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Cross - Polytopes in Nucleic Acids

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Abstract

It is shown that nitrogenous bases are located in two-dimensional coordinate planes of the polytope of the hereditary information with dimension 13, and the number of these planes is exactly equal to the number of possible types of amino acids, i.e. each coordinate plane corresponds to some amino acid. It is not necessary to introduce triplets and the complexities and uncertainties associated with them.

Keywords: Cross-Polytopes, Nucleic Acids, DNA, RNA, Molecular Geometry, Computational Biology, Mathematical Modeling, Structural Biology, Molecular Structure, Biomathematics

Introduction

In single - stranded and double - stranded nucleic acids (RNA, DNA), the constituents of acids (residues of phosphoric acid and sugar molecules) interact with each other [1]. Phosphoric acid residues are connected by divalent metal ions, mainly magnesium ions, due to the interaction of negative charges of phosphoric acid residues with positive charges ions [2]. This interaction is essential for the stability of nucleic acid structures, especially in the ribosomes. Sugar molecules interact with each other due to the hydrogen bond between the nitrogenous bases attached to the sugar molecules. Being geometric forms, the constituents of nucleic acids interact with each other to form new geometric forms - new polytopes of higher dimension – cross-polytopes. Nitrogenous bases are known to be flat structures. However, it is not known how nitrogenous bases are oriented in space of higher dimension, whether their orientation depends on the type of nitrogenous base. Currently there is no information on this. There is also no information on how exactly the metal ions are located, connecting the phosphoric acid residues. It should be remembered here that the adopted three - dimensional model of the components and the nucleic acid molecule itself is only a simplify model for visual perception. As it was shown earlier, the phosphoric acid residue is a polytope of dimension 4, and the sugar molecule has a dimension of 12 [3]. When two phosphoric acid residues or two sugar molecules are combined, the dimension of formation in each case increases. The currently accepted simplified models of complementary double-stranded DNA replication and RNA synthesis on a single DNA strand contradict the multidimensional geometry of the constituent nucleic acids [4, 5]. This leads to misconceptions about the genetic code. This paper demonstrates that there is an exact correspondence between the number of coordinate planes in which pairs of interacting nitrogenous bases can be situated and the number of distinct amino acids.

Connection of Two Five- Carbon Sugar Molecules in a Double-Stranded Nucleic Acid Molecule

A cross-polytope of the lowest higher dimension can be obtained by transforming an arbitrary tetrahedron into another tetrahedron that has antiparallel edges to those of the original one. To do this, it suffices to rotate the original tetrahedron by 180 degrees at about an arbitrary point O. After this rotation, the vertices of the first tetrahedron ABCD are transformed into the vertices of the second tetrahedron A/B/C/D/. Now connect the vertices of the tetrahedrons so that the connecting edges (dotted segments) do not have the same letters. It is easy to see that the connecting edges, together with the edges they join, form parallelograms with antiparallel edges. Together, the two tetrahedrons and the connecting edges form a convex figure centered at point O, with the edges not passing through the center. Such a figure is called a cross-polytope [6, 7].

It was previously shown [8] that the five-carbon sugar molecule has form simplex and 13 vertices in which there are one oxygen

atom, four hydrogen atoms, three hydroxyl groups, four carbon atoms, compound CH2OH. It is known that the dimension of a simplex is one less than the number of its vertices. Therefore, the dimension of the five-carbon sugar molecule equals $n = f_0 - 1 = 12$. The simplex is a simplicial polytope, and all its faces therefore are simplexes. Since all the vertices of a simplex are related to each other, the number of edges is determined by the number of combinations of the number of vertices of two. In this case, the number of edges of the polytope is $f_1 = C_{n+1}^2 = 78$. The number of two - dimensional faces (triangles) of this polytope is $f_2 = C_{n+1}^3 = 286$.

The number of three - dimensional faces (tetrahedrons) of this polytope is $f_3 = C_{n+1}^4 = 715$.
The number of four – dimensional faces (4 – simplexes) of this polytope is $f_4 = C_{n+1}^5 = 1287$.
The number of five – dimensional faces (5 – simplexes) of this polytope is $f_5 = C_{n+1}^6 = 1716$.
The number of six – dimensional faces (6 – simplexes) of this polytope is $f_6 = C_{n+1}^7 = 1716$.
The number of seven – dimensional faces (7 – simplexes) of this polytope is $f_7 = C_{n+1}^8 = 1287$. The number of eight – dimensional faces (8 – simplexes) of this polytope is $f_8 = C_{n+1}^9 = 715$.
The number of nine –dimensional faces (9 – simplexes) of this polytope is $f_9 = C_{n+1}^{10} = 286$.
The number of ten – dimensional faces (10 – simplexes) of this polytope is $f_{10} = C_{n+1}^{11} = 78$.
The number of eleven – dimensional faces (11 – simplexes) of this polytope is $f_{11} = C_{n+1}^{12} = 13$. Substituting the values $f_i, (0 \le i \le 11)$ in the Euler - Poincaré equation (Poincaré, 1895)

$$\sum_{i=0}^{n-1} (-1)^i f_i(P) = 1 + (-1)^{n-1}. \qquad (1)$$

There n is dimension of a polytope P, f i is the number of elements with dimension i in the polytope P.
It can see that for this polytope holds n = 12
13 – 78 + 286 – 715 + 1287 – 1716 + 1716 – 1287 + 715 – 286 + 78 – 13 = 0.
This finally proves that the polytope D - ribose (A) has dimension 12 and a simplex type. Obviously, the polytope D - ribose (B) has the same dimension and type. However, it was shown, that in first approximation form connecting of these two molecules has face.

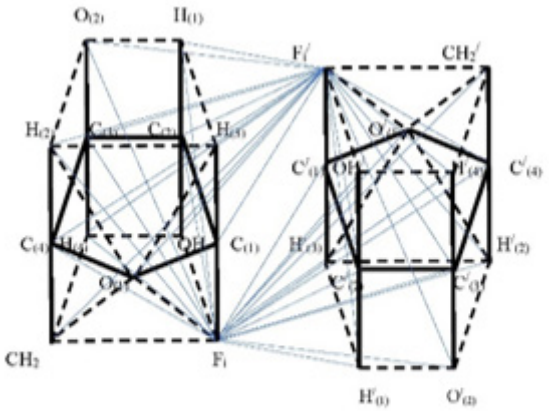


Figure 1

Figure 1: The two sugar molecules with antiparallel edges.

Let us consider in detail the formation of a polytope of two sugar molecules with antiparallel edges. Here, as in the case of the tetrahedron, to form a polytope with antiparallel edges from two sugar molecules, you must have one sugar molecule on one helix to turn this helix together with the sugar molecule and move the sugar molecule along this reversed helix in opposite direction to the original helix direction. When the sugar molecule rotates 180 degrees to the right while moving, then the original sugar molecule and the sugar molecule on the reversed helix are two polytopes with antiparallel edges. Both of these sugar molecules in a simplified form are represented in Figure 1.

When the five - carbon sugar molecule is rotated to the left by 180 degrees, the nitrogenous bases are on opposite sides of both molecules, so that for their connection it is necessary to cross the entire set of atoms of two molecules. This is un existent, therefore this option is not considered. When the sugar molecule is rotated 180 degrees to the left, it is possible to connect the sugar molecules through nitrogenous bases only between two different chains of nucleic acids or in the case of turning the chain itself in the opposite direction.

Polytope of Hereditary Information

In full, the sugar molecules have a dimension of 12, in the corresponding polytope each vertex must have an edge connection with all the other vertices. Knowledge of this now one need. For the formation of a polytope of dimension 13, it is necessary to connect each vertex of one polytope with the vertices of another polytope so that there are no vertex connections with the same letters. All connecting edges break into pairs of antiparallel edges. At the same time, a set of coordinate a two - dimensional planes emanates from the center of the formed polytope as from

the origin of coordinates. Their number is equal to the number of combinations from 13 to 2, i. e. 48 coordinate planes. In order to clarify the possible geometrical circumstances of the connection of helices in double - helix nucleic acid molecules with nitrogenous bases, we are primarily interested in the coordinate planes containing these nitrogenous bases $F_i, F_i^{/}$. There are exactly 12 such coordinate planes in the obtained polytope of dimension 13. They are depicted in Figure 1 by blue solid lines and are indicated below by the vertices of the polytopes contained in them:

$$F_i^{/}H_{(1)} \quad F_i^{/}O_{(2)} \quad F_i^{/}H_{(2)} \quad F_i^{/}C_{(3)} \quad F_i^{/}C_{(2)} \quad F_i^{/}H_{(3)}$$

$$H_{(1)}^{/}F_i \;, \quad O_{(2)}^{/}F_i \;, \quad H_{(2)}^{/}F_i \;, \quad C_{(3)}^{/}F_i \;, \quad C_{(2)}^{/}F_i \;, \quad H_{(3)}^{/}F_i \;,$$

$$F_i^{/}C_{(4)} \quad F_i^{/}H_{(4)} \quad F_i^{/}OH \quad F_i^{/}C_{(1)} \quad F_i^{/}O_{(1)} \quad F_i^{/}CH_2$$

$$C_{(4)}^{/}F_i \;, \quad H_{(4)}^{/}F_i \;, \quad (OH)^{/}F_i \;, \quad C_{(1)}^{/}F_i \;, \quad O_{(1)}^{/}F_i \;, \quad (CH_2)^{/}F_i \;.$$

Other edges of the polytope of dimension 13 are not shown in Figure 1, so as not to ignite the figure. In the center of each parallelogram, indicated by its four vertices, is the origin of coordinates and the corresponding pair of coordinate axes (they are not shown). To identify the different hydrogen and oxygen atoms at vertices of polytope, they indicated by numbers in brackets at the lower indices.

It is surprising that the number of coordinate planes containing vertices is exactly equal to the number of possible compounds of nitrogenous bases 12.

$$A:U, U:A, G:C, C:G, G:U, G:A, U:U, U:C, A\cdot A, A\cdot C, U:G, A:G. \quad (2)$$

Since each coordinate plane designated by the vertices of the parallelograms has a specific atomic environment, it can be assumed that each of the 12 possible compounds of nitrogenous bases is located on one particular coordinate plane out of 12 possible. This solves the question of the possible orientation of the bond of nitrogenous flat bases in nucleic acids using ideas about the high dimensionality of the constituent nucleic acids. It is also surprising that in order to create 13 – cross - polytopes, providing the connection with nitrogenous bases $F_i, F_i^{/}$, nature specially created double - stranded nucleic acids with oppositely directed spirals. This is realized in DNA and RNA when creating regions with inverted helices.

In a variety of nucleic acid molecules, the issue of chain interaction is important. In ribosomes, RNA interacts with each other due to bivalent metal ions (mainly magnesium ions). Positively charged magnesium ions attract negative charges of phosphoric acid residues, ensuring the stability of the ribosomes. In double - stranded nucleic acids, the helices are connected to each other by means of nitrogenous bases complementarily interacting with each other by a hydrogen bond. However, the magnesium ions and nitrogen bases in nucleic acids could not be specifically located. It has been established that magnesium ions and flat nitrogenous bases can be located inside special polytopes of higher dimension. Here knowledge is needed of the higher dimension of phosphoric acid residues and sugar molecules. Such polytopes are polytopes with antiparallel edges, i. e. cross - polytopes of higher dimension. Binding agents are located on the free coordinate planes of these polytopes in the vicinity the center of the polytope.

In this case, the two - dimensional coordinate plane on the boundary of the polytope should contain the objects to be joined. In the case of magnesium ions, there are four specific coordinate planes inside the 5 – cross - polytope, in which an ion can accommodate, combining negative charges. In the case of nitrogenous bases, the existence of 12 coordinate planes inside a cross - polytope of dimension 13, in which flat nitrogenous bases can be located, connecting the helix of nucleic acids, was discovered. Exactly as much as there are options for combining nitrogenous bases. It is given, that each coordinate plane of these 12 planes has a specific environment of atoms. It should be assumed that only one of the 12 possible compounds of nitrogenous bases is placed in each of these planes. It is surprising that the existence of higher - dimensional polytopes with anti - parallel edges is possible only in the case of the opposite direction of interacting helices, and this is exactly what nature provides in the double - helix DNA and in the RNA segments with self - inversion of the helix in the opposite direction.

To build the polytopic of hereditary information, we need four – dimensional polytope with anti – parallel edges to supplement with edges that create a closed and convex figure. In this case, it is not necessary to connect the vertices symmetrically relative to the center of figure with the edges. Each vertex will be connected by an edge to the other vertices. In this case, the polytope will be a cross -polytope and its dimension is equal to half the number of vertices. Indeed, according to, there is a relation between the number of dimension elements i in the cross - polytope and the dimension d of the cross - polytope itself:

$$f_i(d) = 2^{1+i}C_d^{d-1-i} \quad (3)$$

At the vertex i = 0, therefore, according to (3) $f_0 = 2C_d^{d-1} = 2d, d = f_0/2 = 13.$

Thus, the polytope of the hereditary information has dimension 13. When portraying this polytope, we will use the technique that is used in portraying cross-polytopes. We distribute all 26 vertices on the circle so that the vertices opposite in Figure 1 remain opposite and there is no edge between them (Figure 2).

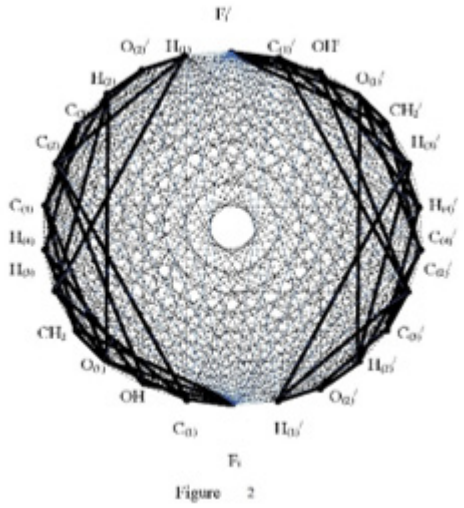


Figure 2: The polytope hereditary information

The edges corresponding to the chemical bonds are indicated in this figure by thick black solid lines. Antiparallel edges highlighting coordinate planes with vertices corresponding to nitrogenous bases are indicated by bluey lines. The remaining edges are indicated by thin dash-dotted black lines. We emphasize that there is a chemical bond between the nitrogenous bases, but it is not covalent. Therefore, this connection is not indicated by an edge.

When the polytope of hereditary information moves along the common axis of the double helix of nucleic acids in accordance with the sequence of bases in DNA, the connection between the vertices $F_i, F_i^{/}$ is carried out by one of the twelve base pairs, which occupies one of the 12 coordinate planes of the polytope. By relation (2), one can determine the number of elements of different dimensions in the polytope of hereditary information. The number of edges is $f_1(13) = 2^2 C_{13}^{11} = 312$, the number of triangles is $f_2(13) = 2^3 C_{13}^{10} = 2288$ the number of tetrahedrons is $f_3(13) = 2^4 C_{13}^{9} = 10560$, the number of fourth-dimensional faces (simplexes) is $f_4(13) = 2^5 C_{13}^{8} = 41184$, the number of fives-dimensional faces (simplexes) is $f_5(13) = 2^6 C_{13}^{7} = 109824$, the number of six-dimensional faces (simplexes) is $f_6(13) = 2^7 C_{13}^{6} = 219648$, the number of seven-dimensional faces (simplexes) is $f_7(13) = 2^8 C_{13}^{5} = 164736$, the number of eight – dimensional faces (simplexes) is $f_8(13) = 2^9 C_{13}^{4} = 183040$, the number of nine-dimensional faces (simplexes) is $f_9(13) = 2^{10} C_{13}^{3} = 292864$, the number of ten-dimensional faces (simplexes) is $f_{10}(13) = 2^{11} C_{13}^{2} = 159744$, the number of eleven-dimensional faces (simplexes) is $f_{11}(13) = 2^{12} C_{13}^{1} = 26624$, the number of twelve-dimensional faces (simplexes) is $f_{12}(13) = 2^{13} = 4096$.

The obtained numbers determine the structure of the polytope of hereditary information.

Now let us recall that in the previous works it was proved [9] that the transmission of hereditary information takes place in a polytope of hereditary information of dimension 13. This polytope has 12 two-dimensional flat coordinate planes. In each of these planes, in principle, pairs of nitrogenous bases connected by a hydrogen bond could be located. However, as follows from the previous geometric analysis, of these 12 coordinate planes, only five planes are free for the location of nitrogenous bases. It is on them that the canonical pairs of nitrogenous bases can be located. Now let us recall that in the previous chapters it was proved that the transmission of hereditary information takes place in a polytope of hereditary information of dimension 13.

This polytope has 12 two-dimensional flat coordinate planes. In each of these planes, in principle, pairs of nitrogenous bases connected by a hydrogen bond could be located [10]. However, as follows from the previous geometric analysis, of these 12 coordinate planes, only five planes are free for the location of nitrogenous bases. It is on them that the canonical pairs of nitrogenous bases can be located, that is, any of the four pairs of nitrogenous bases can be located on each of these coordinate planes. When moving along the nucleotide chain (transition from one polytope of hereditary information to the neighboring polytope of hereditary information), 20 coordinate planes are formed with a characteristic pair of nitrogenous bases. Thus, each of these 20 coordinate planes is characterized by its location in the space of higher dimension and its own pair of nitrogenous bases. There are exactly as many of these coordinate planes as there are types of amino acids [11].

Let us designate the types of amino acids . Let us designate the selected coordinate planes in the polytope of hereditary information . Each amino acid corresponds to a certain coordinate plane . Let's say we have four nucleotide type A, T, C, G. Each nucleotide is paired with another nucleotide from this quadruple .The genetic code in this case consists in determining the correspondence of each of the 20 coordi-

nate planes to one of the 20 amino acids. Suppose one of the chains has a nucleotide A with a certain coordinate plane si plane in the polytope of hereditary information. Let's denote this nucleotide . It connects on this plane to the nucleotide T. Let's denote this nucleotide This connection leads to the synthesis of amino acids . It is easy to understand that in order to form all 20 amino acids, it is necessary to have five A nucleotides on the selected chain on five coordinate planes, five T nucleotides on the other five coordinate planes, five G nucleotides on five more coordinate planes, and five more C nucleotides on other coordinate planes. planes. In this case, all 20 amino acids are formed as a result of the connection of the corresponding nucleotides on 20 coordinate planes. Suppose one of the chains has a nucleotide A with a certain coordinate plane in the polytope of hereditary information. Let's denote this nucleotide F.

It connects on this plane to the nucleotide E. This connection leads to the synthesis of amino acids. It is easy to understand that in order to form all 20 amino acids, it is necessary to have five A nucleotides on the selected chain on five coordinate planes, five T nucleotides on the other five coordinate planes, five P nucleotides on five more coordinate planes, and five more C nucleotides on other coordinate planes. planes. In this case, all 20 amino acids are formed as a result of the connection of the corresponding nucleotides on 20 coordinate planes in the polytope of hereditary information. The introduction of codons (triplets) is not required.

Conclusion

Thus, the number of these variants of coordinate planes is exactly equal to the number of types of amino acids. Each amino acid corresponds to one of the coordinate planes with the corresponding pair of nitrogenous bases. The genetic code within the framework of these ideas consists in establishing a correspondence between the selected amino acid of a certain coordinate plane and a certain pair of nitrogenous bases. Establishing this correspondence should be the task of new experimental studies. Within the framework of these representations, it is not necessary to introduce triplets and the complexities and uncertainties associated with them.

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