Modeling with Simplicial Complexes

(Topology, Geometry, and Algorithms)[1]

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Abstract. Geometric modeling often refers to forming and deforming geometric shape. This paper considers the use of simplicial complexes as a general representation of shapes supporting algorithmic solutions to a variety of geometric modeling problems. At this moment, rather little of the potential of simplicial complexes has been exploited algorithmically, and we concentrate on mathematical results that seem most promising to lead to novel algorithmic methods and ideas.

Keywords. Solid modeling, computational geometry, combinatorial topology, grid generation; simplicial complexes, nerves, Voronoi cells, Delaunay simplicial complexes.

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1 Introduction and Motivation

Unstructured grids in finite element analysis, triangulations in computational geometry, and simplicial complexes in combinatorial topology are one and the same concept. We study this concept from the point of view of using it as a general representation of geometry in solid modeling. The terminology in topology is most advanced and standardized, and it is the one we will mostly use.

Grid generation. In finite element analysis, grids are used to decompose shapes or work-pieces to facilitate the numerical analysis through approximation. The classical approach uses hexahedral elements. Each element has the structure of a cube, with 6 facets, 12 edges, and 8 vertices. These elements are arranged the same way as the cubes in a regular packing, 4 elements around an edge and 8 around a vertex. Indeed, a 3-dimensional array is commonly used as a data structure representing this so-called *structured grid.* This grid implies a homeomorphism between the decomposed shape and a finite portion of a 3-dimensional array. For complicated shapes the construction and maintenance of such a homeomorphism becomes exceedingly difficult [2].

An alternative approach to decomposing shapes uses tetrahedral elements, and the resulting grids are usually referred to a *unstructured* because the number of elements is no longer the same around every interior edge and vertex. In other words, there is no static logical address space that represents the adjacencies between the elements. As a consequence, such a decomposition does not imply any homeomorphism between two possibly very different shapes, and in this respect simplifies the problem. The new challenge is to efficiently handle the less intuitive and less regular structure of a tetrahedral grid. We argue the latter is a challenge that can be met.

Protein structures. Fairly recently, simplicial complexes have been used in the study of proteins and other molecules [5]. The connection between proteins and complexes is less direct than that between shapes and approximating grids. The protein is modeled as a union of balls, one ball per atom, and the complex used is dual to this union [4]. The vertices of the complex are the locations of the atoms in space. Edges, triangles, and tetrahedra are selected on the basis of proximity information. The selection criteria guarantee the dual complex is a subcomplex of the Delaunay simplicial complex of the points, see below. This particular complex plays an important role in our general approach to modeling shapes. It forms a bridge between the globally uniform view of the world using geometry and Euclidean distance and the local view based on decompositions and local neighborhoods.

Dynamical systems. Mechanical systems with several degrees of freedom are commonly mapped to manifolds representing all possible states of the system [1]. Each point of the manifold corresponds to a state. Dynamic change corresponds to a curved traced out on the manifold, which typically lives in a space whose dimension is low but exceeds 3. The intrinsic dimension of the manifold is often much less than that of the embedding space. Such manifolds can be represented by simplicial complexes, which are not restricted to any particular number of dimensions. Simplicial complexes can even model shapes whose intrinsic dimension varies locally.

A particular 3-dimensional modeling problem related to this discussion of dimension is the reconstruction of surfaces. Here the goal is to build a 2-dimensional shape in a 3-dimensional space. With simplicial complexes, there is no principle difference between constructing 3-dimensional grids and 2-dimensional surfaces. In the former problem tetrahedra are fit along triangles, and in the latter triangles are fit along edges. The dimension independent aspect of simplicial complexes makes it possible to generate grids and surfaces with the same tool and format thus bridging the traditional separation between these two problems [8, 14].

Outline. The goal of this paper is to demonstrate the versatility of simplicial complexes as a general representation of geometry. At this moment, limitations of this approach are not well understood and additional research is required to apply this representation to new and old geometric modeling problems.

2 Geometry: Concrete and Abstract

The technical terminology related to decompositions of space and pieces of space is most developed in topology, and in particular in the subarea concerned with combinatorial and algebraic structures within topology [10, 13]. We introduce a few concepts from combinatorial topology relevant to the discussions in this paper. We make an effort to provide intuitive explanations whenever appropriate and possible. The discussion begins with simplices and complexes made up of simplices. Both concepts are geometric in nature, and it is useful to develop abstract counterparts in the form of sets and set systems. The connection between the geometric and the abstract concepts is provided by geometric realizations that map abstract elements to points and sets of elements to simplices.

Simplices. A 2-dimensional simplex is a triangle; it is the simplest 2-dimensional geometric object. A 3-dimensional simplex is a tetrahedron. The author likes to claim the tetrahedron is the simplest 3-dimensional geometric object. It is curious though that a typical high-school curriculum teaches everything about the triangle, and a lot of things about the cube, but little if anything about the tetrahedron. Indeed, mathematical encyclopedia favor a complete treatment of the cube over the discussion of tetrahedra [9]. This is certainly an erroneous path of history.

In general, a k-dimensional simplex, or ***k-simplex***, is the convex hull of $k+1$ points in general position. A k-simplex is inherently k-dimensional and requires at least k dimensions to be embedded. We will primarily be concerned with 3-dimensional real space, $\mathbf{R}^3$, though we would like to remind the reader that there are geometric modeling problems beyond 3 dimensions. In $\mathbf{R}^3$ we have four types of proper simplices: ***vertices*** or 0-simplices, ***edges*** or 1-simplices, ***triangles*** or 2-simplices, and ***tetrahedra*** or 3-simplices. For convenience, the empty set is referred to as a (-1)-simplex. The ***dimension*** of a simplex σ is denoted by $\dim \sigma$; it is one less than the number of vertices. A subset of the vertices spans a lower-dimensional simplex, τ, called a ***face*** of σ. For example, a tetrahedron σ is spanned by 4 vertices, there are four subsets of size 3 and thus 4 triangle faces. A tetrahedron has also 6 edges and 4 vertices as faces. We consider σ itself and $\emptyset$ as improper faces of σ.

Simplicial complexes. A collection of simplices forms a proper decomposition of a geometric object or shape if the simplices have no improver overlap. This means if two simplices overlap then they overlap in a face of both. For example, two triangles may share an edge, or a vertex, or they are disjoint. In the latter case we say they share the empty set, which is considered a face of both and also of all other simplices. Technically, such a collection is referred to as a ***simplicial complex***, $\mathcal{K}$. The formal requirements are (i) if $\sigma \in \mathcal{K}$ and τ is a face of σ then $\tau \in \mathcal{K}$, and (ii) if $\sigma_1, \sigma_2 \in \mathcal{K}$ then $\sigma_1 \cap \sigma_2$ is a face of both. By condition (i), $\sigma_1 \cap \sigma_2$ is also a simplex in $\mathcal{K}$. A ***subcomplex*** is a simplicial complex $\mathcal{L} \subseteq \mathcal{K}$. The ***underlying space*** of $\mathcal{K}$ is $\bigcup \mathcal{K} = \bigcup_{\sigma \in \mathcal{K}} \sigma$. Note that $\bigcup \mathcal{K}$ is a subset of space and thus a geometric object, while $\mathcal{K}$ is a collection of simplices, and thus a combinatorial object. Loose language ignoring the difference between a simplicial complex and its underlying space is however often convenient and frequently used.

Abstract view. There are several reasons why one would want to develop a view that describes simplicial complexes in abstract terms. One is the computational representation of simplices and complexes, which is necessarily symbolic. For example, it is natural to represent a tetrahedron as a set of 4 vertices, or maybe 4 vertex indices. The fact that the tetrahedron is really the convex hull of the 4 points is implicitly understood. This leads to the notions of abstract simplices and abstract simplicial complexes. Let V be a finite set of elements, called ***vertices***. The power set or collection of all subsets of V is denoted by 2^V. A subset $\alpha \subseteq V$ is an ***abstract simplex***, and its dimension is $\dim \alpha = \operatorname{card} \alpha - 1$. A collection $\mathcal{A} \subseteq 2^V$ of abstract simplices is an ***abstract simplicial complex*** if $\alpha \in \mathcal{A}$ and $\beta \subseteq \alpha$ implies $\beta \in \mathcal{A}$. The ***vertex set*** of $\mathcal{A}$ is $\operatorname{vert} \mathcal{A} = \bigcup_{\alpha \in \mathcal{A}} \alpha$.

Abstract simplicial complexes can be constructed directly from finite sets. A particularly important such construction is called the ***nerve*** of the set, A. It consists of all subcollections of sets in A with non-empty common intersection. Formally,

$$\operatorname{nerve} A = \{U \subseteq A \mid \bigcap_{u \in U} u \neq \emptyset\}.$$

nerve A is an abstract simplicial complex. To see this note that the sets in $U \in \operatorname{nerve} A$ have a non-empty intersection, by definition. The intersection of the sets in $T \subseteq U$ contains the intersection of the sets in U and is thus also non-empty. It follows that $T \in$ nerve A, which implies nerve A is indeed an abstract simplicial complex. For example, if A consists of 3 overlapping disks, b_1, b_2, b_3, then nerve $A = \{\emptyset, \{b_1\}, \{b_2\}, \{b_3\}, \{b_1, b_2\}, \{b_2, b_3\}, \{b_3, b_1\}, \{b_1, b_2, b_3\}\}$. This is an abstract representation of a triangle, $\{b_1, b_2, b_3\}$, together with all its faces.

Geometric realization. It is easy to go from a simplicial complex to its abstract counterpart: just replace each simplex by its set of vertices. The other direction is more cumbersome and requires mapping abstract elements to points in some space. Once such a mapping is specified, the other simplices are given as convex hulls of the relevant points. Formally, a map $\varepsilon : \text{vert}\,\mathcal{A} \to \mathbf{R}^d$ defines a simplicial complex if

$$\text{conv}\,\varepsilon(\alpha_1) \cap \text{conv}\,\varepsilon(\alpha_2) = \text{conv}\,\varepsilon(\alpha_1 \cap \alpha_2)$$

for all abstract simplices $\alpha_1, \alpha_2 \in \mathcal{A}$. Given an abstract simplicial complex, a natural question is how many dimensions are needed for a geometric realization. A special case of this problem is to decide whether or not a graph, which is an abstract simplicial complex consisting of vertices and edges, can be drawn in the plane. A realization of a graph in $\mathbf{R}^3$ is always possible simply by placing the vertices so no 4 are coplanar. This way no two edges can cross. In general, the dimension of the space must be at least the largest dimension of any simplex, k, and a general position argument can be used to show that $2k + 1$ dimensions are always sufficient.

There is little incentive in topology to develop methods that use as few dimensions as possible. Still, this question is essential when computing is involved. The complexity of algorithms typically explodes with increasing dimension. General methods that limit the number of dimensions required for geometric realizations are essential in any effort to make topological ideas and results useful in geometric modeling.

3 Grids from Proximity

We use proximity information to obtain geometric realizations of topological concepts. The emphasis is on discreteness and on limiting the number of dimensions. Simplicial complexes seem like the most obvious candidate for discrete encodings of continuous topological information. To limit the number of dimensions we use Voronoi diagrams [17] and Delaunay simplicial complexes [3]. They are based on point set data and proximity in terms of Euclidean distance. After introducing both concepts, we consider a general method for triangulating possibly complicated shapes.

Voronoi cells. Let $S \subseteq \mathbf{R}^3$ be a finite set of points. We use Euclidean distance to measure proximity. For points $x = (\xi_1, \xi_2, \xi_3) \in \mathbf{R}^3$ and $p = (\phi_1, \phi_2, \phi_3) \in S$,

$$|xp| = \left(\sum_{i=1}^{3} (\xi_i - \phi_i)^2\right)^{\frac{1}{2}}$$

is the distance between x and p. For any $x \in \mathbf{R}^3$, we are interested in the point in S nearest to x, or all nearest points in case of a tie. If the points of S are in general position there are at most 4 points of S equidistant from x. Indeed, for any finite set there is an arbitrarily small perturbation so this is the case. Such perturbations can be efficiently simulated, as demonstrated in [6, 18]. For a point $p \in S$, define its *Voronoi cell* as the set of points $x \in \mathbf{R}^3$ so p is nearest to x, that is,

$$V_p = \{x \in \mathbf{R}^3 \mid |xp| \leq |xq|, q \in S\}.$$

The collection of Voronoi cells is $V = V_S = \{V_p \mid p \in S\}$. Clearly, the cells in V_S cover the entire space. Assuming general position, at most 4 Voronoi cells share a common point, namely the point x equidistant from all 4 generators. Two Voronoi cells are either disjoint or they intersect along a 2-dimensional face common to both cells. Similarly, the intersection of three Voronoi cells is either empty or a common edge. The intersection of four Voronoi cells is either empty or a common vertex. Figure 3.1 shows the the Voronoi cells of finitely many points in the plane.

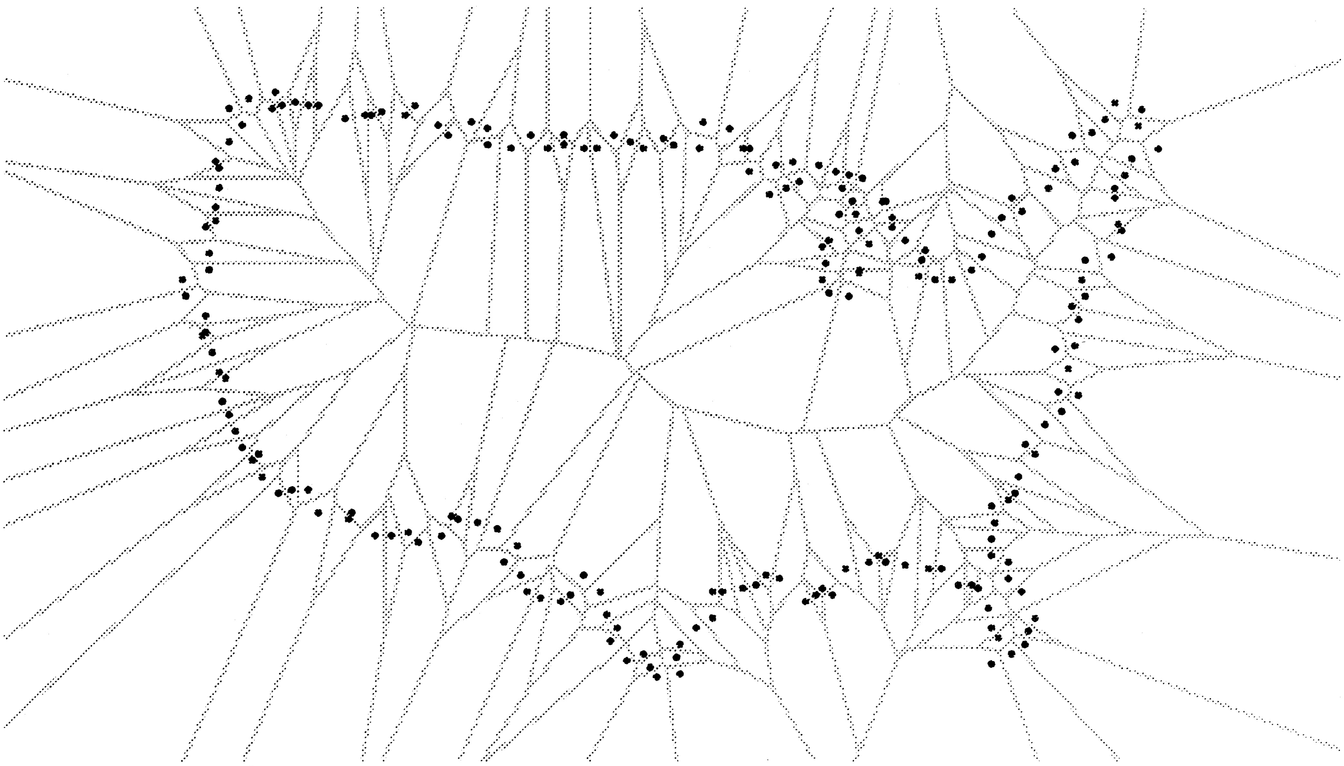

Figure 3.1: The Voronoi cells of a finite set in the plane intersect in pairs and triplets. No higher order intersections occur if general position is assumed.

Delaunay simplicial complexes. Consider the points generating the Voronoi cells, and connect 2 such points by an edge if their cells intersect. Recall that general position implies they intersect along a common 2-dimensional face. Similarly, connect 3 points by a triangle if their cells meet along a common edge, and connect 4 points by a tetrahedron if their cells meet in a common point. The result is a collection of simplices known as the *Delaunay simplicial complex* or *Delaunay triangulation*, $\mathcal{D} = \mathcal{D}_S$, of S, see figure 3.2. A more formal definition can be given using nerves and geometric realizations. The nerve of the set of Voronoi cells, nerve V, contains every subcollection of Voronoi cells with non-empty common intersection. Assuming general position, these subcollections will be of size 1, 2, 3, and 4. nerve V is an abstract simplicial complex. A geometric realization is obtained by mapping each Voronoi cell, V_p, to $p \in S$, see again figure 3.2. This is the Delaunay simplicial complex of S.

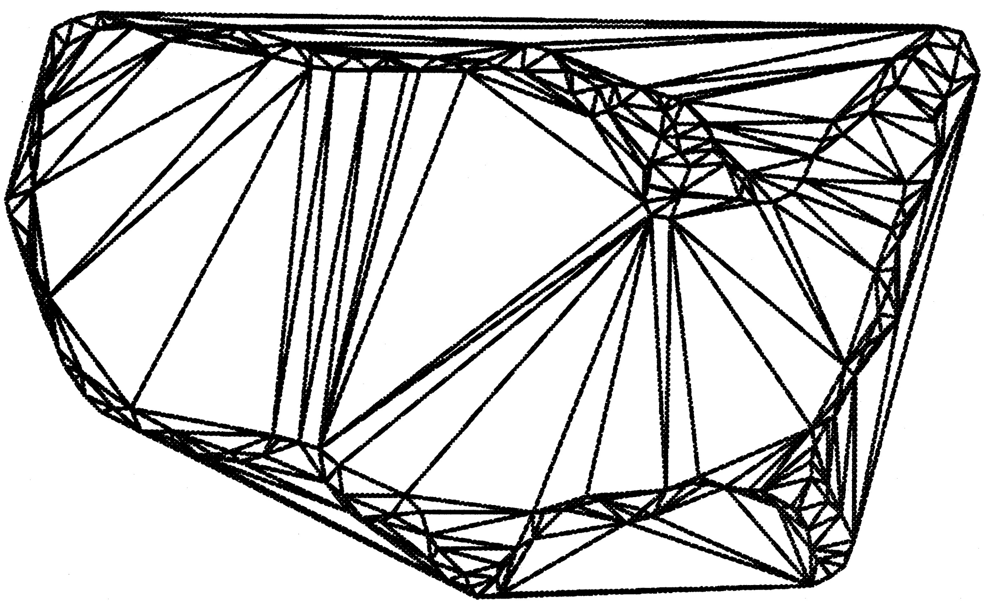

Figure 3.2: The Delaunay simplicial complex of the points generating the Voronoi cells in figure 3.1. The triangles are not shaded although they are genuine elements of the complex.

It is not immediately obvious that the thus realized nerve of V is indeed free of improper intersections and forms a simplicial complex in $\mathbf{R}^3$. To see this is so, one can use the fact that a simplex belongs to $\mathcal{D}$ iff there is a sphere through its vertices so all other points of S lie outside the sphere. There is a long list of nice properties satisfied by Delaunay simplicial complexes, which is the reason they are popular in generating unstructured grids, see e.g. [16].

Restricted cells and complexes. The Delaunay simplicial complex decomposes the entire convex hull of S into tetrahedra. In most applications it is desirable to decompose only a subset $X \subseteq \mathbf{R}^3$, or to find a simplicial complex approximating X. We propose the following mechanism to construct such a simplicial complex.

Let $S \subseteq \mathbf{R}^3$ be a finite point set with Voronoi cells $V = V_S$. S will be the vertex set of the simplicial complex for X, so it makes sense S be a subset of X, but this is not necessary for the construction. Each Voronoi cell, V_p, meets X in a set $V_{p,X} = V_p \cap X$, called the *restricted Voronoi cell* of p and X. The same way unrestricted Voronoi cells define the Delaunay simplicial complex of S, we can use the restricted Voronoi cells to define the *restricted Delaunay simplicial complex*, $\mathcal{D}_X = \mathcal{D}_{X,S}$, of S and X. Let $V_X = \{V_{p,X} \mid p \in S\}$ and consider the nerve,

$$\text{nerve}\, V_X = \{U \subseteq V_X \mid \bigcap_{V_{p,X} \in U} V_{p,X} \neq \emptyset\}.$$

Again we use the natural geometric realization, which maps a cell $V_{p,X}$ to the generator, $p \in S$. The result is $\mathcal{D}_X$, see figure 3.3.

Homeomorphism theorem. The question arises how well the restricted Delaunay simplicial complex represents or approximates the shape X. Somewhat surprisingly, it is possible to specify local conditions on how the Voronoi

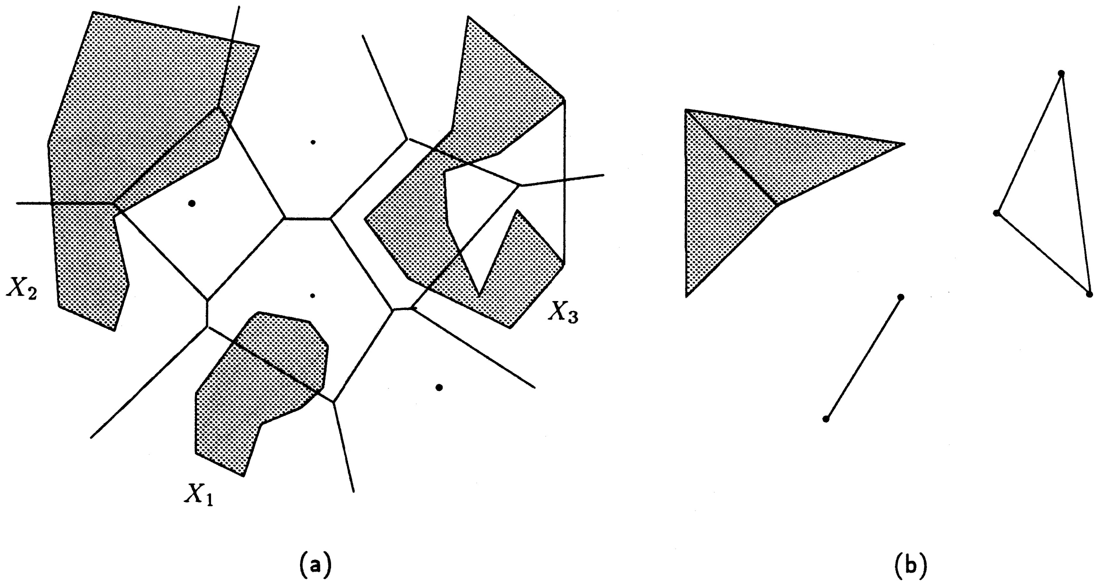

Figure 3.3: By restricting the Voronoi cells to a subset of space, we can specify a subcomplex of the Delaunay simplicial complex suitable to represent the subset. In (a), the Voronoi cells of 10 points decompose 3 shapes, X_1, X_2, X_3. In (b), the corresponding restricted Delaunay simplicial complexes consist of an edge, two triangles sharing an edge, and a cycle *of 3 edges, respectively.*

cells intersect X that imply that X and $\bigcup \mathcal{D}_X$ are homeomorphic. This means there is a bijective map $\varphi : X \to \bigcup \mathcal{D}_X$ so φ and φ^{-1} are both continuous. The existence of a homeomorphism is about the strongest topological requirement between topological spaces such as X and $\bigcup \mathcal{D}_X$. For example, it implies X and $\bigcup \mathcal{D}_X$ are connected the same way (same number and structure of components, tunnels, and voids) and they are locally of the same dimension.

We state the condition under which X and $\bigcup \mathcal{D}_X$ are homeomorphic only for manifolds X. The extension to more general spaces can be found in [7]. X is a ***k*-manifold** if the neighborhood of every point $x \in X$ is homeomorphic to an open k-dimensional ball. In case X has boundary, the neighborhood of every point $y \in \mathrm{bd}\, X$ is homeomorphic to the intersection of an open k-dimensional ball with a closed k-dimensional half-space whose bounding hyperplane passes through the center of the ball. Examples of 2-manifolds are the torus and the sphere, and if open patches with disjoint closures are removed we have 2-manifolds with boundary. An example of a shape $X \subseteq \mathbf{R}^3$ that is not a manifold consists of an edge common to 3 or more triangles. This shape "branches" at the edge, and manifolds are shapes without branching.

We state the condition assuming general position of various kinds. There are arbitrarily small perturbations of S satisfying these assumptions. Intuitively, X and $\bigcup \mathcal{D}_X$ are homeomorphic if all Voronoi cells and common intersections of Voronoi cells meet X and $\mathrm{bd}\, X$ in closed balls. Formally, if all sets of the form

$$\bigcap_{p \in T} V_p \cap X \quad \text{and} \quad \bigcap_{p \in T} V_p \cap \mathrm{bd}\, X,$$

$T \subseteq S$, are closed balls of the appropriate dimension then X and $\bigcup \mathcal{D}_X$ are homeomorphic. See figure 3.3 for examples of homeomorphic and non-homeomorphic restricted Delaunay simplicial complexes.

Alpha complexes. In cases where a shape is specified only by a finite set of points, S, sampled from an object, we can get good triangulations by growing a ball around each point. In other words,

$$X_\alpha = \bigcup_{p \in S} b(p, \alpha),$$

plays the role of the shape. $\alpha \geq 0$ is a parameter and $b(p, \alpha)$ is the closed ball with center p and radius α. The Delaunay simplicial complex restricted by X_α is also known as the *α-complex* of S, $\mathcal{K}_\alpha$, see figure 3.4.

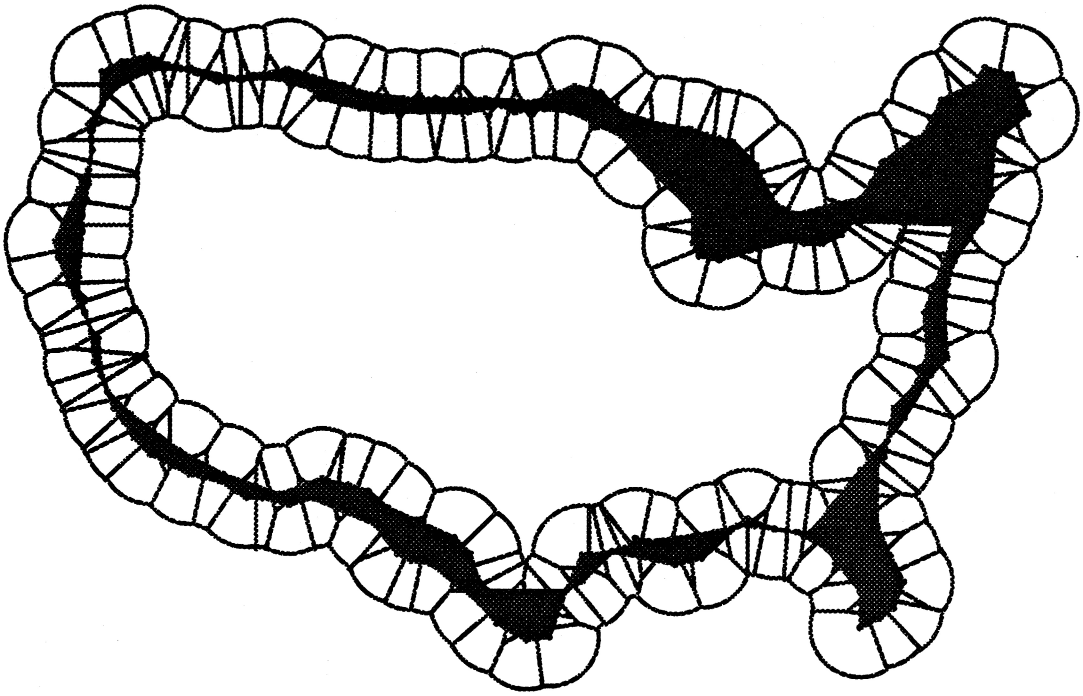

Figure 3.4: The Voronoi cells decompose the union of disks into convex cells. The nerve of the collection of such cells, naturally realized by mapping cells to their generators, is the α-complex. The shaded area in this picture is the underlying space of the α-complex.

Each simplex in the α-complex is also in the Delaunay simplicial complex. In other words, $\mathcal{K}_\alpha$ is a subcomplex of $\mathcal{D}$. More generally, $\mathcal{K}_{\alpha_1} \subseteq \mathcal{K}_{\alpha_2}$ if $\alpha_1 \leq \alpha_2$. By α growing continuously from 0 to $+\infty$, we obtain a nested sequence of complexes, the last one being the Delaunay simplicial complex itself.

An important application of α-complexes is the study of proteins as 3-dimensional structures. Each atom is modeled as a sphere or ball [11, 15]. The size of the sphere depends on the question of interest. For example, the interaction between the protein and a solvent, modeled as a single sphere, can be studied by inflating the atom spheres by the radius of the solvent.

Homotopy equivalence. The decomposition of X_α by Voronoi cells does not always satisfy the closed ball property sufficient for the existence of a homeomorphism. However, all sets of the form

$$\bigcap_{p \in T} V_p \cap X_\alpha,$$

$T \subseteq S$, are convex. The nerve theorem of algebraic topology [12] implies that X_α and $\bigcup \mathcal{K}_\alpha$ are homotopy equivalent. This is weaker than being homeomorphic. Intuitively, it means X_α and $\bigcup \mathcal{K}_\alpha$ are connected the same way, but locally their intrinsic dimension may not agree. For example, a solid torus is homotopy equivalent to a circle in space. It can be shrunk continuously to the circle, but by doing so it loses its 3-dimensionality and is squeezed to a single dimension.

4 Conclusions

The purpose of this paper is to argue and partially demonstrate that simplicial complexes can serve as a general geometric representation for a broad spectrum of modeling problems. This approach has tradition in combinatorial topology, computational geometry, and grid generation. Indeed, the terms 'triangulation' and 'unstructured grid' are often used as synonyms to 'simplicial complex'. The study of simplicial complexes for modeling problems is relatively recent, which is one of the reasons why this paper concentrates on the geometric and topological fundamentals.

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