Formalizing Basic Quaternionic Analysis

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Part I

The core library

(Now part of the HOL Light distribution)

Quaternions

Basic algebraic structure

Complex numbers vs Quaternions

$\mathbb{C}$ $\mathbb{R}$ extended with $\mathbf{i}$

Quaternions

Basic algebraic structure

Complex numbers vs Quaternions

$\mathbb{C}$	$\mathbb{R}$ extended with $\mathbf{i}$
$\mathbb{H}$	$\mathbb{R}$ extended with $\mathbf{i}, \mathbf{j}, \mathbf{k}$

Complex numbers vs Quaternions

$\mathbb{C}$ $\quad$ $\mathbb{R}$ extended with $\mathbf{i}$

$\mathbb{H}$ $\quad$ $\mathbb{R}$ extended with $\mathbf{i}, \mathbf{j}, \mathbf{k}$

Multiplication in $\mathbb{H}$

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \qquad \begin{aligned} \mathbf{ij} &= \mathbf{k} = -\mathbf{ji} \\ \mathbf{jk} &= \mathbf{i} = -\mathbf{kj} \\ \mathbf{ki} &= \mathbf{j} = -\mathbf{ik} \end{aligned}$$

$\mathbb{H}$ is a noncommutative field.

Information encoded in a quaternion

Link with geometry, algebra, hypercomplex analysis

$$q = \underbrace{a}_{\mathrm{Re}\, q} + \underbrace{b\,\mathbf{i} + c\,\mathbf{j} + d\,\mathbf{k}}_{\mathrm{Im}\, q}$$

$$\mathbb{H} = \mathbb{R} \oplus \mathbb{I}$$

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$$
\begin{aligned}
q &= \underbrace{a}_{\mathrm{Re}\, q} + \underbrace{b\,\mathbf{i} + c\,\mathbf{j} + d\,\mathbf{k}}_{\mathrm{Im}\, q} \\
&= \underbrace{a}_{\text{scalar}} + \underbrace{b\,\mathbf{i} + c\,\mathbf{j} + d\,\mathbf{k}}_{\text{3d-vector}}
\end{aligned}
$$

$$\mathbb{H} = \mathbb{R} \oplus \mathbb{I}$$

$$\mathbb{H} \simeq \mathbb{R} \oplus \mathbb{E}^3$$

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$$= \underbrace{a + b\,\mathbf{i}}_{z \in \mathbb{C}} + \underbrace{(c + d\,\mathbf{i})}_{w \in \mathbb{C}}\,\mathbf{j} \qquad \mathbb{H} \simeq \mathbb{C} \oplus \mathbb{C}$$

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$$
\begin{aligned}
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&= \underbrace{a}_{\text{scalar}} + \underbrace{b\,\mathbf{i} + c\,\mathbf{j} + d\,\mathbf{k}}_{\text{3d-vector}} \\
&= \underbrace{a + b\,\mathbf{i}}_{z\in\mathbb{C}} + \underbrace{(c + d\,\mathbf{i})}_{w\in\mathbb{C}}\,\mathbf{j} \\
&= \|q\|\,\big(\cos\theta + \sin\theta\, I\big)
\end{aligned}
$$

$\mathbb{H} = \mathbb{R} \oplus \mathbb{I}$

$\mathbb{H} \simeq \mathbb{R} \oplus \mathbb{E}^3$

$\mathbb{H} \simeq \mathbb{C} \oplus \mathbb{C}$

polar representation

Construction of quaternions

HOL implementation

Implementation based on multivariate analysis (Harison 2007):

$$\texttt{`:quat`} := \texttt{`:real\^{}4`}$$

Principal benefit: we inherit immediately the appropriate

- additive (as $\mathbb{R}$-vector space),
- norm and metric,
- topological,
- analytic

structure.

Construction of quaternions

HOL implementation

```
new_type_abbrev("quat",`:real^4`);;

let quat = new_definition
  `quat (x,y,z,w) = vector [x;y;z;w]:quat`;;
```

```
let quat_mul = new_definition
  `p * q = quat( Re p *  Re q - Im1 p * Im1 q -
                Im2 p * Im2 q - Im3 p * Im3 q,
                 Re p * Im1 q + Im1 p *  Re q +
                Im2 p * Im3 q - Im3 p * Im2 q,
                 Re p * Im2 q - Im1 p * Im3 q +
                Im2 p *  Re q + Im3 p * Im1 q,
                 Re p * Im3 q + Im1 p * Im2 q -
                Im2 p * Im1 q + Im3 p *  Re q)`;;
```

SIMPLE_QUAT_ARITH_TAC

Proving simple algebraic identities

We implemented a very crude automation for proving simple algebraic identities.

```
let SIMPLE_QUAT_ARITH_TAC =
  REWRITE_TAC[QUAT_EQ; QUAT_COMPONENTS; HX_DEF;
              quat_add; quat_neg; quat_sub; quat_mul;
              quat_inv] THEN
  CONV_TAC REAL_FIELD;;
```

It is enough to prove dozens of basic identities.

```
let QUAT_MUL_ASSOC = prove
 (`!x y z:quat. x * (y * z) = (x * y) * z`,
  SIMPLE_QUAT_ARITH_TAC);;
```

Computing with quaternions

A conversion for evaluating literal expressions

We provide a conversion for evaluating algebraic expressions with literal quaternions:

$$\left(1 + 2\mathbf{i} - \frac{1}{2}\mathbf{k}\right)^3 = -\frac{47}{4} - \frac{5}{2}\mathbf{i} + \frac{5}{8}\mathbf{k}$$

```
# RATIONAL_QUAT_CONV
  `(Hx(&1) + Hx(&2) * ii - Hx(&1 / &2) * kk) pow 3`;;
val it : thm =
  |- (Hx(&1) + Hx(&2) * ii - Hx(&1 / &2) * kk) pow 3 =
     -- Hx(&47 / &4) - Hx(&5 / &2) * ii +
       Hx(&5 / &8) * kk
```

QUAT_POLY_CONV

Normal form for quaternionic polynomials

HOL Light has a general procedure for polynomial normalization (SEMIRING_NORMALIZERS_CONV) but it works only for commutative rings.

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Hence we provide our own solution. E.g.,

$$(p+q)^3 = p^3 + q^3 + pq^2 + p^2q + pqp + qp^2 + qpq + q^2p$$

```
# QUAT_POLY_CONV `(x + y) pow 3`;;
val it : thm =
  |- (p + q) pow 3 =
     p pow 3 + q pow 3 + p * q pow 2 + p pow 2 * q +
     p * q * p + q * p pow 2 + q * p * q + q pow 2 * p
```

Vector product and scalar product

The quaternionic product encodes both scalar product and vector product.

Proposition

If $q_1, q_2 \in \mathbb{I}$ then

$$q_1 q_2 = -\underbrace{\langle q_1, q_2 \rangle}_{\textit{scalar product}} + \underbrace{q_1 \wedge q_2}_{\textit{vector product}} \in \mathbb{R} + \mathbb{I}$$

```
QUAT_PURE_IM_DOT_CROSS
|- !q p.
       Re q = &0 /\ Re p = &0
       ==> q * p = --Hx(q dot p) + Hv(HIm q cross HIm p)
```

Geometric conjugation

Geometric conjugation: For $q \neq 0$, define the conjugation map

$$c_q : \mathbb{H} \longrightarrow \mathbb{H}$$
$$c_q(x) := q^{-1}\, x\, q$$

Important property:

$$c_{q_1} \circ c_{q_2} = c_{q_1 q_2}$$

Reflections and orthogonal transformations

- If $q^2 = -1$ then $-c_q \colon \mathbb{R}^3 \to \mathbb{R}^3$ is the reflection w.r.t. $q^\perp$.
- (Cartan–Dieudonné) Any orthogonal transformation $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is the composition of at most n reflections.
- Any orthogonal transformation $f : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ is of the form

$$f = c_q \quad \text{or} \quad f = -c_q, \qquad \|q\| = 1.$$

Limits and continuity

- Theorems (more than 50) to compute limits and continuity.
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- Some are less immediate and require $\epsilon\delta$-reasoning.

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Example: limit of a product

```
LIM_QUAT_MUL
  |- !net f g l m.
        (f --> l) net /\ (g --> m) net
        ==> ((\x. f x * g x) --> l * m) net
```

Example: Continuity of inverse function

```
CONTINUOUS_QUAT_INV
  |- !net f.
         f continuous net /\ ~(f (netlimit net) = Hx (&0))
         ==> (\x. inv (f x)) continuous net
```

The differential structure

We have theorems for computing derivatives:

E.g., **derivative of the product**

$$\frac{\mathrm{d}\big(f(q)g(q)\big)}{\mathrm{d}q}\Big|_{q_0}(x) = f(q_0)\,\mathrm{D}g_{q_0}(x) + \mathrm{D}f_{q_0}(x)g(q_0).$$

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```
QUAT_HAS_DERIVATIVE_MUL_AT
|- !f f' g g' q.
     (f has_derivative f') (at q) /\
     (g has_derivative g') (at q)
     ==> ((\x. f x * g x) has_derivative
          (\x. f q * g' x + f' x * g q)) (at q)
```

Part II

Applications

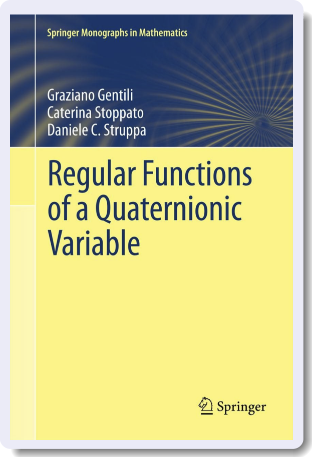
(Take it from `https://bitbucket.org/maggesi/quaternions`)

First application

Slice regular functions

Quaternionic analysis

- Complex holomorphic functions have a quaternionic analogue in the notion of *Cullen regular* functions.
- The development of this theory began in 2006 and is still very active: [Gentili, Stoppato, Struppa 2013].
- It shows a deep analogy between the complex and the quaternionic case.
- We are formalising the very beginning of this theory.
- We formalized some results of this theory, roughly corresponding to the foundational paper of 2006.



Cullen Slices

- Imaginary units form a sphere of pure quaternions

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$$\mathbb{C}_I \stackrel{\text{def}}{=} \mathrm{Span}\{1, I\}$$

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  is called *Cullen-slice*.

- **Key fact:** Quaternionic product is **commutative** when restricted to a slice and

$$\mathbb{C} \simeq \mathbb{C}_I \hookrightarrow \mathbb{H}.$$

Slice Regular functions

- **Slice regular function**: quaternionic function $f : \Omega \subseteq \mathbb{H} \to \mathbb{H}$ which is **holomorphic on cullen slices**.
- Here holomorphic means: satisfy **Cauchy-Riemann equations**

$$\frac{1}{2}\left(\frac{\partial}{\partial x} + I\frac{\partial}{\partial y}\right) f_{\mathbb{C}_I}(x + yI) = 0$$

  on $\mathbb{C}_I$ for each imaginary unit $I \in \mathbb{S}^2$.
- Slice derivative is defined consequently

$$f'(q) = \frac{1}{2}\left(\frac{\partial}{\partial x} - I\frac{\partial}{\partial y}\right) f_{\mathbb{C}_I}(x + yI)$$

Problem: partial derivatives

- **Problem:** Notation for partial derivatives.
- Spivak in his book *Calculus on manifold* notices that if $f(u, v)$ is a function and $u = g(x, y)$ and $v = h(x, y)$, then the chain rule is often written
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x}$$
where f denotes two different functions on the left and on the right.
- **Solution**: use Freché derivative.
- **Basic Idea:**
  - **Complex case:** f is holomorphic if $\mathrm{D}f_{z_0}$ is $\mathbb{C}$-linear;
  - **Quaternionic case:** f is slice regular if its derivative is $\mathbb{H}$-linear on slices in a suitable sense.

Our formalization of Slice Regular functions

Our "alternative" definition of slice regular function

The function f is *slice regular* in $q_0 = x + yI$ if there exists $c \in \mathbb{H}$ such that

$$\mathrm{D}f_{q_0}(x) = xc$$

restricted to the slice $\mathbb{C}_I$. In such case, we write

$$f'(q_0) = c.$$

(And, of course, we have a formal proof that the two definitions are equivalent!)

Abel's theorem for slice regular functions

Power series are slice regular functions:

Theorem (Abel's Theorem)

The quaternionic power series

$$\sum_{n \in \mathbb{N}} q^n a_n \tag{1}$$

is absolutely convergent in the ball $B = B\left(0, 1/\limsup_{n \to +\infty} \sqrt[n]{|a_n|}\right)$ *and uniformly convergent on any compact contained in* B. *Moreover, its sum defines a slice regular function on* B.

Series Expansion

Theorem

Let $f : B(0, R) \to \mathbb{H}$ be a slice regular function. Then

$$f(q) = \sum_{n \in \mathbb{N}} q^n \frac{1}{n!} f^{(n)}(0),$$

where $f^{(n)}$ is the n-th slice derivative of f.

Missing theory

- limit superior and inferior, definition and basic properties;
- root test for series;
- Cauchy-Hadamard formula for the radius of convergences.

Second application

Pythagorean-Hodograph curves

Pythagorean-Hodograph curves

Definition: A parametric curve $\mathbf{r}(t)$ in $\mathbb{R}^n$ is called a *Pythagorean-Hodograph curve* (PH curve) if

- is a polynomial curve
- its parametric speed $\dfrac{ds}{dt} = \left\|\mathbf{r}'(t)\right\|$ is polynomial

PH curves have significant computational advantage because their **arc length can be computed precisely**, i.e., without numerical quadrature.

Quaternionic representation

Spatial PH curves can be conveniently described with quaternions:

The curve

$$\mathbf{r}(t) = x(t)\mathbf{i} + y(t)\mathbf{j} + z(t)\mathbf{k}$$

is PH if and only if there exists a unit vector $\mathbf{u}$ and a quaternionic polynomial $A(t)$ such that

$$\mathbf{r}'(t) = A(t)\mathbf{u}\bar{A}(t)$$

Hermite interpolation problem

Problem

Given the initial and final point $\{\mathbf{p}_i, \mathbf{p}_f\}$ and derivatives $\{\mathbf{d}_i, \mathbf{d}_f\}$, find a PH interpolation for this data set.

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For cubics and quintics spacial PH curves, the problem has been solved by Farouki, Giannelli, Manni, Sestini (2008) by finding a suitable quaternionic polynomial $A(t)$, of degree 1 (for cubics) or 2 (for quintics).

PH cubic interpolant

The cubic case:

- For every initial data set there is a unique "ordinary" cubic interpolant.
- Such curve is PH iff the following conditions hold

$$\mathbf{w} \cdot (\delta_i - \delta_f) = 0$$
$$\left(\mathbf{w} \cdot \frac{\delta_i + \delta_f}{|\delta_i + \delta_f|}\right)^2 + \frac{(\mathbf{w} \cdot \mathbf{z})^2}{|\mathbf{z}|^4} = |\mathbf{d}_i||\mathbf{d}_f|$$

where $\mathbf{w} = 3(\mathbf{p}_f - \mathbf{p}_i) - (\mathbf{d}_i + \mathbf{d}_f)$, $\delta_i = \frac{\mathbf{d}_i}{|\mathbf{d}_i|}$, $\delta_f = \frac{\mathbf{d}_f}{|\mathbf{d}_f|}$ and $\mathbf{z} = \frac{\delta_i \wedge \delta_f}{|\delta_i \wedge \delta_f|}$.

PH cubic interpolant

The quintic case:

- Hermite PH quintic interpolant can be found for every initial data set choosing in the right way the coefficients of the quaternionic polynomial $A(t)$.
- Actually, there is a two-parameter family of such interpolants (Farouki - 2009) and the algebraic expression of $\mathbf{r}(t)$ is substantially more complex with respect to the case of cubics.

Conclusions

- We formalized the basic theory of quaternions in HOL Light
- We also shown two applications:
  - slice regular functions
  - PH curves
- Along the way, we extended other parts of the HOL Light library (limsup/liminf, root test, radius of convergence)

Some statistics:

- 10,000 lines of code
- 600 theorems (350 of which are now part of HOL Light)