Computing interatomic distances using Euclidean, Homogeneous, and Conformal Models*

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Abstract. In computational chemistry, efficiently computing interatomic distances and their derivatives is crucial for advancing our understanding of molecular structures and dynamics. We present a study of two alternative representations of the 3D space in molecular geometry, the homogeneous and the conformal models, against the traditional Euclidean framework. By comparing these models, our research suggests the conformal model as a promising approach in computational chemistry.

1 Distances in the Euclidean Space

We conceptualize a molecule as a sequence of n atoms, delineated by internal coordinates d_i, θ_i, φ_i. Here, d_i denotes the bond length between adjacent atoms at Cartesian positions $x_{i-1}, x_i \in \mathbb{R}^3$, for $i = 2, \ldots, n$. The angle θ_i, formed by consecutive bond vectors b_{i-1} and b_i with $b_i = x_i - x_{i-1}$, for $i = 3, \ldots, n$, and the torsion angle φ_i, indicating the rotation between planes spanned by b_{i-2}, b_{i-1} and b_{i-1}, b_i for $i = 4, \ldots, n$, further describe the molecular structure.

The Cartesian coordinates of the molecule's atoms are derived from these internal coordinates by initially positioning the first three atoms as:

$$x_1 = (0, 0, 0)^t, \quad x_2 = (d_2, 0, 0)^t, \quad x_3 = (d_2 - d_3 \cos\theta_3, d_3 \sin\theta_3, 0)^t.$$

Beyond the third atom, determining the position requires both the angle θ_i and the torsion angle φ_i, encapsulated by the transformation matrix

$$B_i = \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 \\ \sin\theta_i \cos\varphi_i & -\cos\theta_i \cos\varphi_i & -\sin\varphi_i \\ \sin\theta_i \sin\varphi_i & -\cos\theta_i \sin\varphi_i & \cos\varphi_i \end{bmatrix},$$

for $i = 4, \ldots, n$.

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Applying these matrices B_i, with $d_1 = \varphi_1 = \varphi_2 = \varphi_3 = 0$ and $\theta_1 = \theta_2 = \pi$, allows the Cartesian coordinates of all atoms to be expressed via the internal coordinates through

$$x_i = (d_1 B_{[1]} + d_2 B_{[2]} + \cdots + d_i B_{[i]}) e_1,$$

where $e_1 = (1, 0, 0)^t$ and

$$B_{[i]} = B_1 B_2 \cdots B_i,$$

for $i = 1, \ldots, n$.

The distance between any two atoms, i and j, is then computed as:

$$\begin{aligned} r_{i,j} &= \|x_j - x_i\| \\ &= \left\|(d_{i+1} B_{[i+1]} + \cdots + d_j B_{[j]}) e_1\right\| \\ &= \left\| B_{[i+1]} \left(d_{i+1} I_3 + \sum_{s=i+2}^{j} \left(d_s \prod_{m=i+2}^{s} B_m \right) \right) e_1 \right\|, \end{aligned}$$

with I_3 denoting the identity matrix in $\mathbb{R}^{3\times 3}$. Since $B_{[i+1]}$ is an orthogonal matrix, we obtain

$$r_{i,j} = \left\| \left(d_{i+1} I_3 + \sum_{s=i+2}^{j} \left(d_s \prod_{m=i+2}^{s} B_m \right) \right) e_1 \right\|.$$

2 Distances in the Homogeneous Space

The homogeneous coordinate system offers an alternative representation for the 3D space, extending the conventional three-dimensional space into four dimensions. In this model, a point $x = (x_1, x_2, x_3)^t$ in the 3D space is represented by a four-dimensional vector $X \in \mathbb{R}^4$, expressed as:

$$X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ 1 \end{bmatrix}.$$

Thompson [6] suggests leveraging the homogeneous model for converting internal molecular coordinates into Cartesian coordinates, facilitating the consolidation of the atom's three positioning movements (one translation and two rotations) into a singular linear transformation, improving upon traditional methods by simplifying mathematical operations.

In this model, translating a point $x_i \in \mathbb{R}^3$ is represented as

$$\begin{bmatrix} I_3 & d_i e_1 \\ 0 & 1 \end{bmatrix},$$

and the rotations dictated by the bond and torsion angles are integrated into a single matrix:

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

for $i = 1, \ldots, n$, with initial conditions set for simplification.

In contrast to the Euclidean model, where Cartesian coordinates of a point x_i require sequential operations and scaling, the homogeneous model streamlines this to a singular multiplication,

$$X_i = B_{[i]}e_4,$$

where

$$e_4 = (0, 0, 0, 1)^t$$

signifies the origin in 3D space, and $i = 1, \ldots, n$, representing the total atoms in the chain.

Computing the Euclidean distance $r_{i,j}$ between two points x_i and x_j, we have [2]:

$$\begin{aligned} r_{i,j} &= \|(x_j - x_i)\| \\ &= \|(B_1 \cdots B_i \cdots B_j)e_4 - (B_1 \cdots B_i)e_4\| \\ &= \|(B_1 \cdots B_i)\left[(B_{i+1} \cdots B_j)e_4 - Ie_4\right]\| \\ &= \left\|\left(B_{[i+1,j]} - I_4\right)e_4\right\|, \end{aligned}$$

where I_4 is the identity matrix in $\mathbb{R}^{4\times4}$ and $B_{[i,j]} = \prod_{k=i}^{j} B_k$.

3 Distances in the Conformal Space

The conformal model [5] offers a different approach to representing the 3D space [3, 4], where a point $x = (x_1, x_2, x_3)^t$ is mapped to a five-dimensional vector $X \in \mathbb{R}^5$, formulated as

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

After some calculations [1], we obtain

$$X_i = B_{[i]}e_0,$$

with matrices $B_{[i]}$ constructed analogously to those in the homogeneous model, which implies that

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

The advantages of the conformal model become more evident in the calculation of derivatives [1].

For instance, the derivative of the interatomic distance $r_{i,j}$ with respect to an internal coordinate α_k is represented in the Euclidean space as

$$\frac{\partial r_{i,j}}{\partial \alpha_k} = \frac{1}{r_{i,j}} e_1^t \left[\left(d_{i+1} I_3 + \sum_{s=i+2}^{j} d_s B_{[i+2,s]} \right)^t B_{[i+2,k-1]} \frac{\partial B_k}{\partial \alpha_k} \left(d_k I_3 + \sum_{s=k+1}^{j} d_s B_{[k+1,s]} \right) \right] e_1$$

and as

$$\frac{\partial r_{i,j}}{\partial \alpha_k} = \frac{1}{r_{i,j}} e_4^t \left(B_{[i+1,j]}^t B_{[i+1,k-1]} \frac{\partial B_k}{\partial \alpha_k} B_{[k+1,j]} \right) e_4$$

in the homogeneous space.

In the conformal space, we obtain a more succinct expression given by

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

4 Conclusion

In the full version of this work [1], we will provide details of how distance and derivative expressions were obtained with each model.

References

1. Camargo, J., Lavor, C.: Conformal coordinates in molecular geometry. (In preparation)
2. Camargo, J., Lavor, C.: A new perspective on the homogeneous coordinate system for calculating interatomic distances and their derivatives in terms of internal coordinates. (Submitted)
3. Kanatani, K.: Understanding Geometric Algebra: Hamilton, Grassmann, and Clifford for Computer Vision and Graphics. AK Peters/CRC Press (2015)
4. Lavor, C., Souza, M., Aragón, J.: Orthogonality of isometries in the conformal model of the 3d space. Graphical Models **114**, 101100 (2021)
5. Li, H., Hestenes, D., Rockwood, A.: Generalized homogeneous coordinates for computational geometry. In: Sommer, G. (eds), Springer (2001)
6. Thompson, H.B.: Calculation of cartesian coordinates and their derivatives from internal molecular coordinates. The Journal of Chemical Physics **47**(9), 3407–3410 (1967)