III.4 Alpha Complexes

In this section, we use a radius constraint to introduce a family of subcomplexes of the Delaunay complex. These complexes are similar to the Čech complexes but differ from them by having natural geometric realization.

Union of balls. Let S be a finite set of points in $\mathbb{R}^d$ and r a non-negative real number. For each $p \in S$ we let $B_p(r) = p + r\mathbb{B}^d$ be the closed ball with center p and radius r. The union of these balls is the set of points at distance at most r from at least one of the points in S,

$$\text{Union}(r) = \{x \in \mathbb{R}^d \mid \exists p \in S \text{ with } \|x - p\| \leq r\}.$$

To decompose the union, we intersect each ball with the corresponding Voronoi cell, $R_p(r) = B_p(r) \cap V_p$. Since balls and Voronoi cells are convex, the $R_p(r)$ are also convex. Any two of them are disjoint or overlap along a common piece of their boundaries, and together the $R_p(r)$ cover the entire union, as in Figure III.15. The *alpha complex* is isomorphic to the nerve of this cover,

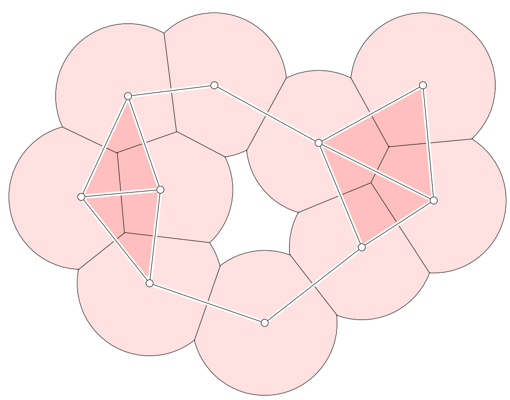

Figure III.15: The union of disks is decomposed into convex regions by the Voronoi cells. The corresponding alpha complex is superimposed.

$$\text{Alpha}(r) = \{\sigma \subseteq S \mid \bigcap_{p \in \sigma} R_p(r) \neq \emptyset\}.$$

Since $R_p(r) \subseteq V_p$, the alpha complex is a subcomplex of the Delaunay complex. It follows that for a set S in general position we get a geometric realization by taking convex hulls, as in Figure III.15. Furthermore, $R_p(r) \subseteq B_p(r)$ which implies $\text{Alpha}(r) \subseteq \check{\text{C}}\text{ech}(r)$. Since the $R_p(r)$ are closed and convex and together they cover the union, the Nerve Theorem implies that $\text{Union}(r)$ and $\text{Alpha}(r)$ have the same homotopy type.

Weighted alpha complexes. For many applications it is useful to permit balls with different sizes. An example of significant importance is the modeling of biomolecules, such as proteins, RNA, and DNA. Each atom is represented by a ball whose radius reflects the range of its van der Waals interactions and thus depends on the atom type. Let therefore S be a finite set of points p with real weights w_p. Same as in Section III.3, we think of p as a ball B_p with center p and radius $r_p = \sqrt{w_p}$. We again consider the union of the balls, which we decompose into convex regions now using weighted Voronoi cells, $R_p = B_p \cap V_p$. This is illustrated in Figure III.16. In complete analogy to the unweighted case

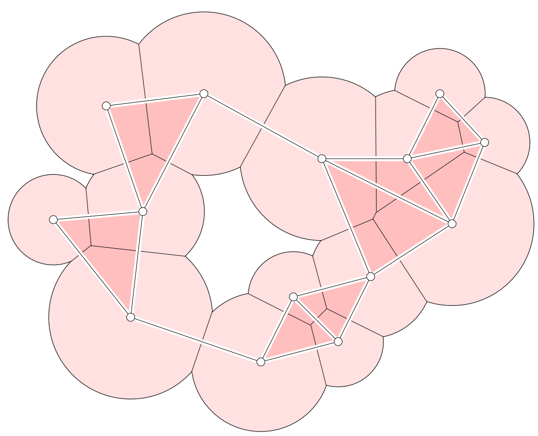

Figure III.16: Convex decomposition of a union of disks and the weighted alpha complex superimposed.

the *weighted alpha complex* of S is defined to be isomorphic to the nerve of the regions R_p, that is, the set of simplices $\sigma \subseteq S$ such that $\bigcap_{p \in \sigma} R_p \neq \emptyset$. The weighted alpha complex is a subcomplex of the weighted Delaunay complex which is isomorphic to the nerve of the collection of weighted Voronoi cells.

We need S to be in general position to guarantee that taking convex hulls of input points gives a geometric realization. Since the points are weighted, the notion of general position is slightly different from the unweighted case. In particular, it needs to imply that $d + 2$ or more Voronoi cells have no non-empty common intersection. To see what this means let $x \in \mathbb{R}^d$ be a point in the common intersection of the weighted Voronoi cells V_p with $p \in \sigma$. By definition, the weighted square distances from x to the points are all the same. It follows there is a weight $w \in \mathbb{R}$ such that $w = \|x - p\| - r_p^2$ for all $p \in \sigma$. If x is outside the balls B_p then this weight is positive and the sphere with center x and radius $r = \sqrt{w}$ is well defined. It is orthogonal to the balls B_p in the sense that $\|x - p\|^2 = r_p^2 + r^2$ for all $p \in \sigma$. The same formula works even if p lies on the boundary or in the interiors of the balls, except that the weight w is then zero or negative. We say a finite set of weighted points is in *general position* if there is no point x with equal weighted square distance to $d + 2$ or more of the points. Equivalently, no $d + 2$ of the balls are orthogonal to a common (possibly imaginary) d-sphere.

Filtration. Given a finite set $S \subseteq \mathbb{R}^d$, we can continuously increase the radius and thus get a 1-parameter family of nested unions. Correspondingly, we get a 1-parameter family of nested alpha complexes. Because they are all subcomplexes of the Delaunay complex, which is finite, only finitely many of the alpha complexes are different. Writing K^i for the i-th alpha complex in the sequence, we get

$$\emptyset = K^0 \subset K^1 \subset \ldots \subset K^m,$$

which we call a *filtration* of $K^m = \text{Delaunay}$. It is a stepwise construction of the final complex in such a way that every set along the way is a complex.

The construction of a filtration is straightforward in the unweighted case and can be extended to the weighted case as follows. Let p be a point with weight w_p. For each $r \in \mathbb{R}$ we let $B_p(r)$ be the ball with center p and radius $\sqrt{w_p + r^2}$ and denote the corresponding alpha complex by $\text{Alpha}(r)$. The collection of such balls, interpreted as weighted points, defines the same weighted Voronoi diagram for any choice of r. It follows that every weighted alpha complex is a subcomplex of the same weighted Delaunay complex. Furthermore, the balls are nested, $B_p(r_0) \subseteq B_p(r)$ for $r_0 \leq r$, so the weighted alpha complexes are nested and define a filtration of the weighted Delaunay complex. We are interested in the difference between two contiguous complexes in the filtration, $K^{i+1} - K^i$. We will see shortly that generically this difference is either a single simplex or a collection that forms an anticollapse.

Collapses. Let K be a simplicial complex. It is convenient to call a simplex in the star a *coface*. A simplex in K is *free* if it has a unique proper coface. The star of a free simplex thus contains exactly two simplices, namely the simplex itself and the unique proper coface. An *elementary collapse* is the operation that removes a free simplex together with its unique proper coface. An *elementary anticollapse* is the inverse of that operation. If the free simplex is τ with dimension $k = \dim \tau$ then the unique proper coface σ has dimension $k+1 = \dim \sigma$ and the elementary collapse that removes τ and σ is called a $(k, k+1)$-*collapse*. Each elementary collapse corresponds to a deformation retraction of the underlying space, which implies that it does not change the homotopy type. Consider the special case in which K is the set of faces of a d-simplex. As illustrated in Figure III.17, this d-simplex can be reduced to a single vertex by a sequence of $2^{d-1}-1$ elementary collapses. Starting with 2^d-1 faces, each elementary collapse removes two, leaving $2^d - 1 - 2(2^{d-1} - 1) = 1$ face, which is necessarily a vertex.

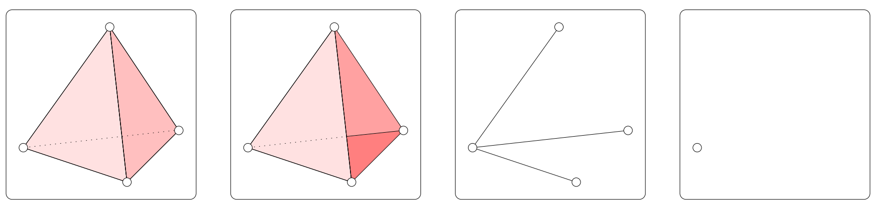

Figure III.17: From left to right: a tetrahedron, the three triangles left after a $(2,3)$-collapse, the three edges left after three $(1,2)$-collapses, the vertex left after three $(0,1)$-collapses.

It is convenient to extend the notion of collapse and consider pairs of simplices $\tau < \sigma$ whose dimensions differ by one or more. Instead of requiring that τ be free, we now require that all cofaces of τ are faces of σ. Letting $k = \dim \tau$ and $\ell = \dim \sigma$ we get $\binom{\ell-k}{i}$ simplices of dimension $i+k$ and therefore a total of $2^{\ell-k} = \sum_{i=0}^{\ell-k} \binom{\ell-k}{i}$ simplices between τ and σ, including the two. They form the structure of an $(\ell-k)$-simplex, which can be collapsed down to a vertex by a sequence of $2^{\ell-k-1} - 1$ elementary collapses. Each $(i, i+1)$-collapse in this sequence corresponds to an $(i+k+1, i+k+2)$-collapse in the sequence that removes the faces of τ. We append a $(k, k+1)$-collapse which finally removes τ together with the last remaining proper coface. We refer to this sequence of $2^{\ell-k-1}$ elementary collapses as a (k, ℓ)-*collapse*. Since elementary collapses preserve the homotopy type so do the more general collapses.

Critical and regular simplices. Let r_i be the smallest radius such that $K^i = \text{Alpha}(r_i)$. A simplex τ belongs to K^{i+1} but not to K^i if the balls with radius r_{i+1} have a non-empty common intersection with the corresponding intersection of Voronoi cells but the balls with radius r_i do not; see Figure

III.18. Assuming general position and $\dim \tau = k$, the intersection of Voronoi cells, $V_\tau = \cap_{p \in \tau} V_p$, is a convex polyhedron of dimension $d - k$. By definition of r_{i+1} the balls $B_p(r_{i+1})$ intersect V_τ in a single point, x.

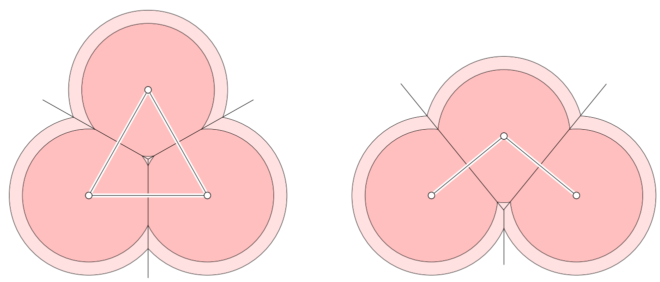

Figure III.18: Left: three points spanning an acute triangle. In the alpha complex evolution, the three edges appear first before the triangle enters as a critical simplex. Right: three points spanning an obtuse triangle. Two edges appear first and the triangle enters together with the third edge.

Consider first the case that x lies on the boundary of V_τ. Then there are other Voronoi polyhedra for which x is the first contact with the union of balls. Assume V_τ is the polyhedron with highest dimension in this collection and let V_σ be the polyhedron with lowest dimension. Correspondingly, τ is the simplex with lowest dimension in $K^{i+1} - K^i$ and σ is the simplex with highest dimension. The other simplices in $K^{i+1} - K^i$ are the faces of σ that are cofaces of τ. In other words, we obtain K^i from K^{i+1} by a (k, ℓ)-collapse, where $k = \dim \tau$ and $\ell = \dim \sigma$. We call all simplices participating in this collapse *regular*.

Consider second the case that x lies in the interior of V_τ and it is not the first contact for any higher-dimensional Voronoi polyhedron. In other words, τ is the only simplex in $K^{i+1} - K^i$. We call τ *critical* because its addition changes the homotopy type of the complex. Since the union of balls has the homotopy type of the complex, we know that also the union changes its type when the radius reaches r_{i+1}.

Bibliographic notes. Alpha complexes have been introduced for points in $\mathbb{R}^2$ by Edelsbrunner, Kirkpatrick, and Seidel [2]. They have been extended to $\mathbb{R}^3$ in [3] and to weighted points in general, fixed dimension in [1]. The three-dimensional software written by Ernst Mücke has been popular in many areas of science and engineering, including structural molecular biology where they serve as an efficient representation of proteins and other biomolecules. Alpha complexes have been the starting point of the work on persistent homology which will be discussed in Chapter V.

The difference between critical and regular simplices reminds us of the difference between critical and regular points of Morse functions, which will be studied in Chapter VI. The connection is direct but made technically difficult because Morse theory has been developed principally for smooth functions [4]. The union of balls is a sublevel set of the continuous but not smooth distance function defined by the data points. An early bridge between the two categories has been built by Marston Morse himself who introduced the concept of topological Morse function [5], of which the distance function on $\mathbb{R}^d$ is an example.

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[3] H. Edelsbrunner and E. P. Mücke. Three-dimensional alpha shapes. *ACM Trans. Graphics* **13** (1994), 43–72.

[4] J. Milnor. *Morse Theory.* Princeton Univ. Press, New Jersey, 1963.

[5] M. Morse. Topologically non-degenerate functions on a compact n-manifold. *J. Analyse Math.* **7** (1959), 189–208.