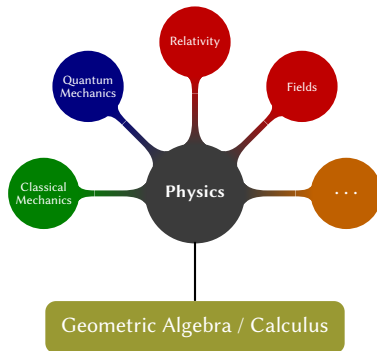


A Tutorial on Geometric Algebra and Geometric Calculus: A Unified Mathematical Language for Physics

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Prologue



Level 1 Goals

Mummy doesn't have to worry about me not being able to understand Maxwell's equations anymore.

I can derive them in just 5 minutes.

Daddy doesn't have to worry about me not being able to do rotations anymore.

I can now handle rotations in spaces of any dimensionality.

Level 2 Goals

Grasp the gist of geometric algebra and geometric calculus.

Appreciate the **unifying**, **simplifying**, and **generalizing** power of geometric algebra and geometric calculus for describing physics in a very natural way.

Level 3 Goals

Use geometric algebra and geometric calculus to solve problems in science with the companion tool **Geomeculus**.

Vector Space \mathbb{R}^n

Let's start with an n -dimensional vector space \mathbb{R}^n with an orthonormal basis denoted by $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$, where \mathbb{R} is the set of real numbers.

An arbitrary vector expanded in terms of the orthonormal basis is given by

$$\mathbf{a} = a_1\mathbf{e}_1 + a_2\mathbf{e}_2 + \dots + a_n\mathbf{e}_n,$$

where $a_1, a_2, \dots, a_n \in \mathbb{R}$.

Vector Space \mathbb{R}^n

A vector space is a set of vectors with two operations: **associative and commutative addition** and **distributive scalar multiplication**.

- ▶ $\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$, commutative addition
- ▶ $(\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c})$, associative addition
- ▶ $a(\mathbf{b} + \mathbf{c}) = a\mathbf{b} + a\mathbf{c}$, scalar multiplication is distributive w.r.t. addition
- ▶ $(a + b)\mathbf{c} = a\mathbf{c} + b\mathbf{c}$, scalar multiplication is distributive w.r.t. addition

Extending \mathbb{R}^n into an Algebra with a Product

Let's define an associative **product** for the unit basis vectors:

$$\mathbf{e}_i \mathbf{e}_j = \begin{cases} \pm 1, 0 & \text{if } i = j, \\ -\mathbf{e}_j \mathbf{e}_i & \text{if } i \neq j. \end{cases}$$

Let's define the product for arbitrary vectors:

$$\begin{aligned} \mathbf{ab} &= (a_1 \mathbf{e}_1 + \cdots + a_n \mathbf{e}_n)(b_1 \mathbf{e}_1 + \cdots + b_n \mathbf{e}_n) \\ &= a_1 b_1 \mathbf{e}_1 \mathbf{e}_1 + a_1 b_2 \mathbf{e}_1 \mathbf{e}_2 + \cdots + a_n b_n \mathbf{e}_n \mathbf{e}_n \end{aligned}$$

Extending Vectors to Multivectors

\mathbb{R}^n can be extended into an algebra \mathbb{G}^n with elements called **multivectors**.

For example, an element of \mathbb{G}^3 can be written as:

$$a_0 + a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3 + a_{12} \mathbf{e}_1 \mathbf{e}_2 + a_{13} \mathbf{e}_1 \mathbf{e}_3 + a_{23} \mathbf{e}_2 \mathbf{e}_3 + a_{123} \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$

- ▶ a_0 is a scalar (0-vector)
- ▶ $a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3$ is a vector (1-vector)
- ▶ $a_{12} \mathbf{e}_1 \mathbf{e}_2 + a_{13} \mathbf{e}_1 \mathbf{e}_3 + a_{23} \mathbf{e}_2 \mathbf{e}_3$ is a bivector (2-vector)
- ▶ $a_{123} \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$ is a trivector (3-vector)

Extending Vectors to Multivectors

Every orthonormal basis in \mathbb{R}^n determines a **standard basis** for \mathbb{G}^n .

A standard basis for \mathbb{G}^3 is defined as:

| | |
|--|---------------------|
| 1 | basis for 0-vectors |
| $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ | basis for 1-vectors |
| $\mathbf{e}_1\mathbf{e}_2, \mathbf{e}_1\mathbf{e}_3, \mathbf{e}_2\mathbf{e}_3$ | basis for 2-vectors |
| $\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$ | basis for 3-vectors |

Extending Vectors to Multivectors

The standard basis for \mathbb{G}^4 :

| | |
|--|---------------------|
| 1 | basis for 0-vectors |
| $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4$ | basis for 1-vectors |
| $\mathbf{e}_1\mathbf{e}_2, \mathbf{e}_1\mathbf{e}_3, \mathbf{e}_1\mathbf{e}_4, \mathbf{e}_2\mathbf{e}_3, \mathbf{e}_2\mathbf{e}_4, \mathbf{e}_3\mathbf{e}_4$ | basis for 2-vectors |
| $\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3, \mathbf{e}_1\mathbf{e}_2\mathbf{e}_4, \mathbf{e}_1\mathbf{e}_3\mathbf{e}_4, \mathbf{e}_2\mathbf{e}_3\mathbf{e}_4$ | basis for 3-vectors |
| $\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3\mathbf{e}_4$ | basis for 4-vectors |

Geometric Algebra

Geometric algebra \mathbb{G} is a **vector space** with a **product**, called the **geometric product**.

The elements of \mathbb{G} are **multivectors**. The **geometric product** of multivectors A and B is written AB . Geometric algebra is closed under the geometric product, that is $AB \in \mathbb{G}$.

Geometric Algebra

For all scalars a ($a \in \mathbb{R}$) and multivectors A , B , and C :

- ▶ $A + B = B + A$, commutative addition.
- ▶ $(A + B) + C = A + (B + C)$, associative addition.
- ▶ $(AB)C = A(BC)$, associative multiplication.
- ▶ $A(B + C) = AB + AC$, $(A + B)C = AC + BC$, multiplication is distributive w.r.t. addition.
- ▶ $a(AB) = (aA)B = A(aB)$, scalars commute with multivectors.
- ▶ $A + 0 = A$, 0 is the additive identity.
- ▶ $1A = A1 = A$, 1 is the multiplicative identity.

Notation

- ▶ Lower case italic symbols denote **scalars**, e.g. a, b, \dots
- ▶ Lower case bold symbols denote **vectors**, e.g. $\mathbf{a}, \mathbf{b}, \dots$
- ▶ Lower case bold \mathbf{e} with a subscript denotes **orthonormal basis vectors**, e.g. $\mathbf{e}_1, \mathbf{e}_2, \dots$
- ▶ Upper case italic symbols denote **multivectors**, e.g. A, B, \dots

Algebra Signature

- ▶ $\mathbf{e}_i \mathbf{e}_i = +1$, positive square
- ▶ $\mathbf{e}_j \mathbf{e}_j = -1$, negative square
- ▶ $\mathbf{e}_k \mathbf{e}_k = 0$, zero square

Algebra signatures:

- ▶ $\mathbb{G}^{p,q,r}$: \mathbb{G} has a basis with p positive squares, q negative squares, r zero squares
- ▶ $\mathbb{G}^{p,q}$: \mathbb{G} has a basis with p positive squares, q negative squares, 0 zero square
- ▶ \mathbb{G}^p : \mathbb{G} has a basis with p positive squares, 0 negative square, 0 zero square

The Companion Tool: Geomeculus

Geomeculus: A program for doing geometric algebra and **Geometric Calculus**

| | On Slides | In Code |
|-------------------|-----------|----------|
| Addition | $A + B$ | $A + B$ |
| Geometric Product | AB | $A * B$ |
| Negation | $-A$ | $-1 * A$ |

We can execute commands interactively in Geomeculus, or we can run batched commands using **Geomeculus** script files (**.gmc**).

Geomeculus Script

```
algebra_signature 3,1
# unnamed expression
e1 * e1
# named expression
F = e1 * e2
# expressions with scalar variables
a = v1 * e1 + v2 * e2 + v3 * e3
A = v11 * e1 + v12 * e2
B = v21 * e1 + v22 * e2
# named exprs can be referenced with $ prefix
C = $A * $B
# assign real number values to the variables
$C; v11=1; v12=2; v21=3; v22=4
# call built-in functions
exponential(0.5 * pi() * $F)
```

gmc script: samples/playground.gmc

Running Geomeculus Scripts

```
./build/release/bin/geomeculus samples/playground.gmc
```

Running Geomeculus Scripts

```
./build/release/bin/geomeculus samples/playground.gmc
```

```
./build/release/bin/geomeculus < samples/playground.gmc
```

Running Geomeculus Scripts

```
./build/release/bin/geomeculus samples/playground.gmc
```

```
./build/release/bin/geomeculus < samples/playground.gmc
```

```
cat samples/playground.gmc | ./build/release/bin/geomeculus
```

Running Geomeculus Scripts

```
./build/release/bin/geomeculus samples/playground.gmc
```

```
./build/release/bin/geomeculus < samples/playground.gmc
```

```
cat samples/playground.gmc | ./build/release/bin/geomeculus
```

```
./build/release/bin/geomeculus  
exec samples/playground.gmc
```

Running Geomeculus Scripts

```
./build/release/bin/geomeculus samples/playground.gmc
```

```
./build/release/bin/geomeculus < samples/playground.gmc
```

```
cat samples/playground.gmc | ./build/release/bin/geomeculus
```

```
./build/release/bin/geomeculus  
exec samples/playground.gmc
```

```
./build/release/bin/geomeculus --import samples/playground.gmc
```

Geometric algebra is unifying, simplifying, and generalizing

- ▶ Number systems
 - Complex numbers, quaternions
- ▶ Vector operations
 - Inner product, outer product, cross product, angular momentum and torque
- ▶ Fields
 - Magnetic field, electromagnetic field → Maxwell's equations
- ▶ Geometric operations
 - Rotations, projective geometry, conformal geometry, molecular geometry problem
- ▶ Quantum mechanics
 - Pauli algebra, Dirac algebra, Schrödinger equation, Dirac equation
- ▶

Complex Numbers

$$I = \mathbf{e}_1 \mathbf{e}_2$$

$$I^2 = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_1 \mathbf{e}_2 = -1$$

$$(a + bI)(c + dI) = (ac - bd) + (ad + bc)I$$

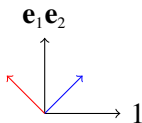
$$e^{I\theta} = \cos \theta + I \sin \theta$$

The complex number system is isomorphic to the subalgebra with form $a + bI$ of \mathbb{G}^2 .

Complex Numbers

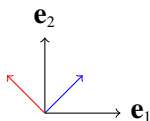
Rotate a vector by θ in the “complex plane” with $\{1, \mathbf{e}_1\mathbf{e}_2\}$ as axes:

$$(1 + \mathbf{e}_1\mathbf{e}_2) \exp(\theta I) = -1 + \mathbf{e}_1\mathbf{e}_2$$



Rotate a vector by θ in the plane with $\{\mathbf{e}_1, \mathbf{e}_2\}$ as axes:

$$(\mathbf{e}_1 + \mathbf{e}_2) \exp(\theta I) = -1 * \mathbf{e}_1 + \mathbf{e}_2$$



In the example, $\theta = \frac{\pi}{2}$
gmc script: `samples/complex.gmc`

Quaternions

$$I = \mathbf{e}_1\mathbf{e}_2, \quad I^2 = -1$$

$$J = \mathbf{e}_2\mathbf{e}_3, \quad J^2 = -1$$

$$K = \mathbf{e}_1\mathbf{e}_3, \quad K^2 = -1$$

$$IJK = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_2\mathbf{e}_3\mathbf{e}_1\mathbf{e}_3 = -1$$

$$(a + bI + cJ + dK)(a - bI - cJ - dK) = a^2 + b^2 + c^2 + d^2$$

Multivectors of form $a + bI + cJ + dK$ are isomorphic to quaternions.

gmc script: `samples/quaternion.gmc`

Inner Product of Vectors

For all vectors **a** and **b** in \mathbb{R}^n ,

$$\mathbf{a} \cdot \mathbf{b} = \frac{1}{2}(\mathbf{ab} + \mathbf{ba}).$$

Outer Product of Vectors

For all vectors **a** and **b** in \mathbb{R}^n ,

$$\mathbf{a} \wedge \mathbf{b} = \frac{1}{2}(\mathbf{ab} - \mathbf{ba}).$$

Geometric Product of Vectors

For all vectors \mathbf{a} and \mathbf{b} in \mathbb{R}^n ,

$$\mathbf{a} \cdot \mathbf{b} = \frac{1}{2}(\mathbf{ab} + \mathbf{ba})$$

$$\mathbf{a} \wedge \mathbf{b} = \frac{1}{2}(\mathbf{ab} - \mathbf{ba})$$

$$\mathbf{ab} = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \wedge \mathbf{b}$$

Cross Product of Vectors

$$I = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$

$$\mathbf{a} = v_{11} \mathbf{e}_1 + v_{12} \mathbf{e}_2 + v_{13} \mathbf{e}_3$$

$$\mathbf{b} = v_{21} \mathbf{e}_1 + v_{22} \mathbf{e}_2 + v_{23} \mathbf{e}_3$$

$$\mathbf{a} \wedge \mathbf{b} = (v_{11}v_{22} - v_{12}v_{21}) \mathbf{e}_1 \mathbf{e}_2 + (v_{11}v_{23} - v_{13}v_{21}) \mathbf{e}_1 \mathbf{e}_3 + (v_{12}v_{23} - v_{13}v_{22}) \mathbf{e}_2 \mathbf{e}_3$$

$$\mathbf{a} \times \mathbf{b} = (v_{11}v_{22} - v_{12}v_{21}) \mathbf{e}_3 - (v_{11}v_{23} - v_{13}v_{21}) \mathbf{e}_2 + (v_{12}v_{23} - v_{13}v_{22}) \mathbf{e}_1$$

$$\mathbf{a} \times \mathbf{b} = -I(\mathbf{a} \wedge \mathbf{b}) \quad \text{or} \quad \mathbf{a} \wedge \mathbf{b} = I(\mathbf{a} \times \mathbf{b})$$

Angular Momentum and Torque

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \qquad \boldsymbol{\tau} = \mathbf{r} \times \mathbf{F}$$

Alternatively, angular momentum and torque can be expressed as outer products:

$$\mathbf{L} = -I(\mathbf{r} \wedge \mathbf{p}) \qquad \boldsymbol{\tau} = -I(\mathbf{r} \wedge \mathbf{F})$$

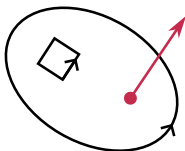
where \mathbf{L} is the angular momentum, $\boldsymbol{\tau}$ is the torque, \mathbf{r} is the position vector, \mathbf{p} is the momentum vector, and \mathbf{F} is the force vector.

Magnetic Field

$$I = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$

$$\mathbf{B} = \mathbf{b}I = I\mathbf{b}$$

where \mathbf{b} is the magnetic field vector, and \mathbf{B} is the magnetic bivector field orthogonal to \mathbf{b} .



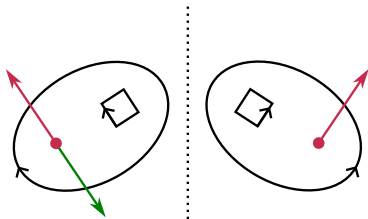
gmc script: `samples/magnetic.gmc`

Magnetic Field

$$I = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$

$$\mathbf{B} = \mathbf{b}I = I\mathbf{b}$$

where \mathbf{b} is the magnetic field vector, and \mathbf{B} is the magnetic bivector field orthogonal to \mathbf{b} .



gmc script: samples/magnetic.gmc

Extending Partial Derivative to Multivector-valued Functions

Let $F : U \subseteq \mathbb{R}^m \rightarrow \mathbb{G}^n$, where U is open. Let $\mathbf{x} \in U$ have coordinates (x_1, \dots, x_m) with respect to an orthonormal basis $\{\mathbf{e}_1, \dots, \mathbf{e}_m\}$. Then the **partial derivative** of F with respect to x_i is

$$\frac{\partial F(\mathbf{x})}{\partial x_i} = \lim_{h \rightarrow 0} \frac{F(\mathbf{x} + h\mathbf{e}_i) - F(\mathbf{x})}{h} = \lim_{h \rightarrow 0} \frac{F(x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + \cdots + (x_i + h)\mathbf{e}_i + \cdots + x_m\mathbf{e}_m) - F(\mathbf{x})}{h}. \quad (1)$$

We will often abbreviate this as $\partial_i F$.

A set $U \subseteq \mathbb{R}^n$ is **open** if every point $x \in U$ has a neighborhood contained in U .

Gradient

Let F be a differentiable multivector function defined on an open set $U \subseteq \mathbb{R}^n$. Let $\{\mathbf{e}_i\}$ be an orthonormal basis for \mathbb{R}^n . Then the **gradient** of F is defined by

$$\nabla F(\mathbf{x}) = \mathbf{e}_i \partial_i F(\mathbf{x}) = \mathbf{e}_1 \partial_1 F(\mathbf{x}) + \mathbf{e}_2 \partial_2 F(\mathbf{x}) + \cdots + \mathbf{e}_n \partial_n F(\mathbf{x}). \quad (2)$$

The product in $\mathbf{e}_i \partial_i F(\mathbf{x})$ is the geometric product.

Magic trick: algebraically, ∇ behaves like a **vector**, and ∂_i behaves like a **scalar**.

$$\begin{aligned} \nabla F &= \nabla \cdot F + \nabla \wedge F \\ \partial_i \partial_j F &= \partial_j \partial_i F \end{aligned}$$

Maxwell's Equations

Maxwell's equation in geometric calculus (natural units):

$$\nabla F = \rho - \mathbf{J}.$$

$$F = \mathbf{e} + \mathbf{B}$$

$$\nabla = \frac{\partial}{\partial t} + \nabla = \partial_t + \mathbf{e}_1 \partial_1 + \mathbf{e}_2 \partial_2 + \mathbf{e}_3 \partial_3$$

ρ : charge density, scalar

\mathbf{J} : current density, vector

The electric vector field \mathbf{e} and the magnetic bivector field \mathbf{B} are combined into a single multivector field F .

Maxwell's Equations

$$\nabla \mathbf{F} = \rho - \mathbf{J}$$

Maxwell's Equations

$$\nabla \mathbf{F} = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + \mathbf{B}) = \rho - \mathbf{J}$$

Maxwell's Equations

$$\nabla \mathbf{F} = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + \mathbf{B}) = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + I\mathbf{b}) = \rho - \mathbf{J}$$

$$I = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$

Maxwell's Equations

$$\nabla F = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + \mathbf{B}) = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + I\mathbf{b}) = \rho - \mathbf{J}$$

$$\frac{\partial}{\partial t}\mathbf{e} + \nabla\mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla\mathbf{b} = \rho - \mathbf{J}$$

$$I = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$$

Maxwell's Equations

$$\nabla F = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + \mathbf{B}) = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + I\mathbf{b}) = \rho - \mathbf{J}$$

$$\frac{\partial}{\partial t}\mathbf{e} + \nabla\mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla\mathbf{b} = \rho - \mathbf{J}$$

$$\frac{\partial}{\partial t}\mathbf{e} + \nabla \cdot \mathbf{e} + \nabla \wedge \mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla \cdot \mathbf{b} + I\nabla \wedge \mathbf{b} = \rho - \mathbf{J}$$

$$I = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$$

Maxwell's Equations

$$\nabla F = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + \mathbf{B}) = \rho - \mathbf{J}$$

$$\left(\frac{\partial}{\partial t} + \nabla\right)(\mathbf{e} + I\mathbf{b}) = \rho - \mathbf{J}$$

$$\frac{\partial}{\partial t}\mathbf{e} + \nabla\mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla\mathbf{b} = \rho - \mathbf{J}$$

$$\frac{\partial}{\partial t}\mathbf{e} + \nabla \cdot \mathbf{e} + \nabla \wedge \mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla \cdot \mathbf{b} + I\nabla \wedge \mathbf{b} = \rho - \mathbf{J}$$

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t}\mathbf{e} + I\nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I\frac{\partial}{\partial t}\mathbf{b} + I\nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

$$I = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} + I \nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} + I \nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

$$\nabla \cdot \mathbf{e} = \rho$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} + I \nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

$$\nabla \cdot \mathbf{e} = \rho$$

$$\frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J}$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} + I \nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

$$\nabla \cdot \mathbf{e} = \rho$$

$$\frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J}$$

$$\nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} = 0$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} + \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} + \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} + I \nabla \cdot \mathbf{b} = \rho - \mathbf{J}$$

$$\nabla \cdot \mathbf{e} = \rho$$

$$\frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J}$$

$$\nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} = 0$$

$$I \nabla \cdot \mathbf{b} = 0$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} = \rho$$

$$\frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J}$$

$$\nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} = 0$$

$$I \nabla \cdot \mathbf{b} = 0$$

Maxwell's Equations

$$\begin{array}{lcl} \nabla \cdot \mathbf{e} = \rho & & \nabla \cdot \mathbf{e} = \rho \\ \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J} & \Rightarrow & -I \nabla \wedge \mathbf{b} = \frac{\partial}{\partial t} \mathbf{e} + \mathbf{J} \\ \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} = 0 & & \nabla \wedge \mathbf{e} = -I \frac{\partial}{\partial t} \mathbf{b} \\ I \nabla \cdot \mathbf{b} = 0 & & \nabla \cdot \mathbf{b} = 0 \end{array}$$

Maxwell's Equations

$$\begin{array}{l} \nabla \cdot \mathbf{e} = \rho \\ \frac{\partial}{\partial t} \mathbf{e} + I \nabla \wedge \mathbf{b} = -\mathbf{J} \\ \nabla \wedge \mathbf{e} + I \frac{\partial}{\partial t} \mathbf{b} = 0 \\ I \nabla \cdot \mathbf{b} = 0 \end{array} \quad \Rightarrow \quad \begin{array}{l} \nabla \cdot \mathbf{e} = \rho \\ -I \nabla \wedge \mathbf{b} = \frac{\partial}{\partial t} \mathbf{e} + \mathbf{J} \\ \nabla \wedge \mathbf{e} = -I \frac{\partial}{\partial t} \mathbf{b} \\ \nabla \cdot \mathbf{b} = 0 \end{array} \quad \Rightarrow \quad \begin{array}{l} \nabla \cdot \mathbf{e} = \rho \\ \nabla \times \mathbf{b} = \frac{\partial}{\partial t} \mathbf{e} + \mathbf{J} \\ \nabla \times \mathbf{e} = -\frac{\partial}{\partial t} \mathbf{b} \\ \nabla \cdot \mathbf{b} = 0 \end{array}$$

Maxwell's Equations

$$\nabla \cdot \mathbf{e} = \rho$$

$$\nabla \times \mathbf{b} = \frac{\partial}{\partial t} \mathbf{e} + \mathbf{J}$$

$$\nabla \times \mathbf{e} = -\frac{\partial}{\partial t} \mathbf{b}$$

$$\nabla \cdot \mathbf{b} = 0$$

Maxwell's Equations

$$\begin{array}{ll} \nabla \cdot \mathbf{e} = \rho & \nabla \cdot \mathbf{E} = \rho \\ \nabla \times \mathbf{b} = \frac{\partial}{\partial t} \mathbf{e} + \mathbf{J} & \nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} \\ \nabla \times \mathbf{e} = -\frac{\partial}{\partial t} \mathbf{b} & \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{b} = 0 & \nabla \cdot \mathbf{B} = 0 \end{array} \Rightarrow$$

Change symbols to **E** and **B** for electric and magnetic fields.

Maxwell's Equations

$$\nabla \cdot \mathbf{E} = \rho$$

$$\nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0$$

Maxwell's Equations

$$\begin{array}{ll} \nabla \cdot \mathbf{E} = \rho & \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \\ \nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} & \nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \\ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} & \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} = 0 & \nabla \cdot \mathbf{B} = 0 \end{array} \quad \Rightarrow$$

From natural units to SI units ($c^2 \epsilon_0 \mu_0 = 1$).

Maxwell's Equation

$$\nabla F = \rho - \mathbf{J}$$

An “Object-Oriented” Approach to Geometry

We can represent geometric entities as “objects” that can be manipulated in a coordinate-free manner.

This can be well demonstrated by doing rotations using geometric algebra.

Rotation

Rotate a vector \mathbf{v} by twice the angle between \mathbf{a} and \mathbf{b} .

$$R = \mathbf{a}\mathbf{b}$$

$$R^\dagger = \mathbf{b}\mathbf{a}$$

$$\mathbf{v}' = R^\dagger \mathbf{v} R$$

Rotation

Rotate a vector \mathbf{v} by twice the angle between \mathbf{a} and \mathbf{b} .

$$R = \mathbf{a}\mathbf{b}$$

$$R^\dagger = \mathbf{b}\mathbf{a}$$

$$\mathbf{v}' = R^\dagger \mathbf{v} R$$

$$\mathbf{v}'' = \frac{\mathbf{v}'}{R^\dagger R}$$

Rotation

Rotate a vector \mathbf{v} by twice the specified angle in the plane P , specified by a bivector.

$$R = e^{\frac{\theta}{2}P}$$

$$R^\dagger = e^{-\frac{\theta}{2}P}$$

$$\mathbf{v}' = R^\dagger \mathbf{v} R$$

Solving Geometric Problem in Higher Dimension

The problem can sometimes be more intuitively solved in a higher dimension.

- ▶ Solving 3D problems in 4D
- ▶ Solving 3D problems in 5D
- ▶ Solving 3D problems in 15D

Geometric algebra provides a unified framework for solving problems in higher dimensions.

Projective Geometric Algebra

Let's represent a 3D point with a 4D vector in $\mathbb{G}^{3,1}$.

A line L passing through two points p and q is represented by the outer product of their corresponding vectors:

$$L = \mathbf{p} \wedge \mathbf{q}$$

A plane P containing three points p , q , and r is represented by the outer product of their corresponding vectors:

$$P = \mathbf{p} \wedge \mathbf{q} \wedge \mathbf{r}$$

Projective Geometric Algebra

Let I be $\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3\mathbf{e}_4$. The intersection of a line L and a plane P is represented by:

$$P \cdot (IL)$$

The intersection of two planes P and Q is represented by:

$$(IP) \cdot Q$$

gmc script: `samples/projective.gmc`

Ref: Geometric algebra for physicists, C. Doran, A. Lasenby

Conformal Geometric Algebra

A 5D conformal geometric algebra can be defined out of $\mathbb{G}^{4,1}$:

$$\mathbf{e}_o = \frac{1}{2}(-\mathbf{e}_4 + \mathbf{e}_5)$$

$$\mathbf{e}_\infty = \frac{1}{2}(\mathbf{e}_4 + \mathbf{e}_5)$$

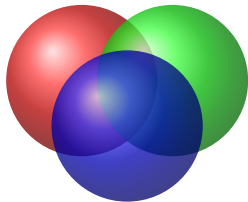
$$I = \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3 \wedge \mathbf{e}_\infty \wedge \mathbf{e}_o$$

$$I^{-1} = \mathbf{e}_o \wedge \mathbf{e}_\infty \wedge \mathbf{e}_3 \wedge \mathbf{e}_2 \wedge \mathbf{e}_1$$

Points, planes, and spheres can be represented by linear combinations of the basis vectors: $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_o, \mathbf{e}_\infty$.

Molecular Distance Geometry Problem

It is to determine a three-dimensional structure of a molecule given an incomplete set of interatomic distances. We can solve the problem based on calculating the intersection points of three spheres in $\mathbb{G}^{4,1}$.



$$\mathbf{p}_i = v_{i1} \mathbf{e}_1 + v_{i2} \mathbf{e}_2 + v_{i3} \mathbf{e}_3$$

$$\mathbf{P}_i = \mathbf{p}_i + \frac{1}{2} \mathbf{p}_i \mathbf{p}_i \mathbf{e}_\infty + \mathbf{e}_o$$

$$\mathbf{S}_i = \mathbf{P}_i - \frac{1}{2} d_i d_i \mathbf{e}_\infty$$

$$\mathbf{Q} = -(\mathbf{S}_1 \wedge \mathbf{S}_2 \wedge \mathbf{S}_3) I^{-1}$$

$$\mathbf{T} = -(\pm \sqrt{\mathbf{Q} \cdot \mathbf{Q}} + \mathbf{Q})(\mathbf{e}_\infty \cdot \mathbf{Q})^{-1}$$

gmc script: `samples/molecular-distance-geometry.gmc`

The power of geometric algebra computing, Dietmar Hildenbrand

Higher Dimensional Geometric Algebra

- ▶ Conics in \mathbb{R}^2 can be represented with $\mathbb{G}^{5,3}$ or $\mathbb{G}^{6,2}$
- ▶ Cubic Curves can be handled with $\mathbb{G}^{9,3}$ or $\mathbb{G}^{4,8}$
- ▶ Quadric surfaces can be represented and constructed intuitively in $\mathbb{G}^{9,6}$

Ref: Quadric conformal geometric algebra of $\mathbb{R}^{9,6}$, Stéphane Breuils et al.

Determinant of Linear Transformation

Let f be a linear transformation on \mathbb{R}^n and $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$ be vectors in \mathbb{R}^n . Then

$$f(\mathbf{v}_1) \wedge f(\mathbf{v}_2) \wedge \dots \wedge f(\mathbf{v}_n) = \det(f)(\mathbf{v}_1 \wedge \mathbf{v}_2 \wedge \dots \wedge \mathbf{v}_n)$$

The determinant of a linear transformation f on \mathbb{R}^n is the factor by which the transformation scales the oriented volumes of n -dimensional parallelograms.

Pauli Algebra

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

| \times | σ_x | σ_y | σ_z |
|------------|--------------|--------------|--------------|
| σ_x | \mathbb{I} | $i\sigma_z$ | $-i\sigma_y$ |
| σ_y | $-i\sigma_z$ | \mathbb{I} | $i\sigma_x$ |
| σ_z | $i\sigma_y$ | $-i\sigma_x$ | \mathbb{I} |

| \times | \mathbf{e}_1 | \mathbf{e}_2 | \mathbf{e}_3 |
|----------------|------------------|------------------|------------------|
| \mathbf{e}_1 | 1 | $I\mathbf{e}_3$ | $-I\mathbf{e}_2$ |
| \mathbf{e}_2 | $-I\mathbf{e}_3$ | 1 | $I\mathbf{e}_1$ |
| \mathbf{e}_3 | $I\mathbf{e}_2$ | $-I\mathbf{e}_1$ | 1 |

where i is the imaginary unit, $I = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$, and \mathbb{I} is the identity matrix. The Pauli algebra generated by three spin operators σ_x , σ_y , and σ_z is isomorphic to the geometric algebra \mathbb{G}^3 .

Dirac Algebra

$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix},$$

$$\gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

where i is the imaginary unit.

Dirac Algebra

| \times | γ^0 | γ^1 | γ^2 | γ^3 |
|------------|--------------|---------------|---------------|---------------|
| γ^0 | \mathbb{I} | | | |
| γ^1 | | $-\mathbb{I}$ | | |
| γ^2 | | | $-\mathbb{I}$ | |
| γ^3 | | | | $-\mathbb{I}$ |

| \times | \mathbf{e}_0 | \mathbf{e}_1 | \mathbf{e}_2 | \mathbf{e}_3 |
|----------------|----------------|----------------|----------------|----------------|
| \mathbf{e}_0 | 1 | | | |
| \mathbf{e}_1 | | -1 | | |
| \mathbf{e}_2 | | | -1 | |
| \mathbf{e}_3 | | | | -1 |

where \mathbb{I} is the identity matrix. The algebra generated by γ^0 , γ^1 , γ^2 , and γ^3 is isomorphic to the geometric algebra $\mathbb{G}^{1,3}$.

Dirac Equation for Hydrogen in $\mathbb{G}^{1,3}$

$$\nabla \psi \mathbf{e}_1 \mathbf{e}_2 - \frac{Ze^2}{4\pi r} \psi + m \mathbf{e}_0 \psi \mathbf{e}_0 = E \psi,$$

where e is the elementary charge, Z is the atomic number, m is the mass of the electron, r is the distance from the nucleus, and E is the energy.

The equation and its observables are in *real* algebra of spacetime, with no need for complex numbers.

Manifold

Here we use the term **manifold** a bit loosely, referring to an m -dimensional object \mathcal{M} that can be locally parametrized by a set of coordinates. The general parameterization of an m -dimensional manifold M in \mathbb{R}^n , $m \leq n$ is given by

$$\mathbf{x}(u_1, u_2, \dots, u_m) = x_i(u_1, u_2, \dots, u_m) \mathbf{e}_i, \quad i = 1, 2, \dots, n.$$

We will call 1-dimensional manifolds *curves*, 2-dimensional manifolds *surfaces*, and 3-dimensional manifolds *solids*.

Tangent Space

There is a tangent space **at every point** of a manifold.

Tangent Space for 1-Dimensional Manifold

Let $\mathbf{x} : A \subseteq \mathbb{R}^1 \rightarrow C \subseteq \mathbb{R}^n$ parameterize a curve C . Fix $t \in A$ and let $\mathbf{p} = \mathbf{x}(t)$. The vector $\mathbf{x}'(t)$, and its scalar multiples, are called **tangent vectors** to the curve C at \mathbf{p} . This 1D span of $\mathbf{x}'(t)$ is called the **tangent space** to C at \mathbf{p} . Denote it $T_{\mathbf{p}}$.

Tangent Space for 2-Dimensional Manifold

Let $\mathbf{x} : A \subseteq \mathbb{R}^2 \rightarrow S \subseteq \mathbb{R}^n$ parameterize a surface S . Fix $\mathbf{q} \in A$ and $\mathbf{w} \in \mathbb{R}^2$. Let $\mathbf{p} = \mathbf{x}(\mathbf{q})$.

$$\partial_{\mathbf{w}}\mathbf{x}(\mathbf{q}) = \lim_{h \rightarrow 0} \frac{\mathbf{x}(\mathbf{q} + h\mathbf{w}) - \mathbf{x}(\mathbf{q})}{h}. \quad (3)$$

The vector $\partial_{\mathbf{w}}\mathbf{x}(\mathbf{q})$ is the **directional derivative** of \mathbf{x} at \mathbf{q} in the direction of \mathbf{w} . The vector is a *tangent vector* to the surface S at \mathbf{p} . The set of **all tangent vectors to S at \mathbf{p}** is a vector space. It is called the **tangent space** to S at \mathbf{p} . Denote it $T_{\mathbf{p}}$.

Tangent Space for m -Dimensional Manifold

The vectors tangent to an m -dimensional manifold M , which is parameterized by $\mathbf{x}(u, v, \dots)$, at a point $\mathbf{p} \in M$ form the **tangent space** to M at \mathbf{p} , which is an m -dimensional vector space $T_{\mathbf{p}}$.

Theorem

$\{\mathbf{x}_u, \mathbf{x}_v, \dots\}$ forms a basis for the tangent space to M at \mathbf{p} , where $\mathbf{x}_u = \frac{\partial \mathbf{x}(u, v, \dots)}{\partial u}$.

Reciprocal Basis

A reciprocal basis $\{\mathbf{x}^u, \mathbf{x}^v, \dots\}$ can always be constructed for a basis $\{\mathbf{x}_u, \mathbf{x}_v, \dots\}$.

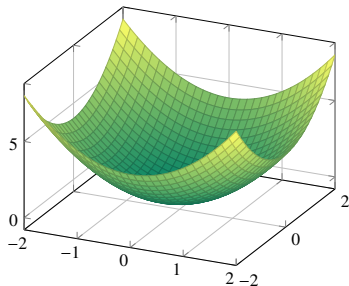
$$\mathbf{x}^u \cdot \mathbf{x}_v = \begin{cases} 1 & \text{if } u = v, \\ 0 & \text{if } u \neq v. \end{cases}$$

Vector Derivative

Let F be a multivector valued function defined on a manifold M , which is parameterized by $\mathbf{x}(u, v, \dots)$. Let $\{\mathbf{x}_u, \mathbf{x}_v, \dots\}$ be a basis for the tangent space $T_{\mathbf{p}}$ at $\mathbf{p} \in M$ and $\{\mathbf{x}^u, \mathbf{x}^v, \dots\}$ be the reciprocal basis. Then the vector derivative $\partial F(\mathbf{x}) = \partial F(\mathbf{x}(u, v, \dots))$ is

$$\partial F(\mathbf{x}(u, v, \dots)) \equiv \mathbf{x}^u \frac{\partial F(\mathbf{x})}{\partial u} + \mathbf{x}^v \frac{\partial F(\mathbf{x})}{\partial v} + \dots = \mathbf{x}^u \partial_u F + \mathbf{x}^v \partial_v F + \dots$$

Vector Derivative



$$\mathbf{x}(v_1, v_2) = v_1 \mathbf{e}_1 + v_2 \mathbf{e}_2 + (v_1^2 + v_2^2) \mathbf{e}_3$$

$$F = (v_2 + 1) \log(v_1)$$

$$\partial F(1, 0) = 0.2 \mathbf{e}_1 + 0.4 \mathbf{e}_2$$

gmc script: samples/basin.gmc

Fundamental Theorem of Geometric Calculus

Let M be an m -dimensional **bounded oriented** manifold in some \mathbb{R}^n ($n \geq m$) with **boundary** ∂M , and let F on $M \cup \partial M$ be continuously differentiable on M and continuous on $M \cup \partial M$, then

$$\int_M d^m \mathbf{x} \, \partial F = \int_{\partial M} d^{m-1} \mathbf{x} \, F$$

The boundary ∂M of M is a manifold of dimension $m - 1$.

Fundamental Theorem of Geometric Calculus

A boundary has no boundary: $\partial(\partial M) = \emptyset$. We can use \oint to signify this:

$$\begin{array}{c}
 \text{vector derivative of } F \\
 \hline
 \int_M \mathbf{d}^m \mathbf{x} \partial F = \oint_{\partial M} \mathbf{d}^{m-1} \mathbf{x} F \\
 \begin{array}{l}
 \text{infinitesimal } m\text{-vector in tangent space} \quad \uparrow \\
 \text{boundary of } M \quad \uparrow
 \end{array}
 \end{array}$$

vector derivative of F
infinitesimal m -vector in tangent space
directed integral
boundary of M

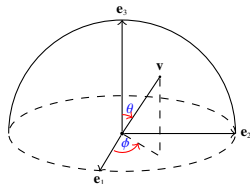
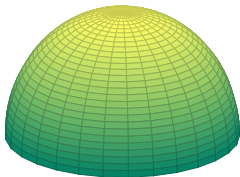
Here, $\mathbf{d}^m \mathbf{x} = \mathbf{I}_m \mathbf{d}^m x$, where $\mathbf{I}_m = \mathbf{I}_m(\mathbf{x})$ is the unit m -vector of the tangent space to M at \mathbf{x} , and $\mathbf{d}^m x$ is the infinitesimal m -volume, which is an infinitesimal scalar.

Directed Integral

Suppose manifold M is parameterized by $\mathbf{x}(u_1, u_2, \dots, u_m) : A \subset \mathbb{R}^m \rightarrow M \subset \mathbb{R}^n$. Then the **directed** integral of F over M is

$$\int_M d^m \mathbf{x} F = \int_A (\mathbf{x}_{u_1} \wedge \mathbf{x}_{u_2} \wedge \dots \wedge \mathbf{x}_{u_m}) F(\mathbf{x}) dA$$

Fundamental Theorem of Geometric Calculus



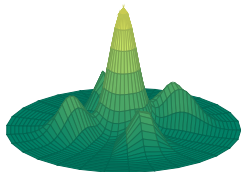
$$\mathbf{x}(\theta, \phi) = \sin(\theta) \cos(\phi) \mathbf{e}_1 + \sin(\theta) \sin(\phi) \mathbf{e}_2 + \cos(\theta) \mathbf{e}_3$$

$$F = \cos(\theta)$$

$$\int_M d^m \mathbf{x} \partial F = \int_{\partial M} d^{m-1} \mathbf{x} F = 0$$

gmc script: `samples/hemisphere.gmc`

Applying Fundamental Theorem to 3D Electronic Structure Problem?



- ▶ Suppose the electronic structure is a 3D manifold M .
- ▶ Assume the chemical property of interest is a function F on M .
- ▶ With carefully designed parametric F and M , we can apply the fundamental theorem to solve the electronic structure problems in 2D or 4D.

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Epilogue

Computational Considerations

- ▶ Matrix representation vs geometric algebra
- ▶ The power of symbolic simplification

Matrix Representation vs Geometric Algebra

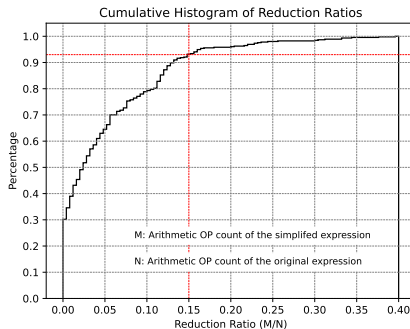
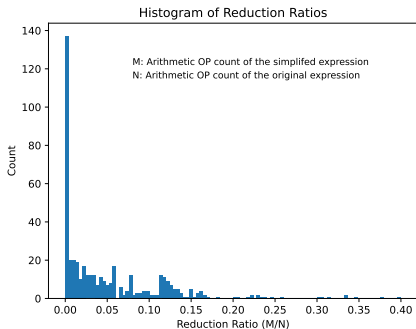
The total dimension of $\mathbb{G}^{p,q}$ is 2^n , where $n = p + q$. If we want to create a matrix representation of the algebra, the matrices will be of the order of $2^{n/2} \times 2^{n/2}$.

For example, the matrix representation of Dirac algebra $G^{1,3}$ requires 4×4 matrices.

Don't be confuse the matrix representation of an algebra with organizing the elements of the algebra in a matrix form.

The Power of Symbolic Simplification: A Case Study

Calculating Hermite coefficients is one of the performance bottlenecks when we implement density functional theory using the McMurchie-Davidson integral scheme.



The arithmetic OP counts of over 93% of the Hermite coefficients calculations are reduced to 15%!

The End