Quaternion Applications

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Siggraph Asia 2012 Tutorial

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

....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

Part I

Introduction to Quaternions:

...Twisting Belts and Rolling Balls...

Explaining Rotation Sequences with Quaternions

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.

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

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 ... "

...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*).

...the author on Broome Bridge...



Yes, I have actually been there!

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.

360 Degree Belt



360 twist: stays twisted, can change DIRECTION!

720 Degree Belt



720 twist: CAN FLATTEN OUT WHOLE BELT!

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!

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 \rightarrow

equator goes counterclockwise

6. small counterclockwise circles \rightarrow

equator goes clockwise

Rolling Ball Scenario





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.



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

Gimbal Lock — Apollo Systems



Red-painted area = Danger of real Gimbal Lock

2D Rotations

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

$$x' = x \cos \theta - y \sin \theta$$
$$y' = x \sin \theta + y \cos \theta$$

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

Frames in 2D

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



Frames in 2D

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Frames in 2D

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Frame Matrix in 2D

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

$$R_{2}(\theta) = \begin{bmatrix} \hat{\mathbf{T}} & \hat{\mathbf{N}} \end{bmatrix}$$
$$= \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

The Belt Trick Says:

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

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

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?

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:

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

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

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!!

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

Frame Evolution in (a, b):

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

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

or

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

2D Quaternion Frames!

Rearranging terms, both \hat{T} and \hat{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.

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

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

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

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

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 $\exp(i\theta/2)!$

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:

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

The Algebra of 2D Rotations

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

$$(a',b') * (a,b) \cong (a'+ib')(a+ib)$$
$$= a'a - b'b + i(a'b+ab')$$
$$\cong (a'a - b'b, a'b+ab')$$
$$= (A, B)$$

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

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.

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{n} , the eigenvector of the rotation matrix:



Quaternion Frames ...

The Matrix $R_3(\theta, \hat{\mathbf{n}})$ giving 3D rotation by θ about axis $\hat{\mathbf{n}}$ 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 $\hat{\mathbf{n}} \cdot \hat{\mathbf{n}} = 1$.

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 $\mathbf{R}(\theta, \hat{\mathbf{n}})$:

$$\begin{bmatrix} a^{2}-b^{2}+(n_{1})^{2}(2b^{2}) & 2b^{2}n_{1}n_{2}-2abn_{3} & 2b^{2}n_{3}n_{1}+2abn_{2} \\ 2b^{2}n_{1}n_{2}+2abn_{3} & a^{2}-b^{2}+(n_{2})^{2}(2b^{2}) & 2b^{2}n_{2}n_{3}-2abn_{1} \\ 2b^{2}n_{3}n_{1}-2abn_{2} & 2b^{2}n_{2}n_{3}+2abn_{1} & a^{2}-b^{2}+(n_{3})^{2}(2b^{2}) \end{bmatrix}$$

Rotations and Quadratic Polynomials

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

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

We find a matrix $R_3(q)$

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

Quaternions and Rotations ...

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

LOOK at

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

THEN we can verify that choosing

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

makes the R_3 equation an *IDENTITY*.

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:

Quaternions and Rotations ...

RESULT: the following multiplication rule

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

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

This is Quaternion Multiplication.

Algebra of Quaternions = 3D Rotations!

2D rotation matrices are represented

by complex multiplication

3D rotation matrices are represented

by quaternion multiplication

Algebraic 2D/3D Rotations

Therefore in 3D, the 2D complex multiplication

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

is replaced by 4D quaternion multiplication:

$$q' * q = (q'_0q_0 - q'_1q_1 - q'_2q_2 - q'_3q_3,$$

$$q'_0q_1 + q'_1q_0 + q'_2q_3 - q'_3q_2,$$

$$q'_0q_2 + q'_2q_0 + q'_3q_1 - q'_1q_3,$$

$$q'_0q_3 + q'_3q_0 + q'_1q_2 - q'_2q_1)$$

Algebra of Quaternions ...

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

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

Now we can SEE quaternions!

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

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

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

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.

360° Belt Trick in Quaternion Form



720° Belt Trick in Quaternion Form



Rolling Ball in Quaternion Form



q vector-only plot.

 (q_0, q_x, q_z) plot



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



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

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

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 :

$$\hat{\mathbf{q}}_{12}(t) = \operatorname{Slerp}(\hat{\mathbf{q}}_1, \hat{\mathbf{q}}_2, t) \\ = \hat{\mathbf{q}}_1 \frac{\sin((1-t)\theta)}{\sin(\theta)} + \hat{\mathbf{q}}_2 \frac{\sin(t\theta)}{\sin(\theta)}$$

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

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*.

Spherical Interpolations



Bezier

Catmull-Rom

Uniform **B**

Quaternion Interpolations



Bezier

Catmull-Rom

Uniform **B**

Exp Form of Quaternion Rotations

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

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

Just set

$$q = (q_0, q_1, q_2, q_3)$$

= $q_0 + iq_1 + jq_2 + kq_3$
= $e^{(\mathbf{I} \cdot \hat{\mathbf{n}} \theta/2)}$

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

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

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

Cute Quaternion Tricks...

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

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

= $2(1+q_0)q$

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

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

Tricks, contd: Lining up $\,\widehat{\mathbf{a}}\,$ and $\,\widehat{\mathbf{b}}\,$

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

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

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

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

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

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 · A = B · B = 1.
- \bullet Create Rotation Matrix ${\bf R}$ and solve for the Quaternion, and you amazingly get THIS:

$$q(\mathbf{A}, \mathbf{B}) = (\mathbf{A} \cdot \mathbf{B}, \mathbf{A} \times \mathbf{B})$$

Clifford Algebra Quaternion Form ...

Why is this a quaternion form?

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

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

Key to Quaternion Intuition

Fundamental Intuition: We know

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

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

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.

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,

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

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
$$\begin{bmatrix} \theta & \theta \end{bmatrix}$$

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

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

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.