Molecular graphs of a finite points set : a generalization of the Delaunay triangulation

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Abstract

The Delaunay triangulation is generated from a points set and a structuring element of type disc. In the Delaunay triangulation definition, replacing the disc by a planar-connected region (we call a molecule), which is a union of a fixed number of discs, allows construction of what we name the molecular graphs. In a finite points set, the molecular graphs record the empty regions which are identical to the molecule, independently of translation, rotation and scaling transforms. The molecular graphs are applied to pattern recognition problem. Knowing a template (an input pattern represented by a molecule), the addressed problem is to identify the existing patterns, whose shapes are similar to the template, in a given input points set. The proposed solution is based on a generalization of the α-shapes ; the disc of radius α in the ordinary α-shape is replaced, in the generalized version, by a template of size depending on α.
Keywords : Pattern Recognition, computational geometry, Delaunay triangulation, molecules.

1 Introduction

In computational geometry, the Delaunay triangulation and its dual the Voronoi diagram are among the most studied concepts. They are both extremely versatile tools for the solution of some fundamental proximity problems and efficient structures to model, detect and manipulate geometrical objects issued from different domains of applications as pattern recognition, computer graphics, and biology. Some complex proximity problems have been solved with efficient algorithms based on generalizations of Voronoi diagram and Delaunay triangulation. Without being exhaustive, they are extended to other geometric objects besides points, such as segments, circles and polygons. Also they are generalized to other distances as the metrics L_1 and L_∞ [8], the convex distance functions [4, 5] and the weighted distances [1, 7]. A complete survey is presented in [2, 3, 10].

There exists some aspects of the Voronoi diagram and Delaunay triangulation generalization which are not yet explored. The Delaunay triangulation of a points set is determined by computing empty discs, the non-explored extension consists in replacing the disc by a more complex geometric object (a planar-connected region).

An efficient algorithm associated to this new generalization will solve some complex proximity problems. An example of these problems is the computation of empty regions, from a finite points set, whose the shapes are identical to the one of a known planar-connected region. Another example consists in computing the largest empty region which has a form of a template. These problems are solved for the region identical to the disc, and the existing solutions are based on the Delaunay triangulation. Specifically, the α-shape algorithm [6] computes the empty discs of radii α, and an algorithm computing the largest empty disc is presented in [11].

The generalization of the Delaunay triangulation, that we propose, is called the molecular graphs. They are generated by a points set and a connected region. The connected region is called a molecule, and is represented by a union of discs arranged according to a fixed configuration. It depends on a unique parameter, which is a positive real number, and represents the radius of the molecule. Varying this radius, the molecule is eroded or dilated. An example is shown in figures 1(a) and 1(d), where a region shaped as a "cross" is defined by eight discs.

Based on a unitary molecule M_1 (a molecule of radius equal to 1), the molecular graphs of a set of points S are the set of polygons (edges, triangles and quadrangles) connecting the points of $T \subset S$, such that there exists an empty molecule M_r of radius r touching the points of T ($M_r \cap S = \emptyset$ and $\partial M_r \cap S = T$). In the case where the molecule M_1 is a disc, the molecular graph of S becomes the Delaunay triangulation of S. Due to the fact that any molecule is a union of discs and the ordinary Voronoi diagram records every thing concerning empty discs, any molecular graph can be computed from the ordinary Voronoi diagram.

The case of two discs-molecules is detailed in this article, the extension to any other molecule needs only some adaptation of the presented computation methods.

Making use of the molecular graphs to pattern recognition, we develop an approach to compute specific-patterns from a cloud of points. This means that we present a method to compute the empty regions (dot-patterns), embedded in a points set, whose the shapes are identical to the form of a known template (specific-pattern to detect). The developed method is based on a generalization of the α-shape concept. The ordinary α-shape computes the empty discs of radii α. And, the proposed extension calculates the empty molecules M_α, where M_α is the dilation or the erosion of a template represented by a unitary molecule M_1. This method is detailed in [9].

2 Molecular graphs concept

Let S be a set of n points in $\mathbb{R}^2$, R_p denotes the Voronoi region of $p \in S$, V is the Voronoi diagram of S and D is the Delaunay triangulation of S. For each $1 \leq k \leq 3$, D_k denotes the set of $\sigma_T = conv(T)$ "convex hull of T", such that T is a subset of S, of size $|T| = k$, and it exists an open disc b such that $b \cap S = \emptyset$ and $\partial b \cap S = T$, where ∂b is the circle bounding b. The Delaunay triangulation of S, can be seen as the set of the triangles in D_3, the edges in D_2 and the vertices in D_1 ($D_1 = S$).

2.1 The molecule notion

A *molecule* is a connected region having a fixed shape and defined by a union of open discs (the number of the discs is fixed).

The simplest molecule is the disc. The molecule shown in figure 1(b) is the union of two discs of different radii; a disc of radius r and one of radius λr, where λ, $0 < \lambda \leq 1$, is a constant. These molecules are $M_r = b(x_1, r) \cup b(x_2, \lambda r)$, where x_1 is the center of the first disc and x_2 is the center of the second disc which belongs to the boundary of the first one ($x_2 \in \partial b(x_1, r)$). Varying r (the radius of the molecule), the molecule is dilated or eroded. Varying the centers x_1 and x_2, the molecule M_r is translated and rotated.

Combining the molecule of type figure 1(c), one can build molecules having complex shapes, most shape can be represented by a molecule. For example, the molecule of figure 1(d) has the shape of a "cross", it is defined as follows : $M_r = \cup_{i=1}^{8} b(x_i, r)$, the centers x_1, x_2, x_3 and x_4 are on the same straight line, the points x_5, x_6, x_7 and x_8 are on a second straight line perpendicular to the first one. Also, we have $x_2x_3 = x_6x_7 = 2r$ and $x_i x_{i+1} = r$, where $i = 1, 3, 5, 7$.

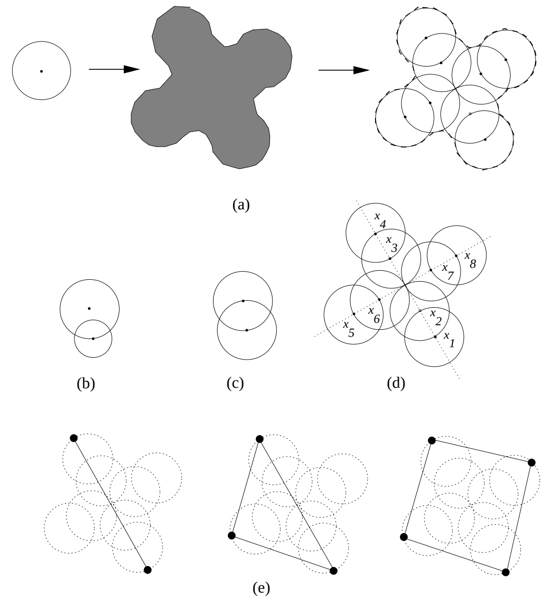

Figure 1: (a) A disc is replaced by a connected region, which is represented by a molecule. (b-d) Some examples of molecules. (e) The hulls σ_T of the points of T (solid discs) are the edge, triangle and quadrangle. Broken discs are those of the molecule.

2.2 Molecular graphs definition

Through this article, we assume that the points of S are in general-position. This means that no five points lie on a common boundary of a molecule.

Definition 3.1.(i) *We say that a molecule M is* empty *iff $M \cap S = \emptyset$.* **(ii)** *Two points $p \in S \cap \partial M$ and $q \in S \cap \partial M$ are* neighbors on ∂M *iff $\widetilde{pq} \cap S = \{p, q\}$. Where M is an empty molecule and $\widetilde{pq}$ is an arc of ∂M connecting p to q* [1]. **(iii)** *Let M be an empty molecule and $T = S \cap \partial M$, the hull of T, we note σ_T, is the polygon of edges $[pq]$ such that the points $p \in T$ and $q \in T$ are neighbors on ∂M.*

Three types of hulls are considered : the edges, triangles and quadrangles. An example is illustrated by figure 1(e). Consider M_1^m a unitary molecule consisting in m discs, the molecular graphs are defined as following :

Definition 3.2. *The molecular graphs of S based on M_1^m, $m > 1$, is the sequence of the graphs $MG_{k,\ell}^m$ defined as following :*

(i) $MG_{2,1}^1 = D_2$ *and* $MG_{3,1}^1 = D_3$.

(ii) $MG_{k,\ell}^m = \{\sigma_T \in MG_{k,\ell}^{m-1} |\ |T| = k,$ there exists $r >$

[1] $\widetilde{pq}$ is one of the two possible arcs

0 such that $M_r^m \cap S = \emptyset$ and $\partial M_r^m \cap S = T\}$, *for* $\ell = 1, \cdots, m-1$ and $k = 2, \cdots, L$.

(iii) $MG_{k,m}^m = \{\sigma_T \notin \cup_{\ell=1}^{m-1} MG_{k,\ell}^{m-1} |\ |T| = k$, there exists $r > 0$ such that $M_r^m \cap S = \emptyset$ and $\partial M_r^m \cap S = T\}$, *for* $k = 2, 3, 4$.

where

$$L = \begin{cases} 3 & \text{if } m = 2 \\ 4 & \text{else} \end{cases}$$

The number of the molecular graphs based on a molecule consisting in m discs is $3m - 1$.

Example. To understand the recurrence relationships of the previous definition, let us develop it for the case where a molecule consisting in three discs is considered ($m = 3$) ; the molecule is $M_r^3 = b(x_1, r) \cup b(x_2, r) \cup b(x_3, r)$ such that the centers x_1, x_2 and x_3 are aligned, and verify $x_1x_2 = x_2x_3$ (see figure 2(a)). The formulas of item (ii) and (iii) become respectively :

$MG_{k,\ell}^3 = \{\sigma_T \in MG_{k,\ell}^2 |\ |T| = k,$ there exists $r > 0$ such that $M_r^3 \cap S = \emptyset$ and $\partial M_r^3 \cap S = T\}$, for $\ell = 1,\ 2$ and $k = 2, 3, 4$.

$MG_{k,3}^3 = \{\sigma_T \notin MG_{k,1}^2 \cup MG_{k,2}^2 |\ |T| = k,$ there exists $r > 0$ such that $M_r^3 \cap S = \emptyset$ and $\partial M_r^3 \cap S = T\}$, for $k = 2, 3, 4$.

The graphs $MG_{k,\ell}^3$ depend on the graphs $MG_{k,\ell}^2$, which are constructed as following: from the molecule M_r^3 is removed a disc to construct a molecule M_r^2 (see figure 2(b)). Thus the graphs $MG_{k,\ell}^2$ are as follows :

$MG_{k,1}^2 = \{\sigma_T \in D_k |\ |T| = k,$ there exists $r > 0$ such that $M_r^2 \cap S = \emptyset$ and $\partial M_r^2 \cap S = T\}$, for $k = 2,\ 3$.

$MG_{k,2}^2 = \{\sigma_T \notin D_2 \cup D_3 |\ |T| = k,$ there exists $r > 0$ such that $M_r^2 \cap S = \emptyset$ and $\partial M_r^2 \cap S = T\}$, for $k = 2,\ 3,\ 4$.

In the notation $MG_{k,\ell}^m$, m is the number of the discs constituting the molecule M_r^m. The integer k indicates the number of the vertices of the polygons σ_T. The integer ℓ means that each σ_T of $MG_{k,\ell}^m$, belongs to $MG_{k,\ell}^\ell$. Two examples of the polygons σ_T are illustrated by figure 2(c). The segment s is common to $MG_{2,1}^3$, $MG_{2,1}^2$ and $MG_{2,1}^1 = D_2$. The triangle TR is not in D_3 but it belongs to $MG_{2,2}^3$ and $MG_{2,2}^2$. If one removes successively a disc from a molecule M_r^m, such that one obtains molecules M_r^{m-1}, M_r^{m-2},..., M_r^1. Then, from the relationship of definition 3.2-item (ii), one deduces an hierarchical relationship between the graphs $MG_{k,\ell}^m$:

$$MG_{k,\ell}^m \subset MG_{k,\ell}^{m-1} \subset MG_{k,\ell}^{m-2} \subset \cdots \subset MG_{k,\ell}^\ell$$

for $\ell = 1, \cdots,\ m-1,$ and $k = 2,\ \cdots,\ L$

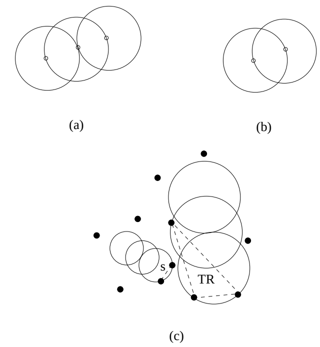

Figure 2: (a) A molecule M_r^3, (b) a molecule M_r^2. (c) The segment s is in $MG_{2,1}^3 \subset MG_{2,1}^2 \subset MG_{2,1}^1 = D_2$. The triangle TR is in $MG_{3,2}^3 \subset MG_{3,2}^2$

The computation of the molecular graphs is detailed in [9].

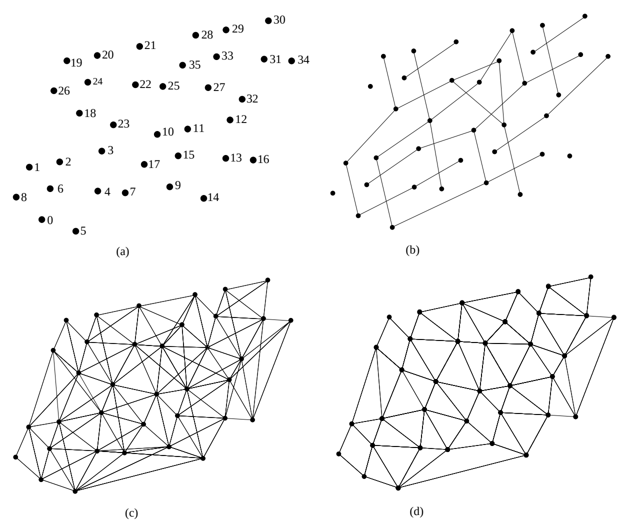

Figure 3: Example of the graphs $MG_{k,\ell}$. (a) A set of points, (b) $MG_{2,2}$, (c) $MG_{3,2}$, (d) $MG_{4,2}$. The graph $MG_{3,1}$ is the Delaunay triangulation of the points set.

3 Conclusion

The molecular graphs are a generalization of the Delaunay triangulation. Given a points set, they allow computing empty planar regions which are similar to a given template. The molecular graphs can be computed from the ordinary Voronoi diagram. This is due to the fact that a molecule is a union of discs. As application of the molecular graphs, a generalization of the α-shape

Triangles of $MG_{3,2}$	Continuation	Continuation	Continuation	Continuation	Continuation
0 5 4	0 6 4	0 6 1	0 8 1	27 35 28	20 21 24
1 2 18	1 26 18	2 3 6	2 4 5	29 30 33	20 22 23
2 6 5	2 26 3	2 3 23	2 18 23	29 31 32	20 22 23
3 4 6	18 26 3	3 4 17	3 7 23	29 33 32	20 24 23
3 17 10	3 23 10	4 7 17	7 9 4	25 35 28	21 22 24
5 14 4	7 14 4	9 14 4	5 7 9	27 32 31	18 26 19
5 14 9	7 9 5	7 17 23	9 14 13	27 33 31	18 24 19
9 15 13	9 15 10	9 17 10	10 11 22	27 33 28	18 24 22
10 11 27	10 25 27	10 23 25	11 25 22	21 22 35	18 23 22
11 12 15	11 12 25	11 12 32	11 27 32	21 25 28	30 31 33
11 13 14	11 15 14	11 25 35	11 27 35	22 25 35	16 34 31
12 13 15	12 27 25	12 32 13	12 16 34	22 23 25	16 32 31
12 32 34	16 32 13	-	-	-	-

Table 1: The triangles of the graph $MG_{3,2}$, depicted by figures 3(c).

Quadrangles of $MG_{4,2}$	Continuation	Continuation
0 5 4 6	0 6 1 8	1 2 18 26
2 3 4 6	2 4 6 5	2 3 18 23
2 26 3 18	2 18 1 26	3 7 17 23
3 4 7 17	3 17 10 23	5 7 9 14
9 14 13 15	9 15 10 17	10 23 22 25
10 11 25 22	10 11 25 27	11 12 13 15
11 12 25 27	11 12 27 32	11 13 14 15
11 25 27 35	12 16 32 34	12 32 13 16
16 32 31 34	18 23 22 24	18 24 19 26
20 21 22 24	20 22 23 24	21 22 25 35
21 25 28 35	27 32 31 33	27 33 28 35
29 31 32 33	29 30 31 33	-

Table 2: The polygons of the graphs $MG_{4,2}$, depicted by figure 3(d).

concept is used to compute empty regions (molecules of size α) similar to a given template.

In ongoing works, we will focus our interest on computation of molecular graphs for higher dimensions data and particularly 3D data. We will also develop the molecular Voronoi diagram.

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