Alpha Shapes: Definition and Software*

Nataraj Akkiraju † Herbert Edelsbrunner ‡ Michael Facello § Ping Fu ¶ Ernst P. Mücke ‖ Carlos Varela **

University of Illinois at Urbana-Champaign

Abstract

The concept of an α-shape of a finite set of points with weights in $\mathbb{R}^d$ is defined and illustrated. It is a polytope uniquely determined by the points, their weights, and a parameter α that controls the desired level of detail. Software that computes such shapes in dimensions 2 and 3 is available via anonymous ftp at `ftp.ncsa.uiuc.edu`.

1 Introduction

The α-shape of a finite point set is a polytope that is uniquely determined by the set and a parameter α. It expresses the intuitive notion of the shape of the point set, and α controls the level of detail reflected by the polytope. The original paper on α-shapes [6] defines the concept in $\mathbb{R}^2$. An extension to $\mathbb{R}^3$ together with an implementation is reported in [8]. In both papers the relationship between α-shapes and Delaunay simplicial complexes [1] is described in detail and used as the basis of an algorithm for constructing alpha shapes.

These algorithms have been implemented and software for 2 and 3 dimensions, complete with graphics interface is publically available. The respective packages can be obtained via ftp at `ftp.ncsa.uiuc.edu` from directory `Visualization/Alpha-shape`. The availability of these implementations, in particular the one in $\mathbb{R}^3$, has led to applications in various areas of science and engineering. Some of these applications are briefly described in [8]. A question that was repeatedly asked in the past is whether it is possible to construct a shape that represents different levels of detail in different parts of space. This is indeed possible by assigning a weight to each point. Intuitively, a large weight favors and a small weight discourages connections to neighboring points. We refer to the resulting concept as the *weighted* alpha shape. If all weights are zero it is the same as the original, unweighted alpha shape. The available software is general enough to handle weights, and this document makes no distinction between weighted and unweighted alpha shapes, unless such a distinction is important.

What are the applications where weights can be beneficial?

(i) A common computational task in biology is modeling molecular structures. It is natural to use α-shapes for this purpose as they are precise duals of the popular sphere models obtained by taking unions of balls, see e.g. [13]. The weights are the radii (e.g. van der Waals radii) of the atoms.

(ii) In reconstructing a surface from scattered point data, it is rarely the case that the points are uniformly dense everywhere on the (unknown) surface. Indeed, the density often varies with the curvature. The assignment of large weights in sparse regions and of small weights in dense regions can be used to counteract the effects resulting from uneven density distributions.

(iii) Another goal that can be achieved by assigning weights is to enforce certain edges or faces. These

*This research is partially supported by the National Science Foundation, under grant ASC-9200301, and under the Alan T. Waterman award, grant CCR-9118874.

†Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA.

‡Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA, and Department of Computer Science, Hong Kong University of Science and Technology, Kowloon, Hong Kong.

§Department of Computer Science and National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA.

¶National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Champaign, Illinois 61820, USA, and Center of Computing Services and Telecommunications, Hong Kong University of Science and Technology, Kowloon, Hong Kong.

‖Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA.

**National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Champaign, Illinois 61820, USA.

might be given as part of the input, but they cannot be processed directly since alpha shapes are defined only for finite point sets and not for other geometric objects.

Outline. Section 2 introduces complexes and shapes via Voronoi decompositions of spherical ball unions. Section 3 defines alpha shapes and their relationship to the (weighted) Delaunay simplicial complex. Section 4 discusses metric, combinatorial, and topological properties computed by the software. Section 5 reviews some of the essential design decisions in the implementations.

2 Complex and Shape

Up front two remarks to avoid any confusion and misconceptions. First, it is more cumbersome to distinguish between $d = 2$ and $d = 3$ dimensions than to phrase all definitions in $\mathbb{R}^d$, for some arbitrary but fixed positive integer d. Second, we use square roots of real numbers as weights. Since negative weight squares do make sense, we choose $\mathbb{R}^{\frac{1}{2}}$ as the domain for all point weights. This is the set of all (positive) square roots of real numbers, and it inherits its linear order from $\mathbb{R}$.

A point $p' \in \mathbb{R}^d$ with weight $p'' \in \mathbb{R}^{\frac{1}{2}}$, is interpreted as a spherical ball

$$p = (p', p'') = \{x \in \mathbb{R}^d \mid |xp'|^2 - p''^2 \leq 0\},$$

where $|yz|$ is the Euclidean distance between points y and z. p' is the *center* and p'' is the *radius* of the ball. All points with non-real weight correspond to empty balls. The shape of a finite set $B \subseteq \mathbb{R}^d \times \mathbb{R}^{\frac{1}{2}}$ of weighted points is defined in terms of a decomposition of the union of balls, $\bigcup B$, into convex sets, see figures 1 and 2. The *(weighted) Voronoi cell* of a ball $p \in B$ is

$$V_p = \{x \in \mathbb{R}^d \mid |xp'|^2 - p''^2 \leq |xq'|^2 - q''^2, q \in B\}.$$

It is a convex polyhedron, and its intersection with the ball union is convex because $\bigcup B \cap V_p = p \cap V_p$. Note that the convex cells have pairwise disjoint interiors, but some of them overlap along common boundary pieces. These pieces of overlap are instrumental in the construction of a set system closed under the subset operation. In topology, such a system is referred to as an *abstract simplicial complex*. Specifically, we define the *nerve* of $C = \{p \cap V_p \mid p \in B\}$ as

$$\mathrm{Nrv}\, C = \{X \subseteq C \mid \bigcap X \neq \emptyset\}.$$

Assuming general position of the points or balls, the largest set in $\mathrm{Nrv}\, C$ is of size $d + 1$: a triple in $\mathbb{R}^2$ and a quadruple in $\mathbb{R}^3$. Under this assumption, $\mathrm{Nrv}\, C$ has a natural geometric realization by mapping each cell $p \cap V_p \in C$ to the point $\varepsilon(p \cap V_p) = p' \in \mathbb{R}^d$. This realization is a (geometric) simplicial complex, $\mathrm{Cpx}\, B$, see e.g. [10]. Each set $X \in \mathrm{Nrv}\, C$ is represented by the convex hull of the corresponding points: the points are the images of the cells in X and their convex hull is a simplex of dimension one less than the cardinality of X. Formally,

$$\mathrm{Cpx}\, B = \{\mathrm{conv}\, \varepsilon(X) \mid X \in \mathrm{Nrv}\, C\}.$$

We refer to this complex as the *dual complex* of $\bigcup B$, and to its *underlying space*, $\bigcup \mathrm{Cpx}\, B = \bigcup_{\sigma \in \mathrm{Cpx}\, B} \sigma$, as the *dual shape*. Examples of a ball union, the decomposition into convex cells, and the dual complex in $\mathbb{R}^2$ are shown in figures 1 through 3.

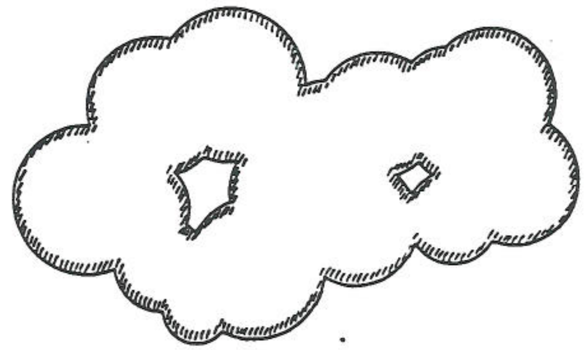

Figure 1: The union of a set of disks in the plane.

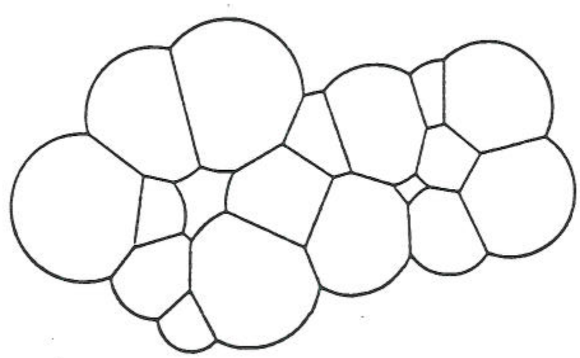

Figure 2: The decomposition of the union using the Voronoi cells of the disks.

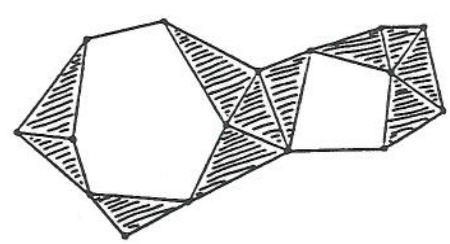

Figure 3: The dual complex of the disk union.

Among the most useful properties of $\mathrm{Cpx}\, B$ are the homotopy equivalence between $\bigcup \mathrm{Cpx}\, B$ and $\bigcup B$, and the fact $\bigcup B$ can be expressed as the alternating sum of common ball intersections, with one term per simplex in Cpx B. This implies short inclusion-exclusion formulas for the d-dimensional volume and other measures of $\bigcup B$, see [5].

3 Filter and Filtration

Suppose we grow all balls $p \in B$ simultaneously without changing Voronoi cells. In this case all cells of the decomposition C of $\bigcup B$ can only grow, and the dual complex can only get larger. The result is a one-parametric family of simplicial complexes.

More formally, let $\alpha \in \mathbb{R}^{\frac{1}{+}}$, $p_\alpha = (p', \sqrt{p''^2 + \alpha^2})$, and $B_\alpha = \{p_\alpha \mid p \in B\}$. For $\alpha = 0$ the radius of p_α is its weight, and for $p'' = 0$ the radius is α. By construction, the Voronoi cell of p_α in B_α is the same as the Voronoi cell of p in B. The *α-complex*, $\text{Cpx}_\alpha B$, is the dual complex of $\bigcup B_\alpha$. The *α-shape* is $\bigcup \text{Cpx}_\alpha B$. By monotonicity of the cells $p_\alpha \cap V_{p_\alpha}$, we have

$$\text{Cpx}_{\alpha_1} B \subseteq \text{Cpx}_{\alpha_2} B$$

whenever $\alpha_1 \leq \alpha_2$. For sufficiently large α, $\text{Cpx}_\alpha B$ geometrically realizes the nerve of the collection of Voronoi cell. We refer to this complex as the *(weighted) Delaunay simplicial complex*, Del B, of B. All $\text{Cpx}_\alpha B$ are subcomplexes of Del B.

Since Del B is a finite complex, there are only finitely many subcomplexes, and the ones we are interested in are naturally ordered by inclusion. We index the complexes from 0 through s, and define $\mathcal{K}_i$ as the ith complex after the trivial complex, $\mathcal{K}_0 = \{\emptyset\}$. The last complex is $\mathcal{K}_s = \text{Del } B$.

The linear structure is essential in obtaining algorithms that efficiently deal with the entire family of alpha complexes and shapes. As a consequence, the most important step in the computation is the construction of Del B. Many efficient algorithms have been described in the literature. The implementation provided as part of our software distribution builds Del B incrementally, adding each point by a sequence of flips [9]. The points are added in random order.

The linear sequence of alpha complexes can be understood as assembling Del B one simplex at a time. This is not quite correct because $\mathcal{K}_i$ and $\mathcal{K}_{i+1}$ may differ by more than only one simplex. In such a case, we can add the simplices in $\mathcal{K}_{i+1} - \mathcal{K}_i$ one by one, lower dimensions first. The resulting sequence of simplices,

$$\emptyset = \sigma_0, \sigma_1, \ldots, \sigma_n,$$

is called a *filter*, and the sequence of complexes,

$$\{\emptyset\} = \mathcal{L}_0, \mathcal{L}_1, \ldots, \mathcal{L}_n = \text{Del } B,$$

$\mathcal{L}_j = \{\sigma_0, \sigma_1, \ldots, \sigma_j\}$, is a *filtration*. For each $0 \leq i \leq s$, there is a $j \geq i$ and an α with $\mathcal{K}_i = \mathcal{L}_j = \text{Cpx}_\alpha B$.

4 Signatures

The filter of Del B implicitly represents all alpha complexes defined by B as prefixes. The availability of this simplex sequence favors incremental algorithms for computing properties of alpha shapes. The software considers metric properties:

> volume, area, and length (defined below),

combinatorial properties:

> number of tetrahedra, triangles, edges, and vertices, distinguishing between simplices on the boundary and in the interior,

and topological properties:

> number of components, independent tunnels, and voids, as expressed by the three betti numbers, β_0, β_1, β_2.

As shown in [11], every additive and continuous map from the set of convex bodies to $\mathbb{R}$ invariant under rigid motion is a linear combination of quermassintegrals, see also [14, chapter 4]. In $\mathbb{R}^3$, the quermassintegrals are basically volume, area, mean width, and the Euler number. Length is defined as an extension of the mean width to non-convex bodies. Specifically, *length* is the sum of edge lengths, each weighted by the (possibly negative) complementary angle. The Euler number is $\chi = \beta_0 - \beta_1 + \beta_2$.

Each property defines a *signature* $f : [s] \to \mathbb{R}$, where $[s] = \{1, 2, \ldots, s\}$. Signatures are useful in studying shapes and convenient in quickly identifying the "interesting" ones in the typically huge family of alpha shapes.

The signatures expressing the above metric and combinatorial properties are straightforward to compute: scan the filter from 0 through n and increment or decrement the current value depending on the next simplex. Such a strategy also works for the three betti numbers, but is less obvious [2].

5 Data Structures

The main two data structures built and used by our software are the Delaunay simplicial complex, Del B, and a filter whose filtration contains all alpha complexes. The filter is accessible through a linear list and an interval tree. The list supports the computation of signatures, and the tree provides fast access to individual shapes. We restrict the discussion to $d = 3$ dimensions.

In $\mathbb{R}^3$, Del B is represented by a triangle-based pointer structure [3]. Each triangle is stored with a pointer each to the 6 neighboring triangles sharing an edge. Following appropriate pointers, each in constant time, it is possible to traverse the triangles around a given edge, or the triangles opposite a given vertex, or all triangles on the convex hull boundary. Further details can be found in [12].

An important ingredient in the construction of Del B, which is synonymous to constructing its triangle-based pointer structure, is the use of exact arithmetic and symbolic computation. The input coordinates and weights are restricted to integers or fixed-point reals.[1] All geometric tests are performed in exact arithmetic so that degenerate cases can be identified without ambiguity. Such degeneracies include 4 points on a common plane, and 5 balls with common orthogonal sphere. All possible degeneracies are reduced to the general case by the use of a simulated perturbation [7]. In the presence of coplanar point on the convex hull boundary, the perturbation results in the construction of infinitesimally thin tetrahedra. As a fortunate consequence of the perturbation scheme in [7] no infinitesimally thin tetrahedra can occur in the interior of the convex hull. The artifacts at the boundary are removed in a post-processing step.

The linear list representation of the filter contains slightly more information than just the sequence of simplices as they enter the alpha complex. Each simplex occurs up to three times: first when it enters the alpha complex, second when the first simplex containing it as a face enters the alpha complex, and third when it becomes completely surrounded by simplices. After the first occurrence the simplex is *singular*, after the second it is *regular*, and after the third it is *interior*. Quite commonly some of the occurrences coincide or vanish. For example, a simplex on the convex hull boundary is never interior, and an entering tetrahedron is right away considered interior.

The additional information available through the multiple occurrences is e.g. useful in selecting the simplices needed for a graphical representation. Only the boundary triangles (singular and regular), the singular edges, and the singular vertices need to be drawn. A triangle belongs to the boundary of all shapes between its first and its third occurrence. Each triangle thus gives rise to an interval of indices in the filtration, and given an index, the corresponding shape is drawn by recovering all triangles whose intervals cover the index. These triangles are located using the interval tree [4] storing their intervals. Except for an additive logarithmic overhead term, it enumerates the desired triangles in constant time each. The same mechanism applies to singular edges and vertices.

[1] A negative weight, $-w$, is interpreted as $w\sqrt{-1}$.

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