Computing interatomic distances using Euclidean, Homogeneous, and Conformal Models

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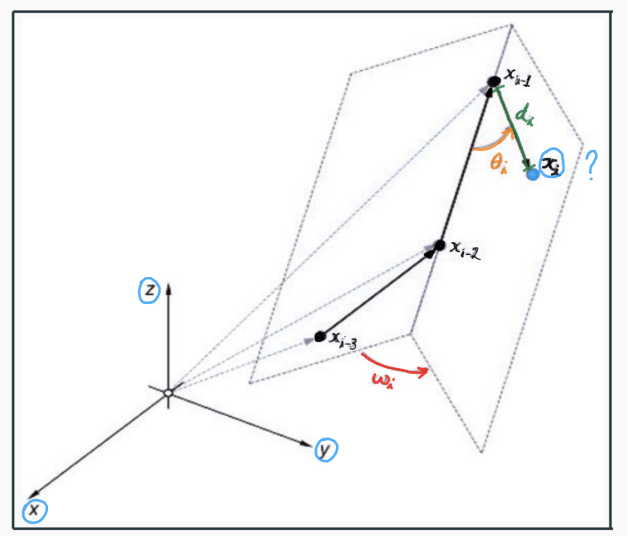
x_{i-1}
d_i
θ_i
x_i
?
x_{i-2}
z
x_{i-3}
ω_i
y
x

- In the homogeneous space:

$$B_{\theta_i} = \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & 0 \\ \sin\theta_i & -\cos\theta_i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \; B_{\omega_i} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\omega_i & -\sin\omega_i & 0 \\ 0 & \sin\omega_i & \cos\omega_i & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

- For the translation,

- In the homogeneous space:

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- For the translation,

$$\begin{bmatrix} 1 & 0 & 0 & d_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

- Combining the matrices,

$$B_i = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\omega_i & -\sin\omega_i & 0 \\ 0 & \sin\omega_i & \cos\omega_i & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & 0 \\ \sin\theta_i & -\cos\theta_i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & d_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Combining the matrices,

$$
\begin{aligned}
B_i &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\omega_i & -\sin\omega_i & 0 \\ 0 & \sin\omega_i & \cos\omega_i & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & 0 \\ \sin\theta_i & -\cos\theta_i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & d_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & -d_i\cos\theta_i \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i & d_i\sin\theta_i\cos\omega_i \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i & d_i\sin\theta_i\sin\omega_i \\ 0 & 0 & 0 & 1 \end{bmatrix}.
\end{aligned}
$$

- With $d_1 = \omega_1 = \omega_2 = \omega_3 = 0$ and $\theta_1 = \theta_2 = \pi$, we get [1]

$$x_1 = B_1 e_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \qquad x_2 = (B_1 B_2) e_4 = \begin{bmatrix} d_2 \\ 0 \\ 0 \\ 1 \end{bmatrix},$$

$$x_3 = (B_1 B_2 B_3) e_4 = \begin{bmatrix} (d_2 - d_3 \cos\theta_3) \\ d_3 \sin\theta_3 \\ 0 \\ 1 \end{bmatrix},$$

$$x_i = (B_1 B_2 B_3 \cdots B_i) e_4,$$

$i = 4, \ldots, n$ and $e_4 = (0, 0, 0, 1)^t$.

[1] Thompson (1967)

- Let us write

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and calculate the Euclidean distance $r_{i,j}$:

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$$\begin{aligned} r_{i,j} &= \|(x_j - x_i)\| \\ &= \|(B_1 \cdots B_i \cdots B_j)e_4 - (B_1 \cdots B_i)e_4\| \\ &= \left\| B_{[1,i]} \left(B_{[i+1,j]} - I \right) e_4 \right\| \end{aligned}$$

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where I is the identity matrix in $\mathbb{R}^{4\times 4}$.

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where I is the identity matrix in $\mathbb{R}^{4\times4}$.

  - In $\mathbb{R}^{3\times3}$:

$$r_{i,j} = \left\| \left(d_{i+1} I + \sum_{s=i+2}^{j} d_s B_{[i+2,s]} \right) e_1 \right\|.$$

- In order to calculate $x_4 = (B_1 B_2 B_3 B_4) e_4$,

$$B_4 e_4 = \begin{bmatrix} -\cos\theta_4 & -\sin\theta_4 & 0 & -d_4\cos\theta_4 \\ \sin\theta_4\cos\omega_4 & -\cos\theta_4\cos\omega_4 & -\sin\omega_4 & d_4\sin\theta_4\cos\omega_4 \\ \sin\theta_4\sin\omega_4 & -\cos\theta_4\sin\omega_4 & \cos\omega_4 & d_4\sin\theta_4\sin\omega_4 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} -d_4\cos\theta_4 \\ d_4\sin\theta_4\cos\omega_4 \\ d_4\sin\theta_4\sin\omega_4 \\ 1 \end{bmatrix}.$$

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Using Geometric Algebra

- With the motor $M_{[i+1,j]}$,

$$r_{i,j}^2 = -2\langle e_0 M_{[i+1,j]} e_0 \left(M_{[i+1,j]}\right)^{-1} \rangle_0$$

- Using internal coordinates $(d_i, \theta_i, \omega_i)$, each atom is "constructed" by one translation and two rotations represented by $f : \mathbb{R}^3 \to \mathbb{R}^3$, given by

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$A \in \mathbb{R}^{3\times3}$, such that $A^{-1} = A^t$, and $b \in \mathbb{R}^3$.

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$A \in \mathbb{R}^{3\times3}$, such that $A^{-1} = A^t$, and $b \in \mathbb{R}^3$.

- Using the homogeneous coordinate system,

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

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

Using the Conformal Model

- In the Conformal Model, [2] [3]

$$\hat{x} = x + e_0 + \frac{1}{2}\|x\|^2 e_\infty,$$

$x \in \mathbb{R}^3$, $\hat{x} \in \mathbb{R}^5$.

- For the isometry f,

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[3] Li, Hestenes, and Rockwood (2001)

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- For the isometry f,

$$\widehat{f(x)} = (Ax + b) + e_0 + \left(\frac{1}{2}\|Ax + b\|^2\right) e_\infty.$$

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- Since

$$\frac{1}{2}\|Ax+b\|^2 = b^t Ax + \frac{\|b\|^2}{2} + \frac{\|x\|^2}{2},$$

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$$\begin{bmatrix} A & b & 0 \\ 0 & 1 & 0 \\ b^t A & \frac{\|b\|^2}{2} & 1 \end{bmatrix} \begin{bmatrix} x \\ 1 \\ \frac{\|x\|^2}{2} \end{bmatrix} = \begin{bmatrix} Ax + b \\ 1 \\ \frac{\|Ax+b\|^2}{2} \end{bmatrix},$$

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

- Recalling that

$$A = \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i \end{bmatrix}, \quad b = \begin{bmatrix} -d_i\cos\theta_i \\ d_i\sin\theta_i\cos\omega_i \\ d_i\sin\theta_i\sin\omega_i \end{bmatrix},$$

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- we get

$$b^t A = \begin{bmatrix} d_i & 0 & 0 \end{bmatrix}$$

and

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- we get

$$b^t A = \begin{bmatrix} d_i & 0 & 0 \end{bmatrix}$$

and

$$||b||^2 = d_i^2.$$

- Thus,

$$U = \begin{bmatrix} A & b & 0 \\ 0 & 1 & 0 \\ b^t A & \frac{\|b\|^2}{2} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & -d_i\cos\theta_i & 0 \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i & d_i\sin\theta_i\cos\omega_i & 0 \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i & d_i\sin\theta_i\sin\omega_i & 0 \\ 0 & 0 & 0 & 1 & 0 \\ d_i & 0 & 0 & \frac{d_i^2}{2} & 1 \end{bmatrix}.$$

- It is easy to check that

$$U^{-1} = I_c U^t I_c$$

and

$$(U^t I_c U = I_c),$$

where

$$I_c = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}.$$

Using I_c,

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Using I_c,

$$\begin{aligned} \hat{x} \cdot \hat{y} &= -\frac{1}{2}\|x - y\|^2 \\ &= \begin{bmatrix} x & 1 & \frac{\|x\|^2}{2} \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} y \\ 1 \\ \frac{\|y\|^2}{2} \end{bmatrix} \\ &= (\hat{x}^t I_c \hat{y}). \end{aligned}$$

$$B_i = \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & -d_i\cos\theta_i & 0 \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i & d_i\sin\theta_i\cos\omega_i & 0 \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i & d_i\sin\theta_i\sin\omega_i & 0 \\ 0 & 0 & 0 & 1 & 0 \\ d_i & 0 & 0 & \frac{d_i^2}{2} & 1 \end{bmatrix}$$

- As we did using the homogeneous model,

$$\hat{x}_i = B_{[i]} e_0,$$

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- e_0 plays the same role as e_4, and

- First, let's write

$$B_{[i+1,j]} = \prod_{k=i+1}^{j} B_k$$

and

$$\color{blue}{B_{[j]}} = B_{[i]} B_{[i+i,j]}.$$

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- From $\hat{x}_i = B_{[i]} e_0$, we obtain

$$\begin{aligned} \hat{x}_j \cdot \hat{x}_i &= \hat{x}_j^t I_c \hat{x}_i \\ &= (e_0^t B_{[j]}^t) I_c (B_{[i]} e_0) \end{aligned}$$

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$$B_{[i+1,j]} = \prod_{k=i+1}^{j} B_k$$

and

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- From $\hat{x}_i = B_{[i]} e_0$, we obtain

$$\begin{aligned}
\hat{x}_j \cdot \hat{x}_i &= \hat{x}_j^t I_c \hat{x}_i \\
&= (e_0^t B_{[j]}^t) I_c (B_{[i]} e_0) \\
&= e_0^t (B_{[i+1,j]})^t (B_{[i]}^t I_c B_{[i]}) e_0 \\
&= e_0^t (B_{[i+1,j]})^t (I_c e_0) \\
&= -e_0^t (B_{[i+1,j]})^t e_\infty \\
&= -e_\infty^t B_{[i+1,j]} e_0,
\end{aligned}$$

- implying that

$$r_{i,j}^2 = 2e_\infty^t(B_{[i+1,j]})e_0.$$

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- Just to compare,

$$r_{i,j}^2 = e_4^t(B_{[i+1,j]}^t B_{[i+1,j]})e_4 - 1$$

and

$$r_{i,j} = \left\| \left(d_{i+1} I + \sum_{s=i+2}^{j} d_s B_{[i+2,s]} \right) e_1 \right\|.$$

Number of operations to calcule $r_{i,j}$

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Model	Number of Operations
Euclidean	$55(j-i)-97$
Homogeneous	$35(j-i)-25$
Conformal	$28(j-i)-45$

Derivatives of $r_{i,j}$

Derivatives of $r_{i,j}$

- Doing the calculations,

$$\begin{aligned}\frac{\partial r_{i,j}}{\partial \alpha_k} &= \frac{1}{2r_{i,j}} \frac{\partial r_{i,j}^2}{\partial \alpha_k} \\ &= \frac{1}{2r_{i,j}} \frac{\partial}{\partial \alpha_k} \left(2 e_\infty^t B_{[i+1,j]} e_0\right) \\ &= \frac{1}{r_{i,j}} e_\infty^t \frac{\partial B_{[i+1,j]}}{\partial \alpha_k} e_0.\end{aligned}$$

- Since

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$$\frac{\partial B_{[i+1,j]}}{\partial \alpha_k} = B_{[i+1,k-1]} \frac{\partial B_k}{\partial \alpha_k} B_{[k+1,j]},$$

implying that

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$$B_{[i+1,j]} = B_{i+1} B_{i+2} \cdots B_j,$$

- we get

$$\frac{\partial B_{[i+1,j]}}{\partial \alpha_k} = B_{[i+1,k-1]} \frac{\partial B_k}{\partial \alpha_k} B_{[k+1,j]},$$

implying that

$$\frac{\partial r_{i,j}}{\partial \alpha_k} = \frac{1}{r_{i,j}} \left(e_\infty^t B_{[i+1,k-1]} \frac{\partial B_k}{\partial \alpha_k} B_{[k+1,j]} e_0 \right).$$

- Similarly,

$$\frac{\partial^2 r_{i,j}}{\partial \beta_l \partial \alpha_k} = \frac{\partial}{\partial \beta_l}\left(\frac{1}{2r_{i,j}}\frac{\partial r_{i,j}^2}{\partial \alpha_k}\right)$$

$$= -\frac{1}{2r_{i,j}^2}\frac{\partial r_{i,j}}{\partial \beta_l}\frac{\partial r_{ij}^2}{\partial \alpha_k} + \frac{1}{2r_{i,j}}\frac{\partial^2 r_{i,j}^2}{\partial \beta_l \partial \alpha_k}$$

$$= \frac{1}{r_{i,j}}\left(\frac{1}{2}\frac{\partial^2 r_{i,j}^2}{\partial \beta_l \partial \alpha_k} - \frac{\partial r_{i,j}}{\partial \beta_l}\frac{1}{2r_{i,j}}\frac{\partial r_{ij}^2}{\partial \alpha_k}\right)$$

$$= \frac{1}{r_{i,j}}\left(\frac{1}{2}\frac{\partial^2 r_{i,j}^2}{\partial \beta_l \partial \alpha_k} - \frac{\partial r_{i,j}}{\partial \beta_l}\frac{\partial r_{ij}}{\partial \alpha_k}\right),$$

- where

$$\frac{1}{2}\frac{\partial^2 r_{i,j}^2}{\partial \beta_l \partial \alpha_k} = \frac{1}{2}\frac{\partial}{\partial \beta_l}\left(2e_\infty^t B_{[i+1,k-1]}\frac{\partial B_k}{\partial \alpha_k}B_{[k+1,j]}e_0\right)$$

$$= e_\infty^t \left(B_{[i+1,l-1]}\frac{\partial B_l}{\partial \beta_l}B_{[l+1,k-1]}\frac{\partial B_k}{\partial \alpha_k}B_{[k+1,j]}\right) e_0.$$

- where

$$\frac{1}{2}\frac{\partial^2 r_{i,j}^2}{\partial\beta_l\partial\alpha_k} = \frac{1}{2}\frac{\partial}{\partial\beta_l}\left(2e_\infty^t B_{[i+1,k-1]}\frac{\partial B_k}{\partial\alpha_k}B_{[k+1,j]}e_0\right)$$
$$= e_\infty^t\left(B_{[i+1,l-1]}\frac{\partial B_l}{\partial\beta_l}B_{[l+1,k-1]}\frac{\partial B_k}{\partial\alpha_k}B_{[k+1,j]}\right)e_0.$$

- Finally,

$$\frac{\partial^2 r_{i,j}}{\partial\beta_l\partial\alpha_k} = \frac{1}{r_{i,j}}\left(\frac{1}{2}\frac{\partial^2 r_{i,j}^2}{\partial\beta_l\partial\alpha_k} - \frac{\partial r_{i,j}}{\partial\beta_l}\frac{\partial r_{ij}}{\partial\alpha_k}\right),$$

for

$$\frac{\partial r_{i,j}}{\partial\alpha_k} = \frac{1}{r_{i,j}}\left(e_\infty^t B_{[i+1,k-1]}\frac{\partial B_k}{\partial\alpha_k}B_{[k+1,j]}e_0\right).$$

Main References

- C.L., M. Souza, & J.L. Aragón, *"Orthogonality of isometries in the conformal model of the 3D space"*, Graphical Models 114 (2021).
- J. Camargo & C.L., *"A new perspective on the homogeneous coordinate system for calculating interatomic distances and their derivatives in terms of internal coordinates"*, Advanced Theory and Simulations (2024).
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Thank you