Diagonals of regular spatial hexagons determined by distance geometry

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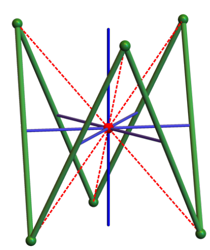
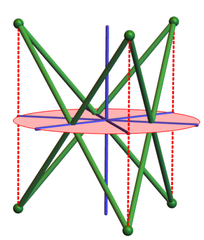
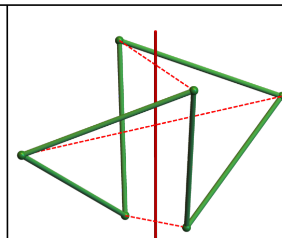
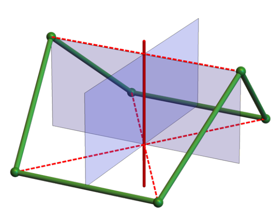
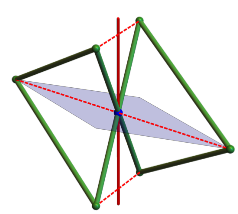
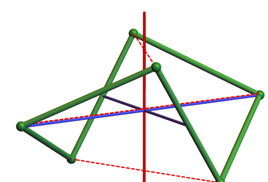
We use the notations and concepts from article ≪Regular spatial hexagons≫ (see also *Elem. Math.*). A regular spatial hexagon (nonplanar equilateral and equiangular 6-gon) with side lengths 1 is briefly called a *hexagon*. Its vertices are sequentially denoted by v_1, v_2, …, v_6, the six diagonals of equal length between a vertex and the next but one by q, and the three diagonals between opposite vertices by x, y, and z, where $x = \overline{v_1 v_4}$, $y = \overline{v_2 v_5}$, and $z = \overline{v_3 v_6}$.

We also refer to the derived symmetry classification and distinguish rigid hexagons with crowns and stars from flexible hexagons with boats, crosses, twists, and lows. The following table shows representatives of the six symmetry classes; in each case, the element of the prime symmetry (exchanging opposite vertices) and the diagonals x, y, and z are indicated in red color and the whole symmetry group is specified by the corresponding Schoenflies symbol (group order in brackets):

 crown D_{3d} (12)	 star D_{3h} (12)	 low C_2 (2)
 boat C_{2v} (4)	 cross C_{2h} (4)	 twist D_2 (4)

In ≪Regular spatial hexagons≫ relations and ranges of the diagonals q, x, y, and z have been determined with the help of vertex coordinates. Here, they are calculated without coordinates, based on results of a relatively young branch of geometry that is called *distance geometry*.

An early approach to distance geometry can be found by Cayley [3] in his very first paper from 1841, wherein he states conditions for distances of five points in space, four points in a plane, and three points on a line. More than 80 years later, in the late 1920s, general and systematic studies were carried out by Menger [5] and subsequently pursued by Blumenthal [2]. Around 1980, distance geometry became important for stereochemistry [4] and in connection with matroid theory [1]. Other applications concern, for instance, sensor networks, statics, robotics, and astronomy. A team of authors published an overview about theory, methods, and applications of distance geometry [6].

Results of distance geometry applied to hexagons

When applying the results of distance geometry to hexagons, we essentially refer to the following symmetric matrix:

$$\mathbf{D} = (d_{ij}) = \begin{pmatrix} 0 & 1 & q^2 & x^2 & q^2 & 1 \\ 1 & 0 & 1 & q^2 & y^2 & q^2 \\ q^2 & 1 & 0 & 1 & q^2 & z^2 \\ x^2 & q^2 & 1 & 0 & 1 & q^2 \\ q^2 & y^2 & q^2 & 1 & 0 & 1 \\ 1 & q^2 & z^2 & q^2 & 1 & 0 \end{pmatrix}, \tag{1}$$

where q, x, y, and z are any positive lengths.

If these lengths are the diagonals of a hexagon with vertices v_1, v_2, $\ldots$, v_6, then the elements d_{ij} of $\mathbf{D}$ are the squared distances between the vertices, i.e., $d_{ij} = \overline{v_i v_j}^2$ $(1 \leq i < j \leq 6)$, and $\mathbf{D}$ is said to be a *distance matrix*[1] of the hexagon.

Distance geometry now provides necessary and sufficient conditions that $\mathbf{D}$ must be met in order to become a distance matrix. These conditions are based on a special kind of determinants as follows: if $\mathbf{D}_k$ is a principal submatrix[2] of $\mathbf{D}$ with k rows and columns $(3 \leq k \leq 6)$, we define:

$$\mathrm{CM}(\mathbf{D}_k) := \det \begin{pmatrix} & & & 1 \\ & \mathbf{D}_k & & \vdots \\ & & & 1 \\ 1 & \ldots & 1 & 0 \end{pmatrix}, \tag{2}$$

which is called a *Cayley-Menger determinant*.

[1] In contrast to this definition and especially in a context different from distance geometry, the entries of a distance matrix are usually defined as distances and not their squares.

[2] A principal submatrix $\mathbf{D}_k$ of $\mathbf{D}$ is obtained by removing $(6-k)$ rows and columns from $\mathbf{D}$ which are symmetric to the main diagonal; evidently it is $\mathbf{D}_6 = \mathbf{D}$.

According to a fundamental theorem of distance geometry, it holds the following:

Theorem 1. *The matrix $\mathbf{D}$ is a distance matrix if and only if there exist principal submatrices $\mathbf{D}_4$ and $\mathbf{D}_3$ of $\mathbf{D}$, where $\mathbf{D}_3$ is a submatrix of $\mathbf{D}_4$, such that the following conditions are satisfied:*

(i) $\mathrm{CM}(\mathbf{D}_4) > 0$ *and* $\mathrm{CM}(\mathbf{D}_3) < 0$,

(ii) $\mathrm{CM}(\mathbf{D}_5) = \mathrm{CM}(\mathbf{D}_5') = 0$, *where $\mathbf{D}_5$ and $\mathbf{D}_5'$ are the two different principal submatrices of $\mathbf{D}$ containing $\mathbf{D}_4$ as a submatrix,*

(iii) $\mathrm{CM}(\mathbf{D}) = 0$.

Consider the hexagon with vertices $v_1, v_2, \ldots, v_6$ determined by the distance matrix $\mathbf{D}$. Any principal submatrix $\mathbf{D}_k$ of $\mathbf{D}$, which is given by the set $\{i_1 \ldots, i_k\}$ of row indices that remain by removing rows (and columns) from $\mathbf{D}$, determines a corresponding simplex with vertices $v_{i_1} \ldots, v_{i_k}$. It can be shown that the Cayley-Menger determinant $\mathrm{CM}(\mathbf{D}_k)$ has a geometrical significance: it is proportional to the square of the $(k-1)$-dimensional volume of this simplex.

The idea behind Theorem 1 can be expressed as follows: condition (i) ensures the existence of a corresponding nondegenerate tetrahedron, where $\mathrm{CM}(\mathbf{D}_4) = 288V^2$ and $\mathrm{CM}(\mathbf{D}_3) = -16A^2$ with V being the volume of the tetrahedron and A the area of the corresponding face triangle; conditions (ii) and (iii) state that the 4- and 5-dimensional simplices containing this tetrahedron must be degenerate, i.e., they have volume 0.

Computation of the diagonals

From the quite extensive computation, we primarily present the results; the verification of detailed calculations requires the use of a computer algebra system. We now specify the possible distance matrices $\mathbf{D}$ from (1) by an (in)equality system without referring to an existential quantifier as it appears in Theorem 1. To do so, it is appropriate to consider a modified version of (i), namely

$$(\mathrm{i}^*) \quad \mathrm{CM}(\mathbf{D}_4) \geq 0 \text{ and } \mathrm{CM}(\mathbf{D}_3) < 0. \tag{3}$$

If $\mathrm{CM}(\mathbf{D}_4) = 0$, the corresponding tetrahedron would be degenerate. With condition (i*) and (ii), (iii) from Theorem 1, as well as an additional condition (iv), we have:

Theorem 2. *Let $\mathcal{L}$ be the set of all quadruples (q, x, y, z) that satisfy the following conditions:*

(i*), (ii) *and* (iii) *with $\mathbf{D}_4$ given by the set $\{1, 2, 3, 4\}$ and $\mathbf{D}_3$ by $\{1, 2, 3\}$,*
and

(iv) $\mathrm{CM}(\mathbf{D}_4') > 0$ *if* $\mathrm{CM}(\mathbf{D}_4) = 0$ *with $\mathbf{D}_4'$ given by* $\{1, 2, 3, 5\}$.

Then $\mathbf{D}$ is a distance matrix if and only if $(q, x, y, z) \in \mathcal{L}$.

Proof. By Theorem 1, the quadruples of $\mathcal{L}$ with $\mathrm{CM}(\mathbf{D}_4) > 0$ evidently yield a distance matrix. A quadruple beyond $\mathcal{L}$ cannot lead to a distance matrix because $\mathrm{CM}(\mathbf{D}_4) < 0$

implies that no corresponding tetrahedron exists (see also [7]). So we still have to examine the quadrupels of $\mathcal{L}$ with $\mathrm{CM}(\mathbf{D}_4) = 0$. Again by Theorem 1, but now based on $\mathbf{D}_4'$ and $\mathbf{D}_3$, there is obtained a distance matrix if $\mathrm{CM}(\mathbf{D}_4') > 0$. It only remains to check that $\mathrm{CM}(\mathbf{D}_5'') = 0$ with $\mathbf{D}_5''$ given by $\{1,2,3,5,6\}$; this is done by calculation. In order to complete the proof, we can exclude quadruples of $\mathcal{L}$ with $\mathrm{CM}(\mathbf{D}_4') < 0$, but also those with $\mathrm{CM}(\mathbf{D}_4) = \mathrm{CM}(\mathbf{D}_4') = 0$. In fact, again by calculation, it is shown that the latter result in the planar hexagon with $q = \sqrt{3}$ and $x = y = z = 2$. $\square$

The set $\mathcal{L}$ therefore comprises exactly all quadruples belonging to an existing hexagon, and we call them *diagonal quadruples*. These will now be determined.

Evaluating the inequalities from (i*) of Theorem 2, it follows

$$q < 2, \;\; |1 - q^2| \leq x \leq \sqrt{1 + 2q^2}. \tag{4}$$

Using $\mathbf{D}_5$ given by $\{1,2,3,4,5\}$ and $\mathbf{D}_5'$ by $\{1,2,3,4,6\}$, we obtain from (ii) two biquadratic equations in y and z, respectively. Calculation leads to the solutions

$$y_1 = z_1 = \sqrt{\frac{f+g}{h}}, \;\; y_2 = z_2 = \sqrt{\frac{f-g}{h}} \;\text{ with} \tag{5}$$

$$\begin{aligned}
f &= -(q^2+1)\,x^4 + 2(q^4+q^2+1)\,x^2 + (q^2-1)^3, \\
g &= 2q\sqrt{\big(x^4 - (q^2+2)x^2 + (q^2-1)^2\big)\big(x^2 - 2q^2 - 1\big)\big(x^2 - (q^2-1)^2\big)}, \\
h &= (x+q+1)(x+q-1)(x-q+1)(-x+q+1).^{3}
\end{aligned}$$

Which values of x from (4) give positive radicands in (5)? By taking into account condition (iv) from Theorem 2, we get a smaller range of q and for $q > 1$ of x:

$$q < \sqrt{3}, \;\; m_1 \leq x \leq \begin{cases} M_1 & \text{for } q \leq 1 \\ M_2 & \text{for } q > 1 \end{cases} \;\text{ with} \tag{6}$$

$$m_1 = |1 - q^2|, \; M_1 = \sqrt{1 + 2q^2}, \; M_2 = \tfrac{1}{2}\big(\sqrt{3}\,q + \sqrt{4 - q^2}\big).$$

For $q = 1$, however, y_2 and z_2 become zero and must therefore be excluded.

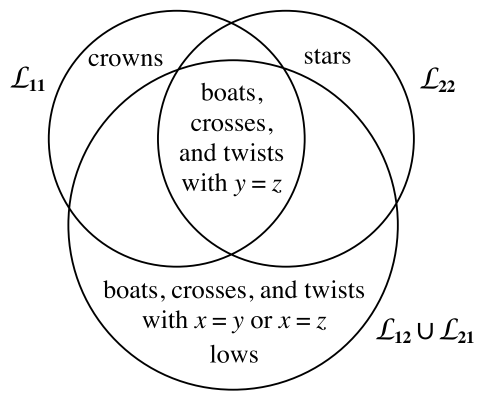
It remains to consider condition (iii). By plugging (5) into (iii), we obtain four subsets of $\mathcal{L}$ as follows:

$$\mathcal{L}_{ij} := \{(q,x,y,z) \mid \text{satisfying (iii) with } y = y_i, z = z_j\} \text{ for } i,j \in \{1,2\}.$$

Calculation shows: $\mathcal{L}_{11}$ and $\mathcal{L}_{22}$ comprise the diagonal quadruples of the rigid hexagons, or more precisely, $\mathcal{L}_{11} \backslash \mathcal{L}_{22}$ gives the crowns and $\mathcal{L}_{22} \backslash \mathcal{L}_{11}$ the stars. $\mathcal{L}_{12}$ and $\mathcal{L}_{21}$ result from the fact that (iii) becomes generally valid in q and x, and the diagonal quadruples of $\mathcal{L}_{12} \cup \mathcal{L}_{21}$ determine the flexible hexagons, i.e., the lows, boats, crosses, and twists.

[3] By the way, $h = -\mathrm{CM}(\mathbf{D}_3)$ with $\mathbf{D}_3$ being the principal submatrix given by $\{1,2,4\}$.

We illustrate with a set diagram:



Summarizing the results of the complete computation, we have:

Theorem 3. *All hexagons are given by diagonal quadruples as follows:*

rigid hexagons by

(q, x, x, x) *with* $q < \sqrt{3}$ *and* $x = \sqrt{1+q^2}$ *for crowns,*
(q, x, x, x) *with* $q < 1$ *and* $x = \sqrt{1-q^2}$ *for stars;*

flexible hexagons by

(q, x, y_1, z_2) *or* (q, x, y_2, z_1)
with $q \neq 1$ *and* x *from* (6), y_1, z_1, y_2, *and* z_2 *from* (5).

In lows the diagonals x, y, *and* z *are pairwise distinct; in boats, crosses* ($q < 1$), *or twists* ($q > 1$) *two of them are equal and the third one is* m_1, M_1, *or* M_2, *respectively.*

The following properties, already derived in ≪Regular spatial hexagons≫, are now an immediate consequence of Theorem 3:

- Rigid hexagons depend on one parameter (here q), and each of them is uniquely determined (up to congruence) by exactly one diagonal quadruple. Flexible hexagons depend on two parameters (here q and x), and a boat, cross, or twist is determined by three, a low even by six distinct diagonal quadruples.
- The resulting range $q < \sqrt{3}$ implies that a hexagon with angle α exists if and only if $\alpha < 120°$. The special angle $\alpha = 60°$ appears only in a crown.
- For a given q ($\neq 1$), the smallest of the diagonals x, y, and z is given by m_1 in a boat, and the largest by M_1 in a cross ($q < 1$) or M_2 in a twist ($q > 1$).
- The diagonal quadruples of hexagons with one double vertex (pentas) result from $q = 1$.

Closing remarks

The coordinate-free approach with distance geometry gives the distance matrix of each hexagon and thus the diagonals. Based on the distance matrix, it would be possible to find the symmetry group and thus the symmetry classification without referring to geometric intuition.

This has been elaborated in [8] for any finite set of points in space as follows: In a first step, the *autometry group*, i.e., the group of the length-preserving point permutations (in the context of hexagons called vertometry group), is generated by means of a canonization algorithm. In a second step, certain Cayley-Menger determinants are used to identify the associated symmetries. This general procedure is then applied to cyclohexane, where the skeleton is a model for all (regular spatial) hexagons with $q = \frac{2}{3}\sqrt{6}$.

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