MATH 529 — Lecture 13 (02/20/2024)

Today: * Varying r_j in weighted alpha complexes
* Empty circle property of Delaunay triangulation
* Witness complexes

Recall: power distance $\pi_{\bar{v}_j}(\bar{x}) = \|\bar{x}-\bar{v}_j\|^2 - w_j$, $w_j = r_j^2$, $W_{\bar{v}_j}$, $R_{\bar{v}_j}(r) = W_{\bar{v}_j} \cap B_{\bar{v}_j}(r)$...

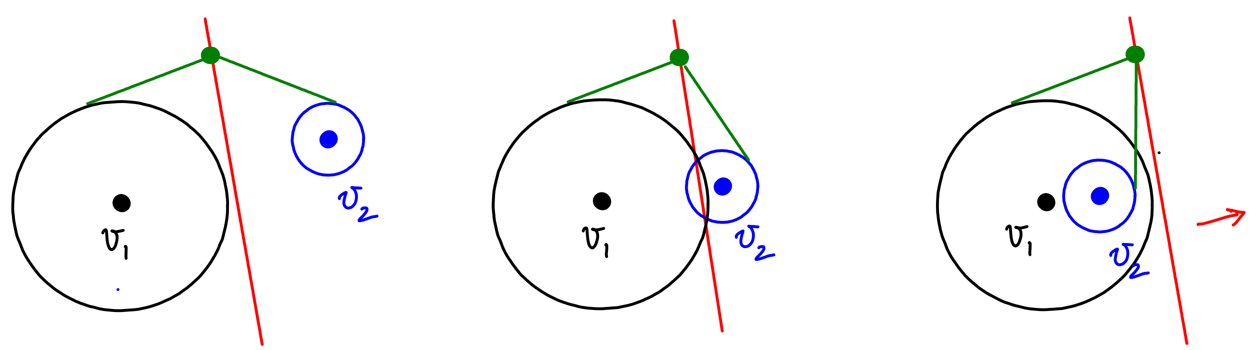
We could "vary" the different radii to get a weighted alpha complex filtration $\phi = K^0 \subseteq \cdots \subseteq K^m$ = weighted Delaunay complex.

Q: How to "vary" the radii? r_j are not same to start with.

1. Set $w_j = r_j^2$, and then increase all radii r_j at the same linear rate, i.e., $r_j \leftarrow r_j + r$ for $r>0$. Then let $r \to \infty$ (uniformly increase all r_j).

But, $W_{\bar{v}_j}$ for different r may not be the same. Hence, it could happen that $K^j \not\subseteq K^{j+1}$ for some j. This situation is best avoided!

Here is an observation: Bisector of two weighted points



Note that the bisector stays a straight line!

Similar to the default alpha complex construction, where the Voronoi cells stay the same while the balls grow, it is desirable to have the weighted Voronoi cells stay same as well.

2. We set $w_j = r_j^2$, and grow the square of the radii uniformly, i.e., set $r_j^2 \leftarrow r_j^2 + r$, as $r \to \infty$.

Since we are using the power distance,

$$\pi_{\bar{v}_j}(\bar{x}) = \pi_{\bar{v}_i}(\bar{x}) \Rightarrow \|\bar{x}-\bar{v}_j\|^2 - (r_j^2 + \cancel{r}) = \|\bar{x}-\bar{v}_i\|^2 - (r_i^2+\cancel{r})$$

Hence, the bisectors using $\pi_{\bar{v}}(\bar{x})$ stay the same as $r \to \infty$. So, the power Voronoi cells remain the same, just like $V_{\bar{v}_j}$.

So, as r increases, $W_{\bar{v}_j}$ remains same. We do get the nesting of simplicial complexes as r increases.

In fact, $W_{\bar{v}_j}$'s here have most of the nice properties that $V_{\bar{v}_j}$, the default Voronoi cells, have. As such, the alpha complex filtration also has most nice properties that the default (same r for each r_j) alpha complexes.

Originally, Edelsbrunner and Mücke (1983) defined the weighted alpha complexes to study structure of biomolecules. The notation, used was $r_j^2 \leftarrow r_j^2 + \alpha$ for the growth parameter α $(-\infty < \alpha < \infty)$. Hence the name alpha complex.

There are efficient algorithms to construct the weighted alpha complexes in 2D and 3D. We will discuss a version in a future lecture.

For large sets of points, all of the complexes we introduced— Čech, VR, alpha, etc., become intensive to compute. We would be better off sampling a subset of points!

Čech and VR complexes grow too large even for moderately large point sets S. For instance, the VR complex of a set with ~2000 points in $\mathbb{R}^3$ could have more than a million triangles! Further, computing Delaunay and alpha complexes are also computationally expensive in high dimensions. We look at a possible alternative now.

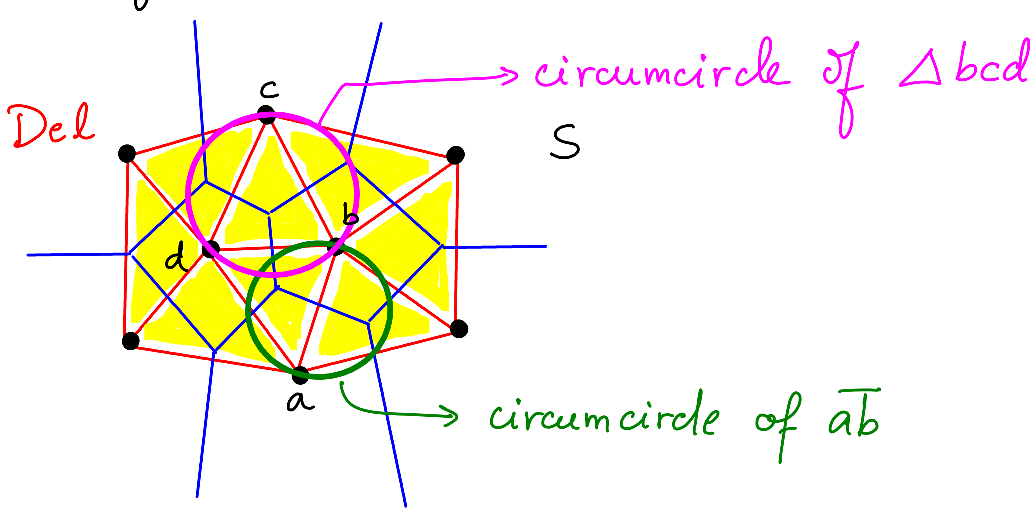
We will now consider two families of complexes that are designed to be much more sparse — they sample from the input point set, and build the complex by generalizing or relaxing some of the conditions used to define the complexes we have already seen.

A crucial property of the Delaunay complex

The **empty circumsphere** property: boundary of miniball

$\sigma \in \mathrm{Del}_S \iff$ circumsphere(σ) has no points of S in its interior.

Of course, with $\sigma = \mathrm{conv}\{\bar{v}_0, \ldots, \bar{v}_k\}$, $\bar{v}_0, \ldots, \bar{v}_k$ lie on the circumsphere, and the center of its circumsphere is in the intersection of the Voronoi cells of $\bar{v}_0, \ldots, \bar{v}_k$.



Witness Complex

Idea: Choose $L \subseteq S$ (L is typically small), and build your complex on L. Use the remaining points in $S \setminus L$ as possible "witnesses" for the simplices in the complex.

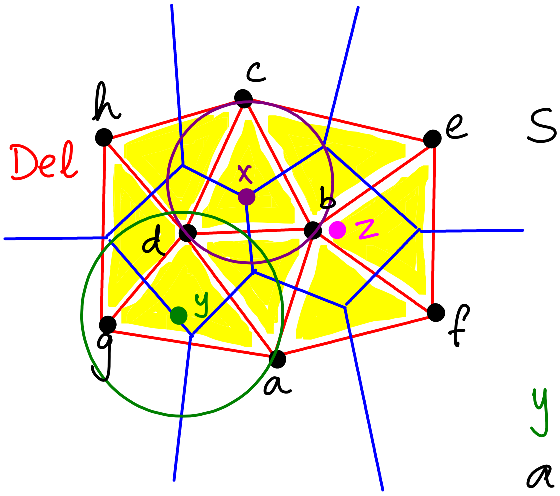
Def Let $\sigma = [\bar{v}_0 \dots \bar{v}_k]$, $\bar{v}_j \in S$, be a k-simplex, where $\bar{v}_j \in \mathbb{R}^d$. $\bar{x} \in \mathbb{R}^d$ is a **weak witness** for σ with respect to S if $\|\bar{x} - \bar{v}\| \leq \|\bar{x} - \bar{u}\|$ $\forall$ $\bar{v} \in \{\bar{v}_0, \dots, \bar{v}_k\}$ and $\bar{u} \in S \setminus \{\bar{v}_0, \dots, \bar{v}_k\}$.

$\bar{x} \in \mathbb{R}^d$ is a **strong witness** for σ w.r.t S if it is a weak witness, and in addition, $\|\bar{x} - \bar{v}_0\| = \|\bar{x} - \bar{v}_1\| = \dots = \|\bar{x} - \bar{v}_k\|$.

Equivalently, we say that σ is weakly (or strongly) witnessed by $\bar{x}$.

We could define the Delaunay complex in terms of existence of strong and weak witnesses for the simplices. Subsequently, we could relax (some of) the requirements to build complexes that are more manageable in size.

We first illustrate weak and strong witness points on the Delaunay complex we have seen previously.



x is a strong witness for Δbcd. Notice that x is the center of the circumcircle of Δbcd, which is also the (point of) intersection of the Voronoi cells of the vertices b, c, and d.

y is a weak witness for $\overline{dg}$, and also for Δadg. Notice that as drawn, $\|y-g\| < \|y-d\| < \|y-a\| < \|y-v\|$ for $v = b, c, e, f, h$.

z is a weak witness for Δabe. Also, Δabe as shown does not have a strong witness. Intuitively, the center of the circumcircle of Δabe lies closer to f than to $a, b,$ and e.

Indeed, every simplex in Del_S will have a strong witness, which is the center of the empty circumsphere of that simplex. Ideally, we want to sample from S, and look for witnesses for simplices in the points not included in the sample. At the same time, looking for a strong witness among a given set of vertices ($\subseteq S$) is futile, as such a point occurs with zero probability. But the following result bails us out.

Result (de Silva, 2003) $\sigma = [v_0 \cdots v_k] \subseteq S$ has a strong witness iff every $\tau \leq \sigma$ (face) has a weak witness.

Notice that one direction is obvious — if σ has a strong witness, the same point is a strong witness for all its faces too, and hence every face has a weak witness. The other direction is more technical — see the paper posted on the course web page for details.

We define witness complexes in the more general setting of a metric space with pairwise distances between points provided.

Let $D = [d_{ij}]$ be the $\ell \times n$ distance matrix between $L \subseteq S$ of landmark points and all points in S. Here, $|L| = \ell$, and $|S| = n$.

Def The (strict) **witness complex** $W_\infty(L,S)$ is the collection of all simplices $\sigma \subseteq L$ whose all subsimplices have weak witnesses in S.

This restriction of all faces having weak witnesses is required to insure that $W_\infty(L,S)$ is a simplicial complex. Notice that we are building simplices on points just from L, and not from all of S.

In particular, if $\sigma = [v_0 \cdots v_k] \in W_\infty(L,S)$, then there exists a j with $1 \leq j \leq n$ such that d_{ij} for $i = v_0, \dots, v_k$ are the $(k+1)$ smallest entries in the j^{th} column of D in some order.

We also say that $\bar{u}_j \in S$ (corresponding to the j^{th} column) is a witness to the existence of σ in $W_\infty(L,S)$.

Relationship to Del_L

Result $\sigma \in \mathrm{Del}_L$ iff σ is strongly witnessed.

(just follows from the empty circumsphere property).

But $\sigma \in W_\infty(L,S)$ implies that σ is strongly witnessed, as all its faces have weak witnesses. Hence, we get that

$$W_\infty(L,S) \subseteq \mathrm{Del}_L.$$

So, we are first choosing a possibly much smaller set L of points from S as landmarks. We then build a complex on L which also has a bound on the dimension of the simplices being included.

Similar to how we defined the Vietoris-Rips complex by relaxing the definition of the Čech complex, we now define an easier to construct version of the strict witness complex by requiring that only edges need to be present for a higher dimensional simplex to be included.

Def The **lazy witness complex** $W_1(L,S) \supseteq W_\infty(L,S)$ has the same 1-skeleton as $W_\infty(L,S)$. After that, $\sigma = [v_0 \cdots v_k] \subseteq L$ is in $W_1(L,S)$ iff all edges of σ are in $W_1(L,S)$.

In practice, we almost always work with the lazy witness complex $W_1(L,S)$, and write $W(L,S)$ to mean $W_1(L,S)$ (and not $W_\infty(L,S)$).

Q: Is $W_1(L,S) \subseteq Del_L$? If not, can you give a counterexample?

Think about it!

How to choose the landmarks L

First decide how many landmarks you want ($|L| = \ell$). Then,

two methods
- random selection (select ℓ points randomly)
- maxmin selection.

Maxmin selection of ℓ landmarks

Choose the first landmark ℓ_1 randomly. After that, inductively, with $\{\ell_1, \ldots \ell_{i-1}\}$ chosen, pick ℓ_i that maximizes the following function:

$$z \mapsto \min\{D(z,\ell_1), D(z,\ell_2) \ldots, D(z,\ell_{i-1})\},$$ where

$D(z,\ell_j)$ is the distance from z to ℓ_j.

Maxmin provides widespread coverage of S, but could also end up picking outliers.

Guidelines for choosing $\ell = |L|$

(de Silva, Carlsson, 2004) for data sampled from surfaces (in 3D), $\ell \leq \frac{n}{20}$ works reasonably well.

Javaplex and Gudhi provide functions to build witness complexes.

https://github.com/appliedtopology and https://gudhi.inria.fr/.

Now that we have seen how to build several simplicial complexes on point sets, we will talk about how to infer the topology of the built complex. We first review basic results from algebra, and use them to define and study groups on the simplicial complex.

Review of Algebra (Groups)

A <u>binary operation</u> $*$ on a set S is a rule that assigns to each ordered pair $(a,b) \in S$ some element in S.

e.g., $a * b = c$, for $c \in S$.

If $a*b = b*a \ \forall a,b \in S$, $*$ is **commutative**.

$(a*b)*c = a*(b*c) \ \forall a,b,c \in S \Rightarrow *$ is **associative**.

A **group** $\langle G, * \rangle$ is a set G with a binary operation $*$ defined on elements of G such that the following conditions hold.

(a) $*$ is associative.

(b) $\exists e \in G$ such that $e*a = a*e = a \ \forall a \in G$.

e is an identity element for $*$ on G.

(c) $\forall a \in G$, $\exists a' \in G$ such that $a*a' = a'*a = e$.

a' is the inverse of a with respect to $*$.

We assume that G is **closed under** $*$ to begin with, i.e., $\forall a,b \in G$, $a*b = c$ for some $c \in G$.

If G is finite, the **order** of the group is $|G|$. Oftentimes, G itself is used to denote the group, with operation $*$ understood.

e.g., $\langle \mathbb{Z}, + \rangle$, $\langle \mathbb{Z}_4, +_4 \rangle$

integers

$\{0,1,2,3\}$

add modulo 4

$\mathbb{Z}_4$	0	1	2	3
0	0	1	2	3
1	1	2	3	0
2	2	3	0	1
3	3	0	1	2

If $*$ is commutative, G is an **Abelian group**. We also say that G is **abelian**.

$\mathbb{Z}$ and $\mathbb{Z}_4$ are both abelian. Also, notice that the order of $\mathbb{Z}_4$ is 4.