Computational Topology

seminar

Alpha shapes

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1. Intuitive definition and applications
2. Formal definition
3. Construction of alpha-shapes (Edelsbrunner's algorithm)
4. Dual definition, union of balls and homotopy equivalence
5. Limitations of classical alpha-shapes
6. Extensions
    - Conformal Alpha-Shapes
    - Weighted-Alpha Shapes

What are α-shapes ?

Originally introduced by:
H. Edelsbrunner, D. G. Kirckpatrick and R. Seidel. ***On the shape of a set of points in the plane***

Approach to formalize the intuitive notion of "shape" for spatial point sets

Generalization of the convex hull of a point set

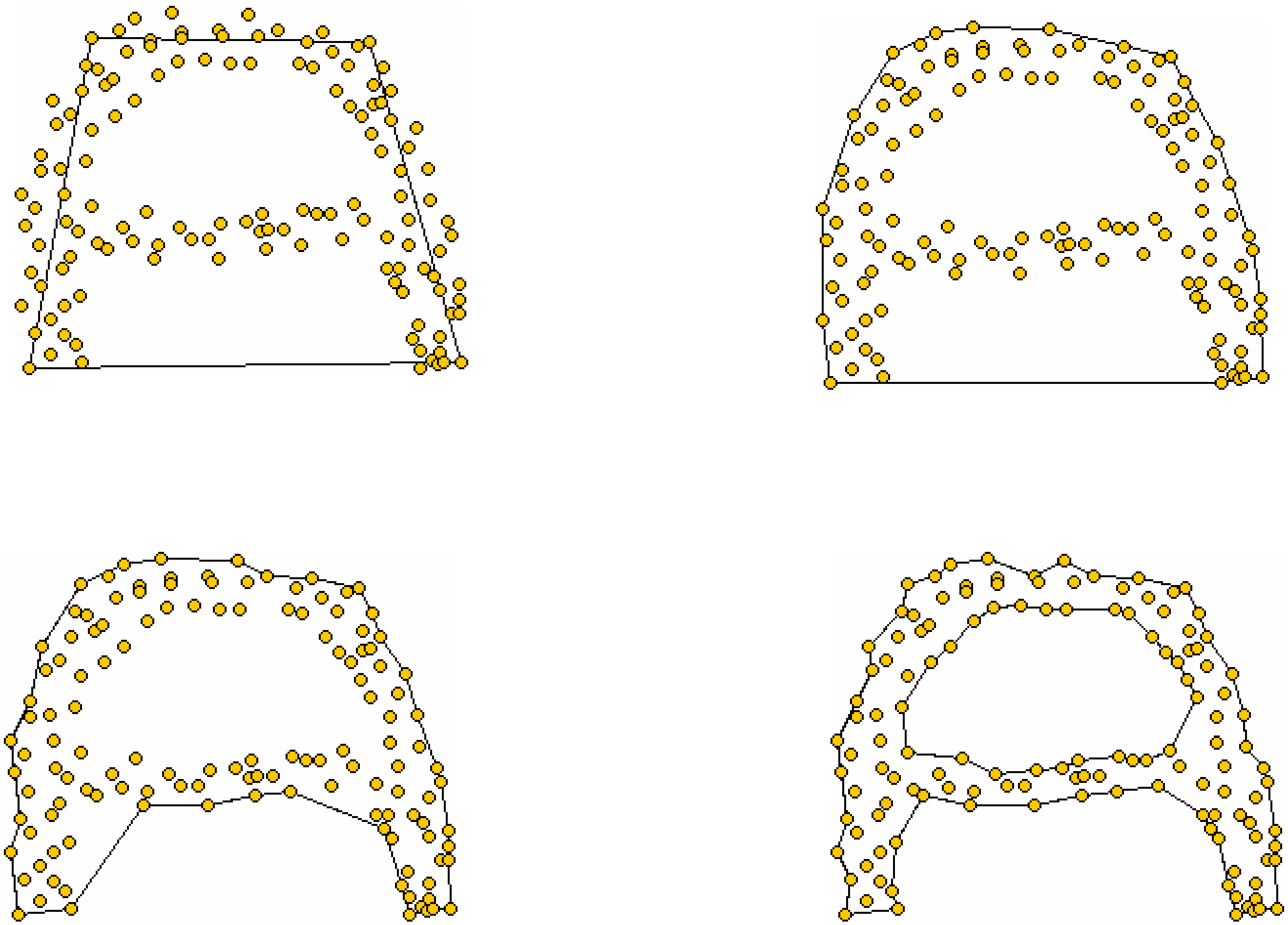
Family of shapes derived from the Delaunay triangulation
parametarized by α

Dual shape* of the union of balls **...**

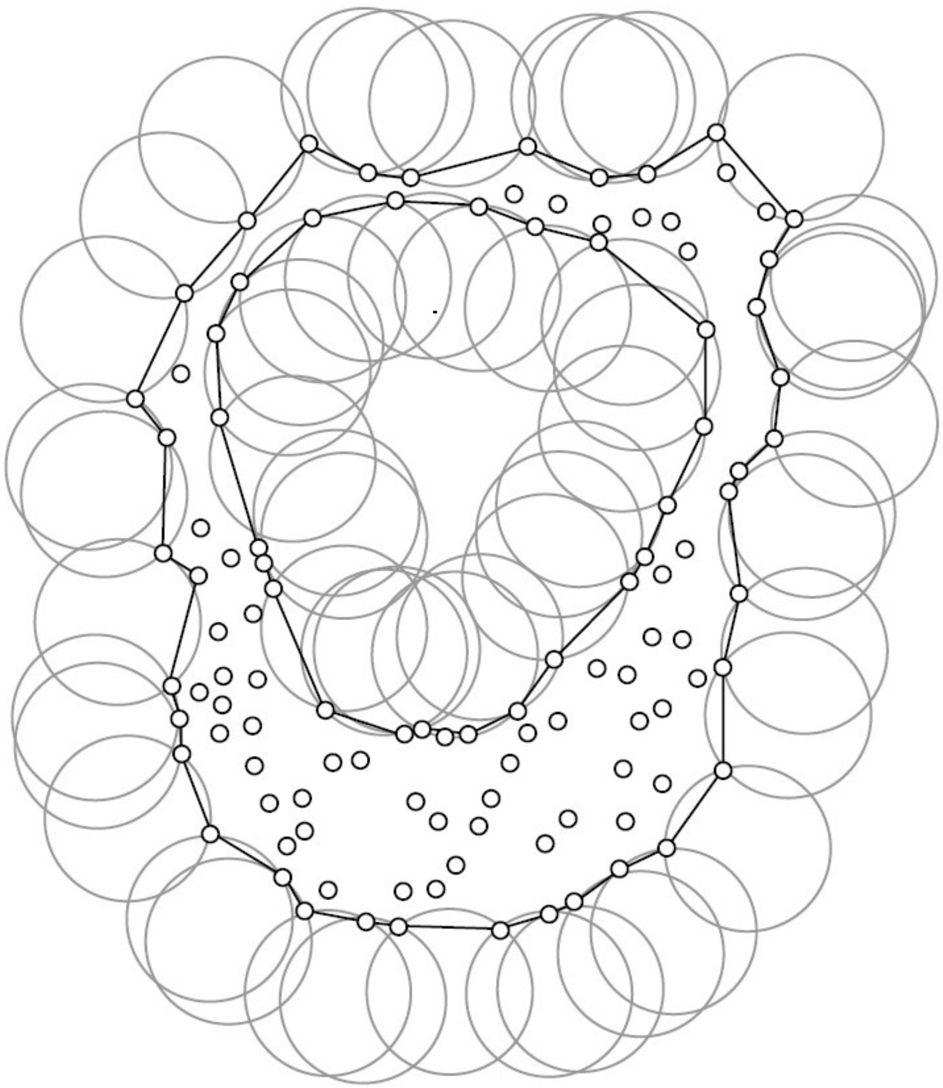
Intuitive definition

Assume a finite set of points in the plane

We have a intuitive notion of the shape formed by these points



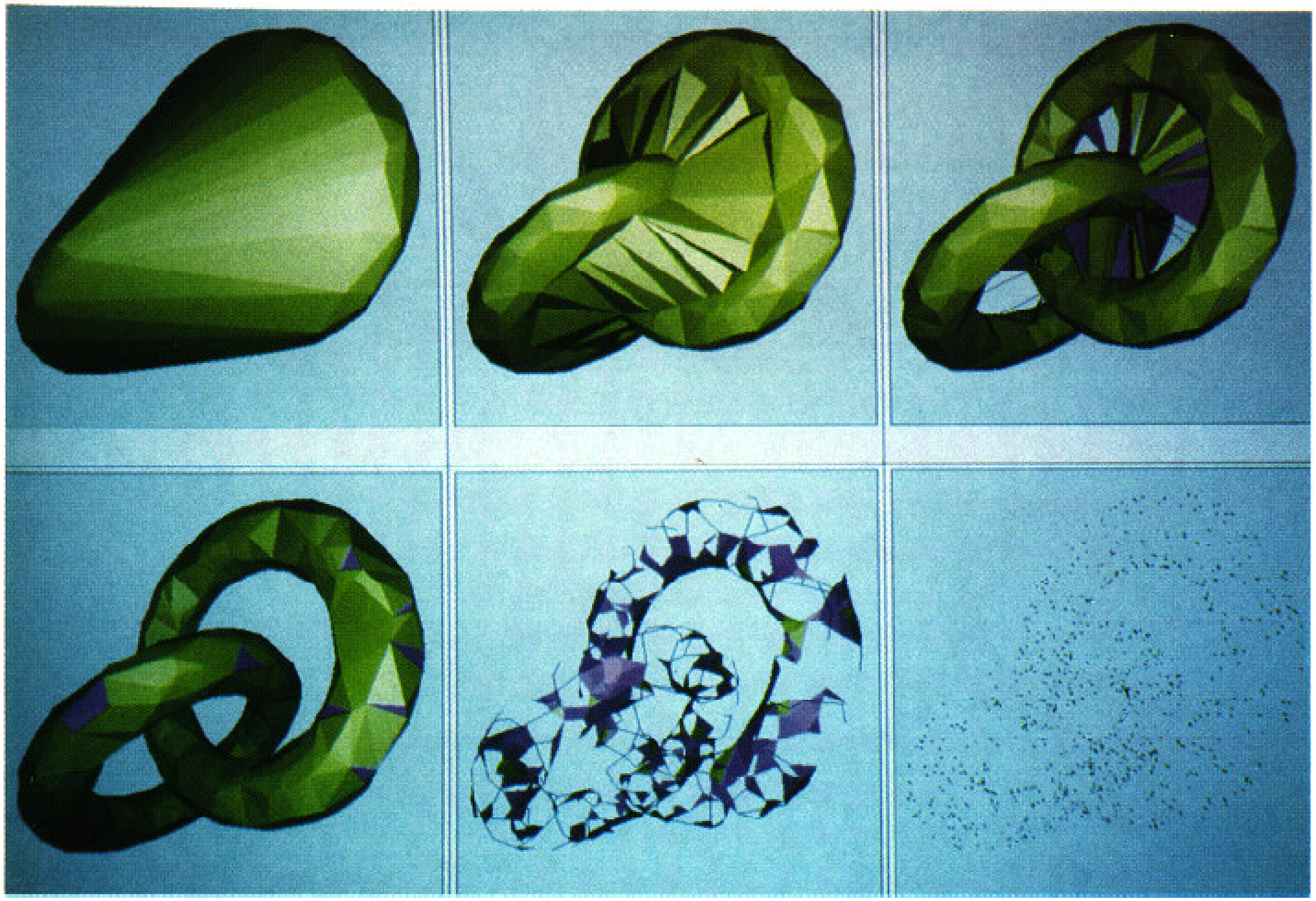
Intuitive definition



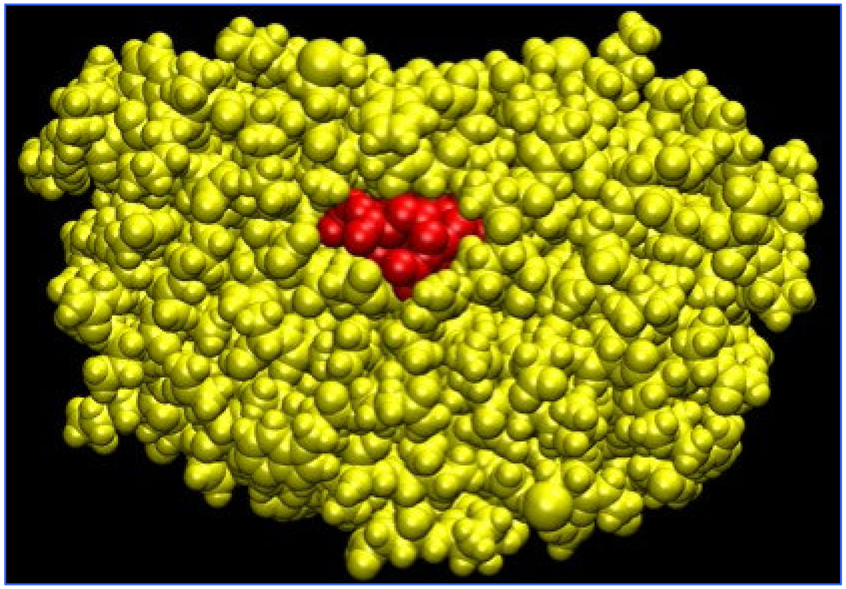
$\alpha \to \infty$

$\alpha \to 0$

- **Surface reconstruction and geometric modeling** (later more)



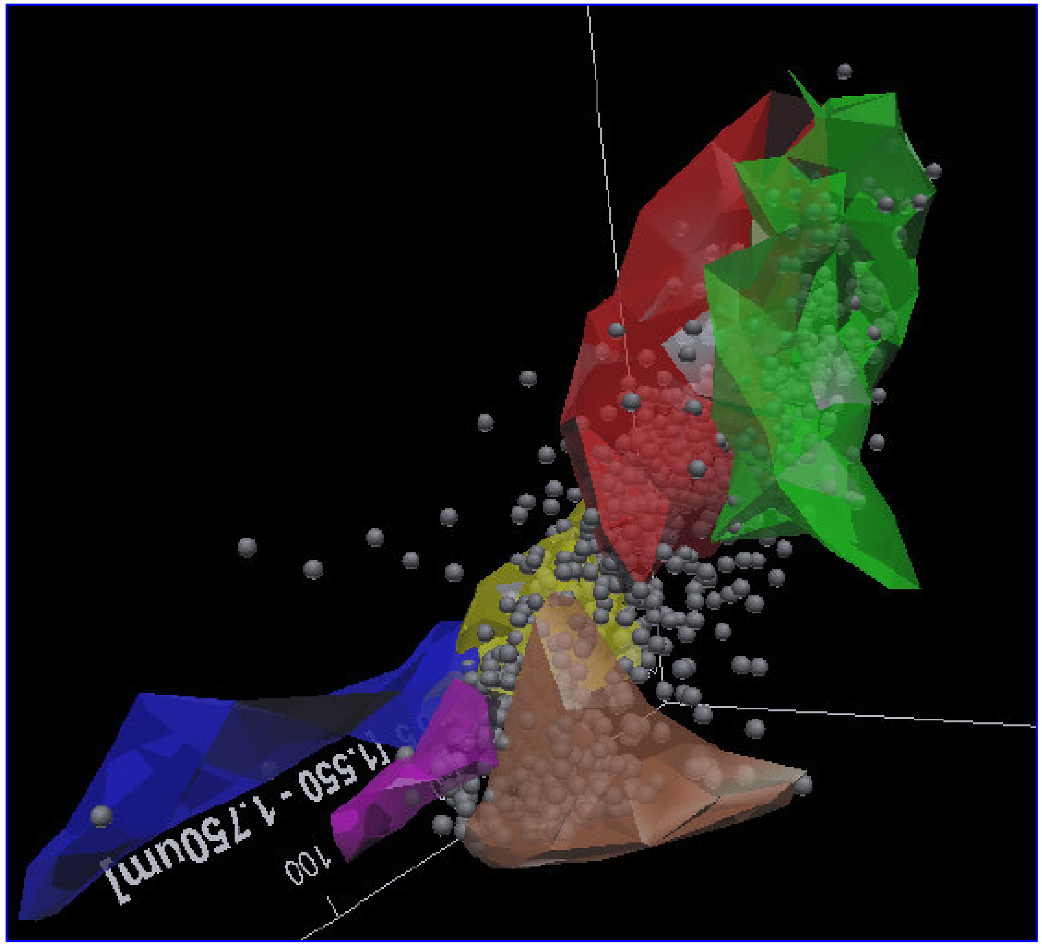
- **Modeling molecular structures** **(later more)**



HIV-1 Protease

Applications

- **Classification and visualization**



- Grid generation
- Medical image analysis
- Visualizing the structure of earthquake data …

Let the points in S be in general position

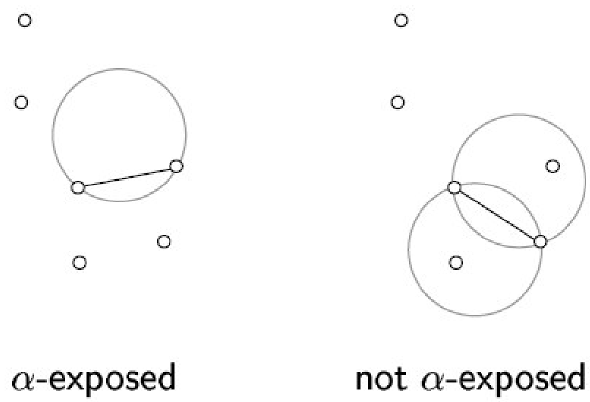
def. In $k\text{-}1$ dimensional hyperplane lie at most k points …

$T \subset S$ **with** $|T| = k+1 \leq d+1$**, the polytope** $\Delta_T = conv T$ **has dimension** k

Then Δ_T **is a** k**-simplex**

Definition. $\alpha - ball$: Open ball with radius α, where ∂b is the surface of the sphere

Definition. k-simplex Δ_T is α-exposed if there exists an empty $\alpha - ball$ with $T = \partial b \cap S$



…analogy with the ice-cream “scenario”?

Let S_α be our alpha-shape

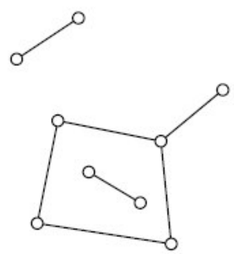
Then the boundary ∂S_α consists of all k-simplices of S, which are α-exposed

$$\partial S_\alpha = \{\Delta_T \mid T \subset S, |T| \le d \text{ and } \Delta_T \text{ is } \alpha-\text{exposed}\}$$

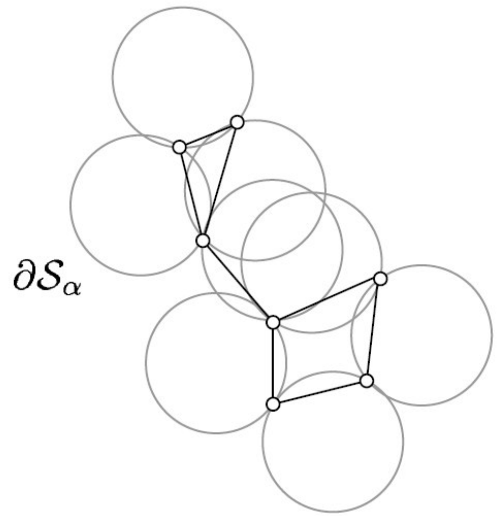
But what exactly is our alpha-shape?
Does it have a structure in space?

Or more formally…

Is there any *polytope* P such that $\partial S_\alpha = \partial P$?



These simplices do not form a boundary.



later …

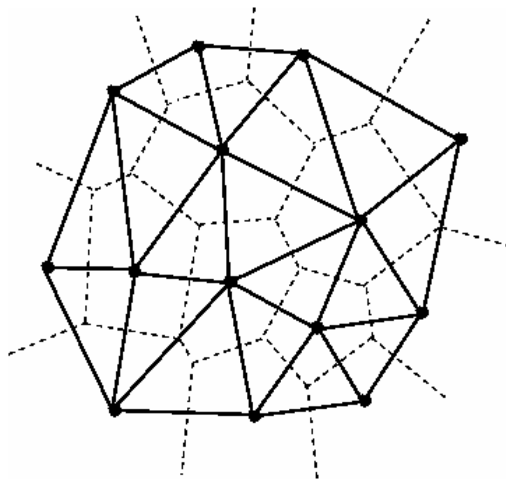
Observation.

$$\lim_{\alpha \to 0} S_\alpha = S \qquad \lim_{\alpha \to \infty} S_\alpha = convS$$

Definiton. The **Delaunay triangulation** of $S \subset R^d$ is the **simplicial complex** $DT(S)$ consisting of:

(i) All d-simplices such that their circumsphere does not contain any other points

(ii) All k-simplices which are faces of other simplices in $DT(S)$



Delaunay triangulation is the dual shape of the Voronoi diagram

Observation.

If Δ_T is an α-exposed simplex of S, then $\Delta_T \in DT(S)$

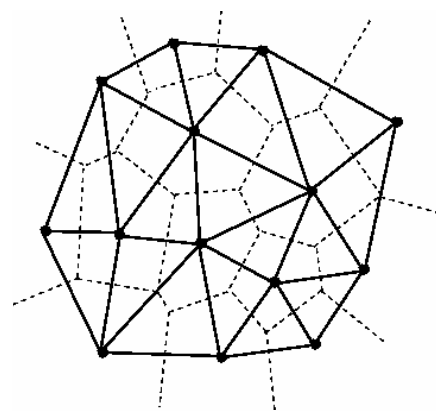
$Proof.$ (black-board)

Observation.

For any $0 \le \alpha \le \infty \quad S_\alpha \subset DT(S)$

This results allows us to construct simple algorithm for computing the alpha-shape

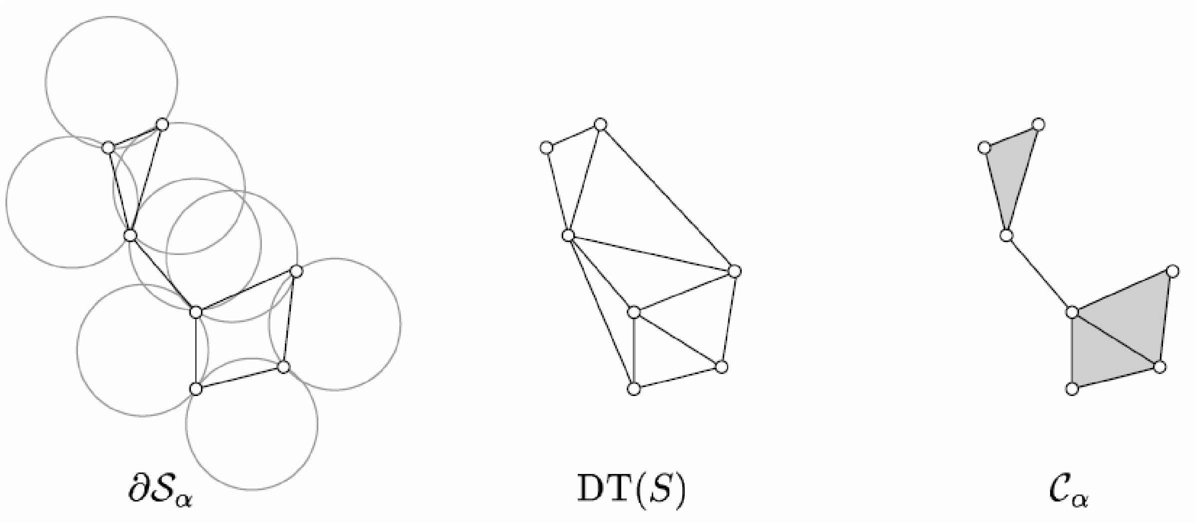
for each $(d\text{-}1)$*-simplex* Δ_T *in* $DT(S)$
if one of its circumspheres with radius α *is empty*
then Δ_T *is* α*-exposed*



…but what about lower dimensional simplices ?
infinitely many α-balls touching it

Definition. The α-complex $C_\alpha(S)$ is a simplicial subcomplex of $DT(S)$.
A simplex $\Delta_T \in DT(S)$ is in $C_\alpha(S)$ if

(i) it's circumsphere is empty and has radius smaller than α, or
(ii) Δ_T is a face of another simplex in $C_\alpha(S)$



We found a simplicial complex with boundary ∂S_α …

Result. The boundary of the α-complex is the boundary of the α-shape
There exist a polytope P, such that $\partial S_\alpha = \partial P$, for all $\infty \geq \alpha \geq 0$

One can prove:

$$\Delta_T \in \partial S_\alpha(S) => \Delta_T \in C_\alpha(S)$$

$$\Delta_T \in \partial S_\alpha(S) => \Delta_T \in \partial C_\alpha(S)$$

$$\Delta_T \in \partial C_\alpha(S) => \Delta_T \in \partial S_\alpha(S)$$

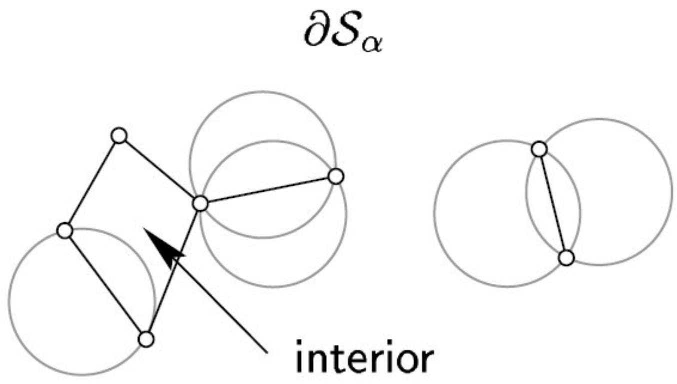
Finally:

$$\partial C_\alpha(S) = \partial S_\alpha(S)$$

$$S_\alpha(S) \leftarrow C_\alpha(S)$$

The α-shape is the α-complex

How to find the interior of an alpha-shape?



The straight-forward way:
Inspect the α-complex structure and check whether there is a d-simplex containing the facet

Another (better) way:
A facet Δ_T bounds the interior iff exactly one of the two α-balls with $T = \partial b \cap S$ is empty

Proof. (black-board)

Observation.

$$\alpha_1 \le \alpha_2 => C_{\alpha_1}(S) \subset C_{\alpha_2}(S) => S_{\alpha_1}(S) \subset S_{\alpha_2}(S)$$

Proof.

According *(i)* $\alpha_1 \le \alpha_2$ implies $C_{\alpha_1}(S) \subset C_{\alpha_2}(S)$

α-complex:

(i)	it's circumsphere is empty and has radius smaller than α, or
(ii)	Δ_T is a face of another simplex in $C_\alpha(S)$

Result.

This shows that for any simplex $\Delta \in DT(S)$ there is an interval $I = [a, \infty]$ and the simplex is in $C_\alpha(S)$ iff $\alpha \in I$

Basis for Edelsbrunner's Algorithm … (next)

1. **Compute the Delaunay triangulation of S knowing that it contains our α-shape**

2. **Compute C_α by inspecting all simplices Δ_T in $DT(S)$:**

   if **its circumsphere is empty with smaller radius than α** *then*
   accept it (as well as all of its faces)

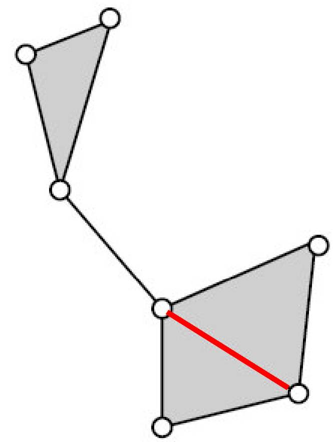
3. **All d-simplices of C_α make up the interior of S_α. All simplices on the boundary ∂C_α form ∂S_α**

We need certain "primitives" to make the algorithm work:

- Delaunay triangulation (easy)
- Test of "emptiness" (easy)
- Whether a simplex lies on the boundary or inside ?

Whether a simplex lies on the boundary or inside ?

1. If $\Delta_T \in \mathrm{conv}S$ then it must lie on the boundary
2. If all d-simplices containing it lie in C_α, then its inside



Let's increase α from 0 to infinity and let $\Delta_T \in DT(S)$,

$$\Delta_T \quad \text{is} \quad \begin{cases} \text{not in } \mathcal{C}_\alpha & (\text{for } \alpha < a) \\ \text{in } \partial\mathcal{C}_\alpha & (\text{for } \alpha \in \boxed{(a,b)}) \\ \text{interior to } \mathcal{C}_\alpha & (\text{for } \alpha \in \boxed{(b,\infty)}) \end{cases} \quad \text{for all } \Delta_T \in DT(S)$$

The algorithm computes all possible α-shapes for S

Case 1: d-dimensional simplex (trivial)

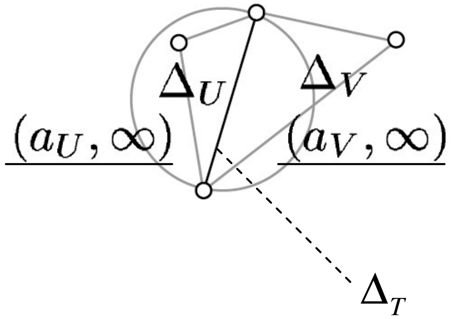
Cannot be on the boundary: a = b = *radius of its circumsphere*

Case 2: k-dimensional simplex ($k<d$)

Idea: compute interval of k-simplex using already computed intervals for $(k+1)$-simplices.

α-complex:

(i) it's circumsphere is empty and has radius smaller than α, or
(ii) Δ_T is a face of another simplex in $C_\alpha(S)$



$$\Delta_T \in \mathcal{C}_\alpha \quad \Leftrightarrow \quad \Delta_U \text{ or } \Delta_V \text{ in } \mathcal{C}_\alpha$$
$$\Leftrightarrow \quad \alpha \in (\min(a_U, a_V), \infty)$$

Observation. Let $\Delta_T \in DT(S)$

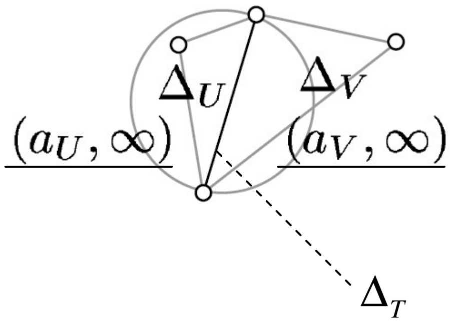
$$a = \min\{a_U \mid B_U = (a_U, b_u),\ \Delta_U\ (k+1)\text{-}Simplex,\ T \subset U\}$$

Then $\Delta_T \in \mathcal{C}_\alpha$ *if and only if* $\alpha \in (a, \infty)$.

α-complex:

(i) it's circumsphere is empty and has radius smaller than α, or
(ii) Δ_T is a face of another simplex in $C_\alpha(S)$

If $\Delta_T \in \mathrm{conv} S$ then it must lie on the boundary



$$\Delta_T \in \mathrm{int}(\mathcal{C}_\alpha) \Leftrightarrow \Delta_U \text{ und } \Delta_V \text{ in } \mathcal{C}_\alpha$$
$$\Leftrightarrow \alpha \in (\max(a_U, a_V), \infty)$$

Observation. Let $\Delta_T \in C_S(\alpha)$

$$b = \max\{a_U \mid B_U = (a_U, b_u),\ B_U \textit{ d-Simplex mit } T \subset U\}$$

Then $\Delta_T \in$ interior of $C_S(\alpha)$ iff $\alpha \in (b, \infty)$

Whether a simplex lies on the boundary or inside

1. If $\Delta_T \in \mathrm{conv} S$ then it must lie on the boundary
2. If all d-simplices containing it lie in C_α , then its inside

Altogether we get the following algorithm:

```
procedure AlphaShape(S,d);
{Given a point-set S ⊂ ℝ^d, computes a list R of simplices Δ_T and}
{two lists B, I of intervals such that Δ_T ∈ ∂𝒮_α if and only if α ∈ B_T}
{and Δ_T ∈ int(𝒮_α) if and only if α ∈ I_T.}
begin
    R:= DT(S);
    for each d-simplex Δ_T ∈ R do
        B_T:= ∅; I_T:= (σ_i, ∞);
    end for;
    for k := d − 1 to 0 by −1 do
        for each k-simplex Δ_T ∈ R do
            if b_T is empty then
                a:= σ_T;
            else
                a:= min {a_U | B_U = (a_U, b_u), Δ_U (k + 1)-Simplex, T ⊂ U
            if Δ_T ∈ ∂ conv(S) then
                b:= ∞;
            else
                b:= max {a_U | B_U = (a_U, b_u), B_U d-Simplex mit T ⊂ U};
            B_T:= (a, b); I_T:= (b, ∞);
        end for;
    end for;
    return (R, B, I);
end AlphaShape;
```

Two dimensions.

Delaunay triangulation doable in $O(n \log n)$ time

The number of simplices (faces) is $O(n)$

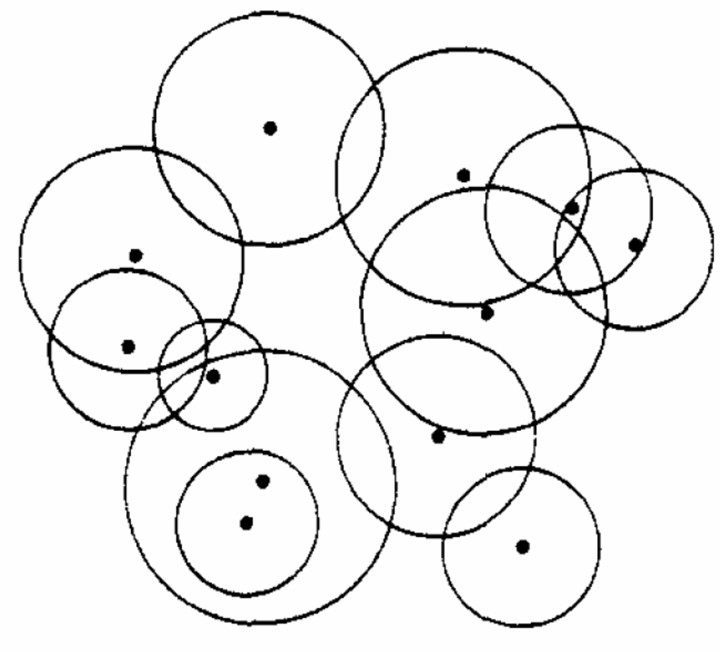
***d* dimensions.**

The number of simplices is $\Theta(n^{\lceil (d-1)/2 \rceil})$!

α–shapes are tightly related to another type of shape: **The union of d-dimensional balls**

Connection to be established soon…

Let B be a set of n d-balls in R^d



Union of balls important for modeling molecules in chemistry and biology

Union of balls – The three primal diagrams

$p_b = \{x \in R^d : \| x - b \| \leq \| x - b' \|, b' \in B\}$ - *voronoi* cell

$q_b = p_b \cap b$ - intersection of the cell with its ball

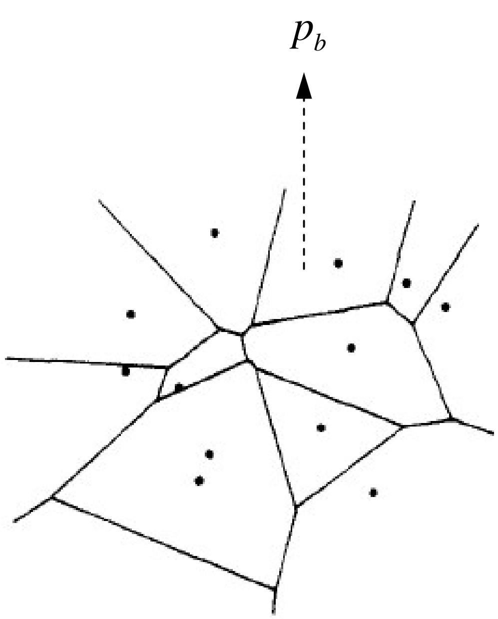
$p_T = \bigcap_{b \in T} p_b$

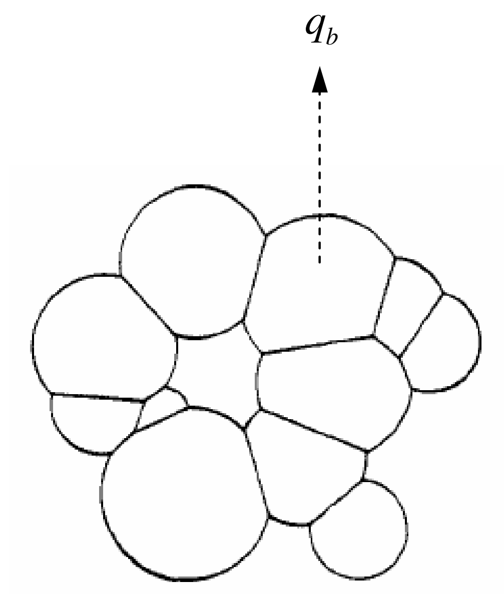
$q_T = \bigcap_{b \in T} q_b$

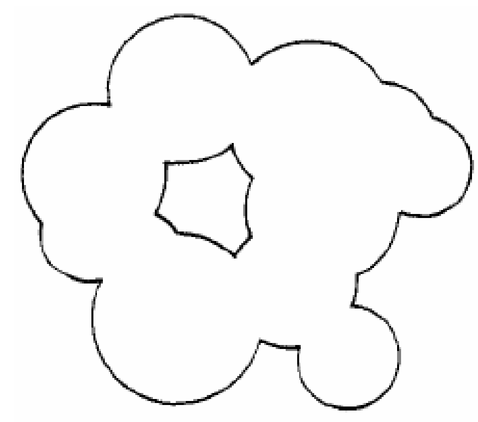
$P = P(B) = \{p_T \mid \emptyset \neq T \subseteq B\}$ The *power diagram* of B (generalization of the Voronoi diagram)

$D = D(B) = \{q_T \mid \emptyset \neq T \subseteq B\}$ *Intersection* of P with U

$U = U(B) = \bigcup_{b \in B} b$ The *union* of the balls







$$P = P(B) = \{ p_T \mid \emptyset \neq T \subseteq B \}$$

$$|P| = \bigcup_{p_T \in P} p_T = R^d$$

$$D = D(B) = \{ q_T \mid \emptyset \neq T \subseteq B \}$$

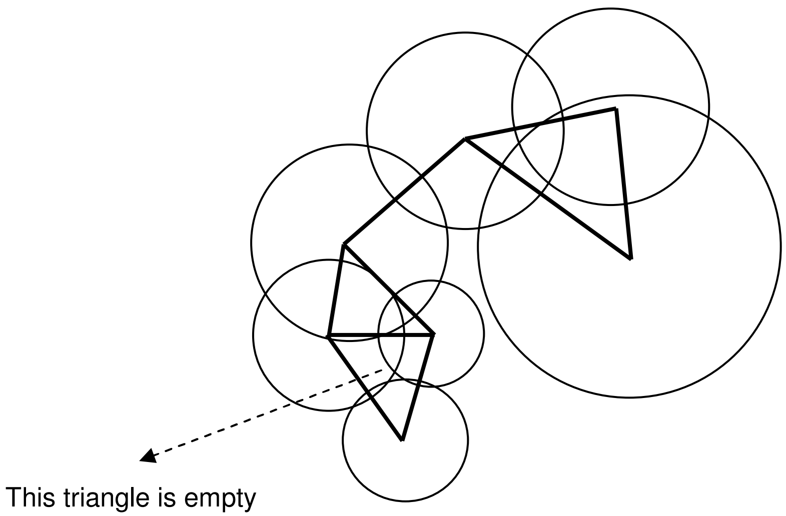
$$|D| = U$$

$$U = U(B) = \bigcup_{b \in B} b$$

Definition. Nerve of a collection of sets A is $N(A) = \{X \subseteq A \mid \bigcap_{a \in X} a \neq \emptyset\}$

All subsets of A with non-empty intersection (thus $N(A)$ is an abstract simplicial complex)

Example: The nerve of B is the collection of all subsets of d-balls with non-empty common intersection



Geometric realization of the nerve of a set of balls

$\sigma_T \equiv$ Convex hull of the centers of the d-balls in T (actually the corresponding simplex $convT$)

$R = R(B) = \{\sigma_T \mid \emptyset \neq p_T \in P\} \cup \{\emptyset\}$ The *regular triangulation* of B (Delaunay triangulation)

$K = K(B) = \{\sigma_T \mid \emptyset \neq q_T \in D\} \cup \{\emptyset\}$ The *dual complex* of D

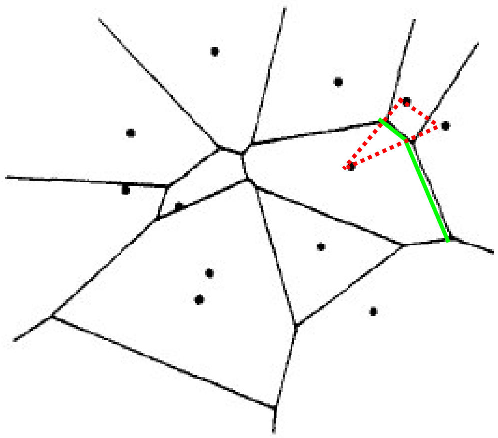
$S = S(B) = |K|$ The *dual shape* of U

R and K are geometric realizations of the nerves of P, D

$P = P(B) = \{p_T \mid \emptyset \neq T \subseteq B\}$

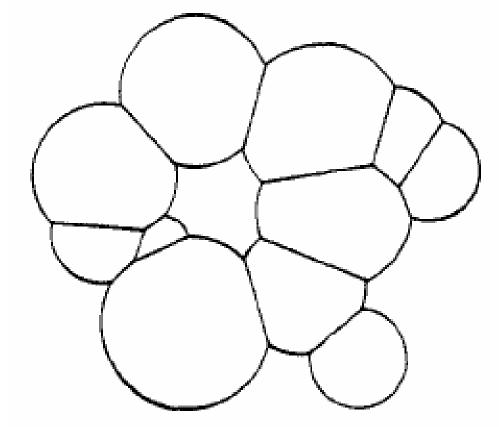
$D = D(B) = \{q_T \mid \emptyset \neq T \subseteq B\}$

$U = U(B) = \bigcup_{b \in B} b$

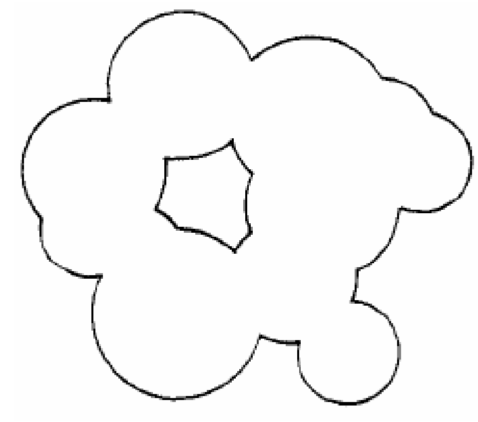


$$P = P(B) = \{ p_T \mid \varnothing \neq T \subseteq B \}$$

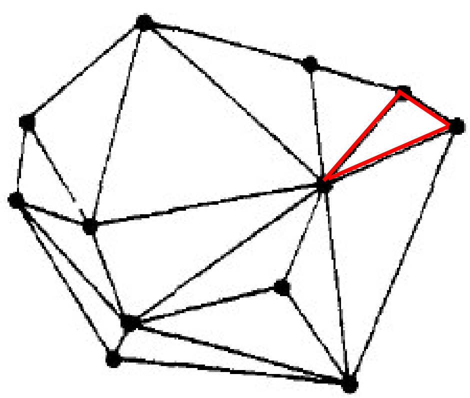
$$p_T \in P \Leftrightarrow \sigma_T \in R$$



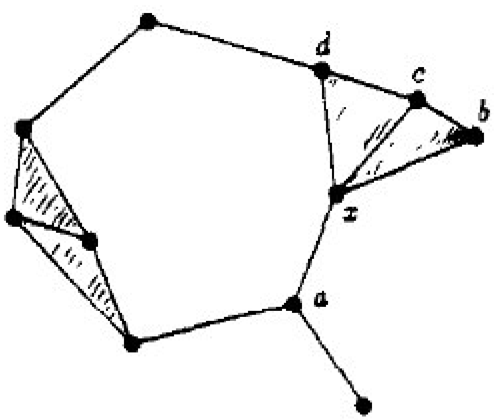
$$D = D(B) = \{ q_T \mid \varnothing \neq T \subseteq B \}$$



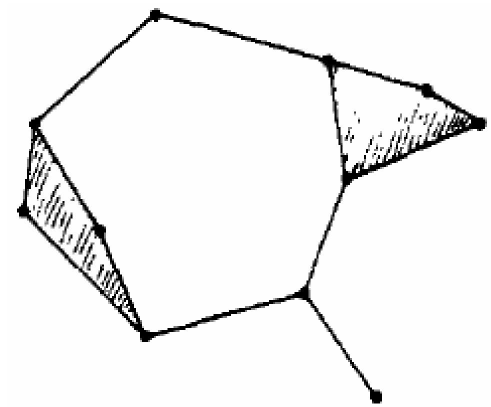
$$U = U(B) = \bigcup_{b \in B} b = |D|$$



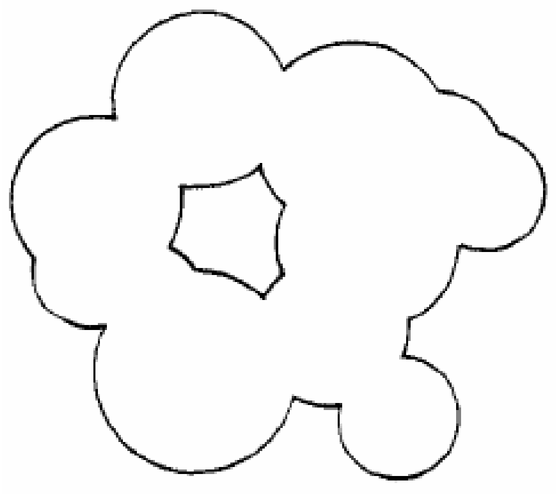
$$R = R(B) = \{ \sigma_T \mid \varnothing \neq p_T \in P \} \cup \{ \varnothing \}$$



$$K = K(B) = \{ \sigma_T \mid \varnothing \neq q_T \in D \} \cup \{ \varnothing \}$$

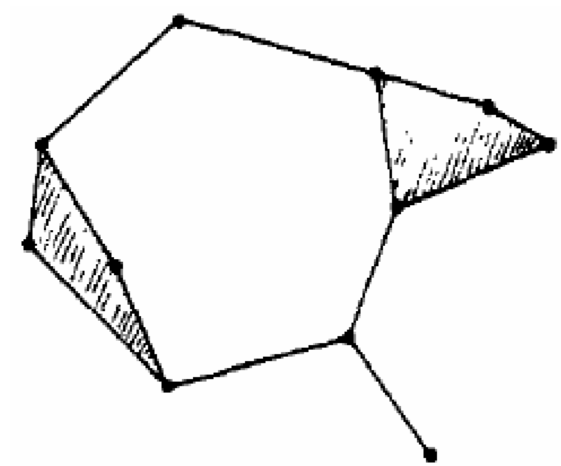


$$S = S(B) = |K|$$



$$U = U(B) = \bigcup_{b \in B} b = |D|$$

dual

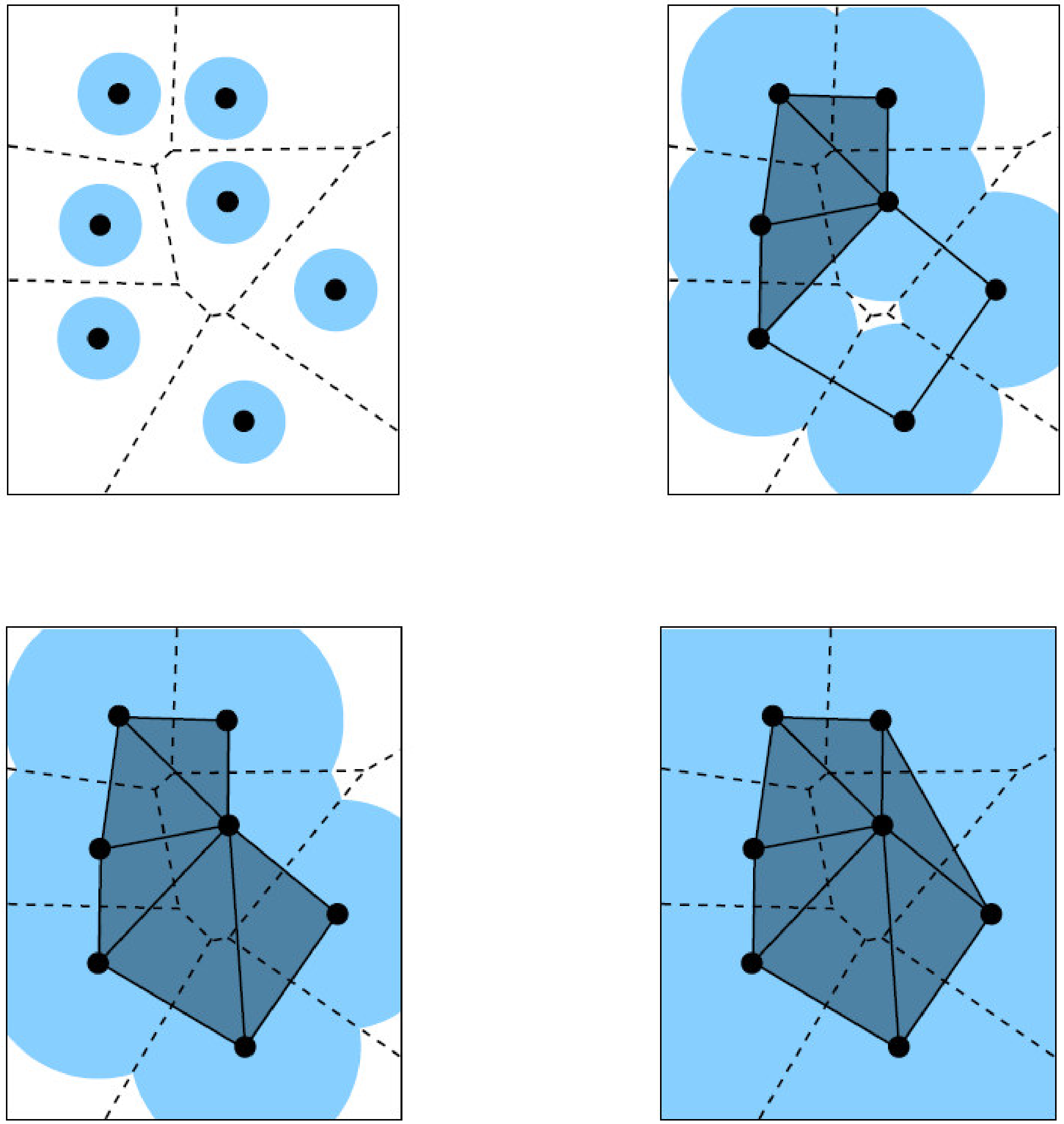


$$S = S(B) = |K|$$

Boundary of this complex is the boundary of an α-shape* !

Alpha shape is the nerve of the union of balls intersected with their respective voronoi cells

Anybody noticing any difference with the previous definition? :-)



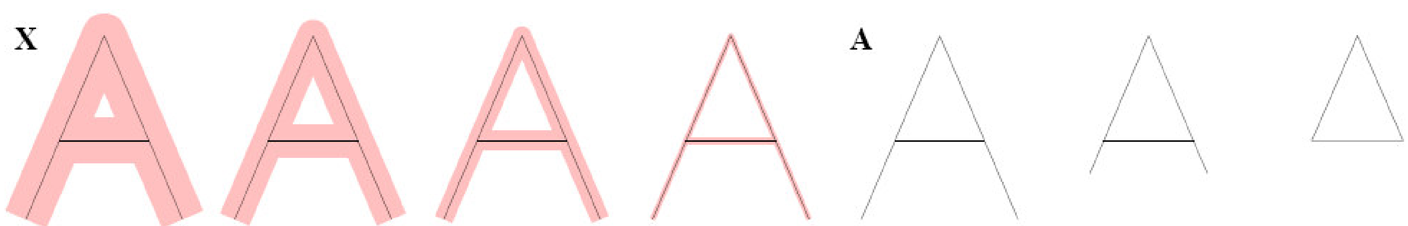
Result. They are homotopy equivalent!

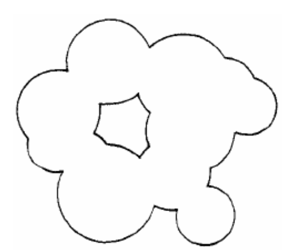
S captures the basic topology of the union (but independently of dimension)

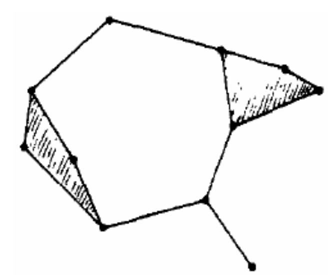
Deformation retraction. S is a deformation retraction of U

Intuitively, continuous deformation of *the space* until becomes *the subspace* without moving…

Special case of homotopy (the requirement of subspace is relaxed here)







For a topological space Y, the k-th homology group $H_k = H_k(Y)$ is an abelian group that expresses the k-dimensional connectivity of Y

Theorem. Two homotopy equivalent topological spaces have isomorphic homology groups.

Fact. There are very well known and efficient algorithms for computing homology groups of simplicial complexes.

Result. We have an efficient algorithm for computing the homology groups for the union of balls!

Union of balls – Algorithmic implications of homotopy equivalence

The Union of balls as a model for various molecules has

- Combinatorial
- Metric
- Topological properties
- Folding, Connectivity …

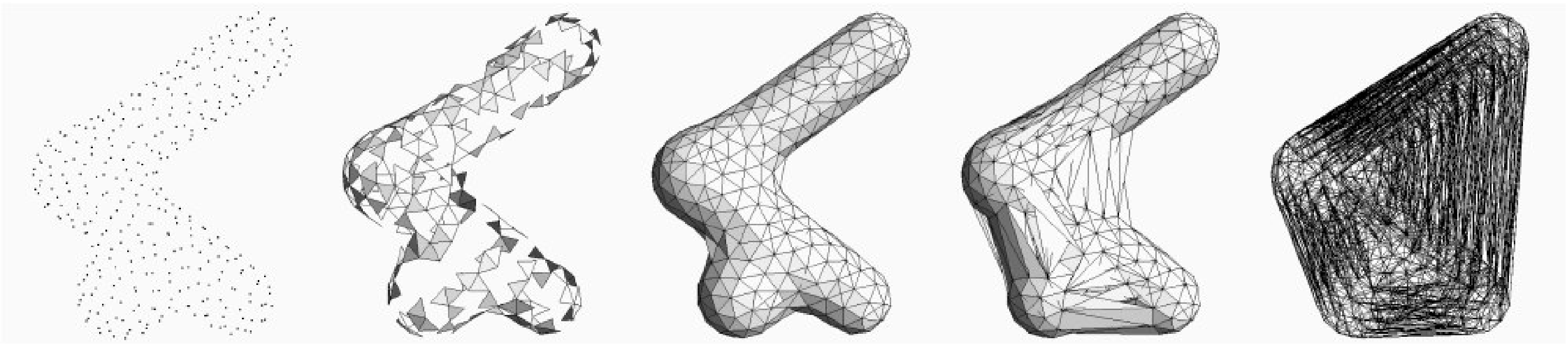
…**directly computable** from the α-shape which is computationally inexpensive

Examples:

- Counting faces of the union of balls
- Measuring the union of balls (ex. volume)
- Physical forces associated with the molecules etc.

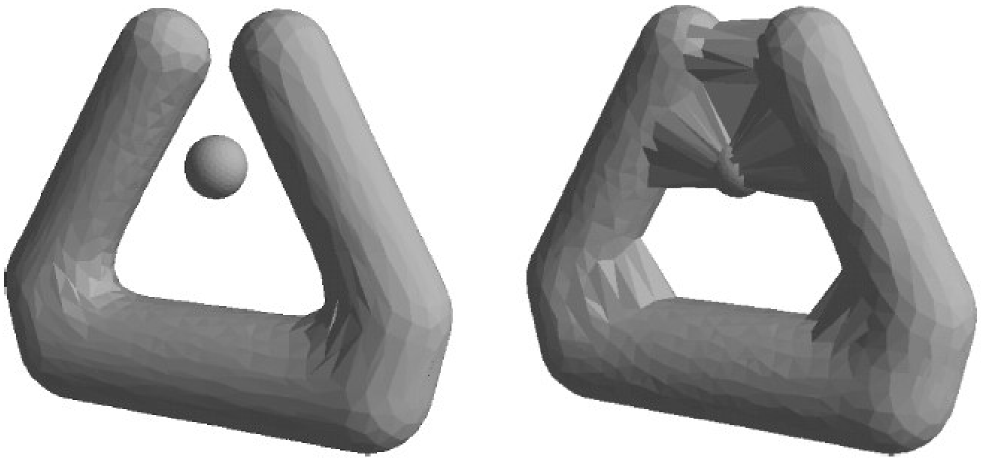
Shape modeling.

Reconstruction of objects which have been sampled by points.



How to determine the “best” α ?

Limitations of classical alpha shapes



There are sets of points for which no satisfying α exists

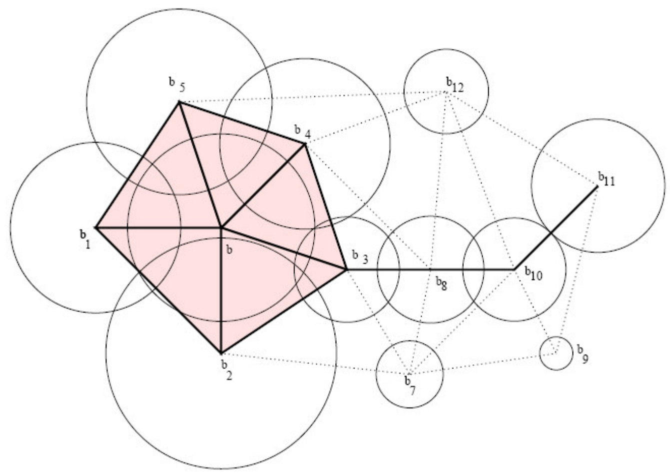
- Low density point-set will require large α in order to connect...
- Non-uniform distribution of points not appropriate

Extensions – weighted alpha shapes

Generalization of α-shapes (the dual of the union of balls)

Each point has a weight assigned, α-shapes: all weights set to 0

Intuitively weights corresponds to radii of the balls



Again weighted alpha shape (again) is a polytope whose boundary is the union of all α-exposed simplices spanned by S

Different definition of α-exposed simplex

Solves the problem of classical α-shapes for non-uniform density of sample points

Problem: How to assign the weights?

Conformal α-shape. Use a local scale parameter $\hat{\alpha}$ instead of the global scale parameter α

Used for reconstructing 3-dimensional smooth surfaces from a finite sampling…

At each point p in S we put a ball of radius α_p determined from its internal alpha scale:

$$\alpha_p(\hat{\alpha}) = \alpha_p^+ \hat{\alpha} + \alpha_p^- \qquad \alpha_p^+ = \| p - p^* \| \quad \alpha_p^- = \alpha_p^1 = 0$$

Let $C_p^{\hat{\alpha}}$ be the intersection of the voronoi cell and the ball at p, and let $C^{\hat{\alpha}}$ be the interior of $\bigcup_{p \in P} C_p^{\hat{\alpha}}$

Then *conformal alpha complex* is the Delaunay triangulation restricted to $C^{\hat{\alpha}}$

Also a filtration of the Delaunay triangulation $DT(S)$

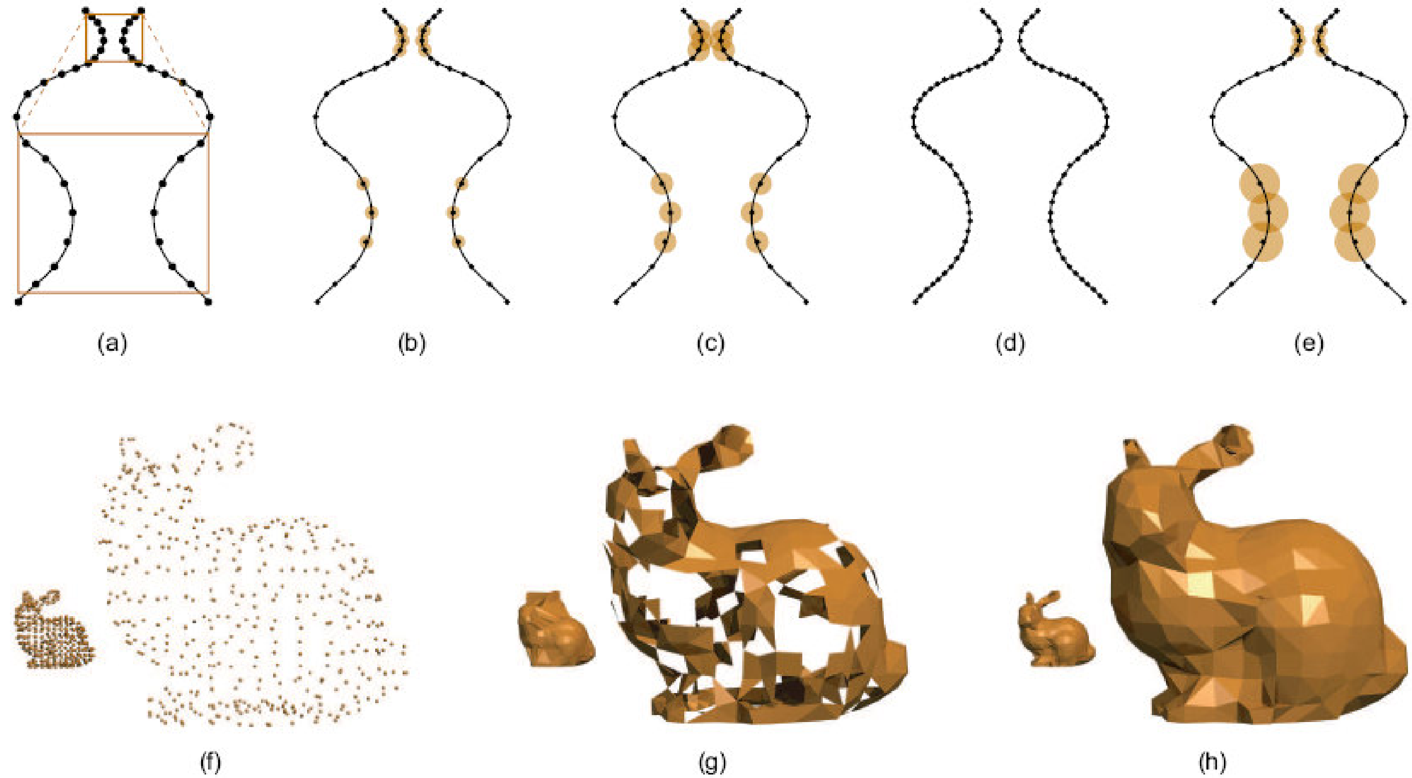


Fig. 5 Adapting the growth of the balls at the sample points as it is done for conformal α-shapes illustrates the superiority of conformal α-shapes (e) over uniform α-shapes (b,c) for curve and surface reconstruction from non-uniform samples (a). Uniform α-shapes would need uniform sampling as in (d). In (f) two scaled versions of a uniform sub-samples of the Stanford Bunny are shown in one scene to illustrate non-uniform sampling on a global scale. An α-shape for this sample is shown in (g) and a conformal α-shape is shown in (h).