On Growth, Form and Yin-Yang

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Abstract

The outer coverings of many virus particles have the rotational symmetry of an icosahedron. How does this external sheath assemble itself? As a simple model we assume each unit or "capsomere" to be represented by a small sphere, attracted to the center of the virus. Geometrically this is similar to studying how a random set of equal spheres would behave if in contact with a given sphere of constant radius, or equivalently a set of N small, equal circles drawn randomly on a fixed sphere. We adopt a "yin-yang" method: first, we jostle the circles in a random manner (the yin phase), and then we allow them expand slightly (the yang phase). When N = 4, 6 or 24 the circles self-assemble to the pattern corresponding to a snub polyhedron, but when N = 60 the densest packing is irregular. When N = 72, as is found in the polyoma virus and other organisms, the packing does not become regular unless the circles are first assembled into a "flower". Each flower has five circles or "petals" surrounding a central circle. When subjected to yin-yang the 12 flowers converge into the observed form. It is inferred that the virus sheath is assembled in this manner.

Introduction

In his classic work "On growth and form" [1] D'Arcy Thompson noted many examples of mathematical patterns occurring in biology. A more recent case was demonstrated by Klug and Finch [2] from micrographs of the human polyoma virus (see figure 1).



Figure 1: Micrographs of human polyoma virus particles (stereographic pairs)

They showed that the outer protein sheath of the virus (like many others) has icosahedral symmetry. It consists of 72 units that all appear to be identical: 12 of these units lie at the vertices of an icosahedron, while the remaining 60 units surround them with the unselfrefexible (cheiral) symmetry of a snub icosahedron.



Figure 2: (a) The snub dodecahedron (= snub icosahedron) and (b) snub cube

A word about the snubs. Among the 15 Archimedean polyhedra (those with regular polygonal faces with the same arrangement of polygons at each vertex [3]) there exist two well-known snubs: the snub dodecahedron (figure 2a) and the snub cube (figure 2b). The snub dodecahedron has one pentagon and four triangles at each vertex; the snub cube has one square and four triangles. The (Wythoff) symbols for these are |235 and |234 respectively. The regular icosahedron, with five triangles at each vertex, can be assigned the symbol |233 and similarly the octahedron |223 and the tetrahedron |222; each "two" corresponds to a digonal symmetry.

The word "snub" means "blunt", see [4], conveying the idea of being rounded or more spherical. Among the Archimedean polyhedra belonging to any symmetry group it is the snubs that have the greatest ratio of edge-length *L* to radius R of the circumscribing sphere. Imagine that at each vertex of an Archimedean solid we draw a small circle centered at that vertex and with radius δ . Then let us enlarge each circle until it touches its nearest neighbors, as in figure 3 and 4. It will be the snubs that can attain the greatest value of δ/R and hence can cover the greatest proportion of the spherical surface.



Figure 3: 60 circles on a unit sphere

Figure 4: 24 circles on a unit sphere

The problem: How did the 72 units or capsomeres in the virus sheath come to have their regular arrangement?

Let us suppose that all of the 72 subunits are modeled as small spheres of equal radius and that each sphere is drawn inwards towards the center of the virus. The process, as the spheres are drawn inward, is geometrically equivalent to an assembly of 72 circles on a fixed sphere being enlarged until they are tightly packed. How can this happen?

The yin-yang method

Let N equal circles be scattered at random on a fixed sphere of unit radius. Reduce the radius of the circles until they do not overlap. Now let the centers of the circles be given random perturbations. (Any perturbation that would cause two circles to overlap is rejected) This is called the relaxation or "yin" phase. Then, if there is still some space between neighboring circles, let the radius of each circle be increased, so that the closest spacing is a certain fraction of the minimum separation. This is the "yang" phase. The yin-yang cycle is then repeated indefinitely. Some examples will make this clearer.



Figure 5: 12 circles placed on a sphere after m yin-yang cycles (a) m = 0 (b) m = 50 (c) m = 5000

N= 12. Suppose we start with a random distribution of just 12 circles (or circular caps) on the surface of the unit sphere (see figure 5) and then apply the yin-yang method. After just 50 cycles the upper hemisphere appears as in figure 5 (b). But after 5,000 cycles it appears as in figure 5 (c). A plot of the radius δ against the number *m* of cycles shows that δ has effectively attained the theoretical value, $\delta = 1/\sqrt{\tau + 2}$, where τ is the golden ratio. That is to say $\delta = 0.55357 = 31.72^{\circ}$



Figure 6: 24 circles placed randomly on a sphere after m yin yang cycles (a) m = 0 (b) m = 100

Next suppose that N = 24, the number of vertices of a snub cube. Robinson [5] has shown that the arrangement of 24 equal circles with centers at the vertices of a snub cube in fact covers the maximum surface area of the sphere. Starting then with 24 random circles as in figure 6 (a) and applying yin-yang we find, after 100 cycles, figure 6 (b).

After 10,000 cycles (figure 7a) adjacent circles do indeed come together and on joining their centers as in figure 7b we find miraculously the outline of a snub cube.



Figure 7: (a) As figures 6a and 6b, but after 10,000 cycles, (b) the results of joining the adjacent center

From the forgoing, we might expect that when N = 60, i.e. the number of vertices of a snub dodecahedron, we would end with a symmetric pattern in the form of the corresponding snub, but this is not the case. The yin-yang method, starting with the randomly chosen arrangement of figure 8 yields,



Figure 8: 60 circles placed randomly on a sphere after m cycles (a) m = 0(b) m = 100,00

after 100,000 cycles, the *irregular* packing of figure 8 (b). This is more closely packed than the *regular* snub arrangement of figure 3, having circles of radius $\delta = 0.2358$, compared with $\delta = 0.2341$ for the regular snub icosahedron. Compare Erber and Hockney [6] who found an irregular arrangement with $\delta = 0.2371$. Sloane, Hardin and Smith [7] quote the value 0.2371. Also see Conway and Sloane [8] and Fejes Toth [9].

Note that a similar result applies to the regular tessellation |236 in which at each vertex there is one hexagon and four triangles. For in the corresponding pattern of circles there is room left for a further circle at the center of each hexagon, so providing a denser arrangement.

We come now to the case N = 72, corresponding to the polyoma virus; see The Introduction. Starting with 72 small circles arranged randomly on the unit sphere, we quickly discover that we do not in general arrive at a regular arrangement of equal circles. How then does nature arrive at the regular patterns in figure 1?

Now in some fruits and their blossoms there frequently occurs 5-fold symmetry, for example in apples and pears as Donald Coxeter liked to demonstrate [10]. Suppose then that we assume that the circular units first grow themselves into small clusters of six, each with five-fold symmetry; see figure 9.



Figure 9: *A* "flower", consisting of with 5 – fold symmetry

Each consists of a central circle surrounded by five circles which we call "petals." Starting with twelve such randomly chosen "flowers" on the surface of a unit sphere as in figure 10 (a), and applying the yin-yang procedure (in which at each yin phase a random perturbation is applied to the center *and* to the orientation of each flower) we find that the pattern develops into figure 10 (b). This is effectively the arrangement of units in figure 1.



Figure 10: *12 flowers placed randomly on a sphere, after m yin-yang cycles: (a)* m = 0 *(b)* m = 10,000

Conclusion

From this yin-yang exercise we may infer that the subunits first assemble themselves into groups of six, each with five-fold symmetry. Then twelve such groups come together to form the sheath. Such a sequence of events was suggested by Casper and Klug [12] on quite different grounds. It is supported by the present purely geometrical argument.

Further details are provided in reference [13], including an account of the method of selecting points randomly on the surface of a sphere, and of generating the random perturbations.

In this work we have effectively created a new kind of mathematics, namely time-dependent, randomized geometry. In so doing we have constructed an intimate link between this subject and the science of virology. Note that Yin-Yang could also be of use to sculptors and artists for the positioning of objects in bounded spaces.

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