Different Models for 3D Space in Molecular Geometry

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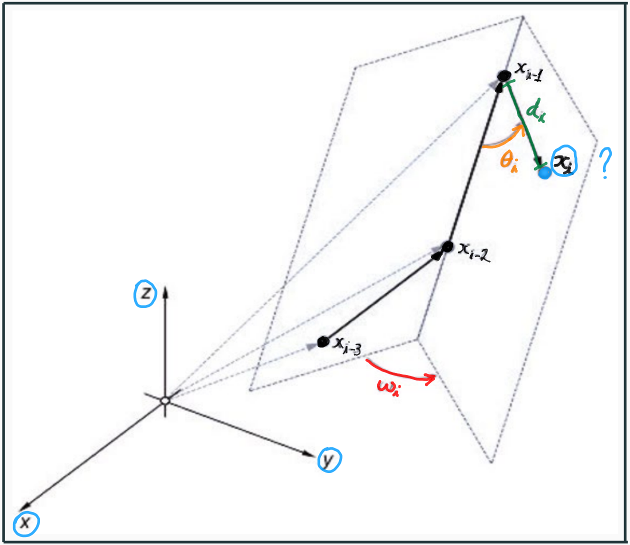

x_{i-1}
d_i
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?
x_{i-2}
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ω_i
z
y
x

Isometries

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For $\alpha \in \mathbb{R}$ and $u, v, w \in \mathbb{R}^3$,

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$$u \cdot (v + w) = (u \cdot v) + (u \cdot w),$$

$$\alpha(u \cdot v) = (\alpha u) \cdot v = u \cdot (\alpha v),$$

and

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and

$$u \neq 0 \Rightarrow u \cdot u > 0.$$

Isometries

An *isometry* in $\mathbb{R}^3$ is a function $f : \mathbb{R}^3 \to \mathbb{R}^3$ such that, $\forall u, v \in \mathbb{R}^3$,

$$||f(u) - f(v)|| = ||u - v||,$$

with

$$||u||^2 = u \cdot u.$$

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An isometry f can also be given by

$$f(u) = Au + b,$$

NONLINEAR !

$A \in \mathbb{R}^{3\times 3}$, $b \in \mathbb{R}^3$, and $A^{-1} = A^T$.

Isometries

Homogeneous Model of the 3D space: an isometry $f(x) = Ax + b$, $A \in \mathbb{R}^{3\times 3}$ and $b \in \mathbb{R}^3$, can be represented linearly in $\mathbb{R}^4$,

$$\begin{bmatrix} A & b \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} = \begin{bmatrix} Ax + b \\ 1 \end{bmatrix}.$$

$x \in \mathbb{R}^3$

The Homogeneous Model

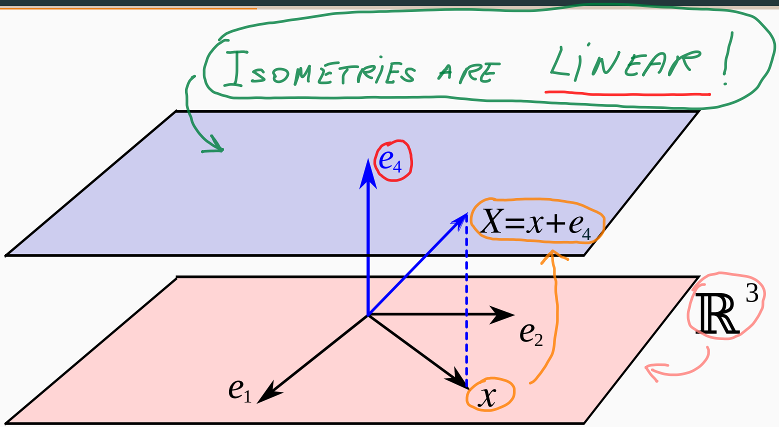

Figure 1: The Homogeneous Model.

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An orthogonal transformation A in $\mathbb{R}^3$ can also be given by, $\forall u, v \in \mathbb{R}^3$,

$$(Au) \cdot (Av) = u \cdot v.$$

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IF there is a constant $k \in \mathbb{R}$ ($\neq 0$) such that, $\forall x, y \in \mathbb{R}^3$,

$$X \cdot Y = k||x - y||^2, \qquad (1)$$

$X, Y \in \mathbb{R}^4$

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A point x of the $3D$ space can also be represented by

$$X = x + x_4 e_4, \quad x_4 \in \mathbb{R} \ (x_4 \neq 0).$$

No solution for $X \cdot Y = k \, \|x - y\|^2$

The Conformal Model

The Conformal Model

In $\mathbb{R}^5$, a point x of the $3D$ space,

$$x = x_1 e_1 + x_2 e_2 + x_3 e_3 + 0 e_4 + 0 e_5,$$

$e_5 \in \mathbb{R}^5$ is orthogonal to $\{e_1, e_2, e_3, e_4\}$, will be represented by

$$X = x + x_4 e_4 + x_5 e_5, \quad x_4, x_5 \in \mathbb{R}.$$

$\mathbb{R}^5$ $\mathbb{R}^3$

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Thus,

$$\begin{aligned} X \cdot X &= 0 \\ &\Rightarrow \\ (x + x_4 e_4 + x_5 e_5) \cdot (x + x_4 e_4 + x_5 e_5) &= 0 \\ &\Rightarrow \\ x_4^2 \overbrace{(e_4 \cdot e_4)}^{1} + x_5^2 (e_5 \cdot e_5) &= \underbrace{-||x||^2}_{<0}. \end{aligned}$$

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$$\begin{aligned} X \cdot X &= 0 \\ &\Rightarrow \\ (x + x_4 e_4 + x_5 e_5) \cdot (x + x_4 e_4 + x_5 e_5) &= 0 \\ &\Rightarrow \\ x_4^2 (e_4 \cdot e_4) + x_5^2 (e_5 \cdot e_5) &= -||x||^2. \end{aligned}$$

$x \neq 0$ and $||e_4|| = 1 \Rightarrow \underline{e_5 \cdot e_5 < 0}$.

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For $\alpha, \beta \in \mathbb{R}$, we have

$$\begin{aligned}(\alpha e_4 + \beta e_5) \cdot (\alpha e_4 + \beta e_5) &= 0 \\ &\Leftrightarrow \\ \alpha^2 (e_4 \cdot e_4) + \beta^2 (e_5 \cdot e_5) &= 0 \\ &\Leftrightarrow \\ \alpha^2 &= \beta^2.\end{aligned}$$

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Defining a new basis for $\mathbb{R}^5$, $\{e_1, e_2, e_3, e_0, e_\infty\}$,

$$e_0 = e_5 - e_4,$$

$$e_\infty = e_5 + e_4,$$

The Conformal Model

Considering a conformal point X using the basis $\{e_1, e_4, e_5\}$,

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we get

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The Conformal Model

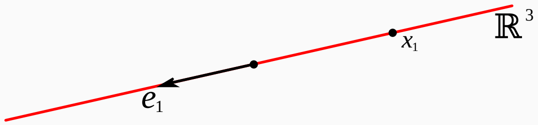

Figure 2: The Conformal Model.

The Conformal Model

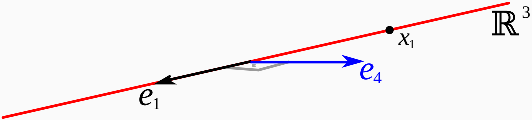

Figure 3: The Conformal Model.

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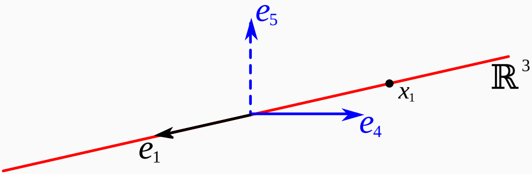

Figure 4: The Conformal Model.

The Conformal Model

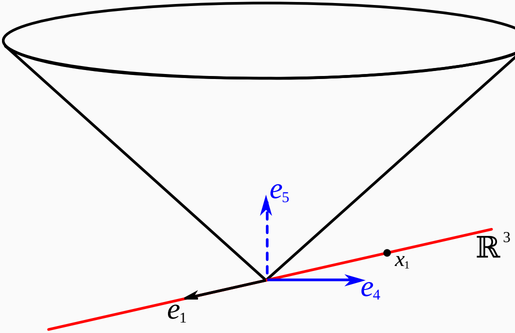

Figure 5: The Conformal Model.

The Conformal Model

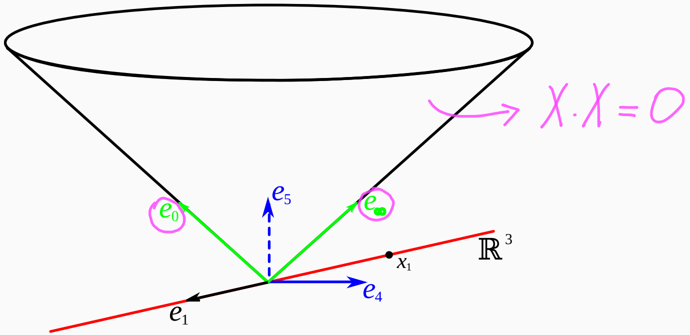

Figure 6: The Conformal Model.

The Conformal Model

To obtain the inner product between

$$X = x + x_0 e_0 + x_\infty e_\infty \text{ and } Y = y + y_0 e_0 + y_\infty e_\infty,$$

for $x_0, x_\infty, y_0, y_\infty \in \mathbb{R}$, we need to calculate

$$e_0 \cdot e_\infty.$$

REMEMBER THAT

$$X \cdot Y = K \|x - y\|^2$$

$$K \neq 0$$

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For

$$e_0 = \frac{e_5 - e_4}{2},$$

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Thus,

$$\begin{aligned} X \cdot Y &= (x + x_0 e_0 + x_\infty e_\infty) \cdot (y + y_0 e_0 + y_\infty e_\infty) \\ &= x \cdot y - (x_0 y_\infty + x_\infty y_0). \end{aligned}$$

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Considering $x_0 = 1$,

$$X = x + e_0 + \frac{1}{2}||x||^2 e_\infty.$$

$$X = \begin{bmatrix} x \\ 1 \\ \frac{1}{2}||x||^2 \end{bmatrix}, \quad x \in \mathbb{R}^3$$

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Considering $x_0 = 1$,

$$X = \underline{x + e_0} + \frac{1}{2}||x||^2 e_\infty.$$

For $x, y \in \mathbb{R}^3$,

$$\begin{aligned} X \cdot Y &= \left(x + e_0 + \frac{1}{2}||x||^2 e_\infty\right) \cdot \left(y + e_0 + \frac{1}{2}||y||^2 e_\infty\right) \\ &= x \cdot y - \left(\frac{1}{2}||x||^2 + \frac{1}{2}||y||^2\right) \\ &= -\frac{1}{2}\underline{||x - y||^2}. \end{aligned}$$

The Conformal Model

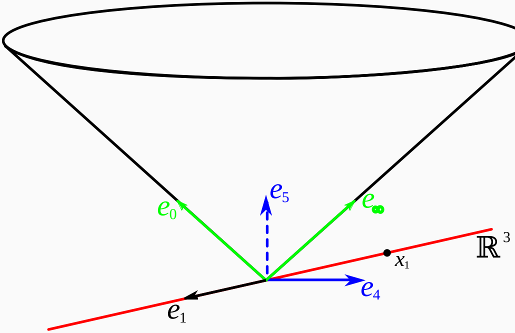

Figure 7: The Conformal Model.

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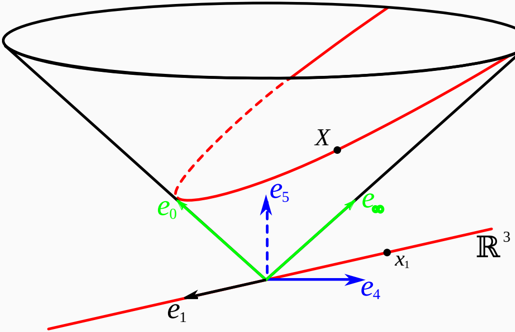

Figure 8: The Conformal Model.

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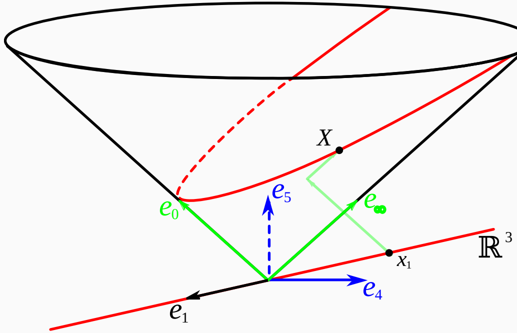

Figure 9: The Conformal Model.

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$\mathbb{R}^5$ with the basis $\{e_1, e_2, e_3, e_0, e_\infty\}$, such that, for $i, j = 1, 2, 3$,

$$e_i \cdot e_j = \delta_{ij},$$

$$e_0 \cdot e_i = 0,$$

$$e_\infty \cdot e_i = 0,$$

and

$$e_0 \cdot e_0 = e_\infty \cdot e_\infty = 0,$$

$$e_0 \cdot e_\infty = -1.$$

C.L., M. Souza, J.L. Aragon, Orthogonality of isometries in the conformal model of the 3D space, *Graphical Models*, 114 (2021).

J.M. Camargo, Geometria de Proteínas no Espaço Conforme, Tese de Doutorado, UNICAMP, 2021.

Questions?

Matrix Representation

If X , Y are the conformal representations of $x, y \in \mathbb{R}^3$,

$$\begin{aligned} UX &= Y \\ &\Leftrightarrow \\ (U^T I_c)UX &= (U^T I_c)Y \\ &\Leftrightarrow \\ X &= (I_c U^T I_c)Y. \end{aligned}$$

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That is,

$$U^{-1} = I_c U^T I_c,$$

with

$$U = \begin{bmatrix} A & b & 0 \\ 0 & 1 & 0 \\ b^T A & \frac{||b||^2}{2} & 1 \end{bmatrix} \text{ and } I_c = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}.$$