit quaternion.

- A pure quaternion is a quaternion with real part zero, $q_{\bar{x}} = (0, \bar{x})$.

- If q is a unit quaternion, then

$$q(\alpha,\hat{n}) \circ q_{\bar{x}} \circ q(\alpha,-\hat{n}) = \left(\cos\frac{\alpha}{2}, \hat{n}\sin\frac{\alpha}{2}\right) \circ (0, \bar{x}) \circ \left(\cos\frac{\alpha}{2}, -\hat{n}\sin\frac{\alpha}{2}\right) =$$

$$= \left(0 - \sin\frac{\alpha}{2}\hat{n}^T\bar{x},\ \cos\frac{\alpha}{2}\bar{x} + 0 + \hat{n}\sin\frac{\alpha}{2} \times \bar{x}\right) \circ \left(\cos\frac{\alpha}{2}, -\hat{n}\sin\frac{\alpha}{2}\right) =$$

$$= \left(-\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\hat{n}^T\bar{x} + \hat{n}\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\bar{x},\ \hat{n}^T\bar{x}\sin^2\frac{\alpha}{2} + \cos^2\frac{\alpha}{2}\bar{x} + \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\hat{n}\times\bar{x} - \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\bar{x}\times\hat{n} + \sin^2\frac{\alpha}{2}(\hat{n}\times\bar{x})\times\hat{n}\right)$$

$$= \left(0,\ (I + [\hat{n}]_\times \sin\alpha + (1-\cos\alpha)[\hat{n}]_\times^2)\bar{x}\right) = \left(0, R(\alpha,\hat{n})\bar{x}\right)$$

The Orthogonal Procrustes Problem

$$A^+ = \begin{cases} (A^TA)^{-1}A^T & \text{if } m \geq n \\ A^T(AA^T)^{-1} & \text{if } m \leq n \end{cases}$$

Suppose $a_1, \dots, a_m \in \mathbb{R}^3$ (or $\mathbb{E}^3$) and $b_k = Ra_k + \varepsilon_k$, and we wish to estimate the rotation R. This is known as the OPP!

- In principle, if there is no noise, we can obtain the correct solution directly by solving $RA = B$ for R, where $A = (a_1 \dots a_m)$ and $B = (b_1 \dots b_m)$.

$$R = BA^+ = BA^T(AA^T)^{-1}$$

$AB^T = USV^T$?

- However, if there is noise, the solution obtained in this way will not be a rotation, but just some other matrix R!

The Orthogonal Procrustes Problem (contd.)

We seek the orthogonal R which minimises

$$\mathcal{E}(R) = \|B - RA\|_F^2 = tr\left((B-RA)(B-RA)^T\right) =$$

$$= tr\left(BB^T - RAB^T - BA^TR^T + RAA^TR^T\right) =$$

$$= tr(BB^T) - tr(RAB^T) - tr(BA^TR^T) + tr(RAA^TR^T) =$$

$$= \underline{tr(BB^T)} - \underbrace{2tr(RAB^T)}_{\text{maximise!}} + \underline{tr(AA^T)} \quad \text{independent of } R!$$

$\|A\|_F$ is the Frobenius norm

$$\|A\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2}$$

$$tr(AA^T) = \|A\|_F^2$$

$$tr(A^TB) = tr(B^TA)$$

$$tr(AB) = tr(BA)$$

Let $AB^T = USV^T$ be an SVD of AB^T. Then

$$tr(RAB^T) = tr(RUSV^T) = tr(\underbrace{V^TRU}_{\text{orthogonal}}S) \quad \text{is maximized when } V^TRU = I$$

$$\Rightarrow R = VU^T$$

The Special OPP

- It can happen that the solution to the OPP is not a proper rotation, but is just another orthogonal matrix (with determinant -1).

- We can "correct" the determinant:

$$\tau = \det U \cdot \det V = \pm 1$$

$$R = U \begin{pmatrix} 1 & & \\ & 1 & \\ & & \tau \end{pmatrix} V^T \Rightarrow \det R = \det U \cdot \det \begin{pmatrix} 1 & & \\ & 1 & \\ & & \tau \end{pmatrix} \cdot \det(V^T) = \tau^2 = 1$$

$\Rightarrow$ R will be a Rotation (not a reflection)!

Estimating Rigid Transformations

Suppose $a_1, \dots, a_m \in \mathbb{R}^3$ (or $\mathbb{E}^3$) and $b_k = Ra_k + t + \varepsilon_k$,

and we wish to estimate the rotation R and the translation t.

Solution: Minimise $\varepsilon(R,t) = \sum_{j=1}^{m} \underbrace{\|b_j - Ra_j - t\|}_{\varepsilon_k}^2 = \sum_{j=1}^{m} (b_j - Ra_j - t)^T (b_j - Ra_j - t) =$

$$= \sum_{j=1}^{m} \Big(b_j^T b_j - 2b_j^T R a_j - 2b_j^T t + \underbrace{2t^T R a_j}_{2(Ra_j)^T t} + (Ra_j)^T R a_j + t^T t \Big)$$

$$\frac{\partial \varepsilon}{\partial t} = \sum_{j=1}^{m} \Big(-\cancel{2} b_j^T + \cancel{2}(Ra_j)^T + \cancel{2} t^T \Big) = 0 \quad \text{solve for } t: \quad t = \overbrace{\frac{1}{m}\sum_{j=1}^{m} b_j}^{\bar{b}} - R \overbrace{\frac{1}{m}\sum_{j=1}^{m} a_j}^{\bar{a}}$$

Optimal $t = \bar{b} - R\bar{a} \Rightarrow b_k = Ra_k + t + \varepsilon_k \Leftrightarrow \overbrace{b_k - \bar{b}}^{\tilde{b}_k} = Ra_k - \cancel{\bar{b} + \bar{b}} - R\bar{a} + \varepsilon_k = R\overbrace{(a_k - \bar{a})}^{\tilde{a}_k} + \varepsilon_k$ OPP!

$\tilde{A}\tilde{B}^T = SVD \dots$