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,

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

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,

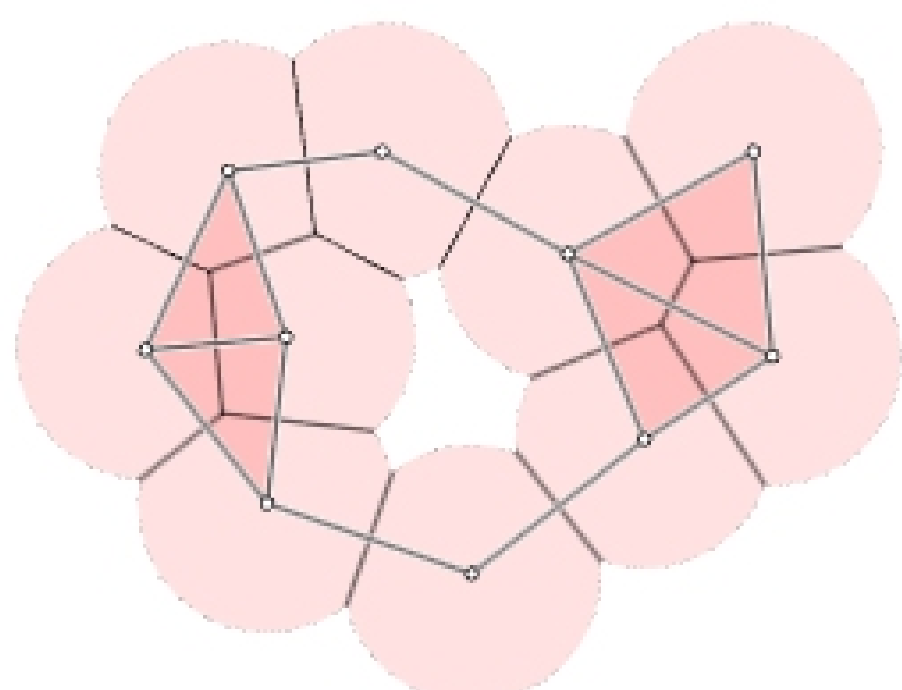

Figure III.15: The union of disks is decomposed into convex regions by the Voronoi cells. The corresponding alpha complex is superimposed.

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

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

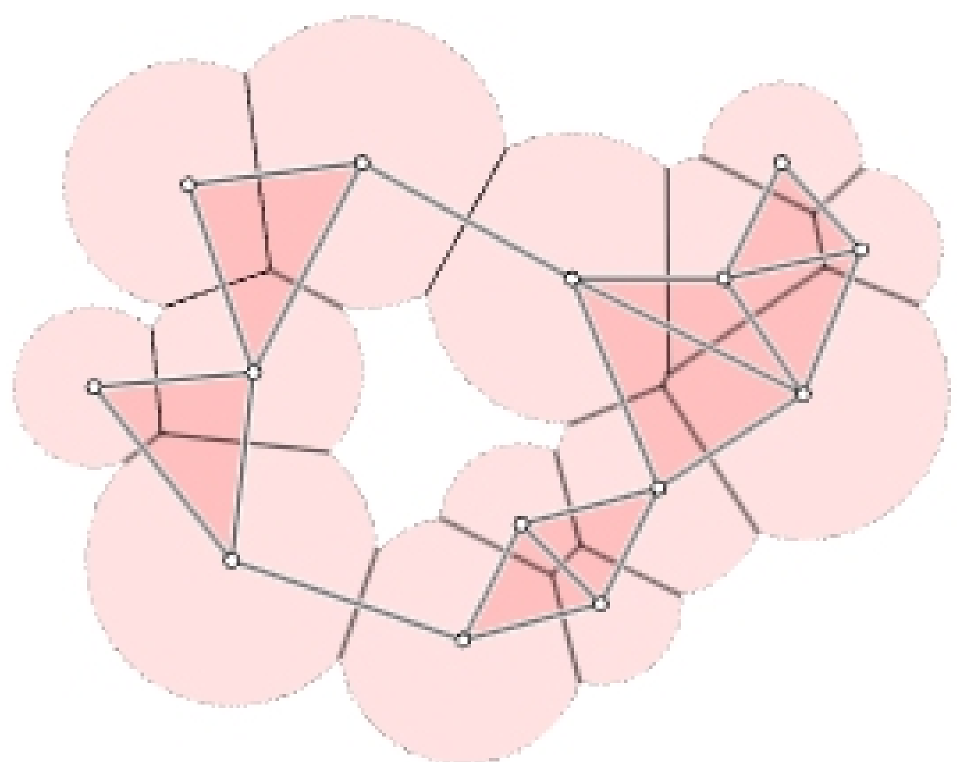

Figure III.16: Convex decomposition of a union of disks and the weighted alpha complex superimposed.

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 nonempty 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 $K^m =$ 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