The Union of Balls and its Dual Shape*

Herbert Edelsbrunner
Department of Computer Science, University of Illinois, Urbana, Illinois 61801, USA.

Abstract

Efficient algorithms are described for computing topological, combinatorial, and metric properties of the union of finitely many balls in $\mathbb{R}^d$. These algorithms are based on a simplicial complex dual to a certain decomposition of the union of balls, and on short inclusion-exclusion formulas derived from this complex. The algorithms are most relevant in $\mathbb{R}^3$ where unions of finitely many balls are commonly used as models of molecules.

1 Introduction

The primary object studied in this paper is the union of finitely many d-balls in $\mathbb{R}^d$. One of the motivations for our considerations is their widespread use in computational chemistry and biology, where a molecule is frequently modeled as the union of 3-balls in $\mathbb{R}^3$ [5, 25]. Each atom is represented by a ball whose size is determined by its van der Waals radius. This model is referred to as the *space filling diagram* of the molecule. As will be seen later, this diagram is related to a certain polytope, called the *dual shape* of the diagram. This paper is part of a larger project [13] that studies such shapes and their applications to problems in science. A declared goal of the project is the implementation of shapes and some of their useful functions. It is therefore essential to find simple algorithms so that the implementation produces a compact system of programs. At the same time, efficiency is essential because typical applications involve thousands of points or balls.

Our study of d-balls requires a variety of concepts whose origins lie in the areas of convex geometry, geometric algorithms, and algebraic topology. We make essential use of power diagrams and regular triangulations, which are generalizations of the more popular Voronoi diagrams and Delaunay triangulations [7, 9, 26]. Important are also polytopes which arise as underlying spaces of certain subcomplexes of a Delaunay or regular triangulation [12, 14, 16]. Topological concepts such as homotopy equivalence and homology groups [1, 23] are instrumental in uncovering the close relationship between these geometric diagrams.

The outline of this paper follows. Section 2 introduces the basic geometric diagrams used in our study. Section 3 establishes the homotopy equivalence of the union of balls and its dual shape; it implies effective algorithms for computing the homology groups of the union. Section 4 shows how the topological insights lead to an efficient algorithm for counting the faces of the union of a set of balls. Section 5 studies variations of the Euler relation for convex polyhedra. Based on these relations, section 6 gives short inclusion-exclusion formulas for measuring the union of balls. Sections 7 and 8 derive another set of such formulas which are decomposable and, among other things, can measure voids formed by the union. Section 9 concludes the paper.

2 Various Diagrams

This section introduces various geometric concepts defined for a finite collection of balls, with the aim to develop tools that can enhance our understanding of the union of these balls.

Basic definitions. Let $|xz|$ denote the Euclidean distance between two points $x, z \in \mathbb{R}^d$. A subset $b \subseteq \mathbb{R}^d$ is a *d-ball* if there is a point $z \in \mathbb{R}^d$ and a real $\varrho > 0$

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so that $b = \{x \in \mathbb{R}^d \mid |xz| \leq \varrho\}$; z is the *center* and ϱ is the *radius* of b. For $0 \leq k \leq d-1$, a *k-ball* is the intersection of a $(k+1)$-ball b with a hyperplane that contains the center of b but not b itself. A *k-sphere* is the boundary of a $(k+1)$-ball b. The center and radius are inherited from b. Note that a 0-ball is a point, a 1-ball is a line segment, and a 2-ball is a disk. A 0-sphere is a pair of points, a 1-sphere is a circle, and a 2-sphere is what in $\mathbb{R}^3$ is commonly called a sphere.

Besides balls and spheres we consider simplices in $\mathbb{R}^d$. For $0 \leq k+1 \leq d+1$, a *k-simplex*, σ, in $\mathbb{R}^d$ is the convex hull of $k+1$ affinely independent points. The *dimension* of σ is $\dim(\sigma) = k$. The convex hull of any $0 \leq \ell+1 \leq k+1$ of these points is an ℓ-simplex and a *face* of σ. For example, the only (-1)-simplex is $\emptyset$, a 0-simplex is a point, a 1-simplex is an edge, a 2-simplex is a triangle, and a 3-simplex is a tetrahedron. An edge has four faces, namely $\emptyset$, its two vertices, and itself, and a triangle has eight faces, namely $\emptyset$, its three vertices, its three edges, and itself.

Different kinds of complexes play an important role in this paper. An *abstract simplicial complex* is a collection A of finite sets so that $X \in A$ and $Y \subseteq X$ implies $Y \in A$. The *k-skeleton* of A is the collection $A^{(k)} = \{X \in A \mid |X| \leq k+1\}$. A *(geometric) simplicial complex* is a collection G of simplices that satisfy the following two conditions. First, if $\sigma \in G$ and σ' is a face of σ then $\sigma' \in G$. Second, if $\sigma_1, \sigma_2 \in G$ then $\sigma_1 \cap \sigma_2$ is a face of both. As a general policy, $\emptyset$ is considered a face of every simplex and is included in all simplicial complexes. The *underlying space* of G is $|G| = \bigcup_{\sigma \in G} \sigma$. A subset $H \subseteq G$ is a *subcomplex* of G if it is a simplicial complex itself, that is, it satisfies the first condition. A special subcomplex is the *k-skeleton* $G^{(k)} = \{\sigma \in G \mid \dim(\sigma) \leq k\}$. G is a *geometric realization* of A if there is a bijection $\phi : A^{(0)} \to G^{(0)}$ so that $X \in A$ iff the convex hull of $\phi(X)$ is a simplex in G.

Furthermore, we consider complexes defined by finite collections of closed and convex bodies with non-empty interior in $\mathbb{R}^d$. We require that the intersection of any $k+1 \leq d+1$ of these bodies is either empty or a $(d-k)$-dimensional body with non-empty ($(d-k)$-dimensional) interior. The *cell complex* defined by such a collection Q is the set of *cells* $\{\bigcap_{q \in T} q \mid T \subseteq Q\}$. Note that for such a complex it is in general not true that the boundary of every cell is the union of other cells. It would be easy to add faces so that this common requirement is satisfied. However, because of general position assumptions these faces will not be necessary. By the *underlying space* of this complex we mean $\bigcup_{q \in Q} q$.

The three primal diagrams. Let B be a set of n d-balls in $\mathbb{R}^d$, see figure 2.1. To simplify the forthcoming discussion we assume the d-balls are in general position. An algorithmic justification of this assumption can be found in [15]. For a subset $T \subseteq B$, with $k+1 = |T| \leq d+1$, the centers of the d-balls in T are affinely independent, by assumption, and therefore define a k-simplex, denoted σ_T.

Consider a d-ball b, with center z and radius ϱ, and a point x. The *power distance* of x from b is $\pi_b(x) = |xz|^2 - \varrho^2$. The *power cell* of $b \in B$ is $p_b = \{x \in \mathbb{R}^d \mid \pi_b(x) \leq \pi_{b'}(x), b' \in B\}$. It is not difficult to see that within its own power cell a ball b contains all other balls of B. That is, for $q_b = p_b \cap b$ and every $b' \in B$ we have $p_b \cap b' \subseteq q_b$. For a subset $T \subseteq B$ define $p_T = \bigcap_{b \in T} p_b$ and $q_T = \bigcap_{b \in T} q_b$. As a generalization of the above observation we have the following result stated without proof.

2.1 For each $T \subseteq B$, $b \in T$, and $b' \in B - T$ we have $q_T = p_T \cap b \supseteq p_T \cap b'$.

Because of general position, p_T is either empty or a $(d-k)$-dimensional convex polyhedral set, where $k+1 = |T|$. Similarly, $q_T \subseteq p_T$ is either empty or a $(d-k)$-dimensional convex set. Hence, the collection of bodies p_b satisfies the requirements for defining a cell complex, and so does the collection of bodies q_b. Now we are ready to define the first three diagrams.

$\mathcal{P} = \mathcal{P}(B) = \{p_T \mid \emptyset \neq T \subseteq B\}$, the *power diagram* of B.

$\mathcal{Q} = \mathcal{Q}(B) = \{q_T \mid \emptyset \neq T \subseteq B\}$, the intersection of $\mathcal{P}$ with $\mathcal{U}$.

$\mathcal{U} = \mathcal{U}(B) = \bigcup_{b \in B} b$, the union of the balls.

Two-dimensional examples of the three diagrams are shown in figure 2.2. The power diagram, $\mathcal{P}$, is a well-known cell complex whose underlying space, $|\mathcal{P}| = \bigcup_{p_T \in \mathcal{P}} p_T$, is equal to the entire space, $\mathbb{R}^d$. Similarly, $\mathcal{Q}$ is a cell complex, and its underlying space is $|\mathcal{Q}| = \mathcal{U}$.

The boundary of $\mathcal{U}$ consists of pieces of spheres of various dimensions. Define $s_b = \mathrm{bd}(b)$, and for each non-empty $T \subseteq B$, $s_T = \bigcap_{b \in T} s_b$. Because of general position, s_T is either empty or a $(d-k-1)$-sphere, where $k+1 = |T| \leq d$. Now define $\dot{q}_b = s_b \cap p_b$, for each $b \in B$, and $\dot{q}_T = s_T \cap p_T = \bigcap_{b \in T} \dot{q}_b$, for each non-empty $T \subseteq B$. Intuitively, $\dot{q}_T$ is the spherical part of $\mathrm{bd}(q_T)$. The components of the $\dot{q}_T$ are the *faces* of $\mathcal{U}$; this includes $\emptyset$ as the only (-1)-face.

The three dual diagrams. The *nerve* of a collection A of sets is $N(A) = \{X \subseteq A \mid \bigcap_{a \in X} a \neq \emptyset\}$. We always have $\emptyset \in N(A)$. The nerve is an abstract simplicial complex because $X \in N(A)$ and $Y \subseteq X$ implies $Y \in N(A)$. For example, the nerve of B, $N(B)$, is the collection of subsets of d-balls with non-empty common intersection. By mapping s_b to b the nerve of $\{s_b \mid b \in B\}$ defines a subset of $N(B)$. Specifically, this is a subset of the $(d-1)$-skeleton $N(B)^{(d-1)}$, because general position implies that no $d+1$ $(d-1)$-sphere have a non-empty common intersection. We define two of the three dual diagrams as geometric realizations of nerves. Recall that σ_T is the convex hull of the centers of the d-balls in T.

> $\mathcal{R} = \mathcal{R}(B) = \{\sigma_T \mid \emptyset \neq p_T \in \mathcal{P}\} \cup \{\emptyset\}$, the *regular triangulation* of B.
>
> $\mathcal{K} = \mathcal{K}(B) = \{\sigma_T \mid \emptyset \neq q_T \in \mathcal{Q}\} \cup \{\emptyset\}$, the *dual complex* of $\mathcal{Q}$.
>
> $\mathcal{S} = \mathcal{S}(B) = |\mathcal{K}|$, the *dual shape* of $\mathcal{U}$.

Examples of the three diagrams are shown in figure 2.3. Note that $\mathcal{R}$ is a geometric realization of the nerve of the collection of (d-dimensional) power cells. By definition, $\mathcal{P}$ and $\mathcal{R}$ are *dual* in the sense that $\emptyset \neq p_T \in \mathcal{P}$ iff $\emptyset \neq \sigma_T \in \mathcal{R}$.

Similarly, $\mathcal{K}$ is a geometric realization of the nerve defined for the family of d-dimensional cells of $\mathcal{Q}$. This definition of $\mathcal{K}$ is different although equivalent to the one in [12]. It should be clear that $\mathcal{K}$ is a subcomplex of $\mathcal{R}$. Indeed, $\sigma_T \in \mathcal{K}$ only if $\sigma_T \in \mathcal{R}$ and $T \in N(B)$, but not necessarily vice versa. The nerve theorem of algebraic topology [22, 27, 28] implies that $\mathcal{U} = |\mathcal{Q}|$ and $\mathcal{S} = |\mathcal{K}|$ are homotopy equivalent. We prefer to give a direct proof of this result in section 3. It will reveal some detailed relations between these diagrams.

Another interesting simplicial complex is the *boundary complex* of $\mathcal{S}$. It consists of all simplices $\sigma \in \mathcal{K}$ contained in $\mathrm{bd}(\mathcal{S})$. Call such a simplex a *face* of $\mathcal{S}$. The faces of $\mathcal{S}$ correspond to the faces of $\mathcal{U}$ in the following manner, see [12].

2.2 For each $T \subseteq B$ with $1 \leq |T| \leq d$, σ_T is a face of $\mathcal{S}$ iff $\dot{q}_T \neq \emptyset$.

3 A Deformation Retraction

Two topological spaces can be homotopy equivalent without being homeomorphic. Intuitively, the main difference between the two notions is that a homeomorphism maintains the intrinsic dimension of a space, and a homotopy equivalence does not. Nevertheless, two homotopy equivalent spaces have the same connectivity as expressed by their homology groups. We begin with some definitions and then prove homotopy equivalence results between $\mathcal{U}$ and $\mathcal{S}$.

Homotopy equivalence and deformation retractions. It will not be necessary to define homotopy equivalence in its full generality. A more restrictive notion is the following. Let $X \subseteq Y$ be two topological spaces. A *retraction* of Y onto X is a continuous map $\phi : Y \to X$ so that $\phi(x) = x$ for all $x \in X$. A *deformation retraction* of Y onto X is a continuous map $\Phi : Y \times [0,1] \to Y$ so that $\Phi(x,t) = x$ for all $x \in X$ and $t \in [0,1]$, Φ is the identity on Y for $t = 0$, and Φ is a retraction of Y onto X for $t = 1$. If such a Φ exists then X is a *deformation retract* of Y.

If X is a deformation retract of Y then X and Y are homotopy equivalent. The reverse is not true, but to show that X and Y are homotopy equivalent it suffices to find a topological space Z and imbeddings $\epsilon : X \to Z$ and $\varepsilon : Y \to Z$ so that both $\epsilon(X)$ and $\varepsilon(Y)$ are deformation retracts of Z. As proved in [18] the existence of Z, ϵ, and ε is also a necessary condition for the homotopy equivalence of X and Y.

A basic property necessary for our construction is $\mathcal{S} \subseteq \mathcal{U}$. Indeed, assuming general position we get $\mathcal{S} \subseteq \mathrm{int}(\mathcal{U})$. It suffices to show the following result.

3.1 If $\sigma_T \in \mathcal{K}$ then $\sigma_T \subseteq \mathrm{int}(\mathcal{U}(T))$.

Proof. The assertion is obviously true for vertices. So let $|T| = k+1 \geq 2$ and assume inductively that the assertion holds for simplices of dimension less than k. In particular, $\sigma_U \subseteq \mathrm{int}(\mathcal{U}(U)) \subseteq \mathrm{int}(\mathcal{U}(T))$ for each proper face σ_U of σ_T. The only possibility for $\sigma_T \not\subseteq \mathrm{int}(\mathcal{U}(T))$ is therefore that the complement of $\mathrm{int}(\mathcal{U}(T)) \cap \mathrm{aff}(T)$ is disconnected. However, $\sigma_T \in \mathcal{K}$ implies that $\mathrm{int}(b_T) = \bigcap_{b \in T} \mathrm{int}(b) \neq \emptyset$, and because b_T lies symmetric with respect to $\mathrm{aff}(T)$ we have $\mathrm{int}(b_T) \cap \mathrm{aff}(T) \neq \emptyset$. Hence, $\mathrm{int}(\mathcal{U}(T)) \cap \mathrm{aff}(T)$ is star-convex which implies that the complement within $\mathrm{aff}(T)$ is connected. Therefore $\sigma_T \subseteq \mathrm{int}(\mathcal{U}(T))$. $\square$

Decomposition with joins. We construct a deformation retraction of $\mathrm{int}(\mathcal{U})$ onto $\mathcal{S}$ based on a natural decomposition of $\mathcal{U}$. Because of general position, the exclusion of $\mathrm{bd}(\mathcal{U})$ does not affect the final result. The cells of this decomposition are joins of simplices of $\mathcal{K}$ and faces of $\mathcal{U}$. In general, the join of two sets $U, V \subseteq \mathbb{R}^d$ exists provided any two edges $u_1v_1 \neq u_2v_2$, with $u_1, u_2 \in U$ and $v_1, v_2 \in V$, are either disjoint or meet at a common endpoint. Then the *join* of U and V is $U * V = \bigcup_{u \in U, v \in V} uv$. For convenience, $U * \emptyset = \emptyset * U = U$.

Consider a subset $T \subseteq B$, with $k+1 = |T| \leq d$, so that $\sigma_T \in \mathcal{K}$. Note that s_T is a $(d-k-1)$-sphere. By 2.2, σ_T is a face of $\mathcal{S}$ iff $\dot{q}_T = s_T \cap \mathrm{bd}(\mathcal{U})$ is non-empty. If $\dot{q}_T = \emptyset$ then $\sigma_T * \emptyset = \sigma_T$ is a cell of the decomposition. In the other case, the affine hull of σ_T is a k-flat, and that of s_T is a $(d-k)$-flat. These two flats are orthogonal and meet in the center of s_T. This implies that the join of σ_T and s_T exists, and therefore also the join of σ_T and any component f of $\dot{q}_T$. For every face σ' of σ_T and every face f' of f, $\sigma' * f'$ exists and is contained in $\sigma_T * f$. Indeed, $\mathrm{bd}(\sigma_T * f)$ is the union of all joins $\sigma' * f'$, $(\sigma', f') \neq (\sigma_T, f)$. Now define

> $\mathcal{J} = \mathcal{J}(B) = \{\sigma_T * f'\}$, where σ_T is any non-empty

simplex in $\mathcal{K}$ and f' is any face of any component of $\dot{q}_T = s_T \cap \mathrm{bd}(\mathcal{U})$.

A two-dimensional example is shown in figure 3.1. We argue that $\mathcal{J}$ is indeed a cell complex with $|\mathcal{J}| = \mathcal{U}$. The following elementary observation will be useful. Consider a subset $T \subseteq B$, $k+1 = |T| \leq d$, so that s_T is a $(d-k-1)$-sphere. Then $y \in \sigma_T$ iff y is the center of a d-ball c with $s_T \subseteq c \subseteq \mathcal{U}(T)$.

3.2 (i) $\bigcup_{j \in \mathcal{J}} j = \mathcal{U}$.
(ii) The cells in $\mathcal{J}$ have pairwise disjoint interiors.

Proof. First, we show that $\mathcal{U}$ is contained in the union of cells of $\mathcal{J}$. We argue that every point $y \in \mathcal{U}$ belongs to some cell $\sigma_T * f \in \mathcal{J}$. This is clear if $y \in |\mathcal{K}| = \mathcal{S}$. So assume $y \in \mathcal{U} - \mathcal{S}$ and let $c(y)$ be the largest d-ball with center y contained in $\mathcal{U}$. Note that $c(y) \cap \mathrm{bd}(\mathcal{U})$ is a unique point v. Let $T = \{b \in B \mid v \in s_b\}$. We claim that the line $l = \mathrm{aff}(\{v, y\})$ intersects σ_T in a unique point u. To see this move a point y' continuously on l starting at y away from v. Stop the motion when $c(y')$ contains s_T and not just a single point of it. At this moment $u = y' \in \sigma_T$, see figure 3.2. This implies that $y \in uv \subseteq \sigma_T * f \in \mathcal{J}$, where f is the component of $\dot{q}_T$ that contains v.

Second, we show that every two cells $\sigma_T * f$ and $\sigma_U * g$ in $\mathcal{J}$, with $f, g \neq \emptyset$, have disjoint interiors. To get a contradiction assume this is not true. Then there are two vertex disjoint edges, $u_1v_1 \in \sigma_T * f$ and $u_2v_2 \in \sigma_U * g$, with $u_1v_1 \cap u_2v_2 \neq \emptyset$. Consider v_1 and v_2, which are points on $\mathrm{bd}(\mathcal{U})$, and define the half-space $h_{ij} = \{x \in \mathbb{R}^d \mid |xv_i| \leq |xv_j|\}$. Notice that $0 = \pi_b(v_1) \leq \pi_b(v_2)$ for each $b \in T$, and $0 = \pi_b(v_2) \leq \pi_b(v_1)$ for each $b \in U$. This implies $\sigma_T \subseteq h_{12}$ and $\sigma_U \subseteq h_{21}$. Since $v_1 \in \mathrm{int}(h_{12})$ and $v_2 \in \mathrm{int}(h_{21})$, the two edges cannot intersect except possibly at the other endpoints. This contradicts the assumption that $u_1 \neq u_2$.

To finish the proof of (ii) we just need to verify that also the interiors of cells $\sigma_T * f \in \mathcal{J}$, $f \neq \emptyset$, and $\sigma_U \in \mathcal{J} \cap \mathcal{K}$ are disjoint. If this were not the case then $\sigma_T * f$ would contain an edge u_1v_1 that intersect a face σ_V of $\mathcal{S}$ at a point u strictly between u_1 and v_1. This is impossible since u is endpoint of some edge uv of at least one other join. By the argument above, u_1v_1 and uv cannot intersect except possibly at a common endpoint. This completes the proof of (ii). By the symmetric argument u_1v_1 cannot intersect $\mathrm{bd}(\mathcal{U})$ at a point strictly between u_1 and v_1. It follows that each cell of $\mathcal{J}$ is contained in $\mathcal{U}$, and therefore $\bigcup_{j \in \mathcal{J}} j = \mathcal{U}$. This completes the proof of (i). ∎

The deformation retraction. We construct a map $\Phi : \mathcal{U} \times [0,1] \to \mathcal{U}$ whose restriction to $\mathrm{int}(\mathcal{U})$ satisfies the requirements of a deformation retraction onto $\mathcal{S}$. We specify Φ for each individual cell of $\mathcal{J}$. Let σ be a simplex in $\mathcal{K}$ and f a face of $\mathcal{U}$ so that $\sigma * f \in \mathcal{J}$. If $f \neq \emptyset$ then for each point $y \in \sigma * f$ there are unique $u \in \sigma$, $v \in f$, and $\lambda \in [0,1]$ so that $y = \lambda u + (1-\lambda)v$. For each $t \in [0,1]$ we define $\Phi(y,t) = (\lambda - \lambda t + t)u + (1-\lambda)(1-t)v$. Intuitively, this means that uv is continuously shortened at v so that at time t its length is $(1-t)|uv|$, see figure 3.3. If $f = \emptyset$ we set $\Phi(y,t) = y$ for all $t \in [0,1]$. The map Φ restricted to $\mathrm{int}(\mathcal{U})$ is continuous because it is continuous within each cell, except possibly at points of $\mathrm{bd}(\mathcal{U})$. Clearly, Φ is the identity on $\mathrm{int}(\mathcal{U})$ for $t = 0$, its restriction to $\mathcal{S}$ is the identity for all $t \in [0,1]$, and $\Phi(\mathrm{int}(\mathcal{U}), 1) : \mathrm{int}(\mathcal{U}) \to \mathcal{S}$ is a retraction.

Remark. The construction of Φ can be modified to get a deformation retraction Φ' of $\mathbb{R}^d - \mathcal{S}$ onto $\mathbb{R}^d - \mathrm{int}(\mathcal{U})$. If $y \in \mathcal{U} - \mathcal{S}$ then $y = \lambda u + (1-\lambda)v$, and we define $\Phi'(y,t) = \lambda(1-t)u + (1-\lambda+\lambda t)v$. For $y \in \mathbb{R}^d - \mathrm{int}(\mathcal{U})$ we set $\Phi'(y,t) = y$ for all t.

Links and unions of caps. A relationship like the one between $\mathcal{U}$ and $\mathcal{S}$ can be shown between some of their substructures. Consider a subset $T \subseteq B$ so that $\sigma_T \in \mathcal{K}$. The *link* of σ_T in $\mathcal{K}$ is $\mathrm{lk}_{\mathcal{K}}(\sigma_T) = \{\sigma \in \mathcal{K} \mid \sigma_T * \sigma \in \mathcal{K}\}$. For example, the link of vertex x in figure 2.3(ii) is $\{\emptyset, a, b, c, d, bc, cd\}$, and the link of edge xc is $\{\emptyset, b, d\}$. Let $1 \leq k+1 = |T|$. Because $\sigma_T \in \mathcal{K}$, s_T is non-empty and thus a $(d-k-1)$-sphere in $\mathbb{R}^d$. Define $\mathcal{K}_T = \mathrm{lk}_{\mathcal{K}}(\sigma_T)$, $\mathcal{S}_T = |\mathcal{K}_T|$, and $\mathcal{U}_T = s_T \cap \mathcal{U}(B - T)$. By definition of link and by 2.2, the spheres $s_{T \cup U}$ in s_T that contain faces of $\mathrm{bd}(\mathcal{U}_T)$ correspond to simplices $\sigma_{T \cup U}$ that are faces of $\mathcal{S}$. Of course, such simplices exist only if σ_T is a face of $\mathcal{S}$.

Unlike $\mathcal{S}$, which is a subset of $\mathrm{int}(\mathcal{U})$, $\mathcal{S}_T$ is usually not contained in $\mathrm{int}(\mathcal{U}_T)$. However, it is possible to imbed $\mathcal{S}_T$ in $\mathrm{int}(\mathcal{U}_T)$. Let x be a point not contained in the k-flat $\mathrm{aff}(T)$. Hence, $\mathrm{aff}(T \cup \{x\})$ is a $(k+1)$-flat and $\mathrm{aff}(T)$ decomposes it into two halves. The half that contains x intersects s_T in a point $\psi_T(x)$. Intuitively, ψ_T projects x into s_T; the center of the projection is $\mathrm{aff}(T)$. The restriction of ψ_T to $|\mathrm{lk}_{\mathcal{R}}(\sigma_T)|$ is continuous and one-to-one. Hence, ψ_T imbeds $\mathcal{S}_T$ in s_T, and using an argument as in 3.1 we see that $\psi_T(\mathcal{S}_T) \subseteq \mathrm{int}(\mathcal{U}_T)$. Similarly, ψ_T imbeds the union of joins $\sigma' * f'$, where $\sigma' = \sigma_U \in \mathcal{K}_T$ and f' is a face of a component of $\dot{q}_{T \cup U}$. The imbedded joins define a complex $\mathcal{J}_T$ that decomposes $\mathcal{U}_T$, analogous to the complex $\mathcal{J}$ which decomposes $\mathcal{U}$. The composition $\psi_T \circ \Phi$ restricted to the joins mentioned above describes a deformation retraction of $\mathrm{int}(\mathcal{U}_T)$ onto $\psi(\mathcal{S}_T)$. If follows that $\mathcal{U}_T$ and $\mathcal{S}_T$ are homotopy equivalent. We summarize the above results.

Thm. 3.3 (i) $\mathcal{S}$ is homotopy equivalent to $\mathcal{U}$.
(ii) For each $T \subseteq B$ with $\sigma_T \in \mathcal{K}$, $\mathcal{S}_T$ is homotopy equivalent to $\mathcal{U}_T$.

Remark. Recall the Φ' is a deformation retraction of $\mathbb{R}^d - \mathcal{S}$ onto $\mathbb{R}^d - \mathrm{int}(\mathcal{U})$. The composition $\psi_T \circ \Phi'$

thus defines a deformation retraction of $s_T - \psi(\mathcal{S}_T)$ onto $s_T - \text{int}(\mathcal{U}_T)$. Intuitively, this means that also the complements of $\mathcal{U}_T$ and $\mathcal{S}_T$ are homotopy equivalent. This will be used in the next section.

Algorithmic implications. The significance of theorem 3.3(i) lies in its algorithmic consequences which concern the homology groups of $\mathcal{U}$. We refer to [23] for an introduction to homology groups of a topological space Y. For each integer k, the *k-th homology group*, $\text{H}_k = \text{H}_k(Y)$, is an abelian group that expresses the k-dimensional connectivity of Y. If the dimension of Y is d then the possibly non-trivial homology groups are H_0 through H_d. An important related numerical value is the *k-th betti number* of Y which is the rank of H_k.

There is a general algorithm for computing H_k, provided Y is given as a finite simplicial complex. Since $\mathcal{S} = |\mathcal{K}|$, this algorithm computes the homology groups of $\mathcal{S}$. An important result from algebraic topology says that two homotopy equivalent topological spaces have isomorphic homology groups. It follows that the algorithm just mentioned also computes the homology groups of $\mathcal{U}$.

Before we say more about this algorithm, let us briefly discuss the complement spaces, $\mathbb{R}^d - \mathcal{U}$ and $\mathbb{R}^d - \mathcal{S}$. We have seen that both spaces are homotopy equivalent and thus have isomorphic homology groups. However, since the underlying space of $\mathcal{R}$ is only a bounded subset of $\mathbb{R}^d$, we do not have a simplicial representation of $\mathbb{R}^d - \mathcal{S}$. This deficiency can be remedied as follows. Call a simplex $\sigma_T \in \mathcal{R}$ a *hull simplex* if $\sigma_T \subseteq \text{bd}(|\mathcal{R}|)$. Add a point ω as a new 0-simplex "at infinity" to $\mathcal{R}$, and for each hull simplex σ_T add $\sigma_{T\cup\{\omega\}}$ to $\mathcal{R}$. Now, $\mathcal{R}$ is a triangulation of $\mathbb{S}^d$ and no further distinction between hull and other simplices is necessary.

The general algorithm for computing homology groups of simplicial complexes is based on computing Smith normal forms of integer matrices, see e.g. [23]. Although no polynomial time bound for this algorithm is known, it is argued that it performs well in practice [10]. Furthermore, improvements of the original Smith normal form algorithm with polynomial behavior have been found, see e.g. [21]. A fast combinatorial algorithm that works for simplicial complexes imbedded in $\mathbb{S}^3$ is described in [8]. For large problem size, which could mean thousands of balls defining $\mathcal{U}$ or similar numbers of simplices constituting $\mathcal{K}$, only the algorithm in [8] performs satisfactorily. This leaves us with the open problem of finding faster algorithms for computing homology groups of cell complexes imbedded in dimensions higher than three.

4 Counting Faces

In this section we consider the algorithmic problem of counting the faces of $\mathcal{U}$. The assumption is that $\mathcal{K}$ is given as a subcomplex of $\mathcal{R}$, and we seek an algorithm that computes the number of ℓ-faces of $\mathcal{U}$, for each $0 \leq \ell \leq d-1$. This problem is related to determining the betti numbers of links in $\mathcal{K}$ because the faces of $\mathcal{U}$ are typically not simply connected. The basic strategy is to consider all ℓ-spheres s_T, $|T| = d - \ell$, with $\sigma_T \in \mathcal{K}$. For each such s_T we compute the number of ℓ-faces of $\mathcal{U}$ it contains, and we take the sum of these numbers. The result is n_ℓ, the number of ℓ-faces of $\mathcal{U}$.

Components of link complements. Recall the definition of $\mathcal{U}_T$: it is the part of s_T contained in d-balls of $B - T$. The complement of $\mathcal{U}_T$, $s_T - \mathcal{U}_T$, is the interior of the union of ℓ-faces contained in s_T. Since we assume general position of the d-balls, the connectivity of the interior is the same as that of its closure. Hence, each component of $s_T - \mathcal{U}_T$ is the interior of an ℓ-face and is to be counted. For each $\sigma_T \in \mathcal{K}$, define $\bar{\mathcal{K}}_T = \text{lk}_{\mathcal{R}}(\sigma_T) - \text{lk}_{\mathcal{K}}(\sigma_T)$, where we assume that $\mathcal{R}$ is extended to a triangulation of $\mathbb{S}^d$ as described at the end of section 3. By the remark after theorem 3.3, the number of components of $s_T - \mathcal{U}_T$ is the same as that of $\bar{\mathcal{K}}_T$. For each $\sigma_T \in \mathcal{K}$ let n_T be the number of components of $\bar{\mathcal{K}}_T$. Then we have the following result.

4.1 For each $0 \leq \ell \leq d-1$, $n_\ell = \sum_{\sigma_T \in \mathcal{K}, |T| = d-\ell} n_T$.

Remark. If $\sigma_T \in \mathcal{K}$ is not a face of $\mathcal{S}$ then $\text{lk}_{\mathcal{K}}(\sigma_T) = \text{lk}_{\mathcal{R}}(\sigma_T)$ is a complete triangulation of $\mathbb{S}^\ell$. Hence, $n_T = 0$ which implies that the equation in 4.1 remains valid if the sum extends only over the simplices of $\mathcal{K}$ that are faces of $\mathcal{S}$.

The algorithm. We assume the following graph representation of $\mathcal{R}$ and $\mathcal{K}$. Algorithms for constructing $\mathcal{R}$ and $\mathcal{K}$ can be found in [12, 17]. The nodes of the graph $\mathcal{R}^*$ are the d-simplices of $\mathcal{R}$, and the arcs of $\mathcal{R}^*$ are the $(d-1)$-simplices of $\mathcal{R}$; this includes the d- and $(d-1)$-simplices incident to ω. Each node or arc is labeled whether or not it belongs to $\mathcal{K}$. The subgraph that consists of the nodes and arcs in $\mathcal{R} - \mathcal{K}$ is denoted $\bar{\mathcal{K}}^*$. Since $\mathcal{K}$ is a proper complex, $\bar{\mathcal{K}}^*$ is a proper graph. Given an arc of $\mathcal{R}^*$, we have access to the two incident nodes in constant time. Similarly, given a node we have access to the incident arcs in constant time. This is a reasonable assumption if d, which is the number of dimensions as well as one less than the node degree, is considered a constant. Furthermore, we assume that given a simplex $\sigma \in \mathcal{R}$ of dimension less than d, we can find an incident node in $\mathcal{R}^*$ in constant time. Starting at this node, all other nodes incident to σ can be enumerated in constant time per node.

The algorithm relies on the fact that the number of components of $\bar{\mathcal{K}}_T$ is also the number of components of the subgraph of $\bar{\mathcal{K}}^*$ induced by the d-simplices $\sigma_U \in \mathcal{R} - \mathcal{K}$ with $T \subseteq U$. Denote this induced subgraph by $\bar{\mathcal{K}}_T^*$. This is because $\sigma_V \in \bar{\mathcal{K}}_T$ iff $\sigma_{T \cup V} \in \mathcal{R} - \mathcal{K}$. In particular, σ_V is an ℓ- or $(\ell-1)$-simplex of $\bar{\mathcal{K}}_T$ iff $\sigma_{T \cup V}$ is a d- or $(d-1)$-simplex of $\mathcal{R} - \mathcal{K}$. The faces of $\mathcal{U}$ can thus be counted by finding components of various induced subgraphs of $\bar{\mathcal{K}}^*$. A more detailed formulation of the algorithm that computes n_ℓ follows. Initially, all nodes of $\mathcal{R}^*$ are unmarked.

```
nℓ := 0;
for each (d − ℓ − 1)-simplex σT ∈ K do
    for each node σU ∈ R* incident to σT do
        if σU is not marked and σU ∉ K then
          mark σU; nℓ := nℓ + 1;
          start a graph search to mark all nodes
                σU' that belong to the same
                component of K̄*T as σU
        endif
    endfor;
    unmark all marked nodes
endfor.
```

As remarked earlier, it is actually sufficient to run the outer for-loop only over all faces of $\mathcal{S}$. In any case, each simplex of $\mathcal{R}$ is touched only a constant number of times, so the entire algorithm runs in time at most proportional to the number of simplices in $\mathcal{R}$. Indeed, also the step that employs graph searching takes only constant time per node it marks, see e.g. [6, chapter VI,23]. We summarize the results of this section.

Thm. 4.2 Given a suitable representation of $\mathcal{K}$ as a subcomplex of $\mathcal{R}$, for $0 \leq \ell \leq d-1$, the number of ℓ-faces of $\mathcal{U}$ can be computed in time proportional to the number of simplices in $\mathcal{R}$.

Remark. Instead of graph searching one can also use union-find data structures, one per $\sigma_T \in \mathcal{R}$, which maintain the components in $\bar{\mathcal{K}}_T^*$. See e.g. [6, chapter V,22] for a description of such data structures. This approach has the advantage that $\mathcal{R} - \mathcal{K}$ can be specified one simplex at a time. The number of ℓ-faces can be updated in time $\alpha(n)$ per simplex, where n is the size of B and α is the inverse of the Ackermann function. In cases where one considers all unions $\mathcal{U}$ obtained by continuously and simultaneously shrinking the d-balls in B, see [12], this allows us to compute the numbers n_ℓ in time $\alpha(n)$ per combinatorially different $\mathcal{U}$.

5 Variations of Euler's Relation

This section derives variations of the Euler relation for convex polyhedra in $\mathbb{R}^d$. For each point $x \in \mathbb{R}^d$ we specify an alternating sum for the faces of a polyhedron visible from x. This sum will be 1 inside the polyhedron and 0 outside. These sums will be used in section 6 to derive short formulas for measuring a polyhedron or its intersection with another body.

Inclusion-exclusion for convex polyhedra. Let H be a finite set of closed half-spaces in $\mathbb{R}^d$ that defines a non-empty convex polyhedron $P = \bigcap_{h \in H} h$. For simplicity we assume general position of the half-spaces. For every $x \in \mathbb{R}^d$ and every $I \in 2^H$ define the characteristic function

$$\gamma_I(x) = \begin{cases} 1 & \text{if } x \notin h \text{ for all } h \in I, \text{ and} \\ 0 & \text{otherwise.} \end{cases}$$

For $L \subseteq 2^H$ define $\Gamma_L(x) = \sum_{I \in L} (-1)^{|I|} \gamma_I(x)$. The general inclusion-exclusion principle implies that

$$\Gamma_{2^H}(x) = \begin{cases} 1 & \text{if } x \in P, \text{ and} \\ 0 & \text{if } x \notin P. \end{cases}$$

A direct proof can easily be given. Define $G = \{h \in H \mid x \notin h\}$. Clearly, $\Gamma_{2^H}(x) = \Gamma_{2^G}(x)$. If $x \in P$ then $G = \emptyset$ and $\Gamma_{2^G}(x) = \gamma_\emptyset(x) = 1$. If $x \notin P$ then $G \neq \emptyset$ and $\Gamma_{2^G}(x) = \sum_{I \in 2^G} (-1)^{|I|} = (1-1)^{|G|} = 0$.

It should be clear that redundant half-spaces can be eliminated, that is, if $P = \bigcap_{h \in G} h$, for some $G \subseteq H$, then $\Gamma_{2^H}(x) = \Gamma_{2^G}(x)$. We claim that a more dramatic reduction of the set 2^H is possible. For $I \in 2^H$ define $f_I = P \cap \bigcap_{h \in I} \mathrm{bd}(h)$. If $f_I \neq \emptyset$ then it is a unique face of P. This includes the case $I = \emptyset$ where $f_I = f_\emptyset = P$. Define $R = R(H) = \{I \in 2^H \mid f_I \neq \emptyset\}$. Observe that R is an abstract simplicial complex, and because of general position any $I \in R$ has cardinality at most d. Figure 5.1 illustrates the following result.

5.1 $\Gamma_R(x) = \begin{cases} 1 & \text{if } x \in P, \text{ and} \\ 0 & \text{if } x \notin P. \end{cases}$

Proof. We use induction over the size of $G = \{h \in H \mid x \notin h\}$. G is empty iff $x \in P$, and indeed we have $\Gamma_R(x) = \gamma_\emptyset(x) = 1$ in this case. So assume $x \notin P$. There is at least one half-space $g \in G$; let $\bar{g}$ be the other half-space bounded by the same hyperplane. Define $H' = H - \{g\}$ and $H'' = H' \cup \{\bar{g}\}$. By induction hypothesis the assertion applies to $P' = \bigcap_{h \in H'} h$ and to $P'' = \bigcap_{h \in H''} h$, see figure 5.2. Define $R' = R(H')$ and $R'' = R(H'')$. We express R, R', and R'' as disjoint unions of smaller sets. By definition, this translates to addition for Γ. For a fixed point $x \notin P$ we have

$$\Gamma_{R'} = \Gamma_{L'} + \Gamma_{X'} + \Gamma_{U'},$$

where $L' = \{I \in R' \mid f_I \subseteq g\}$, $X' = \{I \in R' \mid f_I \cap g \neq \emptyset \text{ and } f_I \cap \bar{g} \neq \emptyset\}$, and $U' = \{I \in R' \mid f_I \subseteq \bar{g}\}$. Similarly,

$$\Gamma_R = \Gamma_{L'} + \Gamma_{X'} + \Gamma_X,$$

where $X = \{I \cup \{g\} \mid I \in X'\}$. Indeed, X' represents all faces of P' that intersect the hyperplane bounding g, and at the same time it represents all faces of P and of P'' that touch this hyperplane. Finally,

$$\Gamma_{R''} = \Gamma_{X'} + \Gamma_{X''} + \Gamma_{U'},$$

where $X'' = \{I \cup \{\bar{g}\} \mid I \in X'\}$. Now we express Γ_R in terms of the other sets:

$$\begin{aligned} \Gamma_R &= \Gamma_{R'} - \Gamma_{U'} + \Gamma_X \\ &= \Gamma_{R'} - \Gamma_{R''} + \Gamma_{X''} + \Gamma_{X'} + \Gamma_X. \end{aligned}$$

We have $x \in P'$ iff $x \in P''$ and therefore $\Gamma_{R'} - \Gamma_{R''} = 0$ by induction hypothesis. Furthermore, $\Gamma_{X''} = 0$ because $x \in \bar{g}$ and each $I \in X''$ contains $\bar{g}$. Finally, $\Gamma_{X'} + \Gamma_X = 0$ because $\gamma_I = \gamma_{I \cup \{g\}}$ and therefore $(-1)^{|I|}\gamma_I + (-1)^{|I|+1}\gamma_{I\cup\{g\}} = 0$ for each $I \in X'$. Therefore $\Gamma_R = 0$ as required. □

Remarks. (1) The following modifications generalize 5.1 and its proof to cover degenerate positions of the half-spaces. First, R is defined so it contains only maximal sets defining faces of P: $R = \{I \in 2^H \mid f_I \neq \emptyset \text{ and } f_I \neq f_J \text{ if } I \subset J\}$. Second, the signs in Γ_R alternate with the codimensions of the faces: $\Gamma_R(x) = \sum_{I \in R} (-1)^{\mathrm{codim}(f_I)} \gamma_I(x)$, where $\mathrm{codim}(f_I) = d - \dim(f_I)$. Third, in the proof we have three additional sets,

$$\begin{aligned} C' &= \{I \in R' \mid f_I \subseteq \mathrm{bd}(g)\}, \\ C &= \{I \cup \{g\} \mid I \in C'\}, \text{ and} \\ C'' &= \{I \cup \{\bar{g}\} \mid I \in C'\}, \end{aligned}$$

which are subsets of R', R, and R'' disjoint from L', U', X', X, X''. In the final expression for Γ_R we get $\Gamma_{C''} - \Gamma_{C'} + \Gamma_C$ as an additional term. It vanishes just as $\Gamma_{X''} + \Gamma_{X'} + \Gamma_X$ does.

(2) Relation 5.1 implies the Euler relation for unbounded convex polyhedra, see e.g. [4, 11, 20]. To see this take x outside all half-spaces. Conversely, another proof of 5.1 can be obtained from the common proof of Euler's relation using the shellability of P [4]: take a line through x that intersects $\mathrm{int}(P)$ and stop the implied line-shelling at x.

Intersection with a convex body. We generalize 5.1 so it makes a statement about points x of a compact convex set A. Define $K = K(A, H) \subseteq R(H)$ so that $I \in K$ iff $f_I \cap \mathrm{int}(A) \neq \emptyset$.

5.2 $$\Gamma_K(x) = \begin{cases} 1 & \text{if } x \in A \cap P, \text{ and} \\ 0 & \text{if } x \in A - P. \end{cases}$$

Proof. We choose a suitable polyhedral approximation of A. Let H_A be a finite collection of closed half-spaces so that $A \subseteq P_A = \bigcap_{h \in H_A} h$ and $K(A,H) = K(P_A, H)$. Such a finite set H_A can be constructed during the following iteration. Find a face f_J disjoint from $\mathrm{int}(A)$ with $f_J \cap \mathrm{int}(H_A) \neq \emptyset$. By convexity of f_J and A there is a separating hyperplane. Add the half-space bounded by this hyperplane that contains A to H_A. The process is finite because P has only finitely many faces.

Define $R_\cap = R(H \cup H_A)$ and use 5.1 to get

$$\Gamma_{R_\cap}(x) = \begin{cases} 1 & \text{if } x \in P_A \cap P, \text{ and} \\ 0 & \text{if } x \notin P_A \cap P. \end{cases}$$

Note that $R_\cap = K \dot{\cup} L$, where $K = K(P_A, H)$ and $L = \{I \in R_\cap \mid I \cap H_A \neq \emptyset\}$. For all $x \in P_A$ and each $I \in L$ we have $\gamma_I(x) = 0$. Hence,

$$\Gamma_K(x) = \Gamma_{R_\cap}(x) - \Gamma_L(x) = \Gamma_{R_\cap}(x)$$

for all $x \in P_A$. The assertion follows because $A \cap P \subseteq P_A \cap P$ and $A - P \subseteq P_A - P$. □

Remark. Relation 5.2 also applies to compact non-convex sets A if the collection of faces considered is determined by the convex hull of A, that is, $K = K(\mathrm{conv}(A), H)$. For example, it applies to the boundary of a compact convex set, and the intersection of this boundary with the boundary of P, etc.

6 Measuring the Union of Balls

This section and the one after the next simplify, improve, and generalize earlier work on algorithms for measuring the union of balls [2, 3]. Based on the correspondences between the various diagrams introduced in section 2, this section derives short inclusion-exclusion formulas for the d-dimensional Lebesgue measure of $\mathcal{U}$ and the total ℓ-dimensional Lebesgue measure of its ℓ-dimensional faces. We begin by studying inclusion-exclusion formulas for convex polyhedra.

Measuring by integration. We measure $A \cap P$ using 5.2. Consider a compact convex set $A \subseteq \mathbb{R}^d$. The d-dimensional measure of $A \cap P$, $\mu_d(A \cap P)$, is the integral of $\Gamma_K(x)$ over all points $x \in A$, where $K = K(A, H)$. We get

$$\begin{aligned} \mu_d(A \cap P) &= \int_{x \in A} \Gamma_K(x) dx \\ &= \int_{x \in A} \sum_{I \in K} (-1)^{|I|} \gamma_I(x) dx \\ &= \sum_{I \in K} (-1)^{|I|} \int_{x \in A} \gamma_I(x) dx. \end{aligned}$$

The integral of $\gamma_I(x)$ over all $x \in A$ is the d-dimensional measure of $A \cap Q_I$, where $Q_I = \bigcap_{h \in I} \bar{h}$.

The same calculation can be done for lower-dimensional sets. We are interested in the sets $\dot{A} \cap$

$P^{(\ell+1)}$, where $\dot{A} = \mathrm{bd}(A)$ and $P^{(\ell+1)}$ is the union of all $(\ell+1)$-dimensional faces of P. Assuming general position these sets are ℓ-dimensional. We state the results.

6.1 (i) $\mu_d(A \cap P) = \sum_{I \in K} (-1)^{|I|} \mu_d(A \cap Q_I)$.
(ii) For $0 \le \ell \le d-1$,
$\mu_\ell(\dot{A} \cap P^{(\ell+1)}) = \sum_{I \in K} (-1)^{|I|} \mu_\ell(\dot{A} \cap Q_I^{(\ell+1)})$.

Remarks. (1) The lowest dimension of any face of Q_I is $d - |I|$. This implies that in 6.1(ii) all terms for sets I with $|I| \le d - \ell - 2$ vanish and can as well be omitted.

(2) The relations in 6.1 are based on the assumption of a uniform density distribution. All results hold without change for any other reasonable density funtion. To see this redefine $\gamma_I(x)$ equal to the density at x, provided $x \notin h$ for all $h \in I$. Otherwise, $\gamma_I(x) = 0$ as before.

(3) Consider a simple special case of 6.1(ii): P is a triangular cone with apex y in $\mathbb{R}^3$, and A is a 3-ball with unit surface area centered at y. By 6.1(ii) the size, μ_2, of the spherical triangle $\dot{A} \cap P$ is $1 - \frac{3}{2} + (\alpha + \beta + \gamma) - \mu_2$, where α, β, γ are the three dihedral angles of P normalized between 0 and 1. This implies the famous formula

$$\mu_2 = \frac{\alpha + \beta + \gamma}{2} - \frac{1}{4}$$

for spherical triangles. In a similar vein it is possible to derive Gram's formulas for convex polyhedra, see e.g. [19].

Inclusion-exclusion with intersections of balls. We write $\mu_d = \mu_d(\mathcal{U})$ for the d-dimensional Lebesgue measure of $\mathcal{U} = \bigcup_{b \in B} b$, and $\mu_\ell = \mu_\ell(\mathcal{U})$ for the total ℓ-dimensional Lebesgue measure of all ℓ-faces of $\mathcal{U}$, for $0 \le \ell \le d-1$. In particular, μ_{d-1} is the size of $\mathrm{bd}(\mathcal{U})$, and μ_0 is the number of vertices of $\mathcal{U}$. We derive formulas that express μ_ℓ in terms of ℓ-dimensional measures of intersections of at most $d+1$ balls from B. These formulas improve similar formulas in [24] in two ways. First, they apply to balls of different sizes, and second, they are shorter because they take K as the index set rather than R.

Call $T \subseteq B$ *independent* if the balls of each subset of T intersect in a unique region with non-empty interior. For example, if σ_T is a simplex in $\mathcal{K}$ then T is independent. Define $b_T = \bigcap_{b \in T} b$. If T is independent then $b_T \ne \emptyset$ and its face structure is dual to that of σ_T, see figure 6.1. We write $\mu_\ell(b_T)$ for the total ℓ-dimensional measure of all ℓ-faces of b_T. Clearly, the lowest dimension of any face of b_T is $d - |T|$, so $\mu_\ell(b_T) = 0$ if $\ell \le d - |T| - 1$. We are ready to state the first set of inclusion-exclusion formulas for $\mathcal{U}$.

Thm. 6.2 (i) $\mu_d(\mathcal{U}) = \sum_{\emptyset \ne \sigma_T \in \mathcal{K}} (-1)^{|T|-1} \mu_d(b_T)$.
(ii) For $0 \le \ell \le d-1$,
$\mu_\ell(\mathcal{U}) = \sum_{\sigma_T \in \mathcal{K}} (-1)^{|T|-d+\ell} \mu_\ell(b_T)$.

Remark. The sets T of size $|T| \le d - \ell - 1$ can be omitted from the sums in theorem 6.2(ii) because their contribution to μ_ℓ is zero anyway. Note that the thus simplified formula for $\ell = 0$ counts 2 for each $(d-1)$-simplex $\sigma_T \in \mathcal{K}$ and then subtracts the number of incident d-simplices that are in $\mathcal{K}$. The result is the same as derived in 4.1.

Proof. We present the detailed argument for (i) using an imbedding of $\mathbb{R}^d$ as a hyperplane Π in $\mathbb{R}^{d+1}$. Let z be a point in $\mathbb{R}^{d+1} - \Pi$ and consider the inversion transform with center z. It maps every point $x \ne z$ to a point x° so that x and x° lie on the same half-line with endpoint z and $|zx^\circ| = \frac{1}{|zx|}$. The image of Π under inversion is a d-sphere Π° that contains z. Furthermore, each d-ball b in Π maps to a spherical cap b° on Π°, see figure 6.2. Let h_b be the halfspace in $\mathbb{R}^{d+1}$ so that $b^\circ = \Pi^\circ \cap \bar{h}_b$.

With an eye on 6.1 we define $A = \mathrm{conv}(\Pi^\circ)$, $\dot{A} = \Pi^\circ$, $H = \{h_b | b \in B\}$, and $P = \bigcap_{b \in B} h_b$. By inversion, $\dot{A} - P$ maps to $\mathrm{int}(\mathcal{U})$. Note that for points on Π°, inversion is the same as stereographic projection into Π centrally from z. The same projection maps the boundary complex of P to the power diagram $\mathcal{P} = \mathcal{P}(B)$. In particular, a face f_I of P maps to $p_T \in \mathcal{P}$ so that $h_b \in I$ iff $b \in T$. Furthermore, $f_I \cap \mathrm{int}(A) \ne \emptyset$ iff $p_T \cap \mathrm{int}(\mathcal{U}) \ne \emptyset$. By assumption of general position the same is true if we replace $\mathrm{int}(A)$ by A and $\mathrm{int}(\mathcal{U})$ by $\mathcal{U}$. Hence, $I \in K(A,H)$ iff $\sigma_T \in \mathcal{K} = \mathcal{K}(B)$.

We derive a formula for the d-dimensional measure of $\dot{A} - P$ using 6.1(ii). For the intersection, $\dot{A} \cap P$, we get

$$\mu_d(\dot{A} \cap P) = \sum_{I \in K(A,H)} (-1)^{|I|} \mu_d(\dot{A} \cap Q_I),$$

where $Q_I = \bigcap_{h \in I} \bar{h}$, as usual. For $\dot{A} - P$ we therefore get

$$\begin{aligned} \mu_d(\dot{A} - P) &= \mu_d(\dot{A}) - \mu_d(\dot{A} \cap P) \\ &= \sum_{\emptyset \ne I \in K(A,H)} (-1)^{|I|-1} \mu_d(\dot{A} \cap Q_I). \end{aligned}$$

To get (i) note that for each $I \in K(A,H)$ the set $\dot{A} \cap Q_I$ is the image under inversion of the corresponding intersection of balls, b_T with $\sigma_T \in \mathcal{K}$. Finally, to get the d-dimensional measure of $\mathcal{U}$ we put a density function on $\dot{A}$ whose image under inversion is the uniform density in Π.

The relations in (ii) are obtained by similar arguments using 6.1(ii) for values of ℓ less than d. The main difference to the above proof for $\ell = d$ is that for $\ell < d$ we compute $\dot{A} \cap P^{(\ell+1)}$ directly, without considering any complement. This explains the inconsistency between the formulas in (i) and (ii). $\square$

7 Lemmas on Simplices

This section proves several elementary results on simplices, which will be used in section 8 where another set of formulas for the measure of $\mathcal{U}$ is derived. The main result is 7.3 which expresses the common intersection of $d+1$ d-balls in terms of the simplex spanned by their centers and common intersections of d or fewer of the d-balls.

Inclusion-exclusion for simplices. Let H be a set of $d+1$ closed half-spaces in $\mathbb{R}^d$ defining a d-simplex $P = \bigcap_{h \in H} h$. Each proper subset $I \subseteq H$ defines a proper face, f_I, of P. Except for the vanishing term $\gamma_H(x)$, 5.1 coincides with the trivial inclusion-exclusion formula,

$$\Gamma_{2^H}(x) = \begin{cases} 1 & \text{if } x \in P, \text{ and} \\ 0 & \text{if } x \notin P. \end{cases}$$

Let R_I contain all index sets in 2^H that contain I. Clearly, $R_I = \{J \cup I \mid J \in 2^{H-I}\}$. Recall that $Q_I = \bigcap_{h \in I} \bar{h}$ and define $P_I = Q_I \cap \bigcap_{h \in H-I} h$, see figure 7.1. We are interested in $\Gamma_{R_I}(x)$ for points $x \in Q_I$. Because Γ_{R_I} coincides with $\Gamma_{2^{H-I}}$ for such points we get the following result.

7.1 $\Gamma_{R_I}(x) = \begin{cases} 1 & \text{if } x \in P_I, \text{ and} \\ 0 & \text{if } x \in Q_I - P_I. \end{cases}$

Intuitively, this means that with respect to inclusion-exclusion P_I behaves in Q_I the same way as P behaves in $\mathbb{R}^d$.

Independent sets of balls. In order to make proper use of 7.1 we need a topological lemma about a set T of $d+1$ d-balls in $\mathbb{R}^d$. For each subset of T consider the region of points contained in the balls of this subset and not contained in any other ball. Recall that T is independent if the balls of each subset intersect in unique region with non-empty interior. In particular, $b_T = \bigcap_{b \in T} b \neq \emptyset$. Since $d+1$ $(d-1)$-spheres decompose $\mathbb{R}^d$ into at most 2^{d+1} d-dimensional components, this implies that each component is connected. Notice that T is independent iff $\mathcal{K}(T)$ consists of σ_T and all its faces.

Write $P = \sigma_T$ and let H be the set of $d+1$ half-spaces so that $P = \bigcap_{h \in H} h$, as before. Each hyperplane $\text{bd}(h)$, $h \in H$, contains the centers of d d-balls in T. For each $I \subseteq H$ let $V = V_I \subseteq T$ contain the d-balls whose centers lie in all hyperplanes bounding half-spaces in I. Define $\bar{V} = \bar{V}_I = T - V$ and note that $|I| = |\bar{V}|$. For a choice of I we are interested in P_I, see figure 7.1. In particular, we claim that within P_I the intersection of the d-balls in $\bar{V}$ is contained in the union of the d-balls in V. To help the discussion we call P_I the *focus* of $\bar{V}$ in T. For example, P is the focus of $\emptyset$ in T, and $\emptyset$ is the focus of T in T. See figure 7.2 for an illustration. The discs around a and b at the right intersect their focus outside the disk around c, but the intersection of the two disks does not. The claim is now formally stated and proved.

7.2 For each $I \subseteq H$, we have $b_{\bar{V}_I} \cap P_I \subseteq \mathcal{U}(V_I)$.

Proof. Note that the assertion holds in $\mathbb{R}^1$, where we have two intersecting 1-balls (intervals) that do not nest. They define a 1-simplex connecting the midpoints of the 1-balls. Assume the assertion inductively for dimensions less than d. Take a subset $I \subseteq H$ and consider the focus, P_I, of $\bar{V} = \bar{V}_I$ in T. If $I \neq H, \emptyset$ then P_I is a proper convex polyhedron which shares the face σ_V with P. By 3.1, this face is contained in $\mathcal{U}(V)$. All other proper faces of P_I are lower-dimensional foci, namely foci of $\bar{U}$ in $\bar{U} \cup U$, where $\bar{U} \subseteq \bar{V}$, $U \subseteq V$, and $\bar{U} \cup U \subset T$. For each choice of $\bar{U}$ and U the assertion holds by induction hypothesis. It follows that $b_{\bar{V}} \cap \text{bd}(P_I) \subseteq \mathcal{U}(V)$.

To get a contradiction, assume the intersection of $b_{\bar{V}}$ with the focus of $\bar{V}$ in T is not contained in $\mathcal{U}(V)$. Choose a point $x \in b_{\bar{V}} \cap P_I$ that is not contained in $\mathcal{U}(V)$. Note that $b_{\bar{V}}$ is symmetric with respect to $a_{\bar{V}} = \text{aff}(\sigma_{\bar{V}})$. Let y be the reflection of x with respect to $a_{\bar{V}}$ and observe that $y \in b_{\bar{V}}$. Similarly, $\mathcal{U}(V)$ is symmetric with respect to $a_V = \text{aff}(\sigma_V)$. By construction, $a_{\bar{V}} \cap P_I = \emptyset$, and thus $y \notin P_I$, by convexity of P_I. Since y is further away from all $b \in V$ than x, we also have $y \notin \mathcal{U}(V)$. Note that x and y belong to the region of the same subset of T, namely $\bar{V}$. Furthermore, $x \in P_I$, $y \notin P_I$, and the region does not intersect $\text{bd}(P_I)$. This implies that the region is diconnected, which contradicts the independence of T. $\square$

Measuring simplices and balls. Using 7.1 and 7.2 we derive a relation for the measure of b_T. We still suppose that T is independent. Hence, $\sigma_T \in \mathcal{K}(T)$, and by 3.1, $\sigma_T \subseteq \mathcal{U}(T)$. For each face σ_U, $U \subseteq T$, let $\varphi_{U,T}$ be the angle at σ_U inside σ_T. We normalize angles between 0 and 1 so that all angles can be visualized as follows. Take a point $x \in \text{int}(\sigma_U)$ and a sufficiently small $(d-1)$-sphere s with center x. Then $\varphi_{U,T}$ is the fraction of s inside σ_T, that is,

$$\varphi_{U,T} = \frac{\mu_{d-1}(s \cap \sigma_T)}{\mu_{d-1}(s)}.$$

For example, $\varphi_{T,T} = 1$, and $\varphi_{U,T} = \frac{1}{2}$ if $|U| = d$. It will be convenient to set $\varphi_{\emptyset,T} = 0$. In $\mathbb{R}^3$, an angle at a vertex is usually referred to as a solid angle, and an angle at an edge as a dihedral angle.

7.3 (i) $\sum_{U \subseteq T} (-1)^{|U|-1} \varphi_{U,T} \cdot \mu_d(b_U) = \mu_d(\sigma_T)$.
(ii) For $0 \leq \ell \leq d-1$,
$\sum_{U \subseteq T} (-1)^{|U|-1} \varphi_{U,T} \cdot \mu_\ell(b_U) = 0$.

Proof. We present the proof of (i) in detail. Recall that $\sigma_T = \bigcap_{h \in H} h$, and that every subset $I \subseteq H$ defines a face $f_I = \sigma_V$, with $V = V_I \subseteq T$. We use 6.1(i) with $P = \sigma_T$ and $A = \mathcal{U}(T)$ and get

$$\mu_d(P) = \mu_d(A \cap P) = \sum_{I \subseteq H} (-1)^{|I|} \mu_d(A \cap Q_I),$$

where $A \cap Q_I$ is the closure of A outside all half-spaces $h \in I$, as before. We first assume the favorable case where $A \cap Q_I = \mathcal{U}(V) \cap Q_I$ for all $I \subseteq H$, see figure 7.2. This case is favorable because all hyperplanes $\mathrm{bd}(h)$, $h \in I$, contain the centers of all $b \in V$ and thus cut these d-balls into equal halves. We use the fact that the angle at σ_V inside P is that same as the opposite angle inside Q_I and get

$$\begin{aligned} \mu_d(A \cap Q_I) &= \mu_d(\mathcal{U}(V) \cap Q_I) \\ &= \varphi_{V,T} \cdot \mu_d(\mathcal{U}(V)) \\ &= \varphi_{V,T} \cdot \sum_{\emptyset \neq U \subseteq V} (-1)^{|U|-1} \mu_d(b_U). \end{aligned}$$

The last line is obtained by straightforward application of the inclusion-exclusion principle. Now we plug the last relation into the earlier one for $\mu_d(P)$ and get

$$\begin{aligned} \mu_d(P) &= \sum_{I \subseteq H} \left((-1)^{|I|} \varphi_{V,T} \sum_{\emptyset \neq U \subseteq V} (-1)^{|U|-1} \mu_d(b_U) \right) \\ &= \sum_{V \subseteq T} \left(\varphi_{V,T} \cdot \sum_{\emptyset \neq U \subseteq V} (-1)^{d-|V|+|U|} \mu_d(b_U) \right) \\ &= \sum_{\emptyset \neq U \subseteq T} \left(\mu_d(b_U) \sum_{V \supseteq U} (-1)^{d-|V|+|U|} \varphi_{V,T} \right) \\ &= \sum_{U \subseteq T} (-1)^{|U|-1} \varphi_{U,T} \cdot \mu_d(b_U). \end{aligned}$$

The last line is obtained by observing that

$$\sum_{V \supseteq U} (-1)^{d-|V|+1} \varphi_{V,T} = \varphi_{U,T}$$

for all $U \subseteq T$, see remark (3) after 6.1. This proves (i) in the favorable case.

With 7.1 and 7.2 we can reduce the unfavorable case to the favorable one. Consider a subset $I \subseteq H$ and $V = V_I$. In the unfavorable case we have $A \cap Q_I \neq \mathcal{U}(V) \cap Q_I$. By 7.2, $b_{\bar{V}}$ intersects P_I at most inside $\mathcal{U}(V)$. By 7.1, within $Q_I - P_I$ all points of $b_{\bar{V}}$ outside $\mathcal{U}(V)$ can be ignored without penalty. After doing this for all $I \subseteq H$ we arrive at the favorable case.

The proof for (ii) is essentially the same using 6.1(ii) instead of 6.1(i). For $\ell \leq d-1$ the right side vanishes because σ_T does not intersect $A = \mathrm{bd}(\mathcal{U}(T))$. □

8 Decomposable Formulas

From theorem 6.2 we derive a second set of inclusion-exclusion formulas for $\mathcal{U}$. In contrast to 6.2, the new formulas have terms that express the contribution of individual simplices of $\mathcal{R}$. This is useful in situations where only a part of $\mathcal{U}$ or its complement is to be measured. Another advantage of the second set of formulas is that its terms correspond to intersections of at most d d-balls, rather than $d+1$ as in 6.2.

Inclusion-exclusion with angle weights. We first make 6.2 more complicated, and then replace or eliminate large parts using 7.3. It will be convenient to cover the part of $\mathcal{U}$ outside $|\mathcal{R}|$ with simplices. This can be done by enlarging B with $d+1$ points (degenerate d-balls) whose convex hull contains $\mathcal{U}$. Consider 6.2(i) and decompose b_T into the parts defined by the d-simplices incident to σ_T. That is, use

$$\mu_d(b_T) = \sum \varphi_{T,S} \cdot \mu_d(b_T),$$

where the sum is taken over all $S \supseteq T$, $|S| = d+1$, so that $\sigma_S \in \mathcal{R}$. We need some notation. For subsets $\mathcal{L}$ and $\mathcal{L}'$ of a simplicial complex in $\mathbb{R}^d$ let $\mathcal{L}^{[d]}$ denote the collection of d-simplices $\sigma_S \in \mathcal{L}$, and let $[\mathcal{L}', \mathcal{L}]$ denote the collection of pairs (σ_T, σ_S) so that $\sigma_T \in \mathcal{L}'$ is a face of $\sigma_S \in \mathcal{L}^{[d]}$. With this notation, theorem 6.2(i) becomes

$$\mu_d(\mathcal{U}) = \sum_{(\sigma_T, \sigma_S) \in [\mathcal{K}, \mathcal{R}]} (-1)^{|T|-1} \varphi_{T,S} \cdot \mu_d(b_T).$$

Now we make a substitution using 7.3(i) whenever $\sigma_S \in \mathcal{K}$, and get the final result stated as theorem 8.1(i). The same derivation works also for $\mu_\ell(\mathcal{U})$, $0 \leq \ell \leq d-1$. In this case, the substitution uses 7.3(ii) and is, in fact, an elimination. We state the resulting second set of formulas for $\mathcal{U}$ and note that the remark after theorem 6.2 also applies to theorem 8.1.

Thm. 8.1 (i) $\mu_d(\mathcal{U}) = \sum_{\sigma_S \in \mathcal{K}^{[d]}} \mu_d(\sigma_S)$
$+ \sum_{(\sigma_T, \sigma_S) \in [\mathcal{K}, \mathcal{R}-\mathcal{K}]} (-1)^{|T|-1} \varphi_{T,S} \cdot \mu_d(b_T)$.
(ii) For $0 \leq \ell \leq d-1$,
$\mu_\ell(\mathcal{U}) = \sum_{(\sigma_T, \sigma_S) \in [\mathcal{K}, \mathcal{R}-\mathcal{K}]} (-1)^{|T|-d+\ell} \varphi_{T,S} \mu_\ell(b_T)$.

How can we interpret theorem 8.1(i) in $\mathbb{R}^2$? It says the area of $\mathcal{U}$ can be computed as follows. First, take the triangles in $\mathcal{K}$ and compute their total area. Second, for each vertex σ_T of $\mathcal{S}$, $T = \{b\}$, compute the angle, φ_T, around σ_T outside $\mathcal{S}$, and add φ_T times the area of $b_T = b$ to the total area. Third, for each edge σ_T of $\mathcal{S}$, $T = \{b, b'\}$, subtract half the area of $b_T = b \cap b'$ if there is one triangle in $\mathcal{R} - \mathcal{K}$ incident to σ_T, and subtract the entire area if there are two such triangles. Similar interpretations apply to theorem 8.1(ii) and in higher dimensions.

Measuring a void. Note that theorem 8.1(i) consists of two sums. The first measures the d-dimensional part of $\mathcal{S}$, and the second measures the *fringe*, $\mathcal{U} - \mathcal{S}$. This relates to the considerations in section 3, where the fringe is deformed in a continuous manner until it disappears. We can also measure the fringe simply by dropping the first sum in 8.1(i). This suggests it should be possible to measure a *void*, that is, a bounded component of $\mathbb{R}^d - \mathcal{U}$. In $\mathbb{R}^3$, measuring voids is of some significance in the study of proteins.

Let $\bar{\mathcal{U}}_0$ be a void of $\mathcal{U}$. As proved in section 3, there is a void $\bar{\mathcal{S}}_0$ of $\mathcal{S}$ that contains $\bar{\mathcal{U}}_0$. Moreover, $\bar{\mathcal{S}}_0$ contains no other void of $\mathcal{U}$, that is, $\bar{\mathcal{U}}_0 = \bar{\mathcal{S}}_0 - \mathcal{U}$. It thus seems natural to collect all simplices $\sigma \in \mathcal{R} - \mathcal{K}$ with $\text{int}(\sigma) \subseteq \bar{\mathcal{S}}_0$ using the ideas described in section 4. Call this set $\bar{\mathcal{K}}_0$ and note that $\bar{\mathcal{K}}_0$ is not a simplicial complex, but $\mathcal{R} - \bar{\mathcal{K}}_0$ is one. To measure $\bar{\mathcal{U}}_0$ we adapt the formulas in theorem 8.1. Recall that $\bar{\mathcal{K}}_0^{[d]}$ is the collection of d-simplices $\sigma_S \in \bar{\mathcal{K}}_0$.

8.2 (i) $\mu_d(\bar{\mathcal{U}}_0) = \sum_{\sigma_S \in \bar{\mathcal{K}}_0^{[d]}} \mu_d(\sigma_S)$
$- \sum_{(\sigma_T,\sigma_S)\in[\mathcal{K},\bar{\mathcal{K}}_0]} (-1)^{|T|-1} \varphi_{T,S} \cdot \mu_d(b_T)$.
(ii) For $0 \le \ell \le d-1$,
$\mu_\ell(\bar{\mathcal{U}}_0) = \sum_{(\sigma_T,\sigma_S)\in[\mathcal{K},\bar{\mathcal{K}}_0]} (-1)^{|T|-d+\ell} \varphi_{T,S} \cdot \mu_\ell(b_T)$.

Proof. We cover the void $\bar{\mathcal{U}}_0$ with finitely many d-balls and consider the difference in measure before and after adding the d-balls. Let B' be the set of d-balls that cover $\bar{\mathcal{U}}_0$, and define $\mathcal{U}' = \mathcal{U}(B \cup B')$ and $\mathcal{K}' = \mathcal{K}(B \cup B')$. We require that (i) B' is finite, (ii) $\mathcal{K}$ is a subcomplex of $\mathcal{K}'$, and (iii) $\bar{\mathcal{U}}_0 = \mathcal{U}' - \mathcal{U}$.

We argue that such a set B' exists. Choose $\varepsilon > 0$ small enough so that $\mathcal{K} = \mathcal{K}(B) = \mathcal{K}(B_\varepsilon)$, where

$$B_\varepsilon = \{b_\varepsilon = (z, \sqrt{\varrho^2 - \varepsilon^2}) \mid b = (z, \varrho) \in B\}.$$

Note that $\mathcal{P}(B) = \mathcal{P}(B_\varepsilon)$, by definition of $\mathcal{P}$, and therefore $\mathcal{R} = \mathcal{R}(B) = \mathcal{R}(B_\varepsilon)$. Since general position of the d-balls in B is assumed, we can find ε small enough so that also the subcomplexes $\mathcal{K} \subseteq \mathcal{R}$ and $\mathcal{K}(B_\varepsilon) \subseteq \mathcal{R}$ coincide. Now let B' be a sufficiently large set of d-balls $b' = (z', \varepsilon)$, with $z' \in \bar{\mathcal{U}}_0$, so that $\bar{\mathcal{U}}_0 \subseteq \bigcup_{b' \in B'} b'$. Since $\bar{\mathcal{U}}_0$ is bounded and $\varepsilon > 0$ we can certainly choose B' finite. We show that (ii) and (iii) are also satisfied. Define B'_ε the same way as B_ε before. The balls of this set are degenerate, that is, B'_ε is a finite point set. Therefore, $\mathcal{K}(B_\varepsilon \cup B'_\varepsilon)$ is just $\mathcal{K}(B_\varepsilon)$ together with finitely many isolated 0-simplices. Hence, $\mathcal{K} = \mathcal{K}(B_\varepsilon) \subseteq \mathcal{K}(B_\varepsilon \cup B'_\varepsilon)$. From this (ii) follows because $\mathcal{K}(B_\varepsilon \cup B'_\varepsilon) \subseteq \mathcal{K}(B \cup B') = \mathcal{K}'$. If σ_T is a simplex in $\mathcal{K}' - \mathcal{K}$ then $T \cap B' \neq \emptyset$. So $\mathcal{S}' - \mathcal{S} \subseteq \bar{\mathcal{S}}_0$, where $\mathcal{S}' = |\mathcal{K}'|$. In fact, $\mathcal{S}' - \mathcal{S} = \bar{\mathcal{S}}_0$ because $\bar{\mathcal{U}}_0 \subseteq \mathcal{U}'$. Condition (iii) follows because the correspondence between $\mathcal{S}'$ and $\mathcal{U}'$ expressed in 2.2 guarantees that $\mathcal{U}'$ and $\mathcal{U}$ coincide outside $\bar{\mathcal{U}}_0$.

So we have $\mu_d(\bar{\mathcal{U}}_0) = \mu_d(\mathcal{U}') - \mu_d(\mathcal{U})$ and $\mu_\ell(\bar{\mathcal{U}}_0) = \mu_\ell(\mathcal{U}) - \mu_\ell(\mathcal{U}')$ for $0 \le \ell \le d-1$. Note that the first sum in (i) is equal to the first sum of 8.1(i) for $\mathcal{U}'$ minus the first sum of 8.1(i) for $\mathcal{U}$. The same is true for the second sum in (i). The sum in (ii) is 8.1(ii) for $\mathcal{U}$ minus 8.1(ii) for $\mathcal{U}'$. ◻

9 Discussion

This paper studies the union of finitely many d-balls in $\mathbb{R}^d$. It is demonstrated that many properties can be computed without explicit construction of the union. Instead, the nerve of the balls intersected with their respective power cells is computed. This is an abstract simplicial complex that can be derived directly from the regular triangulation of the balls. For constant d, the size of this complex is no more than some constant times $n^{\lceil d/2 \rceil}$, where n is the number of balls, and for typical distributions it is much less than that.

Specific algorithms are discussed that compute topological, combinatorial, and metric properties of the union of balls directly from the complex. These methods are relevant to computational problems in chemistry and biology, where molecules are modeled as unions of 3-balls in $\mathbb{R}^3$. For further applications it would be interesting to extend the inclusion-exclusion formulas of 6.2, 8.1, and 8.2 to compute physical forces associated with a molecule.

The most demanding step in obtaining running implementations of the algorithms in this paper is the construction of $\mathcal{K}$. Software for $d \le 3$ is available [13, 16] and algorithms in higher dimensions are described [12, 17]. The time-complexity of these algorithms depends on the distribution of the balls, and typically is roughly of the same order as the number of simplices in $\mathcal{R}$.

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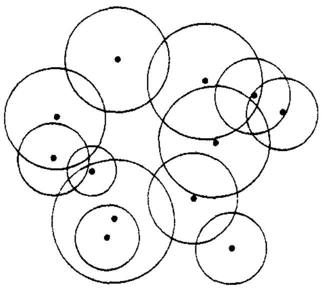
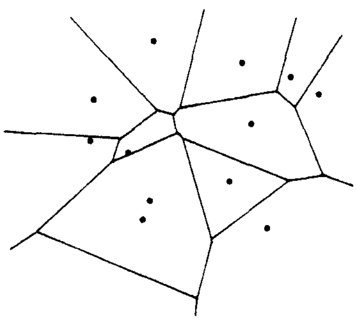
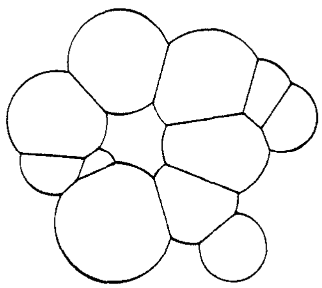


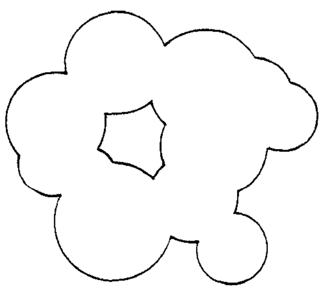
Figure 2.1: This set of 12 disks (2-balls) is used as a running example to illustrate forthcoming definitions.



(i) The power diagram of 12 disks represented by their centers in $\mathbf{R}^2$.

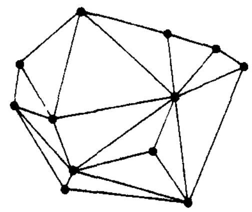


(ii) The decomposition of the union of disks using the power diagram.

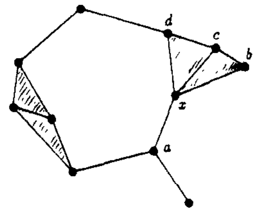


(iii) The union of 12 disks.

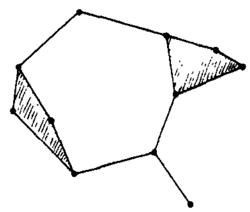
Figure 2.2: The diagrams $\mathcal{P}$, $\mathcal{Q}$, and $\mathcal{U}$ of the 12 disks shown in figure 2.1.



(i) The regular triangulation of 12 disks represented by their centers in $\mathbf{R}^2$.



(ii) A subcomplex of the regular triangulation.



(iii) The underlying space of the subcomplex.

Figure 2.3: The diagrams $\mathcal{R}$, $\mathcal{K}$, and $\mathcal{S}$ of the 12 disks shown in figure 2.1. It is important to note their dual relationship to the corresponding diagrams in figure 2.2.

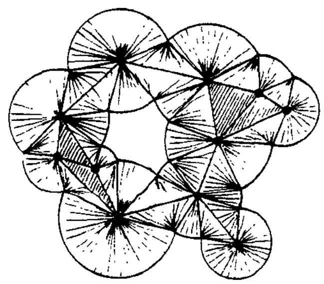


Figure 3.1: The decomposition of $\mathcal{U}$ using joins between simplices of $\mathcal{K}$ and faces of $\mathcal{U}$.

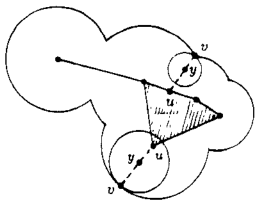


Figure 3.2: Two examples of points y, v, u for 5 of the 12 disks in figure 2.1 are shown. In one example, the join that contains y is between an edge and a point, in the other between a vertex and a piece of a circle.

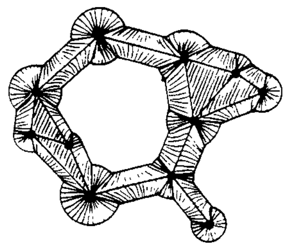


Figure 3.3: This is $\Phi(\mathcal{U}, \frac{1}{2})$: at time $t = \frac{1}{2}$ the fringe is narrowed to half the original width.

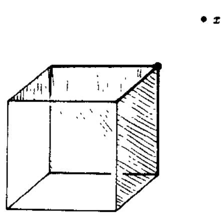


Figure 5.1: The faces f_I of P for which $\gamma_I(x) = 1$ are the ones visible from x. The point x sees the cube itself, three facets, three edges, and one vertex. Hence, $\Gamma_R(x) = 1 - 3 + 3 - 1 = 0$ as claimed.

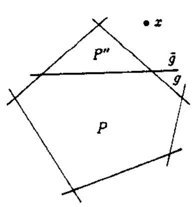


Figure 5.2: P' is the union of P and P''. Since $x \notin P$, by assumption, we have $x \in P'$ iff $x \in P''$.

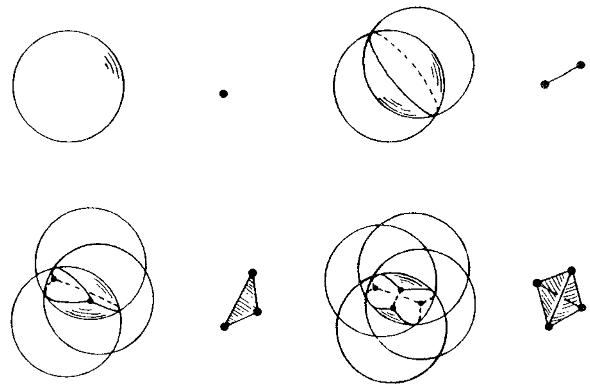


Figure 6.1: The intersection of one, two, three, and four 3-balls. The face structure is dual to that of a vertex, an edge, a triangle, and a tetrahedron.

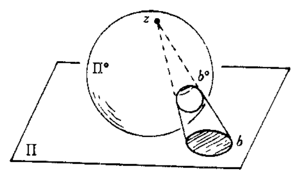


Figure 6.2: Under inversion, the image of a hyperplane is a d-sphere, and every $(d-1)$-sphere in the hyperplane maps to a $(d-1)$-sphere on the d-sphere.

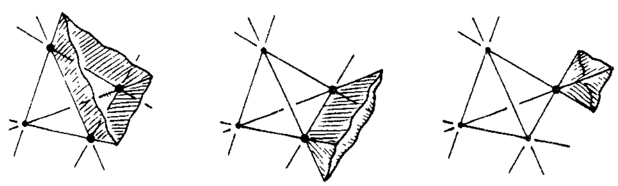


Figure 7.1: Regions P_I of a 3-simplex, with $|I| = 1$ to the left, $|I| = 2$ in the middle, and $|I| = 3$ to the right.

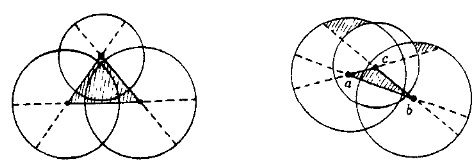


Figure 7.2: The three disks to the left define a favorable case, whereas the disks to the right do not. Indeed, the intersection of the disk around b with the half-plane opposite ac is not covered by the disks around a and c. The same is true for the disk around a and the half-plane opposite bc.