Distance Geometry and Clifford Algebra

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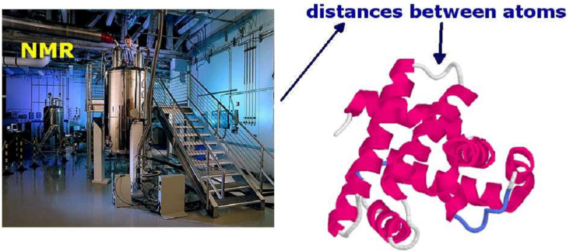

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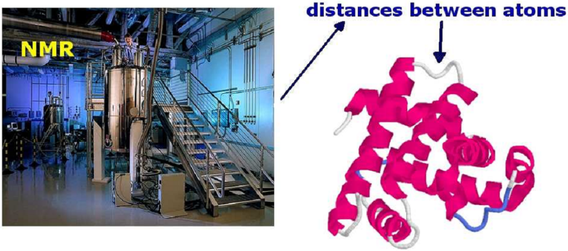

- Model: distance geometry problem (DGP).

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$$\forall \{u, v\} \in E, ||x_u - x_v|| = d_{u,v},$$

where $x_u = x(u)$, $x_v = x(v)$, $d_{u,v} = d(\{u, v\})$.

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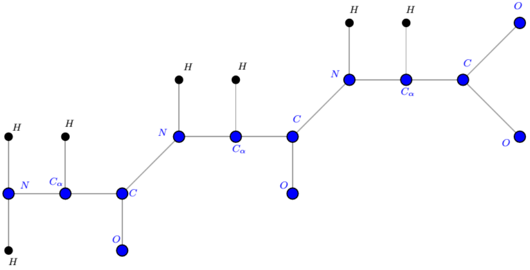

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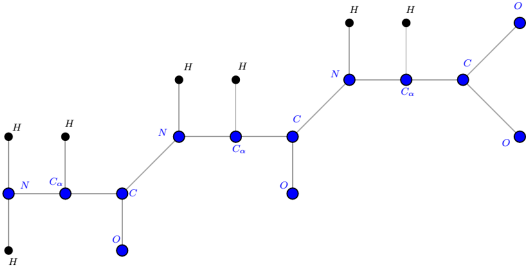

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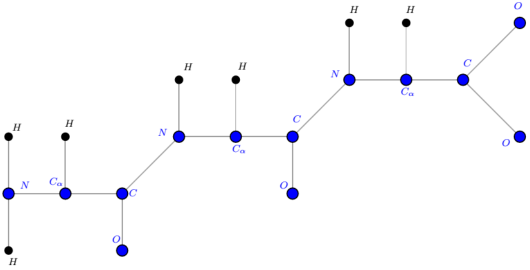
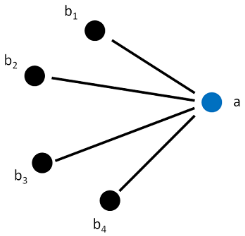


- Simple Geometric Problem:

$$\begin{cases} ||a - b_1|| &= d_{a,b_1} \\ ||a - b_2|| &= d_{a,b_2} \\ ||a - b_3|| &= d_{a,b_3} \\ ||a - b_4|| &= d_{a,b_4} \end{cases}$$



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- **THEN**,
  - Number of solutions: finite;
  - Search space: binary tree;
  - Exact method: Branch & Prune (BP).

- DGP + vertex order: *Discretizable Molecular DGP* (*DMDGP*).

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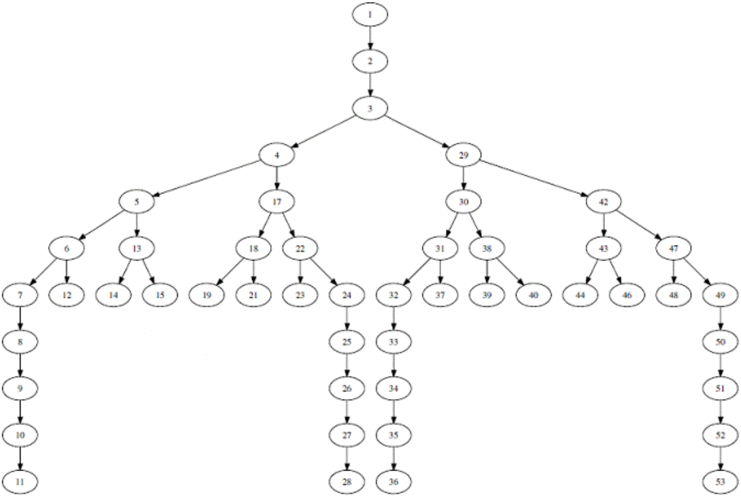

Pruning edges: $N(2) = \{9\}, N(3) = N(4) = \{8, 9, 10\}, N(5) = \{9, 10\}, N(6) = \{10\}, N(7) = \{11\}$.

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- The position for vertex v_i, $i > 3$, is obtained by solving the quadratic system

$$\begin{aligned} ||x_i - x_{i-3}||^2 &= d^2_{i-3,i}, \\ ||x_i - x_{i-2}||^2 &= d^2_{i-2,i}, \\ ||x_i - x_{i-1}||^2 &= d^2_{i-1,i}, \end{aligned}$$

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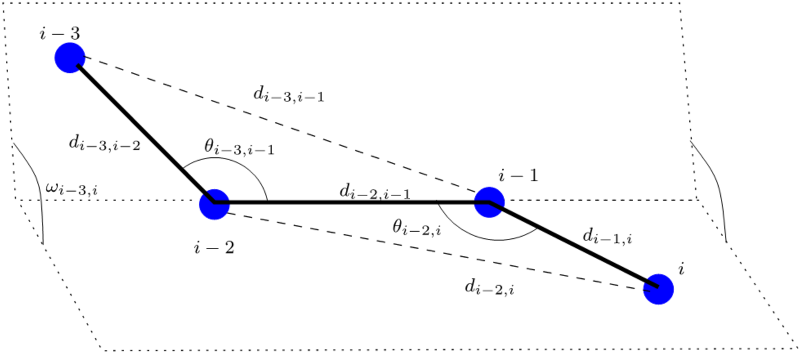
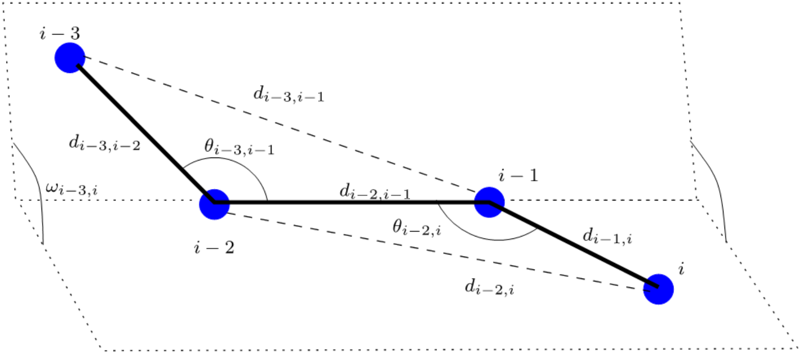
- DMDGP order $\Rightarrow$ replace quadratic systems by matrix multiplications in $\mathbb{R}^4$.



$i-3$
$d_{i-3,i-1}$
$d_{i-3,i-2}$
$\theta_{i-3,i-1}$
$\omega_{i-3,i}$
$i-1$
$d_{i-2,i-1}$
$\theta_{i-2,i}$
$d_{i-1,i}$
$i-2$
i
$d_{i-2,i}$



- DMDGP order $\Rightarrow$ $d_{i-1,i}$, $\theta_{i-2,i}$, $\cos(\omega_{i-3,i})$.

Using homogeneous coordinates:

$$\begin{bmatrix} x_{i_1} \\ x_{i_2} \\ x_{i_3} \\ 1 \end{bmatrix} = B_1 B_2 \cdots B_i \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \ \forall i = 1, \ldots, n,$$

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where

$$B_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \ B_2 = \begin{bmatrix} -1 & 0 & 0 & -d_{1,2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$B_3 = \begin{bmatrix} -\cos\theta_{1,3} & -\sin\theta_{1,3} & 0 & -d_{2,3}\cos\theta_{1,3} \\ \sin\theta_{1,3} & -\cos\theta_{1,3} & 0 & d_{2,3}\sin\theta_{1,3} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

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and $B_i =$

$$\begin{bmatrix} -\cos\theta_{i-2,i} & -\sin\theta_{i-2,i} & 0 & -d_{i-1,i}\cos\theta_{i-2,i} \\ \sin\theta_{i-2,i}\cos\omega_{i-3,i} & -\cos\theta_{i-2,i}\cos\omega_{i-3,i} & -\sin\omega_{i-3,i} & d_{i-1,i}\sin\theta_{i-2,i}\cos\omega_{i-3,i} \\ \sin\theta_{i-2,i}\sin\omega_{i-3,i} & -\cos\theta_{i-2,i}\sin\omega_{i-3,i} & \cos\omega_{i-3,i} & d_{i-1,i}\sin\theta_{i-2,i}\sin\omega_{i-3,i} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

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

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\begin{aligned}
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x_3 &= \begin{bmatrix} -d_{1,2} + d_{2,3}\cos\theta_{1,3} \\ d_{2,3}\sin\theta_{1,3} \\ 0 \end{bmatrix},
\end{aligned}
$$

$$
x_4 = \begin{bmatrix} -d_{1,2} + d_{2,3}\cos\theta_{1,3} - d_{3,4}\cos\theta_{1,3}\cos\theta_{2,4} + d_{3,4}\sin\theta_{1,3}\sin\theta_{2,4}\cos\omega_{1,4} \\ d_{2,3}\sin\theta_{1,3} - d_{3,4}\sin\theta_{1,3}\cos\theta_{2,4} - d_{3,4}\cos\theta_{1,3}\sin\theta_{2,4}\cos\omega_{1,4} \\ \pm d_{3,4}\sin\theta_{2,4}\sqrt{1-\cos^2\omega_{1,4}} \end{bmatrix}.
$$

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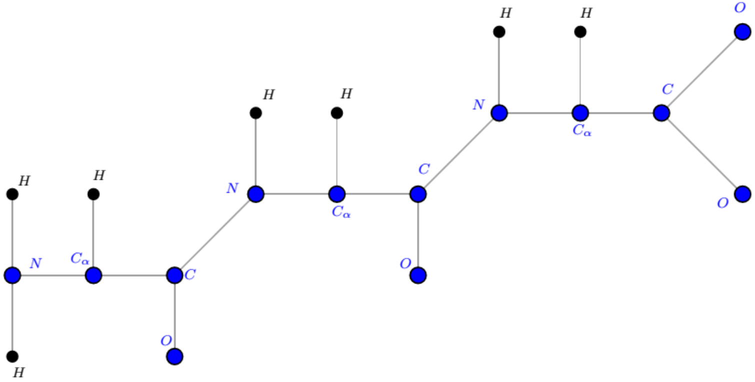

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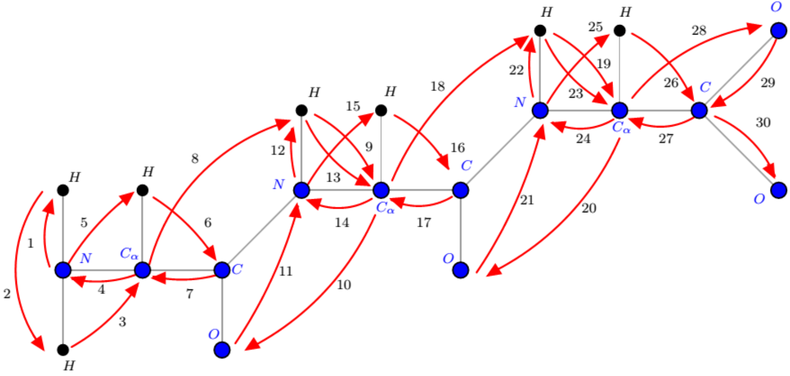

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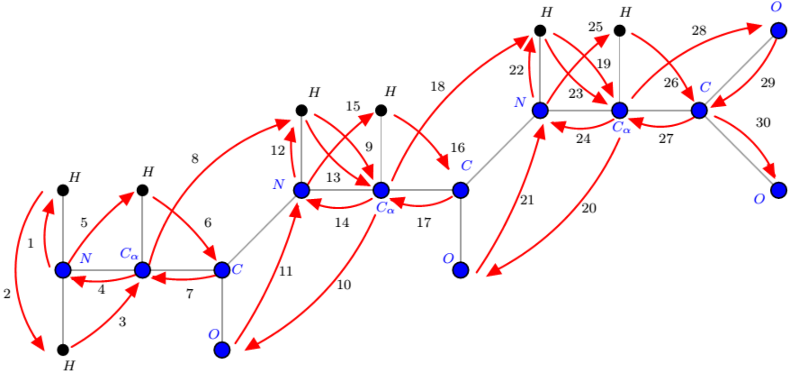

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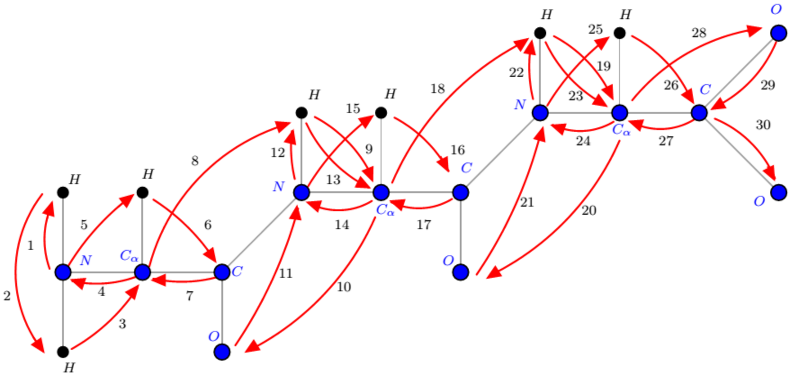

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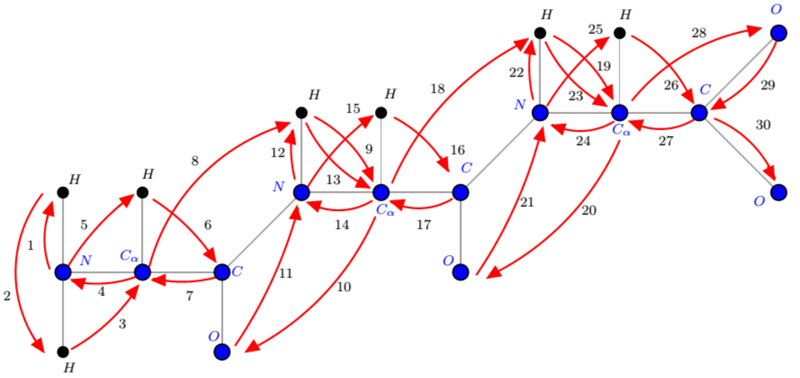

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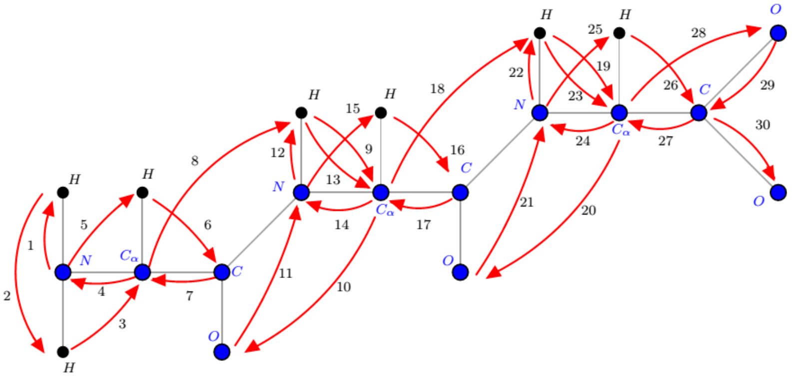

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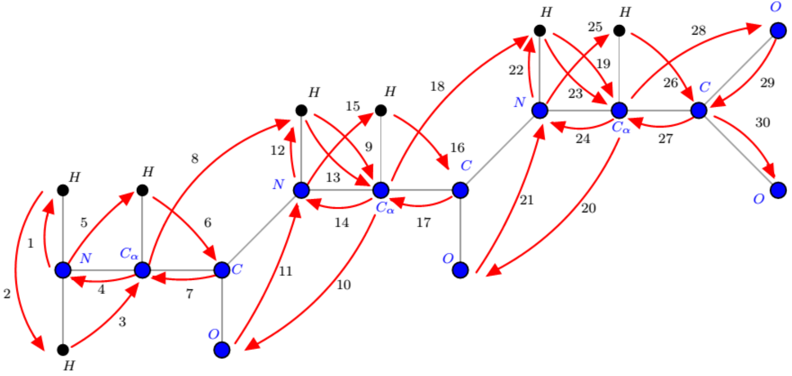

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$$\begin{aligned} e_1 e_2 &= -e_2 e_1, \\ e_2 e_3 &= -e_3 e_2, \\ e_3 e_1 &= -e_1 e_3. \end{aligned}$$

- An element $\mathcal{C}$ of the Clifford algebra, called a **multivector**, has the form

$$\begin{aligned} \mathcal{C} &= \alpha \\ &\quad + a_1 e_1 + a_2 e_2 + a_3 e_3 \\ &\quad + b_1 e_1 e_2 + b_2 e_2 e_3 + b_3 e_3 e_1 \\ &\quad + c e_1 e_2 e_3. \end{aligned}$$

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we get the Hamilton algebra, and defining

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

we get the Grassmann algebra, where $a, b \in \mathbb{R}^3$.

- Using the basis vectors $\{e_1, e_2, e_3\}$, we can write

$$a = a_1 e_1 + a_2 e_2 + a_3 e_3$$

$$b = b_1 e_1 + b_2 e_2 + b_3 e_3$$

to obtain

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to obtain

$$
\begin{aligned}
ab &= a_1 b_1 + a_2 b_2 + a_3 b_3 \\
&\quad + (a_1 b_2 - a_2 b_1) e_1 e_2 \\
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\end{aligned}
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and

- Using the basis vectors $\{e_1, e_2, e_3\}$, we can write

$$a = a_1 e_1 + a_2 e_2 + a_3 e_3$$

$$b = b_1 e_1 + b_2 e_2 + b_3 e_3$$

to obtain

$$\begin{aligned} ab &= a_1 b_1 + a_2 b_2 + a_3 b_3 \\ &+ (a_1 b_2 - a_2 b_1) e_1 e_2 \\ &+ (a_2 b_3 - a_3 b_2) e_2 e_3 \\ &+ (a_3 b_1 - a_1 b_3) e_3 e_1 \end{aligned}$$

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

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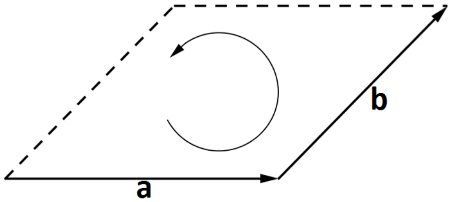

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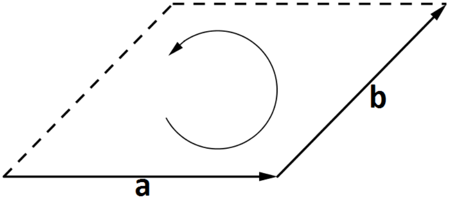

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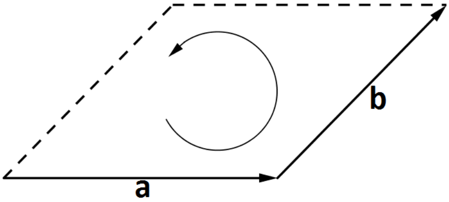

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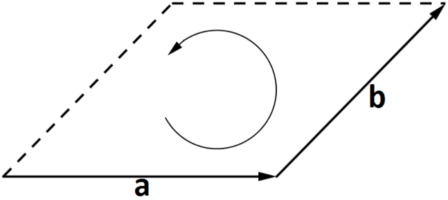

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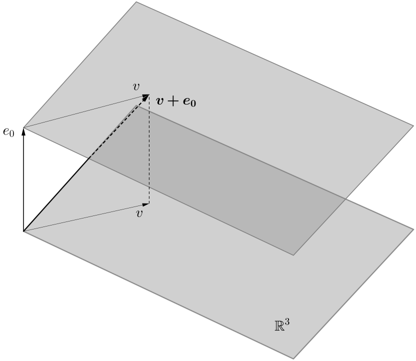

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- Consequence:

<u>inner prod. invariant</u> in $5D \Rightarrow$ <u>distances invariant</u> in $3D$.

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for $i = 1, 2, 3,$

$$\begin{aligned} e_0 e_i &= -e_i e_0, \\ e_\infty e_i &= -e_i e_\infty, \end{aligned}$$

Conformal Clifford Algebra

- **Unified Framework** for objects and transformations.
- For $\{e_1, e_2, e_3\}$:
$$e_i e_j + e_j e_i = 2\delta_{ij}.$$
- For $\{e_0, e_\infty\}$, include:
$$e_0 e_\infty + e_\infty e_0 = -2,$$

for $i = 1, 2, 3,$

$$\begin{aligned} e_0 e_i &= -e_i e_0, \\ e_\infty e_i &= -e_i e_\infty, \end{aligned}$$

and

$$e_0^2 = e_\infty^2 = 0.$$

Basic Objects in the Conformal Clifford Algebra

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$$X_i = e_0 + x_i + \frac{1}{2}||x_i||^2 e_\infty.$$

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- Circle:

$$S_{i-2} \wedge S_{i-1}.$$

- Point Pair:

$$S_{i-3} \wedge S_{i-2} \wedge S_{i-1}.$$

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- Point or $\varnothing$:

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- Rotor:

$$R_i = \cos\left(\frac{\lambda_i}{2}\right) - \sin\left(\frac{\lambda_i}{2}\right) B_i,$$

where

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4. Conformal Clifford Algebra and the DMDGP

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- Basic step of the BP algorithm:

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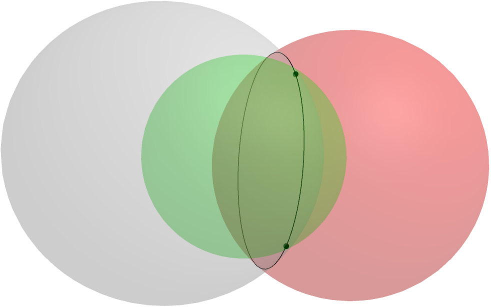
- Geometrically:



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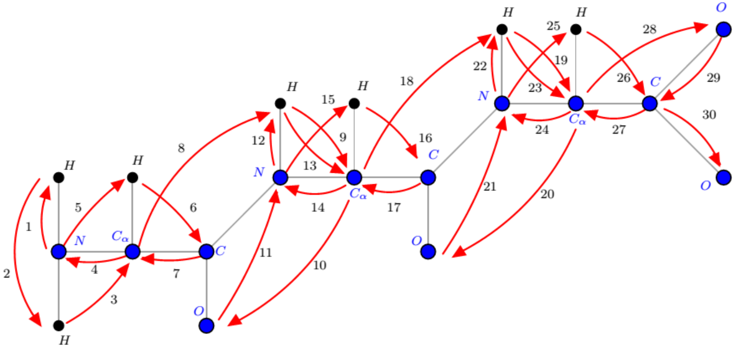

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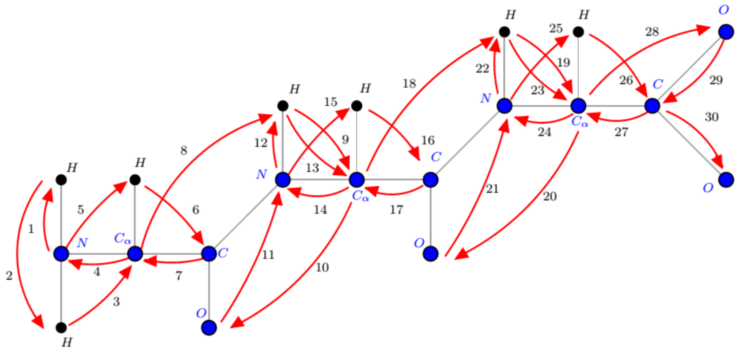

- Chemistry of proteins:
  - $d_{i-1,i}$ and $d_{i-2,i}$ (**precise distances**).

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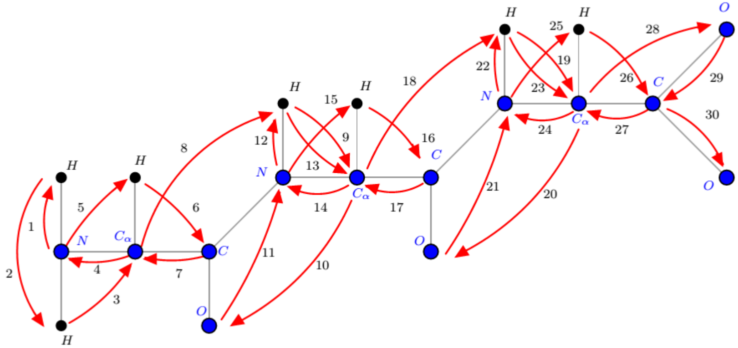

- Chemistry of proteins:
  - $d_{i-1,i}$ and $d_{i-2,i}$ (**precise distances**).
- NMR experiments:
  - $d_{i-3,i}$ (**interval distances**).

- Intersection of two spheres with one spherical shell:

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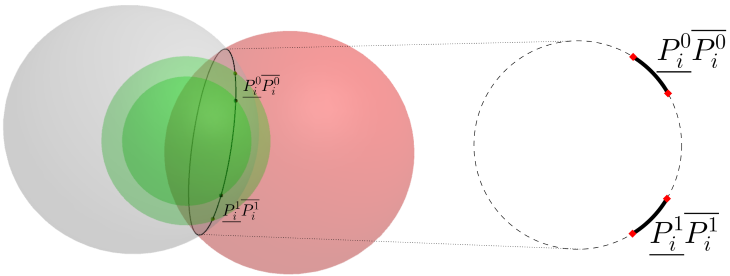
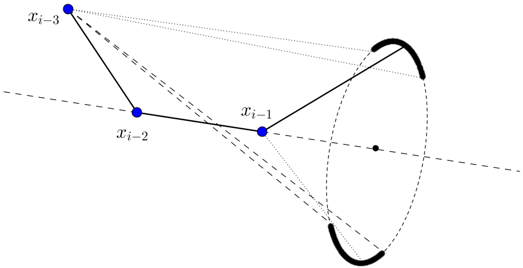


- For $i = 4, ..., n$,



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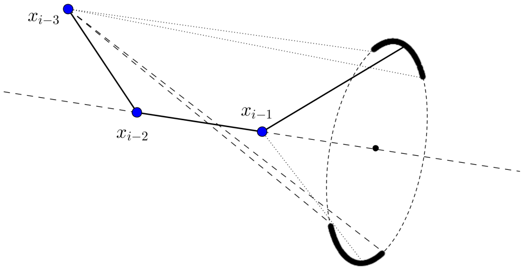
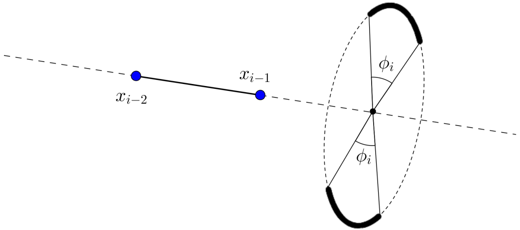


- we can calculate all the angles ϕ_i:



- We define a rotor R_i:

$$R_i = \cos\left(\frac{\lambda_i}{2}\right) + \sin\left(\frac{\lambda_i}{2}\right) z_i^*, \; 0 \leq \lambda_i \leq \phi_i,$$

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Example (distance matrix):

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$$\begin{bmatrix} 0 & 1 & 1.73205 & [1.75, 2.2] & * & * & * \\ & 0 & 1 & 2.3452 & [2.3, 2.5] & * & * \\ & & 0 & 2.3452 & 2.09165 & [1.9, 2.3] & * \\ & & & 0 & 1 & 1.73205 & [2.2, 2.5] \\ & & & & 0 & 1 & 1.73205 \\ & & & & & 0 & 1 \\ & & & & & & 0 \\ \end{bmatrix}.$$

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- The first three atoms can be fixed and the search begins at the fourth level of the BP tree:

$$\begin{aligned} x_1 &= (0, 0, 0)\,, \\ x_2 &= (-1, 0, 0)\,, \\ x_3 &= (-1.5, 0.866025, 0). \end{aligned}$$

Atom x_4

- $\{x_2, d_{2,4}\}$ defines the sphere $S_{2,4}$.

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$$\begin{aligned}
\underline{P_4^0} &= e_0 + 0.719e_1 + 1.57e_2 - 0.287e_3 + 1.53e_\infty, \\
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\end{aligned}$$

$$\begin{aligned}
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\overline{P_4^1} &= e_0 + 0.25e_1 + 1.3e_2 + 1.5e_3 + 2e_\infty.
\end{aligned}$$

- We can also calculate the angle ϕ_4 corresponding to the arcs $\underline{P_4^0}\overline{P_4^0}$ and $\underline{P_4^1}\overline{P_4^1}$:

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given by
$$R_4 = \cos(\tfrac{\lambda_4}{2}) + \sin(\tfrac{\lambda_4}{2})(0.866 e_{13} + 0.5 e_{23} + 0.866 e_3 \wedge e_\infty),$$
for $\lambda_4 \in [0, 0.588]$.

The two possible arcs are giving by

$$
\begin{aligned}
X_4^0(\lambda_4) &= R_4(\lambda_4)\underline{P_4^0}R_4^{-1}(\lambda_4), \\
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For example,

$$x_4^0(\lambda_4) = \begin{bmatrix} 0.719\cos^2(\frac{\lambda_4}{2}) - 0.496\cos(\frac{\lambda_4}{2})\sin(\frac{\lambda_4}{2}) - 3.22\sin^2(\frac{\lambda_4}{2}) \\ 1.57\cos^2(\frac{\lambda_4}{2}) - 0.286\cos(\frac{\lambda_4}{2})\sin(\frac{\lambda_4}{2}) - 0.703\sin^2(\frac{\lambda_4}{2}) \\ -0.286\cos^2(\frac{\lambda_4}{2}) - 4.55\cos(\frac{\lambda_4}{2})\sin(\frac{\lambda_4}{2}) + 0.286\sin^2(\frac{\lambda_4}{2}) \end{bmatrix},$$

for $\lambda_4 \in [0, 0.588]$.

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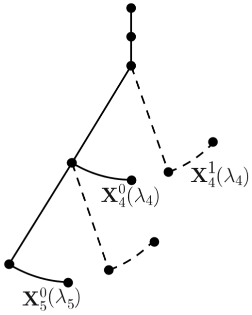

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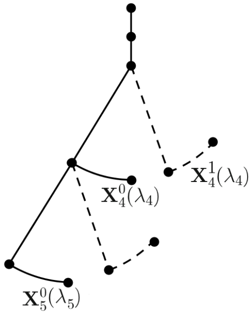

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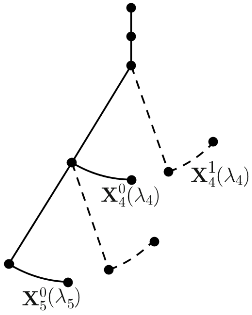

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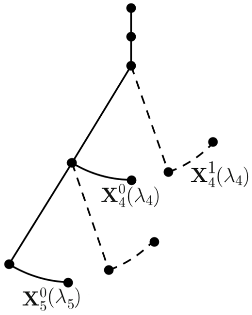

- The rotation axis for R_5,

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also changes when λ_4 varies.

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$$R_5 = \cos(\tfrac{\lambda_5}{2}) + \sin(\tfrac{\lambda_5}{2})z_5^*(\lambda_4), \; 0 \leq \lambda_5 \leq \phi_5,$$

implying that

$$X_5^j(\lambda_4, \lambda_5) = R_5(\lambda_4, \lambda_5) R_4(\lambda_4) \underline{P_5^i} R_4^{-1}(\lambda_4) R_5^{-1}(\lambda_4, \lambda_5).$$

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- That is,

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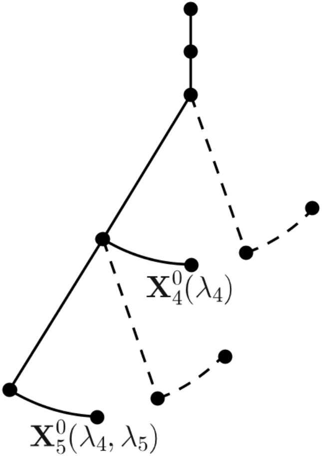

- After some calculations, we get

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$$(x_5)_1 =$$

$$\text{-}1.39 \cos^2\left(\frac{\lambda_4}{2}\right)\cos^2\left(\frac{\lambda_5}{2}\right) - 0.143\cos^2\left(\frac{\lambda_4}{2}\right)\cos\left(\frac{\lambda_5}{2}\right)\sin\left(\frac{\lambda_5}{2}\right) -$$
$$2.34\cos\left(\frac{\lambda_4}{2}\right)\cos^2\left(\frac{\lambda_5}{2}\right)\sin\left(\frac{\lambda_4}{2}\right) -$$
$$3.66\cos\left(\frac{\lambda_4}{2}\right)\cos\left(\frac{\lambda_5}{2}\right)\sin\left(\frac{\lambda_4}{2}\right)\sin\left(\frac{\lambda_5}{2}\right) -$$
$$2.49\cos^2\left(\frac{\lambda_5}{2}\right)\sin^2\left(\frac{\lambda_4}{2}\right) + 1.21\cos\left(\frac{\lambda_5}{2}\right)\sin^2\left(\frac{\lambda_4}{2}\right)\sin\left(\frac{\lambda_5}{2}\right) -$$
$$1.17\cos^2\left(\frac{\lambda_4}{2}\right)\sin^2\left(\frac{\lambda_5}{2}\right) + 2.28\cos\left(\frac{\lambda_4}{2}\right)\sin\left(\frac{\lambda_4}{2}\right)\sin^2\left(\frac{\lambda_5}{2}\right) +$$
$$1.17\sin^2\left(\frac{\lambda_4}{2}\right)\sin\left(\frac{\lambda_5}{2}\right)\cos\left(\frac{\lambda_5}{2}\right) - 0.727\sin^2\left(\frac{\lambda_4}{2}\right)\sin^2\left(\frac{\lambda_5}{2}\right).$$

Atoms x_6 and x_7

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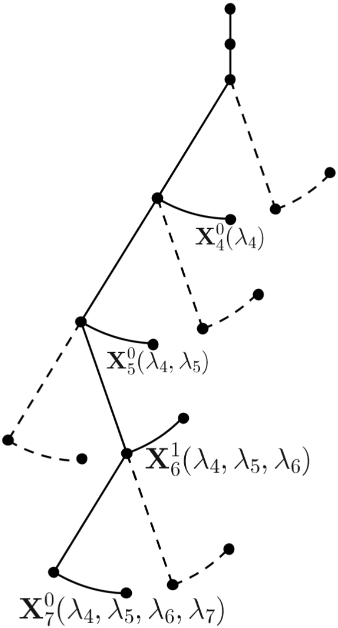

- Additional interval distance $d_{2,6}$:

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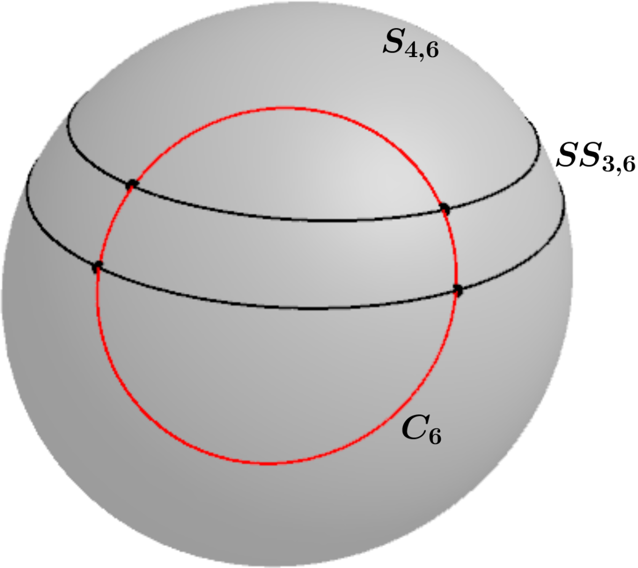

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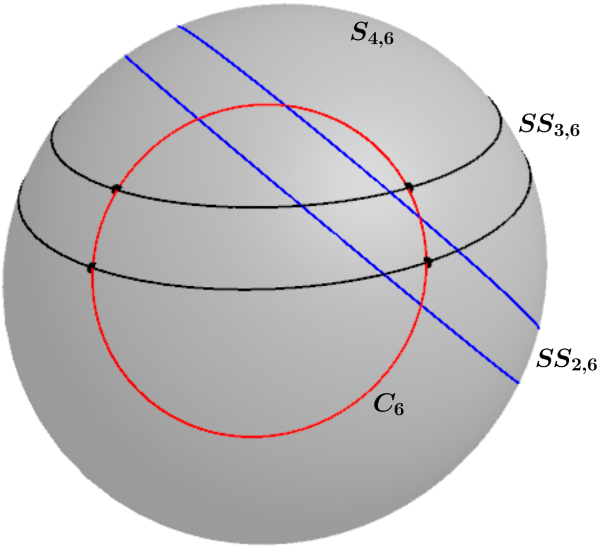

Some References

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