Convex Hulls, Voronoi Diagrams and Delaunay Triangulations

Jean-Daniel Boissonnat

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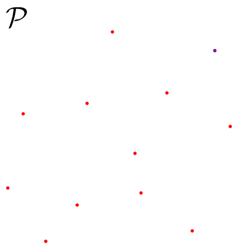
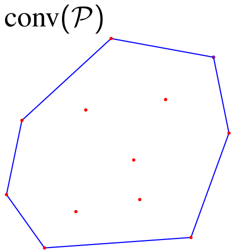
Convex hull





Smallest convex set that contains a finite set of points $\mathcal{P}$

Set of all possible convex combinations of points in $\mathcal{P}$

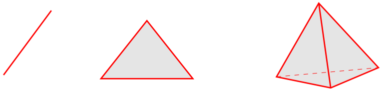
$$\sum \lambda_i p_i,\ \lambda_i \geq 0,\ \sum_i \lambda_i = 1$$

We call polytope the convex hull of a finite set of points

Simplex

The convex hull of $k+1$ points that are affinely independent is called a *k-simplex*

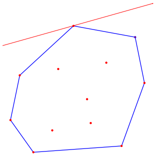
1-simplex = line segment
2-simplex = triangle
3-simplex = tetrahedron



Facial structure of a polytope

Supporting hyperplane

$H \cap C \neq \emptyset$ and C is entirely contained in one of the two half-spaces defined by H



Faces

The faces of a P are the polytopes $P \cap h$, h support. hyp.

The face complex

The faces of P form a cell complex C

- $\forall f \in C$, f is a convex polytope
- $f \in C$, $f \subset g \Rightarrow g \in C$
- $\forall f, g \in C$, either $f \cap g = \emptyset$ or $f \cap g \in C$

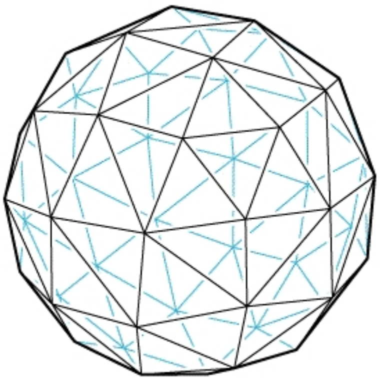
General position

A point set $\mathcal{P}$ is said to be in general position iff no subset of $k + 2$ points lie in a k-flat

If $\mathcal{P}$ is in general position, all the faces of $\mathrm{conv}(\mathcal{P})$ are simplices

The boundary of $\mathrm{conv}(\mathcal{P})$ is a simplicial complex

Two ways of defining polyhedra



Convex hull of n points

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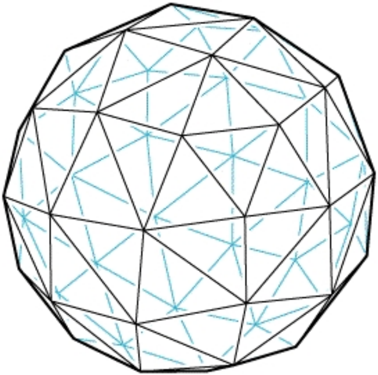
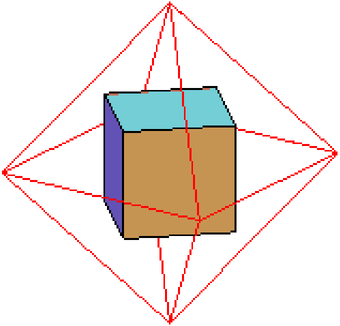


Convex hull of n points



Intersection of n half-spaces

Duality between points and hyperplanes

hyperplane $h : x_d = a \cdot x' - b$ of $\mathbb{R}^d \longrightarrow$ point $h^* = (a, b) \in \mathbb{R}^d$

point $p = (p', p_d) \in \mathbb{R}^d \longrightarrow$ hyperplane $p^* \subset \mathbb{R}^d$
$= \{(a, b) \in \mathbb{R}^d : b = p' \cdot a - p_d\}$

The mapping *

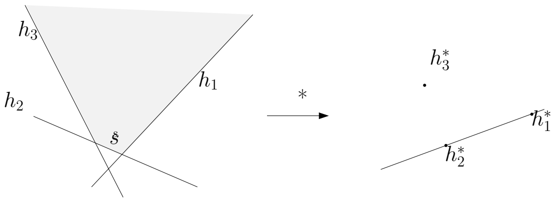
- preserves incidences :

$$
\begin{aligned}
p \in h \quad &\Longleftrightarrow \quad p_d = a \cdot p' - b \Longleftrightarrow b = p' \cdot a - p_d \Longleftrightarrow h^* \in p^* \\
p \in h^+ \quad &\Longleftrightarrow \quad p_d > a \cdot p' - b \Longleftrightarrow b > p' \cdot a - p_d \Longleftrightarrow h^* \in p^{*+}
\end{aligned}
$$

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

Duality between polytopes

Let $h_1, \ldots, h_n$ be n hyperplanes de $\mathbb{R}^d$ and let $P = \cap h_i^+$



A vertex s of P is the intersection of $k \geq d$ hyperplanes $h_1, \ldots, h_k$ lying above all the other hyperplanes

$\Longrightarrow$ s^* is a hyperplane $\ni h_1^*, \ldots, h_k^*$
supporting P^*=conv$^-(h_1^*, \ldots, h_k^*)$

General position :
s is the intersection of d hyperplanes

$\Longrightarrow$ s^* is a $(d-1)$-face (simplex) de P^*

More generally and under the general position assumption, if f is a $(d-k)$-face of P, $f = \cap_{i=1}^{k} h_i$

$$
\begin{aligned}
p \in f \quad \Leftrightarrow \quad & h_i^* \in p^* \ \text{ for } \ i = 1, \dots, k \\
& h_i^* \in p^{*+} \ \text{ for } \ i = k+1, \dots, n \\
\\
\Leftrightarrow \quad & p^* \text{support. hyp. of } \ P^* = \text{conv}(h_1^*, \dots, h_n^*) \\
& \ni h_1^*, \dots, h_k^* \\
\\
\Leftrightarrow \quad & f^* = \text{conv}(h_1^*, \dots, h_k^*) \ \text{ is a } \ (k-1) - \text{face of } \ P^*
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$$\begin{aligned} p \in f \quad \Leftrightarrow \quad & h_i^* \in p^* \ \text{ for } \ i = 1, \ldots, k \\ & h_i^* \in p^{*+} \ \text{ for } \ i = k+1, \ldots, n \\ \\ \Leftrightarrow \quad & p^* \text{support. hyp. of } \ P^* = \text{conv}(h_1^*, \ldots, h_n^*) \\ & \ni h_1^*, \ldots, h_k^* \\ \\ \Leftrightarrow \quad & f^* = \text{conv}(h_1^*, \ldots, h_k^*) \ \text{ is a } \ (k-1) - \text{face of } \ P^* \end{aligned}$$

Duality between P and P^*

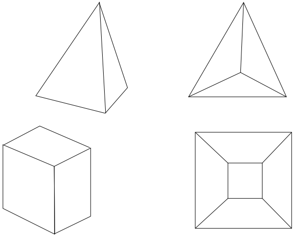
- We have defined an involutive correspondence between the faces of P and P^* s.t. $\forall f, g \in P, f \subset g \Rightarrow g^* \subset f^*$
- As a consequence, computing P reduces to computing a lower convex hull

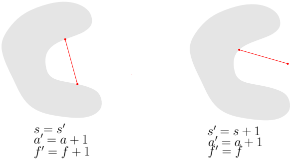
Euler's formula

The numbers of vertices s, edges a and facets f of a polytope of $\mathbb{R}^3$ satisfy

$$s - a + f = 2$$

Schlegel diagram





Euler formula : $s - a + f = 2$

Incidences edges-facets

$$2a \geq 3f \quad \Longrightarrow \quad \begin{array}{l} a \leq 3s - 6 \\ f \leq 2s - 4 \end{array}$$

with equality when all facet are triangles

Beyond the 3rd dimension

Upper bound theorem

[McMullen 1970]

If P is the intersection of n half-spaces of $\mathbb{R}^d$

$$\text{nb faces of } P = \Theta(n^{\lfloor \frac{d}{2} \rfloor})$$

Beyond the 3rd dimension

Upper bound theorem

[McMullen 1970]

If P is the intersection of n half-spaces of $\mathbb{R}^d$

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General position

all vertices of P are incident to d edges (in the worst-case) and have distinct x_d

$\Rightarrow$ the convex hull of $k < d$ edges incident to a vertex p is a k-face of P

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

Proof of the upper bound th.

1. $\geq \lceil \frac{d}{2} \rceil$ edges incident to a vertex p are in $h_p^+ : x_d \geq x_d(p)$ or in h_p^-
   - $\Rightarrow$ p is a x_d-max or x_d-min vertex of at least one $\lceil \frac{d}{2} \rceil$-face of P
   - $\Rightarrow$ # vertices of $P \leq 2 \times$# $\lceil \frac{d}{2} \rceil$-faces of P
2. A k-face is the intersection of $d-k$ hyperplanes defining P
   - $\Rightarrow$ # k-faces $= \binom{n}{d-k} = O(n^{d-k})$
   - $\Rightarrow$ # $\lceil \frac{d}{2} \rceil$-faces $= O(n^{\lfloor \frac{d}{2} \rfloor})$
3. The number of faces incident to p depends on d but not on n

Representation of a convex hull

Adjacency graph (AG) of the facets

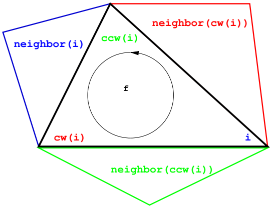
In general position, all the facets are $(d-1)$-simplexes

Vertex

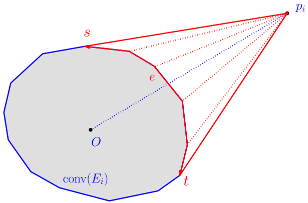
Face*	*v_face*

Face

Vertex*	*vertex*$[d]$
Face*	*neighbor*$[d]$



Incremental algorithm



$\mathcal{P}_i$: set of the i points that have been inserted first

$\mathrm{conv}(\mathcal{P}_i)$: convex hull at step i

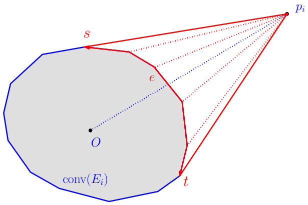
$f = [p_1, ..., p_d]$ is a red facet iff its supporting hyperplane separates p_i from $\mathrm{conv}(\mathcal{P}_i)$

$\iff \texttt{orient}(p_1, ..., p_d, p_i) \times \texttt{orient}(p_1, ..., p_d, O) < 0$

$$\mathrm{orient}(p_0, p_1, ..., p_d) = \begin{vmatrix} 1 & 1 & ... & 1 \\ x_0 & x_1 & ... & x_d \\ y_0 & y_1 & ... & y_d \\ z_0 & z_1 & ... & z_d \end{vmatrix}$$

Update of $\text{conv}(\mathcal{P}_i)$

- Locate : traverse AG to find the red facets and the $(d-2)$-faces on the horizon V
- Update: replace the red facets by the facets $\text{conv}(p_i, e)$, $e \in V$



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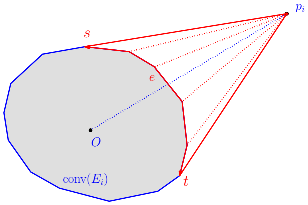
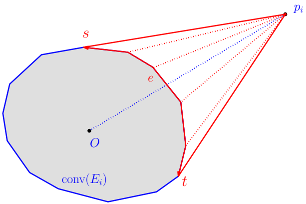


Correctness

- The AG of the red facets is connected
- The new faces are all obtained as above

Complexity analysis

- update proportionnal to the number of red facets
- # new facets $= O(n^{\lfloor \frac{d-1}{2} \rfloor})$
- fast locate : insert the points in lexicographic order and attach a facet to each point



$$
\begin{aligned}
T(n,d) &= O(n\log n) + \textstyle\sum_{i=1}^{n} |\mathrm{conv}(i, d-1)| \\
&= O(n\log n + n \times n^{\lfloor \frac{d-1}{2} \rfloor}) = O(n\log n + n^{\lfloor \frac{d+1}{2} \rfloor})
\end{aligned}
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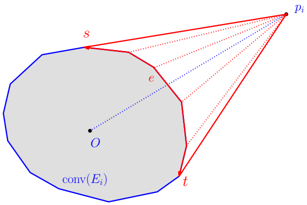

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Optimal in even dimensions

Can be improved to $O(n\log n)$ when $d = 3$

The expected complexity can be improved to $O(n\log n + n^{\lfloor \frac{d}{2} \rfloor})$ by inserting the points in random order (see course 3)

The randomized algorithm can be derandomized [Chazelle 1992]

Delaunay Triangulations

Simplex

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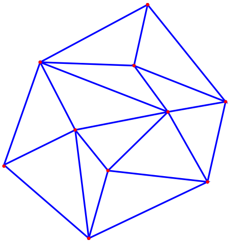
Simplicial complex

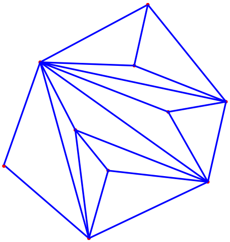
A finite collection of simplices C called the faces of C such that

- $\forall f \in C$, f is a simplex
- $f \in C$, $f \subset g \Rightarrow g \in C$
- $\forall f, g \in C$, either $f \cap g = \emptyset$ or $f \cap g \in C$

Triangulation of a finite set of points

A triangulation $T(\mathcal{P})$ of a finite set of points $\mathcal{P} \in \mathbb{R}^d$ is a d-simplicial complex whose vertices are the points of $\mathcal{P}$ and whose domain is $\mathrm{conv}(\mathcal{P})$





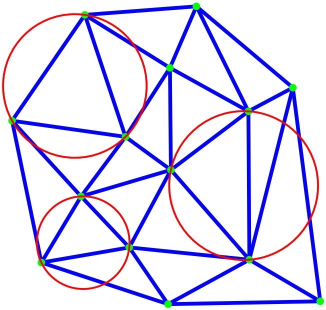
There exists many triangulations of a given set of points

Delaunay triangulation

$\mathcal{P} = \{p_1, p_2 \ldots p_n\}$ set of points in general position ($\nexists\ d+1$ points on a same sphere)

$t \subset \mathcal{P}$ is a Delaunay simplex iff $\exists$ a sphere σ_t s.t.

$\sigma_t(p) = 0\ \forall p \in t$
$\sigma_t(q) > 0\ \forall q \in \mathcal{P} \setminus t$



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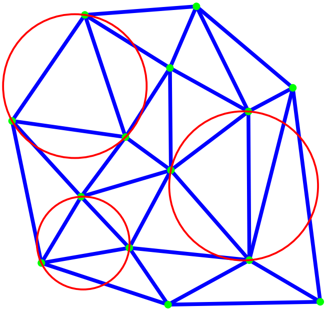
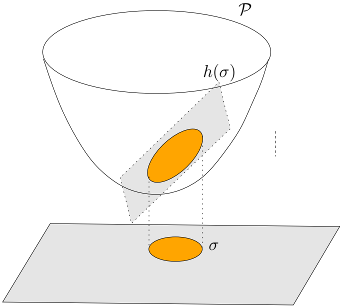


Delaunay theorem

The Delaunay simplices form a triangulation of $\mathcal{P}$, called the Delaunay triangulation of $\mathcal{P}$

Proof of the theorem



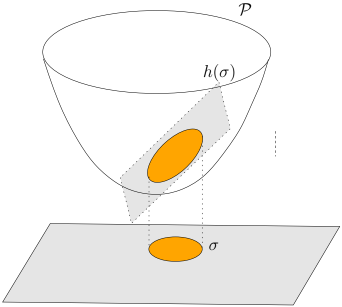
Linearization

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

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

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

Proof of the theorem



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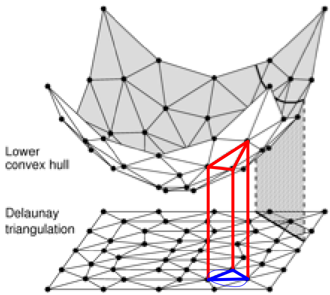
Proof of Delaunay's th.

t a simplex, σ_t its circumscribing sphere

$t \in \mathrm{Del}(\mathcal{P}) \Leftrightarrow \forall i, \hat{p}_i \in h_{\sigma_t}^+$

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

Proof of the theorem



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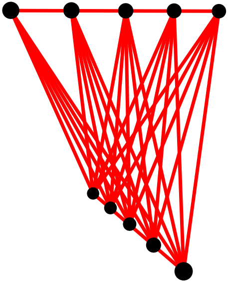
$$\Leftrightarrow \hat{t} \text{ is a face of } \mathrm{conv}^-(\hat{\mathcal{P}})$$

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

Combinatorial complexity

The combinatorial complexity of the Delaunay triangulation diagram of n points of $\mathbb{R}^d$ is the same as the combinatorial complexity of a convex hull of n points of $\mathbb{R}^{d+1}$

Hence, by the Upper Bound Theorem [Mc Mullen 1970]
it is $\Theta\left(n^{\lfloor \frac{d+1}{2} \rfloor}\right)$



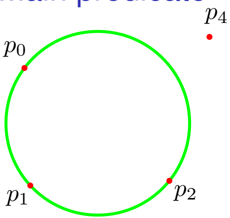
Algorithm for constructing DT

Input : a set $\mathcal{P}$ of n points of $\mathbb{R}^d$

1. Lift the points of $\mathcal{P}$ onto the paraboloid $x_{d+1} = x^2$ of $\mathbb{R}^{d+1}$: $p_i \rightarrow \hat{p}_i = (p_i, p_i^2)$
2. Compute $\mathrm{conv}(\{\hat{p}_i\})$
3. Project the lower hull $\mathrm{conv}^-(\{\hat{p}_i\})$ onto $\mathbb{R}^d$

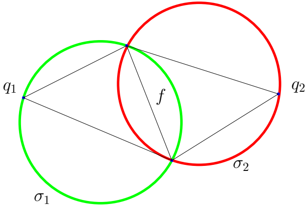
Complexity : $\Theta(n \log n + n^{\lfloor \frac{d+1}{2} \rfloor})$

Main predicate



$$\texttt{insphere}(p_0, \ldots, p_{d+1}) = \texttt{orient}(\hat{p}_0, \ldots, \hat{p}_{d+1}) = \mathrm{sign} \begin{vmatrix} 1 & \ldots & 1 \\ p_0 & \ldots & p_{d+1} \\ p_0^2 & \ldots & p_{d+1}^2 \end{vmatrix}$$

Local characterization



Pair of regular simplices

$$\sigma_2(q_1) \geq 0 \quad \text{and} \quad \sigma_1(q_2) \geq 0$$

$$\Leftrightarrow \hat{c}_1 \in h^+_{\sigma_2} \text{ and } \hat{c}_2 \in h^+_{\sigma_1}$$

Theorem

A triangulation such that all pairs of simplexes are regular is a Delaunay triangulation

Proof

The PL function whose graph is obtained by lifting the triangles is locally convex and has a convex support

Optimality properties of the Delaunay triangulation

Among all possible triangulations of $\mathcal{P}$, $\mathrm{Del}(\mathcal{P})$

1. maximizes the smallest angle (in the plane) [Lawson]
2. minimizes the radius of the maximal smallest ball enclosing a simplex) [Rajan]
3. minimizes the roughness (Dirichlet's energy) [Rippa]

Optimizing the angular vector ($d = 2$)

Angular vector of a triangulation $T(\mathcal{P})$

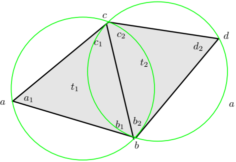
$$\text{ang}\,(T(\mathcal{P})) = (\alpha_1, \ldots, \alpha_{3t}),\ \alpha_1 \leq \ldots \leq \alpha_{3t}$$

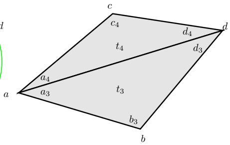
Optimality

Any triangulation of a given point set $\mathcal{P}$ whose angular vector is maximal (for lexicographic order) is a Delaunay triangulation of $\mathcal{P}$

Affects matrix conditioning in FE methods

Constructive proof using flips



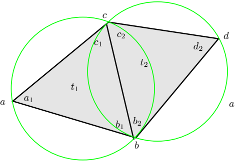


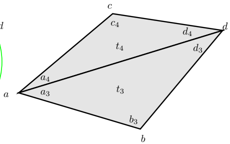
While $\exists$ a non regular pair (t_3, t_4)

/* $t_3 \cup t_4$ is convex */

replace (t_3, t_4) by (t_1, t_2)

Constructive proof using flips





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Regularize $\Leftrightarrow$ improve $\mathrm{ang}\,(T(\mathcal{P}))$

$\mathrm{ang}\,(t_1, t_2) \geq \mathrm{ang}\,(t_3, t_4)$

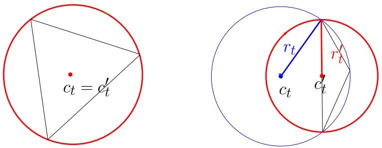
$$a_1 = a_3 + a_4,\ d_2 = d_3 + d_4,$$
$$c_1 \geq d_3,\quad b_1 \geq d_4,\quad b_2 \geq a_4,\quad c_2 \geq a_3$$

- The algorithm terminates since the number of triangulations of $\mathcal{P}$ is finite and $\mathrm{ang}(T(\mathcal{P}))$ cannot decrease
- The obtained triangulation is a Delaunay triangulation of $\mathcal{P}$
- If a triangulation of $\mathcal{P}$ maximixes the angular vector, all its edges are regular; hence, it is a DT of $\mathcal{P}$

Minimizing the maximal min-containment radius [Rajan]

r'_t = radius of the smallest ball containing t

$Q(T) = \max_{t \in T} r'_t$



Th. : for a given $\mathcal{P}$, for all $T(\mathcal{P})$, $Q(\mathrm{Del}(\mathcal{P})) \leq Q(T(\mathcal{P}))$

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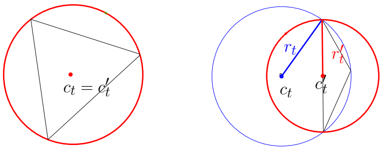


Th. : for a given $\mathcal{P}$, for all $T(\mathcal{P})$, $\quad Q(\mathrm{Del}(\mathcal{P})) \leq Q(T(\mathcal{P}))$

Interpolation error

[Waldron 98]

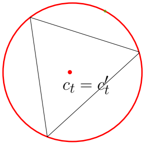
If g is the linear interpolation of f over a simplex t,

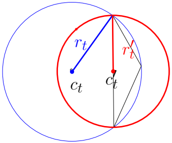
$$\|f - g\|_\infty \leq c_t \, \frac{{r'_t}^2}{2}$$

$c_t =$ bound on the absolute curvature of f in t

Minimizing the maximal min-containment radius

$\max_{t \in \mathrm{Del}} r'_{t \in T} \leq \max_{t \in T} r'_t$



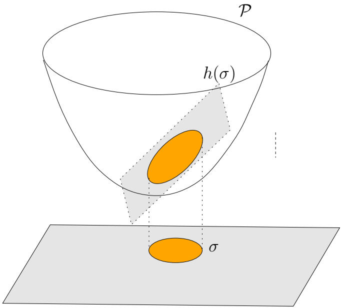


Proof

$\sigma_t(x) = \|x - c_t\|^2 - r_t^2, \qquad \sigma_T(x) = \sigma_t(x)$ if $x \in t \subset T$

1. $\forall x \in \mathrm{conv}(\mathcal{P}) : 0 > \sigma_{\mathrm{Del}}(x) \geq \sigma_T(x)$ see next slide
2. $\min_{x \in t} \sigma_t(x) = -{r'}_t^2 \quad \Leftarrow$ if $c_t \notin t : \sigma_t(x) \geq \|c'_t - c_t\|^2 - r_t^2 = -{r'}_t^2$
3. $x_T = \arg\min \sigma_T(x), \qquad x_{\mathrm{Del}} = \arg\min \sigma_{\mathrm{Del}}(x)$
   $\sigma_T(x_T) = -{r'}_T^2 \leq \sigma_T(x_{\mathrm{Del}}) \leq \sigma_{\mathrm{Del}}(x_{\mathrm{Del}}) = -{r'}_{\mathrm{Del}}^2$

Proof of 1 : $0 > \sigma_{\mathrm{Del}}(x) \geq \sigma_T(x)$



$$\sigma_t(x) = x^2 - 2c_t \cdot x + s \ (s = c_t^2 - r_t^2)$$
$$= f(x) - g(x)$$

where $f(x) = x^2$ and $g_t(x) = 2c_t \cdot x - s$

Geometric interpretation

$\sigma_t(x)$ maximal

$\Leftrightarrow g_t(x)$ minimal
$\Leftrightarrow \mathcal{G}_t = h_{\sigma_t}$ supports $\mathrm{conv}(\hat{\mathcal{P}})$
$\Leftrightarrow \sigma_t$ is empty
$\Leftrightarrow t \in \mathrm{Del}(\mathcal{P})$

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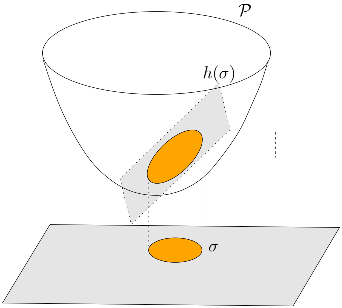

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Minimum roughness of Delaunay triangulations

Input : n points $p_1, ...p_n$ of $\mathbb{R}^2$ and for each p_j a real f_j

Roughness of a triangulation $T(\mathcal{P})$:

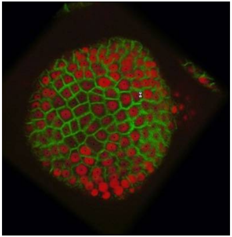
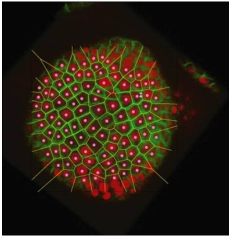
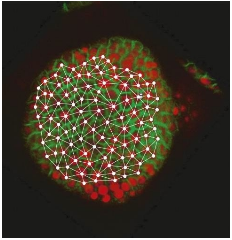
$$R(T) = \sum_i \int_{T_i} \left(\left(\frac{\partial \phi_i}{\partial x} \right)^2 + \left(\frac{\partial \phi_i}{\partial y} \right)^2 \right) dx\, dy$$

$\phi_i =$ linear interpolation of the f_j over triangle $T_i \in T$

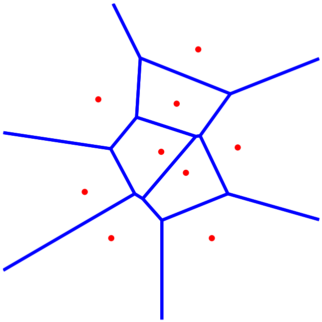
Theorem (Rippa)

Among all possible triangulations of $\mathcal{P}$, $\mathrm{Del}(\mathcal{P})$ is one with minimum roughness

Voronoi Diagrams

Euclidean Voronoi diagrams

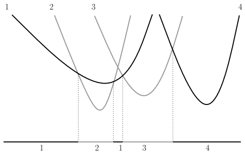


Voronoi cell $\qquad V(p_i) = \{x : \|x - p_i\| \leq \|x - p_j\|, \ \forall j\}$

Voronoi diagram $(\mathcal{P})$ $\qquad = \{$ cell complex whose cells are the $V(p_i)$ and their faces, $p_i \in \mathcal{P}$ $\}$

Voronoi diagrams and polytopes

Vor($p_1, \ldots, p_n$) is the minimization diagram of the n functions $\delta_i(x) = (x - p_i)^2$



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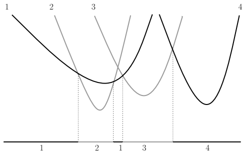

$\arg\min(\delta_i) = \arg\max(h_i)$
where $h_{p_i}(x) = 2\, p_i \cdot x - p_i^2$

The minimization diagram of the δ_i is also the maximization diagram of the affine functions $h_i(x)$

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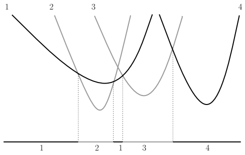

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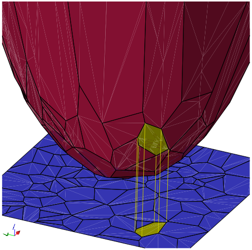

The faces of Vor$(\mathcal{P})$ are the projection of the faces of $\mathcal{V}(\mathcal{P}) = \bigcap_i \; h_{p_i}^+$
$h_{p_i}^+ = \{x : x_{d+1} > 2p_i \cdot x - p_i^2\}$

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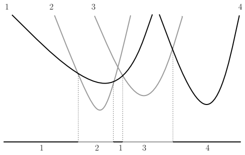

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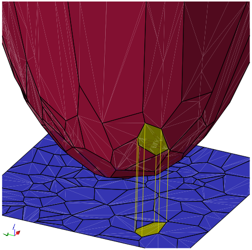

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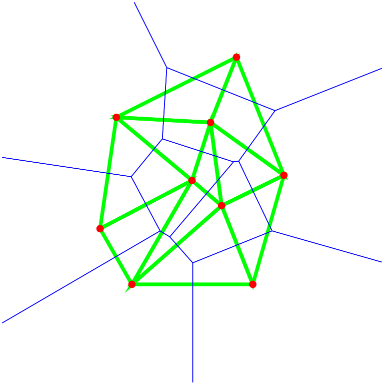
Note !

$h_{p_i}(x) = 0$ is the hyperplane tangent to $\mathcal{Q} : x_{d+1} = x^2$ at (x, x^2)

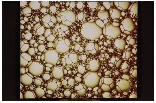
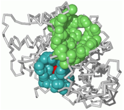
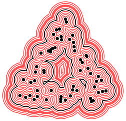
Dual triangulation

$$\begin{array}{ccc} \mathcal{V}(\mathcal{P}) = h_{p_1}^+ \cap \ldots \cap h_{p_n}^+ & \longleftrightarrow & \mathcal{D}(\mathcal{P}) = \mathrm{conv}^-(\{\phi(p_1), \ldots, \phi(p_n)\}) \\ \updownarrow & & \updownarrow \\ \text{Voronoi Diagram of } \mathcal{P} & \longleftrightarrow & \text{Delaunay Triangulation of } \mathcal{P} \end{array}$$



Affine Diagrams

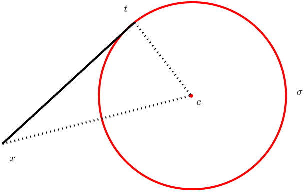
Motivations

- To extend Voronoi diagrams to spheres (or weighted points)
  - molecular biology : how to compute a union of balls ?
  - sampling theory : the offset of a set of points captures topological information on the sapled object (see Course F. Chazal)
  - to improve the quality of a mesh (see Course M. Yvinec)
- To characterize the class of affine diagrams

Power diagrams of spheres

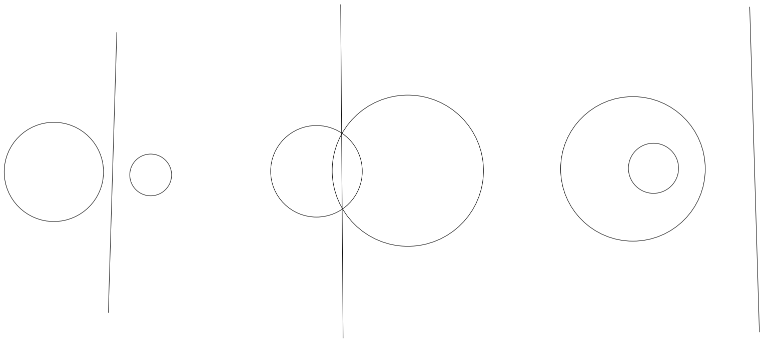
Power of a point to a sphere



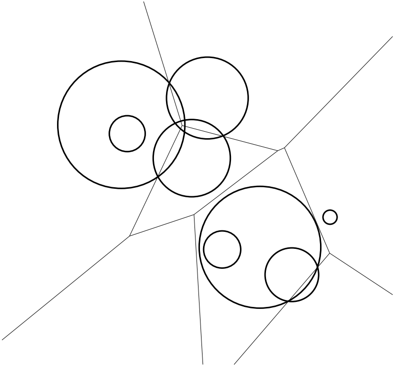
$$\sigma(x) = (x - t)^2 = (x - c)^2 - r^2$$
$$\sigma(x) < 0 \iff x \in \mathrm{int}(\sigma)$$

Bisector of two spheres = hyperplane

$$\sigma_i(x) = \sigma_j(x) \Longleftrightarrow \cancel{x}^2 - 2c_i \cdot x + s_i = \cancel{x}^2 - 2c_j \cdot x + s_j$$



Laguerre (power) diagram



Sites : a set $\mathcal{S}$ of n spheres $\sigma_1, \ldots, \sigma_n$

Distance of a point x to σ_i

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

$\mathrm{Lag}(\mathcal{S})$ is the cell complex whose cells are the

$$\mathrm{Lag}(\sigma_i) = \{x : \sigma_i(x) \leq \sigma_j(x),\ \forall j\}$$

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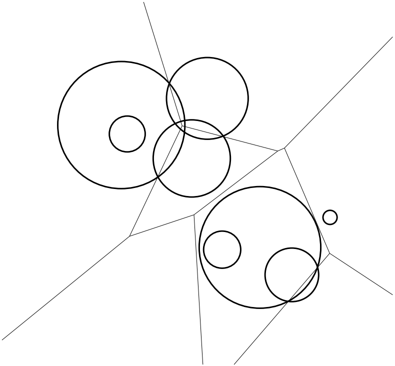

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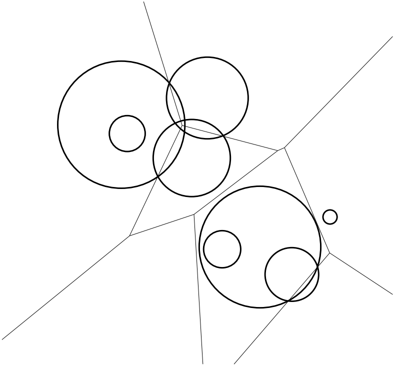
Note !

- $\mathrm{Lag}(\sigma_i)$ may be empty
- c_i may not belong to $\mathrm{Lag}(\sigma_i)$

Laguerre diagrams and polytopes



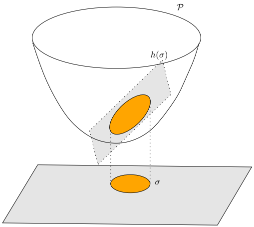
$$\sigma_i(x) = (x - c_i)^2 - r_i^2$$
$$h_{\sigma_i}(x) = 2\, c_i \cdot x - c_i^2 + r_i^2$$

$$\begin{aligned} \arg\min \sigma_i(x) &= \arg\min((x - c_i)^2 - r_i^2) \\ &= \arg\max(h_{\sigma_i}(x)) \\ & \quad h_{\sigma_i}(x) = 2\, c_i \cdot x - c_i^2 + r_i^2) \end{aligned}$$

$\mathrm{Lag}(\mathcal{S})$ is the minimization diagram of the σ_i
$\Leftrightarrow$ the maximization diagram
of the affine functions $h_{\sigma_i}(x)$

- The faces of $\mathrm{Lag}(\mathcal{S})$ are the vertical projections of the faces of $\mathcal{L}(\mathcal{S}) = \bigcap_i h_{\sigma_i}^+$

Space of spheres



σ hypersphere of $\mathbb{R}^d$

$\rightarrow$ point $\hat{\sigma} = (c, s = c^2 - r^2) \in \mathbb{R}^{d+1}$
$\rightarrow$ the polar hyperplane $h_\sigma = \hat{\sigma}^* \subset \mathbb{R}^{d+1}$:

$$x_{d+1} = 2c \cdot x - s$$

1. The spheres of radius 0 are mapped onto the paraboloid

$$\mathcal{Q} : x_{d+1} = x^2$$

2. The vertical projection of $h_{\sigma_i} \cap \mathcal{Q}$ onto $x_{d+1} = 0$ is σ_i

3. $\sigma(x) = x^2 - 2c \cdot x + s$ is the (signed) vertical distance from the lift of x onto h_σ to the lift $\hat{x}$ of x onto $\mathcal{Q}$

4. $\sigma(x) < 0 \Leftrightarrow \hat{x} = (x, x^2) \in h_\sigma^-$

Orthogonality between spheres

A distance between spheres

$$d(\sigma_1, \sigma_2) = \sqrt{(c_1 - c_2)^2 - r_1^2 - r_2^2}$$

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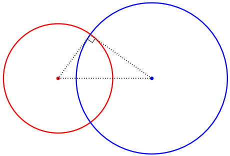
Orthogonality

$$\begin{aligned} d(\sigma_1, \sigma_2) = 0 &\Leftrightarrow (c_1 - c_2)^2 = r_1^2 + r_2^2 \\ &\Leftrightarrow \sigma_1 \perp \sigma_2 \qquad \text{(Pythagore)} \end{aligned}$$



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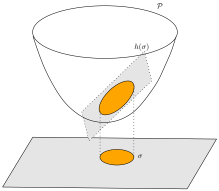

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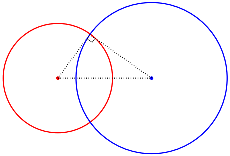

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In the space of spheres

$$\begin{array}{ccccccc} d(\sigma_1, \sigma_2) = 0 & \Leftrightarrow & s_2 = 2\, c_1 \cdot c_2 - c_1^2 & \Leftrightarrow & \hat{\sigma}_2 \in h_{\sigma_1} & & (s_i = c_i^2 - r_i^2) \\ < & & < & & h^-_{\sigma_1} & & \end{array}$$

The vertical projection of the dual complex $\mathcal{R}(\mathcal{S})$ of $\mathcal{L}(\mathcal{S})$ is called the regular triangulation of $\mathcal{S}$

$$
\begin{array}{ccc}
\mathcal{L}(\mathcal{S}) = h^+_{\sigma_1} \cap \ldots \cap h^+_{\sigma_n} & \longleftrightarrow & \mathcal{R}(\mathcal{S}) = \text{conv}^-(\{\hat{\sigma}_1, \ldots, \hat{\sigma}_n\}) \\
\updownarrow & & \updownarrow \\
\text{Laguerre diagram of } \mathcal{S} & \longleftrightarrow & \text{Laguerre triangulation of } \mathcal{S}
\end{array}
$$

$$(\hat{\sigma}_i = h^*_{\sigma_i} = (c_i, c_i^2 - r_i^2) \in \mathbb{R}^{d+1})$$

$\mathcal{S} = \{\sigma_1, ...\sigma_n\}$ where σ_i is the sphere of center c_i and radius r_i

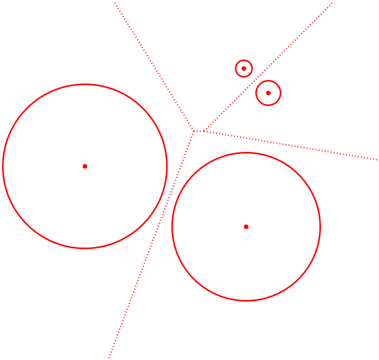
$\mathcal{P} = \{c_1, ..., c_n\}$

Characteristic property

$t \subset \mathcal{P}$ is a simplex of the regular triangulation of $\mathcal{S}$
iff there exists a sphere σ_t s.t.

- $d(\sigma_t, \sigma_i) = 0 \ \forall c_i \in t$ $\qquad$ ($\sigma_t =$ orthosphere of t)
- $d(\sigma_t, \sigma_j) > 0 \ \forall c_j \in \mathcal{P} \setminus t$

Regular triangulation



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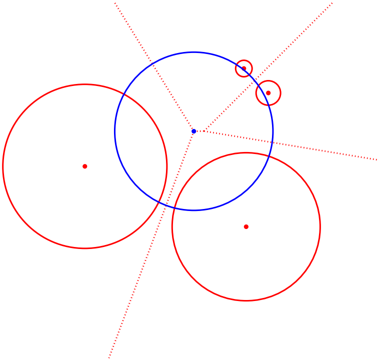
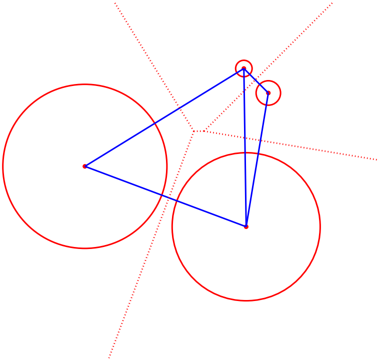


Regular triangulation



Complexity and algorithm

nb of faces $= \Theta\left(n^{\lfloor \frac{d+1}{2} \rfloor}\right)$ (Upper Bound Th.)

can be computed in time $\Theta\left(n \log n + n^{\lfloor \frac{d+1}{2} \rfloor}\right)$

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Main predicate

$$\texttt{power\_test}(\sigma_0, \ldots, \sigma_{d+1}) = \text{sign} \begin{vmatrix} 1 & \ldots & 1 \\ c_0 & \ldots & c_{d+1} \\ c_0^2 - r_0^2 & \ldots & c_{d+1}^2 - r_{d+1}^2 \end{vmatrix}$$

Affine diagrams and regular subdivisions

Definition

Affine diagrams are defined as the maximization diagrams of a finite set of affine functions
They are also called regular subdvisions

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- Voronoi and Laguerre diagrams are affine diagrams
- Any affine Voronoi diagram of $\mathbb{R}^d$ is the Laguerre diagram of a set of spheres of $\mathbb{R}^d$
- Delaunay and Laguerre triangulations are regular triangulations
- Any regular triangulation is a Laguerre triangulation, i.e. dual to a Laguerre diagram

Examples of affine diagrams

1. *The intersection of a power diagram with an affine subspace*

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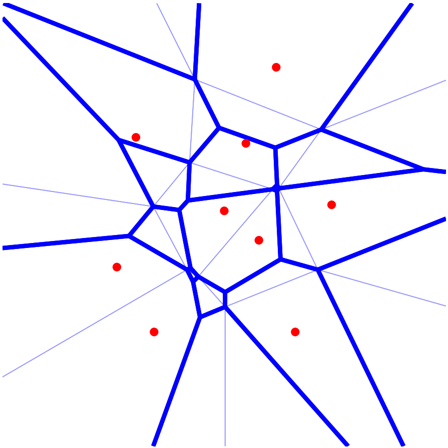
3. k-th order Voronoi diagrams

Order k Voronoi Diagrams



Order 2 Voronoi Diagram

A k-order Voronoi diagram is a power diagram

Let $\mathcal{P}_1, \mathcal{P}_2, \ldots$ denote the subsets of k points of $\mathcal{P}$

$$\sigma_i(x) = \frac{1}{k} \sum_{j \in \mathcal{P}_i} (x - p_j)^2 = x^2 - \frac{2}{k} \sum_{j \in \mathcal{P}_i} p_j \cdot x + \frac{1}{k} \sum_{j \in \mathcal{P}_i} p_j^2$$

The k nearest neighbors of x are the points of $\mathcal{P}_i$ iff

$$\forall j, \quad \sigma_i(x) \leq \sigma_j(x)$$

σ_i is the sphere centered at $\frac{1}{k} \sum_{j=1}^{k} p_{i_j}$

$$\sigma_k(0) = \frac{1}{k} \sum_{j=1}^{k} p_{i_j}^2$$

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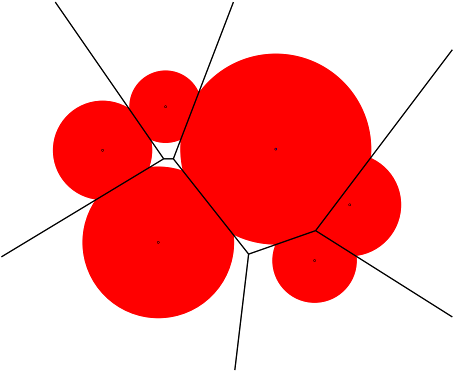
Combinatorial complexity

The number of vertices and faces of the k first Voronoi diagrams is

$$O\left(k^{\lceil \frac{d+1}{2} \rceil} n^{\lfloor \frac{d+1}{2} \rfloor}\right)$$

Molecules



- The union of n balls of $\mathbb{R}^d$ can be represented as a subcomplex of the regular triangulation called the alpha-shape
- It can be computed in time $\Theta(n \log n + n^{\lfloor \frac{d+1}{2} \rfloor})$

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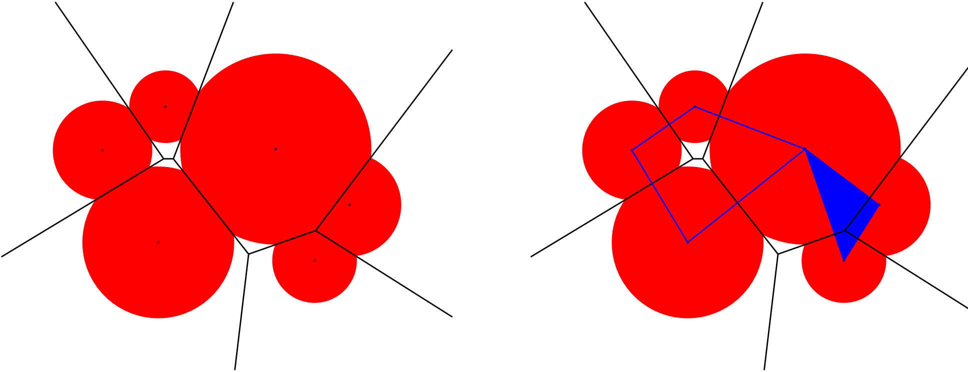

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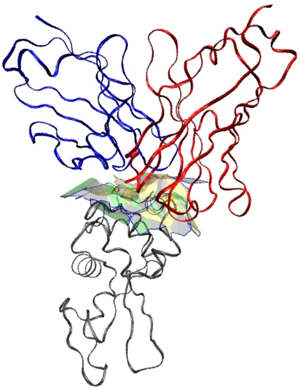
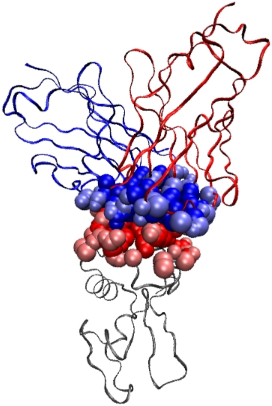
Interfaces entre protéines

[Cazals & Janin 2006]



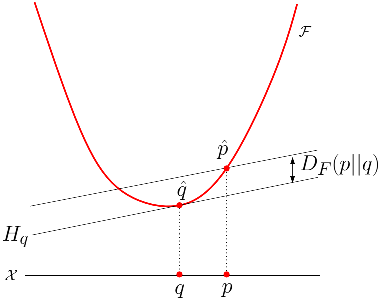


Interface antigène-anticorps

Bregman divergences

F a strictly convex and differentiable function defined over a convex set $\mathcal{X}$

$$D_F(\mathbf{p},\mathbf{q}) = F(\mathbf{p}) - F(\mathbf{q}) - \langle \mathbf{p}-\mathbf{q}, \nabla_F(\mathbf{q})\rangle$$



Not a distance but $D_F(\mathbf{x},\mathbf{y}) \geq 0$ and $D_F(\mathbf{x},\mathbf{y}) = 0 \iff \mathbf{x}=\mathbf{y}$

Examples

- $F(x) = x^2$: Squared Euclidean distance

$$\begin{aligned} D_F(\mathbf{p}, \mathbf{q}) &= F(\mathbf{p}) - F(\mathbf{q}) - \langle \mathbf{p} - \mathbf{q}, \boldsymbol{\nabla}_F(\mathbf{q}) \rangle \\ &= \mathbf{p}^2 - \mathbf{q}^2 - \langle \mathbf{p} - \mathbf{q}, 2\mathbf{q} \rangle = \|\mathbf{p} - \mathbf{q}\|^2 \end{aligned}$$

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- $F(p) = \sum p(x) \log_2 p(x)$ (Shannon entropy)
  $D_F(p, q) = \sum_x p(x) \log_2 \frac{p(x)}{q(x)}$ (K-L divergence)

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- $F(p) = -\sum_x \log p(x)$ (Burg entropy)
  $D_F(p,q) = \sum_x (\frac{p(x)}{q(x)} \log \frac{p(x)}{q(x)} - 1)$ (Itakura-Saito)

Bisectors

$$D_F(\mathbf{p}, \mathbf{q}) = F(\mathbf{p}) - F(\mathbf{q}) - \langle \mathbf{p} - \mathbf{q}, \nabla_F(\mathbf{q}) \rangle$$

Two types of bisectors

$$\begin{aligned} H_{pq} : D_F(\mathbf{x}, \mathbf{p}) &= D_F(\mathbf{x}, \mathbf{q}) \quad \text{(hyperplane)} \\ H^*_{pq} : D_F(\mathbf{p}, \mathbf{x}) &= D_F(\mathbf{q}, \mathbf{x}) \quad \text{(hypersurface)} \end{aligned}$$

Bregman diagrams

- Accordingly, we can define two types of Bregman diagrams
- By Legendre duality : $D_F(\mathbf{x}, \mathbf{y}) = D_{F^*}(\mathbf{y}', \mathbf{x}')$

Bregman Voronoi diagrams

The 1st type Bregman diagram of $\mathcal{P} = \{\mathbf{p}_1, \ldots, \mathbf{p}_n\}$ is the minimization diagram of the n functions $D_F(\mathbf{x}, \mathbf{p}_i)$, $i = 1, \ldots, n$

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Since $\arg\min(D_F(\mathbf{x}, \mathbf{p}_i)) = \arg\max(h_i(\mathbf{x}) = \langle \mathbf{x} - \mathbf{p}_i, \mathbf{p}'_i \rangle - F(\mathbf{p}_i))$

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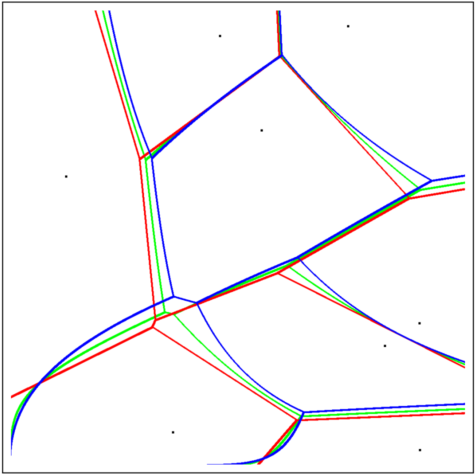
The 2nd type Bregman diagram of $\mathcal{P}$ is the (curved) minimization diagram of the n functions $D_F(\mathbf{p}_i, \mathbf{x})$, $i = 1, \ldots, n$



Bregman Voronoi diagrams from Laguerre diagramms

The 1st type Bregman Voronoi diagram of n sites of $\mathcal{X}$ is identical to the Laguerre diagram of n Euclidean hyperspheres centered at the $\mathbf{p}'_i$

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$$
\begin{aligned}
& D_F(\mathbf{x}, \mathbf{p}_i) \leq D_F(\mathbf{x}, \mathbf{p}_j) \\
\iff \quad & -F(\mathbf{p}_i) - \langle \mathbf{x} - \mathbf{p}_i, \mathbf{p}'_i \rangle) \leq -F(\mathbf{p}_j) - \langle \mathbf{x} - \mathbf{p}_j, \mathbf{p}'_j \rangle) \\
\iff \quad & \langle \mathbf{x}, \mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{p}'_i \rangle - 2F(\mathbf{p}_i) + 2\langle \mathbf{p}_i, \mathbf{p}'_i \rangle \leq \langle \mathbf{x}, \mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{p}'_j \rangle - 2F(\mathbf{p}_j) + 2\langle \mathbf{p}_j, \mathbf{p}'_j \rangle \\
\iff \quad & \langle \mathbf{x} - \mathbf{p}'_i, \mathbf{x} - \mathbf{p}'_i \rangle - r_i^2 \leq \langle \mathbf{x} - \mathbf{p}'_j, \mathbf{x} - \mathbf{p}'_j \rangle - r_j^2
\end{aligned}
$$

where $r_l^2 = \langle \mathbf{p}'_l, \mathbf{p}'_l \rangle + 2(F(\mathbf{p}_l) - \langle \mathbf{p}_l, \mathbf{p}'_l \rangle)$

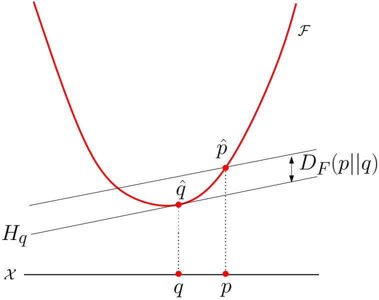
Bregman spheres

$$\sigma(\mathbf{c}, r) = \{\mathbf{x} \in \mathcal{X} \mid D_F(\mathbf{x}, \mathbf{c}) = r\}$$

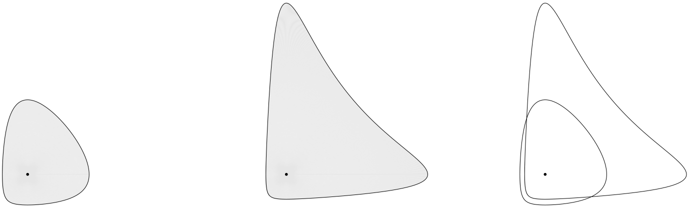
Lemma

The lifted image $\hat{\sigma}$ onto $\mathcal{F}$ of a Bregman sphere σ is contained in a hyperplane H_σ

Conversely, the intersection of any hyperplane H with $\mathcal{F}$ projects vertically onto a Bregman sphere



1st and 2nd types Bregman balls



Bregman triangulations

$\hat{\mathcal{P}}$: the lifted image of $\mathcal{P}$ onto the graph $\mathcal{F}$ of F

$\mathcal{T}$ the lower convex hull of $\hat{\mathcal{P}}$

The vertical projection of $\mathcal{T}$ is called the Bregman triangulation $BT_F(\mathcal{P})$ of $\mathcal{P}$

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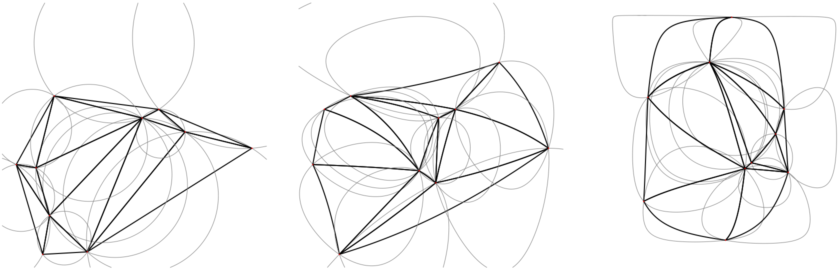
Characteristic property

The Bregman sphere circumscribing any simplex of $BT_F(\mathcal{P})$ does not enclose any point of $\mathcal{P}$

Primal space		Gradient space
1st type $BVD(\mathcal{P})$	=	Laguerre diagram of $(\mathcal{P}')$
		$\updownarrow *$
geodesic $BT(\mathcal{P})$	$\leftrightarrow$	regular triangulation of $(\mathcal{P}')$
$\updownarrow$		
$BT(\mathcal{P})$		



(a) Ordinary Delaunay (b) Exponential loss (c) Hellinger-like divergence

Properties of Bregman triangulations

- $BT(\mathcal{P})$ is the geometric dual of $BD(\mathcal{P})$
- Characteristic property : The Bregman sphere circumscribing any simplex of $BT(\mathcal{P})$ is empty
- Optimality : $BT(\mathcal{P}) = \min_{T \in \mathcal{T}(\mathcal{P})} \max_{\tau \in T} r(\tau)$
  ($r(\tau) =$ radius of the smallest Bregman ball containing τ)

[Rajan]