Computational Topology

seminar

Alpha shapes
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 $\alpha$-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
parametrized by $\alpha$

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

Assume a finite set of points in the plane.
We have an intuitive notion of the shape formed by these points.
Intuitive definition

\[ \alpha \to \infty \]

\[ \alpha \to 0 \]
Applications

- Surface reconstruction and geometric modeling (later more)
Applications

- Modeling molecular structures (later more)

HIV-1 Protease
Applications

• Classification and visualization
Applications

• Grid generation

• Medical image analysis

• Visualizing the structure of earthquake data …
Formal definition – boundary of alpha-shape

Let the points in $S$ be in **general position**

*def.* In $k$-1 dimensional hyperplane lie at most $k$ points …

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

Then $\Delta_T$ is a **$k$-simplex**

**Definition.** $\alpha$–ball : Open ball with radius $\alpha$, where $\partial b$ is the surface of the sphere

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

...analogy with the ice-cream “scenario”?
Formal definition – boundary of alpha-shape

Let $S_\alpha$ be our alpha-shape

Then the boundary $\partial S_\alpha$ consists of all $k$-simplices of $S$, which are $\alpha$-exposed

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

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 …
Formal definition – Convex Hull and Delaunay Triangulation

Observation.

\[
\lim_{\alpha \to 0} S_\alpha = S \quad \lim_{\alpha \to \infty} S_\alpha = \text{conv}S
\]

Definition. The **Delaunay triangulation** of \( S \subset \mathbb{R}^d \) 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 $\Delta_T$ is an $\alpha$-exposed simplex of $S$, then $\Delta_T \in DT(S)$

Proof. (black-board)

Observation.

For any $0 \leq \alpha \leq \infty$, $S_\alpha \subset DT(S)$

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

for each $(d-1)$-simplex $\Delta_T$ in $DT(S)$

  if one of its circumspheres with radius $\alpha$ is empty

  then $\Delta_T$ is $\alpha$-exposed

...but what about lower dimensional simplices?

infinitely many $\alpha$-balls touching it
**Definition.** The $\alpha$-complex $C_\alpha(S)$ is a simplicial subcomplex of $DT(S)$. A simplex $\Delta_T \in DT(S)$ is in $C_\alpha(S)$ if

1. its circumsphere is empty and has radius smaller than $\alpha$, or
2. $\Delta_T$ is a face of another simplex in $C_\alpha(S)$

**We found** a simplicial complex with boundary $\partial S_\alpha$ ... 

**Result.** The boundary of the $\alpha$-complex is the boundary of the $\alpha$-shape

There exist a polytope $P$, such that $\partial S_\alpha = \partial P$, for all $\infty \geq \alpha \geq 0$
One can prove:

\[ \Delta_T \in \partial S_{\alpha}(S) \Rightarrow \Delta_T \in C_{\alpha}(S) \]

\[ \Delta_T \in \partial S_{\alpha}(S) \Rightarrow \Delta_T \in \partial C_{\alpha}(S) \]

\[ \Delta_T \in \partial C_{\alpha}(S) \Rightarrow \Delta_T \in \partial S_{\alpha}(S) \]

Finally:

\[ \partial C_{\alpha}(S) = \partial S_{\alpha}(S) \]

\[ S_{\alpha}(S) \leftarrow C_{\alpha}(S) \]

The \( \alpha \)-shape is the \( \alpha \)-complex
How to find the interior of an alpha-shape?

**The straight-forward way:**
Inspect the $\alpha$-complex structure and check whether there is a $d$-simplex containing the facet.

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

*Proof.* (black-board)
Formal definition

Observation.

\[ \alpha_1 \leq \alpha_2 \Rightarrow C_{\alpha_1}(S) \subseteq C_{\alpha_2}(S) \Rightarrow S_{\alpha_1}(S) \subseteq S_{\alpha_2}(S) \]

Proof.

According (i) \( \alpha_1 \leq \alpha_2 \) implies \( C_{\alpha_1}(S) \subseteq C_{\alpha_2}(S) \)

\( \alpha \)-complex:

(i) it’s circumsphere is empty and has radius smaller than \( \alpha \), or

(ii) \( \Delta_T \) 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)
Edelsbrunner’s Algorithm - Intuitive

1. Compute the Delaunay triangulation of $S$ knowing that it contains our $\alpha$-shape

2. Compute $C_{\alpha}$ by inspecting all simplices $\Delta_T$ in $DT(S)$:
   
   $\text{if its circumsphere is empty with smaller radius than } \alpha$ $\text{then}$
   
   accept it (as well as all of its faces)

3. All d-simplices of $C_{\alpha}$ make up the interior of $S_{\alpha}$. All simplices on the boundary $\partial C_{\alpha}$ form $\partial S_{\alpha}$

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?
Edelsbrunner’s Algorithm

Whether a simplex lies on the boundary or inside?

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

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

\[
\Delta_T \text{ is } \begin{cases} 
\text{not in } C_\alpha & (\text{for } \alpha < a) \\
\text{in } \partial C_\alpha & (\text{for } \alpha \in (a, b)) \\
\text{interior to } C_\alpha & (\text{for } \alpha \in (b, \infty))
\end{cases}
\]

for all $\Delta_T \in DT(S)$

The algorithm computes all possible $\alpha$-shapes for $S$
Edelsbrunner’s Algorithm

**Case 1:** $d$-dimensional simplex (trivial)

Cannot be on the boundary: $a = b = \text{radius of its circumsphere}$

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

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

$\alpha$-complex:

(i) it’s circumsphere is empty and has radius smaller than $\alpha$, or
(ii) $\Delta_r$ is a face of another simplex in $C_\alpha(S)$
**Observation.** Let $\Delta_T \in DT(S)$ 

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

Then $\Delta_T \in C_\alpha$ if and only if $\alpha \in (a, \infty)$.

**$\alpha$-complex:**

1. it's circumsphere is empty and has radius smaller than $\alpha$, or
2. $\Delta_T$ is a face of another simplex in $C_\alpha(S)$
Observation. Let $\Delta_T \in C_S(\alpha)$

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

Then $\Delta_T \in \text{interior of } C_S(\alpha)$ iff $\alpha \in (b, \infty)$
Edelsbrunner’s Algorithm

Altogether we get the following algorithm:

\begin{verbatim}
procedure AlphaShape(S,d);
  \{Given a point-set \( S \subseteq \mathbb{R}^d \), computes a list \( R \) of simplices \( \Delta_T \) and\}
  \{two lists \( B, I \) of intervals such that \( \Delta_T \in \partial S_\alpha \) if and only if \( \alpha \in B_T \)
  \{and \( \Delta_T \in \text{int}(S_\alpha) \) if and only if \( \alpha \in I_T \).\}
  \begin{algorithmic}
    \State \( R := \text{DT}(S) \);
    \For {each \( d \)-simplex \( \Delta_T \in R \)}
      \State \( B_T := \emptyset \); \( I_T := (\sigma_i, \infty) \);
    \EndFor;
    \For {\( k := d - 1 \) to 0 by \(-1 \)}
      \For {each \( k \)-simplex \( \Delta_T \in R \)}
        \If {\( b_T \) is empty}
          \State \( a := \sigma_T \);
        \Else
          \State \( a := \min \{ a_U \mid B_U = (a_U, b_u), \Delta_U (k + 1) \text{-Simplex}, T \subseteq U \} \)
        \EndIf
        \If {\( \Delta_T \in \partial \text{conv}(S) \)}
          \State \( b := \infty \);
        \Else
          \State \( b := \max \{ a_U \mid B_U = (a_U, b_u), B_U \text{-Simplex mit } T \subseteq U \} \);
        \EndIf
        \State \( B_T := (a, b) \); \( I_T := (b, \infty) \);
      \EndFor;
    \EndFor;
    \State \Return \( (R, B, I) \);
  \end{algorithmic}
end AlphaShape;
\end{verbatim}
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 $\Theta(n^{(d-1)/2})$.
$\alpha$-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 $\mathbb{R}^d$

Union of balls important for modeling molecules in chemistry and biology
Union of balls – The three primal diagrams

\[ p_b = \{ x \in \mathbb{R}^d : \| x - b \| \leq \| x - b' \|, b' \in B \} \] - vorontoi 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
Union of balls – The three primal diagrams

\[ P = P(B) = \{ p_T \mid \emptyset \neq T \subseteq B \} \]
\[ |P| = \bigcup_{p_T \in P} p_T = R^d \]

\[ D = D(B) = \{ q_T \mid \emptyset \neq T \subseteq B \} \]
\[ |D| = U \]

\[ U = U(B) = \bigcup_{b \in B} b \]
**Definition.** Nerve of a collection of sets $A$ is $N(A) = \{ X \subseteq A | \bigcap_{a \in X} a \neq \emptyset \}$

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](image)
Union of balls – The three dual diagrams

\[ \sigma_T \equiv \text{Convex hull of the centers of the } d\text{-balls in } T \text{ (actually the corresponding simplex } \text{conv}T) \]

\[ R = R(B) = \{ \sigma_T \mid \emptyset \neq p_T \in P \} \cup \{ \emptyset \} \quad \text{The regular triangulation of } B \text{ (Delaunay triangulation)} \]

\[ K = K(B) = \{ \sigma_T \mid \emptyset \neq q_T \in D \} \cup \{ \emptyset \} \quad \text{The dual complex of } D \]

\[ S = S(B) = \mid K \mid \quad \text{The dual shape of } U \]

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

---

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

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

\[ U = U(B) = \bigcup_{b \in B} b \]
Union of balls – The three dual diagrams

\[ P = P(B) = \{ p_T \mid \emptyset \neq T \subseteq B \} \]
\[ D = D(B) = \{ q_T \mid \emptyset \neq T \subseteq B \} \]
\[ U = U(B) = \bigcup_{b \in B} b \cdot |D| \]

\[ p_T \in P \iff \sigma_T \in R \]

\[ R = R(B) = \{ \sigma_T \mid \emptyset \neq p_T \in P \} \cup \{ \emptyset \} \]

\[ K = K(B) = \{ \sigma_T \mid \emptyset \neq q_T \in D \} \cup \{ \emptyset \} \]

\[ S = S(B) = |K| \]

Computational Topology

Alpha Shapes
Union of balls – Another definition of alpha-shapes

\[ U = U(B) = \bigcup_{b \in B} b \cap D \]

\[ S = S(B) = \partial K \]

Boundary of this complex is the boundary of an \( \alpha \)-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? :-)*
Union of balls – Another definition of alpha-shapes
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!
The Union of balls as a model for various molecules has

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

...directly computable from the $\alpha$-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.
Limitations of classical alpha shapes

Shape modeling.
Reconstruction of objects which have been sampled by points.

How to determine the “best” $\alpha$?
Limitations of classical alpha shapes

There are sets of points for which no satisfying $\alpha$ exists

- Low density point-set will require large $\alpha$ in order to connect...
- Non-uniform distribution of points not appropriate
Extensions – weighted alpha shapes

Generalization of $\alpha$-shapes (the dual of the union of balls)

Each point has a weight assigned, $\alpha$-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 $\alpha$-exposed simplices spanned by $S$

Different definition of $\alpha$-exposed simplex

Solves the problem of classical $\alpha$-shapes for non-uniform density of sample points

Problem: How to assign the weights?
**Extensions – conformal alpha shapes**

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

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

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

$$\alpha_p(\tilde{\alpha}) = \alpha_p^+ \tilde{\alpha} + \alpha_p^-$$

$$\alpha_p^+ = \| p - p^* \|$$

$$\alpha_p^- = \alpha_p^1 = 0$$

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

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

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).