DETERMINATION OF EUCLIDEAN DISTANCES FOR SYMMETRY MOLECULES

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Abstract

This paper represents the geometric analysis of molecular surfaces of the molecules, indicates the blending operation of an atoms constitute to the small molecules. The decision which indicates advantages of Euclidean Voronoi diagram of an atom includes the blending surface among the atoms to make a fundamental study of docking, interactions with macromolecules. The algorithm which proposes the topological part of surfaces discussed through the Euclidean Voronoi Diagram of various accessibility procedures.

Keywords: Euclidean Matrix, Voronoi Diagram, Molecular Surfaces, Non-Rigid Molecules, Melamine

I. INTRODUCTION

Earlier of 20th century, the voronoi methods played a vital role in the topic of chemical structure design through computational geometry [1]. This often referred as *additively weighted voronoi diagram* otherwise called as Euclidean distance metrics. In the design of new material, a similar analysis is fundamental as well. Being study an already existing problem, the new approach has been found out edge tracing algorithm in the order of Depth First search algorithm [2][3]. It is fully implemented on constructing a various voronoi diagram with discussions on various applications. In this paper, we present an algorithmic detail of voronoi diagram of 3D space on solving various biological systems based on Euclidean distances.

The investigation of a molecular structure involves research on its constitution – the number and chemical identity of atoms and bonds joining them along with the configuration in 3D space. he model where every point is assigned to the nearest site is called the Voronoi assignment model. The subdivision induced by this model is called the Voronoi diagram of the set of sites.

II. METHODS

A. Chemical Graphs

In a 3D chemical graph, the vertices denote atom and edge here can indicate the geometric distance. The main difference between these two representations is that the 3D chemical graph is usually weighted by geometrical distance.

B. Distance Geometry

It considered encodes the molecules conformational flexibility within a single graphical representation. Particularly, between the two atoms, each in 3D molecular graph each edge is denoted by a range of distances spanning the maximum and minimum distances. This is specifically imposed by some constraints eg., distances and chiralty. This study means the lower and upper bounds of interatomic distances; the chiralty includes the asymmetric centers in the molecules.

C. Voronoi Diagram

The voronoi diagram is formed by the collection of voronoi cells. For the Hypothetical molecule in Fig. 1, Voronoi cells include the convex polygons bounded all around by dashed lines, as well as the polygons with edges defined by dashed lines, but extending to infinity. A voronoi cell consists of the space around one atom so that the distance of every spatial point in the cell to its atom is less than or equal to the distance to any other atom of the molecule. Across every Voronoi edge separating two neighboring voronoi cells, a line segment connecting the corresponding two atom centers is placed. For every Voronoi vertex where three Voronoi cells intersect, a triangle whose vertices are three atom centers is placed. In this way, the full Delaunay triangulation is obtained by mapping from the Voronoi diagram. That is, both the Delaunay triangulation and the Voronoi diagram contain equivalent information.

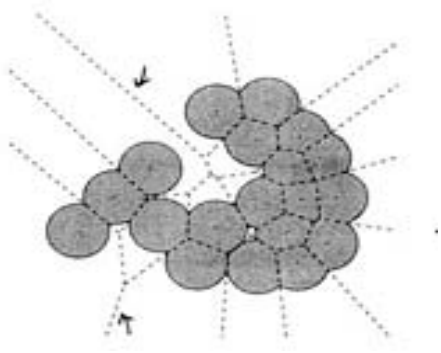


Fig. 1. Illustration of concepts in alpha shape theory. A two-dimensional molecule consisting of disks of uniform radii. The dashed line shows the Voronoi diagram of the molecule. Arrows indicate 2 of the 10 Voronoi edges that are completely outside the molecule.

Let $R = r_1, r_2 \ldots r_n$ be a set of generators where r_i is a three dimensional spherical space. Hence $r_i = (a_i, b_i)$ where $a_i = (m_i, n_i, o_i)$ and b_i denote the coordinate of center and radius of space, respectively. We assume that no space is completely contained inside another space. Associated with each space r_i, there is a region VR_i, called a Voronoi Region of r_i, where $VR_i = \{p|\ \text{dist}\,(p, a_i) - b_i\, \text{dist}\,(p, c_j) - b_j, i \neq j\}$. Then, $VD\,(B) = VR_1, VR_2, \ldots, VRn$ is called a Voronoi Diagram for set B.

D. Voronoi Surfaces

The voronoi surfaces can be defined as $|p - c_i| - r_i = |p - c_j| - r_j$. The principal uses of Voronoi faces are the computations of volumes and boundary areas of Voronoi regions; this represents the two topological factors of the spaces [4]. The topological factors can be determined by, the two spaces are transformed, the center of larger ball is located at the origin and the center of smaller ball is on the positive Z-axis. Then, the Voronoi face between the spaces is always a single-valued function with respect to X and Y. The surface boundary edges were also transformed in the order of rational quadratic Bézier curve form. The surface calculations were made so simple by using this evaluation approach.

E. Molecular Surface

A molecular surface, which is also known as Connolly surface after the name of first researcher defined the surface [5] consists of the most inward points on the probe toward the interior of molecule when the probe is in contact with the same molecule [5] [6]. In other words, the probe can be considered to roll over in any possible direction along the union of atoms without interfering the interior of atoms.

By studying the Molecular surface, we came to know, there are two types of categorized surfaces: Solvent contact surface and reentrant surface. Here, we discussed about reentrant surface. Reentrant surface, is a blending surface among atoms of possibly different sizes, again it consists of two types determined as

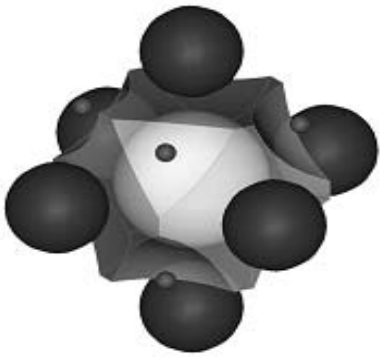


Fig. 2 Voronoi diagram

rolling blending patch and link blending patch [7]. A rolling blending patch is the surface path generated by a probe rolling along two spaces with moving tangentially to both of them. A link blending patch, is created in the positions where a probe tangentially touching three spaces.

F. Creation of Blending Surfaces

The Blending surfaces can be constructed on the molecular surface, requires recognizing the appropriate locations where blending surface patches are to create [8]. The proposed algorithm locates such positions via edge propagations. This employs the accessibility of an edge and face of VD (S).

G. Edge Accessibility

The fixed size of a probe can fly freely through all the corners on an edge with its center placed, the edge called fully accessible for the probe [9]. If probe can fly through only the certain or proper subset of the edge, it refers to partially accessible. Here, we defining three spaces around voronoi edge, the edge accessibility can be identified by comparing the radius

of a probe with the radius of empty space simultaneously tangent

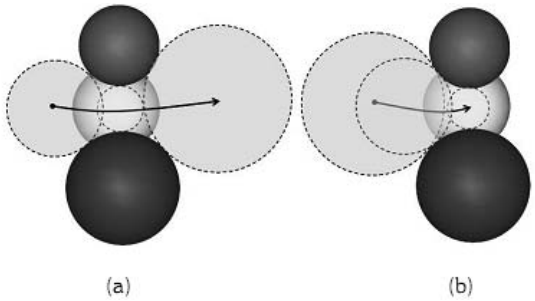


Fig. 3. Empty tangent Spheres of an edge (a) non monotonic edge case (b) mono tonic edge case with reference to gradation of radii of empty tangent spheres.

to three spaces. Although the number of possible empty tangent space is infinite, we can locate empty tangent spheres whose radii are either of the maximum or of the minimum value among the possible empty space. Thus, the edge accessibility can be implemented by computing both minimum and maximum empty tangent spheres, by referring Fig. 3. In this figure, illustrated are also two types of voronoi edges, which are both a monotonic edge and non monotonic edge with regard to the gradation of the radius of empty tangent space. Fig 3 (a). shows that a minimum empty tangent space occurs on one of intermediate points of the edge while maximum empty tangent sphere appears on end vertex. Maximum and minimum empty tangent space appears on start and end vertex, respectively in fig 3 (b). Therefore, if the radius of a probe is smaller than minimum value, the corresponding edge is called fully accessible. If the radius of a probe is larger than maximum value, the edge is non accessible. Otherwise, the edge is partially accessible.

H. Face Accessibility

If all of its boundary edges are fully accessible and the minimum distance between two spheres is larger than the diameter of a probe, the face is fully accessible. If either of two conditions is violated, the corresponding face is partially accessible. If all the boundary edges are non accessible, the face is non accessible.

If the radius of a probe is smaller than minimum radius of current edge, the accessibility of the edge is recognized to be fully accessible and we continue to check the accessibility of incident edges of current edge. If this procedure is repeated for each unbounded Voronoi edge, we can determine the accessibility of every voronoi edge.

I. Definitions Related To Euclidean Distance

The Euclidean distances which plays an essential role to construct a 3D spaces using various algorithms, proposed using Voronoi Diagram, VD(S). The distance between two points defined as the square root of the sum of the squares of the differences between the corresponding coordinates of the points; for example, in two-dimensional Euclidean geometry, the Euclidean distance between two points.

J. Edge Tracing Algorithm

Edge tracing algorithms are expected to achieve a very high success rate besides realizing a rapid and most important thing is changing the dimensions or known as transformations [4]. This expresses tracing only the edge of the objects, desired quickness and performance can be achieved.

The basic idea of the edge-tracing algorithm is quite simple. The algorithm first locates a true Voronoi vertex v_o by computing an empty tangent surface define by four appropriate nearby surfaces. Provided that v_o has been found, four edges e_0, e_1, e_2 and e_3 emanating from v_o can be easily identified and pushed into a stack called Edge-stack. Hence those edges have v_o as their starting vertices. After popping an edge from the stack, the algorithm computes the end vertex of the edge. If an empty tangent space is found, the center of the sphere becomes the end vertex of the popped edge.

Once the end vertex of currently popped edge is found, it is possible to define three more edges emanating from this new vertex. Hence, three edges are created and the new vertex is used as the starting vertex of three new born edges. By computing this Voronoi diagram of a connected graph is completed.

The edge tracing algorithm has a major part to connect the three edges and $O(n_2)$ in the worst case and $O(n)$ on the average, where n is the number of space. Hence we elaborate the details of the algorithm.

K. Edge Tracing Method

The most important information from the edge tracing is the boundaries of the object. Statistical or geometrical characteristic vectors are obtained with the information about boundaries [10].

In order to follow the edge of an object in lines, the important method is rotational transformations [11]. The algorithm can follow the edge of any object as dots. The directions for edge tracing algorithms are discussed below [12].

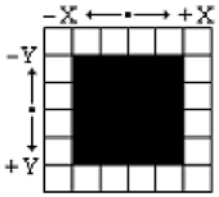


Fig. 4. Directions for edge tracing algorithm on matrix database.

Step 1: The first edge of the object is found by tracing the matrix data-base from the first line in the direction $+x$.

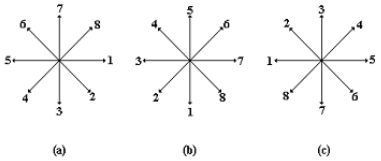


Fig. 4. The edge order of any side points

Step 2: The subsequent points are traced like in fig. 3(a). The first point found during this ordered tracing is accepted as the subsequent point of the object.

Step 3: The coordinates of the edge point found in the second step are processed as follows;

1. If the point is a point in $(+x, +y)$ direction, the tracing order is taken like Fig.3(a).
2. If it is in $-x, +y$ direction, the tracing order in Fig.3(b) is used.
3. If it is in $+x, -y$ direction order, the tracing order in Fig.3(c) is used.
4. If it is in $-x, -y$ direction, the tracing order in Fig.3(b) is used.

Step 4: If there is no point following in any direction, this shows a broken off.

Step 5: The edge tracing process is completed when reached the beginning point by following the steps given above.

Which edge order will be used is decided according to the neighboring positions given in Fig.4.

(x-1,y-1)	(x,y-1)	(x+1,y-1)
(x-1,y)	**(x,y)**	(x+1,y)
(x-1,y+1)	(x,y+1)	(x+1,y+1)

Fig. 5. The neighboring position of any **(x, y)** point

L. Symmetric properties of Non-Rigid Molecules

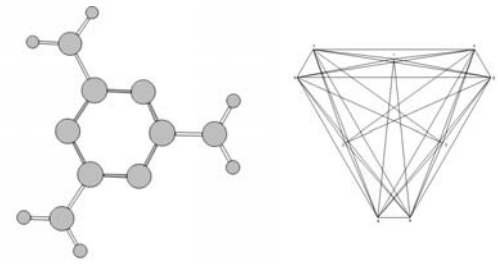
The symmetry of a graph through the automorphism group of the graph depicted in different ways such that its point group symmetry or three dimensional perception may differ but the underlying connectivity symmetry is still the same as characterized by the automorphism group of the graph, which by defining comprises permutation of the vertices of the graph that leave the adjacency matrix invariant [12, 13, 14]. The mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of physical systems. The non-rigid molecule group is strictly defined as the complete set of the molecular conversion operations, which commute with a given nuclear Hamiltonian operator, limited to large amplitude motions [15]. There are physical operations, such as rotations, inversions etc. The study is about the natural investigation of non-rigid molecules.

An automorphism of a graph *G s* a permutation *g* of the vertex set of *G* with the property that, for any vertices *u* and *v*, *ug* and *vg* are adjacent if and only if *u* is adjacent to *v*. The set of all automorphism of a graph *G*, with the operation of composition of permutations, is a permutation group on *VG*, denoted *Aut* (*G*). The symmetry of a graph, also called a topological symmetry, accounts only for the bond relations between atoms. The symmetry of a graph represents the maximal symmetry possessed by the geometrical relization of a given toplogical structure.

By definition, a weighted graph is a graph whose edges and vertices are weighted with different weights. The adjacency matrix of a weighted graph is defined as: $Aij = wij$, if $i \neq j$ and vertices *i* and *j* are connected by an edge with weight *wij*; $Aij = vi$, if $i = j$ and the

weight of the vertex i is vi, and $Aij = 0$. Note that vi can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for nuclei in different equivalence classes and the same weight for the nuclei in the same equivalence classes. Longuet-Higgins has shown a more desirable representation of molecular symmetry using the nuclear permutation and inversion operations, resulting in a group called the Permutation-Inversion (PI) group [16]. The automorphism group of the Euclidean graph of a molecule is the PI group of the molecule [17].

Longuet-Higgins investigated the symmetry groups of non-rigid molecules, where changes from one conformation to another can occur easily. In many cases, these symmetry groups are not isomorphic with any of the familiar symmetry groups of rigid molecules, and their character tables are not known. The importance of this paper to develop easier methods to calculate the classification of wave function and discussing about the f-NRG (full Non rigid group), symmetry of melamine (2, 4, 6-triamino-1, 3, 5-trizaine) it has order of 48 with 10 conjugacy classes.



(a) (b)

Fig. 6. (a) 2,4,6-triamino-1,3,5-triazine molecule(melamine) with D_{3h} point group. (b) The Euclidean graph of melamine.

III. RESULTS AND DISCUSSION

Symmetry operations on a graph are called graph automorphisms [19]. They affect only the labels of vertices by permuting them so that the adjacency matrix of the graph remains unchanged. The graph symmetry is completely determined by all the automorphism it has, i.e., by specifying all the permutations which leave than adjacency matrix intact. A permutation of the vertices of the Euclidean graph under consideration belongs to the permutation representation of an operation in the point group if and only if the corresponding permutation matrix P satisfies $P' DP = D$, where P' is the transpose of permutation matrix P, and D is the adjacency matrix of the graph. All such permutations of the nuclei which preserve the connectivity of the Euclidean graph of the molecule form a group which we call the Euclidean distance group.

Consider the Euclidean graph of melamine and its automorphism group. It suffices to measure the Euclidean distances in terms of the $H - H$ bond lengths and then constructs the Euclidean distance matrix D for Melamine. The original automorphism group of Euclidean graph will always identical to the integer-weighted group of automorphism, this was illustrated by mapping the Euclidean edge, $2.322 \rightarrow 1$, $2.52 \rightarrow 2$, $3.22 \rightarrow 3$, $4.59 \rightarrow 4$, $1.75 \rightarrow 5$, $5.69 \rightarrow 6$, $4.61 \rightarrow 7$ and $6.36 \rightarrow 8$.

The resulting distance matrix D for Melamine is

$$D = \begin{bmatrix} 0 & 1 & 1 & 2 & 3 & 3 & 2 & 4 & 4 \\ 1 & 0 & 1 & 4 & 4 & 2 & 3 & 2 & 3 \\ 1 & 1 & 0 & 3 & 2 & 4 & 4 & 3 & 2 \\ 2 & 4 & 3 & 0 & 5 & 6 & 7 & 8 & 6 \\ 3 & 4 & 2 & 5 & 0 & 8 & 6 & 6 & 7 \\ 3 & 2 & 4 & 6 & 8 & 0 & 5 & 7 & 6 \\ 2 & 3 & 4 & 7 & 6 & 5 & 0 & 6 & 8 \\ 4 & 2 & 3 & 8 & 6 & 7 & 6 & 0 & 5 \\ 4 & 3 & 2 & 6 & 7 & 6 & 8 & 5 & 0 \end{bmatrix}$$

IV. CONCLUSION

Voronoi diagram for surfaces to compute 3D dimensional surfaces in Euclidean Distance has many applications from various disciplines in Sciences especially in constructing chemical structures. This approach is tailor-made and makes an end-user to perform more reliable, efficient and faster.

In this review, we presented properties of edge-tracing algorithm based on euclidean distance of surfaces. This provides $O(mn)$ in the worst-case while initialization, where m and n are number of edges respectively. Here the algorithm provides to compute 3D on $O(n)$ average run to search a number of edges. In an implicit surface, a hyperboloidal surface of voronoi faces also presented with a boundary curves.

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