

Rotations & Quaternions

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CRASH COURSE ON GROUPS

Definition 1 (Group). A *group*, G , is a set with a binary operation, $*$, commonly written as $G(S, *)$ where S is the set. All groups adhere to the four axioms:

(1) Closure:

$$\forall x, y \in G : x * y \in G$$

(2) Associativity:

$$\forall x, y, z \in G : (a * b) * c = a * (b * c)$$

(3) Identity:

$$\exists! e \in G \text{ s.t. } \forall x \in G : x * e = e * x = x$$

(4) Inverse:

$$\forall x \in G, \exists y \in G \text{ s.t. } x * y = y * x = e$$

Some common groups where the objects of interest are matrices and the binary operation is matrix multiplication include, but are not limited to:

(1) General Linear:

$$\mathbf{GL}(n, F) = \{A \in F^{n^2} \mid \det(A) \neq 0\}$$

(2) Special Linear:

$$\mathbf{SL}(n, F) = \{A \in F^{n^2} \mid \det(A) = 1\}$$

(3) Orthogonal:

$$\mathbf{O}(n, F) = \{A \in F^{n^2} \mid A^{-1} = A^T\}$$

(4) Special Orthogonal:

$$\mathbf{SO}(n, F) = \{A \in F^{n^2} \mid A^{-1} = A^T \& \det(A) = 1\}$$

(5) Unitary:

$$\mathbf{U}(n, F) = \{A \in F^{n^2} \mid A^{-1} = A^\dagger\}$$

(6) Special Unitary:

$$\mathbf{SU}(n, F) = \{A \in F^{n^2} \mid A^{-1} = A^\dagger \& \det(A) = 1\}$$

(7) Symplectic:

$$\mathbf{Sp}(2n, F) = \left\{ A \in F^{4n^2} \mid A^T \Omega A = \Omega \text{ where } \Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \right\}$$

where n is the parameter referring to A being a $n \times n$ matrix and F is the field. Typical fields of interest include the integers, real numbers, and complex numbers.

QUATERNIONS

Definition 2 (Quaternion). A *quaternion* is any number that can be written as:

$$q = a + bi + cj + dk \text{ where } a, b, c, d \in \mathbb{R}$$

where a is known as the real part and the rest denotes the imaginary part. Along with this we have:

$$i^2 = j^2 = k^2 = -1$$

$$ij = k \text{ and } ji = -k$$

$$jk = i \text{ and } kj = -i$$

$$ki = j \text{ and } ik = -j$$

Obviously the above is a pain to remember, so instead you can use the cycle below to remember how the multiplication works where reversing the direction throws in a negative sign:



Note that while real and complex numbers are commutative, quaternions in general are not. In addition any quaternion that has a zero valued real part is known as a *pure imaginary quaternion*.

Proposition 1 (Relation to \mathbb{R}^3 Vector Operations). Given any two quaternions that are written down into separate real and imaginary components as:

$$p = p_0 + \vec{p} \text{ and } q = q_0 + \vec{q}$$

their multiplication is defined as:

$$pq = (p_0q_0 - \vec{p} \cdot \vec{q}) + (p_0\vec{q} + q_0\vec{p} + \vec{p} \times \vec{q})$$

where \cdot and \times represent the standard dot product and cross product on \mathbb{R}^3 respectively.

Proof. We start by defining the quaternions as:

$$p = p_0 + p_1i + p_2j + p_3k \text{ and } q = q_0 + q_1i + q_2j + q_3k$$

Now multiplying them gives:

$$\begin{aligned} pq &= (p_0 + p_1i + p_2j + p_3k)(q_0 + q_1i + q_2j + q_3k) \\ &= (p_0q_0 + p_1q_1i^2 + p_2q_2j^2 + p_3q_3k^2) + p_0q_1i + p_0q_2j + p_0q_3k + p_1q_0i \\ &\quad + p_1q_2ij + p_1q_3ik + p_2q_0j + p_2q_1ji + p_2q_3jk + p_3q_0k + p_3q_1ki + p_3q_2kj \\ &= (p_0q_0 - p_1q_1 - p_2q_2 - p_3q_3) + p_0q_1i + p_0q_2j + p_0q_3k + p_1q_0i \\ &\quad + p_1q_2k - p_1q_3j + p_2q_0j - p_2q_1k + p_2q_3i + p_3q_0k + p_3q_1j - p_3q_2i \\ &= (p_0q_0 - p_1q_1 - p_2q_2 - p_3q_3) + p_0(q_1i + q_2j + q_3k) + q_0(p_1i + p_2j + p_3k) \\ &\quad + [(p_2q_3 - p_3q_2)i + (p_3q_1 - p_1q_3)j + (p_1q_2 - p_2q_1)k] \end{aligned}$$

If we vectorize the imaginary component of each quaternion as:

$$\vec{p} = p_1i + p_2j + p_3k \text{ and } \vec{q} = q_1i + q_2j + q_3k$$

then the multiplication takes on the form:

$$pq = (p_0q_0 - \vec{p} \cdot \vec{q}) + (p_0\vec{q} + q_0\vec{p} + \vec{p} \times \vec{q})$$



Definition 3 (Conjugation). Similar to complex numbers, the conjugate of any given quaternion:

$$q = q_0 + q_1i + q_2j + q_3k$$

is defined as:

$$q^* = q_0 - q_1i - q_2j - q_3k$$

Notice that by multiplying the two we arrive at:

$$\|q\|^2 = qq^* = q^*q = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

which defines the square of the norm for any given quaternion.

Proposition 2 (Redefining the Dot and Cross Products of \mathbb{R}^3). Take two pure imaginary quaternions:

$$p = p_1i + p_2j + p_3k \text{ and } q = q_1i + q_2j + q_3k$$

We can now define the dot and cross products as:

$$p \cdot q = \frac{1}{2}(p^*q + q^*p) = \frac{1}{2}(pq^* + qp^*)$$

$$p \times q = \frac{1}{2}(pq - q^*p^*)$$

Proof. To begin consider the fact that for any two quaternions p and q we have:

$$pq = (p_0q_0 - \vec{p} \cdot \vec{q}) + (p_0\vec{q} + q_0\vec{p} + \vec{p} \times \vec{q})$$

Now if we want to talk about pure imaginary quaternions we set $p_0 = q_0 = 0$ to get:

$$pq = \vec{p} \times \vec{q} - \vec{p} \cdot \vec{q}$$

With this can now define:

$$p^*q = (-\vec{p}) \times \vec{q} - (-\vec{p}) \cdot \vec{q}$$

$$= -\vec{p} \times \vec{q} + \vec{p} \cdot \vec{q}$$

$$q^*p = (-\vec{q}) \times \vec{p} - (-\vec{q}) \cdot \vec{p}$$

$$= \vec{p} \times \vec{q} + \vec{p} \cdot \vec{q}$$

Adding these two together and isolating the dot product gives:

$$2\vec{p} \cdot \vec{q} = p^*q + q^*p$$

$$\vec{p} \cdot \vec{q} = \frac{1}{2}(p^*q + q^*p)$$

I now remind you that the dot product will always give back a real number, therefore conjugation will not change the result and so:

$$(\vec{p} \cdot \vec{q})^* = \left[\frac{1}{2}(p^*q + q^*p) \right]^*$$

$$\vec{p} \cdot \vec{q} = \frac{1}{2}(pq^* + qp^*)$$

where the conjugation of the product is equivalent to the product of the conjugations in the same order. Lastly we define:

$$q^*p^* = (-\vec{q}) \times (-\vec{p}) - (-\vec{q}) \cdot (-\vec{p})$$

$$= -\vec{p} \times \vec{q} - \vec{p} \cdot \vec{q}$$

and subtract it from the original multiplication to arrive at the definition of the cross product:

$$2\vec{p} \times \vec{q} = pq - q^*p^*$$

$$\vec{p} \times \vec{q} = \frac{1}{2}(pq - q^*p^*)$$



Definition 4 (Matrix Representations). Any given quaternion:

$$q = q_0 + q_1i + q_2j + q_3k$$

can be written as a 2×2 matrix with inputs consisting of complex numbers:

$$q = \begin{pmatrix} q_0 + q_1i & q_2 + q_3i \\ -q_2 + q_3i & q_0 - q_1i \end{pmatrix}$$

If you do not happen to like imaginary components, then this definition can be easily rewritten as a 4×4 matrix consisting of real numbers as:

$$q = \begin{pmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix}$$

Proposition 3 (Conjugate in Matrix Representation). If we represent a quaternion as a matrix, then the conjugate of the quaternion is equivalent to the conjugate transpose of the matrix.

Proof. Let us define:

$$q = q_0 + q_1i + q_2j + q_3k$$

$$q^* = q_0 - q_1i - q_2j - q_3k$$

where we know that:

$$q = \begin{pmatrix} q_0 + q_1i & q_2 + q_3i \\ -q_2 + q_3i & q_0 - q_1i \end{pmatrix}$$

Now to define the conjugate in terms of a matrix, just place a negative sign in front of the imaginary components:

$$q^* = \begin{pmatrix} q_0 - q_1i & -q_2 - q_3i \\ q_2 - q_3i & q_0 + q_1i \end{pmatrix}$$

which is equivalent to:

$$q^* = \left[\begin{pmatrix} q_0 + q_1i & q_2 + q_3i \\ -q_2 + q_3i & q_0 - q_1i \end{pmatrix} \right]^\dagger = \begin{pmatrix} q_0 - q_1i & -q_2 - q_3i \\ q_2 - q_3i & q_0 + q_1i \end{pmatrix}$$

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Proposition 4 (Norm in Matrix Representation). If we represent a quaternion as a matrix, then the norm squared of the quaternion is equivalent to the determinant of the matrix.

Proof. We note that the square of the norm is already defined as:

$$\|q\|^2 = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

Now taking the determinant of the matrix representation gives:

$$\begin{aligned} \|q\|^2 &= \det \begin{pmatrix} q_0 + q_1i & q_2 + q_3i \\ -q_2 + q_3i & q_0 - q_1i \end{pmatrix} \\ &= (q_0 + q_1i)(q_0 - q_1i) - (q_2 + q_3i)(-q_2 + q_3i) \\ &= q_0^2 + q_1^2 + q_2^2 + q_3^2 \end{aligned}$$

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Definition 5 (Unit Quaternions). Any quaternion q that has a norm equivalent to exactly 1 is known as a *unit quaternion*.

Proposition 5 (Generating a Unit Quaternion). In general given any arbitrary quaternion, q , we can generate a unit quaternion by dividing by the norm:

$$q_u = \frac{q}{\|q\|}$$

Proof. To check we just have to check that the norm of the new quaternion is actually equivalent to 1:

$$\begin{aligned}\|q_u\| &= \sqrt{q_u q_u^*} \\ &= \sqrt{\left(\frac{q}{\|q\|}\right) \left(\frac{q^*}{\|q\|}\right)} \\ &= \sqrt{\frac{qq^*}{\|q\|^2}} \\ &= \sqrt{\frac{qq^*}{qq^*}} \\ &= 1\end{aligned}$$

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Proposition 6 (Quaternion Reciprocal). A quaternion reciprocal can always be defined as:

$$q^{-1} = \frac{q^*}{\|q\|^2} \text{ s.t. } q^{-1}q = qq^{-1} = 1$$

so long as $q \neq 0$.

Proof. In general since quaternions are not commutative, there should exist a distinction between the left and right inverse. Fortunately the definition above abuses the unit quaternions in a way s.t. both inverses are equivalent. To show this just multiply out q with its inverse in both directions to arrive at the same result:

$$\begin{aligned}q^{-1}q &= \left(\frac{q^*}{\|q\|^2}\right)q = \frac{q^*q}{\|q\|^2} = 1 \\ qq^{-1} &= q\left(\frac{q^*}{\|q\|^2}\right) = \frac{qq^*}{\|q\|^2} = 1\end{aligned}$$

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Proposition 7 (Quaternion Representation of \mathbf{S}^3). Pure imaginary quaternions with norm equivalent to 1 form a group isomorphic to \mathbf{S}^3 with the binary operation of quaternion multiplication.

Proof. We have to check the four conditions for being a group:

- (1) We know that multiplying any two quaternions together yields another quaternion. As an add on we also know that if both of the original quaternions have norm equivalent to 1, then so will the final result:

$$\|q_3\| = \|q_1 q_2\| = \|q_1\| \|q_2\| = (1)(1) = 1$$

where the modulus is allowed to be split up under multiplication same as the complex case.

- (2) Even though quaternions are not commutative, it is known that they are associative.
- (3) As for the identity we can define it to be:

$$e = 1$$

- (4) The inverse we define to be the conjugate:

$$q^{-1} = \frac{q^*}{\|q\|^2} = q^*$$

since the norm is taken to be 1.

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Proposition 8 (Useful Identity). Given a pure imaginary quaternion, q , we have the following identity:

$$q^{2n} = (-1)^n \|q\|^{2n} \text{ where } n \in \mathbb{Z}^+$$

Proof. This can easily be proved by induction. For the base case consider $n = 0$ which gives:

$$\begin{aligned} q^0 &= (-1)^0 \|q\|^0 \\ 1 &= 1 \end{aligned}$$

Now we assume that the statement holds true for n and try to show that it holds for $n + 1$:

$$\begin{aligned} q^{2(n+1)} &= q^{2n+2} \\ &= q^{2n} q^2 \\ &= (-1)^n \|q\|^{2n} q^2 \\ &= (-1)^{n+1} \|q\|^{2n} (q)(-q) \\ &= (-1)^{n+1} \|q\|^{2n} (q)(q^*) \\ &= (-1)^{n+1} \|q\|^{2n} \|q\|^2 \\ &= (-1)^{n+1} \|q\|^{2n+2} \\ &= (-1)^{n+1} \|q\|^{2(n+1)} \end{aligned}$$

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Proposition 9 (Euler's Formula). Given a quaternion:

$$p = e^q$$

where q is pure imaginary, we can rewrite p as:

$$p = \cos \|q\| + \frac{q}{\|q\|} \sin \|q\|$$

A consequence of this setup forces p to be a unit quaternion.

Proof. To begin we know that we can expand the exponential as a power series and using the above identity we arrive at:

$$\begin{aligned} p &= \sum_{n=0}^{\infty} \frac{q^n}{n!} \\ &= \sum_{n=0}^{\infty} \frac{q^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{q^{2n+1}}{(2n+1)!} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n \|q\|^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{(-1)^n \|q\|^{2n} q}{(2n+1)!} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n \|q\|^{2n}}{(2n)!} + \frac{q}{\|q\|} \sum_{n=0}^{\infty} \frac{(-1)^n \|q\|^{2n+1}}{(2n+1)!} \\ &= \cos \|q\| + \frac{q}{\|q\|} \sin \|q\| \end{aligned}$$

Now if we want to check the norm of p we have:

$$\begin{aligned} \|p\| &= \sqrt{pp^*} \\ &= \sqrt{(e^q)(e^q)^*} \\ &= \sqrt{(e^q)(e^{q^*})} \\ &= \sqrt{(e^q)(e^{-q})} \\ &= 1 \end{aligned}$$

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ROTATIONS

Proposition 10 (Rodrigues' Rotation Formula). Given a vector $v \in \mathbb{R}^3$ and a unit vector, $\hat{k} \in \mathbb{R}^3$ describing an axis of rotation about which v rotates by an angle θ , according to the right hand rule the resulting vector after rotation is defined as:

$$v' = \cos(\theta)v + \sin(\theta)(\hat{k} \times v) + (1 - \cos(\theta))(\hat{k} \cdot v)\hat{k}$$

Proof. To begin take the vector we want to rotate and split it into components relative to the axis \hat{k} :

$$v = v_{\perp} + v_{\parallel}$$

where the parallel component is nothing more than:

$$v_{\parallel} = (v \cdot \hat{k})\hat{k}$$

and the perpendicular component is:

$$v_{\perp} = v - v_{\parallel} = v - (\hat{k} \cdot v)\hat{k}$$

We now want to use the known identity:

$$(a \cdot c)b - (a \cdot b)c = a \times (b \times c)$$

to rewrite the perpendicular component as:

$$v_{\perp} = -\hat{k} \times (\hat{k} \times v)$$

To continue we note that since we are rotating about the axis \hat{k} , the component parallel to it will not change under the rotation. Therefore, we have:

$$v'_{\parallel} = v_{\parallel}$$

The perpendicular component will transform according to:

$$\begin{aligned} \|v'_{\perp}\| &= \|v_{\perp}\| \\ v'_{\perp} &= \cos(\theta)v_{\perp} + \sin(\theta)(\hat{k} \times v_{\perp}) \end{aligned}$$

which can be simplified because:

$$\hat{k} \times v_{\perp} = \hat{k} \times (v - v_{\parallel}) = \hat{k} \times v - \hat{k} \times v_{\parallel} = \hat{k} \times v$$

giving:

$$v'_{\perp} = \cos(\theta)v_{\perp} + \sin(\theta)(\hat{k} \times v)$$

We know that the above transformation preserves the norm because v_{\perp} and $\hat{k} \times v$ have the same length. Now we can write down the explicit form of the rotated vector as:

$$\begin{aligned} v' &= v'_{\parallel} + v'_{\perp} \\ &= v_{\parallel} + \cos(\theta)v_{\perp} + \sin(\theta)(\hat{k} \times v) \\ &= v_{\parallel} + \cos(\theta)(v - v_{\parallel}) + \sin(\theta)(\hat{k} \times v) \\ &= \cos(\theta)v + (1 - \cos(\theta))v_{\parallel} + \sin(\theta)(\hat{k} \times v) \\ &= \cos(\theta)v + \sin(\theta)(\hat{k} \times v) + (1 - \cos(\theta))(\hat{k} \cdot v)\hat{k} \end{aligned}$$



Proposition 11 (Quaternion Rotation Identity). Given the unit quaternion:

$$q = \cos\left(\frac{\alpha}{2}\right) + u \sin\left(\frac{\alpha}{2}\right)$$

where u is a unit pure imaginary quaternion, the map:

$$w \rightarrow qwq^{-1}$$

defines a counterclockwise rotation about the axis u with angle α where $w \in \mathbb{R}^3$.

Proof. First we note that when talking about unit quaternions we have:

$$q^{-1} = q^*$$

Now by direct calculation:

$$\begin{aligned} qwq^{-1} &= qwq^* \\ &= \left[\cos\left(\frac{\alpha}{2}\right) + u \sin\left(\frac{\alpha}{2}\right) \right] w \left[\cos\left(\frac{\alpha}{2}\right) - u \sin\left(\frac{\alpha}{2}\right) \right] \\ &= w \cos^2\left(\frac{\alpha}{2}\right) + (uw - wu) \sin\left(\frac{\alpha}{2}\right) \cos\left(\frac{\alpha}{2}\right) - uwu \sin^2\left(\frac{\alpha}{2}\right) \\ &= w \cos^2\left(\frac{\alpha}{2}\right) + \left[(u \times w - u \cdot w) - (w \times u - w \cdot u) \right] \sin\left(\frac{\alpha}{2}\right) \cos\left(\frac{\alpha}{2}\right) - \left[(u \times w - u \cdot w)u \right] \sin^2\left(\frac{\alpha}{2}\right) \\ &= w \cos^2\left(\frac{\alpha}{2}\right) + 2(u \times w) \sin\left(\frac{\alpha}{2}\right) \cos\left(\frac{\alpha}{2}\right) - \left[- (u \times w) \cdot u - (u \cdot w)u - u \times (u \times w) \right] \sin^2\left(\frac{\alpha}{2}\right) \\ &= w \cos^2\left(\frac{\alpha}{2}\right) + 2(u \times w) \sin\left(\frac{\alpha}{2}\right) \cos\left(\frac{\alpha}{2}\right) - \left[- (u \cdot w)u - (u \cdot w)u + (u \cdot u)w \right] \sin^2\left(\frac{\alpha}{2}\right) \\ &= w \left[\cos^2\left(\frac{\alpha}{2}\right) - \sin^2\left(\frac{\alpha}{2}\right) \right] + 2(u \times w) \sin\left(\frac{\alpha}{2}\right) \cos\left(\frac{\alpha}{2}\right) - \left[- (u \cdot w)u - (u \cdot w)u \right] \sin^2\left(\frac{\alpha}{2}\right) \\ &= w \cos(\alpha) + (u \times w) \sin(\alpha) + (u \cdot w)u(1 - \cos(\alpha)) \end{aligned}$$

we arrive at Rodrigues' Rotation Formula. ■

APPLICATION OF QUATERNIONS

Definition 6 (Pauli Spin Matrices). In Quantum Mechanics the Pauli spin matrices are defined as:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where:

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = i\sigma_1\sigma_2\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

Now since we are talking about 2×2 matrices with imaginary complex components there is a natural association between the Pauli matrices and quaternions. Specifically we have the map:

$$(1, i, j, k) \rightarrow (I, -i\sigma_1, -i\sigma_2, -i\sigma_3)$$