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Multiple Covers with Balls II: Weighted Averages [1]

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Abstract

Voronoi diagrams and Delaunay triangulations have been extensively used to represent and compute geometric features of point configurations. We introduce a generalization to *poset diagrams* and *poset complexes*, which contain order-k and degree-k Voronoi diagrams and their duals as special cases. Extending a result of Aurenhammer from 1990, we show how to construct poset diagrams as weighted Voronoi diagrams of average balls.

Keywords: Weighted points, Voronoi diagrams, Poset diagrams.

1 Introduction

The work in this paper is motivated by research into the physical organization of DNA in the Eukaryotic cell nucleus. DNA is compartmentalized into segments of roughly the same length, each rolling up into a shape resembling a round ball that deforms if pushed against each other[4]. Modeling the deformation of the balls seems out of reach, which motivates us to consider arrangements of balls

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with overlap. Looking for an optimal arrangement we needed to compute volumes covered by multiple balls, which caused us to look at order-k and degree-k Voronoi diagrams.

Prior work and results. As documented by Aurenhammer [2], Voronoi diagrams have found applications in diverse areas of science. This includes biology, where they assist in the study of proteins in atomic resolution [12] as well as cell cultures on much coarser level of organization [3]. Returning to atomic resolution, Voronoi diagrams have been used to derive inclusion-exclusion formulas for the volume of a union of balls; see Kratky [9] in physics and Naiman and Wynn [10] in statistics. In a companion paper [6], we have recently extended these formulas to the space of points covered by at least k of the balls using order-k Voronoi diagrams [13,7,8] or, alternatively, degree-k Voronoi diagrams [5, page 207].

In this paper, we define cotransitive posets and use them to introduce a family of Euclidean Voronoi diagrams that includes the order-k and degree-k diagrams as special cases. A second contribution is the construction of the diagrams in this family from weighted averages of the given points or balls. This construction is a generalization of a result of Aurenhammer [1], who constructs an order-k Voronoi diagram from the k-fold averages of the given points.

2 Poset Diagrams

This section introduces a common generalization of order-k and degree-k Voronoi diagrams. We begin by recalling the definitions of these diagrams, which we give for weighted points or balls.

Voronoi diagrams. Let $B(x, r)$ be the closed ball with center $x \in \mathbb{R}^n$ and radius $r \geq 0$. Writing $B_i = B(x_i, r_i)$, we let $\mathcal{B} = \{B_1, B_2, \ldots, B_m\}$ be a finite set of balls in $\mathbb{R}^n$. The *weighted distance* from B_i is defined by the function $\pi_i : \mathbb{R}^n \to \mathbb{R}$ that maps a point x to $\pi_i(x) = \|x - x_i\|^2 - r_i^2$. For example, if $r_i = 0$, then $\pi_i(x)$ is the squared Euclidean distance from the center of B_i. Let now Q be a subset of $\mathcal{B}$. Its *Voronoi domain* consists of all points that satisfy $\pi_i(x) \leq \pi_j(x)$ whenever $B_i \in Q$ and $B_j \in \mathcal{B} \setminus Q$. For an integer $1 \leq k \leq m$, the *order-k Voronoi diagram* of $\mathcal{B}$ is the collection of Voronoi domains of all subsets of k balls in $\mathcal{B}$ [13,7,8]. Note that $k = 1$ gives the ordinary Voronoi diagram. We can further subdivide the Voronoi domain of Q depending on which of its balls maximizes the weighted distance. If we do this for all domains in the order-k diagram, we get the *degree-k Voronoi diagram* studied for example in [5, Exercise 13.27]. It decomposes $\mathbb{R}^n$ into regions within which the same ball realizes the k-smallest weighted distance.

Cotransitive posets. We further generalize the notion of Voronoi diagram using posets. Let $U = \{u_1, u_2, \ldots, u_m\}$ be a finite set of nodes and recall that a *partial* *order* on U is a set of pairs $P \subseteq U \times U$ that is reflexive, antisymmetric, and transitive. We write $u_i \leq u_j$ whenever $(u_i, u_j) \in P$ and $u_i < u_j$ if $u_i \leq u_j$ and $u_i \neq u_j$. Nodes u_i and u_j are *comparable* if $u_i \leq u_j$ or $u_j \leq u_i$. Otherwise, they are *incomparable*, which we denote as $u_i \not\sim u_j$. A *chain* of P is a subset of U in which any two nodes are comparable, and a *cochain* is a subset of U in which any two nodes are incomparable. We say P is *cotransitive* if $u_i \not\sim u_j$ and $u_j \not\sim u_k$ implies $u_i \not\sim u_k$.

If two cochains in a cotransitive partial order have a non-empty intersection, then their union is also a cochain. It follows that the maximal cochains partition U. It is therefore possible to order the maximal cochains as

$$U = C_1 \sqcup C_2 \sqcup \ldots \sqcup C_s, \tag{1}$$

such that $P = \bigcup_{i<j} C_i \times C_j$. Indeed, the existence of such a partition characterizes cotransitive partial orders.

Domains and diagrams. Let $\mathcal{B}$ be a set of m balls in $\mathbb{R}^n$ and $P \subseteq U \times U$ a cotransitive poset of m nodes, as before. The P*-domain* of a permutation $\gamma\colon [m] \to [m]$ is the set of points $x \in \mathbb{R}^n$ such that the weighted distances of x from the balls is consistent with the partial order:

$$P(\gamma) = \{x \in \mathbb{R}^n \mid u_i \leq u_j \Rightarrow \pi_{\gamma(i)}(x) \leq \pi_{\gamma(j)}(x)\}. \tag{2}$$

The *poset diagram* of $\mathcal{B}$ and P, denoted as $\mathrm{Pos}(\mathcal{B}, P)$, is the set of P-domains. This diagram shares the fundamental properties with the Voronoi diagram of the balls.

Lemma 2.1 (Structure Lemma) *Let $\mathcal{B}$ be a set of m balls in $\mathbb{R}^n$ and P a cotransitive partial order on m nodes.*

(i) The P-domain of a permutation $\gamma\colon [m] \to [m]$ is either empty or a closed convex polyhedron.
(ii) The P-domains for two different permutations have pairwise disjoint interiors.
(iii) Every point $x \in \mathbb{R}^n$ belongs to the P-domain of at least one permutation.

Proof. (i) is clear from the definition since every inequality of the form $\pi_{\gamma(i)}(x) \leq \pi_{\gamma(j)}(x)$ defines a closed half-space.

(ii) holds because P is transitive as well as cotransitive, which implies that two different permutations either define the same set of inequalities, or at least one inequality is reversed. In the latter case, the two domains lie on different sides of the corresponding bisector.

(iii) follows from the fact that every ordering of the m balls is consistent with the partial order for at least one permutation. $\square$

Examples. Fix an integer $1 \leq k \leq m$ and consider the following cotransitive partial orders on m nodes:

$$P_A = \{u_i \leq u_j \mid 1 \leq i \leq k < j \leq m\}; \tag{3}$$
$$P_B = \{u_i \leq u_k \leq u_j \mid 1 \leq i \leq k \leq j \leq m\}; \tag{4}$$

We note that $\mathrm{Pos}(\mathcal{B}, P_A)$ is the order-k Voronoi diagram, and $\mathrm{Pos}(\mathcal{B}, P_B)$ is the degree-k Voronoi diagram. Referring to the decomposition into maximal cochains in (1), we can describe the poset diagram in general as follows. Letting k_i be the cardinality of the i-th cochain, the diagram decomposes $\mathbb{R}^n$ into the order-k_1 Voronoi domains of the m balls, it refines each domain into the order-k_2 Voronoi domains of the remaining $m - k_1$ balls, and repeats until refining the domain into the order-k_{i-1} Voronoi domains of the remaining $k_{i-1} + k_i$ balls.

3 Average Balls

In this section, we construct the poset diagrams by taking averages of the balls in $\mathcal{B}$. We begin with the introduction of a vector space structure of the set of all balls, including those with negative squared radii.

Vector space of balls. We follow Pedoe [11, Chapter IV], who introduced the vector space to study the geometry of circles in the plane or spheres in higher-dimensions. In particular, we represent the ball $B(x, r)$ by the point $b(x, r) = (x, \|x\|^2 - r^2)$ in $\mathbb{R}^{n+1}$. To have a bijection between the set of balls in $\mathbb{R}^n$ and the set of points in $\mathbb{R}^{n+1}$, we let r^2 range over all real numbers or, equivalently, we let r range over all non-negative real numbers and all positive multiples of the imaginary unit, a set we denote as $\sqrt{\mathbb{R}}$. Borrowing the vector space structure of $\mathbb{R}^{n+1}$, we have a vector space of balls in which addition and multiplication with scalars make sense. More formally, if B_1, B_2 are two balls with corresponding points b_1, b_2, and λ_1, λ_2 are real numbers, then $B_0 = \lambda_1 B_1 + \lambda_2 B_2$ is defined such that the corresponding point satisfies $b_0 = \lambda_1 b_1 + \lambda_2 b_2$ in $\mathbb{R}^{n+1}$. From the centers x_1, x_2 and squared radii r_1^2, r_2^2 of B_1, B_2, we can compute B_0:

$$x_0 = \lambda_1 x_1 + \lambda_2 x_2, \tag{5}$$
$$r_0^2 = \|x_0\|^2 - \lambda_1\big(\|x_1\|^2 - r_1^2\big) - \lambda_2\big(\|x_2\|^2 - r_2^2\big)\,. \tag{6}$$

Assuming $\lambda_1 + \lambda_2 = 1$, we plug the expressions of the center and the squared radius into the formula for the weighted distance of a point $x \in \mathbb{R}^n$ from B_0 and get

$$\pi_0(x) = \lambda_1 \pi_1(x) + \lambda_2 \pi_2(x). \tag{7}$$

Affine combinations. This is an interesting conclusion worth generalizing. We recall that a *linear combination* is a ball $B_0 = \sum_{i=1}^{k} \lambda_i B_i$. It is an *affine combination* if $\sum_i \lambda_i = 1$, and it is a *convex combination* if, in addition, $0 \leq \lambda_i$ for all i. For affine combinations, the weighted distance satisfies a relation that generalizes (7):

Lemma 3.1 (Weighted Distance Lemma) *Let* $B_0 = \sum_{i=1}^{k} \lambda_i B_i$ *with* $\sum_{i=1}^{k} \lambda_i = 1$. *Then* $\pi_0(x) = \sum_{i=1}^{k} \lambda_i \pi_i(x)$, *for every point* $x \in \mathbb{R}^n$.

Proof. For $k = 2$, the claimed relation is the same as (7). For $k > 2$, we decompose the affine combination into two affine combinations of fewer than k balls each:

$$B_0' = \tfrac{1}{\lambda_2 + \ldots + \lambda_k} \left(\lambda_2 B_2 + \ldots + \lambda_k B_k \right), \tag{8}$$

$$B_0 = \lambda_1 B_1 + (\lambda_2 + \ldots + \lambda_k) B_0'. \tag{9}$$

Inductively, we get the claimed relation for the distance from B_0', and combining it with (7), we get the claimed relation for the weighted distance from B_0. □

Weighted averages. As proved in [1], the order-k Voronoi diagram of a finite set of points is the ordinary Voronoi diagram of the k-fold averages. We generalize this result, showing that every poset diagram is an ordinary Voronoi diagram, of course of a different set of balls. To construct this set, we say a function $\lambda \colon [m] \to \mathbb{R}$ is *anti-parallel* to a cotransitive partial order if $\sum \lambda(i) = 1$ and $\lambda(i) > \lambda(j)$ iff $u_i < u_j$. Hence, λ is constant on the nodes in a cochain, and using the ordered partition into maximal cochains (1), there are values $\lambda_1 > \lambda_2 > \ldots > \lambda_s$, such that $\lambda(i) = \lambda_p$ iff $u_i \in C_p$. Given $\mathcal{B}$ and P, the *weighted average ball* of a permutation $\gamma \colon [m] \to [m]$ is

$$A_\gamma = \sum_{i=1}^{m} \lambda(i) B_{\gamma(i)}, \tag{10}$$

and we write $\mathcal{A} = \mathcal{A}(\mathcal{B}, P)$ for the set of all such weighted averages.

Main result. Importantly, the poset diagram of $\mathcal{B}$ and P is equal to the ordinary Voronoi diagram of $\mathcal{A}$.

Theorem 3.2 (Poset Diagram Theorem) *Let* $\mathcal{B}$ *be a finite set of balls in* $\mathbb{R}^n$, *let* P *be a cotransitive partial order on the same number of nodes, and set* $\mathcal{A} = \mathcal{A}(\mathcal{B}, P)$. *Then* $\mathrm{Pos}(\mathcal{B}, P) = \mathrm{Vor}(\mathcal{A})$.

Proof. Fixing a permutation γ, we prove that a point x belongs to the P-domain of γ iff x belongs to the Voronoi domain of A_γ. To see $P(\gamma) \subseteq V(A_\gamma)$, we recall that the weighted distance of x from $B_0 = A_\gamma$ satisfies $\pi_0(x) = \sum_{i=1}^{m} \lambda(i) \pi_{\gamma(i)}(x)$ by Lemma 3.1. Assuming $x \in P(\gamma)$, we have $\pi_{\gamma(i)}(x) \leq \pi_{\gamma(j)}(x)$ as well as

$\lambda(i) > \lambda(j)$ whenever $u_i < u_j$. It follows that the weighted distance to any other weighted average ball is larger. Indeed, this other weighted distance is obtained by switching some of the $\lambda(i)$. We thus go away from the global minimum, which we get by sorting the $\pi_{\gamma(i)}(x)$ and the $\lambda(i)$ in anti-parallel fashion.

Since both the P-domains and the Voronoi domains are interior-disjoint closed convex polyhedra that cover $\mathbb{R}^n$, we have $P(\gamma) = V(A_\gamma)$ for every γ. Indeed, if $P(\gamma)$ were a strict subset of $V(A_\gamma)$, then there would be points in the interior of the Voronoi domain that are not covered by any P-domain. $\square$

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