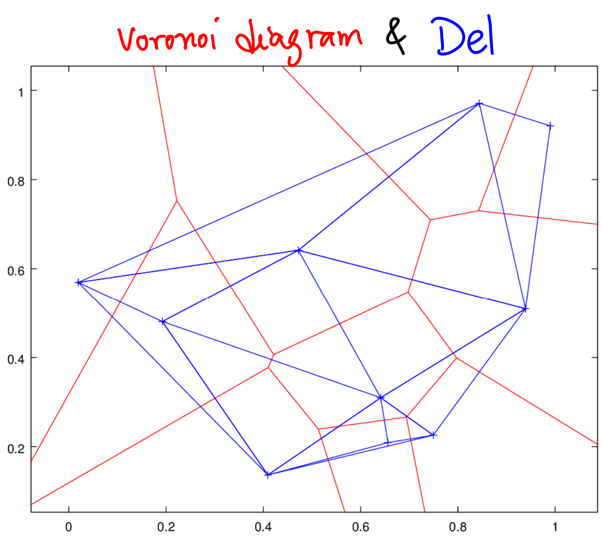
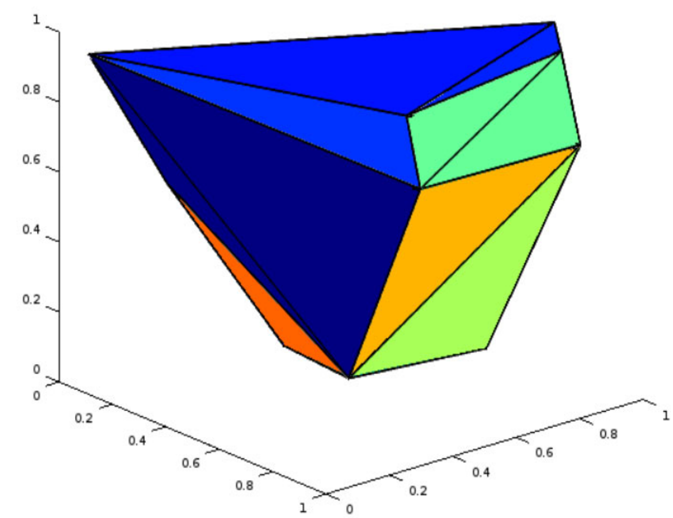
MATH 529 — Lecture 12 (02/15/2024)

Today:
* filtration
* alpha complexes
* weighted alpha complexes

Check out the commands voronoi, delaunay, and delaunayn, as well as related commands in Matlab. Similar commands are available in Python as well.

Here are a couple sample pictures of 2D and 3D Delaunay complexes produced in Matlab. The 2D picture shows the Voronoi diagram as well.

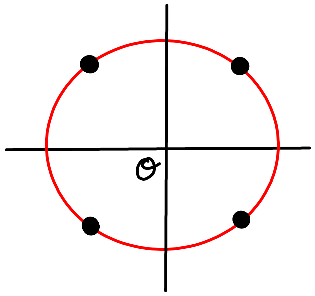




Looks like we only get (upto) triangles here. Recall one of the main motivations we stated for introducing Delaunay complexes — that we wanted to get only upto d-simplices for point sets S in $\mathbb{R}^d$.

Q. Do we always get only triangles in Del_S is 2D?

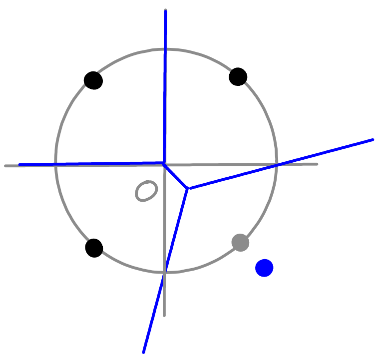
No!



The Voronoi cells V_{v_j} of the four points meet at the central point o (origin) here.

Hence, Del_S contains the tetrahedron!

But, if we move even one of the four points just ever so slightly away from the circle, we can avoid the 4-way intersection of their Voronoi cells.



Mathematically, we need to move only one (out of the four) points by $\varepsilon > 0$ in one of the coordinate directions; ε could be really small, as long as it is > 0.

Def The set of points S in $\mathbb{R}^d$ is in **general position** if no $(d+2)$ points in S lie on a common $(d-1)$-sphere.

e.g., $d=2 \Rightarrow$ no 4 points lie on a circle.

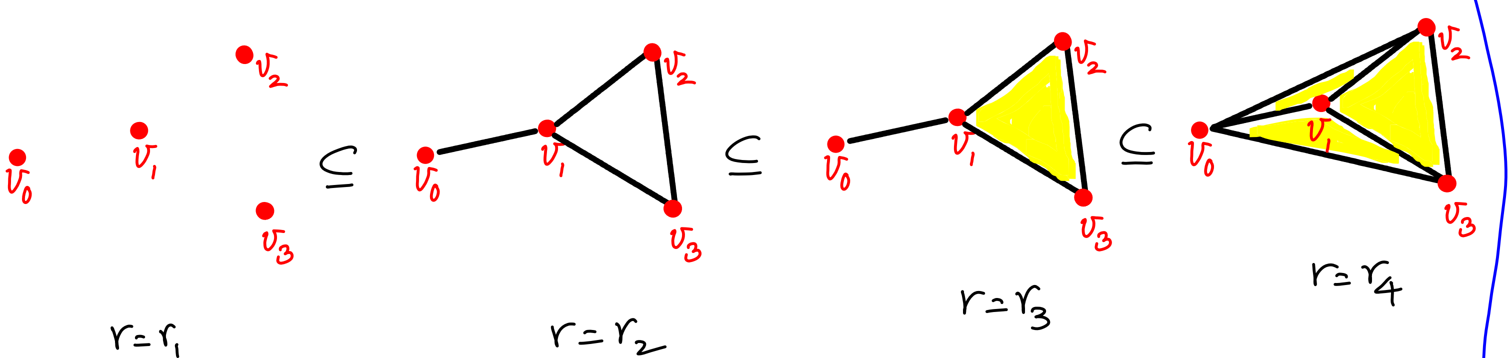
No $(d+2)$ V_{v_j}'s have a common intersection $\Rightarrow$ ($\sigma \in Del_S$ means $\dim \sigma \leq d$)

We assume general position usually. If this condition is not satisfied, we could perturb a single coordinate of a single point from any $(d+2)$ such points by a small $\epsilon > 0$.

There are very efficient (polynomial time) algorithms for constructing Delaunay tessellations, at least in 2D and 3D.

We have seen 3 families of simplicial complexes: $\check{C}ech_S(r)$, $VR_S(r)$, and Del_S. Note that the Delaunay complex is independent of any distance cutoffs (or radii of balls).
But, what do we gain by varying r?

Given S, we could study the family of $\check{C}ech_S(r)$ or $VR_S(r)$ as r varies from 0 to ∞ (or, even from $-\infty$ to $+\infty$).
Since S is finite, we will only a finite number of such complexes.



$\subseteq$ tetrahedron $v_0v_1v_2v_3$ (at $r=r_5$)

→ Since there are only four points here, their tetrahedron is the largest dimensional simplex we get in $\check{C}ech(r)$, even if we keep increasing r beyond r_5.

We capture the fact that v_1, v_2, v_3 are closer to each other than, say, $\{v_2, v_3\}$ are to v_0, since $\Delta v_1v_2v_3$ comes in to $\check{C}ech(r)$ before the other triangles.

We will study such families of complexes in detail.

Def A **filtration** of a simplicial complex K is a nested sequence of subcomplexes of K

$$\phi = K^0 \subseteq K^1 \subseteq \cdots \subseteq K^m = K.$$

The simplicial complex K along with a filtration is a **filtered simplicial complex**.

A **filtration ordering** is a full ordering of all simplices in K such that each prefix of the ordering is a subcomplex.

<u>Filtration ordering: Example</u>

$K =$  $v_0 v_1 v_2 v_3$

a subcomplex

$$v_0 < v_1 < v_2 < v_3 < v_0v_1 < v_0v_2 < v_0v_3 < v_1v_2 \mid < v_1v_3 < v_2v_3$$
$$< v_0v_1v_2 < \cdots < v_0v_1v_2v_3.$$

More generally, '<' could assign the same rank for several simplices, e.g., all vertices < all edges < all triangles < ... . In this case, < is not a full ordering but we can convert it to one by breaking ties arbitrarily.

Q. What do we use filtrations for?

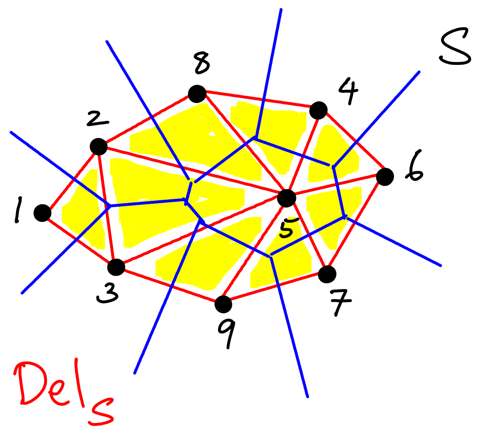
We could study signature functions: $\lambda : \{0, 1, \dots, m\} \longrightarrow \mathbb{R}^d$, $d \geq 1$. λ assigns a value in $\mathbb{R}^d$ for each $k \in \{0, \dots, m\}$. We could compare the signatures for two point sets S_1 and S_2 to distinguish them — by comparing $\lambda(S_1)$ and $\lambda(S_2)$.

For instance, χ (Euler characteristic). We could compute $\chi(K^i)$ for each $i \in \{0, \dots, m\}$, and study the Euler characteristic curve (or vector).

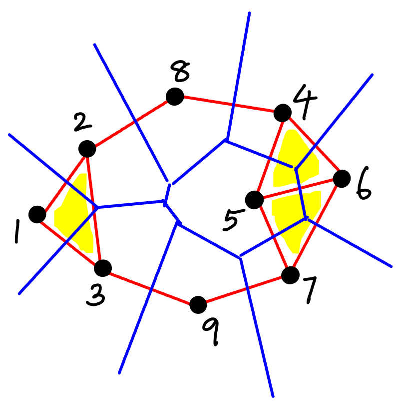
But we will study other more involved signatures soon.

Could we vary r to create a family of nested Delaunay complexes? Equivalently, could we create a filtration for Del_S?

Consider S with 9 points shown here:



Observe: $\{1,2,3\}$ and $\{4,5,6,7\}$ form two clusters of nearby points, which are further away from each other.



A subcomplex of Del_S as shown here would capture the topology of S "better".

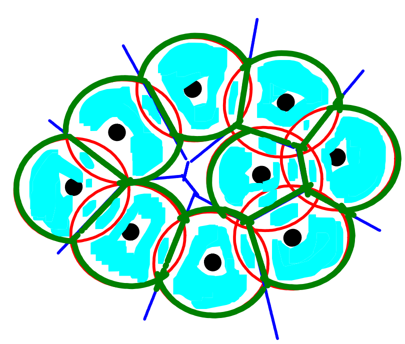
For the given set of 9 points, how do we define the complex shown here?

Alpha Complexes

Let $S = \{\bar{v}_1, \dots, \bar{v}_n\}$, $\bar{v}_j \in \mathbb{R}^d$, $r \geq 0$. Recall that $B_{\bar{v}_j}(r) = \bar{v}_j + r\mathbb{B}^d$ $= \{\bar{x} \in \mathbb{R}^d \mid \|\bar{x} - \bar{v}_j\| \leq r\}$ is the r-ball (d-dimensional) centered at $\bar{v}_j$.

We "combine" balls around the points, and their Voronoi cells. We consider $B_{\bar{v}_j}(r) \cap V_{\bar{v}_j}$.

$\bigcup_{\bar{v}_j \in S} R_{\bar{v}_j}(r)$



Note that there is a "hole" in the union of regions (in the middle).

The idea is to combine the good properties of balls and Voronoi cells – get at most d-simplices, but still get a hierarchy.

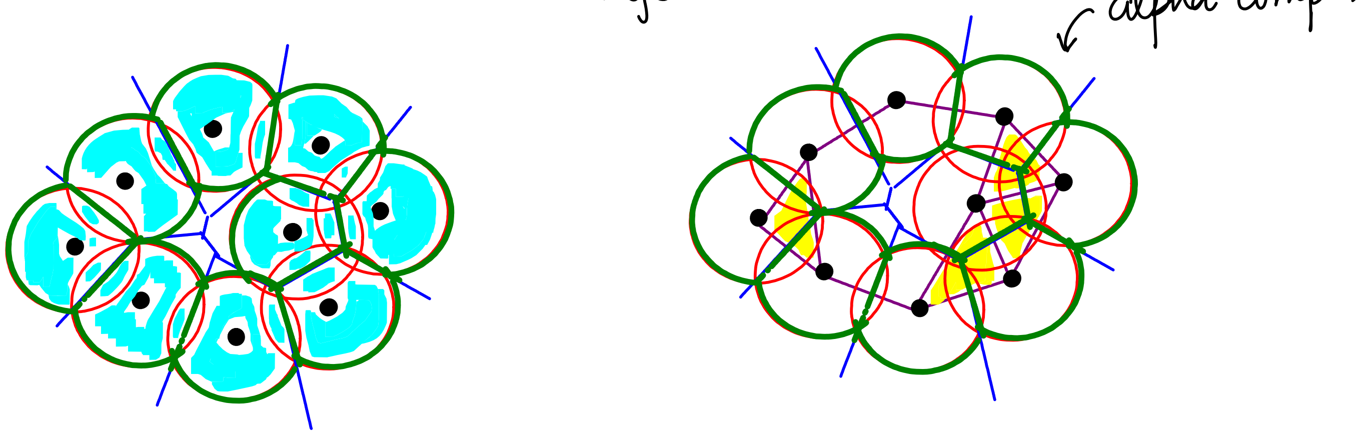
Let $R_{\bar{v}_j}(r) = B_{\bar{v}_j}(r) \cap V_{\bar{v}_j}$. Since both $B_{\bar{v}_j}(r)$ and $V_{\bar{v}_j}$ are convex, so is $R_{\bar{v}_j}(r)$. The regions $R_{\bar{v}_j}(r)$ intersect, if at all, along common boundaries, and together they tile $\bigcup_{\bar{v}_j \in S'} B_{\bar{v}_j}(r)$.

region of $\bar{v}_j$

or, cover

The **alpha complex** is the nerve of this union.

$$\mathrm{Alpha}_S(r) = \{\sigma \subseteq S \mid \bigcap_{\bar{v}_j \in \sigma} R_{\bar{v}_j}(r) \neq \phi\}.$$



$$R_{\bar{v}_j}(r) \subseteq V_{\bar{v}_j} \implies \mathrm{Alpha}(r) \subseteq \mathrm{Del}_S. \quad \text{Also,}$$

$$R_{\bar{v}_j}(r) \subseteq B_{\bar{v}_j}(r) \implies \mathrm{Alpha}(r) \subseteq \check{C}ech_S(r).$$

By the nerve lemma, $\bigcup_{\bar{v}_j \in S} B_{\bar{v}_j}(r) \simeq |\mathrm{Alpha}(r)|$.

By varying r and considering $\mathrm{Alpha}(r)\ \forall r$, we get a filtration of the Delaunay complex.

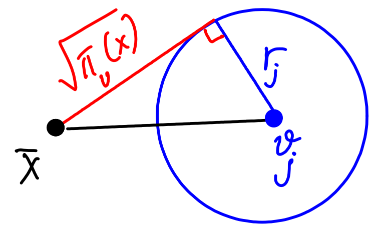
Q: Can we use balls of different radii?

Motivation: modeling proteins – made up of atoms, which could be modeled using balls of different radii.

Weighted Alpha Complexes

Def The weighted squared distance, or the **power distance**, of $\bar{x} \in \mathbb{R}^d$ from $\bar{v}_j$ with weight w_j is

$$\pi_{\bar{v}_j}(\bar{x}) = \|\bar{x}-\bar{v}_j\|^2 - w_j.$$



When $w_j = r_j^2$, we get $\pi_{\bar{v}_j}(\bar{x})$ is the squared length of the tangent from $\bar{x}$ to $B_{\bar{v}_j}(r_j)$.

The **weighted** or **power Voronoi** cell of $\bar{v}_j$ is

$$W_{\bar{v}_j} = \{\bar{x} \in \mathbb{R}^d \mid \pi_{\bar{v}_j}(\bar{x}) \le \pi_{v_i}(\bar{x}) \ \forall \bar{v}_i \in S\}.$$

weighted Voronoi diagram

The **power Voronoi complex** is the collection of $W_{\bar{v}_j}$'s. And the **weighted Delaunay complex** is the nerve of the **weighted Voronoi diagram**.

We could apply the concept of weighted Voronoi diagram also to sets of points where different points have different weights (and not only to cases where the balls are differently sized).

The definition of power distance appears somewhat involved — we will describe the motivation soon!

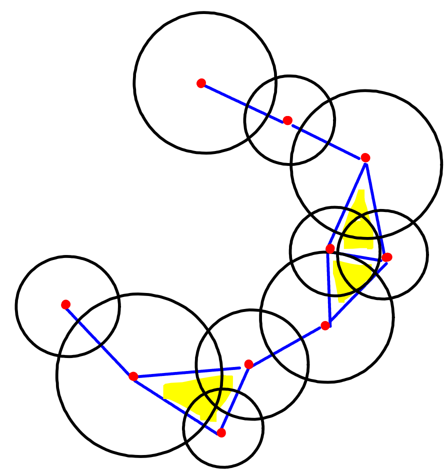
Weighted Alpha Complex

We set $w_j := r_j^2$ and define

$$R^w_{\bar{v}_j}(r) = B_{\bar{v}_j}(r) \cap W_{\bar{v}_j}$$

The **weighted alpha complex** is the nerve of the collection of $R^w_{\bar{v}_j}(r)$. This complex is a subcomplex of the weighted Delaunay complex.

Here is an illustration. The discs could model different atoms, and the weighted alpha complex shown here is one "skeleton" of the protein, which is the collection of atoms.



Here is an illustration of how the weighted alpha complex grows as we increase r_j^2 linearly, i.e., we set $w_j = r_j^2 \leftarrow r_j^2 + r$ and let $r \to \infty$.

A subset of the bigger balls (2D-discs in this case) are shown here for illustration. The extra triangle added to the original nerve is shown in green.