Approximating functions in Clifford algebras: What to do with negative eigenvalues? (Short version)

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Motivation

Functions in Clifford algebras are a special case of matrix functions, as can be seen via representation theory. The square root and logarithm functions, in particular, pose problems for the author of a general purpose library of Clifford algebra functions. This is partly because the *principal* square root and logarithm of a matrix do not exist for a matrix containing a negative eigenvalue.

(Higham 2008)

Problems

1. Define the square root and logarithm of a multivector in the case where the matrix representation has negative eigenvalues.
2. Predict or detect negative eigenvalues.

Topics

- Clifford algebras
- Functions in Clifford algebras
- Dealing with negative eigenvalues
- Predicting negative eigenvalues?
- Detecting negative eigenvalues

Construction of real Clifford algebras

Each real Clifford algebra $\mathbb{R}_{p,q}$ is a real associative algebra generated by $n = p + q$ anticommuting generators, p of which square to 1 and q of which square to -1.

(Braden 1985; Lam and Smith 1989; Porteous 1995; Lounesto 1997)

Start with a group of signed integer sets

Generators: $\{k\}$ where $k \in \mathbb{Z}^*$.

Relations: Element (-1) in the centre.

$$
\begin{aligned}
(-1)^2 &= 1, \\
(-1)\{k\} &= \{k\}(-1) \quad \text{(for all } k\text{)}, \\
\{k\}^2 &= \begin{cases} (-1) & (k < 0), \\ 1 & (k > 0), \end{cases} \\
\{j\}\{k\} &= (-1)\{k\}\{j\} \quad (j \neq k).
\end{aligned}
$$

Canonical ordering:

$$\{j, k, \ell\} := \{j\}\{k\}\{\ell\} \quad (j < k < \ell), \text{ etc.}$$

Product of signed sets is signed XOR.

(Braden 1985; Lam and Smith 1989; Lounesto 1997; Dorst 2001)

Extend to a real linear algebra

Overall vector space $\mathbb{R}_{\mathbb{Z}^*}$:

Real (finite) linear combination of $\mathbb{Z}^*$ sets.

$$v = \sum_{S \subset \mathbb{Z}^*} v_S S.$$

Multiplication: Extends group multiplication.

$$vw = \sum_{S \in \mathbb{Z}^*} v_S S \sum_{T \subset \mathbb{Z}^*} w_T T$$
$$= \sum_{S \in \mathbb{Z}^*} \sum_{T \subset \mathbb{Z}^*} v_S w_T ST.$$

(Braden 1985; Lam and Smith 1989; Wene 1992; Lounesto 1997; Dorst 2001; Ashdown)

Usual notation for real Clifford algebras $\mathbb{R}_{p,q}$

The real Clifford algebra $\mathbb{R}_{p,q}$ uses subsets of $\{-q, \ldots, p\}^*$.

Underlying vector space is $\mathbb{R}^{p,q}$:
real linear combinations of the generators
$\{-q\}, \ldots, \{-1\}, \{1\}, \ldots, \{p\}$.

Conventionally (not always) $\mathrm{e}_1 := \{1\}, \ldots, \mathrm{e}_p := \{p\}$,
$\mathrm{e}_{p+1} := \{-q\}, \ldots, \mathrm{e}_{p+q} := \{-1\}$.

Conventional order of product is then $\mathrm{e}_1^{s_1}\, \mathrm{e}_2^{s_2} \ldots \mathrm{e}_{p+q}^{s_{p+q}}$.

Some examples of Clifford algebras

$$\mathbb{R}_{0,0} \equiv \mathbb{R}.$$

$$\mathbb{R}_{0,1} \equiv \mathbb{R} + \mathbb{R}\{-1\} \equiv \mathbb{C}.$$

$$\mathbb{R}_{1,0} \equiv \mathbb{R} + \mathbb{R}\{1\} \equiv {}^{2}\mathbb{R}.$$

$$\mathbb{R}_{1,1} \equiv \mathbb{R} + \mathbb{R}\{-1\} + \mathbb{R}\{1\} + \mathbb{R}\{-1,1\} \equiv \mathbb{R}(2).$$

$$\mathbb{R}_{0,2} \equiv \mathbb{R} + \mathbb{R}\{-2\} + \mathbb{R}\{-1\} + \mathbb{R}\{-2,-1\} \equiv \mathbb{H}.$$

Matrix representations of Clifford algebras

Each Clifford algebra $\mathbb{R}_{p,q}$ is isomorphic to a matrix algebra over $\mathbb{R}$, ${}^2\mathbb{R} := \mathbb{R} + \mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$ or ${}^2\mathbb{H}$ per the following table, with periodicity of 8. The $\mathbb{R}$ and ${}^2\mathbb{R}$ matrix algebras are highlighted in red.

p \ q	0	1	2	3	4	5	6	7
0	$\mathbb{R}$	$\mathbb{C}$	$\mathbb{H}$	${}^2\mathbb{H}$	$\mathbb{H}(2)$	$\mathbb{C}(4)$	$\mathbb{R}(8)$	${}^2\mathbb{R}(8)$
1	${}^2\mathbb{R}$	$\mathbb{R}(2)$	$\mathbb{C}(2)$	$\mathbb{H}(2)$	${}^2\mathbb{H}(2)$	$\mathbb{H}(4)$	$\mathbb{C}(8)$	$\mathbb{R}(16)$
2	$\mathbb{R}(2)$	${}^2\mathbb{R}(2)$	$\mathbb{R}(4)$	$\mathbb{C}(4)$	$\mathbb{H}(4)$	${}^2\mathbb{H}(4)$	$\mathbb{H}(8)$	$\mathbb{C}(16)$
3	$\mathbb{C}(2)$	$\mathbb{R}(4)$	${}^2\mathbb{R}(4)$	$\mathbb{R}(8)$	$\mathbb{C}(8)$	$\mathbb{H}(8)$	${}^2\mathbb{H}(8)$	$\mathbb{H}(16)$
4	$\mathbb{H}(2)$	$\mathbb{C}(4)$	$\mathbb{R}(8)$	${}^2\mathbb{R}(8)$	$\mathbb{R}(16)$	$\mathbb{C}(16)$	$\mathbb{H}(16)$	${}^2\mathbb{H}(16)$
5	${}^2\mathbb{H}(2)$	$\mathbb{H}(4)$	$\mathbb{C}(8)$	$\mathbb{R}(16)$	${}^2\mathbb{R}(16)$	$\mathbb{R}(32)$	$\mathbb{C}(32)$	$\mathbb{H}(32)$
6	$\mathbb{H}(4)$	${}^2\mathbb{H}(4)$	$\mathbb{H}(8)$	$\mathbb{C}(16)$	$\mathbb{R}(32)$	${}^2\mathbb{R}(32)$	$\mathbb{R}(64)$	$\mathbb{C}(64)$
7	$\mathbb{C}(8)$	$\mathbb{H}(8)$	${}^2\mathbb{H}(8)$	$\mathbb{H}(16)$	$\mathbb{C}(32)$	$\mathbb{R}(32)$	${}^2\mathbb{R}(64)$	$\mathbb{R}(128)$

(Hile and Lounesto 1990; Porteous 1995; Lounesto 1997; Leopardi 2004)

Real representations

A real matrix representation is obtained by representing each complex or quaternion value as a real matrix. Representation is a **linear map**, producing $2^n \times 2^n$ real matrices for some n.

$$\mathbb{R}_{0,1} \equiv \mathbb{C}: \quad \rho(x + y\{-1\}) = \begin{bmatrix} x & -y \\ y & x \end{bmatrix}$$

$$\mathbb{R}_{1,0} \equiv {}^2\mathbb{R}: \quad \rho(x + y\{1\}) = \begin{bmatrix} x & y \\ y & x \end{bmatrix}$$

$$\mathbb{R}_{0,2} \equiv \mathbb{H}:$$

$$\rho(\, w + x\{-2\} + y\{-1\} + z\{-2,-1\}\,) = \begin{bmatrix} w & -y & -x & z \\ y & w & -z & -x \\ x & -z & w & -y \\ z & x & y & w \end{bmatrix}$$

(Cartan and Study 1908; Porteous 1969; Lounesto 1997)

Real chessboard

q → / p ↓	0	1	2	3	4	5	6	7
0	1	2	4	8	8	8	8	16
1	2	2	4	8	16	16	16	16
2	2	4	4	8	16	32	32	32
3	4	4	8	8	16	32	64	64
4	8	8	8	16	16	32	64	128
5	16	16	16	16	32	32	64	128
6	16	32	32	32	32	64	64	128
7	16	32	64	64	64	64	128	128

(Cartan and Study 1908; Porteous 1969; Lounesto 1997)

Why study logarithms in $\mathbb{R}_{p,q}$?

The exponential is common in the study of $\mathbb{R}_{p,q}$.
If $\mathbf{x}$ is a bivector, then $\exp(\mathbf{x}) \in \mathbf{Spin}(p,q)$.
Elements of $\mathbf{Spin}(p,q)$ are called *rotors*.

In general, the exponential can be used to create one-parameter subgroups of the group $\mathbb{R}^{*}_{p,q}$.

The logarithm can then be used to interpolate between group elements – with care because in general $\exp(\mathbf{x}+\mathbf{y}) \neq \exp(\mathbf{x})\exp(\mathbf{y})$.

(Lounesto 1992; Wareham, Cameron and Lasenby 2005)

Definition of matrix functions

For a function f analytic in $\Omega \subset \mathbb{C}$,

$$f(X) := \frac{1}{2\pi i} \int_{\partial\Omega} f(z)\,(zI - X)^{-1}\,dz,$$

where the spectrum $\Lambda(X) \subset \Omega$.

For f analytic on an open disk $D \supset \Lambda(X)$ with $0 \in D$,

$$f(X) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} X^k.$$

For invertible Y, $\quad f(YXY^{-1}) = Y f(X) Y^{-1}$.

(Rinehart 1955; Golub and van Loan 1983, 1996; Horn and Johnson 1994)

Functions in Clifford algebras

For f analytic in $\Omega \subset \mathbb{C}$, $\mathbf{x}$ in a Clifford algebra,

$$f(\mathbf{x}) := \frac{1}{2\pi i} \int_{\partial\Omega} f(z)\,(z - \mathbf{x})^{-1}\,dz,$$

where the spectrum $\Lambda(\rho\mathbf{x}) \subset \Omega$, with $\rho\mathbf{x}$ the matrix representing $\mathbf{x}$.

(Higham 2008)

Principal square root and logarithm

Let $\boldsymbol{X}$ be a matrix in $\mathbb{R}^{n \times n}$ with *no negative (real) eigenvalues.*

The *principal square root* $\sqrt{\boldsymbol{X}}$ is the unique square root of $\boldsymbol{X}$ having all its eigenvalues in the open right half plane of $\mathbb{C}$.

The *principal logarithm* $\log(\boldsymbol{X})$ is the unique logarithm of $\boldsymbol{X}$ having all its eigenvalues in the open strip

$$\{\lambda \mid -\pi < \mathrm{Imag}(\lambda) < \pi\}.$$

Both the principal square root and the principal logarithm are *real matrices*.

Padé approximation

For function f with power series

$$f(z) = \sum_{k=0}^{\infty} f_k z^k,$$

the (m, n) **Padé approximant** is the ratio

$$\frac{a_m(z)}{b_n(z)},$$

of polynomials a_m, b_n of degree m, n such that

$$|f(z)\, b_n(z) - a_m(z)| = \mathrm{O}(z^{m+n+1}).$$

(Padé; Zeilberger 2002)

Padé square root

For $(|z| \leqslant 1)$:

$$\sqrt{1-z} = 1 - \frac{1}{2}z - \frac{1}{8}z^2 - \frac{1}{16}z^3 - \frac{5}{128}z^4 - \ldots$$

For $Z := I - X$ where $\|Z\|$ is "small", use (n, n) Padé approximant

$$\sqrt{X} = \sqrt{I - Z} \simeq a_n(Z) b_n(Z)^{-1}.$$

(Newton; Padé)

Denman–Beavers square root

If X **has no negative eigenvalues**, the iteration

$$M_0 := Y_0 := X,$$
$$M_{k+1} := \frac{M_k + M_k^{-1}}{4} + \frac{I}{2},$$
$$Y_{k+1} := Y_k \, \frac{I + M_k^{-1}}{2}$$

has $Y_k \to \sqrt{X}$ and $M_k \to I$ as $k \to \infty$.

This iteration is **numerically stable**.

(Denman, Beavers 1976; Cheng, Higham, Kenney, Laub 1999)

Cheng–Higham–Kenney–Laub logarithm

$$\log(1-z) = -\sum_{k=1}^{\infty} \frac{z^k}{k} \quad (|z| \leq 1, z \neq 1).$$

Assume X **has no negative eigenvalues**.
Since $\log(X) = 2\log(\sqrt{X})$,

1. iterate square roots until $\|I - X\|$ is “small”,
2. use a Padé approximant to $\log(I - Z)$, where $Z := I - X$,
3. rescale.

C-H-K-L's “incomplete square root cascade”:

- Stop Denman–Beavers iterations early, estimate error in log.

(Cheng, Higham, Kenney, Laub 1999)

The real and complex case

A negative real number does not have a real square root or a real logarithm. Solution: $\mathbb{R} \subset \mathbb{C}$.
For $x < 0$ and complex $c \neq 0$,

$$\sqrt{x} = \sqrt{1/c}\,\sqrt{cx},$$
$$\log(x) = \log(cx) - \log c,$$

For example, if $c = -1$ then,

$$\sqrt{x} = i\sqrt{-x},$$
$$\log(x) = \log(-x) - i\pi,$$

The general multivector case (1)

Only a little more complicated. Each real Clifford algebra $\mathcal{A}$ is a subalgebra of a real Clifford algebra $\mathcal{C}$, containing the pseudoscalar $\mathbf{i}$, such that $\mathbf{i}^2 = -1$ and such that the subalgebra generated by $\mathbf{i}$ is

- the centre $Z(\mathcal{C})$ of $\mathcal{C}$; and
- isomorphic to $\mathbb{C}$ as a real algebra.

Thus $\mathcal{C}$ is isomorphic to an algebra over $\mathbb{C}$.

The general multivector case (2)

For $\mathrm{x} \in \mathcal{A}$ and any $c \in Z(\mathcal{C})$ with $c \neq 0$, if $c\mathrm{x}$ has no negative eigenvalues, we can define

$$\begin{aligned} \mathtt{sqrt}(\mathrm{x}) &:= \sqrt{1/c}\,\sqrt{c\mathrm{x}}, \\ \mathtt{log}(\mathrm{x}) &:= \log(c\mathrm{x}) - \log c, \end{aligned}$$

where the square root and logarithm of $c\mathrm{x}$ on the RHS are principal.

Examples of $\mathcal{A} \subset \mathcal{C}$

$\mathcal{C}$ is an algebra with $\mathbf{i}$: $\mathbf{i}^2 = -\mathbf{1}$, $\mathbf{i}\mathbf{x} = \mathbf{x}\mathbf{i}$ for all $\mathbf{x} \in \mathcal{C}$:
Full $\mathbb{C}$ matrix algebra.

Embeddings:

$$\mathbb{R} \equiv \mathbb{R}_{\mathbf{0},\mathbf{0}} \subset \mathbb{R}_{\mathbf{0},\mathbf{1}} \equiv \mathbb{C}.$$

$$^{\mathbf{2}}\mathbb{R} \equiv \mathbb{R}_{\mathbf{1},\mathbf{0}} \subset \mathbb{R}_{\mathbf{1},\mathbf{2}} \equiv \mathbb{C}(\mathbf{2}).$$

$$\mathbb{R}(\mathbf{2}) \equiv \mathbb{R}_{\mathbf{1},\mathbf{1}} \subset \mathbb{R}_{\mathbf{1},\mathbf{2}} \equiv \mathbb{C}(\mathbf{2}).$$

$$\mathbb{H} \equiv \mathbb{R}_{\mathbf{0},\mathbf{2}} \subset \mathbb{R}_{\mathbf{1},\mathbf{2}} \equiv \mathbb{C}(\mathbf{2}).$$

Real–complex chessboard

p ↓ \ q →	0	1	2	3	4	5	6	7
0	1	2	4	8	8	8	8	16
1	2	2	4	8	16	16	16	16
2	2	4	4	8	16	32	32	32
3	4	4	8	8	16	32	64	64
4	8	8	8	16	16	32	64	128
5	16	16	16	16	32	32	64	128
6	16	32	32	32	32	64	64	128
7	16	32	64	64	64	64	128	128

(Cartan and Study 1908; Porteous 1969; Lounesto 1997)

Example: ${}^2\mathbb{R} \equiv \mathbb{R}_{1,0}$

$$ {}^2\mathbb{R} \equiv \mathbb{R}_{1,0} \subset \mathbb{R}_{1,2} \subset \mathbb{R}_{2,2} \equiv \mathbb{R}(4). $$

$$ \rho(x + y\{1\}) = \begin{bmatrix} x & y & & \\ y & x & & \\ & & x & y \\ & & y & x \end{bmatrix} $$

$$ \mathbf{i} = \begin{bmatrix} & & 1 & 0 \\ & & 0 & -1 \\ -1 & 0 & & \\ 0 & 1 & & \end{bmatrix} $$

(Cartan and Study 1908; Porteous 1969; Lounesto 1997)

Definitions of sqrt and log

When the matrix representing $\mathbf{x}$ has a negative eigenvalue and no imaginary eigenvalues, define

$$\mathtt{sqrt}(\mathbf{x}) := \frac{\mathbf{1} + \mathbf{i}}{\sqrt{\mathbf{2}}} \mathtt{sqrt}(-\mathbf{i}\mathbf{x}),$$

$$\mathtt{log}(\mathbf{x}) := \mathtt{log}(-\mathbf{i}\mathbf{x}) + \mathbf{i}\frac{\boldsymbol{\pi}}{\mathbf{2}},$$

where $\mathbf{i}^2 = -\mathbf{1}$ and $\mathbf{i}\mathbf{x} = \mathbf{x}\mathbf{i}$.

When $\mathbf{x}$ also has imaginary eigenvalues, the real matrix representing $-\mathbf{i}\mathbf{x}$ has negative eigenvalues. Find some ϕ such that $\mathtt{exp}(\mathbf{i}\phi)\mathbf{x}$ does not have negative eigenvalues, and define

$$\mathtt{sqrt}(\mathbf{x}) := \mathtt{exp}\Big(-\mathbf{i}\frac{\phi}{\mathbf{2}}\Big)\mathtt{sqrt}\big(\mathtt{exp}(\mathbf{i}\phi)\mathbf{x}\big),$$

$$\mathtt{log}(\mathbf{x}) := \mathtt{log}\big(\mathtt{exp}(\mathbf{i}\phi)\mathbf{x}\big) - \mathbf{i}\phi.$$

Examples

Let $\mathbf{e_1} := \{1\}$. Eigenvalues of real matrix are -1 and 1.
We have

$$\begin{aligned}\mathtt{sqrt}(\mathbf{e_1}) &= \frac{1}{2} + \frac{1}{2}\{1\} - \frac{1}{2}\{2,3\} + \frac{1}{2}\{1,2,3\},\\ \mathtt{log}(\mathbf{e_1}) &= -\frac{\pi}{2}\{2,3\} + \frac{\pi}{2}\{1,2,3\}.\end{aligned}$$

Check: $\mathtt{sqrt}(\mathbf{e_1}) \times \mathtt{sqrt}(\mathbf{e_1}) = e_1$ and $\mathbf{exp}(\mathtt{log}(\mathbf{e_1})) = e_1$.

Let $v := -2\{1\} + 2\{2\} - 3\{3\} \in \mathbb{R}_{3,0}$. The real matrix has eigenvalues near -4.12311 and 4.12311. We have

$$\begin{aligned}\mathtt{sqrt}(v) :\simeq& 1.015 - 0.4925\{1\} + 0.4925\{2\} - 0.7387\{3\}\\ &+0.7387\{1,2\} + 0.4925\{1,3\} + 0.4925\{2,3\}\\ &+1.015\{1,2,3\},\\ \mathtt{log}(v) :\simeq& 1.417 + 1.143\{1,2\} + 0.7619\{1,3\} + 0.7619\{2,3\}\\ &+1.571\{1,2,3\}.\end{aligned}$$

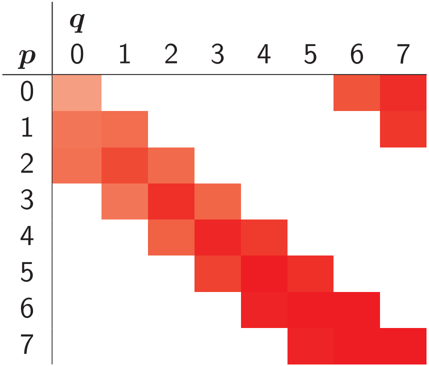
Predicting negative eigenvalues?

In Clifford algebras with a faithful irreducible *complex* or *quaternion* representation, a multivector with independent $N(0,1)$ random coefficients is *unlikely* to have a negative eigenvalue. In large Clifford algebras with an irreducible real representation, such a random multivector is very likely to have a negative eigenvalue.

(Ginibre 1965; Edelman, Kostlan and Shub 1994; Edelman 1997; Forrester and Nagao 2007)

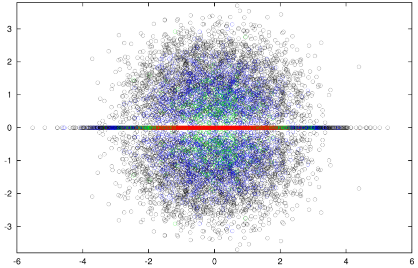
Predicting negative eigenvalues?

Probability of a negative eigenvalue is denoted by shades of red.



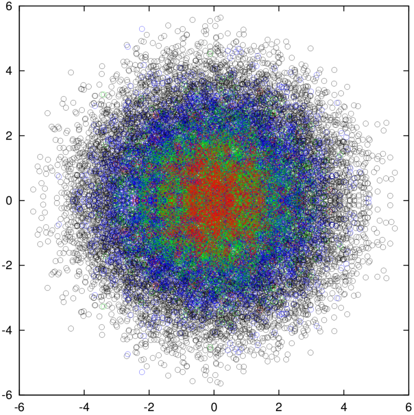
This phenomenon is a direct consequence of the eigenvalue density of the Ginibre ensembles.

Real Ginibre ensemble



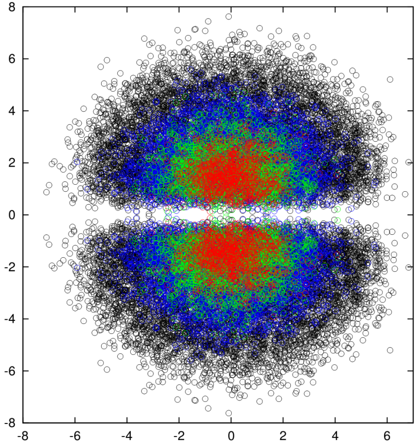
Eigenvalue density of real representations of Real Ginibre ensemble.

Complex Ginibre ensemble



Eigenvalue density of real representations of Complex Ginibre ensemble.

Quaternion Ginibre ensemble



Eigenvalue density of real representations of Quaternion Ginibre ensemble.

Detecting negative eigenvalues

Trying to predict negative eigenvalues using the p and q of $\mathbb{R}_{p,q}$ is futile. Negative eigenvalues are always possible, since $\mathbb{R}_{p,q}$ contains $\mathbb{R}_{p',q'}$ for all $p' \leqslant p$ and $q' \leqslant q$.

The eigenvalue densities of the Ginibre ensembles simply make testing more complicated.

In the absence of an efficient algorithm to detect negative eigenvalues only, it is safest to use a standard algorithm to find all eigenvalues.

(Higham 2008).

Further problem

Devise an algorithm which detects negative eigenvalues only, and is more efficient than standard eigenvalue algorithms.

GluCat — Clifford algebra library

- Generic library of universal Clifford algebra templates.
- C++ template library for use with other libraries.
- Implements algorithms for matrix functions.
- PyCliCal: Prototype Clifford algebra Python extension module.

For details, see **http://glucat.sf.net**

(Lounesto et al. 1987; Lounesto 1992; Raja 1996; Leopardi 2001-2010)