

Quaternion Applications

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OUTLINE

I: (55 min) Introduction to Quaternions:

What are they good for?

Understanding Rotation Sequences!

II a: (15 min) Quaternion Tubing:

Visualizing Framed Space Curves

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...OUTLINE...

II b: (15 min) Quaternion Protein Maps:

Amino Acid Frame Sequences with Quaternions

II c: (20 min) Intro to Dual Quaternions:

Applications to Six-Degrees-of-Freedom

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Part I

Introduction to Quaternions:

...Twisting Belts and Rolling Balls...

Explaining Rotation Sequences with Quaternions

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Where Did Quaternions Come From?

... from the discovery of *Complex Numbers*:

- $z = x + iy$ Complex numbers = realization that $z^2 + 1 = 0$ cannot be solved unless you have an “imaginary” number with $i^2 = -1$.
- **Euler’s formula:** $e^{i\theta} = \cos \theta + i \sin \theta$ allows you to do most of 2D geometry.

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Hamilton

The first to ask “*if you can do 2D geometry with complex numbers, how might you do 3D geometry?*” was William Rowan Hamilton, circa 1840.



Sir William Rowan Hamilton
4 August 1805 — 2 September 1865

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Hamilton's epiphany: 16 October 1843

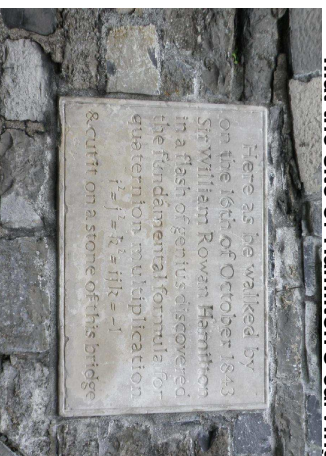
"An electric circuit seemed to close; and a spark flashed forth . . . Nor could I resist the impulse – unphilosophical as it may have been – to cut with a knife on a stone of Brougham Bridge, as we passed it, the fundamental formula with the symbols, i, j, k ; namely,

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

which contains the Solution of the Problem..."

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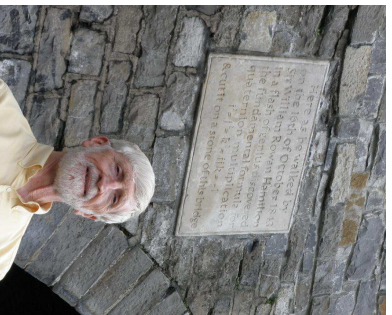
...at the site of Hamilton's carving



The plaque on Broome Bridge in Dublin, Ireland, commemorating the legendary location where Hamilton conceived of the idea of quaternions. (Photo taken July 2012).

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...the author on Broome Bridge...



Yes, I have actually been there!

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The Belt Trick

Quaternion Geometry in our daily lives

- Two people hold ends of a belt.
- Twist the belt either 360 degrees or 720 degrees.
- **Rule:** *Move belt ends any way you like but do not change orientation of either end.*
- Try to straighten out the belt.

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360 Degree Belt



360 twist: stays twisted, can change DIRECTION!

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720 Degree Belt



720 twist: CAN FLATTEN OUT WHOLE BELT!

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The Beltless Trick

Quaternion Geometry is right in your hand!

- Hold a coffee cup (empty is a good idea) in the palm of your hand.
- Keeping the cup vertical, user your hand to twist the handle, first by 360 degrees (painful).
- **Now CONTINUE another 360 degrees**, for a total of 720 degrees.
- ***Your arm is once again STRAIGHT!***

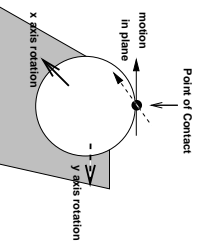
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Rolling Ball Puzzle

1. Put a ball on a flat table.
2. Place hand flat on top of the ball
3. Make circular rubbing motion, as though polishing the tabletop.
4. Watch a point on the equator of the ball.
5. ***small clockwise circles*** → ***equator goes counterclockwise***
6. ***small counterclockwise circles*** → ***equator goes clockwise***

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Rolling Ball Scenario



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Gimbal Lock

- **Gimbal Lock** occurs when a mechanical or computer system experiences an anomaly due to an (x, y, z) -based orientation control sequence.
- ***Mechanical systems cannot avoid all possible gimbal lock situations.***
- ***Computer orientation interpolation systems can avoid gimbal-lock-related glitches by using quaternion interpolation.***

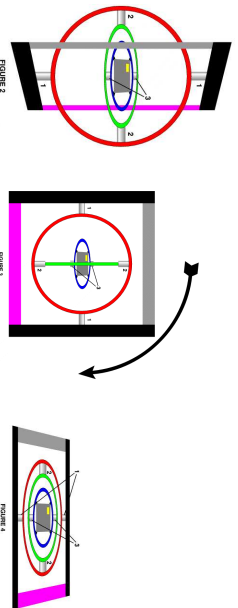
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Gimbal Lock — Apollo Systems



Red-painted area = Danger of real Gimbal Lock

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Mechanical Gimbal Lock: Using x, y, z axes to encode orientation gives singular situations.

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2D Rotations

- 2D rotations \leftrightarrow *complex numbers*.
- Why? $e^{i\theta} (x + iy) = (x' + iy')$

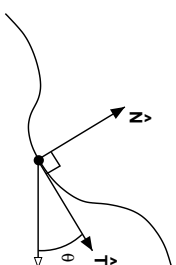
$$\begin{aligned} x' &= x \cos \theta - y \sin \theta \\ y' &= x \sin \theta + y \cos \theta \end{aligned}$$

- **Complex numbers** are a subspace of quaternions — so exploit 2D rotations to **introduce us to quaternions** and their geometric meaning.

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Frames in 2D

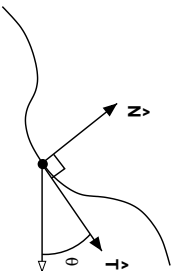
The tangent and normal to 2D curve move continuously along the curve:



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Frames in 2D

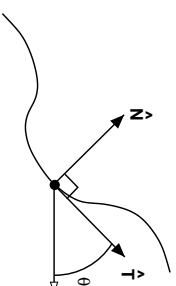
The tangent and normal to 2D curve move continuously along the curve:



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Frames in 2D

The tangent and normal to 2D curve move continuously along the curve:



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Frame Matrix in 2D

This motion is described at each point (or time) by the matrix:

$$\begin{aligned} R_2(\theta) &= \begin{bmatrix} \hat{T} & \hat{N} \end{bmatrix} \\ &= \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}. \end{aligned}$$

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The Belt Trick Says:

There is a Problem...at least in 3D

How do you get $\cos \theta$ to know about 720 degrees?

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The Belt Trick Says:

There is a Problem...at least in 3D

How do you get $\cos \theta$ to know about 720 degrees?

Hmmmm. $\cos(\theta/2)$ knows about 720 degrees, right?

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Half-Angle Transform:

A Fix for the Problem?

Let $a = \cos(\theta/2)$, $b = \sin(\theta/2)$,
(i.e., $\cos \theta = a^2 - b^2$, $\sin \theta = 2ab$),

and parameterize 2D rotations as:

$$R_2(a, b) = \begin{bmatrix} a^2 - b^2 & -2ab \\ 2ab & a^2 - b^2 \end{bmatrix}.$$

where orthonormality implies

$$(a^2 + b^2)^2 = 1$$

which reduces back to $a^2 + b^2 = 1$.

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Frame Evolution in 2D

Examine the time-evolution of a 2D frame (on our way to 3D).

First use $\theta(t)$ coordinates:

$$\begin{bmatrix} \hat{\mathbf{T}} & \hat{\mathbf{N}} \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}.$$

Differentiate to find frame equations:

$$\begin{aligned} \dot{\hat{\mathbf{T}}}(t) &= +\kappa \hat{\mathbf{N}} \\ \dot{\hat{\mathbf{N}}}(t) &= -\kappa \hat{\mathbf{T}}, \end{aligned}$$

where $\kappa(t) = d\theta/dt$ is the **curvature**.

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Frame Evolution in (a, b) :

The basis $(\hat{\mathbf{T}}, \hat{\mathbf{N}})$ is nasty — **Four equations** with **Three constraints** from orthonormality, but just **One** true degree of freedom.

Major Simplification occurs in (a, b) coordinates!!

$$\dot{\hat{\mathbf{T}}} = 2 \begin{bmatrix} a\dot{a} - b\dot{b} \\ a\dot{b} + b\dot{a} \end{bmatrix} = 2 \begin{bmatrix} a & -b \\ b & a \end{bmatrix} \begin{bmatrix} \dot{a} \\ \dot{b} \end{bmatrix}$$

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Frame Evolution in (a, b) :

But this formula for $\dot{\hat{\mathbf{T}}}$ is just $\kappa \hat{\mathbf{N}}$, where

$$\kappa \hat{\mathbf{N}} = \kappa \begin{bmatrix} -2ab \\ a^2 - b^2 \end{bmatrix} = \kappa \begin{bmatrix} a & -b \\ b & a \end{bmatrix} \begin{bmatrix} -b \\ a \end{bmatrix}$$

or

$$\kappa \hat{\mathbf{N}} = \kappa \begin{bmatrix} a & -b \\ b & a \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

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2D Quaternion Frames!

Rearranging terms, *both* $\dot{\hat{\mathbf{T}}}$ and $\dot{\hat{\mathbf{N}}}$ eqns reduce to

$$\begin{bmatrix} \dot{a} \\ \dot{b} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & -\kappa \\ +\kappa & 0 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix}$$

This is the square root of frame equations.

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2D Quaternions . . .

So *one equation* in the two “quaternion” variables (a, b) with the constraint $a^2 + b^2 = 1$ contains *both* the frame equations

$$\dot{\hat{\mathbf{T}}} = +\kappa \hat{\mathbf{N}}$$

$$\dot{\hat{\mathbf{N}}} = -\kappa \hat{\mathbf{T}}$$

\Rightarrow this is much better for computer implementation, etc.

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Rotation as Complex Multiplication

If we let $(a + ib) = \exp(i\theta/2)$ we see that rotation is complex multiplication!

“Quaternion Frames” in 2D are just complex numbers, with

Evolution Eqns = derivative of $\exp(i\theta/2)$!

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Rotation with no matrices!

Due to an extremely deep reason in Clifford Algebras,

$$a + ib = e^{i\theta/2}$$

represents rotations “more nicely” than the matrices $R(\theta)$.

$$(a' + ib')(a + ib) = e^{i(\theta' + \theta)/2} = A + iB$$

where if we want the matrix, we write:

$$R(\theta')R(\theta) = R(\theta' + \theta) = \begin{bmatrix} A^2 - B^2 & -2AB \\ 2AB & A^2 - B^2 \end{bmatrix}$$

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The Algebra of 2D Rotations

The algebra corresponding to 2D rotations is easy: just complex multiplication!!

$$\begin{aligned} (a', b') * (a, b) &\cong (a' + ib')(a + ib) \\ &= a'a - b'b + i(a'b + ab') \\ &\cong (a'a - b'b, a'b + ab') \\ &= (A, B) \end{aligned}$$

2D Rotations are just **complex multiplication**, and take you around the unit circle!

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Quaternion Frames

In 3D, repeat our trick: take square root of the frame, but now use *quaternions*:

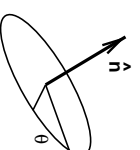
- Write down the 3D frame.
- Write as double-valued quadratic form.
- Rewrite frame evolution equations **linearly** in the new variables.

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The Geometry of 3D Rotations

We begin with a basic fact:

Euler theorem: every 3D frame can be written as a spinning by θ about a fixed axis $\hat{\mathbf{n}}$, the eigenvector of the rotation matrix:



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Quaternion Frames ...

The Matrix $R_3(\theta, \hat{n})$ giving 3D rotation by θ about axis \hat{n} is :

$$\begin{bmatrix} c + (n_1)^2(1-c) & n_1n_2(1-c) - sn_3 & n_3n_1(1-c) + sn_2 \\ n_1n_2(1-c) + sn_3 & c + (n_2)^2(1-c) & n_3n_2(1-c) - sn_1 \\ n_1n_3(1-c) - sn_2 & n_2n_3(1-c) + sn_1 & c + (n_3)^2(1-c) \end{bmatrix}$$

where $c = \cos \theta$, $s = \sin \theta$, and $\hat{n} \cdot \hat{n} = 1$.

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Can we find a 720-degree form?

Remember 2D: $a^2 + b^2 = 1$
then substitute $1 - c = (a^2 + b^2) - (a^2 - b^2) = 2b^2$
to find the remarkable expression for $R(\theta, \hat{n})$:

$$\begin{bmatrix} a^2 - b^2 + (n_1)^2(2b^2) & 2b^2n_1n_2 - 2abn_3 & 2b^2n_3n_1 + 2abn_2 \\ 2b^2n_1n_2 + 2abn_3 & a^2 - b^2 + (n_2)^2(2b^2) & 2b^2n_2n_3 - 2abn_1 \\ 2b^2n_3n_1 - 2abn_2 & 2b^2n_2n_3 + 2abn_1 & a^2 - b^2 + (n_3)^2(2b^2) \end{bmatrix}$$

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Rotations and Quadratic Polynomials

Remember $(n_1)^2 + (n_2)^2 + (n_3)^2 = 1$ and $a^2 + b^2 = 1$; letting

$$q_0 = a = \cos(\theta/2) \quad q = b\hat{n} = \hat{n} \sin(\theta/2)$$

We find a matrix $R_3(q)$

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

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Quaternions and Rotations ...

HOW does $q = (q_0, q)$ represent rotations?

LOOK at

$$R_3(\theta, \hat{n}) \stackrel{?}{=} R_3(q_0, q_1, q_2, q_3)$$

THEN we can verify that choosing

$$q(\theta, \hat{n}) = \left(\cos \frac{\theta}{2}, \hat{n} \sin \frac{\theta}{2} \right)$$

makes the R_3 equation an **IDENTITY**.

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Quaternions and Rotations ...

WHAT happens if you do **TWO** rotations?

EXAMINE the action of two rotations

$$R(q')R(q) = R(Q)$$

EXPRESS in **quadratic forms** in q and LOOK FOR an analog of complex multiplication:

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Quaternions and Rotations ...

RESULT: the following multiplication rule

$q' * q = Q$ yields **exactly** the correct 3×3 rotation matrix $R(Q)$:

$$\begin{bmatrix} Q_0 \\ Q_1 \\ Q_2 \\ Q_3 \end{bmatrix} = \begin{bmatrix} q'_0 * q_0 \\ q'_1 * q_1 \\ q'_2 * q_2 \\ q'_3 * q_3 \end{bmatrix} = \begin{bmatrix} q'_0q_0 - q'_1q_1 - q'_2q_2 - q'_3q_3 \\ q'_0q_1 + q'_1q_0 + q'_2q_3 - q'_3q_2 \\ q'_0q_2 + q'_2q_0 + q'_3q_1 - q'_1q_3 \\ q'_0q_3 + q'_3q_0 + q'_1q_2 - q'_2q_1 \end{bmatrix}$$

This is Quaternion Multiplication.

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Algebra of Quaternions = 3D Rotations!

2D rotation matrices are represented
by **complex multiplication**

3D rotation matrices are represented
by **quaternion multiplication**

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Algebraic 2D/3D Rotations

Therefore in 3D, the 2D complex multiplication

$$(a', b') * (a, b) = (a' a - b' b, a' b + a b')$$

is replaced by 4D quaternion multiplication:

$$\begin{aligned} q' * q &= (q'_0 q_0 - q'_1 q_1 - q'_2 q_2 - q'_3 q_3, \\ & q'_0 q_1 + q'_1 q_0 + q'_2 q_3 - q'_3 q_2, \\ & q'_0 q_2 + q'_2 q_0 + q'_3 q_1 - q'_1 q_3, \\ & q'_0 q_3 + q'_3 q_0 + q'_1 q_2 - q'_2 q_1) \end{aligned}$$

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Algebra of Quaternions ...

The equation is easier to remember by dividing it into a **scalar** piece q_0 and a **vector** piece \vec{q} :

$$\begin{aligned} q' * q &= (q'_0 q_0 - \vec{q}' \cdot \vec{q}, \\ & q'_0 \vec{q} + q_0 \vec{q}' + \vec{q}' \times \vec{q}) \end{aligned}$$

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Now we can SEE quaternions!

Since $(q_0)^2 + q \cdot q = 1$ then

$$q_0 = \sqrt{1 - q \cdot q}$$

Plot just the 3D vector: $q = (q_x, q_y, q_z)$

q_0 is KNOWN! We can also use any other triple: the fourth component is *dependent*.

DEMO

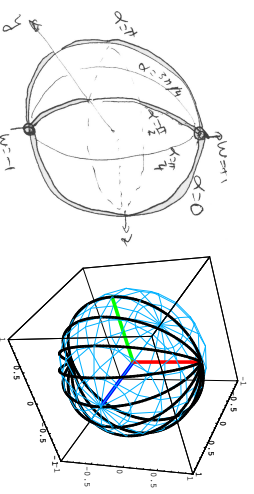
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We can now make a **Quaternion Picture** of each of our favorite tricks

- **360° Belt Trick in Quaternion Form. DEMO:**
- **720° Belt Trick in Quaternion Form.**
- **Rolling Ball in Quaternion Form. DEMO:**
- **Gimbal Lock in Quaternion Form.**

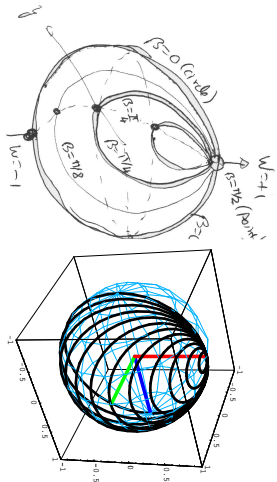
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360° Belt Trick in Quaternion Form



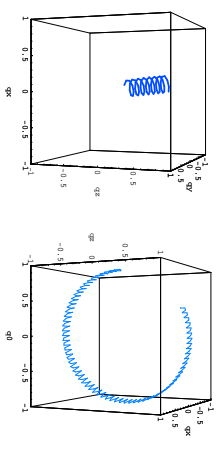
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720° Belt Trick in Quaternion Form



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Rolling Ball in Quaternion Form

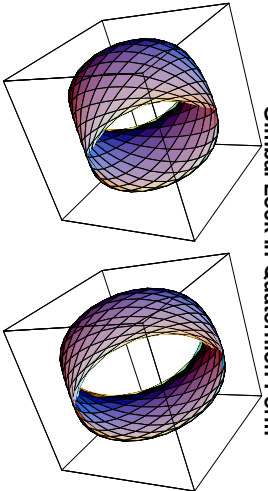


q vector-only plot.

(q_0, q_x, q_z) plot

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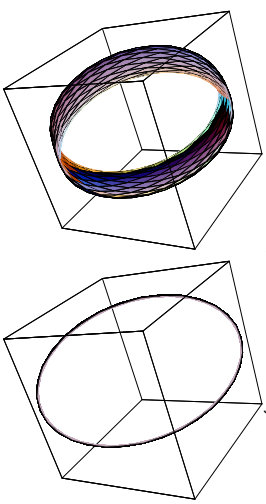
Gimbal Lock in Quaternion Form



Quaternion Plot of the *remaining* orientation degrees of freedom of $R(\theta, \hat{x}) \cdot R(\phi, \hat{y}) \cdot R(\psi, \hat{z})$ at $\phi = 0$ and $\phi = \pi/6$

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Gimbal Lock in Quaternion Form, contd



Choosing ϕ and plotting the *remaining* orientation degrees in the rotation sequence $R(\theta, \hat{x}) \cdot R(\phi, \hat{y}) \cdot R(\psi, \hat{z})$, we see degrees of freedom **decrease from TWO to ONE** as $\phi \rightarrow \pi/2$

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Quaternion Interpolations

- Shoemake (Siggraph '85) proposed using quaternions instead of Euler angles to get smooth frame interpolations without **Gimbal Lock**:

BEST CHOICE: *Animate objects and cameras using rotations represented on S^3 by quaternions*

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Interpolating on Spheres

General quaternion spherical interpolation employs the "SLERP," a constant angular velocity transition between two directions, \hat{q}_1 and \hat{q}_2 :

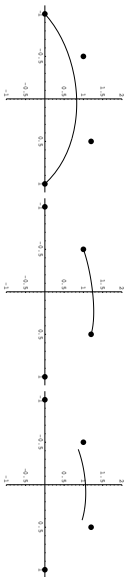
$$\begin{aligned} \hat{q}_{1,2}(t) &= \text{SLerp}(\hat{q}_1, \hat{q}_2, t) \\ &= \hat{q}_1 \frac{\sin((1-t)\theta)}{\sin(\theta)} + \hat{q}_2 \frac{\sin(t\theta)}{\sin(\theta)} \end{aligned}$$

where $\cos \theta = \hat{q}_1 \cdot \hat{q}_2$.

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Plane Interpolations

In Euclidean space, these three basic cubic splines look like this:



Bezier

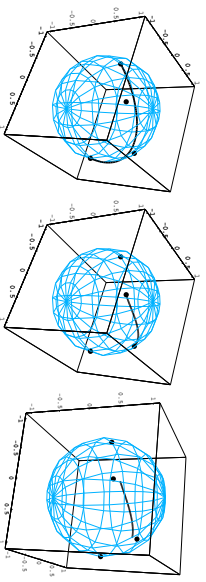
Catmull-Rom

Uniform B

The differences are in the derivatives: Bezier has to start matching all over at every fourth point; Catmull-Rom matches the first derivative; and B-spline is the cadillac, matching **all derivatives** but **no control points**.

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Spherical Interpolations



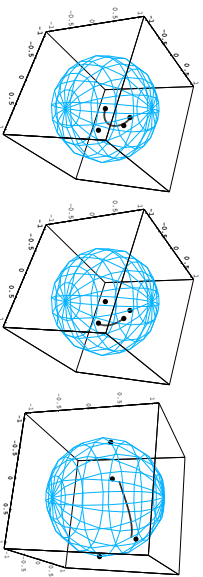
Bezier

Catmull-Rom

Uniform B

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Quaternion Interpolations



Bezier

Catmull-Rom

Uniform B

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Exp Form of Quaternion Rotations

In Hamilton's notation, we can generalize the 2D equation

$$a + ib = e^{i\theta/2}$$

Just set

$$\begin{aligned} q &= (q_0, q_1, q_2, q_3) \\ &= q_0 + iq_1 + jq_2 + kq_3 \\ &= e^{(1 \cdot i\theta/2)} \end{aligned}$$

with $q_0 = \cos(\theta/2)$ and $\vec{q} = \hat{n} \sin(\theta/2)$ and $\mathbf{I} = (i, j, k)$, with $i^2 = j^2 = k^2 = -1$, and $i * j = k$ (cyclic),

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Cute Quaternion Tricks!

Square Roots are cool..

A quaternion p is the **square root** of a quaternion q if

$$p * p = q.$$

A hint: remember that if $c = \cos \theta$, and $\gamma = \cos(\frac{\theta}{2})$, then

$$\gamma = \sqrt{\frac{1+c}{2}} = \frac{1+c}{\sqrt{2(1+c)}}$$

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Cute Quaternion Tricks...

Suppose we now look at $1 + q = (1 + q_0, \mathbf{q})$. Then

$$\begin{aligned} (1 + q) * (1 + q) &= ((1 + q_0)^2 - \mathbf{q} \cdot \mathbf{q}, 2\mathbf{q}(1 + q_0)) \\ &= 2(1 + q_0) \mathbf{q} \end{aligned}$$

Dividing through by $2(1 + q_0)$, we find the **square root**:

$$p = \sqrt{\mathbf{q}} = \frac{1 + \mathbf{q}}{\sqrt{2(1 + q_0)}}$$

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Tricks, contd: Lining up \hat{a} and \hat{b}

A common rotation task is to line up two directions, \hat{a} and \hat{b} . There is a simple **quaternion form** for this operation. Let

$$\hat{a} \cdot \hat{b} = \cos \theta = c, \quad \hat{a} \times \hat{b} = \hat{n} \sin \theta$$

where we assume $\sin \theta > 0$. Then we can compute the rotation from \hat{a} to \hat{b} using, again, the half-angle formula:

$$R(\hat{a}, \hat{b}) = (\cos(\theta/2), \hat{n} \sin(\theta/2)) \\ = \left(\sqrt{\frac{1+c}{2}}, \hat{a} \times \hat{b} \sqrt{\frac{1}{2(1+c)}} \right)$$

where we also used $\sin \theta = 2 \cos(\theta/2) \sin(\theta/2)$.

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Clifford Algebras

- **All Rotations in any dimension are represented by two reflections using Clifford Algebra:**

A and B define the perpendicular directions to two reflection planes, $A \cdot A = B \cdot B = 1$.

- **Create Rotation Matrix R and solve for the Quaternion, and you amazingly get THIS:**

$$q(A, B) = (A \cdot B, A \times B)$$

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Clifford Algebra Quaternion Form ...

Why is this a quaternion form?

$$q \cdot q = (A \cdot B)^2 + (A \times B) \cdot (A \times B) \\ = (A \cdot A) (B \cdot B) \\ \equiv 1$$

If Quaternions are like the Square Roots of Rotations, then Clifford Algebras are like the Square Roots of Quaternions!

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Key to Quaternion Intuition

Fundamental Intuition: We know

$$q_0 = \cos(\theta/2), \quad \vec{q} = \hat{n} \sin(\theta/2)$$

We also know that any coordinate frame M can be written as $M = R(\theta, \hat{n})$.

Therefore

\vec{q} points exactly along the axis we have to rotate around to go from identity I to M , and the length of \vec{q} tells us how much to rotate.

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Summarize Quaternion Properties

- **Unit four-vector.** Take $q = (q_0, q_1, q_2, q_3) = (q_0, \vec{q})$ to obey constraint $q \cdot q = 1$.
- **Multiplication rule.** The quaternion product q and p is $q * p = (q_0 p_0 - \vec{q} \cdot \vec{p}, q_0 \vec{p} + p_0 \vec{q} + \vec{q} \times \vec{p})$, or, alternatively,

$$\begin{bmatrix} [q * p]_0 \\ [q * p]_1 \\ [q * p]_2 \\ [q * p]_3 \end{bmatrix} = \begin{bmatrix} q_0 p_0 - q_1 p_1 - q_2 p_2 - q_3 p_3 \\ q_0 p_1 + q_1 p_0 + q_2 p_3 - q_3 p_2 \\ q_0 p_2 + q_2 p_0 + q_3 p_1 - q_1 p_3 \\ q_0 p_3 + q_3 p_0 + q_1 p_2 - q_2 p_1 \end{bmatrix}$$

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Quaternion Summary ...

- **Rotation Correspondence.** The unit quaternions q and $-q$ correspond to a single 3D rotation R_3 :

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

If

$$q = \left(\cos \frac{\theta}{2}, \hat{n} \sin \frac{\theta}{2} \right),$$

with \hat{n} a unit 3-vector, $\hat{n} \cdot \hat{n} = 1$. Then $R(\theta, \hat{n})$ is usual 3D rotation by θ in the plane \perp to \hat{n} .

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SUMMARY

- Quaternions represent **3D frames**
- Quaternion multiplication represents 3D rotation
- Quaternions are **points on a hypersphere**
- Quaternions paths can be visualized with 3D display
- Belt Trick, Rolling Ball, and Gimbal Lock can be understood as Quaternion Paths.