

Applications of Quaternions in 3D Rotation

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Introduction

Historically, mathematicians have endeavoured to accurately describe the real world around us using mathematics. One of the most fundamental necessities of working with geometry applicable to real life is the ability to reason about mathematical properties in three dimensions. In the modern day, demand for working in three dimensions is ever increasing, with scientific applications in aerodynamic modeling, astrophysics, robotics and computational chemistry, in addition to numerous uses in computer generated imagery (CGI). In all of these use cases, there is a need for a rigorous mathematical framework to represent and manipulate the 3D world.

One of the intuitively simplest, but surprisingly complex aspects of transitioning from a two dimensional space to three dimensional is the problem of rotation. Indeed, there currently exist several competing mathematical models for 3D rotation in common use which bear their own strengths and weaknesses. Of these, some of the most common are 3D “rotation matrices” (which are usually constructed from “Euler angles”), and “quaternions” (Huynh, 2009). Hence, I have chosen the research question “To what extent can quaternions supersede rotation matrices constructed from Euler angles in representing 3D rotation?”

This investigation aims to explore the extent to which quaternions can perform better than rotation matrices constructed from Euler angles in representing 3D rotation, in order to draw conclusions about the applicability and usefulness of different rotation methods in computer graphics and scientific simulations.

As an aspiring computer animator and game developer, this question is of real significance to me as it will provide invaluable experience in the underlying concepts of my field of work for me. The understanding of rotation methods I would gain from this essay will allow me to apply mathematical knowledge to game prototypes I create, especially when programming physics or movement systems. Additionally, from online forums, I have noticed that developers working on the creative part of their work often do not understand mathematical concepts underpinning tools they work with daily, and this leads to ambiguity and confusion when communicating with other developers, or while working. Often, I feel like this could be due to the exaggerated barrier of entry to learning the underlying mathematics, leaving many afraid to investigate in the first place. I hope that this work will help me and others in demystifying how quaternions and rotation matrices work, in addition to showing why and when they are useful in an accessible manner. In order to build intuition for myself and the reader, nearly all of the formulas and proofs in this essay are of my own independent derivation, with some external sources used for inspiration and guidance, which should hopefully demonstrate that one does not need a tertiary education degree to investigate this topic holistically, and I find this very important to making mathematics accessible to everyone.

In order to answer the question, I first build intuition for the reader by examining how rotation works in two dimensions by introducing the concept of rotating axes using two dimensional transformation matrices, and then extend this to the three dimensions. I then introduce and evaluate the concept of Euler angles and link them with how they can be used to construct 3D rotation matrices. Following this, I introduce the concept of quaternions from their original definition and independently develop fundamental rules for operations with them. Finally, I investigate how quaternions can be used to represent 3D rotation and compare various aspects of their performance to rotation matrices constructed from Euler angles in order to draw conclusions about whether one could supersede the other in representing 3D rotation.

1 Rotation Matrices

Rotation matrices are considered one of the most versatile and fundamental ways of doing 3D rotation. They are often used in computer animation and praised for their computational efficiency and versatility. Mathematically, they represent a 3D linear transformation which, when applied to a set of points, describes a 3D rotation.

1.1 In two dimensions

It is worthwhile conceptually exploring what happens in two dimensions first, as this will introduce valuable concepts which will help with understanding how three dimensional rotation matrices work.

Let 2D points be represented as a position vector of the form $\vec{v} = \begin{bmatrix} x \\ y \end{bmatrix}$ where x and y represent the x and y coordinates of the point respective to the origin.

By representing the points as vectors, rotation of a point around the origin would be equivalent to rotating its position vector. Consider the rotation of point $(1, 0)$ by 45 degrees anti-clockwise:

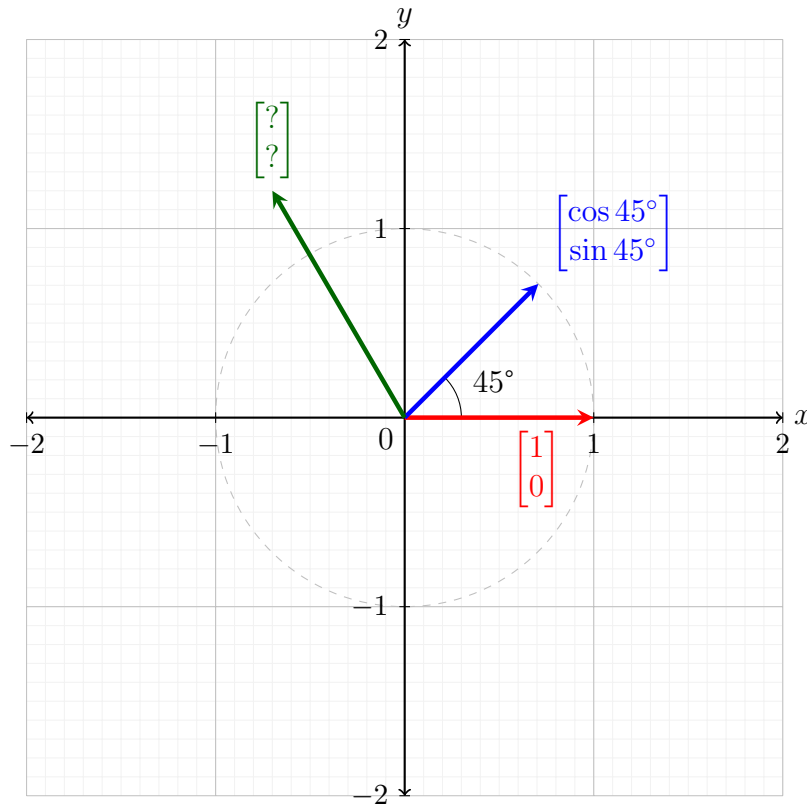


Figure 1: Apparent rotation of red vector $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ by 45° anti-clockwise to form blue vector

From Figure 1, it becomes evident that rotating the red vector of length 1 that lies along the x axis around a unit circle by θ degrees anti-clockwise is equivalent to finding a point on the unit circle at angle of θ degrees to the horizontal. Hence, for any angle θ , the rotation of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is equal to $\begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}$.

Indeed, this is the case for the simple example of a 2D unit vector above, but the applicability of using trigonometric functions to individually compose a vector's components grows increasingly limited as the complexity of the problem at hand increases. For example, consider the case where one would like to rotate several thousand, or millions of points by the same angle, as is often the case in computer graphics. In this case, it would be inefficient (and computationally expensive) to calculate the sine and cosine of the angle to each point individually, and this operation would also be equally expensive to reverse for a large number of points.

Linear transformation using matrices elegantly deals with these problems by introducing one concept - instead of transforming each individual vector, we can transform the axes themselves.

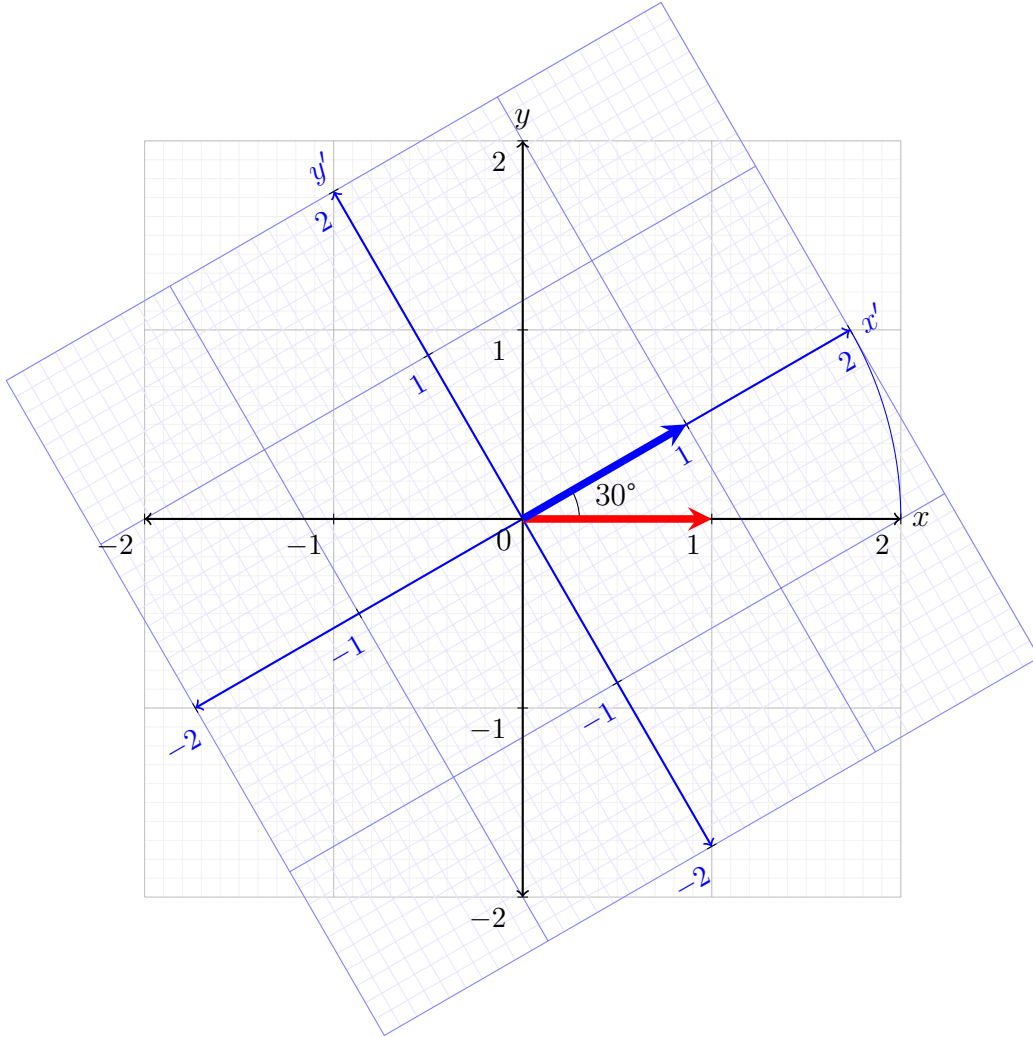


Figure 2: Overlay of new cartesian plane (blue) with axes x' and y' rotated 30° anti-clockwise relative to the original axes.

In Figure 2, the blue vector's coordinates on the rotated axes are identical to the red vector's coordinates on the original axes - both are $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ in their respective axes. In fact, any one point on the original axis has a counterpart on the rotated axis which corresponds to the rotation of that point about the origin by 30° . If we examine the coordinates of the blue vector \vec{b} on the original axes, we find that $\vec{b} = \begin{bmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \cos 30^\circ \\ \sin 30^\circ \end{bmatrix}$, which aligns with findings from the trigonometric method explored earlier above.

In practice, the idea of transforming the axes is integral to the speed of many 3D applications, because linear transformation matrices are not limited to just rotation. As we will soon find, it is possible to scale, warp and reflect a set of point vectors with the very same mathematical method, at no extra computational expense.

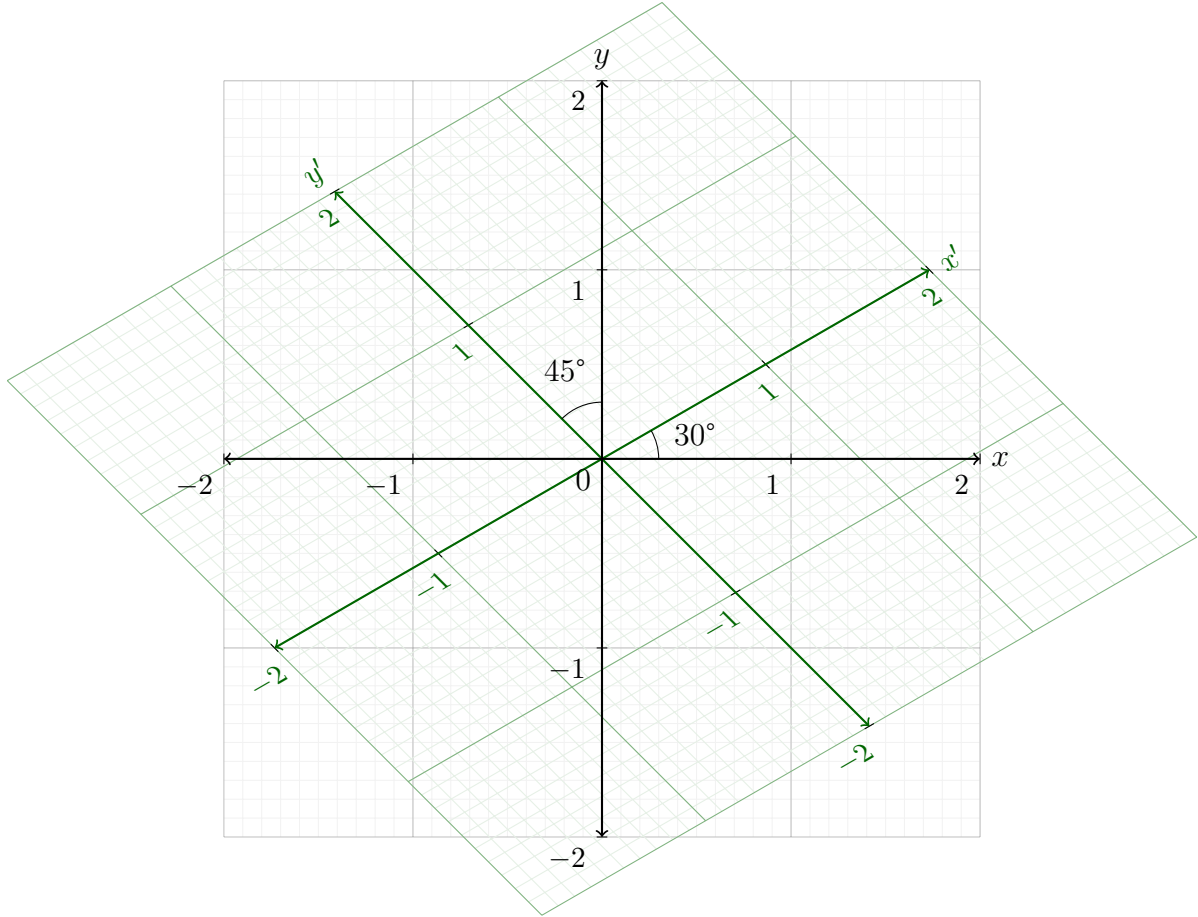


Figure 3: Overlay of new cartesian plane (green) with axes x' and y' rotated 30° anti-clockwise and 45° anti-clockwise respectively.

Figure 3 depicts what is known as a "shear". It occurs when each axis is rotated by a different angle, and results in warping of the transformed vectors, evident by the asymmetric appearance of the graph. Using a particular set of shears, it is technically possible to skew, flip, scale and even rotate any set of points in 2D space. As an aside, one might find it interesting that rotations are nothing more than two shears applied on different axes by an equal angle.

The elegance in this model comes from how one such transformation is actually computed. The first step to this is determining the direction and dilation of the transformed axes by examining what one desires to happen to the vectors $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ after the transformation. Because these vectors each lie in their respective axis, if the magnitude of any one of them changes, that means that that axis has been dilated by a factor of the magnitude. If the direction changes, that means that that axis has been rotated. By knowing the final position of these two vectors after a transformation, the transformation that took place can be reconstructed and applied to more points. This means that if one computes the transformation of just these two vectors once, the transformation can be inexpensively reapplied to a very large number of points, and this is the key reason why transformation matrices are used today.

Now that we understand the theory of axis shifting, we can look at how this can be represented mathematically using “transformation matrices”. Effectively, transformation matrices represent a transformation which can be applied to a set of points. 2D transformation matrices are constructed by taking the “axial vectors” discussed above and storing them in a 2×2 matrix. This allows us to represent any 2D transformation as a matrix multiplication.

Let \vec{x} be the position of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ after transformation: $\vec{x} = \begin{bmatrix} x_x \\ x_y \end{bmatrix}$

Let \vec{y} be the position of $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ after the transformation: $\vec{y} = \begin{bmatrix} y_x \\ y_y \end{bmatrix}$

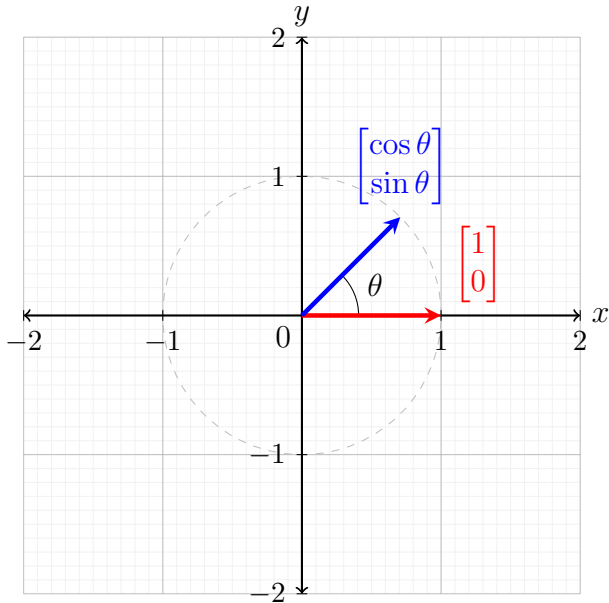
The transformation matrix M is therefore described by $M = \begin{bmatrix} x_x & y_x \\ x_y & y_y \end{bmatrix}$.

The transformation $T_M(\vec{v})$ of point vector $\vec{v} = \begin{bmatrix} v_x \\ v_y \end{bmatrix}$ using M can then be described by

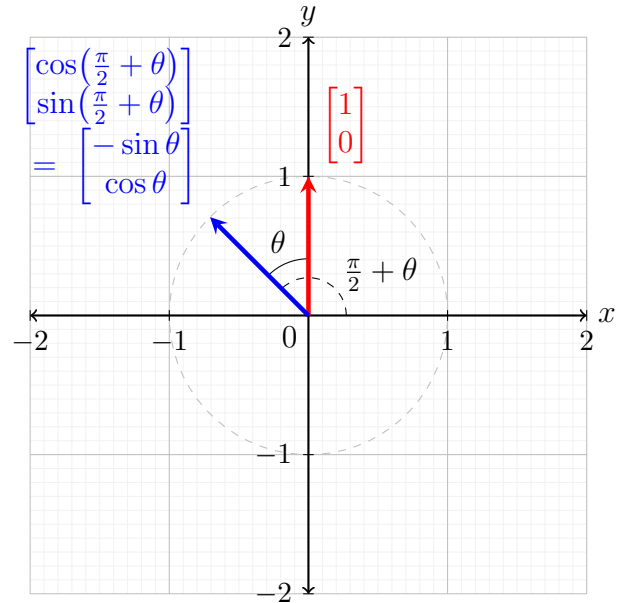
$$T_M(\vec{v}) = M\vec{v} = \begin{bmatrix} x_x & y_x \\ x_y & y_y \end{bmatrix} \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} x_x v_x + y_x v_y \\ x_y v_x + y_y v_y \end{bmatrix}$$

If \vec{x} and \vec{y} do not change after a transformation, they would be equal to $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ respectively. In this state, they are called the “identity vectors” \vec{x}_i and \vec{y}_i . From this, a transformation matrix which does nothing (similarly called the “identity matrix”) I can be constructed in the form $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. In

this case, $T_I(\vec{v}) = \begin{bmatrix} x_{ix} & y_{ix} \\ x_{iy} & y_{iy} \end{bmatrix} \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} (1)v_x + (0)v_y \\ (0)v_x + (1)v_y \end{bmatrix} = \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \vec{v}$.



(a) Rotation of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ by angle θ from the x-axis.



(b) Rotation of $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ by angle θ from the y-axis.

Figure 4: Rotation of the 2D axes by angle θ anti-clockwise.

As seen in Figure 4, on a unit circle, a counter-clockwise rotation of the identity position vector $\vec{x}_i = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ by θ would be represented as $\vec{x} = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}$. Likewise, the rotation of the identity position vector $\vec{y}_i = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ would be equivalent to first rotating by $\frac{\pi}{2}$ and then by θ , hence $\vec{y} = \begin{bmatrix} \cos(\frac{\pi}{2} + \theta) \\ \sin(\frac{\pi}{2} + \theta) \end{bmatrix} = \begin{bmatrix} -\sin \theta \\ \cos \theta \end{bmatrix}$. Hence, a 2D transformation matrix $R(\theta)$ can be constructed so that it rotates the 2D axes by an angle θ using \vec{x} and \vec{y} . This is what is known as a rotation matrix.

$$R(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

You can combine different linear transformations by multiplying a vector by multiple transformation matrices sequentially. For example, you might choose to apply a shear or a scale to your points before rotating them. This property applies to both two and three dimensional transformation matrices. Because of this versatility, transformation matrices are very easy to work with and integrate into more complex applications where multiple transformations need to be chained.

It is important to note that matrix multiplication is not commutative, and hence it is important to always multiply matrices in a right-to-left order: if one wanted to apply the linear transformations $T_1 \rightarrow T_2 \rightarrow T_3$ on vector \vec{v} , the correct multiplication would be $T_3 T_2 T_1 \vec{v}$.

1.2 In three dimensions

Now that we have established basic intuition on what 2D matrices transformation allow us to do, we can extend the established observations to three dimensions.

In 3D, there are now three axes which must be kept track of:

- X (left \leftrightarrow right)
- Y (forward $\swarrow \nearrow$ back)
- Z (up \updownarrow down)

The identity vectors \vec{x}_0 , \vec{y}_0 and \vec{z}_0 in three dimensions, like we saw with 2D, have a magnitude of 1 and lie on the axis they represent.

$$\vec{x}_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \vec{y}_0 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \vec{z}_0 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

A 3D transformation defines the transition from the identity vectors into ones (\vec{x} , \vec{y} and \vec{z}) with potentially different magnitude and direction, signifying reoriented axes.

$$\vec{x} = \begin{bmatrix} x_x \\ y_x \\ z_x \end{bmatrix} \quad \vec{y} = \begin{bmatrix} x_y \\ y_y \\ z_y \end{bmatrix} \quad \vec{z} = \begin{bmatrix} x_z \\ y_z \\ z_z \end{bmatrix}$$

Changing the magnitude and/or direction of these vectors results in various effects on the 3D space, similar to how this works in two dimensions. Individually changing any one or two of these vectors results in the three dimensional equivalent of shear called “deformation” as the three axes would no longer be orthogonal, therefore appearing to “crush” points within them. This property is often used in 3D animation to compress or stretch objects – a ball hitting a wall, or human skin stretching, for example.

As before, constructing a matrix out of these vectors allows us to leverage matrix multiplication to transform points. A 3×3 matrix M can now be constructed to represent a 3D transformation using the above axes. Hence, the identity 3D rotation matrix M_0 can also be defined here.

$$M = \begin{bmatrix} x_x & y_x & z_x \\ x_y & y_y & z_y \\ x_z & y_z & z_z \end{bmatrix} \quad \therefore \quad M_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For a transformation $T_M(\vec{v})$ on $\vec{v} = \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix}$ by matrix M ,

$$T_M(\vec{v}) = M\vec{v} = \begin{bmatrix} x_x & y_x & z_x \\ x_y & y_y & z_y \\ x_z & y_z & z_z \end{bmatrix} \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \begin{bmatrix} x_x v_x + y_x v_y + z_x v_z \\ x_y v_x + y_y v_y + z_y v_z \\ x_z v_x + y_z v_y + z_z v_z \end{bmatrix}$$

Now that we are familiar with the form of a 3D rotation matrix, we can move on to methods of constructing one. In a sense, one could say simply knowing how to use a rotation matrix to transform points is rather useless without knowing how to construct the rotation matrix in the first place. Historically, many construction methods have been invented and used widely, each with their own benefits and shortcomings.

It is interesting to note that while I initially wanted to compare rotation matrices as a whole to quaternion rotation, this fact occurred to me and I realised that it would be more appropriate to compare the most popular construction method of rotation matrices to quaternion rotation instead.

1.3 Construction from Euler angles

1.3.1 Concept

In real life, it is practical to represent rotations with easily measurable metrics, like angles. Aircraft and watercraft make extensive use of yaw, pitch and roll angles in instrumentation to aid their pilots in judging the orientation of the craft. Yaw indicates the left-right angle of the nose, rotating about the vertical axis, somewhat like the “heading” of aircraft. A yaw of 0° indicates the nose is pointing directly north, and a yaw of 90° indicates the nose is pointing directly east, etc. Pitch indicates the angle of the nose relative to the horizon, and roll indicates how much the plane is turned about the forward axis. Figure 5 demonstrates this in terms of an x , y and z axis. In aircraft, y axis here can be considered the “front” of the craft, the z axis the “up” direction and the x axis the “right” direction.

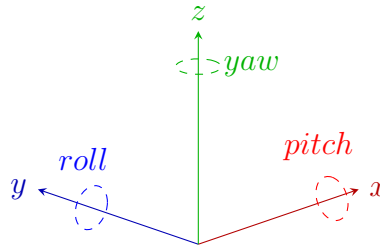


Figure 5: Yaw pitch and roll

Euler angles are based around this concept. A set of Euler angles is a 3D vector containing the yaw, pitch and roll of an object around a reference frame. In the example of aircraft, the reference frame is usually the surface of the Earth. In space, it is usually a prominent constellation or celestial object. If one wishes to encode a rotation as a set of Euler angles, one just needs to measure the angles between the rotated axes and the original axes of the reference frame.

As this system of representing rotation is simple, measurable and intuitive for humans to use, one of the main ways of constructing a rotation matrix is through Euler angles.

1.3.2 Deriving rotation matrices for each angle

Consider rotating the 3D identity axes with vectors \vec{x}_0 , \vec{y}_0 and \vec{z}_0 by θ around the X axis. Let the matrix that describes this rotation in terms of θ be $R_x(\theta)$. After the transformation, let the identity vectors' new positions be \vec{x}_r , \vec{y}_r and \vec{z}_r .

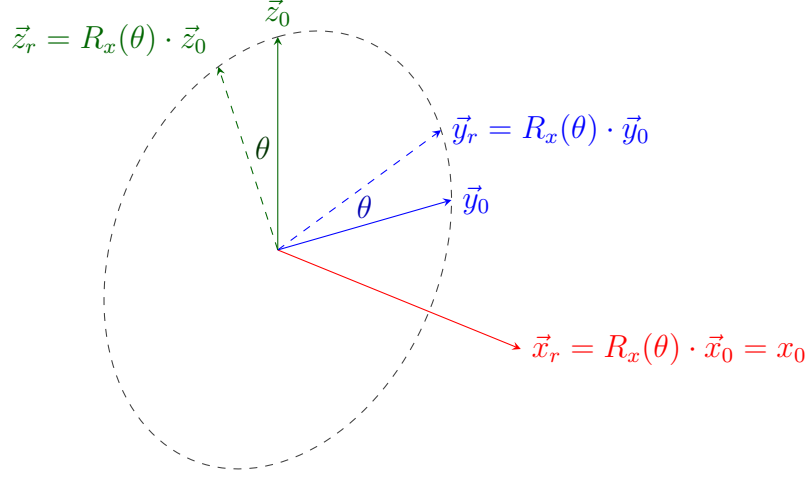


Figure 6: Rotation around the X-axis by angle θ . \vec{x}_r , \vec{y}_r and \vec{z}_r represent the identity vectors after the transformation by $R_x(\theta)$ where $\vec{x}_0 \rightarrow \vec{x}_r$, $\vec{y}_0 \rightarrow \vec{y}_r$ and $\vec{z}_0 \rightarrow \vec{z}_r$.

Considering the components of \vec{x}_r , \vec{y}_r and \vec{z}_r ,

$$\vec{x}_r = \begin{bmatrix} x_{rx} \\ x_{ry} \\ x_{rz} \end{bmatrix} \quad \vec{y}_r = \begin{bmatrix} y_{rx} \\ y_{ry} \\ y_{rz} \end{bmatrix} \quad \vec{z}_r = \begin{bmatrix} z_{rx} \\ z_{ry} \\ z_{rz} \end{bmatrix}$$

Hence, in Figure 6, the rotation $R_x(\theta)$ could be represented as

$$R_x(\theta) = \begin{bmatrix} x_{rx} & y_{rx} & z_{rx} \\ x_{ry} & y_{ry} & z_{ry} \\ x_{rz} & y_{rz} & z_{rz} \end{bmatrix}$$

From Figure 6 it becomes apparent that points that lie along \vec{x}_0 do not move at all, because the rotation is happening around \vec{x}_0 in the first place. Hence,

$$\vec{x}_r = \vec{x}_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Points colinear with the Y axis get rotated around a unit circle in the YZ plane (pictured in Figure 6). Hence, \vec{y}_r is described with the trigonometric functions $\cos \theta$ and $\sin \theta$ as its Y and Z components. The rotation of \vec{z}_r can be derived similarly.

$$\vec{y}_r = \begin{bmatrix} 0 \\ \cos \theta \\ \sin \theta \end{bmatrix} \quad \vec{z}_r = \begin{bmatrix} 0 \\ -\sin \theta \\ \cos \theta \end{bmatrix}$$

Combining \vec{x}_r , \vec{y}_r and \vec{z}_r yields the rotation matrix $R_x(\theta)$ for rotations around the X-axis.

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{bmatrix}$$

A similar process can be followed to derive the rotation matrices by the Y and Z axes, so it has been omitted for brevity. The only thing that changes in the derivation process is that the plane of the circle always lies in the plane described by the two axes perpendicular to the rotation axis.

$$R_y(\theta) = \begin{bmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{bmatrix} \quad R_z(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

1.3.3 Multiplication

It is now possible to compute a rotation matrix in terms of the Euler angles α , β and γ (representing pitch, roll and yaw respectively) by first constructing each individual matrix, then multiplying them. Effectively, this applies the rotation $R_x(\alpha)$ followed by $R_y(\beta)$ and finally $R_z(\gamma)$.

$$\begin{aligned} R(\alpha, \beta, \gamma) &= R_z(\gamma)R_y(\beta)R_x(\alpha) \\ &= \begin{bmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & -\sin \alpha \\ 0 & \sin \alpha & \cos \alpha \end{bmatrix} \\ &= \begin{bmatrix} \cos \beta \cos \gamma & \sin \alpha \sin \beta \cos \gamma - \cos \alpha \sin \gamma & \cos \alpha \sin \beta \cos \gamma + \sin \alpha \sin \gamma \\ \cos \beta \sin \gamma & \sin \alpha \sin \beta \sin \gamma + \cos \alpha \cos \gamma & \cos \alpha \sin \beta \sin \gamma - \sin \alpha \cos \gamma \\ -\sin \beta & \sin \alpha \cos \beta & \cos \alpha \cos \beta \end{bmatrix} \end{aligned}$$

As matrix multiplication does not commute, it is not always the case that rotating by an axis A, then rotating by B would be the same as rotating first by axis B, then by A. Hence, it is important to note that the order of multiplication of R_z , R_y and R_x produces a unique final rotation. For the rest of the investigation, the $x \rightarrow y \rightarrow z$ rotation order seen above will be used. This is alternatively called the ZYX Tait-Bryan order (Wikipedia Contributors, 2023).

It is important to note that traditionally, there has been no set standard defining which rotation order to use - this is left up to choice. In 3D software which uses Euler angles, it is still required to manually specify the order of rotation. When working with large teams of people, such as in an animation and game development studio, or a scientific research team, it is still required to agree on a standard order of Euler angles to avoid ambiguity and misunderstanding, which is potentially a weakness of using the Euler angle system in the first place.

1.4 The gimball lock problem

There is another large problem with constructing rotation matrices from Euler angles. Suppose you rotated an object with the Euler angles α , β and γ , where $\beta = \frac{\pi}{2}$

$$R(\alpha, \frac{\pi}{2}, \gamma) = \begin{bmatrix} \cos \frac{\pi}{2} \cos \gamma & \sin \alpha \sin \frac{\pi}{2} \cos \gamma - \cos \alpha \sin \gamma & \cos \alpha \sin \frac{\pi}{2} \cos \gamma + \sin \alpha \sin \gamma \\ \cos \frac{\pi}{2} \sin \gamma & \sin \alpha \sin \frac{\pi}{2} \sin \gamma + \cos \alpha \cos \gamma & \cos \alpha \sin \frac{\pi}{2} \sin \gamma - \sin \alpha \cos \gamma \\ -\sin \frac{\pi}{2} & \sin \alpha \cos \frac{\pi}{2} & \cos \alpha \cos \frac{\pi}{2} \end{bmatrix}$$

Substituting $\cos \frac{\pi}{2} = 0$ and $\sin \frac{\pi}{2} = 1$:

$$= \begin{bmatrix} 0 & \sin \alpha \cos \gamma - \cos \alpha \sin \gamma & \cos \alpha \cos \gamma + \sin \alpha \sin \gamma \\ 0 & \sin \alpha \sin \gamma + \cos \alpha \cos \gamma & \cos \alpha \sin \gamma - \sin \alpha \cos \gamma \\ -1 & 0 & 0 \end{bmatrix}$$

Applying trigonometric identities:

$$= \begin{bmatrix} 0 & \sin(\alpha - \gamma) & \cos(\alpha - \gamma) \\ 0 & \cos(\alpha - \gamma) & -\sin(\alpha - \gamma) \\ -1 & 0 & 0 \end{bmatrix}$$

Let $\alpha - \gamma = \theta$. The rotation matrix R can now be expressed as $R(\theta) = \begin{bmatrix} 0 & \sin \theta & \cos \theta \\ 0 & \cos \theta & -\sin \theta \\ -1 & 0 & 0 \end{bmatrix}$.

By inspecting this matrix, we find that:

- \vec{x}_0 will always transform to $\begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix} = -\vec{z}_0$. This means that this is the axis around which rotation occurs by angle θ as it remains constant irrespective of the value of θ .
- \vec{y} and \vec{z} revolve around a unit circle in the YX plane by angle θ perpendicularly to the axis of rotation of $-\vec{z}_0$, as seen before in Figure 6.
- This matrix is entirely in terms of θ . When either α or γ is changed, the resulting rotation is always around the $-\vec{z}_0$ axis as it is independent of θ .

Hence, this shows that when $\beta = \frac{\pi}{2}$, the rotation matrix actually loses one degree of rotational freedom entirely as α and γ describe rotation about the same axis because they both contribute to the value of θ . In fact, the same can be shown for the case where one of α , β or γ is equal to $\frac{(2b+1)\pi}{2}$ where $b \in \mathbb{Z}$.

This phenomenon is known as "gimball lock". It is widely considered to be one of the largest issues with using Euler angles for rotation. It is significant because it means that for specific angles of rotation, the system can actually lose the ability to freely rotate, and may even be unable to escape the gimball lock.

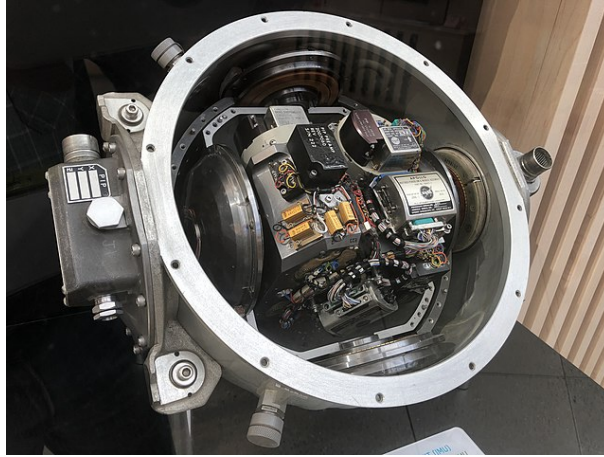


Figure 7: The Apollo 11 "Inertial Measurement Unit" responsible for guidance & orientation of the spacecraft in space.

One of the most famous examples of gimbal lock in action was during the 1969 Apollo 11 manned mission to the moon. The Apollo 11 spacecraft was equipped with an "Inertial Measurement Unit" which was responsible for measuring the orientation of the spacecraft in space. This was done using three gyroscopes, each of which measured the rotation of the spacecraft in terms of yaw, pitch and roll relative to the craft's starting position. Mechanically, these gyroscopes, too undergo gimbal lock when the spacecraft is oriented at specific angles resulting in complete disorientation of the guidance unit. This happened in-flight during the actual mission, meaning that the unit had to be manually moved out of the gimbal lock position using the stars as a reference, in order to regain the lost degree of freedom.

This fundamental flaw with Euler angles demonstrates how despite their simplicity and intuitiveness, they clearly leave a lot to be desired for rigorously representing 3D rotations.

2 Improving on Euler angles with Quaternions

In 1843, Irish mathematician Sir William Rowan Hamilton proposed an alternative way to represent 3D rotation by using four dimensional imaginary numbers called "quaternions". Quaternions allow us to rotate any 3D position vector around any 3D axis by a certain angle with the power of four dimensions (Dam, Koch and Lillholm, 1998). Rotation about an axis is not anything special in particular, in fact, rotating around the X, Y and Z axes individually has already been explored in section 1.3.2.

Quaternions, like rotation matrices constructed from Euler angles, have seen numerous applications in pretty nearly all fields of science and engineering where 3D rotations are required. As we will soon see, quaternions address many of the downsides of Euler angle matrices, and can often be a very efficient alternative to them.

2.1 Hamilton's Definition

Quaternions, like complex numbers, are defined with "real" and "imaginary" parts, and are essentially an extension of the complex numbers to four dimensions. The set of all quaternions is known as \mathbb{H} , named after Hamilton. Algebraically, a quaternion q can be defined in terms of the coefficients of its terms:

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

i , j and k , called "basic quaternions", do not have an explicit definition of their value but are rather defined expressly in terms of the way they interact with each other in that they must satisfy the equality

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

(Dam, Koch and Lillholm, 1998).

2.2 Basic Quaternions

In order to start using quaternions for rotation, we must first explore the details that their definition implies. We must first define how i , j , and k interact algebraically, as this will be the basis for many of the quaternion's properties.

2.2.1 Multiplying by Real Numbers

For any $n \in \mathbb{R}$, it is defined that $in = ni$, $jn = nj$ and $kn = nk$. Hence, for any $q \in \mathbb{H}$, $qn = nq$. Quaternion multiplication by real numbers does, in fact, commute (Dam, Koch and Lillholm, 1998).

2.2.2 Multiplication by other basic quaternions

Hamilton's quaternion definition can then be used to derive the multiplicative interactions between i , j and k :

$ijk = k^2$	$ijk = i^2$
$ijk^2 = k^2k$	$i^2jk = i \cdot i^2$
$ij(-1) = (-1)k$	$(-1)jk = i(-1)$
$ij = k$	$jk = i$
$i = jk$	$k = ij$
$ji = j^2k$	$kj = ij^2$
$ji = -k$	$kj = -i$
$ij = k$	$k = ij$
$kij = k^2$	$ik = i^2j$
$kij^2 = k^2j$	$ik = -j$
$ki(-1) = (-1)j$	
$ki = j$	

An important concept becomes apparent from the above calculations. Like with matrices, quaternion multiplication by other quaternions is not commutative, that is, it can be the case that $q_1q_2 \neq q_2q_1$ where $q_1, q_2 \in \mathbb{H}$. For example, it is seen above that while $ij = k$, $ji = -k$.

The multiplication table of basic quaternions is hence formed, where the column represent the left operand and the row represents the right operand in multiplication.

\times	i	j	k
i	-1	$-k$	j
j	k	-1	$-i$
k	$-j$	i	-1

Table 1: Basic quaternion noncommutative multiplication table

As an aside, it is perhaps interesting that the noncommutativity of quaternions and matrices reflects the noncommutativity of rotations in 3D space. It could be the case that mathematical models used to represent rotations are noncommutative because the order of rotations themselves matters, and what we see as an algebraic constraint is a reflection of what is physically possible.

2.2.3 Associativity

Quaternion multiplication is associative in that $(q_1q_2)q_3 = q_1(q_2q_3)$ where $q_1, q_2, q_3 \in \mathbb{H}$. The same property applies for addition, $(q_1 + q_2) + q_3 = q_1 + (q_2 + q_3)$ where $q_1, q_2, q_3 \in \mathbb{H}$.

This associativity allows for application of useful algebraic techniques like the distributive law.

2.3 Quaternion Operations

2.3.1 Multiplication of non-basic quaternions

Let $q_1 = a_1 + b_1i + c_1j + d_1k$ and $q_2 = a_2 + b_2i + c_2j + d_2k$ where $a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2 \in \mathbb{R}$. The multiplication q_1q_2 can be computed using the distributive law.

$$\begin{aligned}
q_1q_2 &= (a_1 + b_1i + c_1j + d_1k)(a_2 + b_2i + c_2j + d_2k) \\
&= a_1a_2 + a_1b_2i + a_1c_2j + a_1d_2k \\
&\quad + b_1a_2i + b_1b_2i^2 + b_1c_2ij + b_1d_2ik \\
&\quad + c_1a_2j + c_1b_2ji + c_1c_2j^2 + c_1d_2jk \\
&\quad + d_1a_2k + d_1b_2ki + d_1c_2kj + d_1d_2k^2
\end{aligned}$$

Applying the basic quaternion rules then factoring out the real part and i , j , and k ,

$$\begin{aligned}
&= a_1a_2 - b_1b_2 - c_1c_2 - d_1d_2 \\
&\quad + (a_1b_2 + b_1a_2 + c_1d_2 - d_1c_2)i \\
&\quad + (a_1c_2 - b_1d_2 + c_1a_2 + d_1b_2)j \\
&\quad + (a_1d_2 + b_1c_2 - c_1b_2 + d_1a_2)k
\end{aligned}$$

2.3.2 Conjugation

For any quaternion $q = a + bi + cj + dk$ $a, b, c, d \in \mathbb{R}$, its conjugate q^* is defined as $q^* = a - bi - cj - dk$.

2.3.3 Multiplication by Conjugate

Suppose one was to multiply a quaternion q by its conjugate q^* ,

$$\begin{aligned} qq^* &= (a + bi + cj + dk)(a - bi - cj - dk) \\ &= a^2 - abi - acj - adk \\ &\quad + bia - (bi)^2 - bicj - bidk \\ &\quad + cja - cjbi - (cj)^2 - cjdk \\ &\quad + dka - dkbi - dkci - (dk)^2 \end{aligned}$$

Reordering real coefficients and expanding

$$\begin{aligned} &= a^2 - abi - acj - adk \\ &\quad + abi - b^2i^2 - bcij - bdik \\ &\quad + acj - bcji - c^2j^2 - cjdk \\ &\quad + adk - bdk i - cdki - d^2k^2 \end{aligned}$$

Applying basic quaternion rules

$$\begin{aligned} &= a^2 - abi - acj - adk \\ &\quad + abi + b^2 - bck + bdj \\ &\quad + acj + bck + c^2 - cdi \\ &\quad + adk - bdj + cdi + d^2 \end{aligned}$$

Cancelling like terms,

$$= a^2 + b^2 + c^2 + d^2$$

Additionally, given $a, b, c, d \in \mathbb{R}$

$$\therefore a^2 + b^2 + c^2 + d^2 \in \mathbb{R}$$

$$\therefore qq^* \in \mathbb{R}$$

Hence, if you multiply a quaternion by its conjugate, the result will always be a real number and equal to the sum of the squares of its coefficients.

2.3.4 Norm

The norm of a quaternion q is defined as $|q| = \sqrt{qq^*} = \sqrt{a^2 + b^2 + c^2 + d^2}$, corresponding to the length of the quaternion in 4D space, coming from the extension of the Pythagorean theorem in four dimensions. A quaternion of norm 1 is called a unit quaternion. It is hence possible to normalize a quaternion q by dividing it by its norm. If \hat{q} represents the normalization of q , $q \in \mathbb{H}$, $\hat{q} = \frac{q}{|q|}$.

2.3.5 Inverse

The inverse q^{-1} of a quaternion q exists such that $qq^{-1} = 1$, effectively "undoing" any multiplication caused by q . The inverse of a quaternion can be computed using the previously established rules.

$$\begin{aligned} qq^{-1} = 1 &\Rightarrow q^{-1} = \frac{1}{q} \\ \Rightarrow q^{-1} &= \frac{1}{q} \cdot \frac{q^*}{q^*} = \frac{q^*}{qq^*} = \frac{q^*}{a^2 + b^2 + c^2 + d^2} = \frac{q^*}{|q|^2} \end{aligned}$$

In terms of 3D rotations, the inverse of a quaternion allows one to effectively "reverse" or "undo" a rotation similarly to how multiplying by the inverse of a transformation matrix reverses the transformation.

2.4 Rotating position vectors

Although quaternions harbor many different interesting properties, from the very beginning, Hamilton defined them out of the need for unit quaternions to represent 3D rotation in a straightforward manner.

Hamilton's method of rotation involves taking a vector one wishes to rotate, for example $\vec{v} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ and constructing a quaternion p out of it such that $p = xi + yj + zk$. As the real part $\text{Re}(p)$ of p is zero, p is called a "pure quaternion".

Like with rotation matrices, one can then construct a "rotation quaternion" $q = a + bi + cj + dk$ that represents a rotation about an axis $\vec{g} = \begin{bmatrix} b \\ c \\ d \end{bmatrix}$ by an angle θ as follows.

Considering that q is a unit quaternion,

$$|q| = 1 = |q|^2 = a^2 + b^2 + c^2 + d^2$$

$$\text{Given that } \sin^2 \theta + \cos^2 \theta = 1,$$

$$a^2 + (b^2 + c^2 + d^2) = 1 = \sin^2 \theta + \cos^2 \theta$$

From this, one could infer that

$$a = \cos \theta, \sqrt{b^2 + c^2 + d^2} = |\vec{g}| = \sin \theta \quad \text{or} \quad a = \sin \theta, \sqrt{b^2 + c^2 + d^2} = |\vec{g}| = \cos \theta$$

Indeed, both of these formulas work for constructing quaternions from an axis and angle. While the second case works, by convention, the first formula is far more widely used and accepted, so it will be the one used in this investigation hereafter. Hence, $a = \cos \theta$ $|\vec{g}| = \sin \theta$.

Let h equal a quaternion of the form $h = bi + cj + dk$. Let the normalization of h be $\hat{h} = \frac{h}{|h|}$.

$$\begin{aligned} \therefore |\vec{g}| &= |h| = \sqrt{b^2 + c^2 + d^2} \\ \Rightarrow bi + cj + dk &= (bi + cj + dk) \frac{|\vec{g}|}{|\vec{g}|} = \frac{h}{|h|} |\vec{g}| = \hat{h} \sin \theta \end{aligned}$$

Hence, for a rotation by any axis and angle, one can construct a rotation quaternion $q = \cos \theta + \hat{h} \sin \theta$, where θ represents the rotation angle, and \hat{h} represents the normalization of a pure quaternion of the form $xi + yj + zk$ where x , y and z are the components of a 3D vector representing the rotation axis.

When Hamilton was looking into rotation, he discovered that whenever a pure quaternion p is multiplied by a rotation quaternion q from the left (that is, $q \cdot p$), the transformation inevitably distorts it into the fourth dimension.

$$\begin{aligned}
qp &= (a + bi + cj + dk)(xi + yj + zk) \\
&= axi + ayj + azk + bxi^2 + bxi j + bxik + cxji + cyj^2 + cyjk + dxki + dykj + dzk^2 \\
&= axi + ayj + azk - bx + bxx - bxj - cxk - cy + cyi + dxj - dxi - dz \\
\therefore \text{Re}(qp) &= -bx - cy - dz = -(bx + cy + dz) = - \left(\begin{bmatrix} b \\ c \\ d \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} \right) \\
\therefore \text{Re}(qp) &\neq 0 \quad \text{As long as } \begin{bmatrix} b \\ c \\ d \end{bmatrix} \text{ is not parallel to } \begin{bmatrix} x \\ y \\ z \end{bmatrix}.
\end{aligned}$$

That is, the result of the multiplication is no longer a pure quaternion as long as the point being rotated does not lie in the rotation axis (in which case no transformation on it would occur first place as discussed earlier).

Hamilton hence defined the rotation of a pure quaternion p to r by a rotation quaternion q as $r = qpq^{-1} = qpq^*$. By multiplying by q^{-1} , from the right, the change in $\text{Re}(qp)$ is undone,

$$\begin{aligned}
qpq^* &= (a + bi + cj + dk)(xi + yj + zk)(a - bi - cj - dk) \\
&= (axi + ayj + azk - bx + bxx - bxj - cxk - cy + cyi + dxj - dxi - dz)(a - bi - cj - dk) \\
&\text{Expansion of the above has been omitted for brevity, but, notably,} \\
&\text{Re}(qpq^*) = -abx - acy - adz + abx - bcy - bdx + acy + bcy - bcx + cdx + bcx + adz + bdx - cdx \\
&\text{Cancelling opposite terms, } \Rightarrow \text{Re}(qpq^*) = 0
\end{aligned}$$

However, by doing this, $\text{Im}(qpq^*)$ is affected twice, first by $q \cdot p$ and then by $(qp) \cdot q^*$. Effectively, this means that the rotation described by q is applied to the vector represented by pure quaternion p twice, appearing to apply twice the rotation angle.

Knowing this, one can remedy this problem by simply halving the rotation angle. Finally, this leaves us with the following formula for the rotation of a vector $\vec{v} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ around an axis $\vec{g} = \begin{bmatrix} b \\ c \\ d \end{bmatrix}$ by an angle θ using quaternions:

Let $p = xi + yj + zk$ (the point (x, y, z) being rotated)

Let $h = bi + cj + dk$ (the axis $\begin{bmatrix} b \\ c \\ d \end{bmatrix}$ around which the rotation happens)

Let $q = \cos \frac{\theta}{2} + \frac{h}{|h|} \sin \frac{\theta}{2}$ (rotation quaternion q for angle θ)

$r = qpq^{-1}$ (calculating rotated point r)

Evaluating $r = qpq^{-1}$, given that $q = a_q + b_q i + c_q j + d_q k$

$$\begin{aligned} qp &= (-b_q x - c_q y - d_q z) \\ &+ (a_q x + c_q z - d_q y)i \\ &+ (a_q y - b_q z + d_q x)j \\ &+ (a_q z + b_q y - c_q x)k \end{aligned}$$

Let:

$$\begin{aligned} a_{qp} &= -b_q x - c_q y - d_q z, \\ b_{qp} &= a_q x + c_q z - d_q y, \\ c_{qp} &= a_q y - b_q z + d_q x, \\ d_{qp} &= a_q z + b_q y - c_q x \end{aligned}$$

As q is of norm one, $q^{-1} = q^*$

$$\begin{aligned} \therefore qpq^{-1} &= qpq^* = r \\ &= a_{qp}a_q + b_{qp}b_q + c_{qp}c_q + d_{qp}d_q \\ &+ (-a_{qp}b_q + b_{qp}a_q - c_{qp}d_q + d_{qp}c_q)i \\ &+ (-a_{qp}c_q + b_{qp}d_q + c_{qp}a_q - d_{qp}b_q)j \\ &+ (-a_{qp}d_q - b_{qp}c_q + c_{qp}b_q + d_{qp}a_q)k \end{aligned}$$

Knowing that qpq^* must be a pure quaternion, one can extract the final rotated position vector \vec{r} from $\text{Im}(qpq^*)$.

Given

$$\vec{r} = \begin{bmatrix} -a_{qp}b_q + b_{qp}a_q - c_{qp}d_q + d_{qp}c_q \\ -a_{qp}c_q + b_{qp}d_q + c_{qp}a_q - d_{qp}b_q \\ -a_{qp}d_q - b_{qp}c_q + c_{qp}b_q + d_{qp}a_q \end{bmatrix}$$

Substituting a_{qp} , b_{qp} , c_{qp} and d_{qp} :

$$= \begin{bmatrix} (b_q x + c_q y + d_q z)b_q + (a_q x + c_q z - d_q y)a_q \\ (b_q x + c_q y + d_q z)c_q + (a_q x + c_q z - d_q y)d_q \\ (b_q x + c_q y + d_q z)d_q - (a_q x + c_q z - d_q y)c_q \\ -(a_q y - b_q z + d_q x)d_q + (a_q z + b_q y - c_q x)c_q \\ +(a_q y - b_q z + d_q x)a_q - (a_q z + b_q y - c_q x)b_q \\ +(a_q y - b_q z + d_q x)b_q + (a_q z + b_q y - c_q x)a_q \end{bmatrix}$$

Expanding:

$$= \begin{bmatrix} a_q^2 x + 2a_q c_q z - 2a_q d_q y + b_q^2 x + 2b_q c_q y + 2b_q d_q z - c_q^2 x - d_q^2 x \\ a_q^2 y - 2a_q b_q z + 2a_q d_q x - b_q^2 y + 2b_q c_q x + c_q^2 y + 2c_q d_q z - d_q^2 y \\ a_q^2 z + 2a_q b_q y - 2a_q c_q x - b_q^2 z + 2b_q d_q x - c_q^2 z + 2c_q d_q y + d_q^2 z \end{bmatrix}$$

Collecting like terms:

$$= \begin{bmatrix} (a_q^2 + b_q^2 - c_q^2 - d_q^2)x & + & (2b_q c_q - 2a_q d_q)y & + & (2a_q c_q + 2b_q d_q)z \\ (2a_q d_q + 2b_q c_q)x & + & (a_q^2 - b_q^2 + c_q^2 - d_q^2)y & + & (2c_q d_q - 2a_q b_q)z \\ (2b_q d_q - 2a_q c_q)x & + & (2a_q b_q + 2c_q d_q)y & + & (a_q^2 - b_q^2 - c_q^2 + d_q^2)z \end{bmatrix}$$

Factoring out $[x, y, z]$:

$$= \begin{bmatrix} a_q^2 + b_q^2 - c_q^2 - d_q^2 & 2(b_q c_q - a_q d_q) & 2(a_q c_q + b_q d_q) \\ 2(a_q d_q + b_q c_q) & a_q^2 - b_q^2 + c_q^2 - d_q^2 & 2(c_q d_q - a_q b_q) \\ 2(b_q d_q - a_q c_q) & 2(a_q b_q + c_q d_q) & a_q^2 - b_q^2 - c_q^2 + d_q^2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$= \begin{bmatrix} 1 - 2(c_q^2 + d_q^2) & 2(b_q c_q - a_q d_q) & 2(a_q c_q + b_q d_q) \\ 2(a_q d_q + b_q c_q) & 1 - 2(b_q^2 + d_q^2) & 2(c_q d_q - a_q b_q) \\ 2(b_q d_q - a_q c_q) & 2(a_q b_q + c_q d_q) & 1 - 2(b_q^2 + c_q^2) \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Looking at the above result, we can see that the formula for rotation using quaternions can actually also be represented using a linear transformation matrix. This means that, in fact, rotation matrices can be constructed out of quaternions, without suffering from gimbal lock, only because quaternions are not susceptible to it. This is quite interesting, as it further highlights the previously mentioned point about how the usefulness of a rotation matrix depends on how it was constructed in the first place.

2.5 Computational complexity

Although this formula may appear more complicated than the one for deriving rotation matrices from Euler angles to humans, it harbors some invaluable computational savings in computers. The two formulas comprise of the same number of scalar multiplications and additions, and so are roughly equivalent in terms of computational cost. However, as already mentioned, quaternions do not suffer from gimbal lock, and so the formula for deriving rotation matrices from quaternions is actually much more flexible and less prone to errors at no extra cost to the computer.

In terms of raw storage space, however, quaternions are more efficient to store than rotation matrices in a computer's memory. A quaternion is comprised of 4 scalar numbers, whereas a rotation matrix requires 9. Storing precise non-integer numbers, called "floating point numbers" in a computer's memory is computationally expensive, and so in memory constrained environments, quaternions are often a much better option.

However, it is important to note that in such environments, if it is acceptable to incur some of the shortcomings of Euler angles, then they could be a better option for the application as they only require 3 scalar numbers to be stored, but they must be converted to the aforementioned 9-scalar rotation matrix whenever points have to be rotated.

In situations where humans have to interact with 3D rotations directly, and the computer is computationally constrained, for example, like on the Apollo 11 mission Euler angles could prove to be a better option.

2.6 Usability for humans

In terms of usability, quaternions are also much harder to interpret from a human perspective, as it is difficult for the average person to visualise a four dimensional space. Furthermore, they could prove cumbersome to construct by hand, due to the numerous operations required to do so. This is not a negligible issue because, often, the users of 3D softwares are artists or researchers which seek to devote time and attention to their art or research, instead of investing themselves with how quaternions work. To that extent, Euler angles are far easier to understand and could prove more productive to their application in terms of human usability.

However, in most cases, the software that uses quaternions will provide an interface to allow the user to manipulate the axis of rotation, and the angle of rotation, without having to worry about the underlying mathematics. In such cases, quaternions could prove to be a better option, as they are more flexible and do not suffer from some of the problems of Euler angles.

2.7 Spherical Linear Interpolation

Another aspect of rotations which quaternions excel at is spherical linear interpolation - a smooth interpolation of rotation following the shortest arc to the destination on a unit sphere. When interpolating rotation, one cannot naively use linear interpolation with the coefficients of quaternions, as that will result in non-smooth and unexpected jumps.

Suppose that one wishes to interpolate between two unit quaternions q_a to q_b over a time period of t , $0 \leq t \leq 1$. Let the unit quaternion that represents the interpolated rotation at time t be q . Shoemake (1985) proposed a simple and efficient formula for calculating q :

$$q = \frac{\sin((1-t)\theta)}{\sin \theta} q_a + \frac{\sin(t\theta)}{\sin \theta} q_b$$

Although this is relatively straightforward for quaternions, the same cannot be said for rotation matrices constructed from Euler angles. Because Euler angles are, by definition, constrained in $[0, 2\pi]$,

the shortest distance between two rotations may cross over the 2π and 0 boundary, resulting in a noticeable “jump”.

In that regard, quaternions are a much better option in contexts where motion is required, making them convenient for 3D rotation in computer animations, video games, and CGI.

3 Conclusion

In conclusion, quaternions supersede rotation matrices constructed from Euler angles to a partial extent. Euler angles remain a simpler, more intuitive and more human-friendly way to represent rotation, despite their shortcomings such as being prone to gimball lock. Meanwhile, quaternions excel at their flexibility in terms of ability to be smoothly interpolated and represent arbitrary rotations without gimball lock. In terms of performance in computing, both are on a similar level, though quaternions are slightly more efficient in terms of storage space as Euler angles, despite being smaller on their own, require a 3×3 matrix to actually be useful.

Overall, this investigation has revealed why both quaternions and Euler angles are still in use today, and why neither has been completely superseded by the other. It is clear that both have their own strengths and weaknesses, and that the choice of which to use depends on the context of the application, though they are not mutually exclusive - it is often the case that both can be seen available for use as a complement to each other.

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