Parametrization of 3D Rotations Using Quaternions

In 3-dimensional space, according to Euler's rotation theorem, any rotation or sequence of rotations of a rigid body or coordinate system about a fixed point is equivalent to a single rotation by an angle θ about a fixed axis (the Euler axis) shown as $\hat{n}$ which is a unit vector containing the fixed point. Apart from this axis-angle representation, there is another simpler way to encode 3D Rotations using "*Quaternions*" consisting of just four numbers!

A normalized or unit quaternion $Q = \{q_0, q_1, q_2, q_3\} = Q(q_0, \mathbf{q})$, with $q_i \in [-1, 1]$, can be used to uniquely represent homogeneously distributed rotations of a 3D object. In general, a quaternion Q, with its scalar part q_0 and vector part $\mathbf{q}$, can be thought of as an extension of usual complex numbers to four dimensions (three imaginary and one real).

$$Q = q_0 + \mathbf{q} = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \tag{1}$$

Here, the three imaginary numbers $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ follow the property $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1$ and $\mathbf{ij} = \mathbf{k} = -\mathbf{ji}$. The conjugate of Q i.e. $Q^* = Q(q_0, -\mathbf{q})$ is also equal to its inverse Q^{-1} as shown below

$$Q \cdot Q^* = |Q|^2 = q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1 \tag{2}$$

In comparison with the axis-angle representation, the q_0 and $\mathbf{q}$ components of a quaternion contain information about the angle θ and the rotation axis $\hat{n}$ respectively.

$$Q = \cos\frac{\theta}{2} + \hat{n}\sin\frac{\theta}{2} = q_0 + \mathbf{q}$$

An ordinary vector $\mathbf{p} = (p_x, p_y, p_z)$ in 3D space can be thought of as a quaternion with its scalar part equal to zero i.e. $q_p = \{0, p_x, p_y, p_z\}$. These are called pure quaternions or versors. A quaternion $Q = Q(q_0, \mathbf{q})$ and its inverse are used to rotate the vector $\mathbf{p}$ to another vector $\mathbf{p}' = (p'_x, p'_y, p'_z)$ such that $q_{p'} = Q \cdot q_p \cdot Q^{-1}$. The matrix representation of $q_{p'}$ is given as

$$q_{p'} = \begin{bmatrix} 0 \\ \mathbf{p}' \end{bmatrix} = Q \begin{bmatrix} 0 \\ \mathbf{p} \end{bmatrix} Q^{-1}$$

The above-mentioned rotation operation can be described as a matrix multiplication of $\mathbf{p}$ with a 3×3 rotation matrix R_Q to obtain $\mathbf{p}'$ i.e. $\mathbf{p}' = R_Q \cdot \mathbf{p}$. So, the quaternion parametrization of the rotational group $\mathbf{SO}(3)$ can be given by the following 'Quaternion Rotational Matrix' R_Q, with $Q = \{q_0, q_1, q_2, q_3\}$.

$$R_Q = 2\begin{bmatrix} q_0^2 + q_1^2 - 0.5 & q_1q_2 - q_0q_3 & q_0q_2 + q_1q_3 \\ q_0q_3 + q_1q_2 & q_0^2 + q_2^2 - 0.5 & q_2q_3 - q_0q_1 \\ q_1q_3 - q_0q_2 & q_0q_1 + q_2q_3 & q_0^2 + q_3^2 - 0.5 \end{bmatrix} \tag{3}$$

Since the matrix R_Q has the property $R_Q = R_{-Q}$, the quaternions Q and $-Q$ denote the same rotation operation. Hence, the **Quaternion group** is said to be the *double cover* for the $\mathbf{SO}(3)$ group.

Homogeneous Sampling of Rotations

A unit quaternion, a 3D quantity, is a point on the 4D quaternion space (a unit 3-sphere). Thus, to respect the underlying geometry, the components of a quaternion $\tilde{Q}$ are sampled from a *standard normal distribution*. This is then normalized to achieve a unit quaternion $Q = \tilde{Q}/|\tilde{Q}| = \{q_0, q_1, q_2, q_3\}$ which follows Eq. (2).

Distance between two Rotations

The quaternion $Q = (q_0, \mathbf{q})$ for a specific rotation can be transformed into another quaternion $Q' = (q'_0, \mathbf{q}')$, responsible for a different rotation, with the help of a third quaternion $Q' \cdot Q^{-1}$ composed from their product. A group invariant distance measure between these two rotations should only be dependent on the rotation angle (say, δ) of $Q' \cdot Q^{-1}$; which can be obtained from its scalar part $q_0 q'_0 + \mathbf{q} \cdot \mathbf{q}'$ because $\cos(\delta/2) = q_0 q'_0 + \mathbf{q} \cdot \mathbf{q}'$. This measure of the distance can also be written as a function of their Euclidean distance $|Q - Q'|$.

$$\cos(\delta/2) = q_0 q'_0 + \mathbf{q} \cdot \mathbf{q}' = 1 - |Q - Q'|^2/2$$

For a small angle δ, we can expand the cosine term and simplify both sides to get $\delta/2 \approx |Q - Q'|$ which implies that the angular distance between close quaternions is approximately their Euclidean distance.

From Euler Angles to Quaternions

Here, we can relate the quaternion rotational matrix R_Q with the rotational matrix using Euler angles for the same rotation operation. The rotational matrix R_γ for the Euler angle triplet $\gamma = \{\psi, \theta, \phi\}$ can be represented as $R_\gamma = R_Z(\phi) R_Y(\theta) R_Z(\psi)$. For this composite rotation, the corresponding quaternion $Q = \{q_0, q_1, q_2, q_3\}$ is the ordered product of three independent quaternions responsible for three independent rotations along Z, Y, and Z-axes respectively.

$$Q = Q^Z_\phi \cdot Q^Y_\theta \cdot Q^Z_\psi$$

For the quaternion Q^Z_ψ, the rotation is by an angle ψ around the Z-axis. So, its vector part has only the Z-component with a value equal to $\sin(\psi/2)$, and its scalar part is $\cos(\psi/2)$. Similarly, the other two quaternions Q^Y_θ and Q^Z_ϕ are given as

$$Q^Z_\psi = \{\cos\frac{\psi}{2}, 0, 0, \sin\frac{\psi}{2}\} \qquad Q^Y_\theta = \{\cos\frac{\theta}{2}, 0, \sin\frac{\theta}{2}, 0\} \qquad Q^Z_\phi = \{\cos\frac{\phi}{2}, 0, 0, \sin\frac{\phi}{2}\}$$

Thus, the exact expressions for the components of $Q = \{q_0, q_1, q_2, q_3\}$ can be written as

$$\begin{aligned}
q_0 &= \cos\frac{\psi}{2}\cos\frac{\theta}{2}\cos\frac{\phi}{2} - \sin\frac{\psi}{2}\cos\frac{\theta}{2}\sin\frac{\phi}{2} \\
q_1 &= \sin\frac{\psi}{2}\sin\frac{\theta}{2}\cos\frac{\phi}{2} - \cos\frac{\psi}{2}\sin\frac{\theta}{2}\sin\frac{\phi}{2} \\
q_2 &= \cos\frac{\psi}{2}\sin\frac{\theta}{2}\cos\frac{\phi}{2} + \sin\frac{\psi}{2}\sin\frac{\theta}{2}\sin\frac{\phi}{2} \\
q_3 &= \cos\frac{\psi}{2}\cos\frac{\theta}{2}\sin\frac{\phi}{2} + \sin\frac{\psi}{2}\cos\frac{\theta}{2}\cos\frac{\phi}{2}.
\end{aligned}$$

Advantage over other representations

Euler angles suffer from a problem called "Gimbal lock" which occurs when two of the three independent rotation axes (or three gimbals) are in a parallel configuration with each other leaving rotation around one axis unachievable. So, the object under rotation loses one degree of freedom and is locked into rotation in a degenerate two-dimensional space. On the other hand, quaternions are more compact, efficient, and numerically stable and also allow for defining a *distance metric* between two rotations. It is also easier to generate a normalized quaternion which automatically assures an orthogonal rotational matrix.