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

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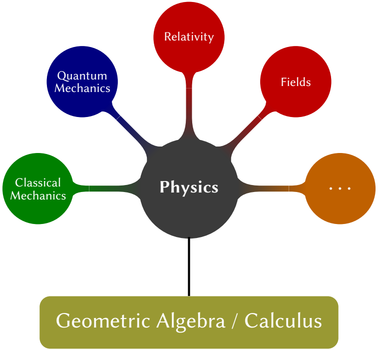
Prologue


Relativity
Quantum Mechanics
Fields
Classical Mechanics
Physics
. . .
Geometric Algebra / Calculus

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 AI for 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 $\{\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_n\}$, where $\mathbb{R}$ is the set of real numbers.

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

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

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

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:

$$\begin{aligned} \mathbf{ab} &= (a_1\mathbf{e}_1 + \cdots + a_n\mathbf{e}_n)(b_1\mathbf{e}_1 + \cdots + b_n\mathbf{e}_n) \\ &= a_1b_1\mathbf{e}_1\mathbf{e}_1 + a_1b_2\mathbf{e}_1\mathbf{e}_2 + \cdots + a_nb_n\mathbf{e}_n\mathbf{e}_n \end{aligned}$$

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

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 **Geome**tric Cal**culus**

	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
# unamed 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

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

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

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

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

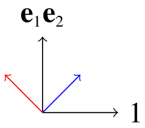
The complex number system is isomorphic to the subalgebra with form $a + bI$ of $\mathbb{G}^2$.

gmc script: samples/complex.gmc

Complex Numbers

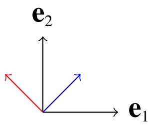
Rotate a vector by θ in the "complex plane" with $\{1, \mathbf{e}_1\mathbf{e}_2\}$ as axes:

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



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

$$I = \mathbf{e}_1\mathbf{e}_2, \;\; I^2 = -1$$
$$J = \mathbf{e}_2\mathbf{e}_3, \;\; J^2 = -1$$
$$K = \mathbf{e}_1\mathbf{e}_3, \;\; K^2 = -1$$

$$IJK = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_2\mathbf{e}_3\mathbf{e}_1\mathbf{e}_3 = -1$$
$$(a + b\,I + c\,J + d\,K)\,(a - b\,I - c\,J - d\,K) = a^2 + b^2 + c^2 + d^2$$

Multivectors of form $a + b\,I + c\,J + d\,K$ are isomorphic to quaternions.

gmc script: samples/quaternion.gmc

Inner Product of Vectors

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

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

gmc script: samples/inner-product.gmc

Outer Product of Vectors

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

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

gmc script: samples/outer-product.gmc

Geometric Product of Vectors

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

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

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

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

Cross Product of Vectors

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

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

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

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

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

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

gmc script: samples/cross-product.gmc

Angular Momentum and Torque

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

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

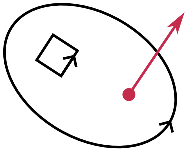
where $\mathbf{L}$ is the angular momentum, $\boldsymbol{\tau}$ is the torque, $\mathbf{r}$ is the position vector, and $\mathbf{p}$ is the momentum vector.

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

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

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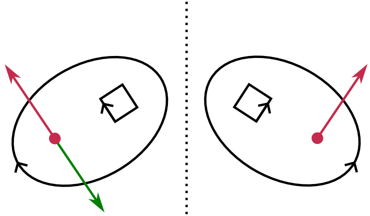
where $\mathbf{b}$ is the magnetic field vector, and $\mathbf{B}$ is the magnetic bivector field orthogonal to $\mathbf{b}$.



gmc script: samples/magnetic.gmc

Extending Partial Derivative to Multivector-valued Functions

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

$$\frac{\partial F(\mathbf{x})}{\partial x_i} = \lim_{h \to 0} \frac{F(\mathbf{x} + h\mathbf{e}_i) - F(\mathbf{x})}{h} = \lim_{h \to 0} \frac{F(x_1, x_2, \ldots, x_i + h, \ldots, x_m) - F(\mathbf{x})}{h}. \tag{1}$$

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.

$$\nabla F = \nabla \cdot F + \nabla \wedge F$$
$$\partial_i \partial_j F = \partial_j \partial_i F$$

Ref: Vector and geometric calculus, A. Macdonald

Maxwell's Equations

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

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

$$\begin{aligned} F &= \mathbf{e} + \mathbf{B} \\ \boldsymbol{\nabla} &= \frac{\partial}{\partial t} + \nabla = \partial_t + \mathbf{e}_1\partial_1 + \mathbf{e}_2\partial_2 + \mathbf{e}_3\partial_3 \\ \rho &: \text{charge density, scalar} \\ \mathbf{J} &: \text{current density, vector} \end{aligned}$$

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

Maxwell's Equations

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

Maxwell's Equations

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

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

Maxwell's Equations

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

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

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

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

Maxwell's Equations

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

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

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

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

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

Maxwell's Equations

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

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

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

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

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

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

Maxwell's Equations

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

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

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

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

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

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

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

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

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

Maxwell's Equations

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

Maxwell's Equations

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

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

$$\nabla \cdot \mathbf{e} = \rho$$
$$\nabla \times \mathbf{b} = \frac{\partial}{\partial t}\mathbf{e} + \mathbf{J}$$
$$\nabla \times \mathbf{e} = -\frac{\partial}{\partial t}\mathbf{b}$$
$$\nabla \cdot \mathbf{b} = 0$$

$$\Rightarrow$$

$$\nabla \cdot \mathbf{E} = \rho$$
$$\nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \cdot \mathbf{B} = 0$$

Change symbols to $\mathbf{E}$ and $\mathbf{B}$ for electric and magnetic fields.

Maxwell's Equations

$$\nabla \cdot \mathbf{E} = \rho$$
$$\nabla \times \mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \cdot \mathbf{B} = 0$$

Ref: Units in electrodynamics, Randy S

Maxwell's Equations

$$
\begin{aligned}
\nabla \cdot \mathbf{E} &= \rho \\
\nabla \times \mathbf{B} &= \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\nabla \cdot \mathbf{E} &= \frac{\rho}{\varepsilon_0} \\
\nabla \times \mathbf{B} &= \mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0
\end{aligned}
$$

From natural units to SI units ($c^2\varepsilon_0\mu_0 = 1$).

Ref: Units in electrodynamics, Randy S

Maxwell's Equation

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

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 $\mathbf{b}$.

$$\begin{aligned} R &= \mathbf{a}\mathbf{b} \\ R^\dagger &= \mathbf{b}\mathbf{a} \\ \mathbf{v}' &= R^\dagger \mathbf{v} R \end{aligned}$$

gmc script: samples/rotation.gmc

Rotation

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

$$
\begin{aligned}
R &= \mathbf{a}\mathbf{b} \\
R^{\dagger} &= \mathbf{b}\mathbf{a} \\
\mathbf{v}' &= R^{\dagger}\mathbf{v}R \\
\mathbf{v}'' &= \frac{\mathbf{v}'}{R^{\dagger}R}
\end{aligned}
$$

gmc script: samples/rotation.gmc

Rotation

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

$$
\begin{aligned}
R &= e^{\frac{\theta}{2}P} \\
R^{\dagger} &= e^{-\frac{\theta}{2}P} \\
\mathbf{v}' &= R^{\dagger}\mathbf{v}R
\end{aligned}
$$

gmc script: samples/rotation.gmc

Solving Geometric Problem in Higher Dimension

The problem can sometimes be more intuively 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 $\mathbb{G}^{4,1}$:

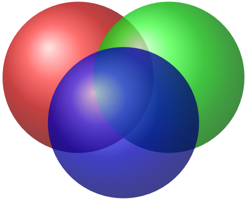
$$
\begin{aligned}
\mathbf{e}_o &= \frac{1}{2}(-\mathbf{e}_4 + \mathbf{e}_5) \\
\mathbf{e}_\infty &= \frac{1}{2}(\mathbf{e}_4 + \mathbf{e}_5) \\
I &= \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3 \wedge \mathbf{e}_\infty \wedge \mathbf{e}_o \\
I^{-1} &= \mathbf{e}_o \wedge \mathbf{e}_\infty \wedge \mathbf{e}_3 \wedge \mathbf{e}_2 \wedge \mathbf{e}_1
\end{aligned}
$$

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

gmc script: samples/conformal.gmc
Foundations of geometric algebra computing, Dietmar Hildenbrand

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 $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ be vectors in $\mathbb{R}^n$. Then

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

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.

gmc script: samples/determinant.gmc
Vector and geometric calculus, A. Macdonald

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 $\mathbb{G}^3$.

gmc script: samples/pauli.gmc

Dirac Algebra

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

$$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \qquad \gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

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 $\mathbb{G}^{1,3}$.

gmc script: samples/dirac.gmc

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.

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

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

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

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 $\mathbf{x} : A \subseteq \mathbb{R}^1 \to C \subseteq \mathbb{R}^n$ 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 $T_{\mathbf{p}}$.

Ref: Vector and geometric calculus, A. Macdonald

Tangent Space for 2-Dimensional Manifold

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

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

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 $T_{\mathbf{p}}$.

Ref: Vector and geometric calculus, A. Macdonald

Tangent Space for m-Dimensional Manifold

The vectors tangent to an m-dimensional manifold M, which is parameterized by $\mathbf{x}(u, v, \cdots)$, 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

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

Ref: Vector and geometric calculus, A. Macdonald

Reciprocal Basis

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

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

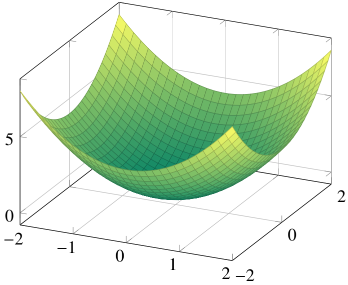
Ref: Vector and geometric calculus, A. Macdonald

Vector Derivative

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

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

Vector Derivative



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

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

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

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

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

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

Vector and geometric calculus, A. Macdonald

Fundamental Theorem of Geometric Calculus

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

vector derivative of F

directed integral

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

infinitesimal m-vector in tangent space

boundary of M

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

Vector and geometric calculus, A. Macdonald

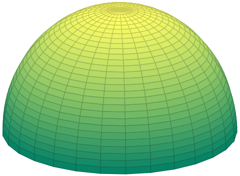
Directed Integral

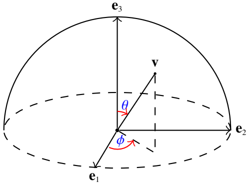
Suppose manifold M is parameterized by $\mathbf{x}(u_1, u_2, \ldots, u_m) : A \subset \mathbb{R}^m \to M \subset \mathbb{R}^n$. Then the directed integral of F over M is

$$\int_M \mathrm{d}^m\mathbf{x}\, F = \int_A (\mathbf{x}_{u_1} \wedge \mathbf{x}_{u_2} \wedge \ldots \wedge \mathbf{x}_{u_m}) F(\mathbf{x})\, \mathrm{d}A$$

Vector and geometric calculus, A. Macdonald

Fundamental Theorem of Geometric Calculus





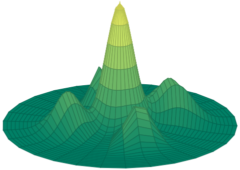
$$\mathbf{x}(\theta,\phi) = \sin(\theta)\cos(\phi)\mathbf{e}_1 + \sin(\theta)\sin(\phi)\mathbf{e}_2 + \cos(\theta)\mathbf{e}_3$$

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

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

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.

References

- Clifford algebra to geometric calculus: A unified language for mathematics and physics, D. Hestenes, G. Sobczyk, 1984
- Geometric algebra for physicists, C. Doran, A. Lasenby, 2003
- Vector and geometric calculus, A. Macdonald, 2012
- Geometric algebra and applications to physics, Venzo De Sabbata and Bidyut Kumar Datta, 2007
- Foundations of geometric algebra computing, Dietmar Hildenbrand, 2013
- The power of geometric algebra computing, Dietmar Hildenbrand, 2022

References

- Molecular distance geometry problem, Encyclopedia of Optimization, 2009
- Fundamental theorem of calculus, Garret Sobczyk, Omar Sanchez, 2011
- A Guided Tour to the Plane-Based Geometric Algebra PGA, Leo Dorst and Steven De Keninck, 2022
- N-dimensional rigid body dynamics, Marc ten Bosch, 2020
- Quadric conformal geometric algebra of $\mathbb{R}^{9,6}$, Stéphane Breuils et al., 2018

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 $2^{n/2} \times 2^{n/2}$.

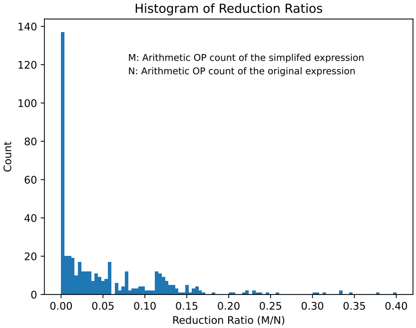
For example, the matrix representation of Dirac algebra $G^{1,3}$ requires 4×4 matrices.

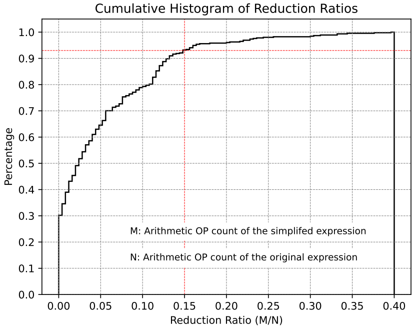
Don't be confuse the matrix representation of an algebra with organizing the elements of the algebra in a matrix form.

N-dimensional rigid body dynamics, Marc ten Bosch
Geometric algebra for physicists, C. Doran, A. Lasenby

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