Lecture 1
Discrete Geometric Structures

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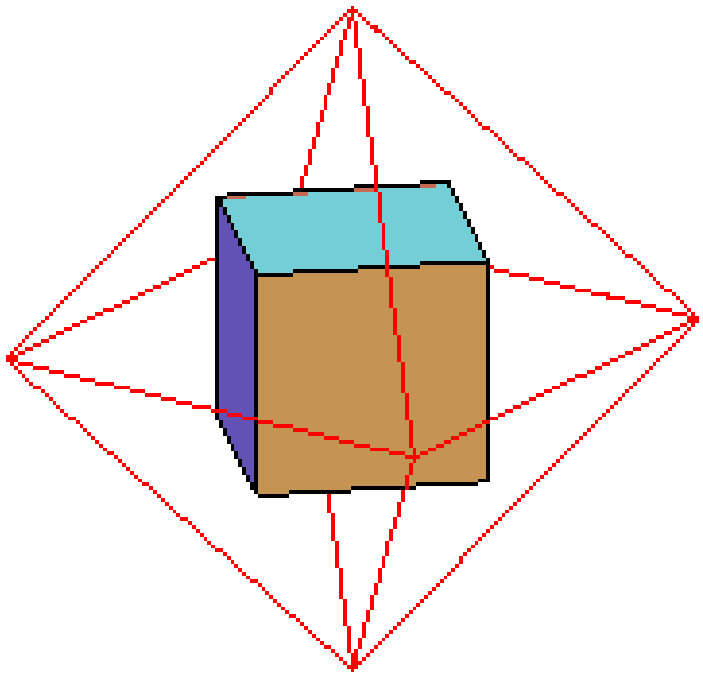
Outline

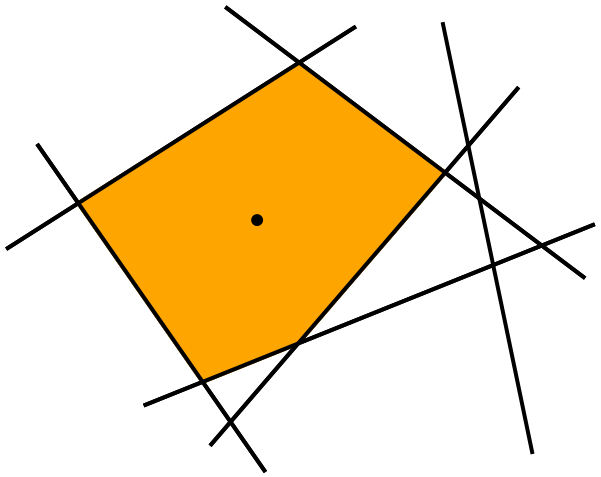
Convex Polytopes



Two ways of defining convex polytopes

Intersection of n half-planes

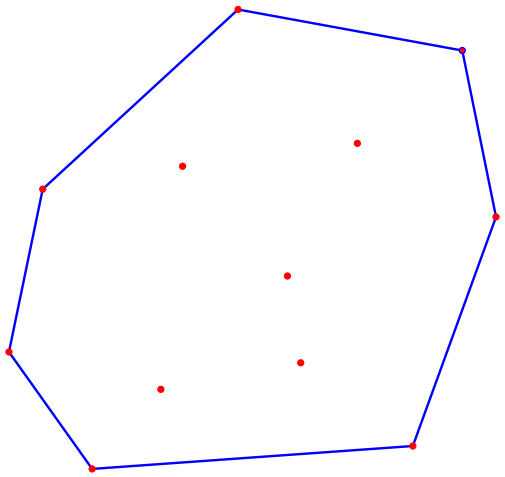
Input : n half-planes $H_i : a_i x + b_i y + c_i \leq 0$, $i = 1, ..., n$



Output : the convex polygon (possibly empty) $H = \bigcap_{i=1}^{n} H_i$

Convex hull of n points

Input : n points $p_1, ..., p_n$ in $\mathbb{R}^2$



Output : the convex polygon $\text{conv}(P) = \sum_i^n \lambda_i p_i$
$\lambda_i \geq 0$
$\sum_i^n \lambda_i = 1$

Equivalently, $\text{conv}(P)$ is the intersection of the halfplanes that

- are bounded by lines passing through 2 points of P
- contain all the points of P

Space of lines and duality

Duality point/line

(non vertical) line $h = \{(x, y) : y = ax - b\} \longrightarrow$ dual point $h^* = (a, b)$

point $p = (a, b) \longrightarrow$ dual line $p^* = \{(x, y) : y = ax - b\}$.

The mapping *

- is an involution and is thus bijective : $h^{**} = h$ and $p^{**} = p$
- preserves incidences :

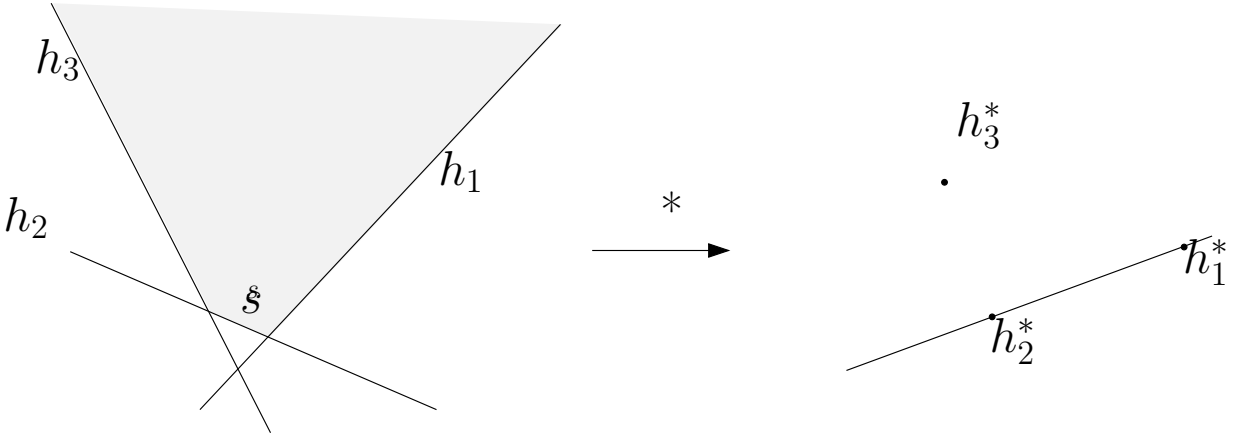
$$p = (x, y) \in h \Longleftrightarrow y = ax - b \Longleftrightarrow b = xa - y \Longleftrightarrow h^* \in p^*.$$

- preserves inclusions

$$p \in h^+ \Longleftrightarrow h^* \in p^{*+} \qquad (h^+ = \{(x, y) : y > ax - b)\}$$

Intersections of halfplanes and convex hulls

Let $h_1, \ldots, h_n$ be n lines and let $H = \cap h_i^+$



A vertex s of H is the intersection point of two lines h_i and h_j lying above all other lines h_k, $k \neq i, j$

$\Longrightarrow s^* = (h_i^* h_j^*)$

s^* is a line supporting $\text{conv}^-(\{h_i^*\})$

From a computational point of view, the two problems are equivalent

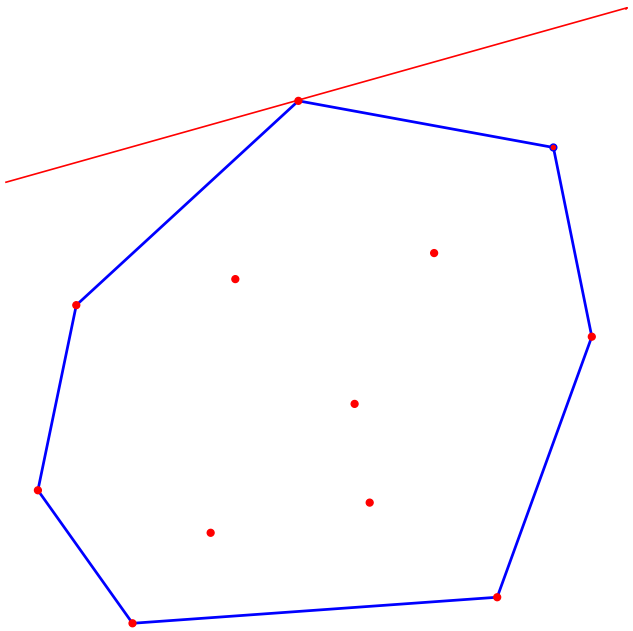
Facial structure of a polytope

Convex polytopes and duality can be defined in very much the same in any fixed dimension

Supporting hyperplane h :
$H \cap \mathcal{P} \neq \emptyset$
$\mathcal{P}$ on one side of h

Faces : $\mathcal{P} \cap h$, h supp. hyp.

Dimension of a face :
the dim. of its affine hull



General position

Points in general position

- P is in general position iff no subset of $k+2$ points lie in a k-flat

$\Rightarrow$ any k-face is the convex hull of $k+1$ point of P, i.e. a k-simplex

conv(P) is called a simplicial polytope

Hyperplanes in general position

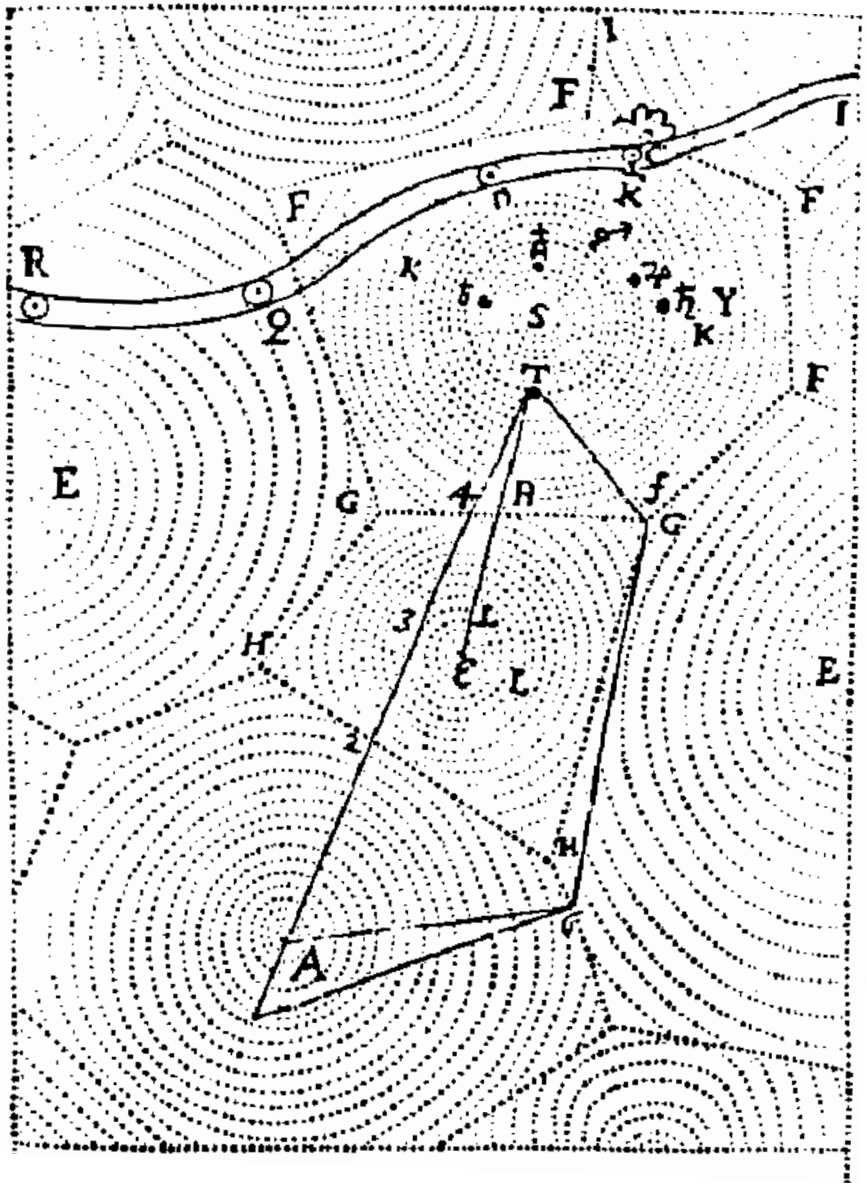
- H is in general position iff the intersection of any subset of $d-k$ hyperplanes intersect in a k-flat

$\Rightarrow$ any k-face is the intersection of $d-k$ hyperplanes

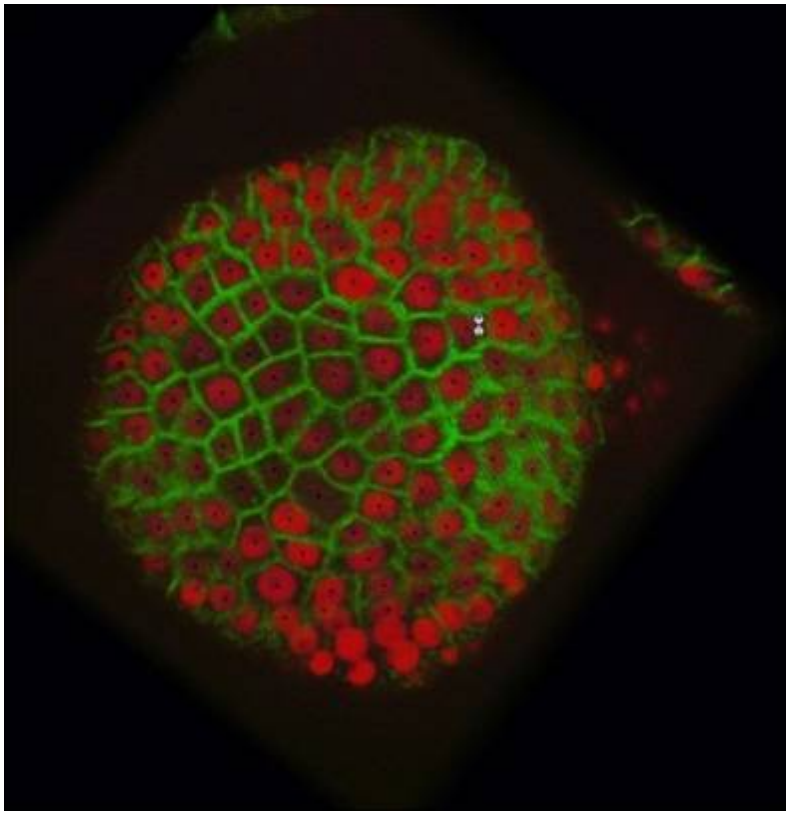
$\bigcap H$ is called a simple polytope

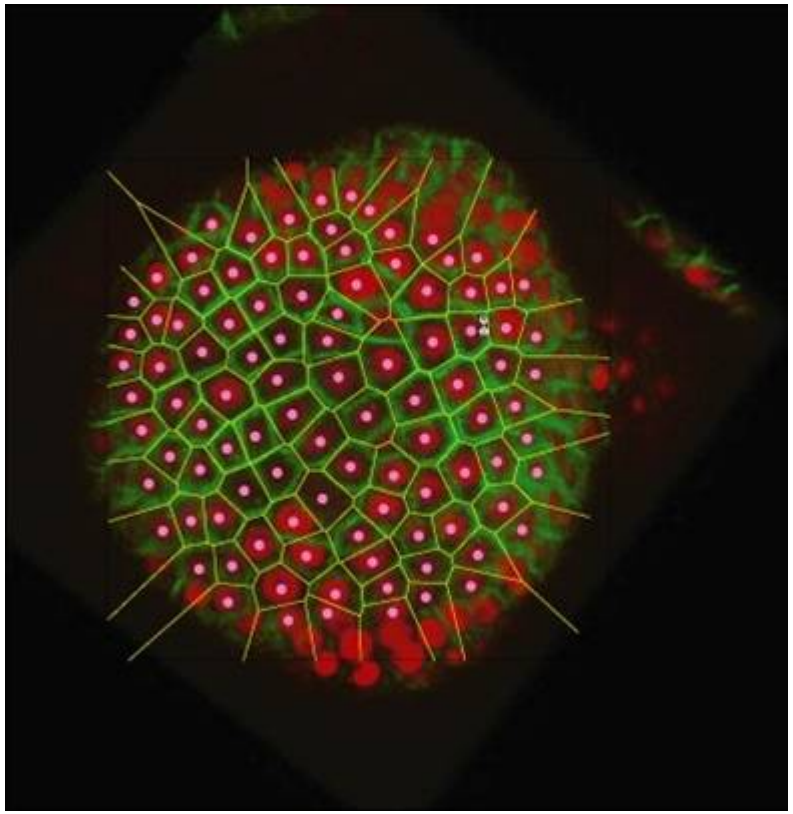
Voronoi diagrams in nature

The solar system (Descartes)

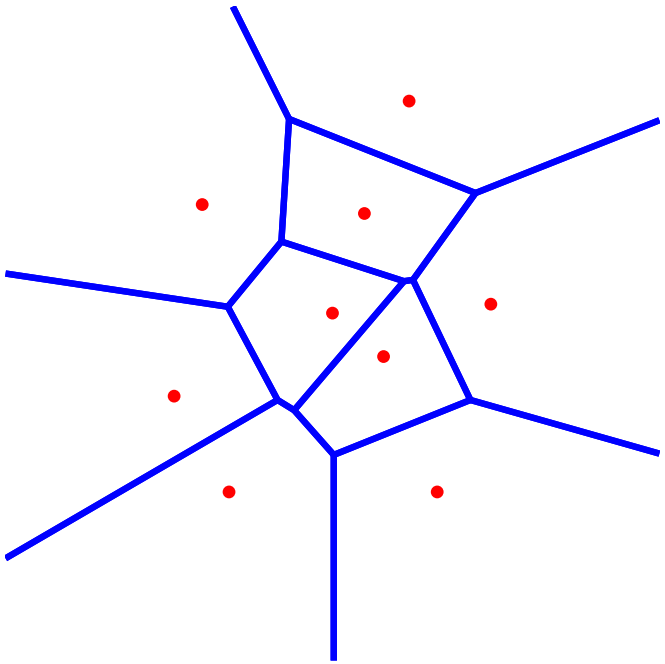


Growth of merystem





Euclidean Voronoi diagrams



Voronoi cell $\quad V(p_i) = \{x : \|x - p_i\| \leq \|x - p_j\|, \ \forall j\}$

Voronoi diagram (P) $\quad = \{$ collection of all cells $V(p_i)$, $p_i \in P$ $\}$

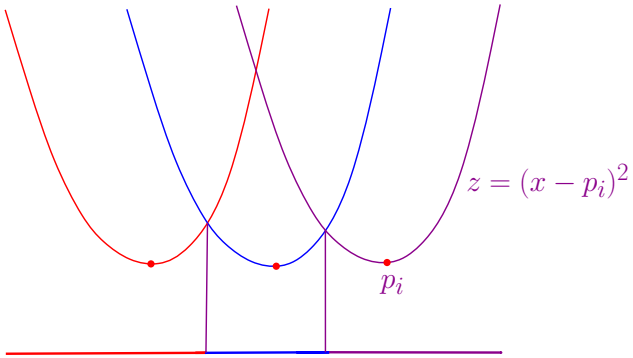
Voronoi diagrams and convex polyhedra

Convex Polyhedron

The intersection of a finite collection of half-spaces : $\mathcal{V} = \bigcap_{i \in I} h_i^+$

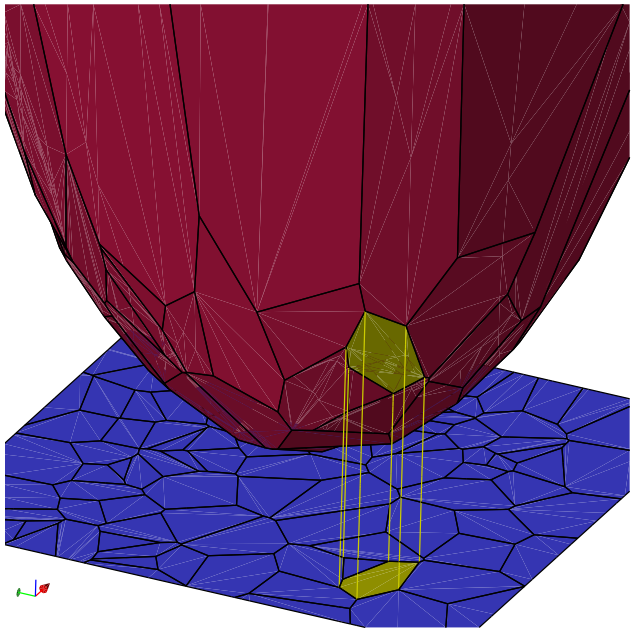
- Each Voronoi cell is a convex polyhedron
- The Voronoi diagram has the structure of a cell complex: two cells either do not intersect or intersect in a common face
- The Voronoi diagram of P is the projection of a convex polyhedron of $\mathbb{R}^{d+1}$

Voronoi diagrams and convex polyhedra



- Vor$(p_1, \ldots, p_n)$ is the minimization diagram of the n functions $\delta_i(x) = (x - p_i)^2$
- $\arg\min(\delta_i) = \arg\max(h_i)$ where $h_{p_i}(x) = 2\, p_i \cdot x - p_i^2$
- The minimization diagram of the δ_i is also the maximization diagram of the affine functions $h_{p_i}(x)$
- The faces of Vor(P) are the projections of the faces of $\mathcal{V}(P) = \bigcap_i \; h^+_{p_i}$

$$h^+_{p_i} = \{x : x_{d+1} > 2p_i \cdot x - p_i^2\}$$



Note !

the graph of $h_{p_i}(x)$ is the hyperplane tangent to $\mathcal{Q}: \quad x_{d+1} = x^2 \quad$ at $\quad (x, x^2)$

Voronoi diagrams and convex polyhedra

Lifting map

The faces of Vor(P) are the projection of the faces of the polytope

$$\mathcal{V}(P) = \bigcap_i \; h^+_{p_i}$$

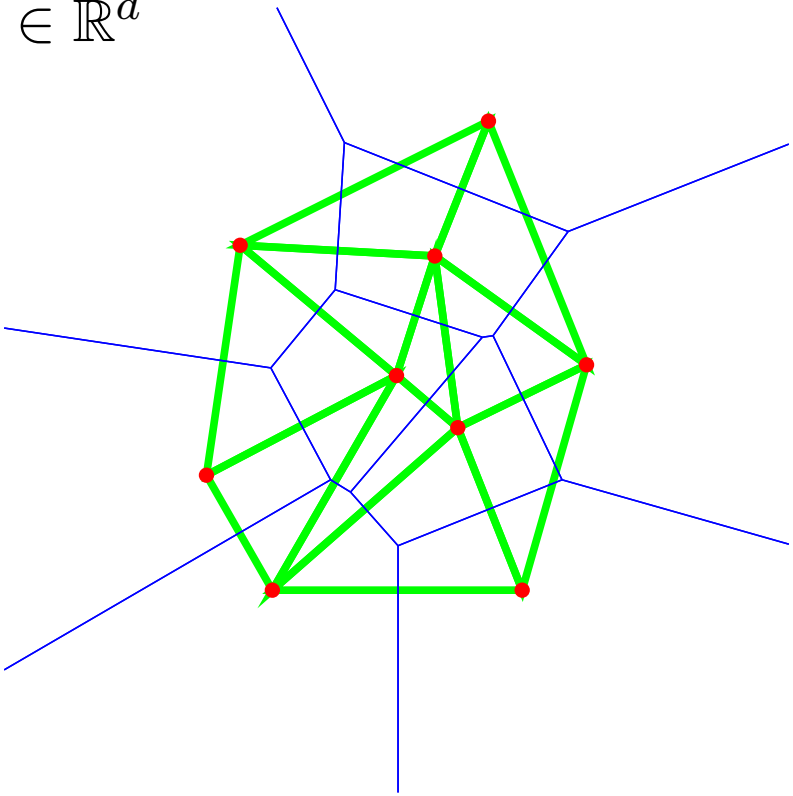
where h_{p_i} is the hyperplane tangent to paraboloid $\mathcal{Q}$ at the lifted point (p_i, p_i^2)

Corollaries

- The size of Vor$(\mathcal{P})$ is the same as the size of $\mathcal{V}(P)$
- Computing Vor$(\mathcal{P})$ reduces to computing $\mathcal{V}(P)$

Voronoi diagram and Delaunay complex

Finite set of points $P \in \mathbb{R}^d$



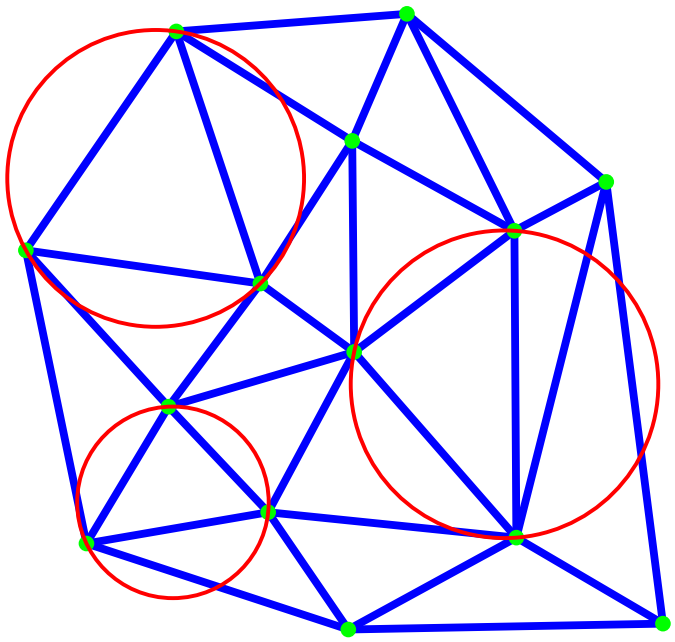
- The Delaunay complex is the nerve of the Voronoi diagram
- It is not always embedded in $\mathbb{R}^d$

Empty circumballs

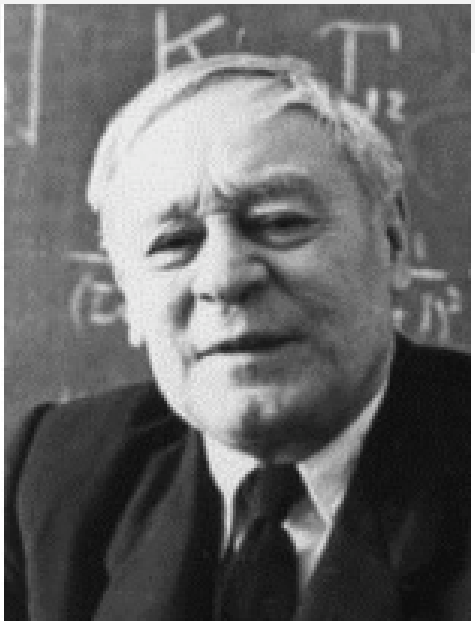
An (open) d-ball B circumscribing a simplex $\sigma \subset \mathcal{P}$ is called empty if

1. $\mathrm{vert}(\sigma) \subset \partial B$
2. $B \cap \mathcal{P} = \emptyset$

$\mathrm{Del}(\mathcal{P})$ is the collection of simplices admitting an empty circumball



Point sets in general position wrt spheres

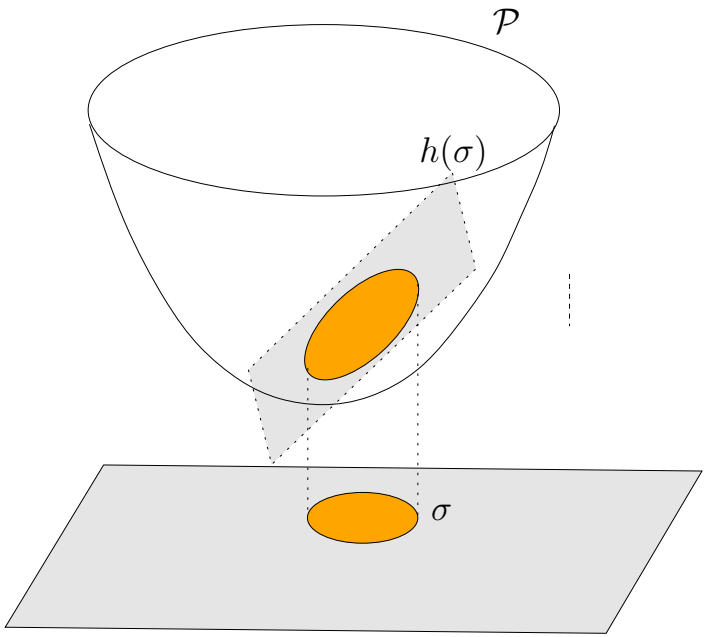


$P = \{p_1, p_2 \dots p_n\}$ is said to be in general position wrt spheres if $\nexists\ d+2$ points of P lying on a same $(d-1)$-sphere

Theorem [Delaunay 1936]

If P is in general position wrt spheres, $\mathrm{Del}(P)$ has a natural realization in $\mathbb{R}^d$ called the Delaunay triangulation of P.

Proof of Delaunay's theorem 1



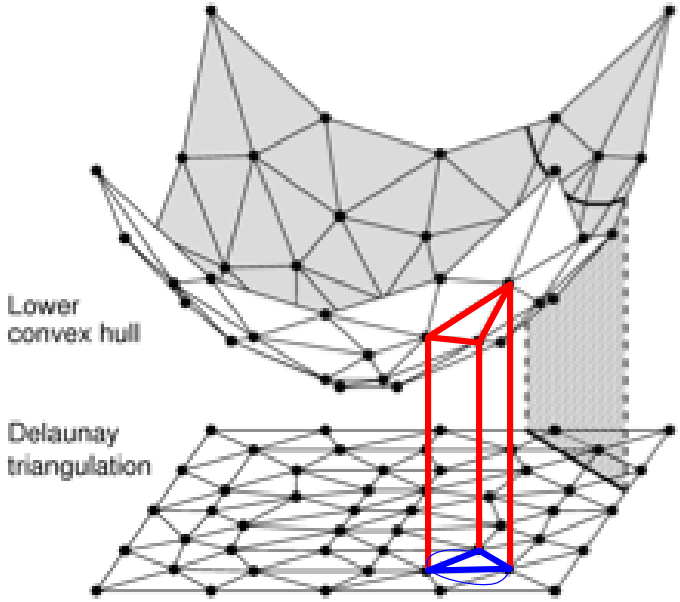
Linearization

$$S(x) = x^2 - 2c \cdot x + s, \quad s = c^2 - r^2$$

$$S(x) < 0 \Leftrightarrow \begin{cases} z < 2c \cdot x - s & (h_S^-) \\ z = x^2 & (\mathcal{P}) \end{cases}$$

$$\Leftrightarrow \hat{x} = (x, x^2) \in h_S^-$$

Proof of Delaunay's theorem 2



Proof of Delaunay's th.

P general position wrt spheres
$\Leftrightarrow \hat{P}$ in general position

σ a simplex, S_σ its circumscribing sphere

$\sigma \in \mathrm{Del}(P) \Leftrightarrow S_\sigma$ empty

$\Leftrightarrow \forall i,\ \hat{p}_i \in h^+_{S_\sigma}$

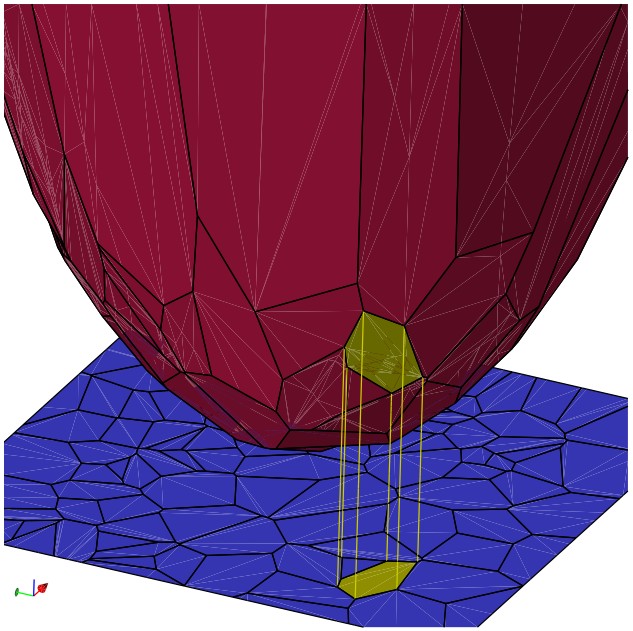
$\Leftrightarrow \hat{\sigma}$ is a face of $\mathrm{conv}^-(\hat{P})$

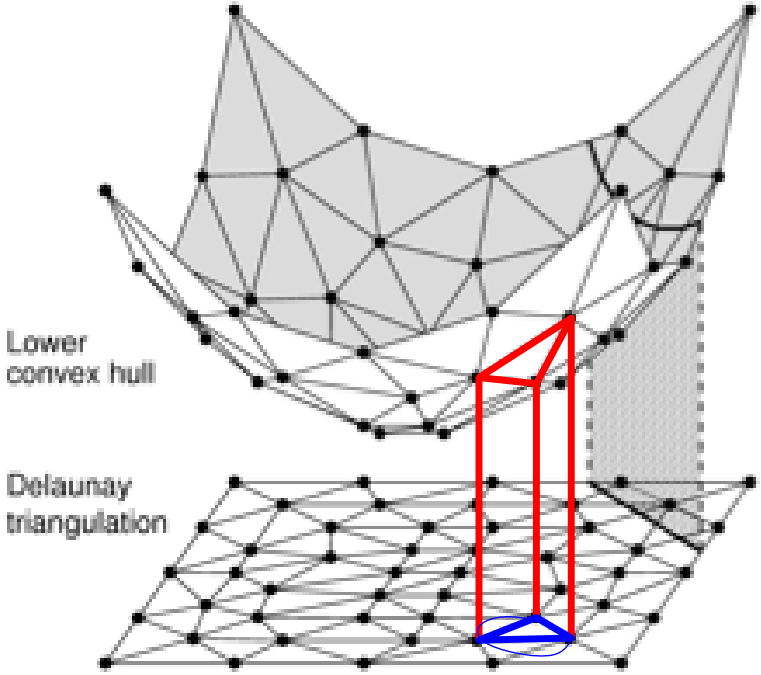
$$\mathrm{Del}(P) = \mathrm{proj}(\mathrm{conv}^-(\hat{P}))$$

VD and DT in the space of spheres

$h_{p_i} : x_{d+1} = 2p_i \cdot x - p_i^2$

$\hat{p}_i = (p_i, p_i^2) = h^*_{p_i}$





$$\mathcal{V}(P) = h^+_{p_1} \cap \ldots \cap h^+_{p_n} \quad \xrightarrow{\text{duality}} \quad \mathcal{D}(P) = \mathsf{conv}^-(\{\hat{p}_1, \ldots, \hat{p}_n\})$$

$$\uparrow \qquad\qquad\qquad\qquad \downarrow$$

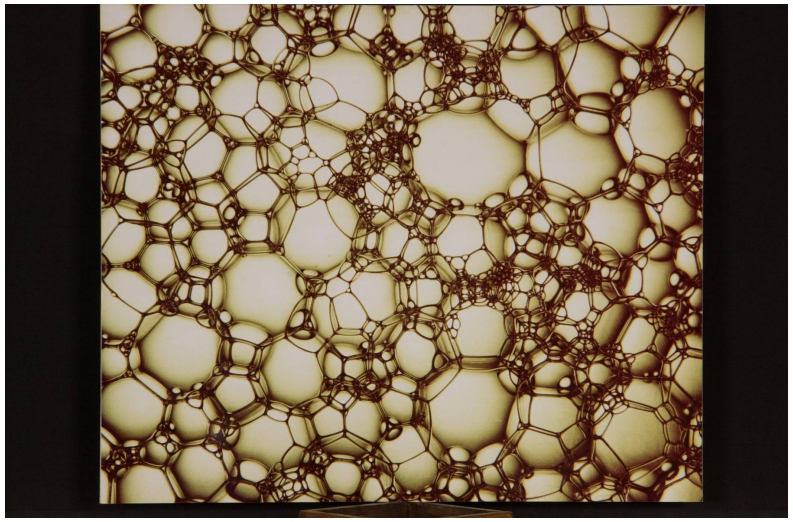
Voronoi Diagram of P $\xrightarrow{\text{nerve}}$ Delaunay Complex of P

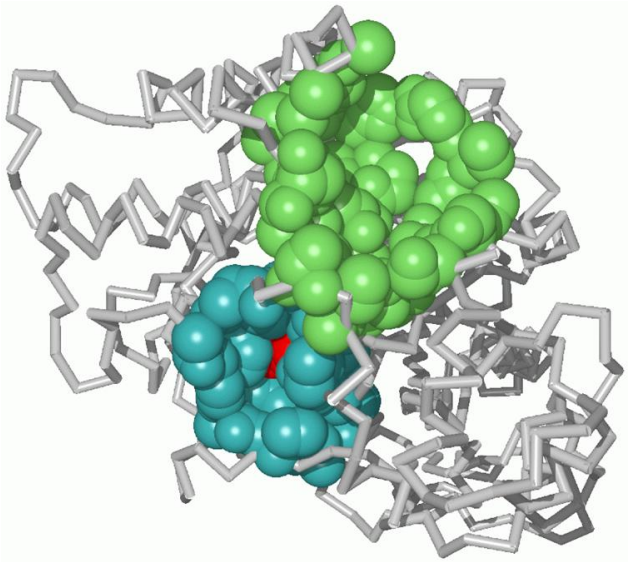
Voronoi diagrams, Delaunay triangulations and polytopes

If P is in general position wrt spheres :

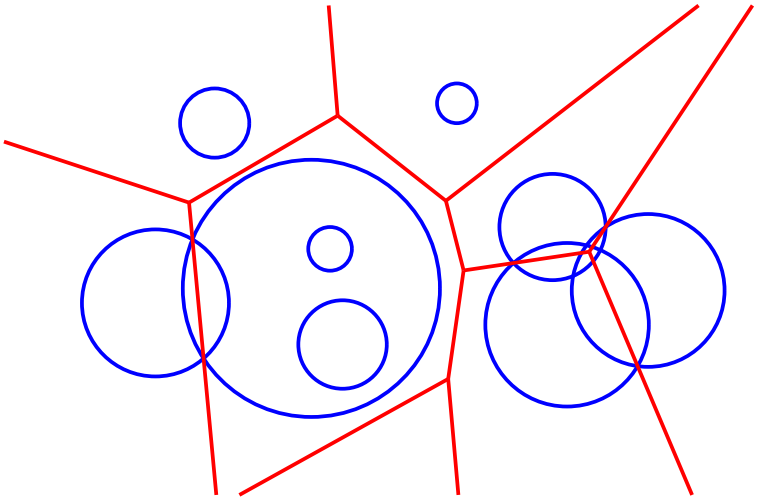
$$\begin{array}{ccc} \mathcal{V}(P) = h^+_{p_1} \cap \ldots \cap h^+_{p_n} & \xrightarrow{\text{duality}} & \mathcal{D}(P) = \mathsf{conv}^-(\{\hat{p}_1, \ldots, \hat{p}_n\}) \\ \uparrow & & \downarrow \\ \text{Voronoi Diagram of } P & \xrightarrow{\text{nerve}} & \text{Delaunay Complex of } P \end{array}$$

Foams, molecules and weighted Voronoi diagrams





Weighted Voronoi (or Power or Laguerre) Diagrams



Sites : n balls $B = \{b_i(p_i, r_i), i = 1, \ldots n\}$

Power distance: $\pi(x, b_i) = (x - p_i)^2 - r_i^2$

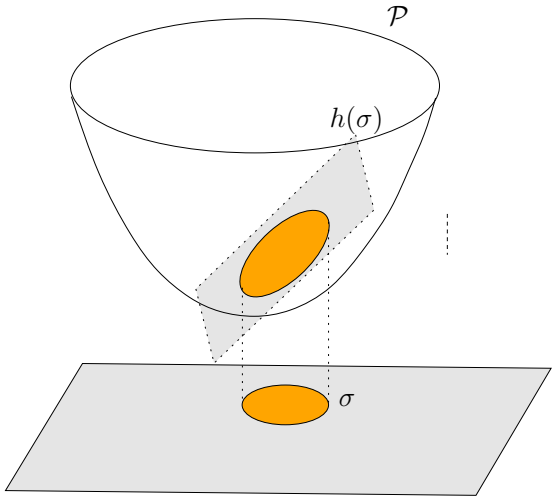
It is not a distance

Power Diagram: Vor(B)
One cell $V(b_i)$ for each site
$V(b_i) = \{x : \pi(x, b_i) \leq \pi(x, b_j). \forall j \neq i\}$

- Each cell is a convex polyhedron
- $V(b_i)$ may be empty
- p_i may not belong to $V(b_i)$

Power diagrams are maximization diagrams

Cell of b_i in the weighed Voronoi diagram Vor(B)



$$\begin{aligned} V(b_i) &= \{x \in \mathbb{R}^d : \pi(x, b_i) \leq \pi(x, b_j). \forall j \neq i\} \\ &= \{x \in \mathbb{R}^d : 2p_i x - s_i = \max_{j \in [1,\ldots n]}\{2p_j x - s_j\}\} \end{aligned}$$

Vor(B) is the maximization diagram of the set of affine functions

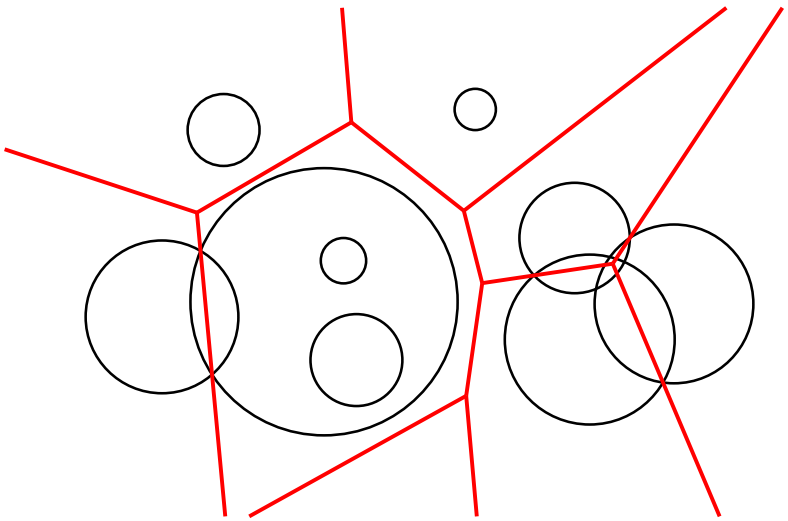
$$\{h_i(x) = 2p_i x - s_i, i = 1, \ldots, n\}$$

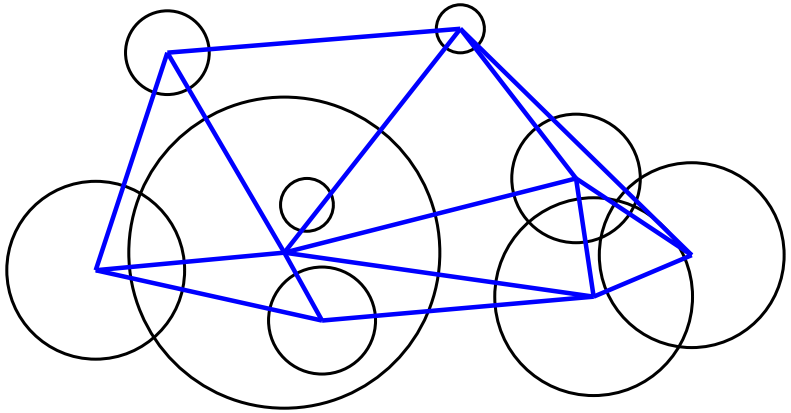
Geometrically : the vertical projection of $\mathcal{P} \cap h_i^-$ is the ball b_i

Weighted Delaunay triangulations

$B = \{b_i(p_i, r_i)\}$ a set of balls

$\mathsf{Del}(B) =$ nerve of $\mathsf{Vor}(B)$





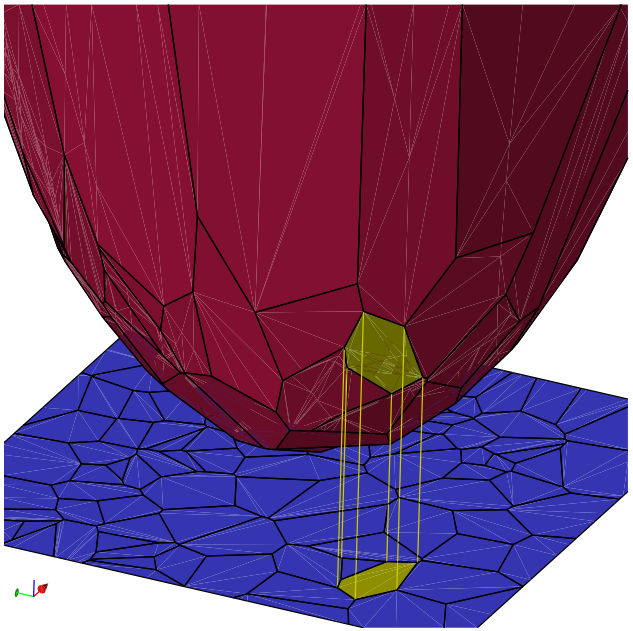
Let $B_\tau = \{b_i(p_i, r_i), i = 0, \ldots k\}\} \subset B$:

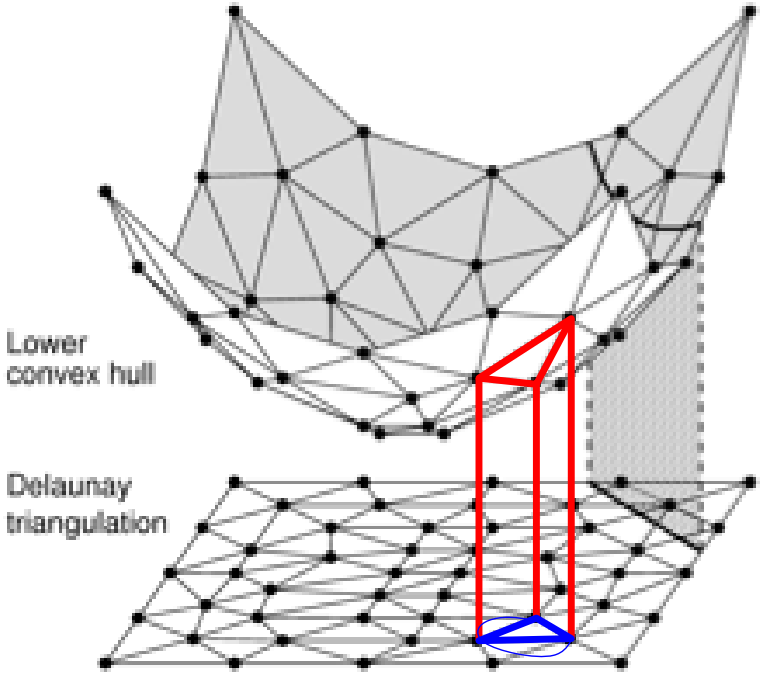
$$B_\tau \in \mathsf{Del}(B) \Longleftrightarrow \bigcap_{b_i \in B_\tau} V(b_i) \neq \emptyset$$

Weighted VD and DT in the space of spheres

$h_{b_i} : x_{d+1} = 2p_i \cdot x - p_i^2 + r_i^2$

$\phi(b_i) = (p_i, p_i^2 - r_i^2) = h^*_{b_i}$





$$\mathcal{V}(B) = h^+_{b_1} \cap \ldots \cap h^+_{b_n} \quad \xrightarrow{\text{duality}} \quad \mathcal{D}(B) = \mathsf{conv}^-(\{\phi(b_1), \ldots, \phi(b_n)\})$$

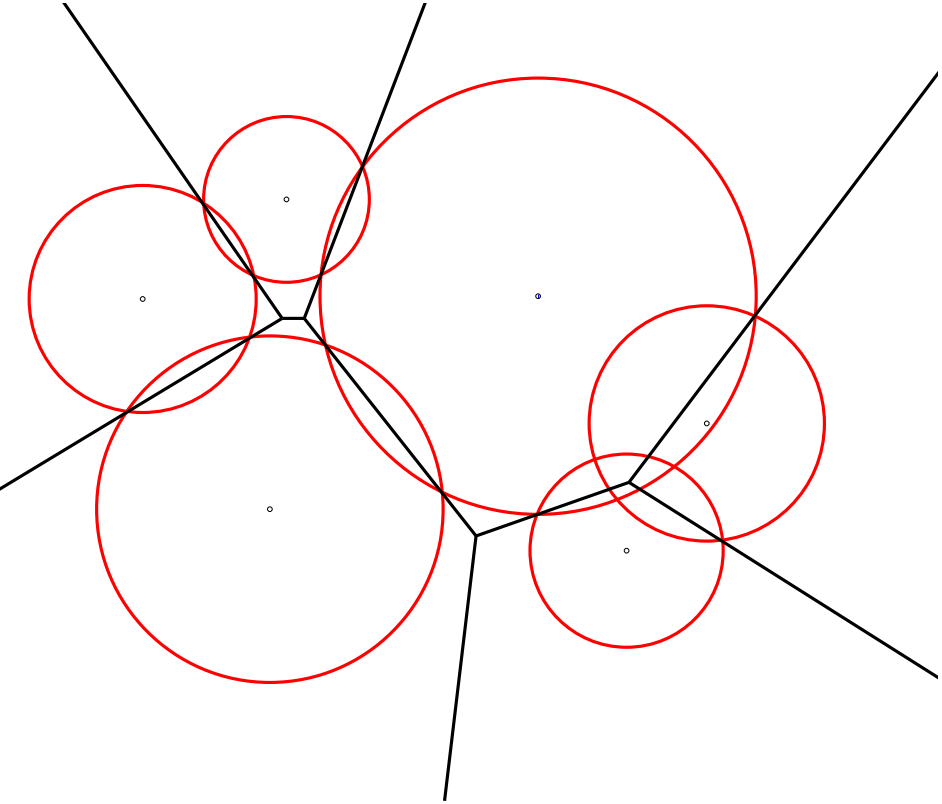
$$\uparrow \qquad\qquad\qquad\qquad \downarrow$$

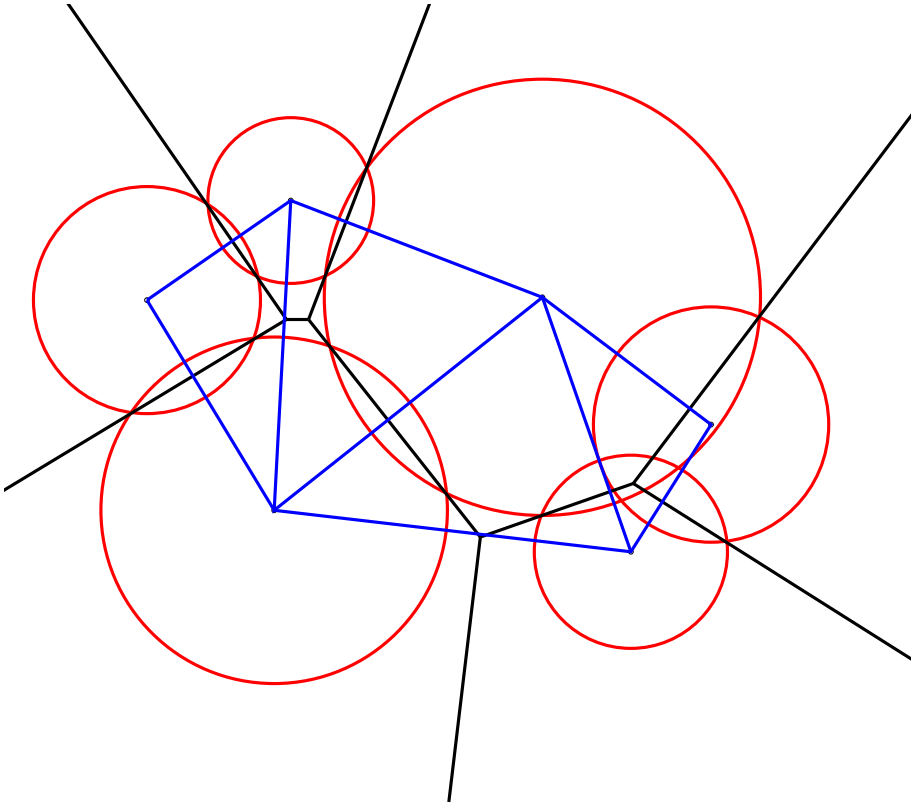
Voronoi Diagram of B $\xrightarrow{\text{nerve}}$ Delaunay Complex of B

Union of balls

- What is the combinatorial complexity of the boundary of the union U of n balls of $\mathbb{R}^d$?
- Compare with the complexity of the arrangement of the bounding hyperspheres
- How can we compute U ?
- What is the image of U in the space of spheres ?

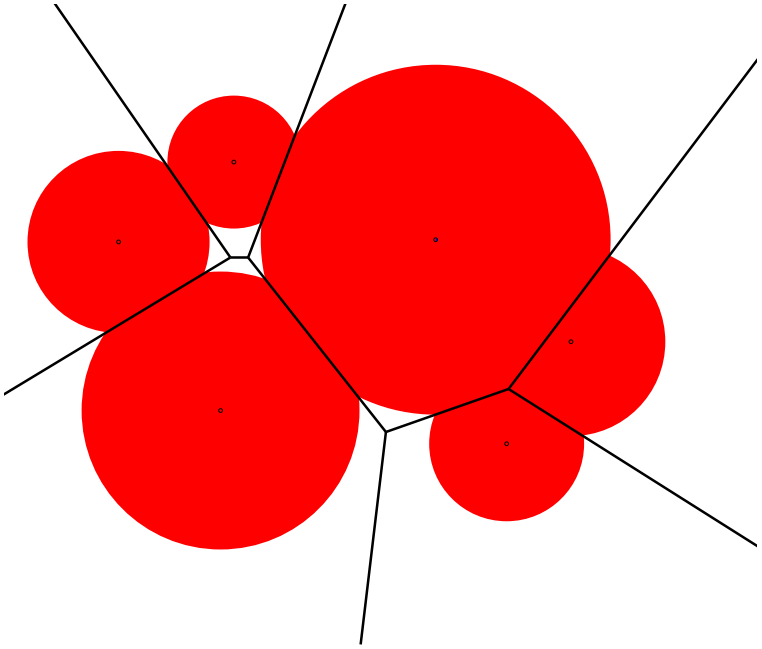
Weighted Voronoi Diagram

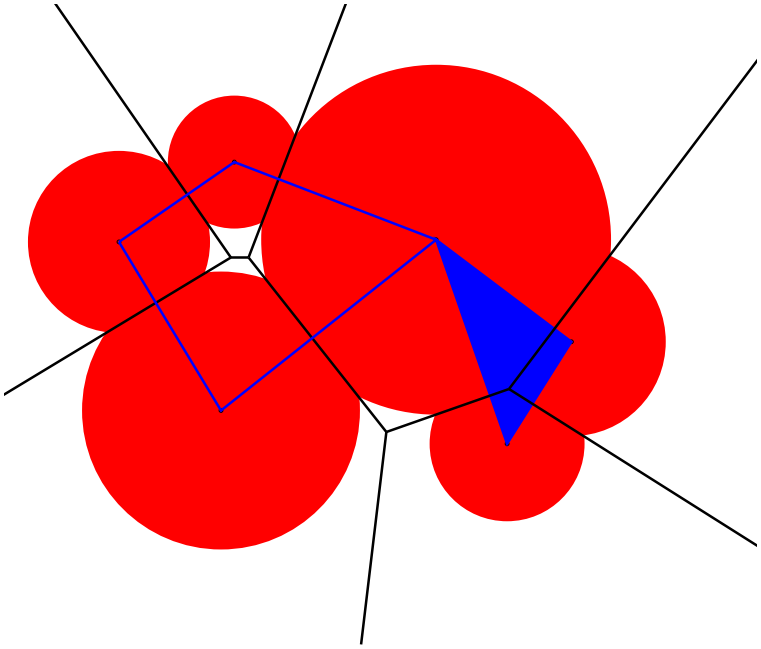




$$\sigma_i(x) = (x - p_i)^2 - r_i^2$$

Restriction of $\mathrm{Del}(B)$ to $U = \bigcup_{b \in B} b$

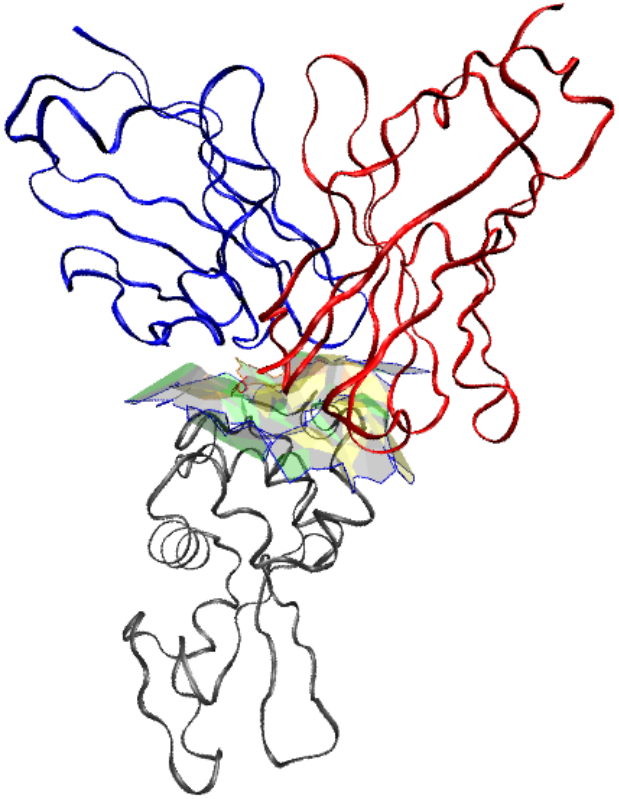


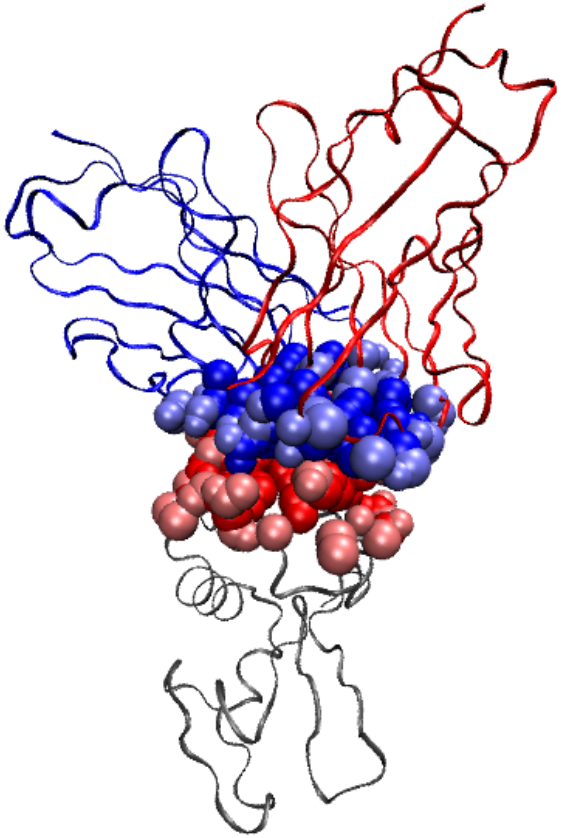


- $U = \bigcup_{b \in B} b \cap V(b)$ and $\partial U \cap \partial b = V(b) \cap \partial b$.
- The nerve of $\mathcal{C}$ is the restriction of $\mathrm{Del}(B)$ to U, i.e. the subcomplex $\mathrm{Del}_{|U}(B)$ of $\mathrm{Del}(B)$ whose faces have a circumcenter in U
- $\forall b,\ \ b \cap V(b)$ is convex and thus contractible
- $\mathcal{C} = \{b \cap V(b), b \in B\}$ is a good cover of U
- The nerve of $\mathcal{C}$ is a deformation retract of U

homotopy equivalent (Nerve theorem)

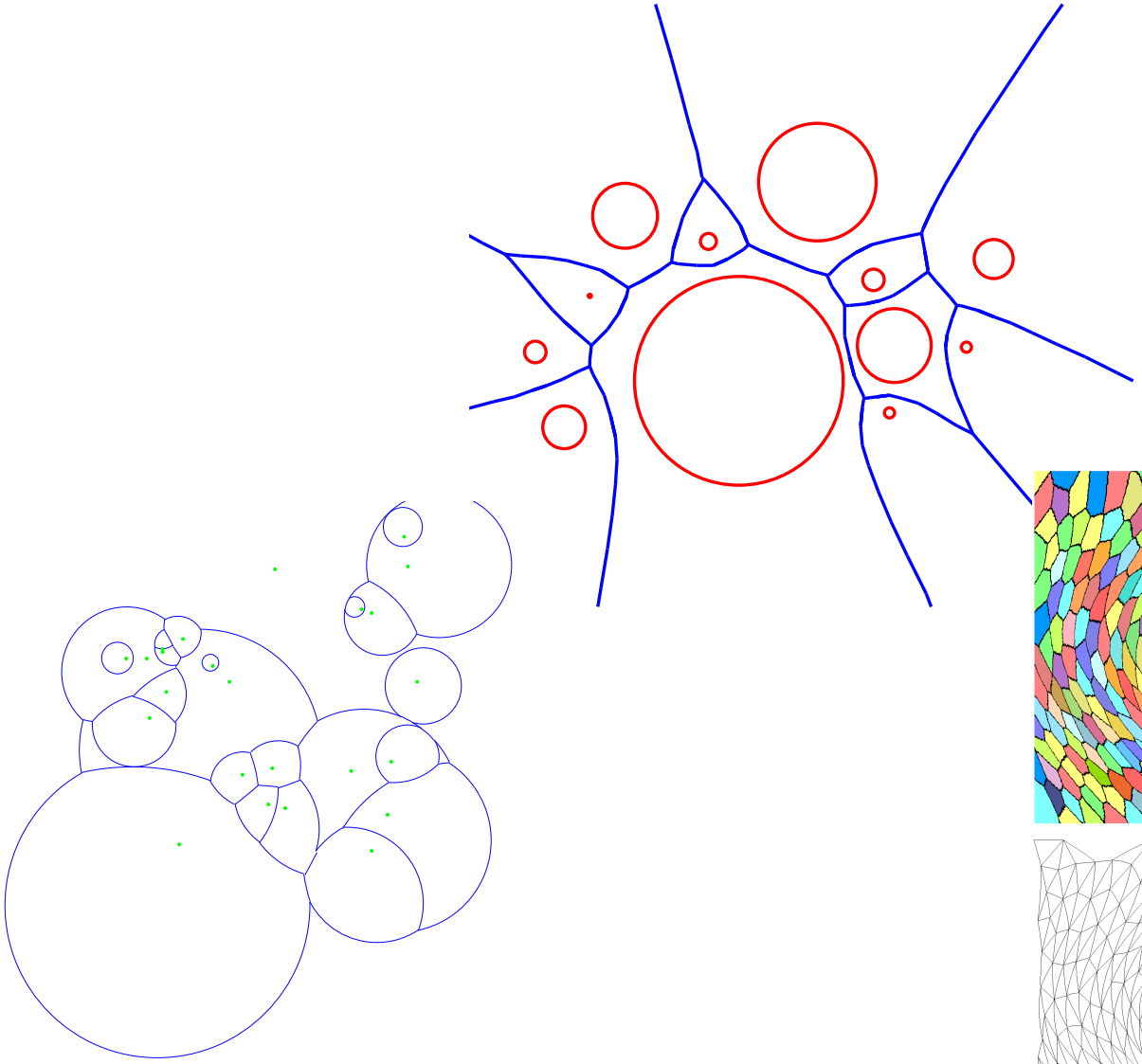
Interfaces between proteins [Cazals & Janin 2006]

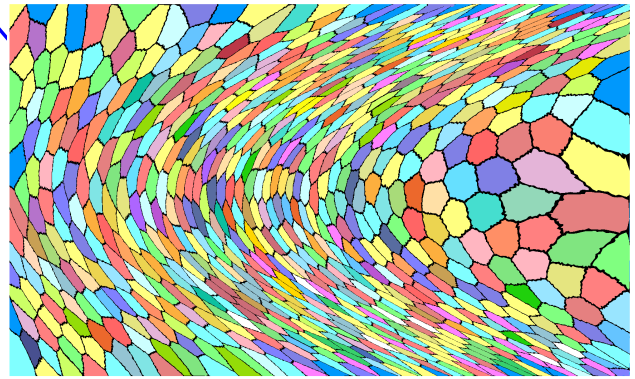


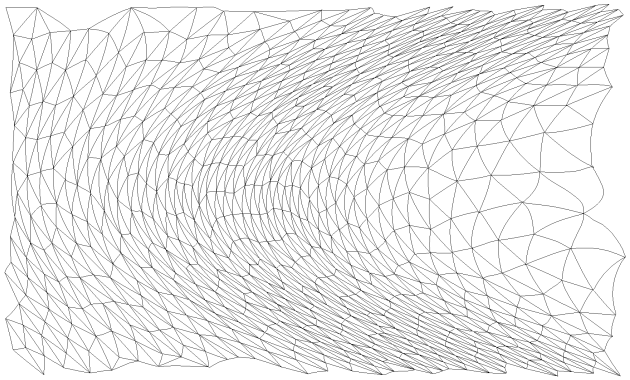


Interface antigen-antibody

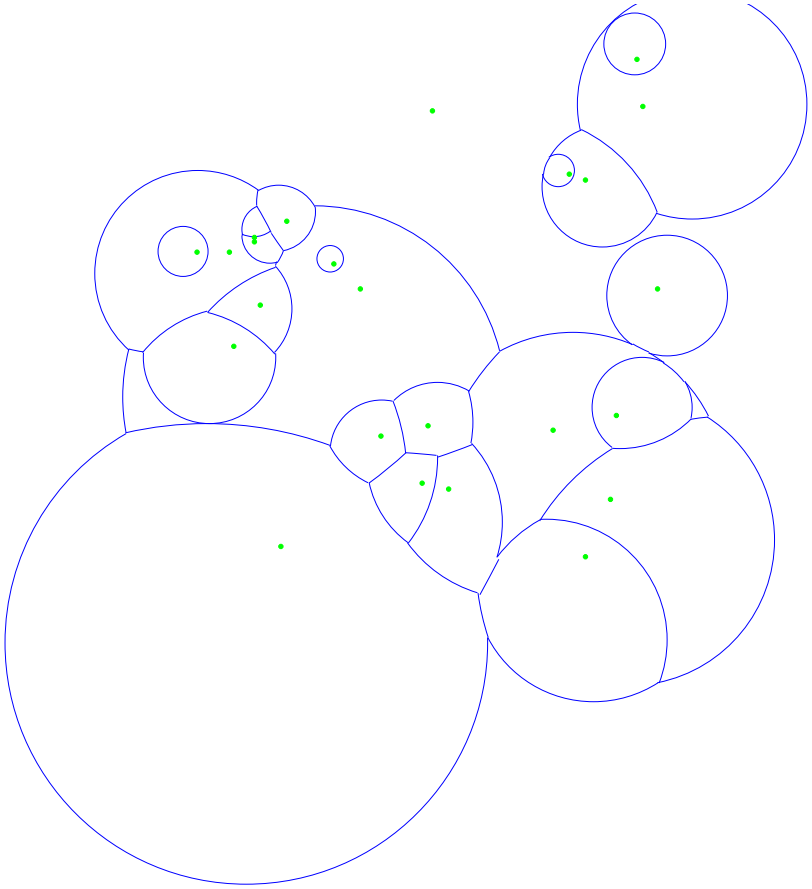
Fonctions distance et modèles de croissance







Möbius Diagrams



$W_i = (p_i, \lambda_i, \mu_i)$

$\delta_M(x, W_i) = \lambda_i \|x - p_i\|^2 - \mu_i$

bisectors are hyperspheres
(hyperplanes or $\emptyset$)

$\text{Mob}(W_i) = \{x, \delta(x, \sigma_i) \leq \delta(x, \sigma_j)\}$

Linearization Lemma

We can associate to each weighted point W_i
a hypersphere Σ_i of $\mathbb{R}^{d+1}$ so that

the faces of the Möbius diagram of the W_i are obtained by

1. computing the Laguerre Diagram of the Σ_i
2. intersecting this diagram with the paraboloid $\mathcal{P}$
3. projecting vertically the faces of this intersection onto $\mathbb{R}^d$

Proof

$$\lambda_i(x-p_i)^2 - \mu_i \leq \lambda_j(x-p_j)^2 - \mu_j$$

$$\begin{aligned}
\iff \quad & (x-\lambda_i p_i)^2 + (x^2 + \tfrac{\lambda_i}{2})^2 - \lambda_i^2 p_i^2 - \tfrac{\lambda_i^2}{4} + \lambda_i p_i^2 - \mu_i \\
& \qquad \leq (x-\lambda_j p_j)^2 + (x^2 + \tfrac{\lambda_j}{2})^2 - \lambda_j^2 p_j^2 - \tfrac{\lambda_j^2}{4} + \lambda_j p_j^2 - \mu_j \\
\iff \quad & (X-C_i)^2 - \rho_i^2 \leq (X-C_j)^2 - \rho_j^2
\end{aligned}$$

where $X = (x, x^2) \in \mathbb{R}^{d+1}$,

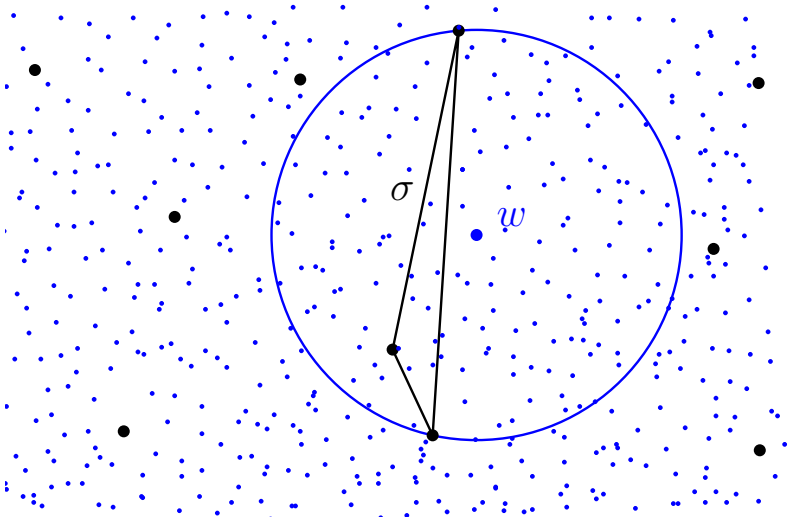
$C_i = (\lambda_i p_i, -\frac{\lambda_i}{2}) \in \mathbb{R}^{d+1}$ and $\rho_i^2 = \lambda_i^2 p_i^2 + \frac{\lambda_i^2}{4} - \lambda_i p_i^2 + \mu_i$

The Möbius diagram of the doubly weighted points W_i is the projection onto $\mathbb{R}^d$ of the restriction to the paraboloid $\mathcal{Q}$ of the Laguerre diagram of the $\Sigma_i = B(C_i, \rho_i)$

Discrete metric spaces : Witness Complex [de Silva]

L a finite set of points (landmarks) — vertices of the complex

W a dense sample (witnesses) — pseudo circumcenters



Let σ be a (abstract) simplex with vertices in L, and let $w \in W$. We say that w is a witness of σ if

$$\|w - p\| \leq \|w - q\| \quad \forall p \in \sigma \text{ and } \forall q \in L \setminus \sigma$$

The witness complex $\mathrm{Wit}(L, W)$ is the complex consisting of all simplexes σ such that for any simplex $\tau \subseteq \sigma$, τ has a witness in W

Easy consequences of the definition

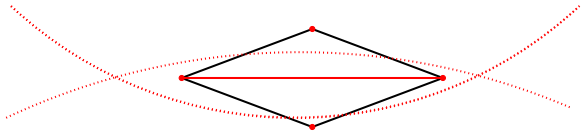
- The witness complex can be defined for any metric space and, in particular, for discrete metric spaces
- If $W' \subseteq W$, then $\mathrm{Wit}(L, W') \subseteq \mathrm{Wit}(L, W)$
- $\mathrm{Del}(L) \subseteq \mathrm{Wit}(L, \mathbb{R}^d)$

Identity of $\mathrm{Del}_{|\Omega}(L)$ and $\mathrm{Wit}(L, \mathbb{R}^d)$ [de Silva 2008]

Theorem : $\mathrm{Wit}(L, W) \subseteq \mathrm{Wit}(L, \mathbb{R}^d) = \mathrm{Del}(L)$

Remarks

- Faces of all dimensions have to be witnessed

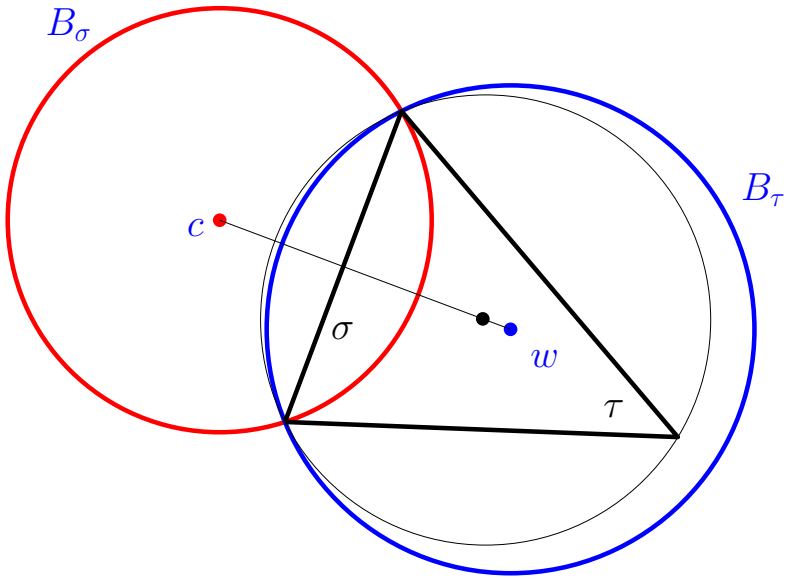


- $\mathrm{Wit}(L, W)$ is embedded in $\mathbb{R}^d$ if L is in general position wrt spheres

Proof of de Silva's theorem

$\tau = [p_0, ..., p_k]$ is a k-simplex of $\mathrm{Wit}(L)$ witnessed by a ball B_τ (i.e. $B_\tau \cap L = \tau$)
We prove that $\tau \in \mathrm{Del}(L)$ by induction on k

Clearly true for $k = 0$



Hyp. : true for $k' \leq k - 1$

$B := B_\tau$

$\sigma := \partial B \cap \tau, \quad l := |\sigma|$

// $\sigma \in \mathrm{Del}(L)$ by the hyp.

while $l + 1 = \dim \sigma < k$ do

$B \leftarrow$ the ball centered on $[cw]$ s.t.

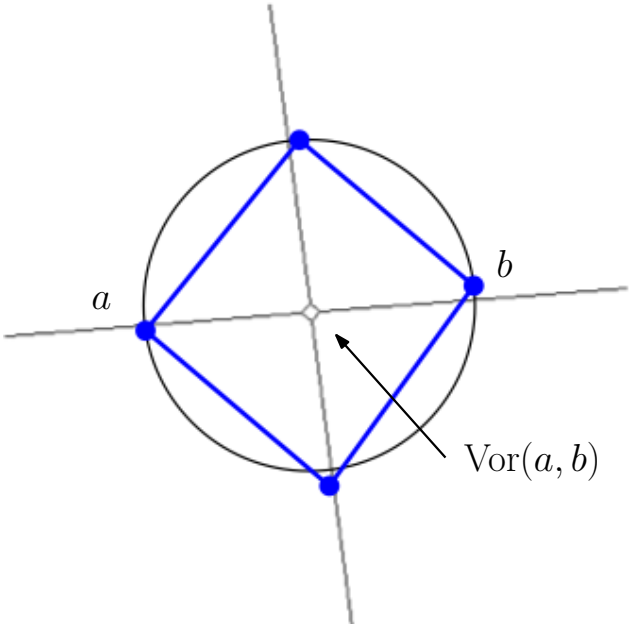
- $\sigma \subset \partial B$,
- B witnesses τ
- $|\partial B \cap \tau| = l + 1$

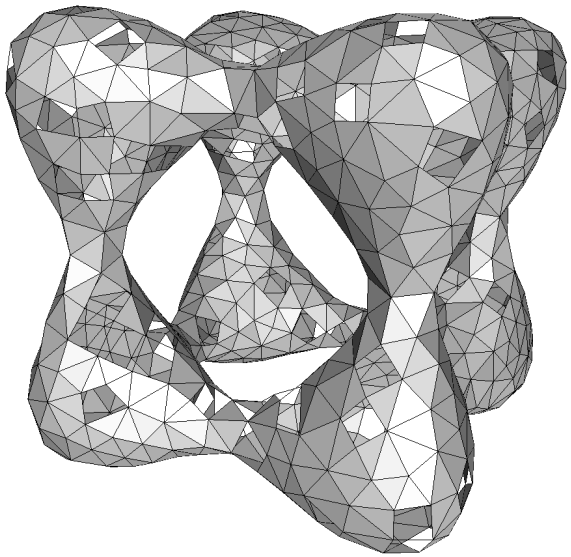
$(B \text{ witnesses } \tau) \wedge (\tau \subset \partial B) \Rightarrow \tau \in \mathrm{Del}(L)$

Case of sampled domains : $\mathrm{Wit}(L, W) \neq \mathrm{Del}(L)$

W a finite set of points $\subset \Omega \subset \mathbb{R}^d$

$\mathrm{Wit}(L, W) \neq \mathrm{Del}(L)$, even if W is a dense sample of Ω





$$[ab] \in \mathrm{Wit}(L, W) \quad \Leftrightarrow \quad \exists p \in W, \ \ \mathsf{Vor}_2(a, b) \cap W \neq \emptyset$$

Relaxed witness complex

Alpha-witness Let σ be a simplex with vertices in L. We say that a point $w \in W$ is an α-witness of σ if

$$\|w - p\| \leq \|w - q\| + \alpha \quad \forall p \in \sigma \quad \text{and} \quad \forall q \in L \setminus \sigma$$

Alpha-relaxed witness complex The α-relaxed witness complex $\mathrm{Wit}^{\alpha}(L, W)$ is the maximal simplicial complex with vertex set L whose simplices have an α-witness in W

$\mathrm{Wit}^{0}(L, W) = \mathrm{Wit}(L, W)$

Filtration : $\alpha \leq \beta \quad \Rightarrow \quad \mathrm{Wit}^{\alpha}(L, W) \subseteq \mathrm{Wit}^{\beta}(L, W)$

Interleaving complexes

Lemma Assume that W is ε-dense in Ω and let $\alpha \geq 2\varepsilon$. Then

$$\mathrm{Wit}(L, W) \subseteq \mathrm{Del}_{|\Omega}(L) \subseteq \mathrm{Wit}^{\alpha}(L, W)$$

Proof

σ : a d-simplex of $\mathrm{Del}(L)$, c_σ its circumcenter
W ε-dense in Ω $\exists w \in W$ s.t. $\|c_\sigma - w\| \leq \varepsilon$
For any $p \in \sigma$ and $q \in L \setminus \sigma$, we then have

$$\begin{aligned} \forall p \in \sigma \text{ and } q \in L \setminus \sigma \quad \|w - p\| &\leq \|c_\sigma - p\| + \|c_\sigma - w\| \\ &\leq \|c_\sigma - q\| + \|c_\sigma - w\| \\ &\leq \|w - q\| + 2\|c_\sigma - w\| \\ &\leq \|w - q\| + 2\varepsilon \end{aligned}$$