Solving Geometric Constraints with Distance-Based Global Coordinate System

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Extended Abstract

Distance geometry has been used in molecular conformation for many years. The classical embedding algorithm requires the full set of distances between all atoms, see book [2]. This is usually impossible or unnecessary in practice. When some of the distances are not provided, two major heuristic approaches have been used to solve the *sparse* distance geometry problem. Recently, another heuristic approach was presented in [3] that requires provided at least $4n-10$ distances and rather severe conditions, e.g. a full set of distances between some four atoms must be given at first. The method was illustrated in [3] by a 7-atom conformation as shown in Fig. 1.

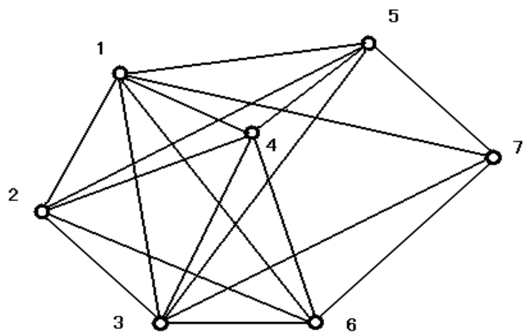

Fig. 1.

Usually, $3n-6$ distances are enough for solving a spatial constraint if these data are independent. In that case the problem is called well-constrained. There are 18 distances given in Fig.1, so the problem is over-constrained. In the present article, a distance-based global coordinate method is proposed in a succinct formulation for solving well-constrained problems without redundant data.

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The classical distance geometry studies metric relations based on the single kind of geometric invariant: *distance* between points. To meet the requirement of geometric computing and reasoning, a generalized frame was developed by the author and his collaborators in 1980s-1990s. In this frame, an *abstract distance* is defined over a configuration of points, hyperplanes and hyperspheres.

The following definition helps solving geometric constraint on a point-plane configuration. Given an n-tuple of points and oriented hyperplanes in an Euclidean space, $P = (p_1, p_2, \cdots, p_n)$, we define a mapping $g : P \times P \to \mathbf{R}$ by letting

- $g(p_i, p_j)$ be the square of the distance between p_i and p_j if both are points,
- $g(p_i, p_j)$ be the signed distance from p_i to p_j, if one is a point and the other an oriented hyperplane,
- $g(p_i, p_j)$ be $-\dfrac{1}{2}\cos(p_i, p_j)$, if both are oriented hyperplanes.

By g_{ij} denote $g(p_i, p_j)$ and G denote the matrix $(g_{ij})_{n\times n}$, and let

$$\delta = (\delta_1, \delta_2, \cdots, \delta_n)$$

where

$$\delta_i = \begin{cases} 1, & \text{if } p_i \text{ is a point} \\ 0, & \text{if } p_i \text{ is a hyperplane} \end{cases}$$

where $i = 1, \ldots, n$. Then, let

$$M(p_1, p_2, \cdots, p_n) = \begin{pmatrix} G & \delta^T \\ \delta & 0 \end{pmatrix}$$

which is called the Cayley-Menger matrix of P, and let

$$D(p_1, p_2, \cdots, p_n) = \begin{vmatrix} G & \delta^T \\ \delta & 0 \end{vmatrix}$$

which is called the Cayley-Menger determinant of P. The following theorem is an extension of the classical result on Cayley-Menger determinant.

Theorem 1. Let $D(p_1, p_2, \cdots, p_n)$ be the Cayley-Menger determinant of an n-tuple of points and oriented hyperplanes in d-dimensional space. If $n \geq d + 2$, then

$$D(p_1, p_2, \cdots, p_n) = 0. \tag{1}$$

The proof will be presented in the full paper, also see [7]. This theorem is essentially the Theorem 1.1 of article [10], and can also be found in earlier articles [8, 9].

By $A_{[i,j]}$ denote the (i,j)th cofactor of a determinant A, i.e. the sub-determinant of A in which the ith row and the jth column have been removed. As a corollary of Theorem 1, we have

Corollary 1. Let D be the Cayley-Menger determinant of an n-tuple of points and oriented hyperplanes in d-dimensional space. If $n \geq d+3$, then

$$D_{[i,j]} = 0 \qquad (\text{ for } i, j = 1, \ldots, n.) \tag{2}$$

Proof. This depends on a lemma on determinants: Given a determinant A, it holds for $i < j$ that

$$A_{[i,i]}A_{[j,j]} - A_{[i,j]}A_{[j,i]} = A\,(A_{[j,j]})_{[i,i]}. \tag{3}$$

Here $(A_{[j,j]})_{[i,i]}$ is the (i,i)th cofactor of $A_{[j,j]}$, simply speaking, that stands for the sub-determinant of A in which the ith, jth rows and ith, jth columns have been removed. The identity (5) was used in Blumenthal's book [1] several times without proof, maybe he thought it well-known, see the pages 100, 102, etc. A proof can be found in [8] or [9]. Applying (5) to the Cayley-Menger determinant D,

$$D_{[i,i]}D_{[j,j]} - D_{[i,j]}D_{[j,i]} = D(D_{[j,j]})_{[i,i]},$$

where clearly $D_{[i,i]}$ is the Cayley-Menger determinant of an $(n-1)$-tuple, by Theorem 1, $D_{[i,i]} = 0, D = 0$ because $n \geq d+3$. Noting D is symmetric, we have $D_{[i,j]} = 0$. Corollary 1 thus holds.

Quartuple coordinate system in $\mathbf{E}^3$

Choose 4 points or oriented planes as a *reference tetrahedron*, say, $\{p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}\}$. For any point or oriented plane p_j, take

$$(\, g(p_j, p_{i_1}),\; g(p_j, p_{i_2}),\; g(p_j, p_{i_3}),\; g(p_j, p_{i_4})\,)$$

as the coordinates of p_j.

Here the choice for the reference tetrahedron may be arbitrarily but the Cayley-Menger determinant of $p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}$ must be non-vanishing, i.e.

$$D(p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}) \neq 0.$$

To solve a constraint problem on a point-plane configuration $\{p_1, \cdots, p_n\}$, we need only find the distance coordinates of every p_i. For any couple (p_i, p_j) with $i < j$, if $g(p_i, p_j)$ is given as a constraint and $\{p_i, p_j\} \cap \{p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}\} = \emptyset$, then we take

$$D(p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}, p_i,\, p_j)_{[5,6]} = 0 \tag{4}$$

as a constraint equation, where $D_{[5,6]}$ stands for the (5,6)th cofactor of D, as defined formerly. Let l be the number of these equations. Furthermore, for every $p_j \notin \{p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}\}$, take

$$D(p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}, p_j) = 0 \tag{5}$$

as a constraint equation, we obtain $n-4$ equations. A complete set of constraint equations with $l+n-4$ members is established in the two ways.

On the other hand, let

$$S_2 = \{(p_i, p_j) \,|\, 1 \leq i < j \leq n, \{p_i, p_j\} \cap \{p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}\} \neq \emptyset\}, \tag{6}$$

then the cardinal number of set S_2 is $4n-10$.

Assume this geometric constraint problem is well-constrained. Then, the number of independent constraints should be $3n-6$ since this is a point-plane configuration. It was known from above argument that exactly l constraints do not concern $p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}$, so exactly $3n-6-l$ constraints concern $p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}$. Therefore, among $4n-10$ distances (or angles) on S_2, there are exactly $3n-6-l$ items are given as constraints, so that $l+n-4$ items are unknown. Thus, the number of unknowns equals that of constraint equations.

As one of the advantages, the quartuple coordinates can uniquely and easily determine the Cartesian coordinates when the reference tetrahedron is fixed.

For example, consider the 7-point conformation shown in Fig.1 but remove 3 segments, say, p_1p_3, p_2p_5, p_2p_6, and then get a well-constrained problem as Fig. 2.

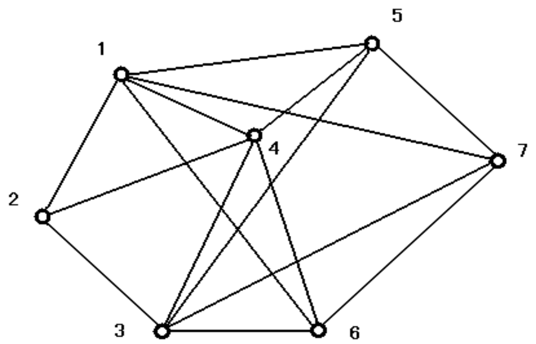

Fig. 2.

The problem cannot be solved by the method of reference [3]. To solve this, choose a quartuple, say $\{p_1, p_3, p_4, p_7\}$, as the reference tetrahedron, this coordinate system yields a complete set of constraint equations consisting of 3 equations,

$$\begin{cases} D(p_1, p_3, p_4, p_7, p_2) = 0, \\ D(p_1, p_3, p_4, p_7, p_5) = 0, \\ D(p_1, p_3, p_4, p_7, p_6) = 0, \end{cases}$$

with 3 unknowns, $g(p_1, p_3), g(p_4, p_7)$ and $g(p_2, p_7)$.

We may, of course, choose another quartuple as the reference tetrahedron, then a different number of equations and unknowns would result.

In fact, we use a short program to yield the constraint equations automatically. Set $x = g(p_1, p_3), y = g(p_4, p_7), z = g(p_2, p_7)$, the computer gives

$$\begin{vmatrix} 0 & x & g_{14} & g_{17} & g_{12} & 1 \\ x & 0 & g_{34} & g_{37} & g_{23} & 1 \\ g_{14} & g_{34} & 0 & y & g_{24} & 1 \\ g_{17} & g_{37} & y & 0 & z & 1 \\ g_{12} & g_{23} & g_{24} & z & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0,$$

$$\begin{vmatrix} 0 & x & g_{14} & g_{17} & g_{15} & 1 \\ x & 0 & g_{34} & g_{37} & g_{35} & 1 \\ g_{14} & g_{34} & 0 & y & g_{45} & 1 \\ g_{17} & g_{37} & y & 0 & g_{57} & 1 \\ g_{15} & g_{35} & g_{45} & g_{57} & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0,$$

$$\begin{vmatrix} 0 & x & g_{14} & g_{17} & g_{16} & 1 \\ x & 0 & g_{34} & g_{37} & g_{36} & 1 \\ g_{14} & g_{34} & 0 & y & g_{46} & 1 \\ g_{17} & g_{37} & y & 0 & g_{67} & 1 \\ g_{16} & g_{36} & g_{46} & g_{67} & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0,$$

where g_{ij} stand for $g(p_i, p_j)$ as defined before. These equations can be briefly written as:

$$c_0 + c_1 y + c_2 z + c_3 yz + c_4 y^2 + c_5 z^2 = 0,$$

$$a_0 + a_1 y + a_2 y^2 = 0,$$
$$b_0 + b_1 y + b_2 y^2 = 0,$$

where all the a_i, b_j, c_k are polynomials in x of degree 2 or less. The system can be easily converted to a triangular set:

$${b_2}^2 {a_0}^2 - 2\, b_2\, a_0\, a_2\, b_0 + {a_2}^2 {b_0}^2 - b_1\, b_2\, a_1\, a_0 - b_1\, a_1\, a_2\, b_0 + a_2\, {b_1}^2\, a_0 + b_0\, b_2\, {a_1}^2 = 0,$$

$$(b_2\, a_1 - a_2\, b_1)\, y + b_2\, a_0 - a_2\, b_0 = 0,$$
$$c_0 + c_1\, y + c_2\, z + c_3\, y\, z + c_4\, y^2 + c5\ z^2 = 0.$$

The first equation is of degree 8 in x since all the a_i, b_j are polynomials in x of degree 2 or less. The second equation is linear in y and the third is quadratic in z, so the problem has 16 isolated solutions for $\{x, y, z\}$ at most.

Another example originated from solving a parallel robot. Two triangles $p_1p_2p_3$ and $p_4p_5p_6$ are not coplanar. The lengths of segments p_1p_4, p_2p_5, p_3p_6 and all the sides of the triangles are provided, as shown in Fig. 3.

There are 6 unknowns, namely,

$$x = g(p_1, p_5), \quad x_1 = g(p_1, p_6), \quad y = g(p_2, p_6),$$

$$y_1 = g(p_2, p_4), \quad z = g(p_3, p_4), \quad z_1 = g(p_3, p_5).$$

If there exist additional conditions as follows,

$$x_1 = m_1 x + n_1, \quad y_1 = m_2 y + n_2, \quad z_1 = m_3 z + n_3,$$

where m_i, n_i are provided, then, combining with the 9 data given in Fig.3, results a well-constrained problem.

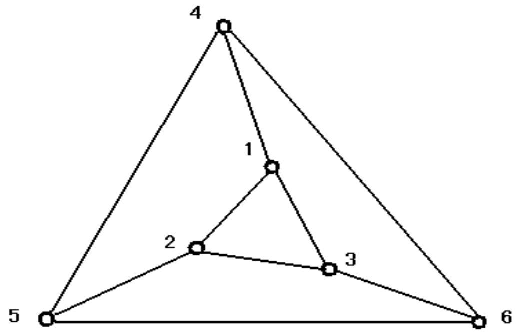

Fig. 3.

To solve this, choose a quartuple, say $\{p_1, p_4, p_5, p_6\}$, as the reference tetrahedron, this coordinate system yields a complete set of constraint equations consisting of 3 equations,

$$\begin{cases} D(p_1, p_4, p_5, p_6, p_2) = 0, \\ D(p_1, p_4, p_5, p_6, p_3) = 0, \\ D(p_1, p_4, p_5, p_6, p_2, p_3)_{[5,6]} = 0, \end{cases}$$

with 3 unknowns, $x = g(p_1, p_6), y = g(p_2, p_6)$ and $z = g(p_3, p_4)$. Here $D(\cdots)_{[5,6]}$ stands for the $(5, 6)$th cofactor of determinant $D(\cdots)$, as introduced formerly. The computer writes them in detail:

$$\begin{vmatrix} 0 & g_{14} & x & x_1 & g_{12} & 1 \\ g_{14} & 0 & g_{45} & g_{46} & y_1 & 1 \\ x & g_{45} & 0 & g_{56} & g_{25} & 1 \\ x_1 & g_{46} & g_{56} & 0 & y & 1 \\ g_{12} & y_1 & g_{25} & y & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0,$$

$$\begin{vmatrix} 0 & g_{14} & x & x_1 & g_{13} & 1 \\ g_{14} & 0 & g_{45} & g_{46} & z & 1 \\ x & g_{45} & 0 & g_{56} & z_1 & 1 \\ x_1 & g_{46} & g_{56} & 0 & g_{36} & 1 \\ g_{13} & z & z_1 & g_{36} & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0,$$

$$\begin{vmatrix} 0 & g_{14} & x & x_1 & g_{12} & 1 \\ g_{14} & 0 & g_{45} & g_{46} & y_1 & 1 \\ x & g_{45} & 0 & g_{56} & g_{25} & 1 \\ x_1 & g_{46} & g_{56} & 0 & y & 1 \\ g_{13} & z & z_1 & g_{36} & g_{23} & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{vmatrix} = 0.$$

Recalling $x_1 = m_1 x + n_1,\ y_1 = m_2 y + n_2,\ z_1 = m_3 z + n_3$, these equations can be briefly written as:

$$a_0 + a_1 y + a_2 y^2 = 0,$$

$$b_0 + b_1 z + b_2 z^2 = 0,$$

$$c_0 + c_1 y + c_2 z + c_3 yz = 0,$$

where all the a_i, b_j, c_k are polynomials in x of degree 2 or less. By a routine method, the system can be converted to a triangular set:

$$\begin{aligned}
&{b_2}^2\,{a_2}^2\,{c_0}^4 - 2\,{a_2}^2\,c_0\,b_0\,{c_2}^3\,b_1 + {b_2}^2\,{a_0}^2\,{c_1}^4 + {a_2}^2\,{b_0}^2\,{c_2}^4 + {c_3}^4\,{b_0}^2\,{a_0}^2\\
&+ 8\,b_2\,a_2\,c_3\,c_0\,b_0\,a_0\,c_1\,c_2 - 2\,b_2\,a_2\,b_0\,a_0\,{c_1}^2\,{c_2}^2 - 2\,{b_2}^2\,a_2\,{c_0}^3\,a_1\,c_1\\
&+ 2\,{b_2}^2\,a_2\,{c_0}^2\,{c_1}^2\,a_0 + {c_3}^2\,{b_0}^2\,{c_2}^2\,{a_1}^2 + {c_3}^2\,{a_0}^2\,{c_1}^2\,{b_1}^2 + {a_2}^2\,{c_0}^2\,{b_1}^2\,{c_2}^2\\
&+ {b_2}^2\,{c_0}^2\,{a_1}^2\,{c_1}^2 + a_2\,{c_3}^2\,{c_0}^2\,a_0\,{b_1}^2 + b_2\,{c_3}^2\,{c_0}^2\,b_0\,{a_1}^2 + a_2\,{b_1}^2\,{c_2}^2\,{c_1}^2\,a_0\\
&+ b_2\,b_0\,{c_2}^2\,{a_1}^2\,{c_1}^2 - c_3\,b_0\,c_1\,{c_2}^2\,{a_1}^2\,b_1 + a_2\,b_0\,{c_2}^3\,c_1\,b_1\,a_1 + b_2\,a_2\,c_3\,{c_0}^3\,a_1\,b_1\\
&+ b_2\,a_0\,{c_1}^3\,c_2\,b_1\,a_1 - a_2\,c_0\,a_1\,{c_2}^2\,c_1\,{b_1}^2 - {c_3}^2\,c_0\,b_0\,c_2\,{a_1}^2\,b_1 + {c_3}^3\,c_0\,b_0\,a_0\,a_1\,b_1\\
&- b_2\,c_0\,{c_1}^2\,c_2\,{a_1}^2\,b_1 - a_2\,c_3\,{c_0}^2\,c_2\,a_1\,{b_1}^2 - b_2\,c_3\,{c_0}^2\,{a_1}^2\,c_1\,b_1 - c_3\,{c_1}^2\,c_2\,a_0\,{b_1}^2\,a_1\\
&+ c_3\,c_0\,c_2\,{a_1}^2\,{b_1}^2\,c_1 - {c_3}^2\,c_0\,a_0\,c_1\,{b_1}^2\,a_1 - 2\,{b_2}^2\,c_0\,a_1\,{c_1}^3\,a_0 + 2\,b_2\,{a_2}^2\,{c_0}^2\,b_0\,{c_2}^2\\
&- 2\,a_2\,c_3\,{b_0}^2\,{c_2}^3\,a_1 - 2\,{c_3}^3\,{b_0}^2\,c_2\,a_0\,a_1 + 2\,a_2\,{c_3}^2\,{b_0}^2\,{c_2}^2\,a_0 - 2\,{c_3}^3\,b_0\,{a_0}^2\,b_1\,c_1\\
&- 2\,b_2\,c_3\,{a_0}^2\,{c_1}^3\,b_1 + 2\,b_2\,{c_3}^2\,b_0\,{a_0}^2\,{c_1}^2 - 2\,b_2\,{a_2}^2\,{c_0}^3\,c_2\,b_1 + 3\,a_2\,c_3\,c_0\,b_0\,{c_2}^2\,a_1\,b_1\\
&- 2\,a_2\,{c_3}^2\,c_0\,b_0\,c_2\,a_0\,b_1 + 3\,b_2\,c_3\,c_0\,a_1\,{c_1}^2\,b_1\,a_0 - 2\,b_2\,a_2\,c_0\,a_0\,b_1\,{c_1}^2\,c_2\\
&- 2\,b_2\,{c_3}^2\,c_0\,b_0\,a_1\,a_0\,c_1 + 3\,b_2\,a_2\,{c_0}^2\,c_1\,b_1\,a_1\,c_2 - 2\,b_2\,a_2\,c_3\,{c_0}^2\,a_0\,b_1\,c_1\\
&- 2\,b_2\,a_2\,c_3\,{c_0}^2\,b_0\,a_1\,c_2 + 3\,{c_3}^2\,b_0\,c_2\,a_0\,c_1\,b_1\,a_1 - 2\,a_2\,c_3\,b_0\,c_1\,{c_2}^2\,a_0\,b_1\\
&- 2\,b_2\,a_2\,c_0\,b_0\,a_1\,{c_2}^2\,c_1 - 2\,b_2\,c_3\,b_0\,{c_1}^2\,c_2\,a_1\,a_0 - 2\,b_2\,a_2\,{c_3}^2\,{c_0}^2\,b_0\,a_0 = 0,
\end{aligned}$$

$$\begin{aligned}
&(-a_2\,b_2\,{c_0}^2\,c_1 - {c_3}^2\,b_0\,a_0\,c_1 + a_2\,b_0\,{c_2}^2\,c_1 - b_2\,{c_1}^3\,a_0 + {c_3}^2\,a_1\,c_0\,b_0 + b_2\,{c_1}^2\,c_0\,a_1\\
&- 2\,c_3\,a_2\,c_0\,b_0\,c_2 + c_3\,a_2\,{c_0}^2\,b_1 + c_3\,{c_1}^2\,b_1\,a_0 - c_3\,c_1\,b_1\,c_0\,a_1)y + a_0\,{c_3}^2\,c_0\,b_0\\
&- b_2\,c_0\,{c_1}^2\,a_0 + b_0\,a_1\,{c_2}^2\,c_1 + b_2\,{c_0}^2\,c_1\,a_1 + a_0\,b_1\,{c_1}^2\,c_2 - a_1\,b_1\,c_0\,c_1\,c_2\\
&+ a_2\,c_2\,{c_0}^2\,b_1 - 2\,b_0\,c_3\,c_2\,a_0\,c_1 - a_2\,b_2\,{c_0}^3 - a_2\,{c_2}^2\,c_0\,b_0 = 0,
\end{aligned}$$

$$(-b_0\,{c_3}^2 + c_1\,b_1\,c_3 - b_2\,{c_1}^2)\,y + (b_2\,c_0\,c_3 - b_2\,c_1\,c_2)\,z - b_2\,c_1\,c_0 - b_0\,c_2\,c_3 + c_3\,b_1\,c_0 = 0.$$

The first equation is of degree 16 in x since all the a_i, b_j, c_k are polynomials in x of degree 2 or less. The second equation is linear in y and the third is linear in z, so the problem has 16 isolated solutions for $\{x, y, z\}$ at most.

See [7] to find more examples, some of which were investigated in [4, 5, 6]. As for a systematic and complete investigation on metric relations of points, hyperplanes and hyperspheres, see [11].

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